Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:20 AM BST

PDB ID	:	2WSE
Title	:	Improved Model of Plant Photosystem I
Authors	:	Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on	:	2009-09-05
Resolution	:	3.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

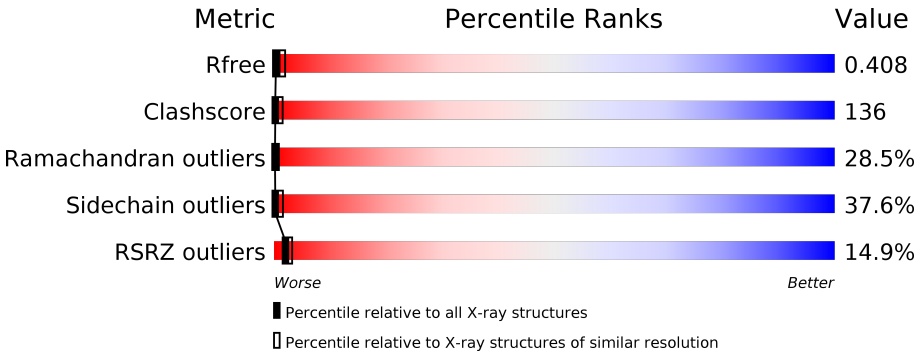
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	241	18% 27% 26% 12% • 32%
2	2	269	14% 7% 20% 25% 13% 35%
3	3	276	23% 17% 18% 17% 6% 42%
4	4	251	10% 6% 18% 26% 17% 34%
5	A	758	11% 6% 47% 34% 9% •
6	B	734	7% 10% 44% 36% 10%

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Mol	Chain	Length	Quality of chain
7	C	81	14% 5% 43% 35% 17%
8	D	212	12% 6% 27% 27% 5% 35%
9	E	143	11% 21% 15% 7% 55%
10	F	231	5% 6% 31% 22% 8% 33%
11	G	167	6% 20% 22% 11% 43%
12	H	144	6% 17% 19% 9% 52%
13	I	40	3% 5% 43% 23% 5% 25%
14	J	44	9% 11% 48% 30% 7% 5%
15	K	131	24% 21% 21% 16% 6% 36%
16	L	216	10% 8% 34% 25% 7% 25%
17	N	170	9% 9% 19% 19% 50%
18	R	53	36% 36% 28%
19	M	2	100%
19	O	2	100%
19	P	2	100%
19	Q	2	100%
19	S	2	100%
19	T	2	100%
19	U	2	100%
19	V	2	100%
19	W	2	100%
19	X	2	100%
19	Y	2	100%
19	Z	2	100%
19	a	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	GLC	M	1	-	-	-	X
19	FRU	M	2	X	-	-	X
19	GLC	O	1	-	-	X	-
19	FRU	O	2	X	-	X	X
19	GLC	P	1	-	-	X	-
19	FRU	P	2	X	-	X	X
19	GLC	Q	1	-	-	-	X
19	FRU	Q	2	X	-	X	X
19	GLC	S	1	-	-	X	-
19	FRU	S	2	X	-	X	-
19	GLC	T	1	-	-	X	-
19	FRU	T	2	X	-	X	-
19	GLC	U	1	-	-	X	-
19	FRU	U	2	X	-	X	-
19	FRU	V	2	X	-	-	-
19	FRU	W	2	X	-	-	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	X
19	GLC	Y	1	-	-	X	-
19	FRU	Y	2	X	-	X	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	GLC	a	1	-	-	-	X
19	FRU	a	2	X	-	-	-
20	CLA	1	201	X	-	-	-
20	CLA	1	202	X	-	X	-
20	CLA	1	203	X	-	-	-
20	CLA	1	204	X	-	-	-
20	CLA	1	205	X	-	-	-
20	CLA	1	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	208	X	-	-	-
20	CLA	1	209	X	-	-	-
20	CLA	1	210	X	-	-	-
20	CLA	1	211	X	-	-	-
20	CLA	1	212	X	-	-	-
20	CLA	1	214	X	-	-	-
20	CLA	1	215	X	-	X	-
20	CLA	1	216	X	-	-	-
20	CLA	2	301	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	306	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	X
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	X
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	315	X	-	-	-
20	CLA	2	316	X	-	-	-
20	CLA	2	322	X	-	X	-
20	CLA	3	301	X	-	-	X
20	CLA	3	302	X	-	X	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	X
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	X
20	CLA	3	310	X	-	-	X
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	X	X
20	CLA	3	316	X	-	-	-
20	CLA	3	317	X	-	-	-
20	CLA	3	318	X	-	-	-
20	CLA	3	319	X	-	-	-
20	CLA	3	320	X	-	-	-
20	CLA	4	302	X	-	X	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	-
20	CLA	4	306	X	-	-	X
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	4	315	X	-	-	-
20	CLA	4	316	X	-	-	-
20	CLA	4	318	X	-	-	-
20	CLA	4	319	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	X
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	X	-
20	CLA	A	806	X	-	X	-
20	CLA	A	807	X	-	X	X
20	CLA	A	808	X	-	X	-
20	CLA	A	809	X	-	X	-
20	CLA	A	810	X	-	-	X
20	CLA	A	811	X	-	X	X
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	X	X
20	CLA	A	815	X	-	X	-
20	CLA	A	816	X	-	X	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	X	X
20	CLA	A	819	X	-	X	X
20	CLA	A	820	X	-	-	X
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	X	-
20	CLA	A	823	X	-	-	X
20	CLA	A	824	X	-	X	-
20	CLA	A	825	X	-	X	-
20	CLA	A	826	X	-	X	X
20	CLA	A	827	X	-	X	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	X
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	X
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	X	-
20	CLA	A	850	X	-	-	-
20	CLA	A	851	X	-	X	-
20	CLA	A	852	X	-	X	-
20	CLA	B	803	X	-	X	X
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	X	-
20	CLA	B	808	X	-	X	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	X	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	X	X
20	CLA	B	815	X	-	X	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	X	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	X	-
20	CLA	B	822	X	-	X	-
20	CLA	B	823	X	-	X	-
20	CLA	B	824	X	-	X	-
20	CLA	B	825	X	-	X	-
20	CLA	B	826	X	-	X	-
20	CLA	B	827	X	-	X	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	X	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	X	-
20	CLA	B	833	X	-	X	X
20	CLA	B	834	X	-	-	X
20	CLA	B	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	836	X	-	X	-
20	CLA	B	837	X	-	X	-
20	CLA	B	838	X	-	X	X
20	CLA	B	839	X	-	X	-
20	CLA	B	840	X	-	-	X
20	CLA	B	849	X	-	X	-
20	CLA	B	850	X	-	X	-
20	CLA	B	851	X	-	X	-
20	CLA	F	204	X	-	-	-
20	CLA	F	205	X	-	-	-
20	CLA	F	206	X	-	-	-
20	CLA	G	102	X	-	-	-
20	CLA	H	101	X	-	X	-
20	CLA	H	102	X	-	-	-
20	CLA	H	103	X	-	-	X
20	CLA	H	109	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	X	-	X	-
20	CLA	J	103	X	-	X	-
20	CLA	K	101	X	-	-	-
20	CLA	K	102	X	-	-	X
20	CLA	K	103	X	-	-	X
20	CLA	K	108	X	-	X	X
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	X	-
20	CLA	L	203	X	-	-	X
20	CLA	L	207	X	-	-	-
20	CLA	L	208	X	-	X	-
20	CLA	L	209	X	-	-	-
20	CLA	R	107	X	-	-	X
20	CLA	R	108	X	-	-	-
21	LMU	1	217	-	-	-	X
21	LMU	1	218	-	-	-	X
21	LMU	2	313	-	-	-	X
21	LMU	2	320	-	-	-	X
21	LMU	4	320	-	-	-	X
21	LMU	A	848	-	-	-	X
21	LMU	A	849	-	-	-	X
21	LMU	A	853	-	-	-	X
21	LMU	A	854	-	-	X	-
21	LMU	A	855	-	-	X	-
21	LMU	B	801	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LMU	B	847	-	-	X	-
21	LMU	E	101	-	-	X	-
21	LMU	H	104	-	-	X	-
21	LMU	H	106	-	-	X	-
21	LMU	H	108	-	-	X	-
21	LMU	K	104	-	-	-	X
21	LMU	K	105	-	-	X	-
21	LMU	K	106	-	-	X	-
21	LMU	L	204	-	-	-	X
21	LMU	N	101	-	-	X	-
21	LMU	R	101	X	-	-	-
21	LMU	R	102	-	-	-	X
21	LMU	R	103	-	-	X	-
21	LMU	R	109	-	-	X	-
22	BCR	3	314	-	-	X	-
22	BCR	A	843	-	-	X	X
22	BCR	A	844	-	-	X	X
22	BCR	A	845	-	-	X	-
22	BCR	A	846	-	-	X	-
22	BCR	A	847	-	-	X	X
22	BCR	B	845	-	-	X	-
22	BCR	B	846	-	-	X	X
22	BCR	F	202	-	-	X	X
22	BCR	F	203	-	-	X	-
22	BCR	I	103	-	-	X	X
22	BCR	J	102	-	-	X	X
22	BCR	L	210	-	-	X	X
23	PQN	A	842	X	-	-	X
23	PQN	B	841	X	-	X	X
24	SF4	A	857	-	-	X	-
24	SF4	C	102	-	-	X	-
24	SF4	C	103	-	-	X	-
25	LMG	B	848	-	-	X	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36461 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	164	Total	C	N	O	S	0	0	0
			1255	817	206	228	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1380	902	229	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	160	Total	C	N	O	S	0	0	0
			1233	811	200	217	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1322	864	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

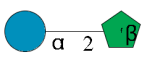
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

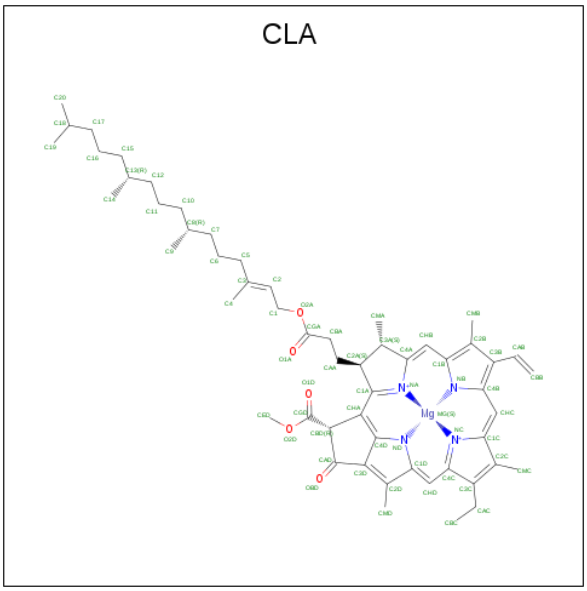
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	M	2	Total C O 23 12 11	0	0	0
19	O	2	Total C O 22 12 10	0	0	0
19	P	2	Total C O 23 12 11	0	0	0
19	Q	2	Total C O 23 12 11	0	0	0
19	S	2	Total C O 23 12 11	0	0	0
19	T	2	Total C O 23 12 11	0	0	0
19	U	2	Total C O 23 12 11	0	0	0
19	V	2	Total C O 23 12 11	0	0	0
19	W	2	Total C O 23 12 11	0	0	0
19	X	2	Total C O 23 12 11	0	0	0
19	Y	2	Total C O 23 12 11	0	0	0
19	Z	2	Total C O 23 12 11	0	0	0
19	a	2	Total C O 23 12 11	0	0	0

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N O 57 47 1 4 5	0	0
20	1	1	Total C Mg N O 47 37 1 4 5	0	0
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 51 41 1 4 5	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N O 61 51 1 4 5	0	0
20	3	1	Total C Mg N O 36 30 1 4 1	0	0
20	3	1	Total C Mg N O 50 40 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 36 30 1 4 1	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 42 34 1 4 3	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 50 40 1 4 5	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N O 65 55 1 4 5	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 50 40 1 4 5	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 46 36 1 4 5	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	4	1	Total C Mg N O 47 37 1 4 5	0	0
20	A	1	Total C Mg N O 46 36 1 4 5	0	0
20	A	1	Total C Mg N 25 20 1 4	0	0
20	A	1	Total C Mg N O 50 40 1 4 5	0	0
20	A	1	Total C Mg N O 55 45 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 55 45 1 4 5	0	0
20	A	1	Total C Mg N O 46 36 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 52 42 1 4 5	0	0
20	A	1	Total C Mg N O 45 35 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 54 44 1 4 5	0	0
20	A	1	Total C Mg N O 54 44 1 4 5	0	0
20	A	1	Total C Mg N O 45 35 1 4 5	0	0
20	A	1	Total C Mg N O 50 40 1 4 5	0	0
20	A	1	Total C Mg N O 54 44 1 4 5	0	0
20	A	1	Total C Mg N O 52 42 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 51 41 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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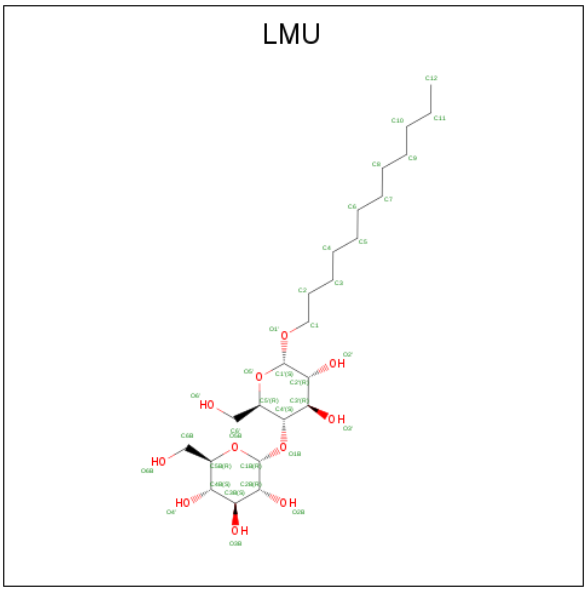
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	2	1	Total C O 35 24 11	0	0
21	2	1	Total C O 35 24 11	0	0
21	2	1	Total C O 35 24 11	0	0
21	3	1	Total C O 35 24 11	0	0
21	3	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 34 23 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	B	1	Total C O 35 24 11	0	0
21	B	1	Total C O 35 24 11	0	0
21	B	1	Total C O 35 24 11	0	0
21	C	1	Total C O 35 24 11	0	0
21	D	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	E	1	Total C O 35 24 11	0	0
21	F	1	Total C O 34 23 11	0	0
21	G	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	N	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0

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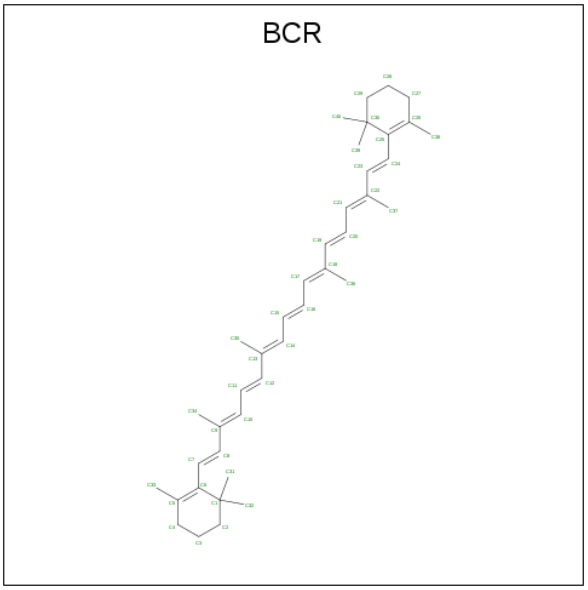
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0

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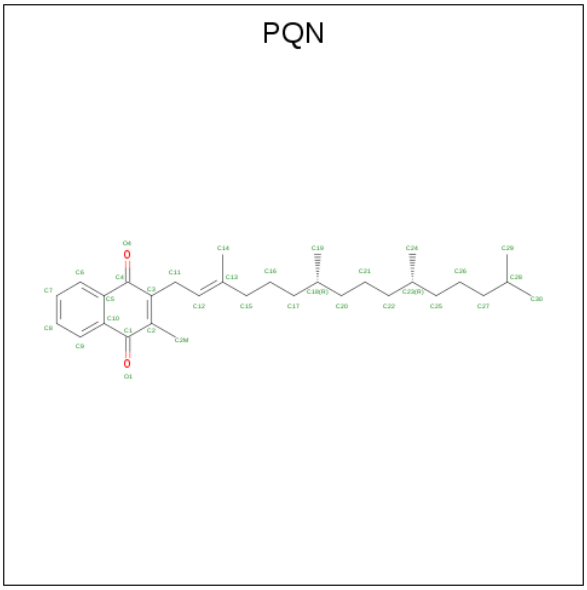
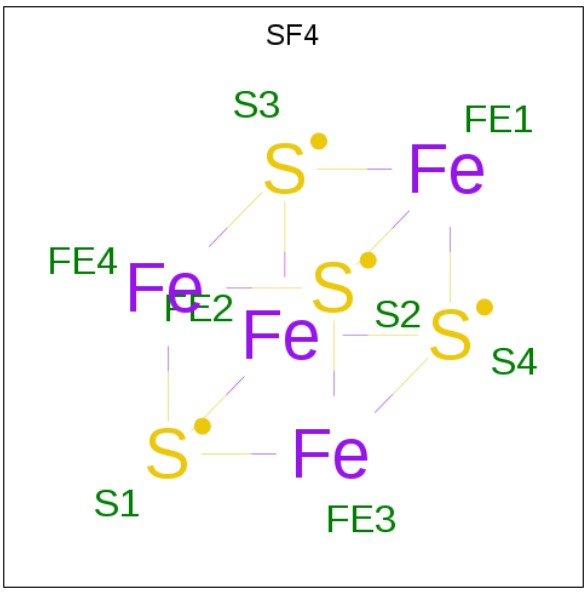
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



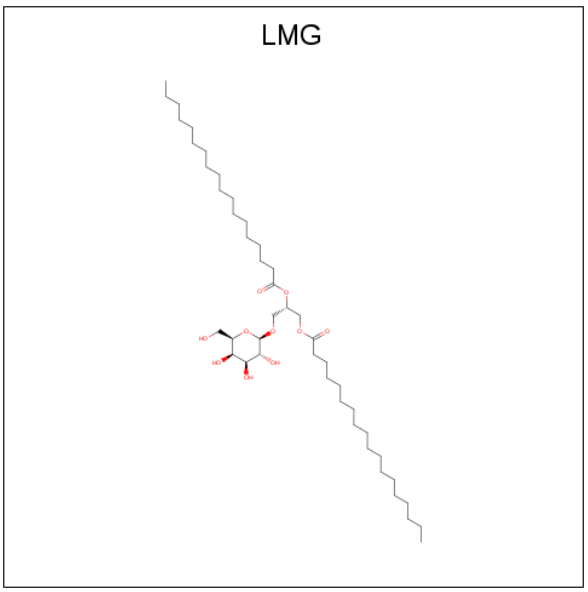
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total Fe S 8 4 4	0	0
24	C	1	Total Fe S 8 4 4	0	0
24	C	1	Total Fe S 8 4 4	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

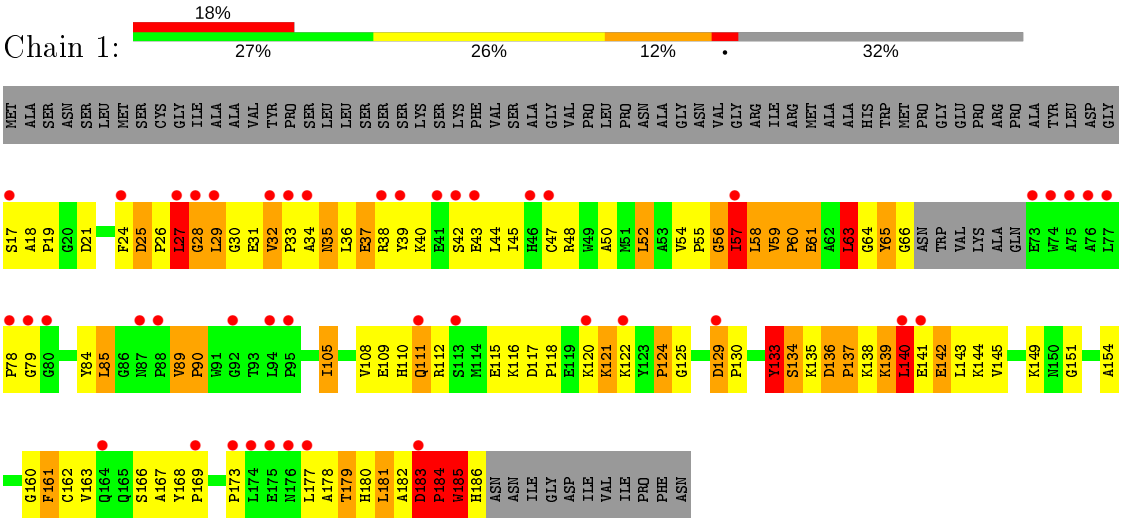
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

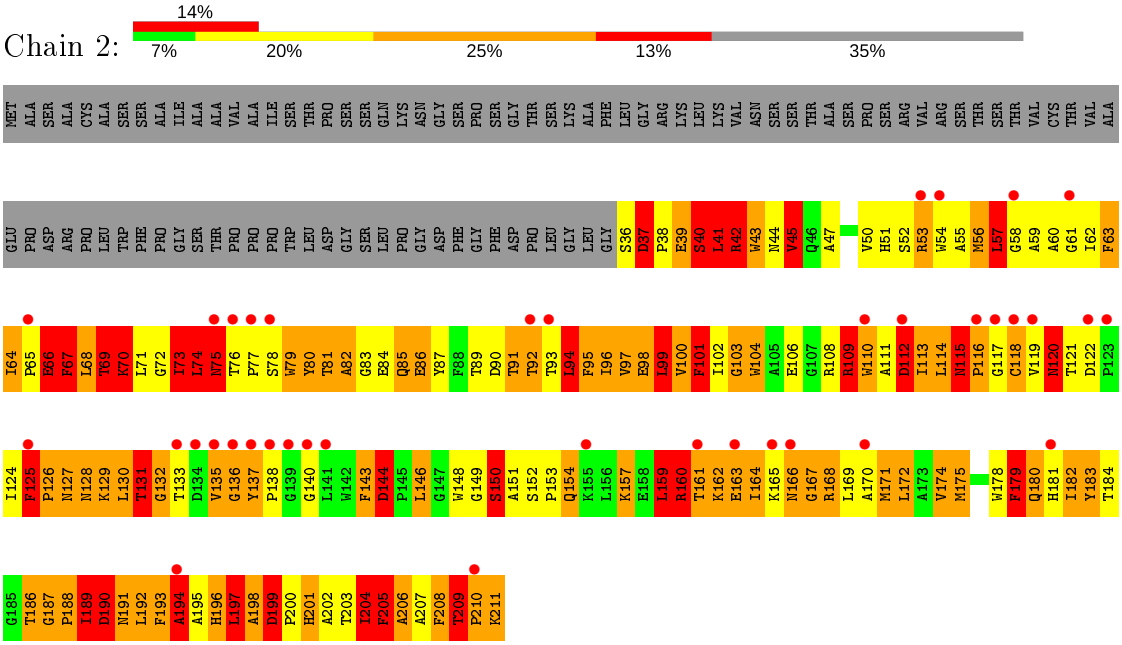
- Molecule 1: AT3G54890

Chain 1:



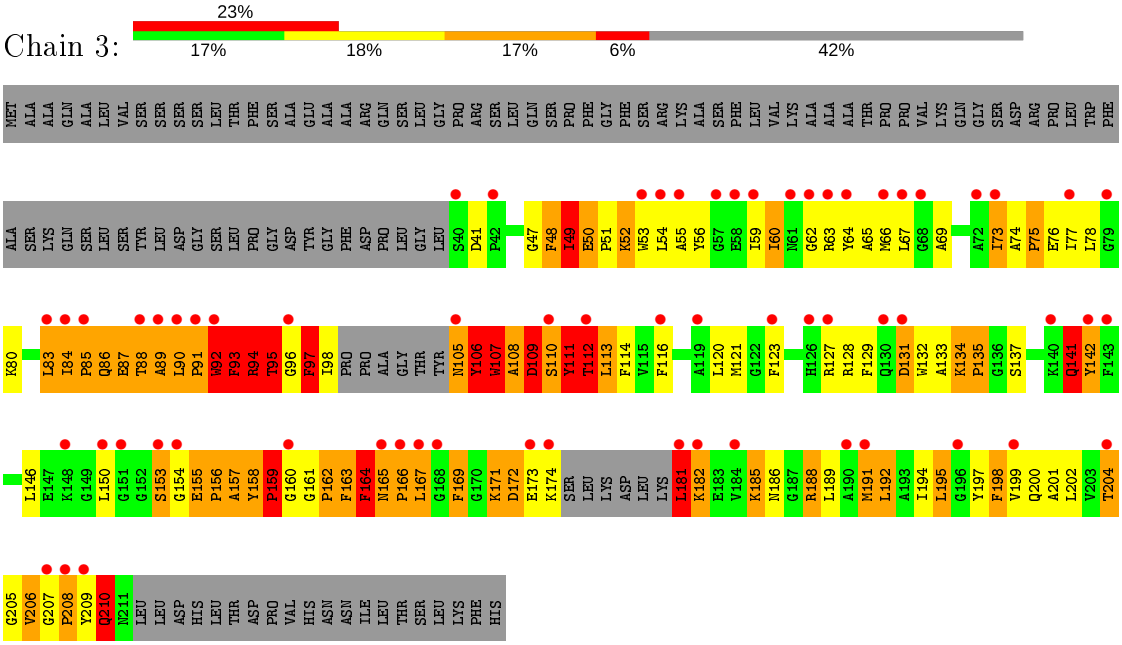
- Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I

Chain 2:



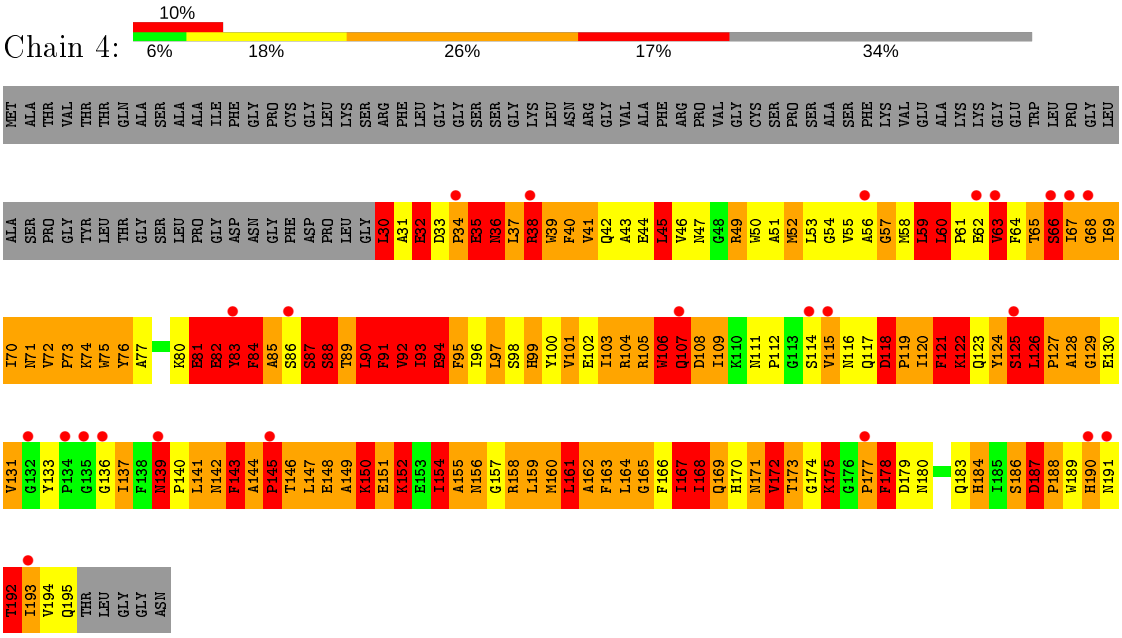
- Molecule 3: LHCA3

Chain 3:



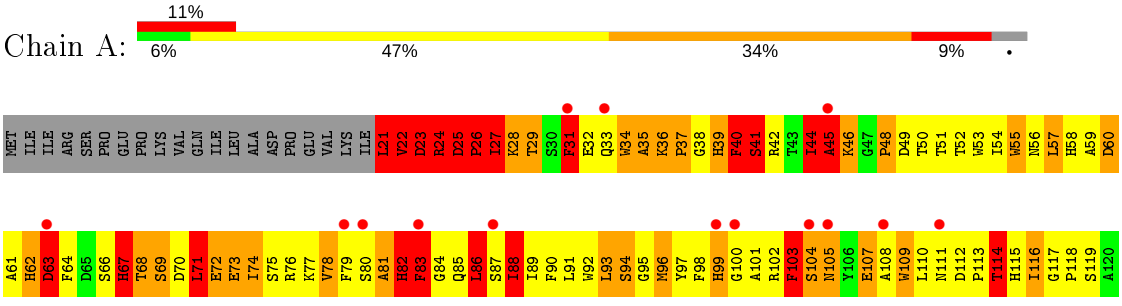
- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

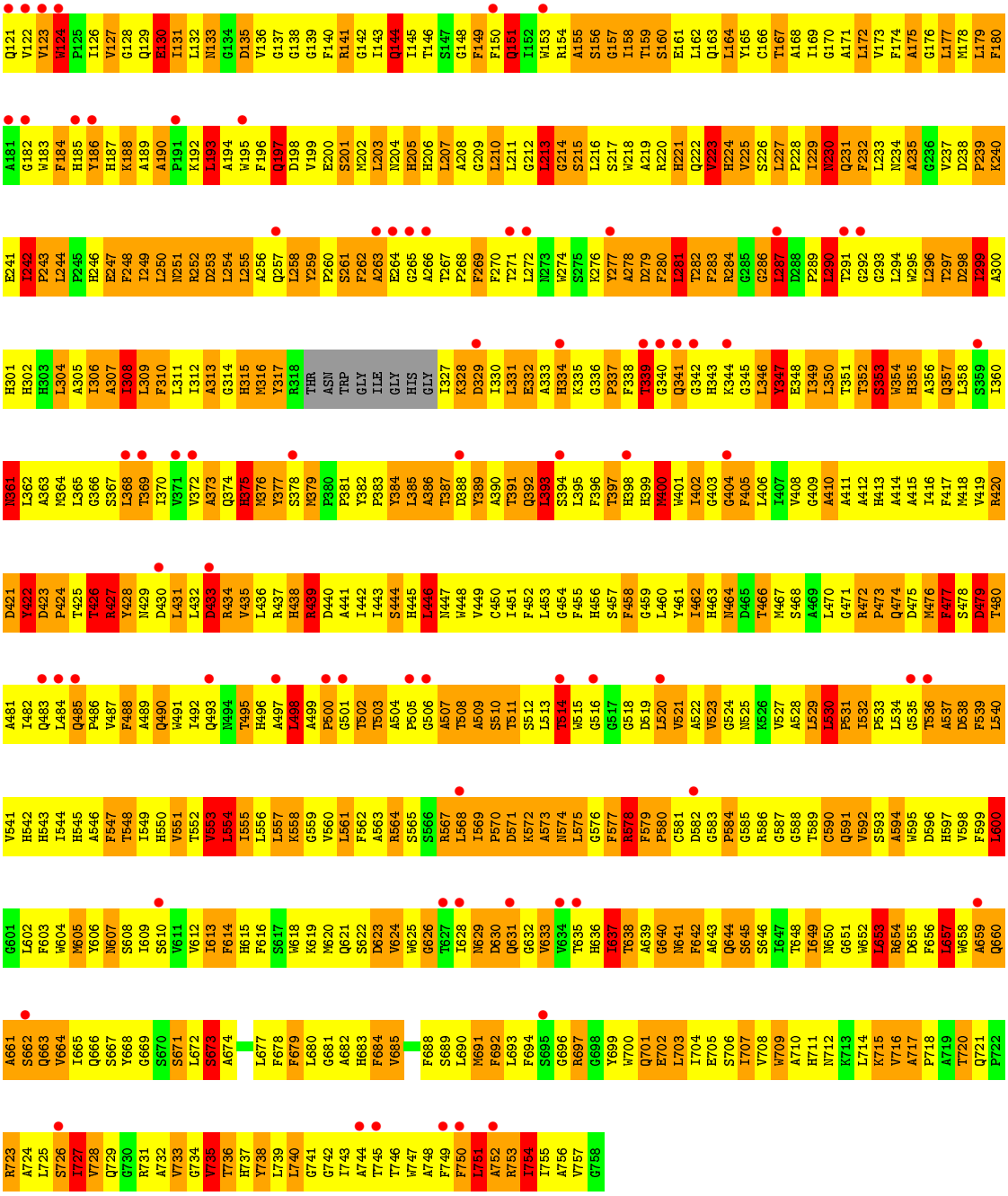
Chain 4:



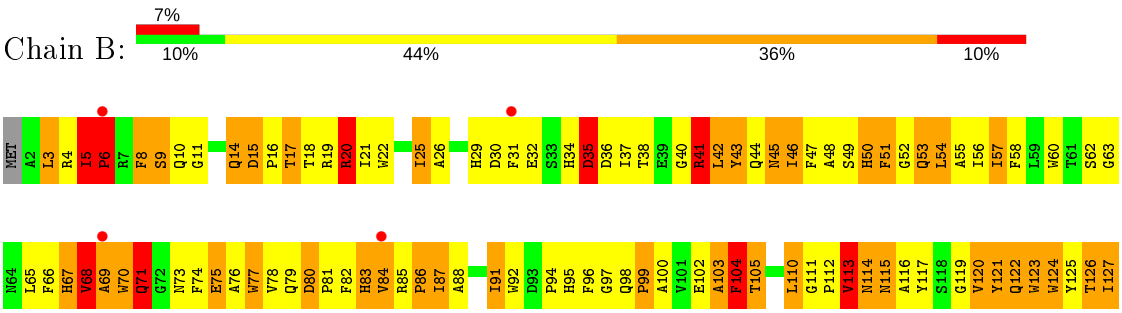
- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

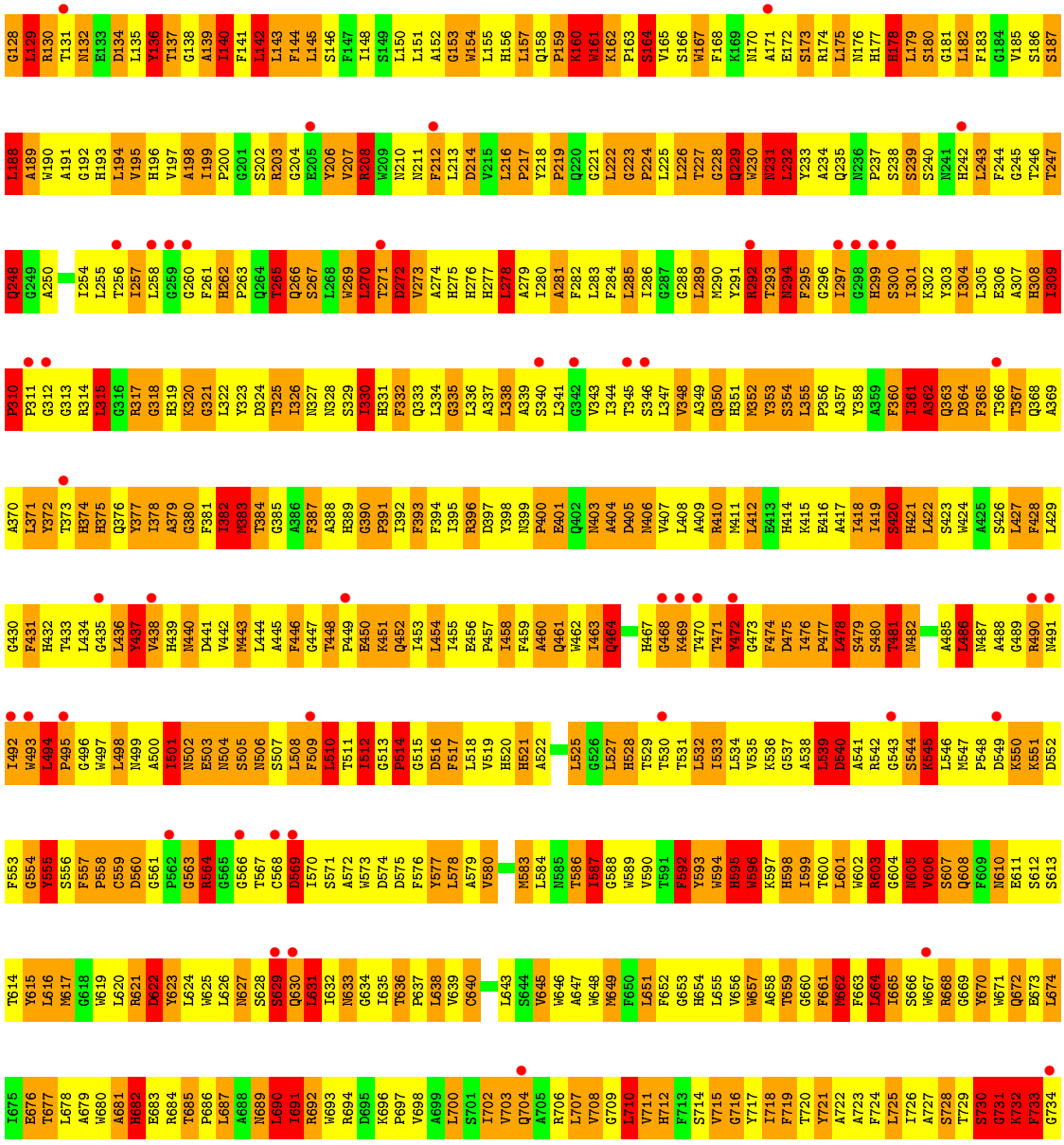
Chain A:



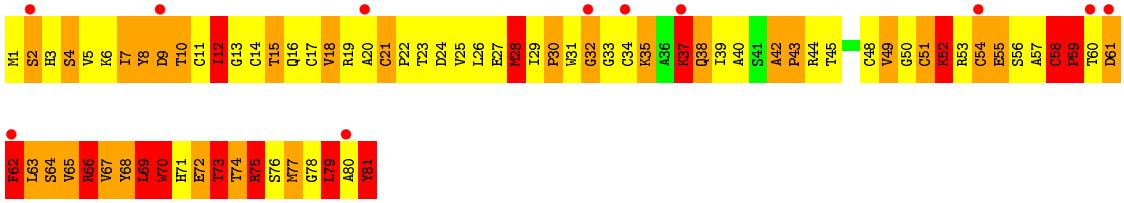


• Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

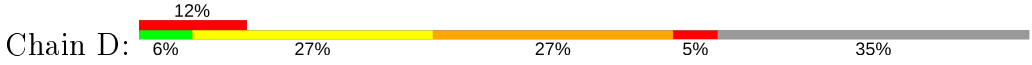


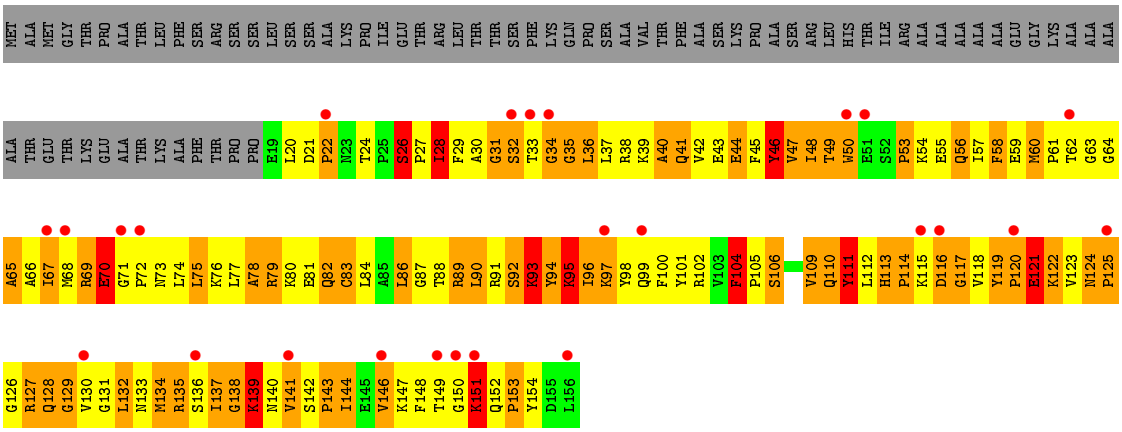


• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



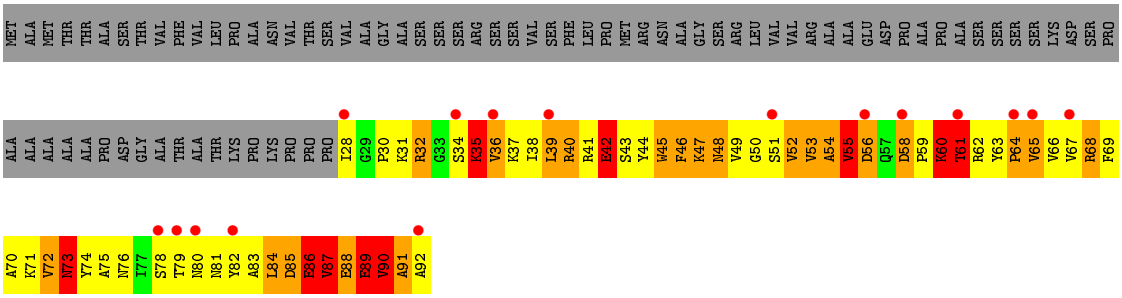
• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC





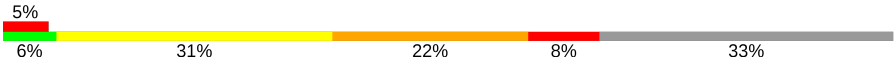
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

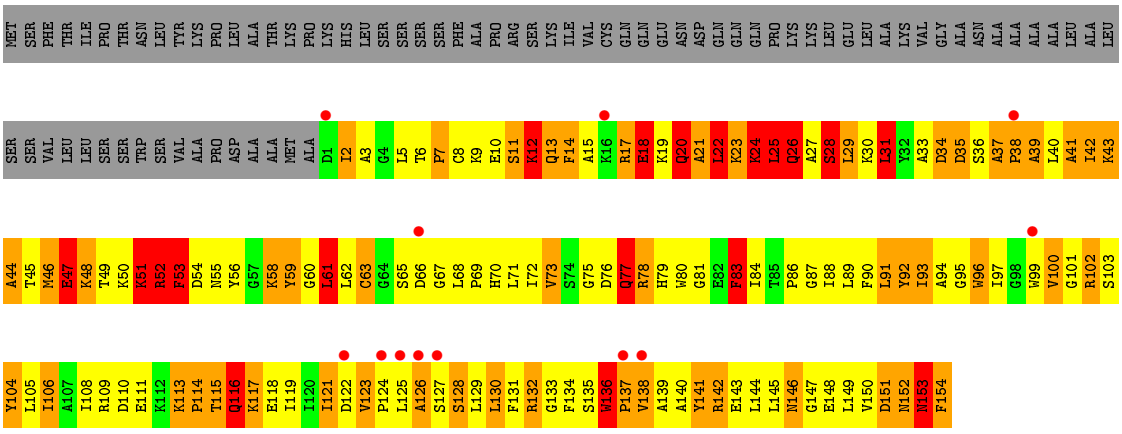
Chain E:



• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

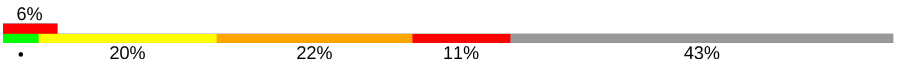
Chain F:

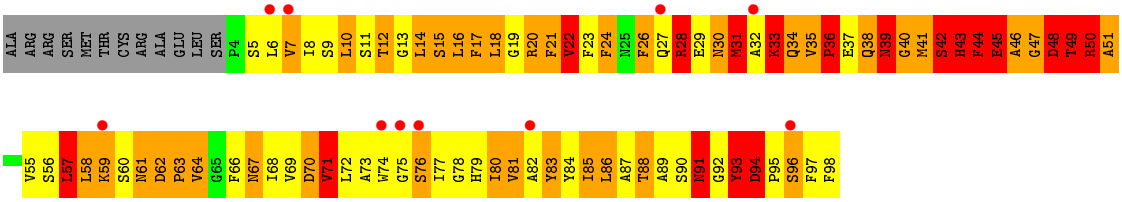




• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

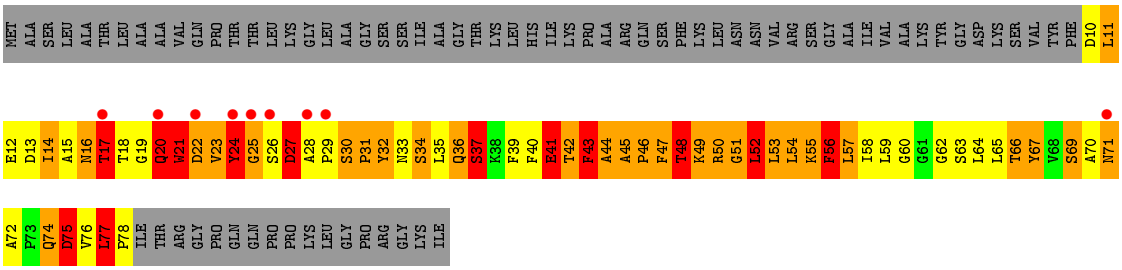
Chain G:





• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC

Chain H:

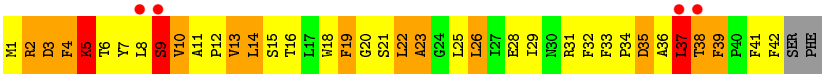


• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII

Chain I:

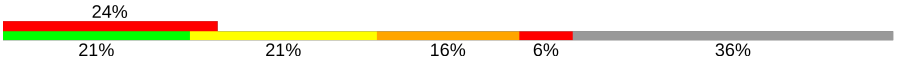
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

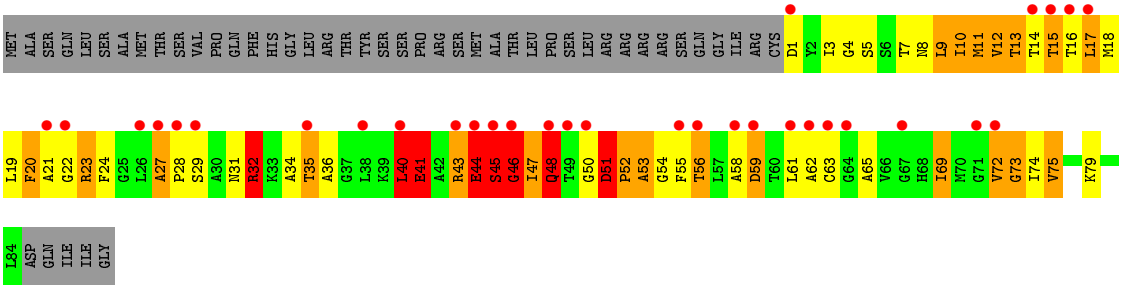
Chain J:



• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

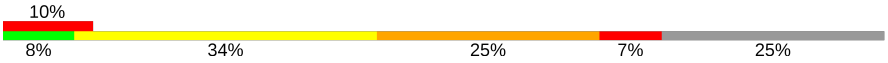
Chain K:

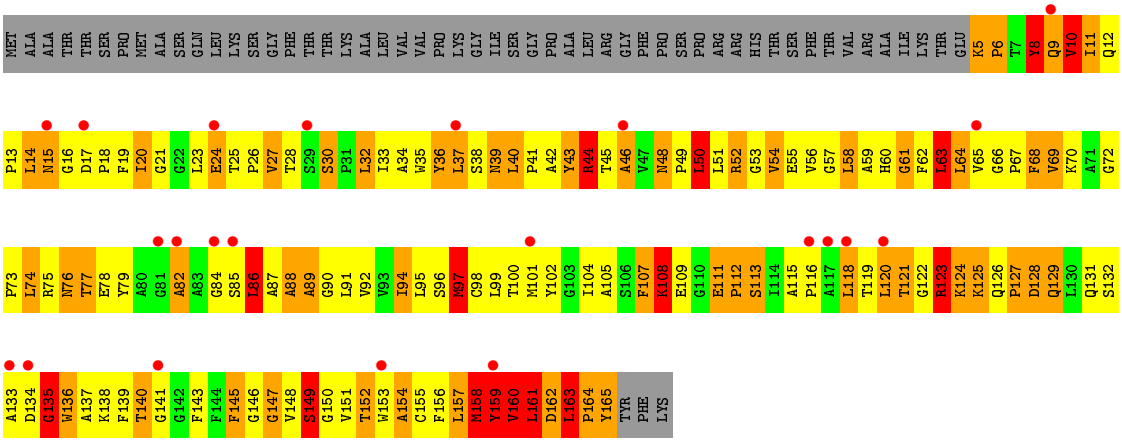




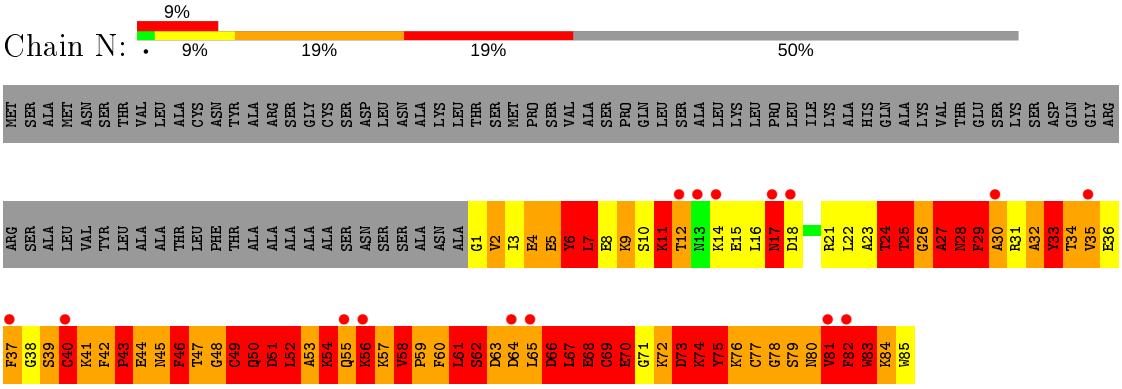
• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

Chain L:

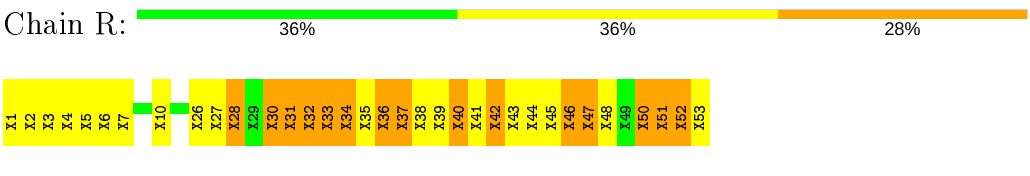




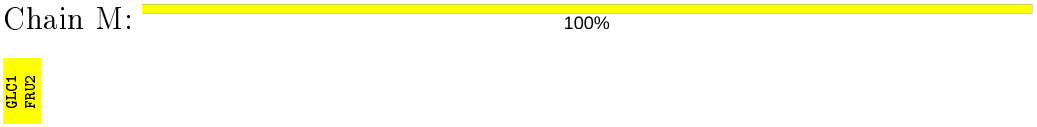
• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



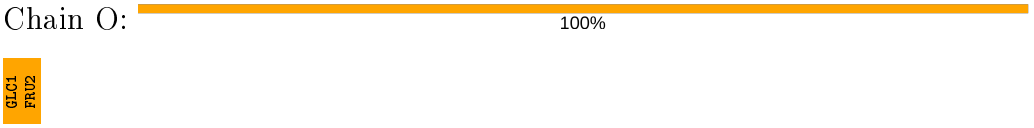
• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

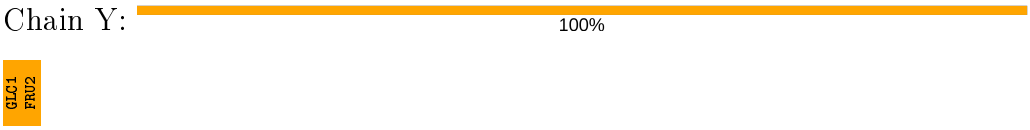
Chain W: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X: 

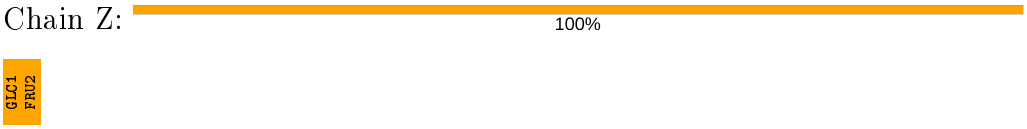
- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y:



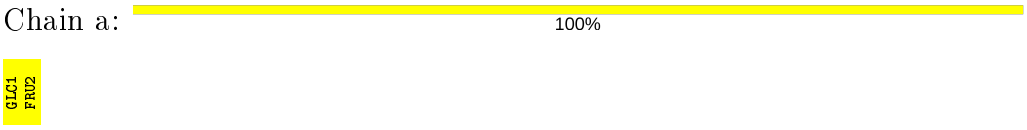
- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z:



- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.49 39.96 – 3.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.49) 90.6 (39.96-3.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.369 , 0.375 0.387 , 0.408	Depositor DCC
R_{free} test set	1334 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	90.9	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 113.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	36461	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, GLC, CLA, PQN, LMU, FRU, UNL, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.62	0/1294	0.89	5/1762 (0.3%)
2	2	1.05	1/1426 (0.1%)	1.32	15/1950 (0.8%)
3	3	0.88	6/1270 (0.5%)	0.96	4/1714 (0.2%)
4	4	1.27	9/1362 (0.7%)	1.35	17/1855 (0.9%)
5	A	0.89	0/5938	1.06	15/8104 (0.2%)
6	B	0.89	2/6058 (0.0%)	1.03	13/8278 (0.2%)
7	C	1.42	7/632 (1.1%)	1.34	5/856 (0.6%)
8	D	1.00	0/1122	1.06	0/1514
9	E	1.10	0/530	1.17	2/718 (0.3%)
10	F	1.05	1/1250 (0.1%)	1.07	3/1687 (0.2%)
11	G	1.04	0/760	1.27	10/1031 (1.0%)
12	H	1.10	0/543	1.20	2/741 (0.3%)
13	I	0.89	0/235	0.98	0/320
14	J	0.93	0/349	1.09	1/475 (0.2%)
15	K	0.63	0/599	1.16	6/810 (0.7%)
16	L	1.02	0/1238	1.14	6/1691 (0.4%)
17	N	1.28	1/699 (0.1%)	1.32	7/936 (0.7%)
All	All	0.97	27/25305 (0.1%)	1.11	111/34442 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	6
2	2	3	22
3	3	0	19
4	4	0	22
5	A	0	30
6	B	0	20

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	3
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	3
16	L	0	5
17	N	0	21
18	R	0	17
All	All	4	217

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.89	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
7	C	72	GLU	CD-OE1	-7.90	1.17	1.25
4	4	83	TYR	CE1-CZ	-7.46	1.28	1.38
3	3	93	PHE	CD2-CE2	7.39	1.54	1.39
7	C	72	GLU	CD-OE2	-6.96	1.18	1.25
7	C	58	CYS	CB-SG	6.87	1.94	1.82
6	B	640	CYS	CB-SG	6.82	1.93	1.82
7	C	81	TYR	CE1-CZ	-6.78	1.29	1.38
3	3	93	PHE	CE2-CZ	6.62	1.50	1.37
7	C	72	GLU	CG-CD	-6.60	1.42	1.51
17	N	70	GLU	CB-CG	6.16	1.63	1.52
4	4	88	SER	C-O	5.83	1.34	1.23
4	4	81	GLU	CG-CD	-5.75	1.43	1.51
4	4	83	TYR	CD1-CE1	-5.73	1.30	1.39
4	4	93	ILE	C-O	5.73	1.34	1.23
4	4	39	TRP	CE3-CZ3	-5.62	1.28	1.38
7	C	54	CYS	CB-SG	-5.61	1.72	1.81
2	2	45	VAL	CB-CG2	-5.61	1.41	1.52
7	C	81	TYR	CD2-CE2	-5.58	1.30	1.39
4	4	39	TRP	CB-CG	5.55	1.60	1.50
4	4	94	GLU	CG-CD	5.45	1.60	1.51
3	3	93	PHE	CD1-CE1	5.39	1.50	1.39
4	4	39	TRP	CA-C	-5.34	1.39	1.52
10	F	47	GLU	CG-CD	5.20	1.59	1.51
3	3	92	TRP	CG-CD1	5.12	1.44	1.36
6	B	401	GLU	CG-CD	5.11	1.59	1.51

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	57	ILE	N-CA-C	9.01	135.32	111.00
5	A	93	LEU	CA-CB-CG	8.09	133.90	115.30
6	B	732	LYS	N-CA-C	-8.08	89.19	111.00
16	L	160	VAL	CB-CA-C	-7.79	96.61	111.40
4	4	39	TRP	C-N-CA	-7.68	102.51	121.70
1	1	59	VAL	CB-CA-C	-7.54	97.07	111.40
6	B	486	LEU	CA-CB-CG	7.44	132.41	115.30
1	1	58	LEU	N-CA-C	-7.42	90.97	111.00
16	L	86	LEU	CA-CB-CG	7.38	132.27	115.30
6	B	315	LEU	CA-CB-CG	7.34	132.18	115.30
17	N	33	TYR	N-CA-C	-7.28	91.34	111.00
1	1	57	ILE	CB-CA-C	-7.26	97.07	111.60
11	G	16	LEU	CA-CB-CG	7.11	131.65	115.30
5	A	530	LEU	CA-CB-CG	7.09	131.60	115.30
6	B	710	LEU	N-CA-C	-7.03	92.03	111.00
4	4	39	TRP	CA-CB-CG	6.95	126.90	113.70
4	4	126	LEU	N-CA-C	6.88	129.59	111.00
5	A	540	LEU	CA-CB-CG	6.88	131.11	115.30
2	2	57	LEU	CA-CB-CG	6.79	130.92	115.30
5	A	554	LEU	CA-CB-CG	6.79	130.92	115.30
3	3	181	LEU	C-N-CA	6.71	138.47	121.70
4	4	92	VAL	O-C-N	-6.68	112.01	122.70
10	F	22	LEU	CB-CG-CD1	-6.60	99.78	111.00
15	K	46	GLY	N-CA-C	-6.57	96.68	113.10
2	2	41	LEU	CA-CB-CG	-6.55	100.24	115.30
2	2	74	LEU	N-CA-C	-6.52	93.39	111.00
3	3	93	PHE	N-CA-CB	-6.41	99.07	110.60
2	2	101	PHE	N-CA-CB	6.40	122.13	110.60
2	2	132	GLY	N-CA-C	6.38	129.06	113.10
11	G	43	HIS	N-CA-C	-6.38	93.78	111.00
9	E	90	VAL	N-CA-C	-6.37	93.79	111.00
4	4	66	SER	N-CA-C	6.35	128.14	111.00
4	4	93	ILE	N-CA-C	6.33	128.08	111.00
4	4	161	LEU	CA-CB-CG	6.32	129.84	115.30
5	A	25	ASP	C-N-CD	-6.29	106.75	120.60
7	C	79	LEU	CA-CB-CG	6.28	129.73	115.30
4	4	143	PHE	N-CA-C	6.27	127.94	111.00
6	B	494	LEU	CA-CB-CG	6.26	129.70	115.30
3	3	95	THR	N-CA-C	6.25	127.86	111.00
5	A	271	THR	N-CA-C	-6.25	94.14	111.00
6	B	338	LEU	CA-CB-CG	6.18	129.51	115.30
17	N	24	THR	N-CA-C	-6.14	94.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	91	ASN	N-CA-C	6.09	127.45	111.00
17	N	27	ALA	N-CA-C	-6.07	94.60	111.00
15	K	51	ASP	N-CA-C	6.05	127.33	111.00
16	L	135	GLY	N-CA-C	-6.04	98.01	113.10
4	4	124	TYR	N-CA-C	-6.01	94.77	111.00
11	G	44	PHE	N-CA-C	-6.01	94.78	111.00
4	4	88	SER	N-CA-C	6.00	127.21	111.00
7	C	69	LEU	CA-CB-CG	5.95	128.99	115.30
14	J	35	ASP	N-CA-C	5.94	127.04	111.00
11	G	57	LEU	CA-CB-CG	5.90	128.87	115.30
6	B	194	LEU	CB-CG-CD1	-5.89	100.98	111.00
4	4	108	ASP	CB-CG-OD2	-5.82	113.06	118.30
4	4	60	LEU	CA-CB-CG	5.80	128.65	115.30
2	2	94	LEU	CA-CB-CG	5.78	128.60	115.30
6	B	380	GLY	N-CA-C	-5.78	98.65	113.10
2	2	175	MET	CB-CA-C	5.77	121.94	110.40
11	G	51	ALA	N-CA-C	5.77	126.58	111.00
5	A	350	LEU	CA-CB-CG	-5.77	102.03	115.30
17	N	31	ARG	N-CA-C	-5.77	95.42	111.00
15	K	53	ALA	C-N-CA	-5.68	110.38	122.30
2	2	172	LEU	CA-CB-CG	-5.67	102.25	115.30
7	C	79	LEU	CB-CG-CD2	5.67	120.63	111.00
7	C	75	ARG	NE-CZ-NH2	5.65	123.12	120.30
4	4	30	LEU	CA-CB-CG	-5.64	102.32	115.30
12	H	27	ASP	N-CA-C	-5.62	95.82	111.00
4	4	145	PRO	N-CA-C	-5.62	97.49	112.10
17	N	62	SER	N-CA-C	-5.62	95.83	111.00
6	B	478	LEU	CA-CB-CG	5.59	128.15	115.30
7	C	75	ARG	CA-CB-CG	5.58	125.67	113.40
17	N	74	LYS	N-CA-C	5.54	125.95	111.00
17	N	6	TYR	N-CA-C	-5.46	96.27	111.00
9	E	60	LYS	N-CA-C	5.45	125.71	111.00
5	A	653	LEU	CA-CB-CG	5.44	127.81	115.30
4	4	41	VAL	CB-CA-C	-5.38	101.18	111.40
6	B	104	PHE	N-CA-C	-5.37	96.50	111.00
16	L	163	LEU	C-N-CD	-5.37	108.80	120.60
11	G	14	LEU	CA-CB-CG	-5.35	102.99	115.30
6	B	631	LEU	CA-CB-CG	5.35	127.61	115.30
2	2	56	MET	N-CA-C	5.34	125.41	111.00
4	4	40	PHE	CB-CA-C	5.33	121.06	110.40
10	F	59	TYR	CB-CA-C	-5.29	99.82	110.40
16	L	50	LEU	CA-CB-CG	5.28	127.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	41	LEU	CB-CG-CD2	-5.27	102.04	111.00
15	K	51	ASP	C-N-CD	-5.26	109.03	120.60
2	2	199	ASP	C-N-CD	-5.25	109.05	120.60
5	A	287	LEU	CA-CB-CG	5.24	127.36	115.30
1	1	63	LEU	CA-CB-CG	-5.24	103.26	115.30
15	K	12	VAL	CB-CA-C	-5.23	101.46	111.40
12	H	52	LEU	N-CA-C	5.19	125.00	111.00
6	B	289	LEU	CA-CB-CG	5.19	127.23	115.30
2	2	43	TRP	N-CA-C	-5.16	97.06	111.00
5	A	626	GLY	N-CA-C	-5.16	100.19	113.10
11	G	21	PHE	N-CA-C	5.15	124.90	111.00
2	2	174	VAL	N-CA-C	5.15	124.90	111.00
4	4	154	ILE	CB-CA-C	-5.14	101.32	111.60
5	A	753	ARG	NE-CZ-NH1	-5.13	117.73	120.30
5	A	600	LEU	CA-CB-CG	5.11	127.05	115.30
16	L	158	MET	N-CA-C	-5.07	97.31	111.00
3	3	111	TYR	CA-CB-CG	5.06	123.02	113.40
5	A	573	ALA	N-CA-C	-5.05	97.35	111.00
15	K	22	GLY	C-N-CA	-5.05	109.06	121.70
2	2	125	PHE	N-CA-C	5.05	124.64	111.00
5	A	385	LEU	CA-CB-CG	5.05	126.92	115.30
5	A	214	GLY	N-CA-C	-5.04	100.49	113.10
11	G	20	ARG	N-CA-C	-5.04	97.38	111.00
6	B	68	VAL	N-CA-C	-5.03	97.43	111.00
11	G	16	LEU	N-CA-C	-5.03	97.43	111.00
2	2	67	PHE	CB-CA-C	5.02	120.44	110.40
10	F	136	TRP	CA-CB-CG	5.01	123.21	113.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	67	PHE	CA
2	2	101	PHE	CA
2	2	174	VAL	CA
11	G	21	PHE	CA

All (217) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	56	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	1	57	ILE	Peptide
1	1	60	PRO	Peptide
1	1	63	LEU	Peptide
2	2	111	ALA	Peptide
2	2	112	ASP	Peptide
2	2	126	PRO	Peptide
2	2	131	THR	Peptide
2	2	144	ASP	Peptide
2	2	166	ASN	Peptide
2	2	189	ILE	Peptide
2	2	194	ALA	Peptide
2	2	197	LEU	Peptide
2	2	201	HIS	Peptide
2	2	209	THR	Peptide
2	2	37	ASP	Peptide
2	2	39	GLU	Peptide
2	2	40	SER	Peptide
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide
2	2	74	LEU	Peptide
2	2	75	ASN	Peptide
2	2	80	TYR	Peptide
2	2	84	GLU	Peptide
2	2	92	THR	Peptide
2	2	99	LEU	Peptide
3	3	105	ASN	Peptide
3	3	106	TYR	Peptide
3	3	107	TRP	Peptide
3	3	109	ASP	Peptide
3	3	111	TYR	Peptide
3	3	112	THR	Peptide
3	3	155	GLU	Peptide
3	3	159	PRO	Peptide
3	3	169	PHE	Peptide
3	3	172	ASP	Peptide
3	3	181	LEU	Peptide
3	3	49	ILE	Peptide
3	3	87	GLU	Peptide
3	3	89	ALA	Peptide
3	3	91	PRO	Peptide
3	3	92	TRP	Peptide
3	3	93	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	3	94	ARG	Peptide
3	3	95	THR	Peptide
4	4	106	TRP	Peptide
4	4	142	ASN	Peptide
4	4	144	ALA	Peptide
4	4	149	ALA	Peptide
4	4	152	LYS	Peptide
4	4	155	ALA	Peptide
4	4	190	HIS	Peptide
4	4	192	THR	Peptide
4	4	30	LEU	Peptide
4	4	35	GLU	Peptide
4	4	36	ASN	Peptide
4	4	37	LEU	Peptide
4	4	38	ARG	Peptide
4	4	63	VAL	Peptide
4	4	65	THR	Peptide
4	4	68	GLY	Peptide
4	4	81	GLU	Peptide
4	4	83	TYR	Peptide
4	4	87	SER	Peptide
4	4	88	SER	Peptide
4	4	89	THR	Peptide
4	4	90	LEU	Peptide
5	A	103	PHE	Peptide
5	A	117	GLY	Peptide
5	A	123	VAL	Peptide
5	A	151	GLN	Peptide
5	A	197	GLN	Peptide
5	A	199	VAL	Peptide
5	A	201	SER	Peptide
5	A	21	LEU	Peptide
5	A	22	VAL	Peptide
5	A	23	ASP	Peptide
5	A	24	ARG	Peptide
5	A	240	LYS	Peptide
5	A	242	ILE	Peptide
5	A	26	PRO	Peptide
5	A	27	ILE	Peptide
5	A	315	HIS	Peptide
5	A	347	TYR	Peptide
5	A	37	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	A	393	LEU	Peptide
5	A	41	SER	Peptide
5	A	427	ARG	Peptide
5	A	44	ILE	Peptide
5	A	45	ALA	Peptide
5	A	482	ILE	Peptide
5	A	502	THR	Peptide
5	A	55	TRP	Peptide
5	A	551	VAL	Peptide
5	A	573	ALA	Peptide
5	A	67	HIS	Peptide
5	A	81	ALA	Peptide
6	B	104	PHE	Peptide
6	B	126	THR	Peptide
6	B	232	LEU	Peptide
6	B	265	THR	Peptide
6	B	304	ILE	Peptide
6	B	310	PRO	Peptide
6	B	362	ALA	Peptide
6	B	377	TYR	Peptide
6	B	390	GLY	Peptide
6	B	404	ALA	Peptide
6	B	481	THR	Peptide
6	B	510	LEU	Peptide
6	B	563	GLY	Peptide
6	B	595	HIS	Peptide
6	B	622	ASP	Peptide
6	B	728	SER	Peptide
6	B	730	SER	Peptide
6	B	731	GLY	Peptide
6	B	732	LYS	Peptide
6	B	99	PRO	Peptide
7	C	42	ALA	Peptide
7	C	51	CYS	Peptide
7	C	79	LEU	Peptide
8	D	104	PHE	Peptide
8	D	111	TYR	Peptide
8	D	113	HIS	Peptide
8	D	117	GLY	Peptide
8	D	141	VAL	Peptide
8	D	90	LEU	Peptide
9	E	59	PRO	Peptide

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Mol	Chain	Res	Type	Group
9	E	85	ASP	Peptide
9	E	86	GLU	Peptide
9	E	87	VAL	Peptide
9	E	88	GLU	Peptide
9	E	89	GLU	Peptide
10	F	136	TRP	Peptide
10	F	148	GLU	Peptide
10	F	18	GLU	Peptide
10	F	20	GLN	Peptide
10	F	22	LEU	Peptide
10	F	24	LYS	Peptide
10	F	26	GLN	Peptide
10	F	28	SER	Peptide
10	F	31	LEU	Peptide
10	F	41	ALA	Peptide
10	F	51	LYS	Peptide
10	F	56	TYR	Peptide
11	G	15	SER	Peptide
11	G	22	VAL	Peptide
11	G	26	PHE	Peptide
11	G	36	PRO	Peptide
11	G	39	ASN	Peptide
11	G	40	GLY	Peptide
11	G	42	SER	Peptide
11	G	43	HIS	Peptide
11	G	44	PHE	Peptide
11	G	45	GLU	Peptide
11	G	47	GLY	Peptide
11	G	48	ASP	Peptide
11	G	49	THR	Peptide
11	G	50	ARG	Peptide
11	G	90	SER	Peptide
11	G	94	ASP	Peptide
12	H	12	GLU	Peptide
12	H	20	GLN	Peptide
12	H	21	TRP	Peptide
12	H	22	ASP	Peptide
12	H	25	GLY	Peptide
12	H	27	ASP	Peptide
12	H	43	PHE	Peptide
12	H	48	THR	Peptide
12	H	51	GLY	Peptide

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Mol	Chain	Res	Type	Group
15	K	45	SER	Peptide
15	K	46	GLY	Peptide
15	K	50	GLY	Peptide
16	L	157	LEU	Mainchain
16	L	160	VAL	Peptide
16	L	161	LEU	Peptide
16	L	162	ASP	Peptide
16	L	82	ALA	Peptide
17	N	12	THR	Peptide
17	N	15	GLU	Peptide
17	N	17	ASN	Peptide
17	N	23	ALA	Peptide
17	N	26	GLY	Peptide
17	N	28	ASN	Peptide
17	N	29	PHE	Peptide
17	N	30	ALA	Peptide
17	N	32	ALA	Peptide
17	N	43	PRO	Peptide
17	N	44	GLU	Peptide
17	N	46	PHE	Peptide
17	N	52	LEU	Peptide
17	N	53	ALA	Peptide
17	N	54	LYS	Peptide
17	N	56	LYS	Peptide
17	N	67	LEU	Peptide
17	N	7	LEU	Peptide
17	N	70	GLU	Peptide
17	N	73	ASP	Peptide
17	N	75	TYR	Peptide
18	R	27	UNK	Peptide
18	R	28	UNK	Peptide
18	R	30	UNK	Peptide
18	R	31	UNK	Peptide
18	R	32	UNK	Peptide
18	R	33	UNK	Peptide
18	R	34	UNK	Peptide
18	R	36	UNK	Peptide
18	R	37	UNK	Peptide
18	R	40	UNK	Peptide
18	R	42	UNK	Peptide
18	R	46	UNK	Peptide
18	R	47	UNK	Peptide

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Mol	Chain	Res	Type	Group
18	R	48	UNK	Peptide
18	R	50	UNK	Peptide
18	R	51	UNK	Peptide
18	R	52	UNK	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1255	0	1222	206	0
2	2	1380	0	1341	486	0
3	3	1233	0	1199	283	12
4	4	1322	0	1287	744	8
5	A	5745	0	5595	1666	0
6	B	5848	0	5653	1490	13
7	C	619	0	608	234	0
8	D	1095	0	1112	222	0
9	E	520	0	528	154	0
10	F	1221	0	1246	306	1
11	G	740	0	709	304	11
12	H	529	0	514	122	0
13	I	229	0	252	63	0
14	J	338	0	340	78	0
15	K	593	0	618	120	0
16	L	1203	0	1213	369	8
17	N	685	0	670	447	11
18	R	265	0	65	65	0
19	M	23	0	21	0	0
19	O	22	0	18	11	0
19	P	23	0	21	19	0
19	Q	23	0	21	14	0
19	S	23	0	21	7	0
19	T	23	0	21	7	0
19	U	23	0	21	21	0
19	V	23	0	21	2	0
19	W	23	0	18	5	0
19	X	23	0	21	10	0
19	Y	23	0	20	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	23	0	21	13	0
19	a	23	0	21	0	0
20	1	606	0	376	166	1
20	2	672	0	513	141	0
20	3	659	0	382	132	0
20	4	710	0	463	175	0
20	A	2449	0	2260	988	1
20	B	2360	0	2255	834	0
20	F	130	0	86	31	0
20	G	51	0	40	20	0
20	H	225	0	201	66	0
20	I	60	0	58	12	0
20	J	109	0	95	55	0
20	K	210	0	177	43	1
20	L	322	0	277	113	0
20	R	115	0	106	22	0
21	1	175	0	230	46	0
21	2	175	0	230	25	3
21	3	70	0	92	12	0
21	4	174	0	224	23	5
21	A	210	0	276	84	0
21	B	105	0	138	45	30
21	C	35	0	46	0	0
21	D	35	0	40	12	0
21	E	35	0	41	30	0
21	F	34	0	41	19	0
21	G	35	0	46	19	0
21	H	175	0	230	110	0
21	K	140	0	183	95	0
21	L	105	0	138	10	0
21	N	35	0	45	36	0
21	R	245	0	321	84	5
22	3	40	0	54	19	28
22	A	200	0	269	214	0
22	B	240	0	321	144	0
22	F	80	0	108	76	0
22	I	80	0	108	64	0
22	J	40	0	52	41	0
22	L	40	0	54	51	0
23	A	33	0	46	15	0
23	B	33	0	46	32	0
24	A	8	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	16	0	0	8	0
25	B	49	0	71	30	0
26	H	23	0	0	2	0
All	All	36461	0	35177	9737	69

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 136.

All (9737) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:TRP:CZ3	2:2:125:PHE:CG	1.81	1.63
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.30	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CE1	1.88	1.61
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.24	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CZ	1.85	1.60
2:2:43:TRP:CZ3	2:2:125:PHE:CD1	1.89	1.59
16:L:164:PRO:HD2	16:L:165:TYR:CE2	1.36	1.59
1:1:27:LEU:HD21	6:B:314:ARG:CG	1.25	1.59
20:A:807:CLA:C3B	22:J:102:BCR:C33	1.76	1.59
20:A:819:CLA:H92	22:A:845:BCR:C37	1.16	1.57
4:4:122:LYS:HB2	4:4:143:PHE:CD2	1.31	1.57
21:F:201:LMU:C2	21:F:201:LMU:H82	1.34	1.57
21:K:105:LMU:H22	21:K:105:LMU:C7	1.34	1.56
2:2:43:TRP:CZ2	2:2:125:PHE:CE1	1.87	1.55
20:B:810:CLA:HAC2	20:B:811:CLA:CBB	1.12	1.55
2:2:43:TRP:HH2	2:2:125:PHE:CE2	1.17	1.55
4:4:69:ILE:CD1	4:4:175:LYS:CG	1.81	1.55
1:1:179:THR:CG2	4:4:87:SER:HB3	1.32	1.55
20:1:202:CLA:H8	20:1:202:CLA:C4	1.35	1.55
3:3:132:TRP:CZ3	3:3:155:GLU:HG2	1.37	1.55
23:B:841:PQN:C19	22:B:846:BCR:H10C	1.34	1.55
3:3:132:TRP:CH2	3:3:155:GLU:CD	1.76	1.55
16:L:163:LEU:HB3	16:L:164:PRO:CG	1.35	1.55
2:2:42:ARG:CD	2:2:45:VAL:HG21	1.37	1.54
20:A:819:CLA:C9	22:A:845:BCR:H373	1.32	1.53
6:B:25:ILE:HG21	22:L:210:BCR:C29	1.09	1.53
20:A:822:CLA:C4C	22:A:845:BCR:H19C	1.32	1.53
23:B:841:PQN:H162	22:B:846:BCR:C33	1.28	1.53
20:B:810:CLA:CAC	20:B:811:CLA:CBB	1.84	1.51
17:N:62:SER:HB3	17:N:66:ASP:CB	1.39	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:202:CLA:H41	20:1:202:CLA:C8	1.35	1.51
20:L:201:CLA:C2	20:L:201:CLA:HED1	1.30	1.51
2:2:43:TRP:CZ2	2:2:125:PHE:CZ	1.95	1.51
11:G:45:GLU:CG	11:G:49:THR:HG23	1.38	1.51
5:A:744:ALA:CB	22:A:847:BCR:H391	1.41	1.50
21:A:855:LMU:H91	21:A:855:LMU:C2	1.41	1.50
2:2:205:PHE:CD1	2:2:206:ALA:N	1.77	1.50
5:A:103:PHE:CE1	20:A:807:CLA:O1D	1.64	1.50
20:1:215:CLA:H43	20:1:215:CLA:C11	1.42	1.50
3:3:132:TRP:CZ3	3:3:155:GLU:CG	1.91	1.50
17:N:45:ASN:ND2	17:N:54:LYS:HG2	1.24	1.49
5:A:328:LYS:CE	5:A:332:GLU:HG3	1.40	1.49
4:4:107:GLN:CA	20:4:302:CLA:HMA3	1.40	1.48
18:R:32:UNK:CB	18:R:33:UNK:CB	1.85	1.48
16:L:164:PRO:HB2	16:L:165:TYR:CB	1.39	1.48
4:4:36:ASN:HB2	4:4:39:TRP:CZ3	1.48	1.48
21:B:847:LMU:C6B	21:B:847:LMU:H3'	1.42	1.48
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.01	1.48
6:B:732:LYS:HG2	6:B:733:PHE:C	1.21	1.48
6:B:732:LYS:CG	6:B:734:GLY:N	1.75	1.47
3:3:181:LEU:N	3:3:182:LYS:HG3	1.16	1.46
6:B:25:ILE:CG2	22:L:210:BCR:C29	1.94	1.46
20:1:215:CLA:HED3	20:1:215:CLA:C1A	1.45	1.46
21:K:106:LMU:H32	21:K:106:LMU:C5'	1.43	1.46
21:A:854:LMU:H81	21:A:854:LMU:C2	1.44	1.46
5:A:308:ILE:CD1	20:A:816:CLA:H91	1.44	1.46
20:L:201:CLA:HAA1	20:L:201:CLA:CGD	1.44	1.46
21:K:105:LMU:C6'	21:K:105:LMU:H32	1.42	1.45
4:4:34:PRO:CA	4:4:35:GLU:HB2	1.46	1.45
4:4:69:ILE:CD1	4:4:175:LYS:CB	1.90	1.45
20:1:202:CLA:HED3	20:1:202:CLA:C2A	1.47	1.45
1:1:112:ARG:HH12	20:1:209:CLA:CGD	1.24	1.45
20:4:304:CLA:CED	20:4:304:CLA:HAA2	1.45	1.45
21:K:106:LMU:C2'	21:K:106:LMU:H22	1.36	1.44
20:1:202:CLA:HMA2	20:1:202:CLA:CGA	1.45	1.44
16:L:164:PRO:HD2	16:L:165:TYR:CZ	1.52	1.43
15:K:44:GLU:CG	15:K:45:SER:N	1.71	1.43
7:C:14:CYS:HA	7:C:17:CYS:SG	1.56	1.43
4:4:40:PHE:HB3	4:4:43:ALA:CB	1.48	1.43
5:A:368:LEU:HD21	20:A:818:CLA:C9	1.49	1.43
20:A:838:CLA:H141	22:A:847:BCR:C2	1.48	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:103:CLA:HED3	20:J:103:CLA:C1A	1.47	1.43
2:2:43:TRP:CH2	2:2:125:PHE:CD1	2.03	1.42
11:G:48:ASP:CB	11:G:49:THR:HG22	1.45	1.42
16:L:164:PRO:HG2	16:L:165:TYR:CD1	1.55	1.41
6:B:732:LYS:CG	6:B:733:PHE:C	1.82	1.41
17:N:45:ASN:HD22	17:N:54:LYS:CG	1.28	1.41
11:G:93:TYR:HA	11:G:94:ASP:CB	1.42	1.41
2:2:103:GLY:N	20:2:311:CLA:HBB2	1.33	1.41
21:B:847:LMU:H112	21:B:847:LMU:C6	1.48	1.41
20:B:836:CLA:H152	22:F:203:BCR:C31	1.51	1.41
20:A:815:CLA:HAA1	20:A:815:CLA:CED	1.47	1.41
4:4:122:LYS:HB3	4:4:143:PHE:CB	1.51	1.40
2:2:43:TRP:CH2	2:2:125:PHE:CE2	1.98	1.40
4:4:194:VAL:HG12	4:4:195:GLN:CB	1.51	1.40
7:C:54:CYS:HB2	24:C:102:SF4:S3	1.61	1.40
5:A:23:ASP:CG	5:A:24:ARG:HD3	1.42	1.40
17:N:48:GLY:HA2	17:N:49:CYS:SG	1.62	1.39
4:4:149:ALA:HB3	4:4:151:GLU:CG	1.52	1.39
20:K:101:CLA:CED	20:K:108:CLA:HMB2	1.49	1.39
20:A:822:CLA:CHD	22:A:845:BCR:H19C	1.51	1.39
4:4:40:PHE:CB	4:4:43:ALA:HB2	1.52	1.39
20:L:201:CLA:H2	20:L:201:CLA:CED	1.51	1.39
4:4:36:ASN:HB2	4:4:39:TRP:CE3	1.57	1.38
17:N:61:LEU:HD11	17:N:63:ASP:C	1.40	1.38
3:3:132:TRP:CH2	3:3:155:GLU:OE2	1.68	1.38
16:L:163:LEU:CG	16:L:164:PRO:HB3	1.51	1.38
20:2:322:CLA:H41	20:2:322:CLA:C7	1.49	1.38
3:3:84:ILE:CB	20:3:302:CLA:O1A	1.69	1.38
2:2:42:ARG:CG	2:2:45:VAL:HG21	1.48	1.38
4:4:128:ALA:HB2	4:4:143:PHE:CE2	1.56	1.38
6:B:732:LYS:HB3	6:B:733:PHE:CA	1.48	1.38
4:4:93:ILE:HA	4:4:96:ILE:CD1	1.53	1.37
17:N:58:VAL:HB	17:N:59:PRO:CD	1.47	1.37
21:N:101:LMU:H51	21:N:101:LMU:C6'	1.51	1.37
20:1:202:CLA:HBA2	20:1:202:CLA:CED	1.54	1.37
20:A:815:CLA:CBC	20:A:815:CLA:HMC1	1.51	1.37
4:4:37:LEU:C	4:4:39:TRP:HB3	1.39	1.37
17:N:62:SER:HB3	17:N:66:ASP:CG	1.45	1.37
5:A:744:ALA:HB2	22:A:847:BCR:C39	1.53	1.36
17:N:45:ASN:ND2	17:N:54:LYS:CG	1.82	1.36
9:E:52:VAL:O	9:E:53:VAL:CG2	1.73	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:102:CLA:CHD	20:G:102:CLA:HBC3	1.52	1.36
20:4:307:CLA:CBA	20:4:307:CLA:HMA2	1.55	1.36
17:N:72:LYS:HB3	17:N:73:ASP:CA	1.48	1.36
2:2:43:TRP:CH2	2:2:125:PHE:CD2	2.13	1.36
20:A:814:CLA:C4B	22:A:843:BCR:H19C	1.55	1.36
17:N:72:LYS:HG3	17:N:74:LYS:CB	1.56	1.35
20:A:826:CLA:H203	22:J:102:BCR:C17	1.55	1.35
2:2:42:ARG:HA	2:2:45:VAL:CG2	1.54	1.35
14:J:31:ARG:HH22	20:J:103:CLA:C4B	1.38	1.35
3:3:194:ILE:CD1	20:3:304:CLA:HMC2	1.54	1.35
4:4:121:PHE:CE2	4:4:122:LYS:O	1.79	1.35
16:L:164:PRO:HB2	16:L:165:TYR:CA	1.44	1.35
21:1:219:LMU:C6B	21:1:219:LMU:H3'	1.55	1.34
21:E:101:LMU:H32	21:E:101:LMU:C7	1.52	1.34
16:L:161:LEU:HD12	16:L:162:ASP:CA	1.54	1.34
21:N:101:LMU:H121	21:N:101:LMU:C8	1.56	1.34
17:N:61:LEU:HD11	17:N:63:ASP:CA	1.56	1.34
17:N:47:THR:HG21	17:N:54:LYS:NZ	1.37	1.34
4:4:122:LYS:CB	4:4:143:PHE:CD2	2.07	1.34
16:L:164:PRO:HD2	16:L:165:TYR:CD2	1.60	1.34
1:1:27:LEU:CD2	6:B:314:ARG:CG	2.04	1.34
4:4:101:VAL:HG13	4:4:104:ARG:NH2	1.40	1.34
19:U:2:FRU:H11	19:U:2:FRU:C6	1.55	1.34
20:A:839:CLA:CBC	20:A:839:CLA:HHD	1.55	1.34
21:K:106:LMU:H5'	21:K:106:LMU:C3	1.58	1.33
1:1:185:TRP:HB2	1:1:186:HIS:CE1	1.63	1.33
20:3:313:CLA:CMC	20:3:313:CLA:HBC3	1.50	1.33
21:K:109:LMU:H81	21:K:109:LMU:C4	1.47	1.33
20:B:821:CLA:HMC1	20:B:821:CLA:CBC	1.59	1.33
20:4:304:CLA:C20	20:4:304:CLA:H151	1.58	1.32
11:G:6:LEU:HB3	11:G:9:SER:CB	1.59	1.32
13:I:11:LEU:CD1	22:I:103:BCR:H10C	1.60	1.32
2:2:205:PHE:HD1	2:2:206:ALA:N	1.15	1.32
20:2:322:CLA:H72	20:2:322:CLA:C4	1.58	1.32
9:E:52:VAL:O	9:E:53:VAL:HG23	1.23	1.32
2:2:42:ARG:CA	2:2:45:VAL:HG23	1.58	1.32
4:4:107:GLN:C	20:4:302:CLA:CMA	1.96	1.32
5:A:316:MET:HG2	5:A:317:TYR:CD1	1.62	1.32
20:A:839:CLA:HBA1	20:A:839:CLA:CMA	1.55	1.32
20:1:215:CLA:CBC	20:1:215:CLA:HHD	1.55	1.32
20:J:101:CLA:HBA2	20:J:101:CLA:CBD	1.58	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:24:LYS:CA	10:F:24:LYS:HE2	1.47	1.32
16:L:163:LEU:HB3	16:L:164:PRO:CB	1.59	1.31
16:L:163:LEU:HD22	16:L:164:PRO:CA	1.58	1.31
4:4:102:GLU:OE2	20:4:314:CLA:C3B	1.75	1.31
16:L:163:LEU:CD1	16:L:164:PRO:HB3	1.60	1.31
21:N:101:LMU:C9	21:N:101:LMU:H52	1.44	1.31
20:1:201:CLA:CMC	20:1:201:CLA:HBC3	1.46	1.31
4:4:194:VAL:HB	4:4:195:GLN:C	1.50	1.31
21:F:201:LMU:C7	21:F:201:LMU:H31	1.45	1.30
17:N:66:ASP:C	17:N:67:LEU:HD12	1.49	1.30
4:4:94:GLU:HB3	4:4:95:PHE:CE1	1.64	1.30
2:2:55:ALA:HB3	2:2:56:MET:CE	1.60	1.30
5:A:316:MET:HB3	5:A:317:TYR:CB	1.62	1.30
1:1:57:ILE:HD13	1:1:58:LEU:N	1.47	1.30
21:H:106:LMU:C2B	21:H:106:LMU:H31	1.60	1.30
1:1:112:ARG:NH1	20:1:209:CLA:CGD	1.91	1.29
5:A:567:ARG:NH1	8:D:35:GLY:HA2	1.48	1.29
4:4:149:ALA:HB3	4:4:151:GLU:CD	1.52	1.29
20:3:313:CLA:H142	20:3:313:CLA:C10	1.62	1.29
23:B:841:PQN:C16	22:B:846:BCR:C33	2.10	1.29
21:B:847:LMU:C3'	21:B:847:LMU:H5B	1.63	1.29
20:L:201:CLA:CBC	20:L:201:CLA:HHD	1.61	1.29
20:B:836:CLA:H93	20:B:836:CLA:CBB	1.61	1.29
20:H:101:CLA:HMC1	20:H:101:CLA:CBC	1.58	1.29
20:3:313:CLA:HAA2	20:3:313:CLA:CED	1.60	1.29
5:A:24:ARG:C	5:A:26:PRO:HG2	1.53	1.29
21:A:855:LMU:C3	21:A:855:LMU:H82	1.61	1.29
11:G:45:GLU:CG	11:G:49:THR:CG2	2.10	1.29
22:A:844:BCR:C40	22:A:844:BCR:H23C	1.60	1.28
20:A:814:CLA:C3B	22:A:843:BCR:H19C	1.61	1.28
3:3:205:GLY:N	5:A:252:ARG:HH22	1.30	1.28
21:K:106:LMU:C9	21:K:106:LMU:H31	1.61	1.28
20:L:201:CLA:C1	20:L:201:CLA:HED1	1.62	1.28
5:A:711:HIS:CD2	20:A:837:CLA:HBC1	1.67	1.28
11:G:6:LEU:CB	11:G:9:SER:HB3	1.60	1.28
20:4:319:CLA:HED2	20:4:319:CLA:C2A	1.61	1.28
16:L:163:LEU:HD22	16:L:164:PRO:CB	1.62	1.28
2:2:128:ASN:C	2:2:130:LEU:H	1.30	1.28
21:A:855:LMU:H21	21:A:855:LMU:C9	1.60	1.28
20:A:822:CLA:CBB	22:A:845:BCR:C35	2.10	1.27
20:3:313:CLA:HMC1	20:3:313:CLA:CBC	1.63	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:314:BCR:H23C	22:3:314:BCR:C39	1.55	1.27
21:F:201:LMU:C3	21:F:201:LMU:H82	1.62	1.27
2:2:118:CYS:O	2:2:119:VAL:HG13	1.18	1.27
17:N:65:LEU:HD23	17:N:65:LEU:C	1.53	1.27
5:A:331:LEU:CD2	5:A:343:HIS:O	1.81	1.27
6:B:732:LYS:CB	6:B:733:PHE:HA	1.63	1.27
21:E:101:LMU:H72	21:E:101:LMU:C3	1.55	1.27
16:L:161:LEU:HD12	16:L:162:ASP:N	1.50	1.27
3:3:132:TRP:CH2	3:3:155:GLU:CG	2.12	1.27
7:C:17:CYS:HB2	7:C:58:CYS:SG	1.74	1.27
12:H:20:GLN:HB3	12:H:22:ASP:CB	1.64	1.27
4:4:147:LEU:HD21	4:4:148:GLU:CG	1.63	1.27
4:4:37:LEU:N	4:4:39:TRP:HB2	1.46	1.27
17:N:67:LEU:HB2	17:N:68:GLU:CG	1.65	1.27
20:A:824:CLA:HED1	20:A:825:CLA:C2D	1.65	1.26
20:4:307:CLA:CGD	20:4:307:CLA:HAA2	1.66	1.26
20:4:319:CLA:H2A	20:4:319:CLA:CED	1.65	1.26
20:1:202:CLA:H92	20:1:202:CLA:C12	1.58	1.26
12:H:25:GLY:CA	12:H:27:ASP:H	1.47	1.26
21:A:855:LMU:C9	21:A:855:LMU:H41	1.64	1.26
17:N:45:ASN:ND2	17:N:54:LYS:CB	1.99	1.26
21:R:102:LMU:C5B	21:R:102:LMU:H6E	1.64	1.26
5:A:79:PHE:CE2	5:A:185:HIS:CD2	2.24	1.26
21:K:106:LMU:C3'	21:K:106:LMU:H22	1.64	1.25
17:N:41:LYS:HB2	17:N:42:PHE:CB	1.66	1.25
4:4:40:PHE:O	4:4:43:ALA:HB3	1.34	1.25
17:N:67:LEU:CB	17:N:68:GLU:HG2	1.66	1.25
21:N:101:LMU:C1'	21:N:101:LMU:H32	1.64	1.25
20:A:819:CLA:CMD	20:A:821:CLA:HBB2	1.66	1.25
20:A:839:CLA:C12	20:A:839:CLA:H71	1.47	1.25
20:4:306:CLA:CMC	20:4:306:CLA:HBC2	1.59	1.25
17:N:72:LYS:CG	17:N:74:LYS:HG3	1.67	1.25
20:2:302:CLA:O1A	20:2:302:CLA:H42	1.37	1.25
11:G:93:TYR:CA	11:G:94:ASP:HB2	1.64	1.25
15:K:7:THR:CA	15:K:10:ILE:HD13	1.55	1.25
20:1:215:CLA:H43	20:1:215:CLA:C10	1.67	1.25
21:K:106:LMU:H82	21:K:106:LMU:C3	1.66	1.25
3:3:74:ALA:HA	20:3:307:CLA:C3D	1.68	1.24
4:4:104:ARG:HH11	4:4:105:ARG:CB	1.47	1.24
4:4:94:GLU:HG2	4:4:95:PHE:CD1	1.72	1.24
22:I:103:BCR:C31	22:I:103:BCR:HC8	1.61	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:105:LMU:H22	21:K:105:LMU:C6	1.58	1.24
20:1:201:CLA:CBC	20:1:201:CLA:HMC1	1.64	1.24
5:A:25:ASP:N	5:A:26:PRO:HG2	1.52	1.24
4:4:34:PRO:CB	4:4:35:GLU:HB2	1.67	1.24
22:F:203:BCR:C8	22:F:203:BCR:H321	1.55	1.24
3:3:181:LEU:N	3:3:182:LYS:CG	2.01	1.24
4:4:149:ALA:CB	4:4:151:GLU:HG2	1.66	1.24
21:H:108:LMU:H32	21:H:108:LMU:C10	1.67	1.24
1:1:27:LEU:CD2	6:B:314:ARG:HG2	1.60	1.24
4:4:39:TRP:C	4:4:40:PHE:HD1	1.38	1.24
21:G:101:LMU:C6B	21:G:101:LMU:H3'	1.66	1.24
20:1:215:CLA:H41	20:1:215:CLA:C8	1.66	1.24
4:4:121:PHE:O	4:4:122:LYS:HD2	1.36	1.24
4:4:192:THR:HG22	4:4:193:ILE:O	1.35	1.23
15:K:11:MET:SD	15:K:12:VAL:HA	1.76	1.23
20:4:304:CLA:CAA	20:4:304:CLA:HED3	1.68	1.23
20:4:318:CLA:CED	20:4:318:CLA:H12	1.67	1.23
6:B:732:LYS:CB	6:B:733:PHE:CA	2.14	1.23
12:H:20:GLN:CB	12:H:22:ASP:HB3	1.65	1.23
21:N:101:LMU:H92	21:N:101:LMU:C5	1.67	1.23
4:4:102:GLU:OE2	20:4:314:CLA:C4B	1.85	1.23
21:A:854:LMU:H81	21:A:854:LMU:C3	1.69	1.23
21:H:108:LMU:H81	21:H:108:LMU:C3	1.66	1.23
21:K:105:LMU:C2	21:K:105:LMU:H71	1.69	1.23
20:4:306:CLA:HMC1	20:4:306:CLA:CBC	1.58	1.23
20:K:108:CLA:H3A	20:K:108:CLA:O1A	1.38	1.23
7:C:62:PHE:CE2	9:E:42:GLU:OE1	1.90	1.23
6:B:25:ILE:CG2	22:L:210:BCR:C28	2.16	1.23
4:4:147:LEU:CD1	4:4:148:GLU:H	1.52	1.23
21:N:101:LMU:H6E	21:N:101:LMU:C5	1.68	1.22
21:K:109:LMU:C8	21:K:109:LMU:H42	1.67	1.22
6:B:25:ILE:CG2	22:L:210:BCR:H292	1.59	1.22
3:3:74:ALA:HA	20:3:307:CLA:C2D	1.67	1.22
20:A:826:CLA:C20	22:J:102:BCR:H17C	1.68	1.22
21:R:104:LMU:H2'	21:R:104:LMU:C2	1.65	1.22
6:B:732:LYS:HG2	6:B:734:GLY:N	0.90	1.22
21:A:855:LMU:C6B	21:A:855:LMU:H2B	1.65	1.22
7:C:7:ILE:O	7:C:8:TYR:O	1.55	1.22
4:4:68:GLY:O	4:4:71:ASN:HB2	1.34	1.22
21:H:106:LMU:C1B	21:H:106:LMU:H31	1.68	1.22
5:A:342:GLY:CA	5:A:430:ASP:HB2	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:807:CLA:C1	20:A:809:CLA:HED3	1.69	1.22
4:4:30:LEU:CA	4:4:31:ALA:HB3	1.69	1.22
21:H:108:LMU:C8	21:H:108:LMU:H32	1.68	1.22
4:4:144:ALA:HB3	4:4:147:LEU:O	1.38	1.22
6:B:517:PHE:O	6:B:517:PHE:CD2	1.93	1.22
4:4:124:TYR:O	4:4:127:PRO:HD2	1.36	1.22
5:A:331:LEU:HD11	5:A:346:LEU:CB	1.68	1.21
20:A:824:CLA:HED2	20:A:825:CLA:CAD	1.70	1.21
20:A:824:CLA:HED1	20:A:825:CLA:C3D	1.69	1.21
21:H:108:LMU:H92	21:H:108:LMU:C5	1.49	1.21
20:L:201:CLA:C2	20:L:201:CLA:CED	2.13	1.21
2:2:43:TRP:CH2	2:2:125:PHE:CG	2.18	1.21
4:4:170:HIS:O	4:4:171:ASN:O	1.58	1.21
21:B:847:LMU:C11	21:B:847:LMU:H61	1.69	1.21
21:H:108:LMU:H101	21:H:108:LMU:C3	1.69	1.21
16:L:163:LEU:CD2	16:L:164:PRO:HB3	1.71	1.21
5:A:328:LYS:CG	5:A:332:GLU:HB2	1.70	1.21
20:R:107:CLA:C1A	20:R:107:CLA:HED3	1.68	1.21
5:A:21:LEU:HD12	5:A:21:LEU:O	1.38	1.21
20:4:302:CLA:HHD	20:4:302:CLA:CBC	1.71	1.21
17:N:57:LYS:CG	17:N:58:VAL:H	1.52	1.21
21:R:102:LMU:H5B	21:R:102:LMU:C6'	1.70	1.21
5:A:316:MET:HB3	5:A:317:TYR:CG	1.74	1.21
20:4:307:CLA:CMA	20:4:307:CLA:HBA1	1.55	1.21
1:1:179:THR:HG21	4:4:87:SER:CB	1.70	1.21
20:A:822:CLA:CBB	22:A:845:BCR:H351	1.71	1.21
18:R:41:UNK:CB	18:R:42:UNK:HA	1.68	1.21
20:1:215:CLA:HED3	20:1:215:CLA:C2A	1.69	1.21
4:4:171:ASN:O	4:4:173:THR:N	1.74	1.21
3:3:48:PHE:CD2	3:3:49:ILE:HG22	1.74	1.21
17:N:61:LEU:HD12	17:N:62:SER:C	1.62	1.21
5:A:76:ARG:NH1	5:A:192:LYS:HG2	1.56	1.20
9:E:86:GLU:HG3	9:E:87:VAL:N	1.49	1.20
4:4:122:LYS:CB	4:4:143:PHE:HD2	1.46	1.20
20:A:815:CLA:CAA	20:A:815:CLA:HED2	1.69	1.20
4:4:94:GLU:HG2	4:4:95:PHE:CE1	1.75	1.20
17:N:45:ASN:ND2	17:N:54:LYS:HB2	1.53	1.20
20:A:839:CLA:HMA2	20:A:839:CLA:CBA	1.66	1.20
6:B:403:ASN:O	6:B:406:ASN:CB	1.89	1.20
20:B:836:CLA:C15	22:F:203:BCR:C31	2.18	1.20
17:N:79:SER:HA	17:N:80:ASN:O	1.37	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:120:VAL:HA	6:B:123:TRP:CD1	1.75	1.20
21:F:201:LMU:H22	21:F:201:LMU:C8	1.72	1.20
4:4:118:ASP:OD1	4:4:123:GLN:HB2	1.38	1.20
4:4:147:LEU:CG	4:4:148:GLU:H	1.53	1.20
1:1:179:THR:CG2	4:4:87:SER:CB	2.20	1.19
17:N:70:GLU:OE2	17:N:72:LYS:O	1.58	1.19
4:4:104:ARG:HD2	20:4:313:CLA:C2C	1.71	1.19
21:A:854:LMU:H32	21:A:854:LMU:C9	1.72	1.19
1:1:63:LEU:HD22	1:1:63:LEU:C	1.50	1.19
4:4:107:GLN:HA	20:4:302:CLA:CMA	1.70	1.19
20:4:318:CLA:HED3	20:4:318:CLA:C1	1.71	1.19
4:4:192:THR:HG22	4:4:193:ILE:C	1.60	1.19
11:G:46:ALA:N	11:G:48:ASP:HB3	1.56	1.19
5:A:301:HIS:NE2	20:A:816:CLA:O1D	1.76	1.19
18:R:52:UNK:HA	18:R:53:UNK:CB	1.69	1.19
20:1:210:CLA:CAD	20:1:210:CLA:HED2	1.66	1.19
5:A:541:VAL:HG11	5:A:615:HIS:CD2	1.78	1.19
20:B:823:CLA:HBB1	20:B:837:CLA:CMB	1.73	1.19
20:G:102:CLA:HHD	20:G:102:CLA:CBC	1.71	1.19
20:1:215:CLA:HBA1	20:1:215:CLA:CGD	1.71	1.19
17:N:48:GLY:CA	17:N:49:CYS:SG	2.30	1.19
21:R:103:LMU:C1'	21:R:103:LMU:H31	1.67	1.19
5:A:331:LEU:O	5:A:331:LEU:HD23	1.42	1.18
20:B:821:CLA:C1A	20:B:821:CLA:H43	1.72	1.18
22:3:314:BCR:C23	22:3:314:BCR:H393	1.67	1.18
6:B:25:ILE:CG2	22:L:210:BCR:H282	1.72	1.18
10:F:24:LYS:HE2	10:F:24:LYS:N	1.56	1.18
2:2:169:LEU:HD22	20:2:305:CLA:CAB	1.72	1.18
22:F:203:BCR:C27	22:F:203:BCR:H403	1.52	1.18
5:A:342:GLY:HA3	5:A:430:ASP:CB	1.73	1.18
21:G:101:LMU:H6'2	21:G:101:LMU:C3'	1.74	1.18
1:1:25:ASP:H	6:B:314:ARG:NH2	1.40	1.18
4:4:34:PRO:HA	4:4:35:GLU:CB	1.70	1.18
1:1:57:ILE:C	1:1:57:ILE:HD13	1.62	1.18
22:A:847:BCR:C31	20:A:852:CLA:C14	2.20	1.18
20:B:821:CLA:H151	20:B:821:CLA:C10	1.65	1.18
11:G:45:GLU:HG2	11:G:49:THR:HG23	1.19	1.17
21:H:108:LMU:H32	21:H:108:LMU:C9	1.73	1.17
3:3:132:TRP:CZ3	3:3:155:GLU:CD	2.06	1.17
20:B:823:CLA:HHD	20:B:823:CLA:CBC	1.74	1.17
16:L:163:LEU:CB	16:L:164:PRO:HG3	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:57:LYS:HG3	17:N:58:VAL:N	1.44	1.17
20:A:824:CLA:HED1	20:A:825:CLA:CMD	1.74	1.17
14:J:31:ARG:NH2	20:J:103:CLA:C4B	2.06	1.17
4:4:107:GLN:CA	20:4:302:CLA:CMA	2.21	1.17
20:B:836:CLA:HBB2	20:B:836:CLA:C9	1.75	1.17
7:C:1:MET:H2	7:C:3:HIS:N	1.42	1.17
20:A:822:CLA:C4C	22:A:845:BCR:C19	2.23	1.17
17:N:72:LYS:CB	17:N:73:ASP:HA	1.73	1.17
20:A:824:CLA:H72	20:A:825:CLA:CED	1.73	1.16
15:K:10:ILE:HA	15:K:13:THR:CG2	1.72	1.16
16:L:164:PRO:CG	16:L:165:TYR:CG	2.28	1.16
4:4:147:LEU:CD2	4:4:148:GLU:HG3	1.75	1.16
4:4:30:LEU:HD12	4:4:30:LEU:O	1.45	1.16
5:A:79:PHE:CE2	5:A:185:HIS:NE2	2.13	1.16
17:N:41:LYS:CB	17:N:42:PHE:HB3	1.75	1.16
5:A:702:GLU:OE2	6:B:550:LYS:NZ	1.76	1.16
3:3:132:TRP:HH2	3:3:155:GLU:OE2	0.82	1.16
6:B:25:ILE:HG21	22:L:210:BCR:C28	1.70	1.16
4:4:194:VAL:CG1	4:4:195:GLN:HB2	1.75	1.16
20:B:836:CLA:H161	22:F:203:BCR:H313	1.24	1.16
20:B:850:CLA:C9	20:B:851:CLA:H91	1.75	1.16
11:G:46:ALA:N	11:G:49:THR:HG21	1.58	1.16
20:L:209:CLA:HBC3	20:L:209:CLA:HHD	1.20	1.16
3:3:132:TRP:HH2	3:3:155:GLU:CD	1.21	1.16
5:A:81:ALA:CB	20:A:804:CLA:CMA	2.24	1.16
11:G:33:LYS:CE	11:G:33:LYS:HA	1.66	1.16
24:A:857:SF4:S3	24:A:857:SF4:S2	2.44	1.16
21:H:104:LMU:O3B	19:Y:2:FRU:H5	1.37	1.16
20:G:102:CLA:H3A	20:G:102:CLA:O2A	1.44	1.16
17:N:63:ASP:H	17:N:64:ASP:CB	1.57	1.16
17:N:70:GLU:O	17:N:72:LYS:HD3	1.41	1.16
5:A:81:ALA:CB	20:A:804:CLA:HMA1	1.75	1.15
3:3:110:SER:C	3:3:111:TYR:HD2	1.48	1.15
4:4:36:ASN:OD1	4:4:37:LEU:HA	1.44	1.15
1:1:179:THR:CB	4:4:87:SER:HB3	1.77	1.15
20:H:102:CLA:HAC2	22:I:103:BCR:HC31	1.28	1.15
16:L:163:LEU:HD13	16:L:164:PRO:HB3	1.27	1.15
20:R:108:CLA:C9	21:R:109:LMU:O4'	1.94	1.15
2:2:110:TRP:HD1	2:2:113:ILE:HG21	1.11	1.15
5:A:316:MET:CG	5:A:317:TYR:CD1	2.30	1.15
6:B:87:ILE:HA	6:B:115:ASN:HA	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:672:GLN:HA	6:B:672:GLN:HE21	1.09	1.15
8:D:134:MET:N	8:D:134:MET:SD	2.19	1.15
21:R:104:LMU:H21	21:R:104:LMU:C2'	1.59	1.15
21:A:854:LMU:H21	21:A:854:LMU:C8	1.75	1.15
21:R:101:LMU:H11	21:R:101:LMU:H62	1.17	1.15
19:Y:2:FRU:C6	19:Y:2:FRU:H12	1.71	1.15
4:4:94:GLU:CB	4:4:95:PHE:CE1	2.29	1.15
4:4:174:GLY:O	4:4:175:LYS:HG3	1.47	1.15
4:4:38:ARG:HG3	4:4:39:TRP:N	1.48	1.15
5:A:160:SER:O	5:A:163:GLN:HG2	1.44	1.15
4:4:36:ASN:CB	4:4:39:TRP:CE3	2.29	1.15
23:B:841:PQN:C19	22:B:846:BCR:C10	2.24	1.15
7:C:1:MET:CB	7:C:4:SER:OG	1.94	1.15
21:N:101:LMU:H32	21:N:101:LMU:O5'	1.47	1.15
20:1:202:CLA:HED3	20:1:202:CLA:C1A	1.77	1.14
3:3:194:ILE:HD11	20:3:304:CLA:HMC2	1.26	1.14
4:4:36:ASN:C	4:4:39:TRP:HB2	1.66	1.14
16:L:164:PRO:CD	16:L:165:TYR:CE2	2.29	1.14
21:H:104:LMU:O3B	19:Y:2:FRU:C5	1.77	1.14
11:G:33:LYS:HE3	11:G:33:LYS:HA	1.24	1.14
1:1:185:TRP:CB	1:1:186:HIS:CE1	2.29	1.14
4:4:89:THR:O	4:4:92:VAL:HB	1.48	1.14
5:A:316:MET:HB3	5:A:317:TYR:CD1	1.82	1.14
12:H:25:GLY:HA3	12:H:27:ASP:N	1.60	1.14
21:1:217:LMU:H3'	21:1:217:LMU:H12	1.21	1.14
20:3:313:CLA:HBA1	20:3:313:CLA:HED1	1.19	1.14
20:A:816:CLA:HBC3	20:A:816:CLA:HMC1	1.30	1.14
20:A:824:CLA:HBA2	20:A:836:CLA:HED1	1.28	1.14
22:A:844:BCR:H403	22:A:844:BCR:H23C	1.28	1.14
21:B:847:LMU:C7	21:B:847:LMU:H112	1.77	1.14
21:F:201:LMU:H31	21:F:201:LMU:C8	1.77	1.14
17:N:72:LYS:HG3	17:N:74:LYS:CG	1.78	1.14
4:4:99:HIS:CE1	4:4:103:ILE:CD1	2.30	1.14
20:B:807:CLA:HBB2	20:B:807:CLA:C9	1.77	1.14
20:J:101:CLA:HBD	20:J:101:CLA:CBA	1.76	1.14
2:2:102:ILE:C	20:2:311:CLA:HBB2	1.66	1.14
20:A:830:CLA:H52	22:B:846:BCR:H343	1.19	1.14
20:A:824:CLA:C4B	22:A:846:BCR:H373	1.77	1.14
6:B:493:TRP:O	6:B:495:PRO:HD3	1.48	1.14
20:B:803:CLA:HMD3	22:F:202:BCR:HC41	1.20	1.14
16:L:164:PRO:CG	16:L:165:TYR:CD1	2.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:92:TRP:HA	3:3:93:PHE:CD1	1.80	1.14
2:2:43:TRP:HH2	2:2:125:PHE:CD2	1.56	1.14
20:A:822:CLA:CHD	22:A:845:BCR:C19	2.25	1.14
6:B:22:TRP:NE1	20:B:838:CLA:HBB1	1.60	1.14
16:L:163:LEU:CD2	16:L:164:PRO:HA	1.76	1.14
4:4:74:LYS:N	4:4:75:TRP:HA	1.50	1.13
5:A:76:ARG:CZ	5:A:192:LYS:HG2	1.77	1.13
21:A:853:LMU:O2B	21:A:853:LMU:H3'	1.47	1.13
16:L:27:VAL:HA	20:L:203:CLA:HMA3	1.17	1.13
17:N:61:LEU:C	17:N:61:LEU:HD12	1.65	1.13
5:A:435:VAL:O	5:A:438:HIS:O	1.66	1.13
20:B:821:CLA:H102	20:B:821:CLA:C15	1.76	1.13
20:R:108:CLA:H92	21:R:109:LMU:O4'	1.49	1.13
21:4:320:LMU:H5B	21:4:320:LMU:O3'	1.45	1.13
5:A:251:ASN:O	5:A:253:ASP:N	1.80	1.13
5:A:316:MET:CB	5:A:317:TYR:CD1	2.30	1.13
24:A:857:SF4:S4	24:A:857:SF4:S2	2.46	1.13
20:B:827:CLA:CBC	20:B:827:CLA:HMC1	1.77	1.13
15:K:9:LEU:HD23	15:K:9:LEU:N	1.53	1.13
21:N:101:LMU:H121	21:N:101:LMU:H82	1.26	1.13
2:2:169:LEU:CD2	20:2:305:CLA:CBB	2.27	1.13
24:A:857:SF4:S4	24:A:857:SF4:S1	2.46	1.13
20:B:810:CLA:CAC	20:B:811:CLA:HBB2	1.60	1.13
2:2:38:PRO:HB2	2:2:40:SER:OG	1.45	1.13
4:4:94:GLU:CG	4:4:95:PHE:CE1	2.30	1.13
19:Q:2:FRU:H62	19:Q:2:FRU:C1	1.69	1.13
2:2:39:GLU:N	2:2:40:SER:HB2	1.63	1.13
4:4:104:ARG:HH11	4:4:105:ARG:HB2	1.13	1.13
4:4:37:LEU:O	4:4:39:TRP:HB3	1.48	1.13
22:A:847:BCR:H313	20:A:852:CLA:C14	1.76	1.13
6:B:596:TRP:CH2	6:B:612:SER:O	2.02	1.13
7:C:14:CYS:CA	7:C:17:CYS:SG	2.36	1.13
3:3:110:SER:O	3:3:111:TYR:HD2	1.31	1.13
20:B:819:CLA:HHD	20:B:819:CLA:HBC2	1.13	1.13
19:P:2:FRU:C1	19:P:2:FRU:H62	1.75	1.13
19:P:2:FRU:H62	19:P:2:FRU:H11	1.27	1.13
5:A:423:ASP:HB3	5:A:424:PRO:HD3	1.20	1.13
5:A:402:ILE:HG13	20:A:827:CLA:HBB2	1.29	1.13
16:L:66:GLY:HA3	20:L:209:CLA:CHC	1.79	1.13
17:N:61:LEU:HD12	17:N:62:SER:N	1.63	1.13
22:F:203:BCR:HC8	22:F:203:BCR:C32	1.66	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:164:PRO:CD	16:L:165:TYR:CZ	2.32	1.12
20:1:210:CLA:O1D	20:1:210:CLA:HAA2	1.46	1.12
20:3:310:CLA:CHA	20:3:318:CLA:CBC	2.27	1.12
5:A:451:ILE:HD12	20:A:830:CLA:HED3	1.29	1.12
20:B:836:CLA:C16	22:F:203:BCR:H313	1.78	1.12
19:T:1:GLC:H5	19:T:2:FRU:O1	1.49	1.12
24:A:857:SF4:S4	24:A:857:SF4:S3	2.46	1.12
2:2:40:SER:O	2:2:41:LEU:HD22	1.45	1.12
5:A:590:CYS:SG	24:A:857:SF4:S4	2.47	1.12
15:K:11:MET:SD	15:K:12:VAL:CA	2.36	1.12
17:N:58:VAL:CB	17:N:59:PRO:HD2	1.77	1.12
19:Z:1:GLC:O2	19:Z:2:FRU:H5	1.48	1.12
20:1:215:CLA:O2D	20:1:215:CLA:HBA1	1.47	1.12
15:K:10:ILE:O	15:K:13:THR:HG23	1.50	1.12
2:2:41:LEU:C	2:2:41:LEU:HD23	1.64	1.12
4:4:122:LYS:CB	4:4:143:PHE:HB2	1.79	1.12
4:4:89:THR:N	4:4:90:LEU:HD22	1.64	1.12
5:A:316:MET:HG2	5:A:317:TYR:CE1	1.83	1.12
6:B:58:PHE:HB2	6:B:146:SER:HB3	1.27	1.12
6:B:403:ASN:O	6:B:406:ASN:HB3	0.96	1.12
17:N:61:LEU:CD1	17:N:63:ASP:HB2	1.79	1.12
17:N:75:TYR:O	17:N:76:LYS:O	1.68	1.12
4:4:91:PHE:CD2	20:4:312:CLA:C3C	2.31	1.12
20:4:305:CLA:HAA1	20:F:206:CLA:H42	1.30	1.12
21:1:219:LMU:H6'2	21:1:219:LMU:C3'	1.78	1.12
3:3:158:TYR:HB3	3:3:159:PRO:HD2	1.31	1.12
4:4:107:GLN:C	20:4:302:CLA:HMA3	1.61	1.12
6:B:131:THR:HB	6:B:134:ASP:HB2	1.16	1.12
21:F:201:LMU:C3	21:F:201:LMU:C8	2.28	1.12
22:I:103:BCR:C4	22:I:103:BCR:H322	1.59	1.12
2:2:168:ARG:O	2:2:172:LEU:HD12	1.50	1.11
20:H:101:CLA:HMC1	20:H:101:CLA:HBC3	1.20	1.11
22:B:846:BCR:H382	22:B:846:BCR:H23C	1.22	1.11
20:4:302:CLA:HHD	20:4:302:CLA:HBC2	1.21	1.11
20:4:305:CLA:HMC1	20:4:305:CLA:HBC3	1.11	1.11
4:4:33:ASP:HB3	4:4:34:PRO:HD3	1.32	1.11
20:A:824:CLA:CED	20:A:825:CLA:HMD1	1.80	1.11
23:B:841:PQN:H191	22:B:846:BCR:C10	1.78	1.11
15:K:17:LEU:HG	15:K:56:THR:OG1	1.49	1.11
16:L:164:PRO:CB	16:L:165:TYR:CA	2.28	1.11
20:L:201:CLA:HHD	20:L:201:CLA:HBC3	1.18	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:147:LEU:HD22	4:4:148:GLU:N	1.65	1.11
6:B:608:GLN:HA	6:B:608:GLN:HE21	1.01	1.11
21:B:847:LMU:C5B	21:B:847:LMU:H3'	1.80	1.11
21:H:105:LMU:C5	21:H:105:LMU:H91	1.68	1.11
19:X:1:GLC:C1	19:X:2:FRU:C5	2.27	1.11
5:A:331:LEU:HD11	5:A:346:LEU:HB3	1.22	1.11
21:A:854:LMU:C6	21:A:854:LMU:H22	1.57	1.11
10:F:25:LEU:CD2	10:F:46:MET:HB3	1.80	1.11
11:G:12:THR:HG22	11:G:72:LEU:HG	1.20	1.11
11:G:45:GLU:C	11:G:49:THR:HG21	1.69	1.11
2:2:44:ASN:ND2	14:J:1:MET:SD	2.22	1.11
16:L:164:PRO:CD	16:L:165:TYR:CD2	2.33	1.11
20:1:202:CLA:HED1	20:1:202:CLA:H2	1.29	1.11
21:A:855:LMU:H92	21:A:855:LMU:H41	1.13	1.11
20:B:827:CLA:HBC2	20:B:827:CLA:HMC1	1.27	1.11
21:H:104:LMU:O4'	19:Y:2:FRU:H3	1.38	1.11
21:K:106:LMU:C8	21:K:106:LMU:H31	1.81	1.11
20:A:839:CLA:H122	20:A:839:CLA:C7	1.79	1.11
10:F:22:LEU:CD1	10:F:22:LEU:H	1.64	1.11
11:G:43:HIS:CA	11:G:44:PHE:HB3	1.79	1.11
21:K:106:LMU:H52	21:K:106:LMU:C1	1.72	1.11
17:N:67:LEU:C	17:N:68:GLU:HG3	1.71	1.11
18:R:46:UNK:CB	18:R:47:UNK:CB	2.28	1.11
3:3:52:LYS:O	3:3:56:TYR:CD2	2.03	1.11
21:A:854:LMU:H61	21:A:854:LMU:H22	1.25	1.11
8:D:113:HIS:NE2	8:D:118:VAL:HG11	1.63	1.11
20:L:201:CLA:CGA	20:L:201:CLA:CED	2.29	1.10
17:N:62:SER:CB	17:N:66:ASP:CB	2.28	1.10
17:N:72:LYS:HG3	17:N:74:LYS:CA	1.79	1.10
4:4:128:ALA:CB	4:4:143:PHE:CE2	2.32	1.10
4:4:69:ILE:HG22	4:4:70:ILE:H	0.97	1.10
4:4:94:GLU:CG	4:4:95:PHE:CD1	2.34	1.10
20:A:839:CLA:HBC2	20:A:839:CLA:HHD	1.27	1.10
22:A:843:BCR:H402	22:A:843:BCR:H23C	1.32	1.10
7:C:66:ARG:HH21	7:C:66:ARG:HG2	1.16	1.10
18:R:38:UNK:O	18:R:42:UNK:HA	1.48	1.10
4:4:122:LYS:HB3	4:4:143:PHE:HB2	1.26	1.10
20:A:814:CLA:HHC	22:A:843:BCR:H17C	1.31	1.10
21:A:854:LMU:H32	21:A:854:LMU:C8	1.80	1.10
21:B:847:LMU:C3'	21:B:847:LMU:C5B	2.29	1.10
2:2:42:ARG:CD	2:2:45:VAL:CG2	2.29	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:208:ALA:HA	5:A:310:PHE:O	1.50	1.10
5:A:308:ILE:CD1	20:A:816:CLA:C9	2.30	1.10
18:R:34:UNK:CB	18:R:35:UNK:CB	2.29	1.10
5:A:331:LEU:HD21	5:A:343:HIS:O	0.94	1.10
6:B:189:ALA:CB	20:B:826:CLA:H203	1.80	1.10
19:Y:2:FRU:H61	19:Y:2:FRU:H12	1.31	1.10
20:1:215:CLA:HBC3	20:1:215:CLA:HHD	1.23	1.10
2:2:211:LYS:HA	2:2:211:LYS:HE2	1.33	1.10
5:A:25:ASP:HB3	5:A:26:PRO:HD2	1.10	1.10
5:A:98:PHE:CZ	20:A:807:CLA:HMD3	1.87	1.10
20:A:815:CLA:HBA1	20:A:815:CLA:CHA	1.75	1.10
6:B:247:THR:CA	6:B:250:ALA:HB2	1.80	1.10
20:1:215:CLA:C2A	20:1:215:CLA:CED	2.29	1.10
4:4:93:ILE:HA	4:4:96:ILE:HD12	1.20	1.10
5:A:581:CYS:HB2	5:A:590:CYS:HA	1.22	1.10
5:A:81:ALA:HB2	20:A:804:CLA:CMA	1.79	1.10
20:A:815:CLA:HBC3	20:A:815:CLA:CMC	1.70	1.10
21:A:855:LMU:C9	21:A:855:LMU:C4	2.29	1.10
10:F:22:LEU:N	10:F:22:LEU:HD12	1.52	1.10
11:G:48:ASP:CB	11:G:49:THR:CG2	2.28	1.10
21:H:105:LMU:C5	21:H:105:LMU:C9	2.30	1.10
21:K:106:LMU:C8	21:K:106:LMU:C3	2.30	1.10
22:A:845:BCR:H23C	22:A:845:BCR:H382	1.19	1.10
21:A:854:LMU:C2	21:A:854:LMU:C8	2.30	1.10
6:B:531:THR:HG22	20:B:823:CLA:HMC2	1.16	1.10
9:E:86:GLU:CG	9:E:87:VAL:H	1.65	1.10
16:L:163:LEU:CB	16:L:164:PRO:CB	2.29	1.10
17:N:72:LYS:HG2	17:N:74:LYS:HG3	1.32	1.10
20:A:839:CLA:H71	20:A:839:CLA:H121	1.29	1.10
11:G:42:SER:HB2	11:G:45:GLU:CD	1.72	1.10
20:K:101:CLA:CED	20:K:108:CLA:CMB	2.30	1.10
17:N:54:LYS:HB3	17:N:57:LYS:HE2	1.19	1.10
5:A:25:ASP:CB	5:A:26:PRO:HD2	1.71	1.10
20:A:814:CLA:HMB2	22:A:843:BCR:H382	1.34	1.10
21:A:854:LMU:C3	21:A:854:LMU:C8	2.29	1.10
20:4:304:CLA:CED	20:4:304:CLA:CAA	2.29	1.09
5:A:365:LEU:HD23	20:A:805:CLA:HED3	1.25	1.09
20:A:814:CLA:C4B	22:A:843:BCR:C19	2.28	1.09
21:B:847:LMU:C7	21:B:847:LMU:C11	2.30	1.09
21:E:101:LMU:C5	21:E:101:LMU:C1	2.29	1.09
21:H:104:LMU:H41	21:H:104:LMU:C8	1.80	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:106:LMU:C2	21:K:106:LMU:C2'	2.30	1.09
21:K:106:LMU:H91	21:K:106:LMU:C3	1.81	1.09
21:1:219:LMU:C6B	21:1:219:LMU:C3'	2.30	1.09
4:4:94:GLU:HB3	4:4:95:PHE:CD1	1.86	1.09
5:A:25:ASP:HB3	5:A:26:PRO:CD	1.78	1.09
5:A:316:MET:HB3	5:A:317:TYR:HB2	1.20	1.09
5:A:335:LYS:HG2	5:A:336:GLY:H	1.12	1.09
21:A:855:LMU:C8	21:A:855:LMU:C4	2.30	1.09
6:B:58:PHE:CB	6:B:146:SER:HB3	1.81	1.09
20:1:215:CLA:C1A	20:1:215:CLA:CED	2.29	1.09
4:4:35:GLU:HB3	4:4:36:ASN:HB3	1.32	1.09
20:B:850:CLA:H93	20:B:851:CLA:H91	1.13	1.09
10:F:47:GLU:HG3	10:F:51:LYS:HE3	1.16	1.09
21:H:108:LMU:H81	21:H:108:LMU:C4	1.82	1.09
20:L:201:CLA:CAA	20:L:201:CLA:CGD	2.29	1.09
18:R:41:UNK:CB	18:R:42:UNK:CA	2.29	1.09
20:1:202:CLA:CMA	20:1:202:CLA:CGA	2.30	1.09
20:A:839:CLA:H122	20:A:839:CLA:H71	1.18	1.09
21:B:847:LMU:C3'	21:B:847:LMU:C6B	2.30	1.09
9:E:52:VAL:HG12	9:E:53:VAL:H	1.16	1.09
21:H:106:LMU:H3'	21:H:106:LMU:O5B	1.35	1.09
12:H:69:SER:HB2	20:H:109:CLA:H61	1.10	1.09
15:K:7:THR:HA	15:K:10:ILE:HD13	1.11	1.09
2:2:42:ARG:CG	2:2:45:VAL:CG2	2.29	1.09
4:4:151:GLU:C	4:4:154:ILE:H	1.56	1.09
20:A:801:CLA:HMC1	20:A:801:CLA:HBC2	1.23	1.09
5:A:103:PHE:HE1	20:A:807:CLA:O1D	1.00	1.09
20:A:824:CLA:CED	20:A:825:CLA:CAD	2.29	1.09
15:K:20:PHE:HD2	15:K:21:ALA:N	1.50	1.09
20:1:202:CLA:CED	20:1:202:CLA:C2A	2.30	1.09
4:4:94:GLU:CB	4:4:95:PHE:CD1	2.33	1.09
4:4:95:PHE:CZ	20:4:315:CLA:NC	1.97	1.09
5:A:328:LYS:HG2	5:A:332:GLU:HB2	1.32	1.09
20:A:804:CLA:H12	20:A:811:CLA:H61	1.23	1.09
6:B:103:ALA:O	6:B:104:PHE:HB2	1.48	1.09
14:J:11:ALA:HB1	14:J:12:PRO:HD2	1.34	1.09
20:R:107:CLA:HED3	20:R:107:CLA:CHA	1.83	1.09
2:2:38:PRO:C	2:2:40:SER:HB2	1.71	1.09
2:2:41:LEU:HG	2:2:42:ARG:N	1.49	1.09
2:2:73:ILE:H	2:2:73:ILE:HD12	1.00	1.09
21:A:855:LMU:C3	21:A:855:LMU:C8	2.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:588:GLY:CA	6:B:668:ARG:HD3	1.82	1.09
20:H:102:CLA:CAC	22:I:103:BCR:HC31	1.81	1.09
21:K:106:LMU:C1	21:K:106:LMU:C5	2.30	1.09
16:L:164:PRO:HB2	16:L:165:TYR:CG	1.87	1.09
17:N:72:LYS:CG	17:N:74:LYS:CG	2.31	1.09
20:1:210:CLA:CAD	20:1:210:CLA:CED	2.31	1.09
20:1:215:CLA:C4	20:1:215:CLA:C11	2.29	1.09
20:1:215:CLA:CHD	20:1:215:CLA:CBC	2.29	1.09
21:G:101:LMU:C6B	21:G:101:LMU:C3'	2.30	1.09
17:N:54:LYS:HB3	17:N:57:LYS:CE	1.82	1.09
17:N:72:LYS:CG	17:N:74:LYS:CB	2.31	1.09
20:A:824:CLA:CED	20:A:825:CLA:CMD	2.30	1.09
22:B:845:BCR:H23C	22:B:845:BCR:H382	1.30	1.09
5:A:308:ILE:HD11	20:A:816:CLA:C9	1.81	1.09
21:H:106:LMU:C3	21:H:106:LMU:C1B	2.30	1.09
21:H:108:LMU:H52	21:H:108:LMU:C9	1.81	1.09
20:K:101:CLA:HED1	20:K:108:CLA:HMB2	1.17	1.09
5:A:27:ILE:O	5:A:28:LYS:HG3	1.52	1.08
5:A:472:ARG:HH12	16:L:74:LEU:HG	1.06	1.08
8:D:117:GLY:O	8:D:118:VAL:HG23	1.52	1.08
10:F:102:ARG:HG2	10:F:106:ILE:HD11	1.12	1.08
16:L:161:LEU:CD1	16:L:162:ASP:CA	2.30	1.08
18:R:39:UNK:C	18:R:41:UNK:CB	2.30	1.08
5:A:328:LYS:CE	5:A:332:GLU:CG	2.30	1.08
16:L:163:LEU:CB	16:L:164:PRO:CG	2.29	1.08
20:2:322:CLA:C10	20:2:322:CLA:H152	1.54	1.08
20:3:313:CLA:CAA	20:3:313:CLA:CED	2.30	1.08
20:4:319:CLA:HMC1	20:4:319:CLA:HBC3	1.21	1.08
6:B:119:GLY:HA3	20:B:826:CLA:HED1	1.11	1.08
6:B:282:PHE:HZ	20:B:814:CLA:C1	1.67	1.08
20:1:215:CLA:C4	20:1:215:CLA:C10	2.30	1.08
20:2:302:CLA:HMC1	20:2:302:CLA:CBC	1.82	1.08
20:A:830:CLA:H161	22:L:210:BCR:H361	1.31	1.08
20:B:821:CLA:CMC	20:B:821:CLA:HBC3	1.65	1.08
20:4:307:CLA:CGA	20:4:307:CLA:HMA2	1.82	1.08
4:4:52:MET:HG3	4:4:160:MET:HG3	1.35	1.08
4:4:30:LEU:CA	4:4:31:ALA:CB	2.30	1.08
20:1:202:CLA:CBA	20:1:202:CLA:CED	2.30	1.08
3:3:107:TRP:CD1	3:3:108:ALA:N	2.21	1.08
20:A:815:CLA:O2D	20:A:815:CLA:H2A	1.54	1.08
20:B:810:CLA:CAC	20:B:811:CLA:HBB1	1.58	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:201:LMU:C7	21:F:201:LMU:C3	2.29	1.08
17:N:51:ASP:C	17:N:52:LEU:HD23	1.73	1.08
19:X:1:GLC:C1	19:X:2:FRU:H5	1.83	1.08
15:K:11:MET:SD	15:K:11:MET:C	2.30	1.08
16:L:163:LEU:CD2	16:L:164:PRO:CA	2.29	1.08
1:1:27:LEU:HD21	6:B:314:ARG:CD	1.83	1.08
4:4:147:LEU:HD13	4:4:148:GLU:N	1.68	1.08
4:4:99:HIS:CE1	4:4:103:ILE:HD12	1.89	1.08
20:A:803:CLA:H42	20:A:838:CLA:H61	1.08	1.08
20:B:823:CLA:HHD	20:B:823:CLA:HBC2	1.14	1.08
21:H:108:LMU:C3	21:H:108:LMU:C9	2.30	1.08
19:U:1:GLC:H3	19:U:2:FRU:O5	1.52	1.08
4:4:119:PRO:HG3	20:4:313:CLA:C2D	1.82	1.08
21:F:201:LMU:C2	21:F:201:LMU:C8	2.30	1.08
21:K:105:LMU:C3	21:K:105:LMU:H6D	1.83	1.08
16:L:164:PRO:CB	16:L:165:TYR:CB	2.30	1.08
21:R:109:LMU:O6B	21:R:109:LMU:H1B	1.50	1.08
3:3:198:PHE:HA	3:3:201:ALA:HB2	1.36	1.07
4:4:128:ALA:N	4:4:143:PHE:HZ	1.49	1.07
20:A:825:CLA:HBC2	20:A:825:CLA:HMC1	1.31	1.07
21:K:105:LMU:C3	21:K:105:LMU:C6'	2.30	1.07
2:2:169:LEU:HD23	20:2:305:CLA:HBB2	1.33	1.07
6:B:302:LYS:O	6:B:303:TYR:HB2	1.50	1.07
22:I:103:BCR:C8	22:I:103:BCR:H313	1.74	1.07
21:N:101:LMU:H2B	21:N:101:LMU:O3'	1.54	1.07
20:A:839:CLA:CHD	20:A:839:CLA:CBC	2.30	1.07
6:B:22:TRP:HE1	20:B:838:CLA:CBB	1.66	1.07
21:B:847:LMU:H6'2	21:B:847:LMU:H3'	1.18	1.07
7:C:54:CYS:CB	24:C:102:SF4:S3	2.42	1.07
10:F:23:LYS:HB2	10:F:24:LYS:HZ1	1.18	1.07
20:J:103:CLA:CHA	20:J:103:CLA:HED3	1.83	1.07
20:A:823:CLA:OBD	20:A:823:CLA:H92	1.51	1.07
20:K:102:CLA:HBC2	20:K:102:CLA:HMC1	1.35	1.07
13:I:7:LEU:CD1	22:I:103:BCR:H333	1.83	1.07
15:K:10:ILE:C	15:K:13:THR:HG23	1.75	1.07
5:A:511:THR:HG23	20:A:817:CLA:O1A	1.52	1.07
21:A:855:LMU:H32	21:A:855:LMU:C8	1.85	1.07
6:B:594:TRP:O	6:B:595:HIS:HB3	1.49	1.07
6:B:729:THR:O	6:B:729:THR:HG22	1.53	1.07
20:B:821:CLA:H2A	20:B:821:CLA:O2D	1.52	1.07
10:F:42:ILE:HG13	10:F:43:LYS:H	1.14	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:45:GLU:HG3	11:G:49:THR:CG2	1.78	1.07
4:4:75:TRP:CD1	20:4:311:CLA:HMD3	1.90	1.07
5:A:210:LEU:CD1	20:A:813:CLA:HMB2	1.85	1.07
20:A:833:CLA:CBC	22:A:846:BCR:HC31	1.83	1.07
11:G:46:ALA:HA	11:G:48:ASP:OD2	1.54	1.07
4:4:107:GLN:O	20:4:302:CLA:CMA	1.99	1.07
21:A:855:LMU:H32	21:A:855:LMU:H82	1.13	1.07
17:N:45:ASN:HD22	17:N:54:LYS:CB	1.64	1.07
20:2:322:CLA:H41	20:2:322:CLA:C8	1.84	1.07
2:2:99:LEU:HD22	20:2:311:CLA:HMC3	1.10	1.07
21:H:108:LMU:H101	21:H:108:LMU:H31	1.34	1.07
21:R:103:LMU:C3	21:R:103:LMU:H1'	1.81	1.07
2:2:120:ASN:HB3	2:2:121:THR:HB	1.34	1.07
2:2:169:LEU:CD2	20:2:305:CLA:CAB	2.32	1.07
20:2:322:CLA:C10	20:2:322:CLA:C15	2.28	1.07
4:4:194:VAL:CG1	4:4:195:GLN:CB	2.28	1.07
20:A:825:CLA:HMC1	20:A:825:CLA:CBC	1.84	1.07
5:A:402:ILE:CG1	20:A:827:CLA:HBB2	1.85	1.07
21:H:106:LMU:H12	21:H:106:LMU:O2'	1.45	1.07
21:H:108:LMU:C8	21:H:108:LMU:C3	2.30	1.07
21:H:108:LMU:C8	21:H:108:LMU:C4	2.30	1.07
17:N:48:GLY:HA3	17:N:49:CYS:O	1.53	1.07
3:3:93:PHE:N	3:3:93:PHE:CD2	2.22	1.06
4:4:123:GLN:O	4:4:143:PHE:CD1	2.07	1.06
6:B:58:PHE:HB2	6:B:146:SER:CB	1.83	1.06
23:B:841:PQN:C16	22:B:846:BCR:H333	1.79	1.06
9:E:87:VAL:HG12	9:E:87:VAL:O	1.54	1.06
21:G:101:LMU:H3'	21:G:101:LMU:H6'2	1.08	1.06
16:L:64:LEU:HB3	16:L:68:PHE:HE1	1.17	1.06
4:4:36:ASN:CG	4:4:39:TRP:CD2	2.28	1.06
20:A:819:CLA:HMD3	20:A:821:CLA:HBB2	1.12	1.06
22:A:847:BCR:C31	20:A:852:CLA:H142	1.84	1.06
21:A:855:LMU:O3B	21:A:855:LMU:H6'1	1.46	1.06
20:B:805:CLA:O1A	20:B:805:CLA:H62	1.54	1.06
6:B:310:PRO:HG3	20:B:821:CLA:HMA1	1.12	1.06
21:H:104:LMU:H12	21:H:104:LMU:C5	1.82	1.06
17:N:52:LEU:N	17:N:52:LEU:HD23	1.65	1.06
2:2:91:THR:O	2:2:94:LEU:HB3	1.55	1.06
20:A:824:CLA:CBC	20:A:824:CLA:HHD	1.85	1.06
10:F:5:LEU:HG	10:F:6:THR:N	1.66	1.06
4:4:36:ASN:CG	4:4:39:TRP:CE2	2.29	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:105:LMU:H5'	21:K:105:LMU:O2B	1.54	1.06
20:L:209:CLA:CBC	20:L:209:CLA:HHD	1.83	1.06
21:R:102:LMU:C6'	21:R:102:LMU:C5B	2.29	1.06
20:4:318:CLA:CED	20:4:318:CLA:C1	2.29	1.06
6:B:25:ILE:HG23	22:L:210:BCR:H282	1.37	1.06
11:G:28:ARG:HG2	11:G:28:ARG:HH21	1.20	1.06
20:L:201:CLA:CBC	20:L:201:CLA:CHD	2.32	1.06
20:3:313:CLA:H142	20:3:313:CLA:H101	1.07	1.06
5:A:368:LEU:CD2	20:A:818:CLA:C9	2.32	1.06
6:B:202:SER:O	6:B:245:GLY:HA2	1.52	1.06
20:B:829:CLA:HHD	20:B:829:CLA:HBC2	1.35	1.06
21:B:847:LMU:C11	21:B:847:LMU:C6	2.30	1.06
21:D:201:LMU:C3	21:E:101:LMU:C12	2.34	1.06
4:4:147:LEU:CD2	4:4:148:GLU:CG	2.30	1.06
20:H:101:CLA:H2	20:H:101:CLA:HMA2	1.30	1.06
16:L:164:PRO:CB	16:L:165:TYR:CG	2.37	1.06
20:3:318:CLA:H12	20:3:318:CLA:HMA2	1.28	1.06
4:4:122:LYS:HB3	4:4:143:PHE:CG	1.90	1.06
20:4:316:CLA:HBA1	20:4:316:CLA:HBD	1.37	1.06
20:A:822:CLA:CAB	22:A:845:BCR:H351	1.85	1.06
20:A:852:CLA:HMD3	6:B:578:LEU:HD23	1.09	1.06
21:A:854:LMU:C6	21:A:854:LMU:C2	2.29	1.06
21:H:105:LMU:H51	21:H:105:LMU:H91	1.34	1.06
13:I:11:LEU:HD12	22:I:103:BCR:C10	1.83	1.06
13:I:7:LEU:HD12	22:I:103:BCR:C33	1.86	1.06
16:L:164:PRO:C	16:L:165:TYR:CD2	2.29	1.06
5:A:249:ILE:HG12	5:A:250:LEU:N	1.67	1.06
5:A:267:THR:O	5:A:269:PHE:HD2	1.39	1.06
20:B:810:CLA:C3C	20:B:811:CLA:HBB1	1.84	1.06
20:B:823:CLA:HBB1	20:B:837:CLA:HMB3	1.35	1.06
16:L:27:VAL:HA	20:L:203:CLA:CMA	1.84	1.06
17:N:58:VAL:CB	17:N:59:PRO:CD	2.30	1.06
17:N:65:LEU:HD23	17:N:65:LEU:O	1.53	1.06
5:A:605:MET:HA	5:A:608:SER:OG	1.56	1.06
20:A:833:CLA:HMA2	20:A:839:CLA:HBB1	1.37	1.06
20:1:215:CLA:HHD	20:1:215:CLA:HBC2	1.33	1.05
21:H:108:LMU:H32	21:H:108:LMU:H81	1.25	1.05
14:J:2:ARG:HH12	14:J:8:LEU:HD13	1.21	1.05
21:K:106:LMU:H91	21:K:106:LMU:H31	1.07	1.05
20:4:304:CLA:H151	20:4:304:CLA:H202	1.25	1.05
20:4:304:CLA:H203	20:4:304:CLA:H151	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:44:ARG:HH21	8:D:127:ARG:HB3	1.19	1.05
9:E:72:VAL:O	9:E:73:ASN:HB3	1.55	1.05
10:F:24:LYS:CA	10:F:24:LYS:CE	2.34	1.05
17:N:45:ASN:HD22	17:N:57:LYS:NZ	1.52	1.05
17:N:46:PHE:O	17:N:47:THR:HG23	1.54	1.05
2:2:203:THR:O	2:2:204:ILE:HG23	1.54	1.05
20:3:313:CLA:HAA2	20:3:313:CLA:HED2	1.09	1.05
4:4:93:ILE:CA	4:4:96:ILE:HD12	1.87	1.05
5:A:454:GLY:H	5:A:457:SER:HB3	1.16	1.05
6:B:474:PHE:HE2	6:B:476:ILE:HG13	1.19	1.05
6:B:560:ASP:OD1	6:B:561:GLY:N	1.89	1.05
7:C:1:MET:HG2	7:C:4:SER:HB3	1.36	1.05
11:G:43:HIS:O	11:G:45:GLU:HB2	1.56	1.05
12:H:25:GLY:HA3	12:H:27:ASP:H	1.00	1.05
16:L:161:LEU:C	16:L:161:LEU:HD12	1.58	1.05
19:U:2:FRU:C1	19:U:2:FRU:H62	1.85	1.05
4:4:193:ILE:HG22	4:4:194:VAL:H	1.13	1.05
20:A:814:CLA:CHC	22:A:843:BCR:C19	2.35	1.05
22:A:847:BCR:C31	22:A:847:BCR:HC8	1.85	1.05
6:B:663:PHE:O	6:B:664:LEU:HB2	1.50	1.05
15:K:11:MET:SD	15:K:12:VAL:N	2.29	1.05
1:1:39:TYR:HB3	20:1:209:CLA:OBD	1.54	1.05
21:1:217:LMU:O6B	21:1:217:LMU:H1B	1.51	1.05
5:A:116:ILE:HG23	5:A:137:GLY:HA3	1.39	1.05
5:A:370:ILE:HG22	5:A:400:MET:HA	1.38	1.05
1:1:27:LEU:CD2	6:B:314:ARG:HG3	1.85	1.05
11:G:42:SER:OG	11:G:45:GLU:HB2	1.56	1.05
11:G:46:ALA:H	11:G:48:ASP:CB	1.69	1.05
20:H:102:CLA:C4C	22:I:103:BCR:HC22	1.85	1.05
20:4:304:CLA:C20	20:4:304:CLA:C15	2.28	1.05
4:4:39:TRP:C	4:4:40:PHE:CD1	2.29	1.05
5:A:51:THR:HG21	20:A:837:CLA:HBB2	1.35	1.05
20:B:821:CLA:HAA1	20:B:821:CLA:H43	1.38	1.05
21:E:101:LMU:H51	21:E:101:LMU:C1	1.87	1.05
20:2:322:CLA:H102	20:2:322:CLA:C15	1.85	1.05
4:4:117:GLN:O	4:4:122:LYS:O	1.72	1.05
5:A:365:LEU:HD23	20:A:805:CLA:CED	1.85	1.05
20:A:824:CLA:H72	20:A:825:CLA:HED2	1.30	1.05
22:A:844:BCR:H23C	22:A:844:BCR:H402	1.38	1.05
20:B:823:CLA:CED	20:B:824:CLA:HMD1	1.87	1.05
11:G:68:ILE:CG2	11:G:72:LEU:HD13	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:107:LMU:O2'	21:H:107:LMU:H12	1.57	1.05
20:4:304:CLA:H2A	20:4:304:CLA:O1D	1.56	1.05
5:A:197:GLN:HA	5:A:197:GLN:HE21	0.91	1.05
5:A:425:THR:HG21	8:D:59:GLU:OE2	1.54	1.05
20:1:210:CLA:OBD	20:1:210:CLA:HED2	1.56	1.05
20:A:824:CLA:HHD	20:A:824:CLA:HBC2	1.07	1.05
20:B:829:CLA:HHD	20:B:829:CLA:CBC	1.87	1.05
22:B:846:BCR:H17C	20:B:850:CLA:H101	1.39	1.05
20:1:202:CLA:CED	20:1:202:CLA:H2	1.87	1.05
4:4:193:ILE:HG22	4:4:195:GLN:O	1.57	1.05
5:A:27:ILE:O	5:A:27:ILE:HG23	1.55	1.05
10:F:130:LEU:HG	10:F:131:PHE:H	1.13	1.05
21:N:101:LMU:H121	21:N:101:LMU:H81	1.37	1.05
2:2:205:PHE:C	2:2:205:PHE:CD1	2.29	1.04
4:4:30:LEU:HA	4:4:31:ALA:CB	1.87	1.04
23:B:841:PQN:H192	22:B:846:BCR:H10C	1.35	1.04
7:C:1:MET:HB3	7:C:4:SER:OG	1.54	1.04
10:F:23:LYS:O	10:F:26:GLN:HB2	1.57	1.04
12:H:25:GLY:HA3	12:H:27:ASP:CB	1.86	1.04
13:I:11:LEU:HG	22:I:103:BCR:C7	1.86	1.04
15:K:10:ILE:HD12	15:K:10:ILE:H	1.19	1.04
5:A:599:PHE:CE2	5:A:735:VAL:HG21	1.92	1.04
6:B:65:LEU:HD22	6:B:124:TRP:HE3	1.20	1.04
11:G:12:THR:CG2	11:G:72:LEU:HG	1.85	1.04
4:4:122:LYS:CB	4:4:143:PHE:CB	2.33	1.04
21:A:854:LMU:H51	21:A:854:LMU:H6'	1.19	1.04
6:B:11:GLY:HA3	7:C:71:HIS:HD2	1.18	1.04
6:B:340:SER:HA	20:B:824:CLA:H51	1.37	1.04
10:F:151:ASP:O	10:F:154:PHE:HB3	1.56	1.04
21:F:201:LMU:C3	21:F:201:LMU:H71	1.83	1.04
22:I:103:BCR:HC42	22:I:103:BCR:H322	1.09	1.04
16:L:164:PRO:HB2	16:L:165:TYR:HA	1.35	1.04
2:2:41:LEU:CG	2:2:42:ARG:N	2.14	1.04
5:A:29:THR:O	5:A:29:THR:HG23	1.57	1.04
5:A:281:LEU:HD12	20:A:816:CLA:HED2	1.37	1.04
9:E:85:ASP:O	9:E:86:GLU:HB3	1.52	1.04
20:1:202:CLA:HED1	20:1:202:CLA:C2	1.86	1.04
21:H:106:LMU:H2B	21:H:106:LMU:H31	1.34	1.04
5:A:269:PHE:CE1	15:K:14:THR:HG21	1.91	1.04
16:L:165:TYR:N	16:L:165:TYR:HD2	1.54	1.04
21:N:101:LMU:C3	21:N:101:LMU:C1'	2.30	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD11	17:N:63:ASP:N	1.73	1.04
19:Q:2:FRU:H11	19:Q:2:FRU:H62	1.06	1.04
3:3:110:SER:O	3:3:111:TYR:CD2	2.10	1.04
20:H:102:CLA:CAC	22:I:103:BCR:C3	2.36	1.04
20:1:215:CLA:CBA	20:1:215:CLA:CGD	2.35	1.04
5:A:394:SER:HB2	20:A:826:CLA:HMA1	1.38	1.04
20:A:819:CLA:HMD3	20:A:821:CLA:CBB	1.86	1.04
20:B:807:CLA:H92	20:B:807:CLA:CBB	1.86	1.04
20:B:836:CLA:H152	22:F:203:BCR:H312	1.08	1.04
23:B:841:PQN:C16	22:B:846:BCR:H331	1.86	1.04
8:D:78:ALA:HB3	8:D:82:GLN:HE22	1.16	1.04
10:F:24:LYS:HE2	10:F:24:LYS:HA	1.40	1.04
1:1:179:THR:HG21	4:4:87:SER:HB3	1.18	1.04
20:A:814:CLA:HMB2	22:A:843:BCR:C38	1.87	1.04
6:B:310:PRO:HG2	6:B:311:PRO:HD2	1.38	1.04
2:2:43:TRP:CE3	2:2:125:PHE:CD1	2.46	1.04
20:A:839:CLA:HBC3	20:A:839:CLA:HHD	1.29	1.04
20:J:101:CLA:HBC2	20:J:101:CLA:HMC1	1.39	1.04
21:K:105:LMU:C7	21:K:105:LMU:C2	2.30	1.04
16:L:164:PRO:C	16:L:165:TYR:HD2	1.58	1.04
20:3:313:CLA:C14	20:3:313:CLA:C10	2.33	1.03
4:4:34:PRO:CA	4:4:35:GLU:CB	2.28	1.03
4:4:69:ILE:HD11	4:4:175:LYS:HB2	1.09	1.03
20:A:807:CLA:CAA	20:A:807:CLA:C1	2.34	1.03
5:A:401:TRP:CD1	20:A:826:CLA:HHC	1.93	1.03
20:A:838:CLA:C14	22:A:847:BCR:C2	2.36	1.03
20:G:102:CLA:CHD	20:G:102:CLA:CBC	2.30	1.03
21:K:106:LMU:C8	21:K:106:LMU:C4	2.30	1.03
20:1:202:CLA:HED1	20:1:202:CLA:CBA	1.85	1.03
20:1:215:CLA:C4	20:1:215:CLA:C8	2.35	1.03
20:3:313:CLA:HBA1	20:3:313:CLA:CED	1.88	1.03
20:4:318:CLA:CED	20:4:318:CLA:CGA	2.36	1.03
4:4:98:SER:O	4:4:102:GLU:HG3	1.55	1.03
6:B:708:VAL:O	6:B:712:HIS:HB2	1.56	1.03
12:H:20:GLN:HB3	12:H:22:ASP:HB3	1.04	1.03
20:3:313:CLA:CMC	20:3:313:CLA:CBC	2.30	1.03
16:L:163:LEU:HD13	16:L:164:PRO:CB	1.86	1.03
22:F:203:BCR:C27	22:F:203:BCR:C40	2.30	1.03
2:2:118:CYS:O	2:2:119:VAL:CG1	2.06	1.03
2:2:54:TRP:CZ2	2:2:109:ARG:HD2	1.93	1.03
4:4:95:PHE:CZ	20:4:315:CLA:C1C	2.34	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:810:CLA:C3C	20:B:811:CLA:CBB	2.36	1.03
11:G:68:ILE:HG23	11:G:72:LEU:HD13	1.34	1.03
1:1:63:LEU:O	1:1:63:LEU:HD13	1.57	1.03
9:E:51:SER:HB3	9:E:68:ARG:CZ	1.89	1.03
20:H:101:CLA:HED3	20:H:101:CLA:OBD	1.59	1.03
20:2:322:CLA:H91	20:2:322:CLA:C15	1.89	1.03
3:3:205:GLY:H	5:A:252:ARG:NH2	1.55	1.03
4:4:158:ARG:HA	4:4:161:LEU:HD12	1.39	1.03
20:4:305:CLA:HMC1	20:4:305:CLA:CBC	1.88	1.03
4:4:72:VAL:HG13	4:4:72:VAL:O	1.56	1.03
5:A:707:ILE:HG22	5:A:711:HIS:NE2	1.74	1.03
20:A:839:CLA:C12	20:A:839:CLA:C7	2.31	1.03
22:A:843:BCR:HC8	22:A:843:BCR:H311	1.05	1.03
6:B:419:ILE:O	6:B:420:SER:OG	1.77	1.03
4:4:194:VAL:CB	4:4:195:GLN:C	2.26	1.03
11:G:44:PHE:N	11:G:45:GLU:HB2	1.71	1.03
2:2:128:ASN:C	2:2:130:LEU:N	2.04	1.03
22:F:203:BCR:H271	22:F:203:BCR:H403	1.04	1.03
10:F:24:LYS:O	10:F:27:ALA:HB2	1.59	1.03
20:H:102:CLA:C3C	22:I:103:BCR:C2	2.36	1.03
21:N:101:LMU:C6'	21:N:101:LMU:C5	2.30	1.03
20:R:108:CLA:HBA2	20:R:108:CLA:HBD	1.39	1.03
20:1:202:CLA:C9	20:1:202:CLA:C12	2.30	1.02
20:1:202:CLA:HED1	20:1:202:CLA:HBA2	1.07	1.02
4:4:149:ALA:CB	4:4:151:GLU:CG	2.30	1.02
6:B:382:ILE:HG22	6:B:383:MET:H	1.24	1.02
9:E:45:TRP:CH2	9:E:78:SER:OG	2.11	1.02
11:G:47:GLY:H	11:G:48:ASP:CB	1.72	1.02
11:G:48:ASP:HB3	11:G:49:THR:CG2	1.88	1.02
17:N:72:LYS:HB3	17:N:73:ASP:C	1.79	1.02
4:4:117:GLN:O	4:4:121:PHE:CE2	2.12	1.02
20:A:815:CLA:CAA	20:A:815:CLA:CED	2.29	1.02
16:L:163:LEU:CG	16:L:164:PRO:CB	2.36	1.02
20:A:851:CLA:HMB3	20:B:849:CLA:H18	1.42	1.02
20:B:803:CLA:CMD	22:F:202:BCR:HC41	1.89	1.02
10:F:23:LYS:C	10:F:24:LYS:HE2	1.78	1.02
20:H:101:CLA:CMA	20:H:101:CLA:H61	1.90	1.02
16:L:108:LYS:O	16:L:132:SER:HB2	1.58	1.02
1:1:63:LEU:HD22	1:1:63:LEU:O	1.55	1.02
2:2:42:ARG:HB3	2:2:43:TRP:HA	1.37	1.02
5:A:355:HIS:ND1	5:A:416:ILE:HG21	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:803:CLA:H42	20:A:838:CLA:C6	1.89	1.02
5:A:382:TYR:OH	20:A:827:CLA:H42	1.58	1.02
16:L:88:ALA:C	16:L:90:GLY:H	1.55	1.02
3:3:84:ILE:H	20:3:302:CLA:C4	1.72	1.02
4:4:69:ILE:CD1	4:4:175:LYS:HB3	1.84	1.02
4:4:69:ILE:HD11	4:4:175:LYS:HB3	1.39	1.02
5:A:281:LEU:CD1	20:A:816:CLA:HED2	1.88	1.02
5:A:390:ALA:HB2	5:A:754:ILE:HB	1.41	1.02
11:G:45:GLU:HG3	11:G:49:THR:HG23	1.08	1.02
4:4:34:PRO:HB3	4:4:35:GLU:HB2	1.40	1.02
20:2:322:CLA:H152	20:2:322:CLA:C8	1.88	1.02
20:4:318:CLA:HBC2	20:4:318:CLA:HHD	1.36	1.02
22:A:847:BCR:C31	20:A:852:CLA:H143	1.86	1.02
24:A:857:SF4:S3	24:A:857:SF4:S1	2.58	1.02
17:N:76:LYS:HG3	17:N:77:CYS:H	1.22	1.02
4:4:74:LYS:H	4:4:75:TRP:CA	1.72	1.02
20:A:813:CLA:HBA1	20:A:823:CLA:H41	1.40	1.02
20:K:101:CLA:HED2	20:K:108:CLA:CMB	1.90	1.02
21:K:105:LMU:O3'	21:K:105:LMU:H1B	1.57	1.02
15:K:1:ASP:HA	15:K:5:SER:HB3	1.40	1.02
20:1:215:CLA:C4	20:1:215:CLA:C7	2.29	1.02
20:1:215:CLA:H8	20:1:215:CLA:H41	1.40	1.02
20:3:310:CLA:CHA	20:3:318:CLA:HBC2	1.90	1.02
22:B:846:BCR:H19C	20:B:850:CLA:H151	1.40	1.02
16:L:122:GLY:C	16:L:124:LYS:H	1.61	1.02
17:N:61:LEU:CD1	17:N:63:ASP:CB	2.37	1.02
20:R:108:CLA:CBD	20:R:108:CLA:HBA2	1.90	1.02
20:2:303:CLA:HBC2	20:2:303:CLA:HHD	1.41	1.02
4:4:37:LEU:C	4:4:39:TRP:CB	2.27	1.02
6:B:558:PRO:HG2	6:B:703:VAL:HB	1.38	1.02
21:N:101:LMU:C12	21:N:101:LMU:C8	2.30	1.02
20:1:215:CLA:H43	20:1:215:CLA:H112	1.40	1.01
2:2:169:LEU:CD2	20:2:305:CLA:HBB2	1.90	1.01
20:3:310:CLA:CHA	20:3:318:CLA:HBC1	1.87	1.01
20:B:836:CLA:H152	22:F:203:BCR:H313	1.42	1.01
11:G:43:HIS:HA	11:G:44:PHE:CB	1.89	1.01
2:2:44:ASN:HD21	14:J:1:MET:HB2	1.24	1.01
21:1:213:LMU:H1'	21:1:213:LMU:O6'	1.54	1.01
2:2:182:ILE:O	2:2:204:ILE:O	1.78	1.01
5:A:239:PRO:HA	5:A:242:ILE:CD1	1.90	1.01
20:A:806:CLA:H43	20:A:828:CLA:H11	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:807:CLA:C1	20:A:809:CLA:CED	2.38	1.01
20:A:838:CLA:C14	22:A:847:BCR:HC22	1.90	1.01
2:2:41:LEU:HG	2:2:42:ARG:H	1.10	1.01
20:3:310:CLA:C2A	20:3:318:CLA:HAC2	1.89	1.01
5:A:368:LEU:CD2	20:A:818:CLA:H92	1.87	1.01
20:B:811:CLA:HMC1	20:B:811:CLA:HBC3	1.39	1.01
17:N:45:ASN:ND2	17:N:53:ALA:O	1.92	1.01
21:R:103:LMU:H22	21:R:103:LMU:H62	1.06	1.01
1:1:185:TRP:HA	1:1:185:TRP:CE3	1.93	1.01
4:4:192:THR:CG2	4:4:193:ILE:C	2.29	1.01
5:A:412:ALA:HB2	5:A:598:VAL:HG11	1.42	1.01
20:B:823:CLA:HED1	20:B:824:CLA:HMD1	1.42	1.01
17:N:18:ASP:CB	17:N:22:LEU:HG	1.90	1.01
20:2:302:CLA:CGA	20:2:302:CLA:H42	1.90	1.01
2:2:103:GLY:N	20:2:311:CLA:CBB	2.22	1.01
5:A:249:ILE:HG12	5:A:250:LEU:H	0.90	1.01
5:A:328:LYS:HE2	5:A:332:GLU:HG3	1.39	1.01
20:A:833:CLA:CMA	20:A:839:CLA:HBB1	1.90	1.01
20:B:821:CLA:H42	20:B:821:CLA:C4A	1.90	1.01
7:C:1:MET:HB3	7:C:4:SER:HG	1.25	1.01
21:1:217:LMU:O2'	21:1:217:LMU:H11	1.55	1.01
4:4:149:ALA:HB3	4:4:151:GLU:HG2	1.23	1.01
4:4:36:ASN:ND2	4:4:39:TRP:CE2	2.29	1.01
6:B:361:ILE:HG23	6:B:368:GLN:OE1	1.61	1.01
11:G:43:HIS:C	11:G:45:GLU:HB2	1.80	1.01
17:N:54:LYS:CG	17:N:57:LYS:HZ3	1.73	1.01
4:4:75:TRP:CE3	4:4:76:TYR:N	2.28	1.01
20:A:824:CLA:C7	20:A:825:CLA:CED	2.38	1.01
20:B:835:CLA:HBC3	20:B:835:CLA:HMC1	1.43	1.01
11:G:12:THR:HG22	11:G:72:LEU:CG	1.88	1.01
6:B:247:THR:HA	6:B:250:ALA:HB2	1.05	1.01
7:C:8:TYR:O	7:C:60:THR:HA	1.59	1.01
21:1:219:LMU:H6'2	21:1:219:LMU:H3'	1.05	1.01
2:2:43:TRP:CZ3	2:2:125:PHE:CD2	2.41	1.01
2:2:203:THR:O	2:2:204:ILE:HG12	1.60	1.01
4:4:154:ILE:HG13	4:4:155:ALA:H	1.21	1.01
22:J:102:BCR:H393	22:J:102:BCR:H23C	1.03	1.01
17:N:1:GLY:O	17:N:2:VAL:HG13	1.58	1.01
17:N:42:PHE:CD1	17:N:43:PRO:N	2.29	1.01
20:B:850:CLA:H93	20:B:851:CLA:C9	1.91	1.01
11:G:48:ASP:HB3	11:G:49:THR:HG22	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:108:LMU:C10	21:H:108:LMU:C3	2.30	1.01
2:2:110:TRP:HA	2:2:113:ILE:HG23	1.42	1.00
3:3:181:LEU:N	3:3:182:LYS:HE2	1.74	1.00
3:3:64:TYR:HB3	20:3:311:CLA:C4	1.90	1.00
4:4:149:ALA:HB3	4:4:151:GLU:OE1	1.58	1.00
5:A:368:LEU:HD21	20:A:818:CLA:H93	1.40	1.00
21:H:108:LMU:C5	21:H:108:LMU:C9	2.29	1.00
21:A:855:LMU:H6'2	21:A:855:LMU:C2B	1.87	1.00
15:K:17:LEU:O	15:K:17:LEU:HD23	1.59	1.00
16:L:163:LEU:HB3	16:L:164:PRO:HG3	1.06	1.00
21:1:218:LMU:H1B	21:1:218:LMU:O6B	1.56	1.00
3:3:48:PHE:HD2	3:3:49:ILE:HG22	0.85	1.00
4:4:71:ASN:C	4:4:73:PRO:HD3	1.81	1.00
9:E:83:ALA:O	9:E:86:GLU:HG2	1.60	1.00
10:F:23:LYS:C	10:F:24:LYS:CE	2.29	1.00
16:L:164:PRO:HD2	16:L:165:TYR:CE1	1.95	1.00
20:A:824:CLA:CHD	20:A:824:CLA:HBC2	1.91	1.00
20:A:830:CLA:H161	22:L:210:BCR:C36	1.91	1.00
17:N:62:SER:HB3	17:N:66:ASP:HB3	1.39	1.00
21:1:213:LMU:H6D	21:1:213:LMU:C2'	1.82	1.00
2:2:96:ILE:HG13	2:2:97:VAL:H	1.26	1.00
22:A:847:BCR:C8	22:A:847:BCR:H311	1.83	1.00
20:B:808:CLA:H41	22:I:101:BCR:C23	1.90	1.00
10:F:22:LEU:O	10:F:25:LEU:HB2	1.57	1.00
12:H:58:ILE:HD11	16:L:97:MET:SD	2.00	1.00
20:K:101:CLA:HMD1	20:K:108:CLA:NA	1.75	1.00
17:N:18:ASP:HB2	17:N:22:LEU:HG	1.40	1.00
4:4:192:THR:HG21	4:4:195:GLN:N	1.76	1.00
22:A:843:BCR:HC8	22:A:843:BCR:C31	1.89	1.00
20:B:821:CLA:C4	20:B:821:CLA:C4A	2.30	1.00
9:E:39:LEU:H	9:E:40:ARG:NH1	1.58	1.00
16:L:160:VAL:O	16:L:160:VAL:HG13	1.61	1.00
5:A:81:ALA:HB1	20:A:804:CLA:HMA1	1.40	1.00
17:N:62:SER:CB	17:N:66:ASP:CG	2.28	1.00
17:N:72:LYS:HB3	17:N:74:LYS:N	1.77	1.00
17:N:70:GLU:C	17:N:72:LYS:H	1.65	1.00
22:A:847:BCR:H313	20:A:852:CLA:H142	1.42	1.00
6:B:530:THR:HG21	20:B:823:CLA:HAC1	1.40	1.00
16:L:82:ALA:CB	16:L:86:LEU:HD13	1.92	1.00
17:N:61:LEU:CD1	17:N:63:ASP:C	2.30	1.00
1:1:179:THR:HG23	4:4:87:SER:HB3	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:23:ASP:OD2	5:A:24:ARG:HG2	1.62	1.00
10:F:26:GLN:HA	10:F:26:GLN:OE1	1.61	1.00
15:K:7:THR:HA	15:K:10:ILE:CD1	1.91	1.00
5:A:217:SER:HA	22:A:843:BCR:H351	1.43	1.00
5:A:368:LEU:HD21	20:A:818:CLA:H92	1.43	1.00
5:A:365:LEU:CD2	20:A:805:CLA:HED3	1.92	1.00
20:A:818:CLA:H121	20:A:818:CLA:HBB2	1.41	1.00
10:F:102:ARG:CG	10:F:106:ILE:HD11	1.91	1.00
21:H:104:LMU:H41	21:H:104:LMU:H82	1.41	1.00
21:R:103:LMU:C6	21:R:103:LMU:H22	1.92	1.00
1:1:39:TYR:CB	20:1:209:CLA:OBD	2.07	0.99
4:4:36:ASN:ND2	4:4:39:TRP:CZ2	2.29	0.99
20:A:825:CLA:O1D	20:A:825:CLA:HBA1	1.62	0.99
20:J:103:CLA:HBC3	20:J:103:CLA:HHD	1.41	0.99
3:3:74:ALA:HB3	3:3:75:PRO:HD3	1.45	0.99
4:4:107:GLN:O	20:4:302:CLA:HMA1	1.59	0.99
22:A:847:BCR:HC8	22:A:847:BCR:H311	1.00	0.99
16:L:37:LEU:O	16:L:42:ALA:HB3	1.62	0.99
21:N:101:LMU:H1'	21:N:101:LMU:H32	1.40	0.99
17:N:32:ALA:HB1	17:N:35:VAL:HG22	1.44	0.99
17:N:55:GLN:O	17:N:56:LYS:HG3	1.60	0.99
20:A:833:CLA:C3A	20:A:839:CLA:HBB1	1.91	0.99
6:B:560:ASP:HB2	7:C:66:ARG:NE	1.76	0.99
11:G:48:ASP:HB2	11:G:49:THR:CG2	1.89	0.99
11:G:46:ALA:H	11:G:49:THR:CG2	1.73	0.99
4:4:118:ASP:HA	4:4:123:GLN:N	1.78	0.99
20:J:103:CLA:CHA	20:J:103:CLA:CED	2.40	0.99
17:N:66:ASP:C	17:N:67:LEU:CD1	2.29	0.99
21:R:101:LMU:H11	21:R:101:LMU:C6	1.90	0.99
5:A:304:LEU:HD22	20:A:816:CLA:HBB2	1.44	0.99
5:A:370:ILE:HG23	5:A:403:GLY:HA3	1.43	0.99
5:A:451:ILE:CD1	20:A:830:CLA:CED	2.40	0.99
16:L:164:PRO:HG2	16:L:165:TYR:CG	1.93	0.99
17:N:47:THR:OG1	17:N:54:LYS:HD3	1.61	0.99
21:R:103:LMU:H1'	21:R:103:LMU:H31	0.99	0.99
2:2:39:GLU:CA	2:2:40:SER:HB2	1.92	0.99
3:3:84:ILE:HB	20:3:302:CLA:CGA	1.92	0.99
4:4:128:ALA:HB2	4:4:143:PHE:CZ	1.98	0.99
6:B:608:GLN:HA	6:B:608:GLN:NE2	1.78	0.99
21:B:847:LMU:H5B	21:B:847:LMU:O3'	1.63	0.99
4:4:102:GLU:OE2	20:4:314:CLA:CHC	2.10	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:91:PHE:CG	20:4:312:CLA:C3C	2.45	0.99
5:A:328:LYS:HE3	5:A:332:GLU:CG	1.91	0.99
5:A:672:LEU:O	5:A:674:ALA:N	1.95	0.99
7:C:39:ILE:HG12	7:C:40:ALA:H	1.26	0.99
21:E:101:LMU:O2B	21:E:101:LMU:H5B	1.63	0.99
12:H:44:ALA:CB	16:L:145:PHE:HD1	1.75	0.99
21:R:103:LMU:H41	21:R:103:LMU:C6'	1.92	0.99
19:S:1:GLC:C2	19:S:2:FRU:H11	1.92	0.99
2:2:128:ASN:O	2:2:130:LEU:N	1.95	0.99
4:4:128:ALA:CB	4:4:143:PHE:HE2	1.74	0.99
20:A:851:CLA:H11	6:B:616:LEU:HG	1.45	0.99
20:K:101:CLA:HED2	20:K:108:CLA:HMB2	1.41	0.99
20:R:108:CLA:HBA2	20:R:108:CLA:CGD	1.92	0.99
20:2:316:CLA:H192	20:2:316:CLA:H152	1.43	0.99
20:3:313:CLA:CBA	20:3:313:CLA:CED	2.41	0.99
4:4:118:ASP:HA	4:4:122:LYS:C	1.81	0.99
5:A:170:GLY:O	5:A:173:VAL:HG22	1.62	0.99
20:B:836:CLA:C15	22:F:203:BCR:H313	1.88	0.99
2:2:42:ARG:HD3	2:2:45:VAL:HG21	1.43	0.98
5:A:355:HIS:CE1	5:A:416:ILE:HG21	1.98	0.98
6:B:269:TRP:HB2	6:B:497:TRP:HH2	1.23	0.98
1:1:89:VAL:O	11:G:77:ILE:CD1	2.11	0.98
22:I:103:BCR:C31	22:I:103:BCR:C8	2.28	0.98
2:2:128:ASN:O	2:2:130:LEU:HD13	1.63	0.98
5:A:204:ASN:O	5:A:205:HIS:HB2	1.62	0.98
5:A:381:PRO:HB2	20:A:818:CLA:HAA2	1.45	0.98
5:A:114:THR:OG1	5:A:525:ASN:HB2	1.63	0.98
10:F:22:LEU:H	10:F:22:LEU:HD12	0.83	0.98
11:G:45:GLU:CA	11:G:49:THR:HG21	1.91	0.98
20:A:807:CLA:HMB1	22:J:102:BCR:HC7	1.44	0.98
20:K:102:CLA:O1A	20:K:102:CLA:HMA2	1.63	0.98
20:4:307:CLA:O1D	20:4:307:CLA:HAA2	1.62	0.98
4:4:36:ASN:CB	4:4:39:TRP:CZ3	2.43	0.98
4:4:94:GLU:HB3	4:4:95:PHE:HE1	1.18	0.98
16:L:164:PRO:CB	16:L:165:TYR:HA	1.88	0.98
4:4:34:PRO:HA	4:4:35:GLU:HB2	1.22	0.98
20:A:814:CLA:CHC	22:A:843:BCR:H19C	1.92	0.98
5:A:442:ILE:HG23	20:A:829:CLA:HMC3	1.43	0.98
4:4:128:ALA:HB2	4:4:143:PHE:HE2	1.26	0.98
4:4:30:LEU:HA	4:4:31:ALA:HB3	0.98	0.98
5:A:316:MET:CB	5:A:317:TYR:HB2	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:451:ILE:CD1	20:A:830:CLA:HED3	1.93	0.98
20:B:805:CLA:H2	20:B:805:CLA:O1A	1.19	0.98
9:E:68:ARG:C	9:E:68:ARG:HE	1.66	0.98
19:U:2:FRU:C6	19:U:2:FRU:C1	2.30	0.98
2:2:196:HIS:CE1	19:O:1:GLC:O3	2.15	0.98
4:4:37:LEU:CA	4:4:39:TRP:CB	2.41	0.98
5:A:197:GLN:NE2	5:A:197:GLN:HA	1.71	0.98
20:B:836:CLA:HBB2	20:B:836:CLA:H93	0.99	0.98
11:G:42:SER:HB2	11:G:45:GLU:OE1	1.64	0.98
11:G:42:SER:CB	11:G:45:GLU:CD	2.30	0.98
16:L:161:LEU:CD1	16:L:162:ASP:C	2.31	0.98
17:N:51:ASP:C	17:N:52:LEU:CD2	2.32	0.98
18:R:52:UNK:CA	18:R:53:UNK:CB	2.36	0.98
21:4:320:LMU:H3'	21:4:320:LMU:O5B	1.61	0.98
5:A:23:ASP:CG	5:A:24:ARG:CD	2.30	0.98
20:A:838:CLA:H141	22:A:847:BCR:HC21	1.44	0.98
11:G:44:PHE:HD2	11:G:44:PHE:O	1.46	0.98
17:N:63:ASP:CA	17:N:64:ASP:C	2.30	0.98
5:A:246:HIS:O	5:A:248:PHE:HD2	1.45	0.98
20:B:814:CLA:HHD	20:B:814:CLA:HBC2	1.44	0.98
6:B:421:HIS:NE2	20:B:829:CLA:ND	2.11	0.98
22:B:846:BCR:H19C	20:B:850:CLA:H112	1.42	0.98
8:D:44:GLU:HB2	8:D:46:TYR:HE2	1.25	0.98
15:K:17:LEU:C	15:K:17:LEU:CD2	2.30	0.98
17:N:45:ASN:ND2	17:N:57:LYS:HZ1	1.61	0.98
20:1:202:CLA:O1A	20:1:202:CLA:HMA2	1.63	0.98
4:4:147:LEU:HD13	4:4:148:GLU:H	1.18	0.98
20:A:833:CLA:HBC2	22:A:846:BCR:HC31	1.43	0.98
20:B:805:CLA:O1A	20:B:805:CLA:C2	2.11	0.98
20:B:851:CLA:H43	20:B:851:CLA:HHB	1.45	0.98
3:3:173:GLU:HG2	3:3:174:LYS:H	1.29	0.98
4:4:194:VAL:HG12	4:4:195:GLN:CA	1.94	0.98
5:A:210:LEU:HD13	20:A:813:CLA:HMB2	1.45	0.98
5:A:302:HIS:O	5:A:306:ILE:HG12	1.64	0.98
20:A:852:CLA:HMD3	6:B:578:LEU:CD2	1.94	0.98
6:B:493:TRP:CH2	20:B:833:CLA:HMA2	1.98	0.98
20:B:826:CLA:H142	22:B:844:BCR:H10C	1.43	0.98
10:F:5:LEU:HG	10:F:6:THR:H	0.84	0.98
22:J:102:BCR:C39	22:J:102:BCR:H23C	1.90	0.98
17:N:61:LEU:CD1	17:N:62:SER:C	2.32	0.98
2:2:55:ALA:CB	2:2:56:MET:HE2	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:87:GLU:C	22:3:314:BCR:C38	2.33	0.97
4:4:104:ARG:HH11	4:4:105:ARG:HB3	1.24	0.97
21:A:854:LMU:H61	21:A:854:LMU:C2	1.91	0.97
6:B:247:THR:HA	6:B:250:ALA:CB	1.93	0.97
10:F:5:LEU:CG	10:F:6:THR:H	1.74	0.97
6:B:122:GLN:O	6:B:126:THR:OG1	1.81	0.97
20:H:101:CLA:HMC1	20:H:101:CLA:HBC2	1.40	0.97
13:I:26:LEU:HA	13:I:29:GLU:O	1.63	0.97
21:K:105:LMU:H2B	21:K:105:LMU:H3'	1.44	0.97
16:L:82:ALA:HB2	16:L:86:LEU:CD1	1.93	0.97
17:N:61:LEU:CD1	17:N:63:ASP:CA	2.42	0.97
2:2:54:TRP:CZ2	2:2:109:ARG:CD	2.47	0.97
4:4:58:MET:O	4:4:61:PRO:HD2	1.63	0.97
2:2:99:LEU:CD2	20:2:311:CLA:HMC3	1.94	0.97
5:A:21:LEU:N	5:A:22:VAL:HB	1.80	0.97
5:A:40:PHE:HE1	5:A:53:TRP:CD1	1.82	0.97
22:A:844:BCR:C40	22:A:844:BCR:C23	2.36	0.97
5:A:87:SER:HB2	5:A:178:MET:O	1.63	0.97
10:F:24:LYS:CE	10:F:24:LYS:N	2.26	0.97
20:J:103:CLA:CED	20:J:103:CLA:C1A	2.42	0.97
2:2:55:ALA:HB3	2:2:56:MET:HE2	0.98	0.97
5:A:21:LEU:N	5:A:22:VAL:HG12	1.80	0.97
20:A:824:CLA:CED	20:A:825:CLA:C3D	2.42	0.97
21:A:855:LMU:H6'2	21:A:855:LMU:H2B	0.98	0.97
6:B:292:ARG:NE	6:B:292:ARG:HA	1.79	0.97
6:B:588:GLY:O	6:B:592:PHE:HB2	1.62	0.97
7:C:44:ARG:NH2	8:D:127:ARG:HB3	1.78	0.97
6:B:174:ARG:HB2	20:B:811:CLA:HBC2	1.41	0.97
6:B:295:PHE:H	6:B:295:PHE:HD2	1.07	0.97
6:B:461:GLN:O	6:B:464:GLN:HG2	1.65	0.97
22:B:846:BCR:C19	20:B:850:CLA:H151	1.94	0.97
17:N:79:SER:HA	17:N:80:ASN:C	1.83	0.97
24:A:857:SF4:S1	24:A:857:SF4:S2	2.62	0.97
6:B:269:TRP:HB2	6:B:497:TRP:CH2	2.00	0.97
17:N:65:LEU:C	17:N:65:LEU:CD2	2.30	0.97
17:N:70:GLU:O	17:N:72:LYS:CD	2.12	0.97
19:W:1:GLC:H5	19:W:1:GLC:O2	1.62	0.97
5:A:79:PHE:HE2	5:A:185:HIS:CD2	1.80	0.97
6:B:608:GLN:HE21	6:B:608:GLN:CA	1.78	0.97
16:L:160:VAL:O	16:L:160:VAL:HG22	1.60	0.97
21:N:101:LMU:C12	21:N:101:LMU:H81	1.82	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:101:LMU:C3	21:N:101:LMU:H1'	1.91	0.97
17:N:72:LYS:HB3	17:N:73:ASP:HA	0.98	0.97
6:B:87:ILE:CA	6:B:115:ASN:HA	1.93	0.97
20:B:815:CLA:H52	20:B:824:CLA:HMB1	1.45	0.97
20:1:201:CLA:CBC	20:1:201:CLA:CMC	2.29	0.97
4:4:100:TYR:HA	4:4:103:ILE:HD11	1.47	0.97
4:4:33:ASP:HB3	4:4:34:PRO:CD	1.95	0.97
11:G:94:ASP:N	11:G:95:PRO:HD3	1.80	0.97
21:H:106:LMU:C2B	21:H:106:LMU:C3	2.42	0.97
5:A:79:PHE:CZ	5:A:185:HIS:NE2	2.32	0.96
20:A:841:CLA:HMD3	22:B:846:BCR:HC31	1.44	0.96
17:N:63:ASP:HA	17:N:64:ASP:O	1.65	0.96
2:2:42:ARG:HD2	2:2:45:VAL:HG21	1.43	0.96
4:4:122:LYS:CB	4:4:143:PHE:CG	2.46	0.96
21:A:855:LMU:H82	21:A:855:LMU:C4	1.74	0.96
21:E:101:LMU:H12	21:E:101:LMU:H51	1.45	0.96
20:B:836:CLA:C16	22:F:203:BCR:C31	2.40	0.96
20:L:201:CLA:CHD	20:L:201:CLA:HBC3	1.91	0.96
1:1:63:LEU:CD2	1:1:63:LEU:C	2.30	0.96
4:4:40:PHE:CG	4:4:43:ALA:HB2	2.00	0.96
11:G:60:SER:HA	11:G:63:PRO:HD2	1.48	0.96
17:N:57:LYS:N	17:N:60:PHE:O	1.87	0.96
2:2:66:GLU:O	2:2:69:THR:N	1.97	0.96
4:4:147:LEU:CD2	4:4:148:GLU:N	2.28	0.96
4:4:40:PHE:HB3	4:4:43:ALA:HB2	0.98	0.96
20:A:807:CLA:C4A	20:A:807:CLA:HBA1	1.93	0.96
6:B:390:GLY:O	22:B:845:BCR:HC42	1.65	0.96
6:B:586:THR:O	6:B:588:GLY:N	1.99	0.96
16:L:164:PRO:CD	16:L:165:TYR:CE1	2.48	0.96
20:1:201:CLA:HMA2	20:1:201:CLA:HBA1	1.46	0.96
20:1:215:CLA:H43	20:1:215:CLA:H111	1.47	0.96
4:4:30:LEU:N	4:4:31:ALA:HB2	1.79	0.96
4:4:69:ILE:HG22	4:4:70:ILE:N	1.79	0.96
5:A:114:THR:HG22	5:A:115:HIS:CE1	1.98	0.96
5:A:345:GLY:O	5:A:347:TYR:N	1.96	0.96
22:B:845:BCR:C38	22:B:845:BCR:H23C	1.92	0.96
2:2:38:PRO:C	2:2:40:SER:CB	2.34	0.96
2:2:39:GLU:N	2:2:40:SER:CB	2.28	0.96
4:4:107:GLN:HA	20:4:302:CLA:HMA3	0.98	0.96
11:G:44:PHE:N	11:G:45:GLU:CB	2.29	0.96
20:A:824:CLA:CHC	22:A:846:BCR:H373	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:826:CLA:C20	22:J:102:BCR:C17	2.35	0.96
1:1:25:ASP:N	6:B:314:ARG:HH22	1.62	0.96
6:B:50:HIS:HD2	20:B:805:CLA:HAA2	1.28	0.96
7:C:62:PHE:HE2	9:E:42:GLU:OE1	1.46	0.96
10:F:61:LEU:HD23	10:F:69:PRO:HB2	1.46	0.96
20:G:102:CLA:O1D	20:G:102:CLA:H2A	1.66	0.96
11:G:47:GLY:N	11:G:48:ASP:CB	2.29	0.96
12:H:20:GLN:CB	12:H:22:ASP:CB	2.34	0.96
2:2:110:TRP:O	2:2:113:ILE:HG12	1.65	0.96
20:A:836:CLA:HBC3	20:A:836:CLA:HMC1	1.48	0.96
6:B:732:LYS:CG	6:B:734:GLY:CA	2.43	0.96
9:E:56:ASP:HB2	9:E:64:PRO:HB3	1.46	0.96
10:F:100:VAL:HA	10:F:103:SER:OG	1.64	0.96
16:L:161:LEU:CD1	16:L:161:LEU:C	2.30	0.96
17:N:62:SER:CB	17:N:66:ASP:HB3	1.93	0.96
20:2:307:CLA:CAD	20:2:307:CLA:CED	2.44	0.96
5:A:452:PHE:CE1	20:A:835:CLA:HBB2	2.01	0.96
5:A:98:PHE:HZ	20:A:807:CLA:HMD3	1.31	0.96
20:B:803:CLA:H2A	20:B:803:CLA:HED3	1.48	0.96
7:C:52:LYS:HG3	7:C:52:LYS:O	1.66	0.96
7:C:63:LEU:HG	7:C:64:SER:N	1.77	0.96
9:E:52:VAL:O	9:E:53:VAL:HG22	1.63	0.96
20:B:803:CLA:H191	10:F:104:TYR:HB3	1.46	0.96
20:B:836:CLA:C15	22:F:203:BCR:H312	1.92	0.96
17:N:54:LYS:CB	17:N:57:LYS:NZ	2.28	0.96
1:1:59:VAL:HG12	1:1:60:PRO:O	1.65	0.96
2:2:129:LYS:O	2:2:132:GLY:N	1.99	0.96
20:4:318:CLA:HED1	20:4:318:CLA:O1A	1.64	0.96
5:A:328:LYS:HE3	5:A:332:GLU:HG3	0.98	0.96
17:N:62:SER:HB3	17:N:66:ASP:CA	1.96	0.96
21:1:213:LMU:H6D	21:1:213:LMU:O3'	1.65	0.95
2:2:203:THR:C	2:2:204:ILE:CG1	2.32	0.95
3:3:74:ALA:HA	20:3:307:CLA:C4D	1.96	0.95
4:4:122:LYS:CG	4:4:143:PHE:HB2	1.95	0.95
20:4:304:CLA:H203	20:4:304:CLA:C15	1.94	0.95
4:4:91:PHE:CD2	4:4:92:VAL:N	2.34	0.95
6:B:715:VAL:HG23	6:B:719:PHE:CD2	2.01	0.95
20:B:823:CLA:CHD	20:B:823:CLA:HBC2	1.95	0.95
17:N:67:LEU:N	17:N:67:LEU:HD12	1.79	0.95
5:A:331:LEU:HD21	5:A:343:HIS:C	1.85	0.95
22:A:843:BCR:C8	22:A:843:BCR:H311	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:850:CLA:HBB2	20:B:851:CLA:C1B	1.96	0.95
11:G:94:ASP:N	11:G:95:PRO:CD	2.29	0.95
21:R:109:LMU:H1'	21:R:109:LMU:O6'	1.64	0.95
20:A:852:CLA:CMD	6:B:578:LEU:HD23	1.96	0.95
11:G:43:HIS:HA	11:G:44:PHE:HB3	0.97	0.95
17:N:54:LYS:CG	17:N:57:LYS:NZ	2.29	0.95
1:1:185:TRP:CB	1:1:186:HIS:ND1	2.30	0.95
21:2:318:LMU:O2'	21:2:318:LMU:H12	1.65	0.95
20:4:316:CLA:HBC3	20:4:316:CLA:HHD	1.46	0.95
21:4:320:LMU:H5B	21:4:320:LMU:C3'	1.96	0.95
20:A:808:CLA:CHC	20:A:809:CLA:HMD2	1.96	0.95
21:H:104:LMU:O4'	19:Y:2:FRU:C3	1.97	0.95
1:1:63:LEU:N	1:1:63:LEU:CD1	2.30	0.95
4:4:192:THR:CG2	4:4:195:GLN:N	2.29	0.95
4:4:74:LYS:H	4:4:75:TRP:HA	1.07	0.95
5:A:335:LYS:HG2	5:A:336:GLY:N	1.82	0.95
21:K:105:LMU:H6D	21:K:105:LMU:H32	0.97	0.95
16:L:161:LEU:HD12	16:L:162:ASP:HA	1.43	0.95
17:N:66:ASP:O	17:N:67:LEU:HG	1.67	0.95
5:A:21:LEU:N	5:A:22:VAL:CB	2.29	0.95
5:A:246:HIS:O	5:A:248:PHE:N	2.00	0.95
5:A:588:GLY:HA3	6:B:668:ARG:HD3	1.44	0.95
20:A:826:CLA:HBA1	20:A:826:CLA:H43	1.49	0.95
7:C:1:MET:HG2	7:C:4:SER:CB	1.96	0.95
21:H:106:LMU:C3	21:H:106:LMU:H2B	1.96	0.95
13:I:12:VAL:O	13:I:17:PRO:HD3	1.64	0.95
20:L:201:CLA:HAA1	20:L:201:CLA:O2D	1.65	0.95
21:N:101:LMU:C9	21:N:101:LMU:C5	2.30	0.95
1:1:64:GLY:O	1:1:65:TYR:HB2	1.66	0.95
20:2:302:CLA:HBC3	20:2:302:CLA:HMC1	1.49	0.95
3:3:110:SER:C	3:3:111:TYR:CD2	2.40	0.95
4:4:93:ILE:CA	4:4:96:ILE:CD1	2.41	0.95
5:A:103:PHE:HE1	20:A:807:CLA:CGD	1.77	0.95
5:A:328:LYS:HE2	5:A:332:GLU:CG	1.94	0.95
6:B:127:ILE:HD13	6:B:198:ALA:HB2	1.49	0.95
6:B:119:GLY:CA	20:B:826:CLA:HED1	1.97	0.95
6:B:11:GLY:HA3	7:C:71:HIS:CD2	2.01	0.95
17:N:52:LEU:N	17:N:52:LEU:CD2	2.29	0.95
1:1:144:LYS:NZ	20:1:201:CLA:OBD	1.99	0.95
20:2:307:CLA:CGD	20:2:307:CLA:CBA	2.43	0.95
9:E:68:ARG:HH21	9:E:69:PHE:HA	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:206:CLA:HED2	20:F:206:CLA:OBD	1.66	0.95
20:H:101:CLA:HMA2	20:H:101:CLA:O1A	1.65	0.95
15:K:24:PHE:CD1	15:K:52:PRO:HG2	2.01	0.95
17:N:72:LYS:CB	17:N:73:ASP:CA	2.30	0.95
3:3:194:ILE:HG13	20:3:304:CLA:CMC	1.97	0.95
5:A:331:LEU:CD1	5:A:346:LEU:HB3	1.95	0.95
5:A:547:PHE:O	5:A:551:VAL:HG13	1.64	0.95
21:D:201:LMU:C4	21:E:101:LMU:C12	2.40	0.95
11:G:46:ALA:H	11:G:48:ASP:HB3	1.17	0.95
2:2:37:ASP:OD2	3:3:41:ASP:CG	2.05	0.95
4:4:30:LEU:N	4:4:31:ALA:CB	2.30	0.95
20:4:318:CLA:HED1	20:4:318:CLA:H12	1.47	0.95
16:L:161:LEU:CD1	16:L:162:ASP:N	2.29	0.95
16:L:164:PRO:HB2	16:L:165:TYR:HB3	1.48	0.95
17:N:56:LYS:O	17:N:60:PHE:HD1	1.50	0.95
17:N:72:LYS:CB	17:N:74:LYS:N	2.29	0.95
18:R:40:UNK:N	18:R:41:UNK:CB	2.30	0.95
19:Y:1:GLC:H5	19:Y:1:GLC:O2	1.64	0.95
1:1:185:TRP:HB3	1:1:186:HIS:CG	2.02	0.94
2:2:110:TRP:CD1	2:2:113:ILE:HG21	2.01	0.94
5:A:81:ALA:HB1	20:A:804:CLA:CMA	1.92	0.94
20:A:815:CLA:HED2	20:A:815:CLA:HAA1	0.95	0.94
20:B:839:CLA:HMC1	20:B:839:CLA:HBC2	1.47	0.94
20:B:836:CLA:HBC1	10:F:83:PHE:CZ	2.01	0.94
15:K:10:ILE:N	15:K:10:ILE:HD12	1.82	0.94
15:K:44:GLU:HG3	15:K:45:SER:N	0.75	0.94
17:N:67:LEU:C	17:N:68:GLU:CG	2.32	0.94
1:1:57:ILE:CD1	1:1:58:LEU:N	2.30	0.94
20:3:318:CLA:H122	20:3:318:CLA:H172	1.49	0.94
4:4:101:VAL:CG1	4:4:104:ARG:NH2	2.28	0.94
4:4:147:LEU:HD22	4:4:148:GLU:CA	1.97	0.94
5:A:25:ASP:N	5:A:26:PRO:CG	2.30	0.94
20:B:819:CLA:CHD	20:B:819:CLA:HBC2	1.95	0.94
10:F:23:LYS:CB	10:F:24:LYS:NZ	2.30	0.94
11:G:13:GLY:HA2	11:G:16:LEU:HG	1.48	0.94
11:G:28:ARG:HG2	11:G:29:GLU:N	1.80	0.94
21:K:106:LMU:C3'	21:K:106:LMU:C2	2.45	0.94
17:N:51:ASP:O	17:N:52:LEU:HD22	1.66	0.94
17:N:61:LEU:CD1	17:N:62:SER:N	2.29	0.94
4:4:38:ARG:CG	4:4:39:TRP:N	2.30	0.94
5:A:599:PHE:CE2	5:A:731:ARG:HB3	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:824:CLA:HED3	20:A:825:CLA:HMD1	1.46	0.94
7:C:73:THR:OG1	7:C:76:SER:HB3	1.67	0.94
20:H:102:CLA:HAC1	22:I:103:BCR:C3	1.98	0.94
22:I:103:BCR:C32	22:I:103:BCR:C4	2.38	0.94
20:J:103:CLA:O1A	20:J:103:CLA:H143	1.67	0.94
3:3:194:ILE:CG1	20:3:304:CLA:HMC2	1.97	0.94
5:A:162:LEU:O	5:A:165:TYR:HB3	1.66	0.94
20:A:824:CLA:H2	20:A:825:CLA:HED3	1.50	0.94
6:B:124:TRP:NE1	6:B:129:LEU:HD22	1.83	0.94
6:B:612:SER:HA	6:B:615:TYR:HE1	1.30	0.94
21:K:106:LMU:H82	21:K:106:LMU:C2	1.96	0.94
21:K:106:LMU:H52	21:K:106:LMU:H12	1.46	0.94
20:L:201:CLA:HBC2	20:L:201:CLA:HHD	1.47	0.94
2:2:41:LEU:CD2	2:2:41:LEU:N	2.29	0.94
4:4:147:LEU:CD2	4:4:148:GLU:H	1.81	0.94
4:4:32:GLU:O	4:4:33:ASP:OD1	1.83	0.94
4:4:37:LEU:N	4:4:39:TRP:CB	2.30	0.94
21:K:106:LMU:C9	21:K:106:LMU:C3	2.40	0.94
12:H:44:ALA:HB2	16:L:145:PHE:CD1	2.01	0.94
2:2:43:TRP:CE2	2:2:125:PHE:CE1	2.56	0.94
3:3:181:LEU:N	3:3:181:LEU:CD1	2.30	0.94
5:A:340:GLY:O	5:A:343:HIS:HB2	1.68	0.94
5:A:462:ILE:HD11	20:B:850:CLA:H51	1.47	0.94
20:B:823:CLA:CBB	20:B:837:CLA:HMB3	1.97	0.94
18:R:34:UNK:N	18:R:36:UNK:CB	2.30	0.94
20:1:215:CLA:C4	20:1:215:CLA:H112	1.94	0.94
2:2:167:GLY:O	2:2:170:ALA:N	2.00	0.94
5:A:361:ASN:HD21	20:A:805:CLA:CED	1.79	0.94
20:A:803:CLA:C4	20:A:838:CLA:H61	1.97	0.94
6:B:266:GLN:O	6:B:267:SER:HB3	1.66	0.94
7:C:1:MET:H1	7:C:4:SER:N	1.66	0.94
11:G:46:ALA:CA	11:G:48:ASP:CG	2.36	0.94
20:4:319:CLA:HMC1	20:4:319:CLA:CBC	1.97	0.94
4:4:96:ILE:O	4:4:99:HIS:HB3	1.66	0.94
5:A:114:THR:HG22	5:A:115:HIS:ND1	1.82	0.94
5:A:626:GLY:HA3	5:A:636:HIS:HA	1.49	0.94
20:B:823:CLA:HED1	20:B:824:CLA:CMD	1.97	0.94
16:L:163:LEU:HD22	16:L:164:PRO:HA	1.36	0.94
3:3:181:LEU:N	3:3:182:LYS:CE	2.30	0.94
5:A:358:LEU:HD11	5:A:413:HIS:CG	2.02	0.94
20:3:302:CLA:HMC3	20:A:814:CLA:HBA2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:39:LYS:HD2	8:D:42:VAL:CG1	1.98	0.94
21:D:201:LMU:H32	21:E:101:LMU:C12	1.97	0.94
16:L:82:ALA:HB2	16:L:86:LEU:HD13	0.97	0.94
21:R:103:LMU:H41	21:R:103:LMU:O6'	1.67	0.94
2:2:203:THR:C	2:2:204:ILE:HG12	1.87	0.94
2:2:98:GLU:HG3	2:2:99:LEU:CD1	1.97	0.94
3:3:74:ALA:CA	20:3:307:CLA:C2D	2.46	0.94
4:4:165:GLY:O	4:4:169:GLN:HG2	1.67	0.94
4:4:34:PRO:HG3	4:4:35:GLU:OE1	1.67	0.94
4:4:34:PRO:HA	4:4:35:GLU:CG	1.96	0.94
5:A:21:LEU:N	5:A:22:VAL:CG1	2.30	0.94
21:A:855:LMU:C9	21:A:855:LMU:C2	2.30	0.94
6:B:422:LEU:HD13	6:B:535:VAL:HG11	1.47	0.94
11:G:46:ALA:N	11:G:48:ASP:CB	2.30	0.94
16:L:164:PRO:HD2	16:L:165:TYR:CG	2.02	0.94
17:N:72:LYS:NZ	17:N:74:LYS:HG2	1.82	0.94
4:4:100:TYR:HA	4:4:103:ILE:CD1	1.98	0.94
5:A:316:MET:CB	5:A:317:TYR:HD1	1.76	0.94
20:A:808:CLA:H142	22:J:102:BCR:C14	1.98	0.94
6:B:556:SER:C	6:B:558:PRO:HD2	1.88	0.94
21:K:106:LMU:C5'	21:K:106:LMU:C3	2.30	0.94
15:K:9:LEU:CD2	15:K:9:LEU:N	2.30	0.94
20:1:215:CLA:CHD	20:1:215:CLA:HBC3	1.96	0.93
21:1:219:LMU:H3'	21:1:219:LMU:C5B	1.98	0.93
2:2:203:THR:CG2	2:2:204:ILE:N	2.30	0.93
2:2:50:VAL:O	2:2:54:TRP:HD1	1.51	0.93
4:4:147:LEU:CG	4:4:148:GLU:N	2.29	0.93
20:4:307:CLA:HMA2	20:4:307:CLA:HBA1	0.95	0.93
17:N:47:THR:HG21	17:N:54:LYS:HZ3	0.88	0.93
20:R:108:CLA:HBA2	20:R:108:CLA:O1D	1.65	0.93
5:A:100:GLY:HA3	5:A:153:TRP:CH2	2.03	0.93
5:A:23:ASP:OD1	5:A:24:ARG:HD3	1.66	0.93
6:B:22:TRP:HE1	20:B:838:CLA:HBB1	0.79	0.93
6:B:517:PHE:O	6:B:517:PHE:HD2	1.36	0.93
11:G:93:TYR:CA	11:G:94:ASP:CB	2.30	0.93
16:L:163:LEU:CB	16:L:164:PRO:HB3	1.96	0.93
17:N:63:ASP:H	17:N:64:ASP:HB3	1.32	0.93
17:N:61:LEU:CD1	17:N:63:ASP:N	2.30	0.93
20:1:215:CLA:H41	20:1:215:CLA:C7	1.83	0.93
20:2:322:CLA:H41	20:2:322:CLA:H72	0.95	0.93
4:4:36:ASN:O	4:4:39:TRP:HB2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:819:CLA:C9	22:A:845:BCR:C37	2.11	0.93
22:A:845:BCR:H23C	22:A:845:BCR:C38	1.98	0.93
22:F:203:BCR:C8	22:F:203:BCR:C32	2.30	0.93
1:1:57:ILE:HD13	1:1:58:LEU:H	1.25	0.93
21:A:854:LMU:H51	21:A:854:LMU:O6'	1.66	0.93
6:B:732:LYS:HG2	6:B:734:GLY:H	1.24	0.93
10:F:42:ILE:HG13	10:F:43:LYS:N	1.80	0.93
16:L:164:PRO:CD	16:L:165:TYR:CG	2.51	0.93
19:P:2:FRU:C6	19:P:2:FRU:H11	1.99	0.93
19:Q:2:FRU:C6	19:Q:2:FRU:C1	2.39	0.93
4:4:93:ILE:HA	4:4:96:ILE:HD11	1.48	0.93
20:A:814:CLA:HHC	22:A:843:BCR:C17	1.97	0.93
20:A:850:CLA:HAA1	20:B:849:CLA:HBB2	1.49	0.93
20:B:850:CLA:C9	20:B:851:CLA:C9	2.46	0.93
7:C:5:VAL:C	7:C:65:VAL:HG22	1.87	0.93
20:K:101:CLA:CMD	20:K:108:CLA:NA	2.30	0.93
21:K:104:LMU:H5'	21:K:104:LMU:O2'	1.66	0.93
16:L:118:LEU:HD12	16:L:119:THR:H	1.30	0.93
2:2:169:LEU:HD23	20:2:305:CLA:CBB	1.92	0.93
3:3:84:ILE:H	20:3:302:CLA:H43	1.32	0.93
5:A:328:LYS:HG2	5:A:332:GLU:CB	1.99	0.93
20:A:822:CLA:C1D	22:A:845:BCR:H19C	1.99	0.93
20:L:201:CLA:HAA1	20:L:201:CLA:O1D	1.69	0.93
20:1:215:CLA:C4	20:1:215:CLA:H71	1.99	0.93
21:2:317:LMU:H22	21:2:317:LMU:O2'	1.69	0.93
3:3:84:ILE:HB	20:3:302:CLA:O1A	0.76	0.93
4:4:147:LEU:CD1	4:4:148:GLU:N	2.30	0.93
5:A:331:LEU:HD11	5:A:346:LEU:HB2	1.49	0.93
20:A:833:CLA:H3A	20:A:839:CLA:CBB	1.98	0.93
9:E:61:THR:HG22	9:E:62:ARG:H	1.34	0.93
21:K:106:LMU:H3'	21:K:106:LMU:C2	1.99	0.93
20:2:322:CLA:HED3	20:2:322:CLA:OBD	1.67	0.93
2:2:44:ASN:ND2	14:J:1:MET:HB2	1.83	0.93
21:3:322:LMU:O2'	21:3:322:LMU:H11	1.68	0.93
20:4:302:CLA:CHD	20:4:302:CLA:CBC	2.42	0.93
22:A:844:BCR:C23	22:A:844:BCR:H402	1.96	0.93
8:D:124:ASN:HB3	8:D:125:PRO:HD3	1.51	0.93
11:G:46:ALA:N	11:G:49:THR:CG2	2.30	0.93
5:A:73:GLU:O	5:A:76:ARG:N	2.02	0.93
20:A:826:CLA:C7	22:A:847:BCR:C37	2.47	0.93
20:B:820:CLA:HBC2	20:B:821:CLA:HBA1	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:68:ILE:O	11:G:72:LEU:HB3	1.68	0.93
21:H:106:LMU:H1B	21:H:106:LMU:O1'	1.68	0.93
1:1:89:VAL:O	11:G:77:ILE:HD13	1.68	0.93
4:4:104:ARG:NH1	4:4:105:ARG:CB	2.29	0.93
6:B:353:TYR:CG	6:B:594:TRP:HZ3	1.86	0.93
2:2:116:PRO:O	2:2:131:THR:HB	1.67	0.92
5:A:239:PRO:HA	5:A:242:ILE:HD11	1.49	0.92
6:B:525:LEU:O	6:B:525:LEU:HD22	1.69	0.92
6:B:279:ALA:O	20:B:814:CLA:HMB3	1.67	0.92
2:2:61:GLY:O	2:2:65:PRO:HG2	1.69	0.92
2:2:73:ILE:HD12	2:2:73:ILE:N	1.83	0.92
2:2:70:LYS:HG3	2:2:73:ILE:HG13	1.50	0.92
4:4:71:ASN:O	4:4:73:PRO:HD3	1.69	0.92
3:3:87:GLU:O	22:3:314:BCR:H381	1.69	0.92
4:4:74:LYS:N	4:4:75:TRP:CA	2.29	0.92
20:A:838:CLA:H141	22:A:847:BCR:HC22	0.94	0.92
22:A:843:BCR:H402	22:A:843:BCR:C23	1.94	0.92
6:B:648:TRP:CZ3	22:B:846:BCR:H392	2.03	0.92
11:G:93:TYR:HA	11:G:94:ASP:CG	1.89	0.92
22:J:102:BCR:H393	22:J:102:BCR:C23	1.93	0.92
19:U:2:FRU:H11	19:U:2:FRU:H62	0.93	0.92
1:1:179:THR:OG1	4:4:87:SER:CB	2.17	0.92
3:3:84:ILE:H	20:3:302:CLA:C3	1.82	0.92
5:A:478:SER:HB3	5:A:644:GLN:OE1	1.69	0.92
6:B:142:LEU:CD2	22:B:844:BCR:H333	2.00	0.92
21:F:201:LMU:H31	21:F:201:LMU:H71	0.94	0.92
2:2:42:ARG:HG3	2:2:45:VAL:HG21	1.46	0.92
5:A:24:ARG:O	5:A:26:PRO:HG2	1.68	0.92
10:F:40:LEU:HA	10:F:42:ILE:HG12	1.50	0.92
11:G:47:GLY:H	11:G:48:ASP:CA	1.82	0.92
11:G:45:GLU:HG2	11:G:49:THR:CG2	1.86	0.92
2:2:127:ASN:HD21	14:J:7:TYR:HA	1.33	0.92
20:A:830:CLA:C16	22:L:210:BCR:C36	2.47	0.92
4:4:194:VAL:HG12	4:4:195:GLN:HB2	0.94	0.92
5:A:472:ARG:HE	5:A:474:GLN:HG3	1.31	0.92
20:A:824:CLA:O1A	20:A:824:CLA:H2	1.68	0.92
6:B:596:TRP:HH2	6:B:612:SER:O	1.48	0.92
7:C:1:MET:CG	7:C:4:SER:OG	2.16	0.92
11:G:40:GLY:O	11:G:41:MET:SD	2.28	0.92
11:G:7:VAL:CG2	11:G:8:ILE:H	1.83	0.92
15:K:9:LEU:HD23	15:K:9:LEU:H	1.25	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:TRP:HZ2	2:2:125:PHE:CZ	1.84	0.92
4:4:166:PHE:O	4:4:169:GLN:HB2	1.69	0.92
7:C:79:LEU:HD22	7:C:81:TYR:O	1.70	0.92
20:R:107:CLA:CED	20:R:107:CLA:CHA	2.47	0.92
4:4:101:VAL:HG13	4:4:104:ARG:HH21	1.11	0.92
22:A:847:BCR:H313	20:A:852:CLA:H143	1.48	0.92
22:B:846:BCR:C38	22:B:846:BCR:H23C	1.98	0.92
22:F:203:BCR:H271	22:F:203:BCR:C40	1.95	0.92
20:A:826:CLA:H203	22:J:102:BCR:H17C	0.92	0.92
2:2:162:LYS:NZ	20:2:305:CLA:OBD	2.02	0.92
21:4:320:LMU:C5B	21:4:320:LMU:C3'	2.47	0.92
4:4:60:LEU:HG	4:4:61:PRO:HD3	1.49	0.92
4:4:88:SER:O	4:4:90:LEU:HA	1.70	0.92
6:B:369:ALA:O	6:B:725:LEU:HD11	1.70	0.92
6:B:351:HIS:HB3	20:B:815:CLA:HED1	1.49	0.92
8:D:102:ARG:NH1	8:D:104:PHE:CE1	2.38	0.92
10:F:23:LYS:C	10:F:24:LYS:HZ3	1.73	0.92
19:S:1:GLC:O2	19:S:2:FRU:H11	1.70	0.92
1:1:163:VAL:HA	1:1:166:SER:HB3	1.51	0.92
3:3:93:PHE:H	3:3:95:THR:H	1.10	0.92
20:4:302:CLA:CHD	20:4:302:CLA:HBC2	1.99	0.92
20:A:815:CLA:CBC	20:A:815:CLA:CMC	2.30	0.92
8:D:111:TYR:HD2	8:D:114:PRO:HB3	1.33	0.92
17:N:61:LEU:HD11	17:N:63:ASP:CB	1.98	0.92
17:N:72:LYS:NZ	17:N:74:LYS:CG	2.33	0.92
1:1:39:TYR:CG	20:1:209:CLA:OBD	2.22	0.91
20:A:822:CLA:NC	22:A:845:BCR:H19C	1.84	0.91
6:B:602:TRP:O	6:B:604:GLY:N	2.01	0.91
11:G:46:ALA:C	11:G:48:ASP:CG	2.29	0.91
2:2:40:SER:C	2:2:41:LEU:HD22	1.89	0.91
4:4:117:GLN:O	4:4:121:PHE:HE2	1.49	0.91
20:A:830:CLA:H52	22:B:846:BCR:C34	2.00	0.91
20:H:101:CLA:HBC3	20:H:101:CLA:CMC	2.00	0.91
20:K:108:CLA:CGA	20:K:108:CLA:H3A	2.00	0.91
21:R:104:LMU:C2'	21:R:104:LMU:C2	2.31	0.91
20:1:215:CLA:CAA	20:1:215:CLA:CGD	2.49	0.91
2:2:54:TRP:CE2	2:2:109:ARG:HD2	2.04	0.91
5:A:259:TYR:HB3	5:A:260:PRO:HD2	1.51	0.91
5:A:411:ALA:HB2	22:A:846:BCR:H392	1.52	0.91
6:B:382:ILE:CG2	6:B:383:MET:H	1.83	0.91
16:L:123:ARG:HA	16:L:123:ARG:CZ	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:102:LMU:H5B	21:R:102:LMU:H6E	1.30	0.91
21:R:103:LMU:H62	21:R:103:LMU:C2	1.97	0.91
1:1:37:GLU:HA	1:1:40:LYS:HB2	1.49	0.91
2:2:203:THR:HG22	2:2:204:ILE:N	1.84	0.91
3:3:83:LEU:HA	20:3:302:CLA:H43	1.50	0.91
6:B:65:LEU:HD22	6:B:124:TRP:CE3	2.05	0.91
21:K:105:LMU:H22	21:K:105:LMU:H71	0.93	0.91
8:D:30:ALA:O	16:L:18:PRO:HB2	1.71	0.91
17:N:72:LYS:CG	17:N:74:LYS:HB2	2.00	0.91
20:3:311:CLA:H2A	20:3:311:CLA:O1D	1.71	0.91
6:B:172:GLU:O	6:B:176:ASN:HB2	1.70	0.91
23:B:841:PQN:H191	22:B:846:BCR:H10C	0.91	0.91
7:C:5:VAL:HB	7:C:65:VAL:HA	1.52	0.91
11:G:45:GLU:CB	11:G:49:THR:HG21	1.99	0.91
21:K:106:LMU:H22	21:K:106:LMU:O2'	1.68	0.91
4:4:143:PHE:HB2	4:4:150:LYS:HE2	1.52	0.91
21:4:320:LMU:H3'	21:4:320:LMU:C5B	2.00	0.91
5:A:248:PHE:H	5:A:248:PHE:HD2	1.11	0.91
20:A:822:CLA:C1D	22:A:845:BCR:C19	2.47	0.91
21:A:854:LMU:H81	21:A:854:LMU:H21	0.93	0.91
6:B:142:LEU:HD22	22:B:844:BCR:H333	1.52	0.91
17:N:47:THR:CG2	17:N:54:LYS:HZ3	1.81	0.91
1:1:59:VAL:HG13	1:1:60:PRO:HD2	1.53	0.91
6:B:561:GLY:HA3	7:C:52:LYS:HG2	1.51	0.91
7:C:78:GLY:O	7:C:81:TYR:HE1	1.53	0.91
12:H:25:GLY:HA2	12:H:27:ASP:OD2	1.69	0.91
16:L:95:LEU:HD13	22:L:210:BCR:C31	2.01	0.91
16:L:30:SER:OG	16:L:32:LEU:HB2	1.67	0.91
5:A:648:THR:HG23	5:A:651:GLY:H	1.34	0.91
6:B:442:VAL:HG21	20:B:831:CLA:HAC2	1.51	0.91
2:2:41:LEU:O	2:2:42:ARG:CD	2.19	0.91
4:4:91:PHE:C	4:4:91:PHE:CD2	2.39	0.91
6:B:492:ILE:H	6:B:492:ILE:HD13	1.36	0.91
21:B:801:LMU:C6	21:B:801:LMU:H101	1.99	0.91
20:H:101:CLA:H2	20:H:101:CLA:O1A	1.68	0.91
17:N:54:LYS:CB	17:N:57:LYS:HZ1	1.83	0.91
17:N:72:LYS:CG	17:N:74:LYS:N	2.33	0.91
22:3:314:BCR:H311	22:3:314:BCR:C8	1.99	0.91
3:3:87:GLU:C	22:3:314:BCR:H381	1.91	0.91
3:3:205:GLY:N	5:A:252:ARG:NH2	2.14	0.91
5:A:301:HIS:CD2	20:A:816:CLA:O1D	2.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:815:CLA:CAA	20:A:815:CLA:H42	1.99	0.91
6:B:120:VAL:HA	6:B:123:TRP:NE1	1.85	0.91
20:B:808:CLA:HBB2	20:B:850:CLA:H13	1.53	0.91
20:L:209:CLA:HAA1	20:L:209:CLA:CGD	1.99	0.91
4:4:93:ILE:C	4:4:96:ILE:HD12	1.92	0.90
6:B:5:ILE:HB	6:B:6:PRO:HD2	1.51	0.90
20:B:823:CLA:CHD	20:B:823:CLA:CBC	2.45	0.90
19:Q:1:GLC:H5	19:Q:2:FRU:O5	1.71	0.90
5:A:328:LYS:HG3	5:A:332:GLU:HB2	1.50	0.90
11:G:46:ALA:H	11:G:49:THR:HG21	1.32	0.90
20:H:101:CLA:H3A	20:H:101:CLA:CGA	2.00	0.90
21:H:108:LMU:H41	21:H:108:LMU:H81	1.51	0.90
5:A:453:LEU:HB3	5:A:547:PHE:HB2	1.53	0.90
5:A:659:ALA:O	5:A:662:SER:OG	1.87	0.90
5:A:304:LEU:HD22	20:A:816:CLA:CBB	2.01	0.90
6:B:672:GLN:HE21	6:B:672:GLN:CA	1.84	0.90
21:K:106:LMU:H3'	21:K:106:LMU:H22	1.51	0.90
15:K:52:PRO:O	15:K:56:THR:HG22	1.71	0.90
17:N:47:THR:CG2	17:N:54:LYS:NZ	2.32	0.90
1:1:24:PHE:CD2	6:B:314:ARG:NH2	2.39	0.90
1:1:89:VAL:HB	1:1:90:PRO:HD3	1.52	0.90
6:B:282:PHE:CZ	20:B:814:CLA:C1	2.53	0.90
6:B:362:ALA:HB2	6:B:368:GLN:HG2	1.53	0.90
6:B:382:ILE:O	6:B:384:THR:N	2.05	0.90
21:H:104:LMU:H4O1	19:Y:2:FRU:H3	1.32	0.90
13:I:12:VAL:HG21	20:I:102:CLA:O1A	1.71	0.90
16:L:64:LEU:HB3	16:L:68:PHE:CE1	2.07	0.90
3:3:181:LEU:HD12	3:3:181:LEU:N	1.85	0.90
4:4:121:PHE:O	4:4:122:LYS:CD	2.19	0.90
20:A:809:CLA:CBB	20:B:831:CLA:HMD2	2.01	0.90
6:B:167:TRP:HB2	11:G:41:MET:HE2	1.49	0.90
11:G:42:SER:HB2	11:G:45:GLU:OE2	1.70	0.90
20:H:109:CLA:O2A	20:H:109:CLA:HMA2	1.71	0.90
18:R:33:UNK:C	18:R:36:UNK:CB	2.50	0.90
1:1:63:LEU:N	1:1:63:LEU:HD13	1.84	0.90
2:2:196:HIS:O	2:2:197:LEU:HB2	1.70	0.90
2:2:41:LEU:N	2:2:41:LEU:HD23	1.85	0.90
2:2:73:ILE:O	2:2:74:LEU:HD23	1.72	0.90
3:3:64:TYR:HB3	20:3:311:CLA:H42	1.50	0.90
20:A:824:CLA:C6	20:A:825:CLA:HED1	2.02	0.90
20:A:824:CLA:C7	20:A:825:CLA:HED1	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:50:HIS:CD2	20:B:805:CLA:HAA2	2.06	0.90
6:B:732:LYS:CB	6:B:733:PHE:C	2.39	0.90
8:D:48:ILE:HB	8:D:100:PHE:HB3	1.52	0.90
20:1:206:CLA:HHD	20:1:206:CLA:CBC	2.01	0.90
4:4:36:ASN:O	4:4:39:TRP:CE3	2.25	0.90
6:B:119:GLY:HA3	20:B:826:CLA:CED	2.00	0.90
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.36	0.90
20:B:833:CLA:HMB1	22:B:845:BCR:H292	1.53	0.90
20:B:850:CLA:HBB2	20:B:851:CLA:CHB	2.00	0.90
11:G:48:ASP:HB2	11:G:49:THR:HG22	0.92	0.90
20:H:101:CLA:HAA2	20:H:101:CLA:O1D	1.69	0.90
15:K:20:PHE:CD2	15:K:20:PHE:C	2.43	0.90
15:K:74:ILE:HG22	15:K:75:VAL:HG22	1.54	0.90
16:L:66:GLY:HA3	20:L:209:CLA:HHC	1.52	0.90
2:2:43:TRP:CZ3	2:2:125:PHE:CB	2.55	0.90
4:4:69:ILE:CG2	4:4:70:ILE:H	1.84	0.90
6:B:697:PRO:O	7:C:79:LEU:CD1	2.19	0.90
20:B:821:CLA:C2	20:B:821:CLA:H71	1.99	0.90
13:I:8:PHE:HB2	20:I:102:CLA:OBD	1.72	0.90
17:N:40:CYS:SG	17:N:40:CYS:O	2.29	0.90
17:N:63:ASP:HA	17:N:64:ASP:C	1.91	0.90
1:1:57:ILE:CD1	1:1:58:LEU:H	1.85	0.90
4:4:124:TYR:O	4:4:127:PRO:CD	2.20	0.90
4:4:39:TRP:CG	4:4:40:PHE:N	2.27	0.90
4:4:75:TRP:HE3	4:4:76:TYR:H	1.18	0.90
20:A:823:CLA:HMD2	20:A:823:CLA:H142	1.52	0.90
6:B:5:ILE:HB	6:B:6:PRO:CD	2.01	0.90
20:B:806:CLA:O1D	20:B:806:CLA:H2A	1.72	0.90
20:B:836:CLA:H161	22:F:203:BCR:C31	2.02	0.90
21:K:106:LMU:H82	21:K:106:LMU:H31	1.45	0.90
2:2:42:ARG:HG3	2:2:45:VAL:CB	2.02	0.90
20:A:824:CLA:C6	20:A:825:CLA:CED	2.50	0.90
24:A:857:SF4:S4	24:A:857:SF4:FE1	1.64	0.90
6:B:551:LYS:NZ	8:D:140:ASN:O	2.05	0.90
2:2:64:ILE:O	2:2:68:LEU:HB2	1.71	0.89
20:2:307:CLA:CGD	20:2:307:CLA:HBA1	2.01	0.89
6:B:504:ASN:HD22	6:B:504:ASN:H	1.14	0.89
21:B:847:LMU:H112	21:B:847:LMU:H61	0.91	0.89
21:F:201:LMU:H22	21:F:201:LMU:H82	0.91	0.89
15:K:20:PHE:CD2	15:K:21:ALA:N	2.41	0.89
1:1:179:THR:OG1	4:4:87:SER:HB3	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:302:CLA:CGA	20:2:302:CLA:C4	2.50	0.89
3:3:84:ILE:N	20:3:302:CLA:H43	1.88	0.89
4:4:193:ILE:HG22	4:4:194:VAL:N	1.87	0.89
5:A:545:HIS:ND1	20:A:834:CLA:HBB2	1.87	0.89
22:A:847:BCR:H23C	22:A:847:BCR:H393	1.52	0.89
6:B:621:ARG:O	6:B:625:TRP:HB3	1.71	0.89
5:A:470:LEU:CD1	6:B:95:HIS:HB3	2.02	0.89
3:3:92:TRP:CZ2	5:A:250:LEU:HD12	2.08	0.89
4:4:52:MET:CE	4:4:156:ASN:HB2	2.02	0.89
5:A:472:ARG:NH1	16:L:74:LEU:HG	1.87	0.89
19:P:1:GLC:H3	19:P:2:FRU:O5	1.72	0.89
2:2:55:ALA:CB	2:2:56:MET:CE	2.48	0.89
6:B:635:ILE:O	6:B:636:THR:O	1.91	0.89
6:B:693:TRP:HD1	20:B:838:CLA:C2D	1.86	0.89
8:D:102:ARG:HE	8:D:110:GLN:HB2	1.38	0.89
5:A:567:ARG:HH11	8:D:35:GLY:HA2	1.37	0.89
10:F:93:ILE:O	10:F:96:TRP:HD1	1.55	0.89
21:G:101:LMU:H4'	21:G:101:LMU:O6B	1.73	0.89
2:2:98:GLU:CG	2:2:99:LEU:CD1	2.51	0.89
4:4:121:PHE:O	4:4:122:LYS:HB2	1.73	0.89
3:3:205:GLY:H	5:A:252:ARG:HH22	0.92	0.89
20:A:804:CLA:HBB2	20:A:806:CLA:C3D	2.02	0.89
6:B:574:ASP:HA	6:B:577:TYR:HB3	1.52	0.89
20:B:811:CLA:H41	20:B:816:CLA:CBC	2.03	0.89
6:B:87:ILE:HA	6:B:115:ASN:CA	2.03	0.89
21:H:108:LMU:O3B	21:H:108:LMU:H6'1	1.73	0.89
20:2:307:CLA:OBD	20:2:307:CLA:HED3	1.71	0.89
2:2:94:LEU:O	2:2:98:GLU:HB3	1.71	0.89
5:A:578:ARG:CZ	5:A:578:ARG:HB2	2.02	0.89
5:A:714:LEU:HD13	22:F:203:BCR:C39	2.01	0.89
20:B:823:CLA:H52	20:B:837:CLA:CAD	2.03	0.89
20:A:807:CLA:CAB	22:J:102:BCR:C33	2.50	0.89
17:N:45:ASN:HB2	17:N:57:LYS:HZ2	1.35	0.89
1:1:63:LEU:HD23	1:1:64:GLY:C	1.93	0.89
2:2:164:ILE:O	2:2:167:GLY:HA3	1.72	0.89
2:2:41:LEU:O	2:2:42:ARG:CB	2.21	0.89
20:3:313:CLA:C14	20:3:313:CLA:H102	2.03	0.89
5:A:368:LEU:HD11	20:A:825:CLA:H61	1.51	0.89
5:A:711:HIS:NE2	20:A:837:CLA:CAC	2.35	0.89
6:B:91:ILE:HG21	20:B:808:CLA:HMD1	1.54	0.89
20:B:811:CLA:H41	20:B:816:CLA:HBC3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:101:CLA:HED1	20:K:108:CLA:CMB	1.96	0.89
16:L:164:PRO:CD	16:L:165:TYR:CD1	2.56	0.89
2:2:43:TRP:HZ3	2:2:125:PHE:CB	1.86	0.89
20:3:313:CLA:CBA	20:3:313:CLA:HED1	2.00	0.89
3:3:74:ALA:HA	20:3:307:CLA:C1D	2.02	0.89
4:4:122:LYS:HB3	4:4:143:PHE:HB3	1.55	0.89
4:4:95:PHE:HZ	20:4:315:CLA:NC	1.63	0.89
20:A:807:CLA:CMB	22:J:102:BCR:HC7	2.01	0.89
20:A:839:CLA:H91	15:K:61:LEU:HD13	1.54	0.89
20:A:822:CLA:CBB	22:A:845:BCR:H353	2.02	0.89
9:E:68:ARG:O	9:E:68:ARG:NE	2.05	0.89
19:P:1:GLC:O2	19:P:2:FRU:H12	1.70	0.89
20:2:322:CLA:H91	20:2:322:CLA:C16	2.03	0.89
4:4:40:PHE:CB	4:4:43:ALA:CB	2.29	0.89
5:A:25:ASP:CB	5:A:26:PRO:CD	2.46	0.89
5:A:327:ILE:O	5:A:328:LYS:O	1.90	0.89
5:A:355:HIS:ND1	5:A:416:ILE:CG2	2.35	0.89
5:A:131:ILE:O	5:A:671:SER:HA	1.73	0.89
6:B:25:ILE:CG2	22:L:210:BCR:H291	2.01	0.89
6:B:292:ARG:O	6:B:293:THR:OG1	1.91	0.89
21:H:106:LMU:H3'	21:H:106:LMU:C5B	2.03	0.89
5:A:81:ALA:HB2	20:A:804:CLA:HMA2	1.55	0.88
6:B:393:PHE:HD2	6:B:397:ASP:OD1	1.55	0.88
6:B:91:ILE:HD12	6:B:104:PHE:HE2	1.37	0.88
4:4:99:HIS:HE1	4:4:103:ILE:HD12	1.35	0.88
20:4:304:CLA:CGD	20:4:304:CLA:C2A	2.51	0.88
4:4:90:LEU:H	4:4:91:PHE:HB3	1.38	0.88
20:A:822:CLA:CAB	22:A:845:BCR:C35	2.48	0.88
21:B:802:LMU:O3'	21:B:802:LMU:H1B	1.65	0.88
20:4:311:CLA:C10	20:4:311:CLA:H41	2.02	0.88
20:A:824:CLA:HMB3	22:A:846:BCR:C18	2.03	0.88
3:3:98:ILE:HB	17:N:61:LEU:HB2	1.55	0.88
20:A:824:CLA:C7	20:A:825:CLA:HED2	2.01	0.88
20:B:814:CLA:CBC	20:B:814:CLA:HHD	2.02	0.88
20:J:103:CLA:C16	20:J:103:CLA:H2	2.04	0.88
20:2:307:CLA:HBD	20:2:307:CLA:HBA1	1.55	0.88
2:2:99:LEU:HD22	20:2:311:CLA:CMC	2.01	0.88
20:A:839:CLA:O1A	20:A:839:CLA:HED1	1.74	0.88
20:B:807:CLA:H92	20:B:807:CLA:HBB2	0.90	0.88
2:2:165:LYS:O	2:2:168:ARG:N	2.05	0.88
4:4:104:ARG:NH1	4:4:105:ARG:HB3	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:304:CLA:C15	20:4:304:CLA:H202	1.99	0.88
5:A:27:ILE:O	5:A:27:ILE:HD12	1.72	0.88
5:A:711:HIS:CD2	20:A:837:CLA:CBC	2.56	0.88
22:B:845:BCR:H321	22:B:845:BCR:HC8	1.56	0.88
7:C:14:CYS:HA	7:C:17:CYS:HG	1.01	0.88
17:N:32:ALA:CB	17:N:35:VAL:HG22	2.04	0.88
1:1:185:TRP:CA	1:1:186:HIS:ND1	2.37	0.88
5:A:267:THR:O	5:A:269:PHE:CD2	2.25	0.88
5:A:711:HIS:CE1	20:A:837:CLA:HAC1	2.08	0.88
1:1:27:LEU:HD21	6:B:314:ARG:HG2	0.90	0.88
6:B:70:TRP:CD1	6:B:71:GLN:OE1	2.27	0.88
20:B:821:CLA:C7	20:B:821:CLA:C2	2.50	0.88
12:H:69:SER:CB	20:H:109:CLA:H61	2.01	0.88
20:H:109:CLA:HBB2	13:I:13:GLY:O	1.74	0.88
20:A:826:CLA:H171	22:J:102:BCR:H15C	1.54	0.88
17:N:67:LEU:HB2	17:N:68:GLU:HG2	0.91	0.88
5:A:581:CYS:CB	5:A:590:CYS:HA	2.04	0.88
20:A:824:CLA:C5	20:A:825:CLA:HED1	2.03	0.88
24:A:857:SF4:FE4	24:A:857:SF4:S2	1.64	0.88
6:B:230:TRP:CH2	11:G:11:SER:HB2	2.09	0.88
21:H:105:LMU:C9	21:H:105:LMU:H52	2.01	0.88
16:L:56:VAL:HG13	20:L:208:CLA:CED	2.04	0.88
20:1:207:CLA:HMC1	20:1:207:CLA:HBC3	1.53	0.88
6:B:531:THR:O	6:B:535:VAL:HG12	1.74	0.88
8:D:113:HIS:H	8:D:114:PRO:HD2	1.38	0.88
15:K:10:ILE:CA	15:K:13:THR:HG23	2.04	0.88
2:2:103:GLY:CA	20:2:311:CLA:HBB2	2.03	0.88
5:A:207:LEU:HA	5:A:211:LEU:HG	1.54	0.88
5:A:358:LEU:HD11	5:A:413:HIS:CB	2.03	0.88
20:A:839:CLA:CHD	20:A:839:CLA:HBC2	2.00	0.88
6:B:275:HIS:O	6:B:279:ALA:N	2.05	0.88
6:B:732:LYS:HG2	6:B:733:PHE:CA	2.04	0.88
21:H:106:LMU:O5B	21:H:106:LMU:H31	1.72	0.88
13:I:11:LEU:CD1	22:I:103:BCR:C10	2.45	0.88
17:N:48:GLY:HA2	17:N:49:CYS:HG	1.05	0.88
1:1:184:PRO:C	1:1:185:TRP:HE3	1.77	0.87
3:3:112:THR:OG1	3:3:113:LEU:N	2.04	0.87
4:4:95:PHE:HD1	4:4:95:PHE:N	1.72	0.87
5:A:24:ARG:O	5:A:26:PRO:HB2	1.74	0.87
20:A:815:CLA:HAA1	20:A:815:CLA:HED1	1.52	0.87
20:A:839:CLA:O2D	20:A:839:CLA:HAA1	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:805:CLA:H151	22:A:843:BCR:H393	1.55	0.87
21:A:855:LMU:C3	21:A:855:LMU:C9	2.49	0.87
12:H:25:GLY:HA3	12:H:27:ASP:CA	2.03	0.87
16:L:115:ALA:H	16:L:116:PRO:HD2	1.36	0.87
20:A:835:CLA:H192	20:L:202:CLA:HBB1	1.55	0.87
18:R:39:UNK:HA	18:R:42:UNK:CB	2.04	0.87
5:A:425:THR:HG1	5:A:428:TYR:HE1	0.93	0.87
20:A:833:CLA:C3A	20:A:839:CLA:CBB	2.52	0.87
17:N:32:ALA:HB1	17:N:35:VAL:CG2	2.05	0.87
5:A:356:ALA:HB2	5:A:417:PHE:HD2	1.39	0.87
6:B:732:LYS:CG	6:B:733:PHE:CA	2.49	0.87
6:B:527:LEU:HD12	20:B:823:CLA:C1D	2.03	0.87
15:K:10:ILE:CD1	15:K:10:ILE:H	1.87	0.87
17:N:72:LYS:HG3	17:N:74:LYS:N	1.87	0.87
20:1:202:CLA:HBA2	20:1:202:CLA:O2D	1.72	0.87
2:2:168:ARG:NH2	2:2:171:MET:HB2	1.88	0.87
20:2:322:CLA:HED2	20:J:101:CLA:HMA3	1.54	0.87
4:4:106:TRP:C	4:4:108:ASP:H	1.78	0.87
4:4:38:ARG:HG3	4:4:39:TRP:CA	2.05	0.87
5:A:370:ILE:CG2	5:A:400:MET:HA	2.04	0.87
6:B:137:THR:HA	6:B:140:ILE:HG13	1.55	0.87
6:B:732:LYS:HG2	6:B:734:GLY:CA	2.04	0.87
7:C:1:MET:N	7:C:3:HIS:C	2.27	0.87
20:H:101:CLA:C3A	20:H:101:CLA:CGA	2.51	0.87
17:N:48:GLY:CA	17:N:49:CYS:CB	2.50	0.87
2:2:42:ARG:CA	2:2:45:VAL:CG2	2.30	0.87
5:A:331:LEU:C	5:A:331:LEU:HD23	1.94	0.87
5:A:349:ILE:HG23	5:A:352:THR:O	1.73	0.87
24:A:857:SF4:FE4	24:A:857:SF4:S3	1.66	0.87
6:B:310:PRO:CG	6:B:311:PRO:HD2	2.04	0.87
25:B:848:LMG:O3	7:C:70:TRP:CZ2	2.26	0.87
19:X:1:GLC:C1	19:X:2:FRU:C4	2.51	0.87
20:4:307:CLA:CGD	20:4:307:CLA:CAA	2.51	0.87
4:4:37:LEU:O	4:4:39:TRP:CD1	2.27	0.87
4:4:75:TRP:CG	20:4:311:CLA:HMD3	2.09	0.87
5:A:249:ILE:CG1	5:A:250:LEU:H	1.83	0.87
5:A:151:GLN:NE2	5:A:384:TYR:O	2.07	0.87
5:A:361:ASN:HD21	20:A:805:CLA:HED3	1.39	0.87
8:D:113:HIS:NE2	8:D:118:VAL:CG1	2.37	0.87
10:F:23:LYS:HB2	10:F:24:LYS:NZ	1.89	0.87
10:F:24:LYS:CA	10:F:26:GLN:H	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:217:SER:CA	22:A:843:BCR:H351	2.03	0.87
20:A:816:CLA:HBA2	20:A:816:CLA:H2	1.54	0.87
20:A:819:CLA:C3C	20:A:825:CLA:H172	2.03	0.87
20:A:839:CLA:HBC3	20:A:839:CLA:CHD	2.01	0.87
20:A:805:CLA:H42	22:A:844:BCR:H313	1.56	0.87
6:B:189:ALA:HB2	20:B:826:CLA:H203	1.54	0.87
7:C:1:MET:CG	7:C:4:SER:CB	2.53	0.87
9:E:42:GLU:HG2	9:E:43:SER:N	1.90	0.87
12:H:21:TRP:H	12:H:22:ASP:HA	1.38	0.87
5:A:309:LEU:HD21	20:A:819:CLA:CMC	2.05	0.87
22:A:847:BCR:C8	22:A:847:BCR:C31	2.46	0.87
6:B:110:LEU:HD12	6:B:111:GLY:H	1.40	0.87
6:B:317:ARG:NH1	6:B:405:ASP:O	2.08	0.87
21:K:106:LMU:H41	21:K:106:LMU:C8	1.94	0.87
12:H:44:ALA:CB	16:L:145:PHE:CD1	2.58	0.87
20:A:830:CLA:C16	22:L:210:BCR:H361	2.05	0.87
17:N:4:GLU:O	17:N:4:GLU:HG3	1.72	0.87
20:R:108:CLA:H91	21:R:109:LMU:O4'	1.72	0.87
21:1:213:LMU:C6'	21:1:213:LMU:C2'	2.47	0.87
4:4:106:TRP:HD1	20:4:302:CLA:O1D	1.53	0.87
4:4:36:ASN:OD1	4:4:39:TRP:CG	2.27	0.87
6:B:427:LEU:HD23	6:B:431:PHE:CZ	2.10	0.87
13:I:11:LEU:HD12	22:I:103:BCR:H10C	0.87	0.87
21:K:106:LMU:H3'	21:K:106:LMU:C3	2.04	0.87
2:2:178:TRP:C	2:2:182:ILE:HG13	1.95	0.86
4:4:169:GLN:NE2	4:4:169:GLN:HA	1.87	0.86
5:A:661:ALA:O	5:A:664:VAL:HG22	1.75	0.86
6:B:216:LEU:HD21	6:B:221:GLY:HA2	1.57	0.86
6:B:474:PHE:CE2	6:B:476:ILE:HG13	2.10	0.86
20:B:823:CLA:CBB	20:B:837:CLA:HHB	2.05	0.86
6:B:86:PRO:O	6:B:87:ILE:HG13	1.73	0.86
21:H:108:LMU:H41	21:H:108:LMU:C8	2.02	0.86
13:I:24:LEU:C	13:I:26:LEU:H	1.78	0.86
15:K:10:ILE:CA	15:K:13:THR:CG2	2.53	0.86
20:1:202:CLA:O2A	20:1:202:CLA:HMA2	1.74	0.86
20:2:302:CLA:HBC2	20:2:302:CLA:HMC1	1.54	0.86
4:4:100:TYR:HA	4:4:103:ILE:CG1	2.05	0.86
5:A:194:ALA:O	5:A:198:ASP:N	2.07	0.86
5:A:393:LEU:HG	5:A:394:SER:H	1.40	0.86
22:A:846:BCR:HC8	22:A:846:BCR:C33	2.05	0.86
16:L:95:LEU:HD13	22:L:210:BCR:H312	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD11	17:N:63:ASP:O	1.76	0.86
17:N:63:ASP:H	17:N:64:ASP:CA	1.88	0.86
5:A:606:TYR:O	5:A:610:SER:HB2	1.76	0.86
20:A:807:CLA:C2B	22:J:102:BCR:C33	2.53	0.86
21:K:104:LMU:O6'	21:K:104:LMU:H1B	1.75	0.86
20:L:201:CLA:CGA	20:L:201:CLA:HED1	1.98	0.86
2:2:168:ARG:HH21	2:2:171:MET:HB2	1.36	0.86
4:4:121:PHE:CD2	4:4:122:LYS:O	2.27	0.86
6:B:203:ARG:HG2	6:B:204:GLY:N	1.89	0.86
6:B:469:LYS:HG2	6:B:471:THR:OG1	1.76	0.86
7:C:14:CYS:SG	7:C:18:VAL:O	2.32	0.86
11:G:68:ILE:O	11:G:72:LEU:CB	2.22	0.86
21:K:105:LMU:H61	21:K:105:LMU:C2	2.00	0.86
15:K:44:GLU:HG3	15:K:45:SER:CA	2.05	0.86
4:4:84:PHE:O	4:4:85:ALA:HB3	1.75	0.86
5:A:452:PHE:HE1	20:A:835:CLA:CBB	1.87	0.86
17:N:58:VAL:HG23	17:N:60:PHE:CE1	2.11	0.86
20:H:101:CLA:CMA	20:H:101:CLA:H2	2.06	0.86
17:N:5:GLU:OE1	17:N:6:TYR:CG	2.29	0.86
1:1:185:TRP:C	1:1:186:HIS:CG	2.44	0.86
2:2:171:MET:SD	2:2:171:MET:C	2.54	0.86
2:2:174:VAL:O	2:2:178:TRP:CD1	2.29	0.86
2:2:178:TRP:O	2:2:182:ILE:HG13	1.75	0.86
2:2:188:PRO:O	2:2:190:ASP:N	2.09	0.86
3:3:132:TRP:HZ3	3:3:155:GLU:HG2	1.07	0.86
4:4:122:LYS:HG2	4:4:143:PHE:HB2	1.55	0.86
4:4:149:ALA:HB1	4:4:151:GLU:HG2	1.55	0.86
4:4:152:LYS:HD3	4:4:154:ILE:HD11	1.55	0.86
4:4:169:GLN:NE2	20:4:305:CLA:HHD	1.91	0.86
5:A:195:TRP:CZ2	20:A:810:CLA:HMA1	2.10	0.86
10:F:20:GLN:NE2	10:F:20:GLN:C	2.29	0.86
3:3:63:ARG:HH22	3:3:189:LEU:HD23	1.40	0.86
4:4:36:ASN:O	4:4:39:TRP:CB	2.23	0.86
5:A:356:ALA:HB2	5:A:417:PHE:CD2	2.09	0.86
1:1:24:PHE:HD2	6:B:314:ARG:NH2	1.71	0.86
20:B:815:CLA:CAD	20:B:824:CLA:HBB2	2.06	0.86
20:A:830:CLA:C5	22:B:846:BCR:H343	2.05	0.86
16:L:163:LEU:CD2	16:L:164:PRO:CB	2.30	0.86
17:N:45:ASN:ND2	17:N:57:LYS:NZ	2.20	0.86
17:N:5:GLU:OE1	17:N:6:TYR:CD1	2.29	0.86
17:N:70:GLU:HB3	17:N:72:LYS:N	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:99:HIS:ND1	4:4:103:ILE:CD1	2.38	0.86
5:A:197:GLN:HE21	5:A:197:GLN:CA	1.84	0.86
5:A:599:PHE:CE2	5:A:735:VAL:CG2	2.59	0.86
5:A:723:ARG:HH11	5:A:723:ARG:CG	1.88	0.86
20:A:815:CLA:HAA2	20:A:815:CLA:H42	1.57	0.86
20:A:841:CLA:CMD	22:B:846:BCR:HC31	2.05	0.86
20:L:201:CLA:H2	20:L:201:CLA:HED3	1.58	0.86
2:2:73:ILE:H	2:2:73:ILE:CD1	1.79	0.86
4:4:52:MET:HE3	4:4:156:ASN:HB2	1.57	0.86
20:A:832:CLA:CBC	20:A:832:CLA:HMC1	2.06	0.86
6:B:438:VAL:CG2	20:B:831:CLA:HMC1	2.05	0.86
7:C:59:PRO:O	24:C:103:SF4:S3	2.33	0.86
10:F:153:ASN:HD22	10:F:153:ASN:C	1.79	0.86
20:B:836:CLA:H121	22:F:203:BCR:H312	1.57	0.86
20:1:215:CLA:O1D	20:1:215:CLA:HBA1	1.74	0.85
2:2:211:LYS:HG2	3:3:113:LEU:HD11	1.57	0.85
4:4:118:ASP:CG	4:4:123:GLN:HB2	1.96	0.85
6:B:348:VAL:HA	20:B:816:CLA:H42	1.58	0.85
20:B:836:CLA:C20	22:F:203:BCR:HC41	2.04	0.85
10:F:20:GLN:CD	10:F:21:ALA:H	1.77	0.85
17:N:63:ASP:N	17:N:64:ASP:CB	2.38	0.85
1:1:185:TRP:C	1:1:186:HIS:ND1	2.29	0.85
20:2:307:CLA:CGD	20:2:307:CLA:HBA2	2.06	0.85
4:4:128:ALA:N	4:4:143:PHE:CZ	2.40	0.85
4:4:36:ASN:OD1	4:4:39:TRP:CD2	2.29	0.85
5:A:269:PHE:HE1	15:K:14:THR:HG21	1.38	0.85
6:B:438:VAL:HG22	20:B:831:CLA:CMC	2.05	0.85
7:C:63:LEU:HG	7:C:64:SER:H	1.39	0.85
10:F:23:LYS:C	10:F:24:LYS:NZ	2.28	0.85
4:4:124:TYR:CB	4:4:143:PHE:HD1	1.89	0.85
4:4:107:GLN:C	20:4:302:CLA:HMA2	1.93	0.85
4:4:38:ARG:HG3	4:4:39:TRP:H	1.38	0.85
20:A:826:CLA:H72	22:A:847:BCR:H371	1.57	0.85
20:B:807:CLA:H102	20:B:807:CLA:H142	1.58	0.85
23:B:841:PQN:H162	22:B:846:BCR:H333	0.87	0.85
12:H:45:ALA:O	12:H:48:THR:N	2.08	0.85
20:A:841:CLA:H201	16:L:64:LEU:HD21	1.57	0.85
17:N:61:LEU:CG	17:N:62:SER:N	2.33	0.85
2:2:59:ALA:HB1	2:2:172:LEU:HD22	1.59	0.85
3:3:132:TRP:CH2	3:3:155:GLU:HG3	2.08	0.85
4:4:124:TYR:HB3	4:4:143:PHE:CD1	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:36:ASN:O	4:4:39:TRP:HE3	1.60	0.85
4:4:69:ILE:HD12	4:4:175:LYS:HG2	0.86	0.85
5:A:316:MET:CB	5:A:317:TYR:CB	2.49	0.85
20:A:807:CLA:HAA1	20:A:807:CLA:C1	2.04	0.85
20:A:811:CLA:HMC1	20:A:811:CLA:HBC3	1.58	0.85
20:A:824:CLA:H52	20:A:825:CLA:HED1	1.56	0.85
6:B:167:TRP:CZ2	20:B:811:CLA:HAC1	2.12	0.85
7:C:74:THR:OG1	7:C:80:ALA:HB2	1.75	0.85
20:4:305:CLA:HAA1	20:F:206:CLA:C4	2.05	0.85
10:F:93:ILE:HG21	22:F:202:BCR:H371	1.58	0.85
13:I:1:MET:O	13:I:2:ILE:HG22	1.75	0.85
21:1:219:LMU:H6'2	21:1:219:LMU:O2'	1.76	0.85
4:4:30:LEU:HD13	21:4:317:LMU:H121	1.57	0.85
5:A:402:ILE:CD1	20:A:827:CLA:HBB2	2.05	0.85
6:B:594:TRP:O	6:B:595:HIS:CB	2.24	0.85
20:B:825:CLA:O1D	20:B:826:CLA:HMA1	1.76	0.85
9:E:35:LYS:NZ	9:E:89:GLU:OE2	2.08	0.85
10:F:23:LYS:CB	10:F:24:LYS:HZ1	1.89	0.85
12:H:21:TRP:H	12:H:22:ASP:CA	1.88	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CD2	2.30	0.85
4:4:106:TRP:CD1	20:4:302:CLA:O1D	2.30	0.85
4:4:154:ILE:HG13	4:4:155:ALA:N	1.92	0.85
5:A:349:ILE:HG22	5:A:349:ILE:O	1.74	0.85
6:B:571:SER:OG	6:B:574:ASP:OD1	1.95	0.85
6:B:661:PHE:HB2	20:B:851:CLA:CMC	2.05	0.85
20:B:829:CLA:H12	20:B:829:CLA:HMA2	1.55	0.85
21:E:101:LMU:O3'	21:E:101:LMU:H6E	1.76	0.85
9:E:39:LEU:N	9:E:40:ARG:NH1	2.24	0.85
1:1:184:PRO:O	1:1:185:TRP:CE3	2.29	0.85
2:2:41:LEU:O	2:2:42:ARG:HB2	1.76	0.85
3:3:80:LYS:HD3	3:3:105:ASN:HB2	1.59	0.85
3:3:181:LEU:CD1	3:3:182:LYS:HE2	2.06	0.85
20:A:833:CLA:HBC1	22:A:846:BCR:HC31	1.58	0.85
21:A:855:LMU:O6'	21:A:855:LMU:H1'	1.75	0.85
9:E:58:ASP:OD2	9:E:60:LYS:HG2	1.75	0.85
16:L:56:VAL:HA	20:L:208:CLA:HED2	1.56	0.85
21:R:102:LMU:O6'	21:R:102:LMU:H5B	1.76	0.85
5:A:53:TRP:HA	5:A:56:ASN:HB2	1.59	0.85
20:A:819:CLA:H92	22:A:845:BCR:H371	1.51	0.85
6:B:353:TYR:CG	6:B:594:TRP:CZ3	2.64	0.85
6:B:388:ALA:C	6:B:391:PRO:HD2	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:20:GLN:CD	10:F:21:ALA:N	2.29	0.85
16:L:56:VAL:HA	20:L:208:CLA:CED	2.06	0.85
17:N:42:PHE:H	17:N:43:PRO:CD	1.88	0.85
4:4:69:ILE:HD12	4:4:175:LYS:CG	1.74	0.85
5:A:567:ARG:HH12	8:D:35:GLY:HA2	1.37	0.85
24:A:857:SF4:FE3	24:A:857:SF4:S2	1.67	0.85
6:B:432:HIS:HE1	20:B:830:CLA:NB	1.73	0.85
10:F:130:LEU:HG	10:F:131:PHE:N	1.92	0.85
20:L:209:CLA:HBC3	20:L:209:CLA:CHD	2.05	0.85
1:1:24:PHE:HB3	6:B:314:ARG:HH21	1.41	0.85
2:2:116:PRO:HB2	2:2:136:GLY:HA2	1.59	0.85
4:4:90:LEU:N	4:4:91:PHE:HB3	1.91	0.85
4:4:93:ILE:HG22	4:4:94:GLU:N	1.91	0.85
5:A:581:CYS:HB2	5:A:590:CYS:CA	2.05	0.85
5:A:308:ILE:HD11	20:A:816:CLA:H91	0.85	0.85
20:A:838:CLA:C14	22:A:847:BCR:HC21	2.01	0.85
20:B:821:CLA:CMC	20:B:821:CLA:CBC	2.31	0.85
10:F:96:TRP:HZ3	10:F:134:PHE:HB2	1.42	0.85
15:K:51:ASP:OD1	15:K:55:PHE:CG	2.30	0.85
17:N:5:GLU:OE2	17:N:5:GLU:HA	1.74	0.85
20:1:215:CLA:CHD	20:1:215:CLA:HBC2	2.02	0.84
4:4:194:VAL:N	4:4:195:GLN:C	2.30	0.84
5:A:207:LEU:HD21	5:A:314:GLY:HA2	1.59	0.84
5:A:58:HIS:HE1	20:A:803:CLA:ND	1.75	0.84
5:A:368:LEU:CD1	20:A:825:CLA:H61	2.06	0.84
20:A:830:CLA:O1A	20:A:841:CLA:H11	1.76	0.84
21:K:105:LMU:C2	21:K:105:LMU:C6	2.29	0.84
4:4:75:TRP:CD1	20:4:311:CLA:CMD	2.60	0.84
9:E:60:LYS:HG3	9:E:61:THR:H	1.40	0.84
21:K:109:LMU:H42	21:K:109:LMU:H81	0.85	0.84
22:L:210:BCR:H403	22:L:210:BCR:H271	1.59	0.84
16:L:63:LEU:HD22	16:L:64:LEU:H	1.40	0.84
3:3:158:TYR:HB3	3:3:159:PRO:CD	2.06	0.84
4:4:91:PHE:HD2	4:4:91:PHE:C	1.79	0.84
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.57	0.84
6:B:464:GLN:CD	6:B:469:LYS:HD3	1.96	0.84
20:B:821:CLA:HMD2	20:B:822:CLA:CBB	2.06	0.84
16:L:124:LYS:NZ	16:L:124:LYS:HB2	1.91	0.84
16:L:163:LEU:HD23	16:L:164:PRO:HA	1.57	0.84
10:F:24:LYS:C	10:F:26:GLN:N	2.30	0.84
16:L:48:ASN:HB3	16:L:49:PRO:HD2	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:841:CLA:C20	16:L:64:LEU:HD21	2.07	0.84
21:1:213:LMU:H2'	21:1:213:LMU:H6D	1.58	0.84
5:A:110:LEU:HD11	5:A:239:PRO:HG2	1.57	0.84
20:A:807:CLA:C1	20:A:807:CLA:HAA2	2.04	0.84
6:B:427:LEU:HD23	6:B:431:PHE:HZ	1.41	0.84
7:C:62:PHE:CZ	9:E:42:GLU:OE1	2.31	0.84
20:1:210:CLA:CGD	20:1:210:CLA:HAA2	2.06	0.84
2:2:162:LYS:C	2:2:162:LYS:HD3	1.98	0.84
20:3:313:CLA:HED2	20:3:313:CLA:CAA	1.96	0.84
5:A:133:ASN:ND2	5:A:142:GLY:HA2	1.92	0.84
5:A:207:LEU:HD12	5:A:310:PHE:HD1	1.42	0.84
6:B:202:SER:HB3	6:B:270:LEU:HD11	1.60	0.84
21:B:801:LMU:C6	21:B:801:LMU:C10	2.49	0.84
11:G:16:LEU:HD23	11:G:68:ILE:CG2	2.07	0.84
20:J:101:CLA:O1D	20:J:101:CLA:H12	1.77	0.84
4:4:124:TYR:HB2	4:4:143:PHE:HD1	1.43	0.84
4:4:39:TRP:O	4:4:40:PHE:CD1	2.30	0.84
4:4:57:GLY:O	4:4:60:LEU:HD23	1.78	0.84
5:A:108:ALA:HB1	5:A:138:GLY:HA3	1.58	0.84
5:A:393:LEU:HG	5:A:394:SER:N	1.91	0.84
20:A:833:CLA:HMA2	20:A:839:CLA:CBB	2.07	0.84
12:H:25:GLY:HA3	12:H:27:ASP:HB2	1.57	0.84
20:J:101:CLA:CGD	20:J:101:CLA:CGA	2.54	0.84
20:J:101:CLA:OBD	20:J:101:CLA:HED2	1.78	0.84
20:2:307:CLA:HED2	20:2:307:CLA:CAD	2.07	0.84
4:4:75:TRP:HE3	4:4:75:TRP:H	1.26	0.84
11:G:44:PHE:CD2	11:G:44:PHE:O	2.30	0.84
12:H:20:GLN:CA	12:H:22:ASP:HB3	2.07	0.84
12:H:28:ALA:N	12:H:29:PRO:HD3	1.89	0.84
20:1:215:CLA:O2A	20:1:215:CLA:H51	1.76	0.84
1:1:27:LEU:HD22	6:B:314:ARG:HG3	1.59	0.84
2:2:41:LEU:O	2:2:41:LEU:HD23	1.78	0.84
4:4:147:LEU:CD1	4:4:148:GLU:HB2	2.08	0.84
4:4:158:ARG:HA	4:4:161:LEU:CD1	2.07	0.84
20:A:801:CLA:O1D	20:A:801:CLA:HBA2	1.77	0.84
24:A:857:SF4:S4	24:A:857:SF4:FE2	1.69	0.84
6:B:167:TRP:HB2	11:G:41:MET:CE	2.08	0.84
6:B:391:PRO:HB3	6:B:538:ALA:HA	1.59	0.84
11:G:26:PHE:HB2	11:G:27:GLN:HE21	1.41	0.84
16:L:14:LEU:HA	16:L:24:GLU:HG3	1.59	0.84
20:1:202:CLA:CED	20:1:202:CLA:CAA	2.54	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:322:CLA:C4	20:2:322:CLA:C7	2.30	0.84
4:4:121:PHE:CZ	4:4:122:LYS:O	2.29	0.84
5:A:286:GLY:C	5:A:287:LEU:HD22	1.98	0.84
5:A:373:ALA:HB1	5:A:396:PHE:HD1	1.43	0.84
5:A:470:LEU:HD11	6:B:95:HIS:HB3	1.60	0.84
15:K:10:ILE:HA	15:K:13:THR:HG21	1.59	0.84
21:1:217:LMU:H3'	21:1:217:LMU:C1	2.07	0.83
5:A:397:THR:HB	5:A:613:ILE:CG1	2.08	0.83
20:A:816:CLA:CBC	20:A:816:CLA:HMC1	2.08	0.83
20:A:851:CLA:CAD	20:A:851:CLA:HED2	2.07	0.83
6:B:310:PRO:HG3	20:B:821:CLA:CMA	2.04	0.83
21:B:801:LMU:H61	21:B:801:LMU:H101	1.58	0.83
21:E:101:LMU:C5	21:E:101:LMU:H11	2.05	0.83
20:1:215:CLA:HED1	20:1:215:CLA:HMA3	1.59	0.83
4:4:124:TYR:CB	4:4:143:PHE:CD1	2.62	0.83
5:A:393:LEU:CD1	5:A:750:PHE:CE1	2.60	0.83
6:B:732:LYS:HG3	6:B:733:PHE:C	1.97	0.83
20:B:807:CLA:H141	20:B:825:CLA:H91	1.60	0.83
20:B:821:CLA:C4	20:B:821:CLA:C1A	2.40	0.83
6:B:370:ALA:O	20:B:825:CLA:HMA1	1.77	0.83
17:N:67:LEU:O	17:N:68:GLU:HG3	1.77	0.83
17:N:59:PRO:HB3	17:N:75:TYR:HE1	1.42	0.83
4:4:147:LEU:HD21	4:4:148:GLU:HG3	0.85	0.83
4:4:106:TRP:HE3	20:4:314:CLA:HMA1	1.43	0.83
6:B:310:PRO:CG	20:B:821:CLA:HMA1	2.04	0.83
22:B:846:BCR:H19C	20:B:850:CLA:C11	2.08	0.83
3:3:87:GLU:HB2	22:3:314:BCR:H382	1.57	0.83
4:4:105:ARG:HG3	4:4:105:ARG:O	1.75	0.83
4:4:192:THR:HG21	4:4:195:GLN:H	1.40	0.83
5:A:497:ALA:HB2	5:A:515:TRP:HB2	1.59	0.83
6:B:516:ASP:O	6:B:520:HIS:HB2	1.79	0.83
20:B:812:CLA:HMB2	22:B:844:BCR:C8	2.08	0.83
21:K:105:LMU:H32	21:K:105:LMU:C5'	2.08	0.83
18:R:41:UNK:CB	18:R:42:UNK:CB	2.56	0.83
3:3:80:LYS:HD3	3:3:105:ASN:CB	2.07	0.83
5:A:558:LYS:HZ2	6:B:674:LEU:HB3	1.43	0.83
20:A:826:CLA:H71	22:A:847:BCR:H372	1.58	0.83
22:B:844:BCR:C8	22:B:844:BCR:H331	2.06	0.83
7:C:7:ILE:HG22	7:C:65:VAL:CG2	2.08	0.83
10:F:61:LEU:HD23	10:F:69:PRO:CB	2.07	0.83
20:H:102:CLA:C3C	22:I:103:BCR:HC22	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:108:LMU:H52	21:H:108:LMU:H92	0.84	0.83
4:4:119:PRO:CG	20:4:313:CLA:C2D	2.56	0.83
5:A:100:GLY:HA3	5:A:153:TRP:HH2	1.40	0.83
5:A:693:LEU:HD21	5:A:735:VAL:H	1.43	0.83
20:A:814:CLA:C3B	22:A:843:BCR:C19	2.53	0.83
1:1:25:ASP:H	6:B:314:ARG:HH22	0.84	0.83
20:L:202:CLA:H52	20:L:203:CLA:HHB	1.60	0.83
4:4:69:ILE:CD1	4:4:175:LYS:HB2	1.83	0.83
5:A:21:LEU:HD12	5:A:21:LEU:C	1.90	0.83
5:A:692:PHE:CE2	20:A:838:CLA:HBC3	2.14	0.83
8:D:124:ASN:CB	8:D:125:PRO:HD3	2.08	0.83
21:E:101:LMU:H51	21:E:101:LMU:H11	1.57	0.83
10:F:62:LEU:HG	10:F:72:ILE:HD13	1.59	0.83
17:N:18:ASP:HB2	17:N:22:LEU:CG	2.09	0.83
3:3:132:TRP:HZ3	3:3:155:GLU:CG	1.60	0.83
12:H:20:GLN:HB3	12:H:22:ASP:HB2	1.60	0.83
17:N:56:LYS:O	17:N:60:PHE:CD1	2.31	0.83
21:R:109:LMU:O5B	21:R:109:LMU:H6D	1.79	0.83
19:S:1:GLC:H2	19:S:2:FRU:H11	1.61	0.83
4:4:149:ALA:CB	4:4:151:GLU:OE1	2.27	0.83
4:4:73:PRO:O	4:4:74:LYS:HG3	1.79	0.83
22:A:847:BCR:C39	22:A:847:BCR:H23C	2.09	0.83
6:B:212:PHE:HE1	20:B:812:CLA:HHD	1.42	0.83
6:B:414:HIS:CD2	20:B:828:CLA:HMA3	2.13	0.83
20:B:836:CLA:H121	22:F:203:BCR:C31	2.09	0.83
11:G:8:ILE:O	11:G:8:ILE:HG13	1.77	0.83
2:2:38:PRO:O	2:2:40:SER:HB2	1.77	0.83
5:A:373:ALA:HB1	5:A:396:PHE:CD1	2.14	0.83
5:A:451:ILE:CD1	20:A:830:CLA:HED1	2.09	0.83
20:A:824:CLA:CHC	22:A:846:BCR:C37	2.56	0.83
6:B:230:TRP:HB3	20:B:814:CLA:HED3	1.59	0.83
20:H:101:CLA:O1D	20:H:101:CLA:H2A	1.79	0.83
20:H:101:CLA:HMA2	20:H:101:CLA:H61	1.58	0.83
15:K:20:PHE:HD2	15:K:20:PHE:C	1.80	0.83
16:L:163:LEU:HD22	16:L:165:TYR:HA	1.61	0.83
17:N:48:GLY:HA3	17:N:49:CYS:CB	2.07	0.83
3:3:89:ALA:HB1	3:3:90:LEU:HG	1.61	0.82
4:4:42:GLN:OE1	4:4:120:ILE:HA	1.79	0.82
4:4:47:ASN:HB3	4:4:161:LEU:HD23	1.59	0.82
6:B:464:GLN:OE1	6:B:469:LYS:HD3	1.78	0.82
6:B:711:VAL:HG12	6:B:711:VAL:O	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:TYR:O	8:D:95:LYS:HG2	1.77	0.82
12:H:25:GLY:C	12:H:27:ASP:H	1.74	0.82
20:L:209:CLA:CBC	20:L:209:CLA:CHD	2.55	0.82
16:L:88:ALA:C	16:L:90:GLY:N	2.30	0.82
17:N:58:VAL:HB	17:N:59:PRO:HD2	0.83	0.82
5:A:141:ARG:HH21	5:A:141:ARG:HG3	1.42	0.82
22:A:847:BCR:H312	20:A:852:CLA:H143	1.61	0.82
23:B:841:PQN:H161	22:B:846:BCR:H331	1.60	0.82
8:D:78:ALA:HB3	8:D:82:GLN:NE2	1.93	0.82
20:H:102:CLA:C3C	22:I:103:BCR:HC21	2.08	0.82
21:K:104:LMU:H1B	21:K:104:LMU:O6B	1.76	0.82
3:3:157:ALA:C	3:3:158:TYR:HD2	1.83	0.82
4:4:36:ASN:CB	4:4:39:TRP:CD2	2.62	0.82
4:4:75:TRP:CD1	20:4:311:CLA:C2D	2.62	0.82
5:A:746:THR:HA	5:A:749:PHE:HB3	1.61	0.82
6:B:278:LEU:HD12	20:B:814:CLA:CMA	2.09	0.82
7:C:2:SER:O	7:C:69:LEU:HB2	1.79	0.82
7:C:17:CYS:CB	7:C:58:CYS:SG	2.66	0.82
8:D:39:LYS:HD2	8:D:42:VAL:HG13	1.59	0.82
17:N:63:ASP:N	17:N:64:ASP:C	2.33	0.82
2:2:85:GLN:OE1	2:2:85:GLN:HA	1.79	0.82
21:A:854:LMU:H91	21:A:854:LMU:H32	1.60	0.82
6:B:131:THR:HB	6:B:134:ASP:CB	2.06	0.82
6:B:664:LEU:C	6:B:667:TRP:HZ3	1.81	0.82
21:H:108:LMU:H42	21:H:108:LMU:O1'	1.67	0.82
16:L:118:LEU:CD1	16:L:119:THR:H	1.92	0.82
21:R:102:LMU:O6B	21:R:102:LMU:H6E	1.79	0.82
21:2:317:LMU:O5B	21:2:317:LMU:H5'	1.74	0.82
20:4:318:CLA:HBC2	20:4:318:CLA:CHD	2.09	0.82
5:A:349:ILE:CG2	5:A:349:ILE:O	2.27	0.82
20:A:801:CLA:CMC	20:A:801:CLA:HBC2	2.09	0.82
24:A:857:SF4:S4	24:A:857:SF4:FE3	1.69	0.82
6:B:337:ALA:HA	20:B:822:CLA:HAA1	1.61	0.82
6:B:374:HIS:HB2	20:B:825:CLA:C1B	2.09	0.82
20:B:823:CLA:HBB1	20:B:837:CLA:HMB2	1.58	0.82
20:B:823:CLA:HMB3	22:B:845:BCR:C35	2.10	0.82
14:J:31:ARG:NH2	20:J:103:CLA:CHC	2.42	0.82
14:J:9:SER:O	14:J:10:VAL:HB	1.80	0.82
2:2:43:TRP:HZ3	2:2:125:PHE:CG	1.55	0.82
20:3:302:CLA:HMA2	20:3:302:CLA:HBA2	1.61	0.82
5:A:244:LEU:HD22	5:A:247:GLU:OE2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:747:TRP:CD2	22:A:847:BCR:C40	2.62	0.82
24:A:857:SF4:FE2	24:A:857:SF4:S3	1.71	0.82
11:G:16:LEU:HD12	11:G:17:PHE:CE2	2.14	0.82
11:G:47:GLY:H	11:G:48:ASP:HB3	1.43	0.82
17:N:48:GLY:CA	17:N:49:CYS:O	2.28	0.82
17:N:61:LEU:C	17:N:61:LEU:CD1	2.37	0.82
1:1:57:ILE:HD13	1:1:57:ILE:O	1.80	0.82
4:4:36:ASN:HB2	4:4:39:TRP:CH2	2.14	0.82
4:4:36:ASN:OD1	4:4:37:LEU:CA	2.28	0.82
4:4:73:PRO:O	4:4:74:LYS:CG	2.27	0.82
20:A:804:CLA:H2A	20:A:804:CLA:O2D	1.80	0.82
5:A:207:LEU:CB	20:A:819:CLA:HBB2	2.09	0.82
5:A:370:ILE:HD11	20:A:824:CLA:C3D	2.09	0.82
20:B:851:CLA:O2A	20:B:851:CLA:H3A	1.79	0.82
12:H:50:ARG:HH12	12:H:53:LEU:C	1.83	0.82
20:1:204:CLA:HMC1	20:1:204:CLA:HBC3	1.62	0.82
4:4:194:VAL:H	4:4:195:GLN:C	1.83	0.82
5:A:239:PRO:HA	5:A:242:ILE:HD13	1.62	0.82
20:A:824:CLA:CHB	22:A:846:BCR:H363	2.09	0.82
6:B:53:GLN:C	6:B:55:ALA:H	1.83	0.82
9:E:45:TRP:HH2	9:E:78:SER:OG	1.63	0.82
20:H:101:CLA:CAD	20:H:101:CLA:HED3	2.06	0.82
14:J:23:ALA:O	14:J:26:LEU:HB3	1.80	0.82
20:1:201:CLA:HMA2	20:1:201:CLA:CBA	2.08	0.82
4:4:37:LEU:CA	4:4:39:TRP:HB3	2.08	0.82
5:A:545:HIS:O	5:A:549:ILE:HG13	1.80	0.82
20:A:815:CLA:HAA2	20:A:815:CLA:H11	1.61	0.82
20:A:824:CLA:HBA2	20:A:836:CLA:CED	2.10	0.82
5:A:401:TRP:CD1	20:A:826:CLA:CHC	2.62	0.82
11:G:16:LEU:HD23	11:G:68:ILE:HG23	1.61	0.82
17:N:67:LEU:HB2	17:N:68:GLU:CB	2.09	0.82
21:1:218:LMU:O6B	21:1:218:LMU:C1B	2.28	0.82
2:2:162:LYS:O	2:2:162:LYS:HD3	1.80	0.82
2:2:54:TRP:CG	20:2:311:CLA:O1D	2.33	0.82
4:4:169:GLN:CG	20:4:305:CLA:HAC2	2.10	0.82
20:A:834:CLA:HBD	20:A:834:CLA:HBA2	1.59	0.82
8:D:44:GLU:HB2	8:D:46:TYR:CE2	2.14	0.82
9:E:60:LYS:HG3	9:E:61:THR:N	1.95	0.82
20:4:305:CLA:CAA	20:F:206:CLA:H42	2.09	0.82
11:G:60:SER:OG	11:G:63:PRO:HB2	1.80	0.82
21:H:104:LMU:H41	21:H:104:LMU:H81	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:205:LMU:C1	21:L:205:LMU:O2'	2.28	0.82
21:R:102:LMU:O6'	21:R:102:LMU:C1B	2.28	0.82
1:1:24:PHE:HD2	6:B:314:ARG:HH21	1.22	0.81
2:2:171:MET:SD	2:2:172:LEU:HG	2.19	0.81
2:2:42:ARG:HB3	2:2:43:TRP:CA	2.04	0.81
20:A:814:CLA:HMC2	22:A:843:BCR:C16	2.10	0.81
9:E:43:SER:HB2	9:E:82:TYR:HE1	1.44	0.81
21:G:101:LMU:C6B	21:G:101:LMU:C4'	2.58	0.81
19:Y:2:FRU:O6	19:Y:2:FRU:H12	1.80	0.81
5:A:567:ARG:NH1	8:D:35:GLY:CA	2.38	0.81
5:A:711:HIS:NE2	20:A:837:CLA:HAC1	1.93	0.81
5:A:370:ILE:CD1	20:A:824:CLA:CAD	2.58	0.81
7:C:74:THR:C	7:C:76:SER:N	2.30	0.81
10:F:20:GLN:NE2	10:F:21:ALA:N	2.28	0.81
6:B:294:ASN:HB3	11:G:36:PRO:HD2	1.59	0.81
11:G:43:HIS:C	11:G:45:GLU:N	2.29	0.81
12:H:53:LEU:HG	12:H:54:LEU:H	1.44	0.81
16:L:122:GLY:C	16:L:124:LYS:N	2.31	0.81
17:N:47:THR:HB	17:N:52:LEU:O	1.78	0.81
17:N:47:THR:HG21	17:N:54:LYS:HZ2	1.41	0.81
20:2:322:CLA:C9	20:2:322:CLA:C15	2.58	0.81
20:4:318:CLA:HED3	20:4:318:CLA:O2A	1.79	0.81
20:A:851:CLA:C3B	6:B:589:TRP:HH2	1.93	0.81
6:B:395:ILE:HD12	6:B:396:ARG:HG2	1.62	0.81
20:B:819:CLA:HHD	20:B:819:CLA:CBC	2.00	0.81
10:F:22:LEU:O	10:F:25:LEU:CB	2.28	0.81
10:F:26:GLN:O	10:F:27:ALA:HB3	1.80	0.81
19:P:1:GLC:C3	19:P:2:FRU:O5	2.28	0.81
19:Q:2:FRU:C6	19:Q:2:FRU:O1	2.28	0.81
18:R:36:UNK:O	18:R:38:UNK:CB	2.28	0.81
1:1:63:LEU:HD12	1:1:63:LEU:H	1.45	0.81
4:4:98:SER:CB	4:4:102:GLU:OE1	2.29	0.81
4:4:114:SER:OG	4:4:120:ILE:HD11	1.81	0.81
4:4:95:PHE:N	4:4:95:PHE:CD1	2.43	0.81
6:B:304:ILE:HD11	20:B:817:CLA:CED	2.11	0.81
20:B:803:CLA:C19	10:F:104:TYR:HB3	2.10	0.81
20:K:102:CLA:O1A	20:K:102:CLA:CMA	2.27	0.81
21:L:204:LMU:O3'	21:L:204:LMU:H1B	1.78	0.81
17:N:72:LYS:HZ2	17:N:74:LYS:CG	1.90	0.81
1:1:179:THR:HG21	4:4:87:SER:CA	2.09	0.81
20:1:215:CLA:HED3	20:1:215:CLA:NA	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:312:CLA:HBC3	20:2:312:CLA:HMC1	1.62	0.81
5:A:621:GLN:HG2	5:A:637:ILE:HD12	1.60	0.81
20:A:801:CLA:HMC1	20:A:801:CLA:CBC	2.10	0.81
5:A:103:PHE:CZ	20:A:807:CLA:O1D	2.33	0.81
6:B:255:LEU:HD13	6:B:275:HIS:HB2	1.62	0.81
25:B:848:LMG:O3	7:C:70:TRP:CE2	2.32	0.81
9:E:88:GLU:O	9:E:90:VAL:CB	2.29	0.81
21:K:106:LMU:O5'	21:K:106:LMU:H32	1.80	0.81
21:R:103:LMU:O6'	21:R:103:LMU:C2	2.29	0.81
1:1:184:PRO:C	1:1:185:TRP:CE3	2.53	0.81
22:3:314:BCR:H311	22:3:314:BCR:HC8	1.61	0.81
4:4:98:SER:O	4:4:102:GLU:CG	2.28	0.81
6:B:294:ASN:OD1	11:G:38:GLN:N	2.13	0.81
6:B:546:LEU:HD11	6:B:567:THR:HG22	1.60	0.81
20:B:808:CLA:H41	22:I:101:BCR:H23C	1.62	0.81
20:2:322:CLA:HED2	20:J:101:CLA:CMA	2.10	0.81
2:2:137:TYR:CD1	2:2:138:PRO:HD2	2.15	0.81
4:4:154:ILE:CG1	4:4:155:ALA:H	1.94	0.81
5:A:284:ARG:HA	5:A:284:ARG:CZ	2.09	0.81
5:A:362:LEU:HB3	5:A:410:ALA:HB2	1.62	0.81
5:A:596:ASP:HA	5:A:599:PHE:HB3	1.62	0.81
6:B:334:LEU:HG	6:B:334:LEU:O	1.79	0.81
6:B:373:THR:HA	6:B:376:GLN:HB2	1.62	0.81
20:B:827:CLA:H62	25:B:848:LMG:H182	1.62	0.81
20:B:851:CLA:CGA	20:B:851:CLA:H3A	2.11	0.81
10:F:47:GLU:CG	10:F:51:LYS:HE3	2.08	0.81
11:G:45:GLU:CG	11:G:49:THR:HG21	2.11	0.81
17:N:72:LYS:CD	17:N:72:LYS:N	2.41	0.81
17:N:72:LYS:HZ3	17:N:74:LYS:HG2	1.43	0.81
20:1:215:CLA:H43	20:1:215:CLA:H102	1.62	0.81
4:4:144:ALA:HB3	4:4:148:GLU:O	1.81	0.81
21:A:854:LMU:C3	21:A:854:LMU:O6'	2.29	0.81
6:B:560:ASP:HB2	7:C:66:ARG:HE	1.40	0.81
7:C:74:THR:OG1	7:C:80:ALA:CB	2.29	0.81
11:G:19:GLY:C	11:G:21:PHE:N	2.28	0.81
21:H:106:LMU:C1	21:H:106:LMU:O5B	2.29	0.81
20:K:102:CLA:C3A	20:K:102:CLA:O1A	2.29	0.81
17:N:5:GLU:OE2	17:N:6:TYR:CB	2.28	0.81
17:N:66:ASP:O	17:N:67:LEU:CG	2.28	0.81
21:R:104:LMU:H2'	21:R:104:LMU:H21	0.82	0.81
19:Z:1:GLC:HO2	19:Z:1:GLC:H5	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:219:LMU:O2'	21:1:219:LMU:C6B	2.29	0.81
2:2:98:GLU:CG	2:2:99:LEU:HD11	2.10	0.81
4:4:99:HIS:CE1	4:4:103:ILE:HD11	2.16	0.81
20:4:318:CLA:O2D	20:4:318:CLA:CGA	2.29	0.81
4:4:36:ASN:C	4:4:39:TRP:CB	2.46	0.81
6:B:331:HIS:CE1	6:B:392:ILE:HG21	2.16	0.81
11:G:17:PHE:O	11:G:20:ARG:HB2	1.81	0.81
20:H:101:CLA:O1A	20:H:101:CLA:C3A	2.29	0.81
21:K:106:LMU:H82	21:K:106:LMU:H21	1.61	0.81
17:N:50:GLN:CA	17:N:51:ASP:O	2.28	0.81
19:Q:1:GLC:C5	19:Q:2:FRU:O5	2.28	0.81
2:2:181:HIS:CE1	20:2:304:CLA:C4D	2.64	0.81
2:2:196:HIS:NE2	19:O:1:GLC:O3	2.14	0.81
4:4:93:ILE:O	4:4:96:ILE:HD12	1.79	0.81
20:A:818:CLA:H202	20:A:825:CLA:H3A	1.62	0.81
6:B:317:ARG:NE	6:B:317:ARG:HA	1.94	0.81
7:C:26:LEU:H	7:C:43:PRO:HG3	1.46	0.81
12:H:65:LEU:HD23	20:H:109:CLA:H52	1.63	0.81
20:J:103:CLA:CHD	20:J:103:CLA:HBC3	2.11	0.81
15:K:69:ILE:HA	15:K:72:VAL:HG12	1.63	0.81
16:L:165:TYR:N	16:L:165:TYR:CD2	2.29	0.81
20:L:201:CLA:O2D	20:L:201:CLA:CGA	2.29	0.81
17:N:4:GLU:O	17:N:4:GLU:CG	2.28	0.81
21:R:102:LMU:C6'	21:R:102:LMU:O5B	2.29	0.81
2:2:203:THR:O	2:2:204:ILE:CG2	2.28	0.81
20:2:307:CLA:OBD	20:2:307:CLA:CED	2.29	0.81
2:2:73:ILE:O	2:2:74:LEU:CG	2.29	0.81
20:4:304:CLA:O1D	20:4:304:CLA:C2A	2.29	0.81
20:A:826:CLA:C7	22:A:847:BCR:H371	2.10	0.81
6:B:404:ALA:C	6:B:406:ASN:H	1.84	0.81
10:F:26:GLN:CA	10:F:26:GLN:OE1	2.28	0.81
21:G:101:LMU:H6'2	21:G:101:LMU:C4'	2.10	0.81
17:N:34:THR:OG1	17:N:36:GLU:HB3	1.79	0.81
20:2:322:CLA:CED	20:2:322:CLA:OBD	2.30	0.80
2:2:96:ILE:HG13	2:2:97:VAL:N	1.96	0.80
4:4:145:PRO:O	4:4:147:LEU:CA	2.29	0.80
20:4:302:CLA:HBC3	20:4:302:CLA:HHD	1.61	0.80
4:4:99:HIS:O	4:4:103:ILE:CD1	2.30	0.80
5:A:248:PHE:CD2	5:A:248:PHE:N	2.49	0.80
20:A:833:CLA:CMA	20:A:839:CLA:CBB	2.58	0.80
21:A:854:LMU:C1	21:A:854:LMU:O6'	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:857:SF4:FE4	24:A:857:SF4:S1	1.72	0.80
6:B:128:GLY:HA2	6:B:130:ARG:HE	1.44	0.80
6:B:131:THR:O	6:B:135:LEU:N	2.14	0.80
20:B:821:CLA:HAA1	20:B:821:CLA:H12	1.61	0.80
21:B:847:LMU:C11	21:B:847:LMU:H72	2.09	0.80
8:D:102:ARG:NH1	8:D:104:PHE:CD1	2.47	0.80
21:E:101:LMU:O3'	21:E:101:LMU:C6'	2.28	0.80
20:H:101:CLA:CMA	20:H:101:CLA:O1A	2.29	0.80
21:H:107:LMU:O2B	21:H:107:LMU:C5'	2.29	0.80
2:2:99:LEU:HB3	20:2:311:CLA:HBB1	1.62	0.80
4:4:37:LEU:O	4:4:39:TRP:CB	2.27	0.80
5:A:393:LEU:O	5:A:397:THR:HG23	1.81	0.80
20:A:841:CLA:HBB2	20:B:838:CLA:HMD1	1.63	0.80
21:A:854:LMU:C1'	21:A:854:LMU:O6'	2.29	0.80
21:B:801:LMU:O6'	21:B:801:LMU:H1B	1.81	0.80
21:B:801:LMU:C1B	21:B:801:LMU:O6'	2.29	0.80
20:B:807:CLA:HMC2	22:B:846:BCR:H281	1.61	0.80
20:B:823:CLA:CED	20:B:824:CLA:OBD	2.29	0.80
20:B:839:CLA:H102	13:I:21:MET:SD	2.21	0.80
16:L:164:PRO:HD2	16:L:165:TYR:CD1	2.15	0.80
17:N:66:ASP:O	17:N:67:LEU:CD1	2.29	0.80
20:1:202:CLA:O2A	20:1:202:CLA:CMA	2.30	0.80
1:1:60:PRO:O	1:1:61:GLU:HB3	1.81	0.80
3:3:86:GLN:HB2	3:3:88:THR:HB	1.60	0.80
4:4:128:ALA:HB1	4:4:141:LEU:HD23	1.62	0.80
20:4:318:CLA:HED1	20:4:318:CLA:CGA	2.07	0.80
5:A:599:PHE:HD1	5:A:600:LEU:HD23	1.44	0.80
6:B:398:TYR:HD1	6:B:542:ARG:HH21	1.27	0.80
6:B:85:ARG:O	6:B:86:PRO:O	1.98	0.80
7:C:63:LEU:CG	7:C:64:SER:H	1.95	0.80
8:D:104:PHE:HB3	8:D:106:SER:H	1.47	0.80
16:L:161:LEU:HD11	16:L:162:ASP:C	2.01	0.80
20:L:201:CLA:C1	20:L:201:CLA:CED	2.54	0.80
21:L:205:LMU:C1'	21:L:205:LMU:O6'	2.29	0.80
17:N:54:LYS:CB	17:N:57:LYS:CE	2.59	0.80
19:S:1:GLC:O2	19:S:2:FRU:C1	2.30	0.80
3:3:83:LEU:CA	20:3:302:CLA:H43	2.11	0.80
5:A:308:ILE:O	5:A:312:ILE:N	2.15	0.80
21:A:853:LMU:C3'	21:A:853:LMU:O2B	2.29	0.80
6:B:661:PHE:HB2	20:B:851:CLA:HMC3	1.63	0.80
21:H:106:LMU:C1B	21:H:106:LMU:O1'	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:108:LMU:O3'	21:H:108:LMU:C6B	2.30	0.80
17:N:45:ASN:HD21	17:N:54:LYS:CB	1.93	0.80
19:T:1:GLC:C5	19:T:2:FRU:O1	2.29	0.80
3:3:80:LYS:HB2	20:3:306:CLA:C3D	2.12	0.80
4:4:128:ALA:CB	4:4:143:PHE:CZ	2.61	0.80
4:4:71:ASN:O	4:4:73:PRO:CD	2.29	0.80
4:4:75:TRP:CZ3	4:4:76:TYR:HB3	2.16	0.80
5:A:27:ILE:CD1	5:A:27:ILE:O	2.30	0.80
6:B:278:LEU:HD12	20:B:814:CLA:HMA2	1.63	0.80
5:A:588:GLY:H	6:B:668:ARG:NH1	1.79	0.80
20:B:824:CLA:C8	22:B:845:BCR:H14C	2.11	0.80
7:C:73:THR:OG1	7:C:76:SER:CB	2.30	0.80
7:C:7:ILE:O	7:C:8:TYR:C	2.18	0.80
9:E:51:SER:HB3	9:E:68:ARG:NH1	1.96	0.80
20:B:830:CLA:HBB2	22:F:202:BCR:H272	1.64	0.80
10:F:22:LEU:O	10:F:25:LEU:CD1	2.29	0.80
11:G:46:ALA:CA	11:G:48:ASP:OD2	2.30	0.80
21:H:106:LMU:C3	21:H:106:LMU:O5B	2.29	0.80
16:L:123:ARG:HA	16:L:123:ARG:NE	1.95	0.80
17:N:51:ASP:O	17:N:52:LEU:CD2	2.29	0.80
17:N:61:LEU:CD1	17:N:63:ASP:O	2.29	0.80
21:R:102:LMU:O6'	21:R:102:LMU:C2B	2.29	0.80
20:R:108:CLA:CBA	20:R:108:CLA:O1D	2.29	0.80
18:R:33:UNK:O	18:R:36:UNK:CB	2.29	0.80
1:1:185:TRP:HB3	1:1:186:HIS:CD2	2.16	0.80
20:1:215:CLA:C2A	20:1:215:CLA:O2D	2.29	0.80
20:1:215:CLA:O2A	20:1:215:CLA:C5	2.30	0.80
20:4:307:CLA:CAA	20:4:307:CLA:O1D	2.29	0.80
4:4:89:THR:O	4:4:92:VAL:CB	2.29	0.80
5:A:23:ASP:OD2	5:A:24:ARG:HD3	1.80	0.80
5:A:423:ASP:CB	5:A:424:PRO:HD3	2.09	0.80
5:A:747:TRP:CE3	22:A:847:BCR:C40	2.65	0.80
6:B:382:ILE:HG22	6:B:383:MET:N	1.96	0.80
6:B:586:THR:C	6:B:588:GLY:H	1.85	0.80
6:B:693:TRP:CD1	20:B:838:CLA:C2D	2.65	0.80
9:E:85:ASP:O	9:E:86:GLU:CB	2.30	0.80
11:G:67:ASN:HA	11:G:70:ASP:OD2	1.81	0.80
11:G:73:ALA:O	11:G:75:GLY:N	2.14	0.80
18:R:26:UNK:O	18:R:28:UNK:CB	2.30	0.80
4:4:69:ILE:HD13	4:4:175:LYS:HB3	1.62	0.80
20:1:206:CLA:HAA1	21:4:301:LMU:O3'	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:839:CLA:CAA	20:A:839:CLA:O2D	2.30	0.80
6:B:172:GLU:O	6:B:176:ASN:CB	2.30	0.80
10:F:24:LYS:O	10:F:27:ALA:CB	2.30	0.80
21:H:104:LMU:O3'	21:H:104:LMU:H2B	1.80	0.80
12:H:25:GLY:CA	12:H:27:ASP:OD2	2.30	0.80
15:K:62:ALA:O	15:K:65:ALA:N	2.14	0.80
20:L:201:CLA:CBA	20:L:201:CLA:O2D	2.29	0.80
20:L:208:CLA:HMC1	20:L:208:CLA:HBC3	1.62	0.80
17:N:65:LEU:CD2	17:N:65:LEU:O	2.30	0.80
18:R:38:UNK:O	18:R:42:UNK:CA	2.29	0.80
1:1:63:LEU:O	1:1:63:LEU:CD2	2.29	0.80
3:3:107:TRP:CG	3:3:108:ALA:N	2.38	0.80
4:4:147:LEU:HD11	4:4:148:GLU:HB2	1.62	0.80
4:4:81:GLU:O	4:4:82:GLU:CG	2.30	0.80
5:A:210:LEU:HD12	20:A:813:CLA:HMB2	1.64	0.80
20:A:824:CLA:O1A	20:A:825:CLA:HED3	1.82	0.80
6:B:557:PHE:N	6:B:558:PRO:CD	2.44	0.80
8:D:46:TYR:HE1	8:D:80:LYS:HE2	1.45	0.80
9:E:88:GLU:O	9:E:90:VAL:CA	2.29	0.80
10:F:12:LYS:HG2	10:F:13:GLN:N	1.97	0.80
21:G:101:LMU:O6B	21:G:101:LMU:C3'	2.30	0.80
21:H:108:LMU:C4	21:H:108:LMU:C9	2.60	0.80
21:K:105:LMU:C3	21:K:105:LMU:O6'	2.29	0.80
21:R:103:LMU:C1'	21:R:103:LMU:O6'	2.30	0.80
21:R:103:LMU:C3	21:R:103:LMU:O6'	2.30	0.80
18:R:35:UNK:O	18:R:38:UNK:CB	2.29	0.80
19:Z:1:GLC:O2	19:Z:2:FRU:C5	2.29	0.80
4:4:151:GLU:O	4:4:154:ILE:N	2.03	0.80
5:A:684:PHE:C	5:A:684:PHE:CD2	2.55	0.80
21:A:854:LMU:C7	21:A:854:LMU:H112	2.12	0.80
6:B:454:LEU:HD11	10:F:69:PRO:O	1.80	0.80
21:B:802:LMU:O3'	21:B:802:LMU:C1B	2.29	0.80
8:D:93:LYS:HB3	8:D:93:LYS:NZ	1.96	0.80
9:E:90:VAL:CG1	9:E:90:VAL:O	2.29	0.80
5:A:715:LYS:HD2	10:F:153:ASN:OD1	1.82	0.80
11:G:7:VAL:HG22	11:G:8:ILE:H	1.46	0.80
20:H:101:CLA:O1D	20:H:101:CLA:C2A	2.30	0.80
21:H:106:LMU:C1	21:H:106:LMU:O2'	2.29	0.80
13:I:8:PHE:CB	20:I:102:CLA:OBD	2.29	0.80
20:K:102:CLA:O1A	20:K:102:CLA:C2A	2.30	0.80
20:A:841:CLA:C9	22:L:210:BCR:H321	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:8:TYR:HE1	16:L:11:ILE:HG23	1.47	0.80
17:N:48:GLY:C	17:N:49:CYS:SG	2.58	0.80
17:N:62:SER:CB	17:N:66:ASP:OD1	2.29	0.80
17:N:72:LYS:HG2	17:N:74:LYS:CG	2.04	0.80
19:O:1:GLC:O2	19:O:2:FRU:C5	2.29	0.80
20:R:108:CLA:CGA	20:R:108:CLA:O1D	2.29	0.80
19:Y:2:FRU:O6	19:Y:2:FRU:C1	2.30	0.80
2:2:203:THR:O	2:2:204:ILE:CG1	2.29	0.80
5:A:107:GLU:OE1	5:A:161:GLU:HG3	1.82	0.80
5:A:24:ARG:O	5:A:26:PRO:CG	2.30	0.80
20:A:824:CLA:CMA	20:A:825:CLA:O1A	2.30	0.80
6:B:323:TYR:CE1	20:B:822:CLA:HBC1	2.17	0.80
21:B:847:LMU:O6B	21:B:847:LMU:C3'	2.29	0.80
11:G:42:SER:OG	11:G:45:GLU:CB	2.29	0.80
11:G:43:HIS:O	11:G:45:GLU:CB	2.29	0.80
21:H:106:LMU:C3	21:H:106:LMU:H1B	2.09	0.80
21:N:101:LMU:C4	21:N:101:LMU:O6'	2.30	0.80
17:N:63:ASP:N	17:N:65:LEU:N	2.30	0.80
19:P:1:GLC:C1	19:P:1:GLC:O6	2.29	0.80
21:R:103:LMU:O6'	21:R:103:LMU:H1'	1.82	0.80
18:R:34:UNK:O	18:R:38:UNK:CB	2.29	0.80
1:1:185:TRP:O	1:1:186:HIS:CB	2.30	0.79
20:3:313:CLA:O2D	20:3:313:CLA:CAA	2.30	0.79
20:4:318:CLA:CED	20:4:318:CLA:O2A	2.30	0.79
5:A:711:HIS:HB3	5:A:717:ALA:HB2	1.63	0.79
5:A:726:SER:O	5:A:728:VAL:N	2.15	0.79
6:B:415:LYS:HE3	6:B:539:LEU:O	1.81	0.79
20:B:821:CLA:O2D	20:B:821:CLA:C2A	2.30	0.79
7:C:1:MET:H2	7:C:3:HIS:CA	1.94	0.79
9:E:44:TYR:CE1	9:E:73:ASN:HA	2.17	0.79
20:H:101:CLA:CAA	20:H:101:CLA:O1D	2.30	0.79
22:I:101:BCR:H392	20:I:102:CLA:H142	1.63	0.79
21:K:106:LMU:C2	21:K:106:LMU:O2'	2.30	0.79
16:L:124:LYS:C	16:L:126:GLN:H	1.85	0.79
16:L:148:VAL:O	16:L:149:SER:HB3	1.80	0.79
2:2:40:SER:O	2:2:41:LEU:CD2	2.30	0.79
2:2:45:VAL:O	2:2:45:VAL:CG1	2.29	0.79
4:4:73:PRO:O	4:4:74:LYS:CB	2.29	0.79
5:A:207:LEU:O	5:A:310:PHE:HB3	1.80	0.79
5:A:452:PHE:CE1	20:A:835:CLA:CBB	2.63	0.79
5:A:496:HIS:HB3	5:A:515:TRP:CE3	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:747:TRP:CE3	22:A:847:BCR:H401	2.16	0.79
20:A:815:CLA:C2A	20:A:815:CLA:O2D	2.30	0.79
20:A:819:CLA:C2C	20:A:825:CLA:C17	2.60	0.79
6:B:120:VAL:HA	6:B:123:TRP:HD1	1.45	0.79
20:B:827:CLA:H72	25:B:848:LMG:H311	1.64	0.79
10:F:30:LYS:O	10:F:31:LEU:HB2	1.80	0.79
11:G:30:ASN:O	11:G:33:LYS:NZ	2.15	0.79
15:K:8:ASN:O	15:K:12:VAL:HG23	1.81	0.79
17:N:1:GLY:O	17:N:2:VAL:CG1	2.29	0.79
19:P:1:GLC:O2	19:P:2:FRU:C2	2.30	0.79
1:1:63:LEU:O	1:1:63:LEU:CD1	2.29	0.79
2:2:120:ASN:CB	2:2:121:THR:HB	2.12	0.79
2:2:73:ILE:O	2:2:74:LEU:CD2	2.29	0.79
3:3:194:ILE:CD1	20:3:304:CLA:CMC	2.50	0.79
4:4:103:ILE:O	4:4:106:TRP:HB3	1.82	0.79
4:4:104:ARG:NE	4:4:105:ARG:N	2.29	0.79
5:A:62:HIS:HB2	20:A:828:CLA:HBA1	1.63	0.79
20:A:819:CLA:HAA2	20:A:823:CLA:HBB2	1.65	0.79
20:A:824:CLA:O2A	20:A:836:CLA:O2D	2.00	0.79
5:A:78:VAL:O	5:A:82:HIS:HB2	1.82	0.79
5:A:545:HIS:CG	20:A:834:CLA:HBB2	2.16	0.79
20:A:814:CLA:HMC2	22:A:843:BCR:C17	2.13	0.79
21:A:855:LMU:O6'	21:A:855:LMU:C1'	2.28	0.79
6:B:120:VAL:CA	6:B:123:TRP:CD1	2.63	0.79
6:B:414:HIS:HD2	20:B:828:CLA:HMA3	1.44	0.79
6:B:672:GLN:HA	6:B:672:GLN:NE2	1.94	0.79
9:E:52:VAL:HG12	9:E:53:VAL:N	1.97	0.79
10:F:103:SER:C	10:F:105:LEU:H	1.86	0.79
21:G:101:LMU:O6B	21:G:101:LMU:C4'	2.29	0.79
20:H:101:CLA:CBC	20:H:101:CLA:CMC	2.39	0.79
21:H:107:LMU:O2B	21:H:107:LMU:C6'	2.30	0.79
12:H:21:TRP:N	12:H:22:ASP:HB3	1.96	0.79
21:K:104:LMU:O6'	21:K:104:LMU:C1B	2.30	0.79
21:K:105:LMU:O2B	21:K:105:LMU:C5'	2.30	0.79
15:K:10:ILE:HA	15:K:13:THR:HG23	1.57	0.79
20:L:201:CLA:O1A	20:L:201:CLA:CED	2.30	0.79
17:N:29:PHE:CD1	17:N:32:ALA:HB3	2.18	0.79
21:R:102:LMU:O6'	21:R:102:LMU:C5B	2.30	0.79
1:1:184:PRO:O	1:1:185:TRP:HE3	1.63	0.79
2:2:70:LYS:HG3	2:2:73:ILE:CG1	2.12	0.79
5:A:157:GLY:HA2	5:A:229:ILE:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:826:CLA:H71	22:A:847:BCR:C37	2.10	0.79
20:B:812:CLA:HMA1	22:B:844:BCR:H313	1.63	0.79
21:F:201:LMU:C6'	21:F:201:LMU:O5B	2.30	0.79
20:G:102:CLA:O1D	20:G:102:CLA:C2A	2.30	0.79
11:G:45:GLU:CB	11:G:49:THR:CG2	2.59	0.79
11:G:88:THR:OG1	11:G:92:GLY:HA3	1.82	0.79
21:H:104:LMU:H12	21:H:104:LMU:H51	1.64	0.79
21:K:105:LMU:C4	21:K:105:LMU:O6'	2.29	0.79
21:R:102:LMU:O6'	21:R:102:LMU:C3B	2.30	0.79
1:1:185:TRP:O	1:1:186:HIS:HB2	1.81	0.79
2:2:110:TRP:HD1	2:2:113:ILE:CG2	1.92	0.79
2:2:42:ARG:HG3	2:2:45:VAL:CG2	2.05	0.79
4:4:33:ASP:CB	4:4:34:PRO:HD3	2.12	0.79
4:4:92:VAL:HG12	4:4:93:ILE:N	1.98	0.79
6:B:374:HIS:HB2	20:B:825:CLA:NB	1.97	0.79
7:C:1:MET:N	7:C:4:SER:N	2.30	0.79
10:F:102:ARG:HG2	10:F:106:ILE:CD1	2.05	0.79
22:F:203:BCR:HC8	22:F:203:BCR:H321	0.83	0.79
12:H:25:GLY:CA	12:H:27:ASP:N	2.27	0.79
20:B:839:CLA:C19	13:I:21:MET:HB3	2.11	0.79
20:J:103:CLA:C14	20:J:103:CLA:O1A	2.30	0.79
21:K:104:LMU:C5'	21:K:104:LMU:O2'	2.29	0.79
16:L:152:THR:O	16:L:156:PHE:N	2.11	0.79
21:R:102:LMU:O6'	21:R:102:LMU:H3B	1.82	0.79
19:U:1:GLC:O6	19:U:1:GLC:C1	2.29	0.79
21:1:213:LMU:C6'	21:1:213:LMU:O3'	2.30	0.79
21:1:217:LMU:C1	21:1:217:LMU:O2'	2.30	0.79
3:3:158:TYR:O	3:3:160:GLY:N	2.16	0.79
4:4:34:PRO:CG	4:4:35:GLU:OE1	2.29	0.79
5:A:23:ASP:OD2	5:A:24:ARG:CG	2.30	0.79
5:A:581:CYS:SG	24:A:857:SF4:S2	2.79	0.79
21:A:854:LMU:C5	21:A:854:LMU:O6'	2.29	0.79
12:H:23:VAL:O	12:H:23:VAL:CG1	2.30	0.79
22:I:103:BCR:H313	22:I:103:BCR:HC8	0.83	0.79
20:K:108:CLA:HMC1	20:K:108:CLA:HBC2	1.65	0.79
21:1:218:LMU:H1B	21:1:218:LMU:H6B	1.48	0.79
4:4:193:ILE:CG2	4:4:195:GLN:O	2.29	0.79
5:A:331:LEU:CD2	5:A:331:LEU:C	2.51	0.79
20:B:824:CLA:H122	22:B:845:BCR:C14	2.12	0.79
17:N:45:ASN:CB	17:N:57:LYS:NZ	2.46	0.79
17:N:60:PHE:CA	17:N:61:LEU:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD13	17:N:63:ASP:HB2	1.64	0.79
17:N:62:SER:O	17:N:63:ASP:CB	2.30	0.79
19:U:1:GLC:C3	19:U:2:FRU:O5	2.30	0.79
21:1:219:LMU:O5B	21:1:219:LMU:C3'	2.28	0.79
4:4:168:ILE:O	4:4:168:ILE:HG13	1.83	0.79
20:4:304:CLA:CAA	20:4:304:CLA:O2D	2.30	0.79
20:A:819:CLA:C1C	20:A:825:CLA:H171	2.13	0.79
20:B:821:CLA:HAA2	20:B:821:CLA:HBD	1.65	0.79
20:B:805:CLA:H43	22:B:843:BCR:H313	1.63	0.79
20:F:206:CLA:OBD	20:F:206:CLA:CED	2.31	0.79
20:H:101:CLA:CED	20:H:101:CLA:OBD	2.30	0.79
20:H:102:CLA:HAC1	22:I:103:BCR:HC32	1.64	0.79
20:A:807:CLA:C4B	22:J:102:BCR:C33	2.60	0.79
20:L:201:CLA:O2D	20:L:201:CLA:CAA	2.30	0.79
20:A:831:CLA:H41	16:L:64:LEU:HD23	1.64	0.79
17:N:79:SER:CA	17:N:80:ASN:O	2.27	0.79
19:P:1:GLC:O2	19:P:2:FRU:C1	2.30	0.79
20:1:215:CLA:C3	20:1:215:CLA:H112	2.12	0.79
3:3:92:TRP:HA	3:3:93:PHE:CG	2.18	0.79
4:4:104:ARG:NH1	4:4:105:ARG:HB2	1.90	0.79
4:4:90:LEU:HD22	4:4:90:LEU:N	1.98	0.79
5:A:381:PRO:CB	20:A:818:CLA:HAA2	2.13	0.79
21:A:854:LMU:C4	21:A:854:LMU:O6'	2.30	0.79
21:A:855:LMU:C6B	21:A:855:LMU:O3B	2.30	0.79
24:A:857:SF4:FE1	24:A:857:SF4:S2	1.71	0.79
21:H:105:LMU:H92	21:H:105:LMU:H52	1.64	0.79
20:L:201:CLA:C2	20:L:201:CLA:O1A	2.30	0.79
19:W:1:GLC:C5	19:W:1:GLC:O2	2.27	0.79
20:2:322:CLA:H102	20:2:322:CLA:H151	1.64	0.79
5:A:40:PHE:HE1	5:A:53:TRP:HD1	1.28	0.79
5:A:491:TRP:CD1	5:A:492:ILE:HG23	2.18	0.79
20:A:824:CLA:CHD	20:A:824:CLA:CBC	2.52	0.79
20:A:832:CLA:OBD	20:A:833:CLA:HAC1	1.83	0.79
25:B:848:LMG:HC61	7:C:70:TRP:CH2	2.17	0.79
20:F:205:CLA:HHD	20:F:205:CLA:HBC2	1.64	0.79
17:N:62:SER:O	17:N:63:ASP:HB2	1.79	0.79
21:R:103:LMU:H41	21:R:103:LMU:H6D	1.65	0.79
18:R:3:UNK:O	18:R:4:UNK:CB	2.31	0.79
21:H:104:LMU:H3O1	19:Y:2:FRU:H5	1.48	0.79
1:1:161:PHE:H	20:1:203:CLA:CBB	1.95	0.78
1:1:59:VAL:CG1	1:1:60:PRO:O	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:163:PHE:O	4:4:166:PHE:HB3	1.82	0.78
4:4:44:GLU:O	4:4:47:ASN:N	2.15	0.78
5:A:27:ILE:O	5:A:28:LYS:CG	2.30	0.78
20:A:839:CLA:CED	20:A:839:CLA:O1A	2.31	0.78
21:A:854:LMU:C2	21:A:854:LMU:O6'	2.30	0.78
6:B:438:VAL:HG22	20:B:831:CLA:HMC3	1.64	0.78
6:B:596:TRP:CD1	6:B:623:TYR:HB2	2.17	0.78
20:B:817:CLA:OBD	20:B:820:CLA:HBC3	1.83	0.78
7:C:39:ILE:CG1	7:C:40:ALA:H	1.92	0.78
10:F:94:ALA:HA	10:F:97:ILE:HG12	1.65	0.78
21:H:106:LMU:C2	21:H:106:LMU:O5B	2.30	0.78
21:K:106:LMU:C5	21:K:106:LMU:H11	2.12	0.78
21:N:101:LMU:O2B	21:N:101:LMU:H5B	1.82	0.78
17:N:45:ASN:HB2	17:N:57:LYS:NZ	1.99	0.78
17:N:70:GLU:HB3	17:N:72:LYS:H	1.46	0.78
19:T:1:GLC:H5	19:T:2:FRU:HO1	1.46	0.78
21:1:219:LMU:C2'	21:1:219:LMU:H6'2	2.12	0.78
20:3:313:CLA:CBA	20:3:313:CLA:O2D	2.31	0.78
5:A:269:PHE:CD1	15:K:14:THR:HG21	2.18	0.78
6:B:317:ARG:HE	6:B:317:ARG:HA	1.47	0.78
6:B:558:PRO:CG	6:B:703:VAL:HB	2.13	0.78
8:D:48:ILE:HG22	8:D:83:CYS:HB2	1.64	0.78
10:F:147:GLY:CA	10:F:150:VAL:HB	2.13	0.78
11:G:28:ARG:NH2	11:G:28:ARG:HG2	1.95	0.78
8:D:32:SER:O	16:L:21:GLY:HA2	1.83	0.78
21:R:103:LMU:O6'	21:R:103:LMU:C4	2.30	0.78
20:R:108:CLA:CBA	20:R:108:CLA:HBD	2.14	0.78
2:2:126:PRO:HG2	2:2:129:LYS:H	1.47	0.78
4:4:71:ASN:C	4:4:73:PRO:CD	2.52	0.78
5:A:29:THR:CG2	5:A:29:THR:O	2.30	0.78
5:A:624:VAL:O	5:A:636:HIS:CD2	2.36	0.78
24:A:857:SF4:FE3	24:A:857:SF4:S1	1.74	0.78
6:B:124:TRP:O	6:B:129:LEU:HB3	1.84	0.78
17:N:54:LYS:HB2	17:N:57:LYS:HZ1	1.47	0.78
17:N:5:GLU:OE1	17:N:6:TYR:CE1	2.36	0.78
19:Y:2:FRU:C6	19:Y:2:FRU:C1	2.49	0.78
2:2:38:PRO:CB	2:2:40:SER:OG	2.29	0.78
2:2:41:LEU:C	2:2:41:LEU:CD2	2.28	0.78
4:4:145:PRO:O	4:4:147:LEU:HA	1.84	0.78
5:A:146:THR:O	20:A:826:CLA:HMA2	1.82	0.78
20:A:804:CLA:HMC3	20:A:806:CLA:O2D	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:353:TYR:CD2	6:B:594:TRP:CZ3	2.70	0.78
6:B:189:ALA:HB1	20:B:826:CLA:H203	1.64	0.78
20:B:827:CLA:HMC1	20:B:827:CLA:HBC3	1.65	0.78
10:F:33:ALA:HA	10:F:36:SER:HB2	1.64	0.78
20:G:102:CLA:O2A	20:G:102:CLA:C3A	2.30	0.78
11:G:46:ALA:HA	11:G:48:ASP:CG	2.01	0.78
11:G:93:TYR:HA	11:G:94:ASP:HB2	0.78	0.78
21:H:108:LMU:O3B	21:H:108:LMU:C6B	2.29	0.78
14:J:11:ALA:CB	14:J:12:PRO:HD2	2.14	0.78
17:N:5:GLU:OE2	17:N:5:GLU:CA	2.29	0.78
19:U:2:FRU:O6	19:U:2:FRU:C1	2.30	0.78
19:X:1:GLC:C1	19:X:2:FRU:O4	2.30	0.78
20:1:215:CLA:O2D	20:1:215:CLA:CBA	2.29	0.78
21:3:322:LMU:C1	21:3:322:LMU:O2'	2.29	0.78
4:4:128:ALA:HB1	4:4:141:LEU:CD2	2.13	0.78
21:4:320:LMU:C5B	21:4:320:LMU:O3'	2.29	0.78
6:B:25:ILE:HG21	22:L:210:BCR:H291	1.53	0.78
5:A:555:ILE:HG21	20:B:851:CLA:HMD1	1.65	0.78
22:B:852:BCR:H23C	22:B:852:BCR:H383	1.64	0.78
20:F:206:CLA:HED2	20:F:206:CLA:CAD	2.13	0.78
20:G:102:CLA:CAD	20:G:102:CLA:HED3	2.13	0.78
21:N:101:LMU:O6'	21:N:101:LMU:C5	2.30	0.78
17:N:46:PHE:O	17:N:47:THR:CG2	2.28	0.78
2:2:126:PRO:CD	2:2:129:LYS:HB2	2.14	0.78
2:2:59:ALA:HB3	2:2:172:LEU:HD13	1.66	0.78
20:4:307:CLA:CMA	20:4:307:CLA:CBA	2.30	0.78
4:4:34:PRO:HB3	4:4:35:GLU:CB	2.14	0.78
5:A:197:GLN:HE22	5:A:351:THR:HB	1.49	0.78
5:A:700:TRP:O	5:A:704:ILE:HB	1.83	0.78
6:B:160:LYS:HG3	6:B:161:TRP:H	1.47	0.78
6:B:475:ASP:HA	6:B:480:SER:O	1.84	0.78
6:B:656:VAL:HG22	20:B:839:CLA:HMB3	1.66	0.78
11:G:21:PHE:O	11:G:23:PHE:HB2	1.82	0.78
20:H:101:CLA:O1A	20:H:101:CLA:C2A	2.31	0.78
20:R:107:CLA:CED	20:R:107:CLA:C1A	2.57	0.78
5:A:242:ILE:HG12	5:A:243:PRO:HD3	1.64	0.78
5:A:24:ARG:C	5:A:26:PRO:CG	2.46	0.78
5:A:402:ILE:HG13	20:A:827:CLA:CBB	2.12	0.78
6:B:280:ILE:HA	6:B:283:LEU:HD12	1.64	0.78
6:B:353:TYR:O	6:B:354:SER:OG	2.01	0.78
5:A:697:ARG:NH2	6:B:566:GLY:O	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:697:PRO:O	7:C:79:LEU:HD13	1.82	0.78
6:B:438:VAL:HG21	20:B:831:CLA:HMC1	1.65	0.78
21:E:101:LMU:H72	21:E:101:LMU:H32	0.79	0.78
16:L:99:LEU:CD1	22:L:210:BCR:HC7	2.14	0.78
2:2:42:ARG:CB	2:2:45:VAL:CG2	2.61	0.78
4:4:37:LEU:O	4:4:39:TRP:HD1	1.67	0.78
5:A:259:TYR:CB	5:A:260:PRO:HD2	2.13	0.78
20:A:852:CLA:H11	6:B:431:PHE:CE1	2.18	0.78
6:B:409:ALA:O	6:B:411:MET:N	2.16	0.78
20:B:814:CLA:HED2	20:B:814:CLA:CBA	2.13	0.78
9:E:44:TYR:CD1	9:E:73:ASN:HB2	2.18	0.78
14:J:31:ARG:NH2	20:J:103:CLA:C3B	2.46	0.78
22:I:103:BCR:H391	22:L:210:BCR:H401	1.64	0.78
17:N:45:ASN:HD22	17:N:54:LYS:HG2	0.80	0.78
21:R:103:LMU:O3B	21:R:103:LMU:C6B	2.28	0.78
4:4:123:GLN:O	4:4:143:PHE:CG	2.37	0.78
4:4:39:TRP:O	4:4:40:PHE:HD1	1.64	0.78
5:A:308:ILE:HG22	5:A:309:LEU:N	1.99	0.78
5:A:327:ILE:O	5:A:328:LYS:C	2.16	0.78
20:A:804:CLA:C1	20:A:811:CLA:H61	2.10	0.78
6:B:354:SER:O	6:B:355:LEU:HD13	1.84	0.78
7:C:79:LEU:CD2	7:C:81:TYR:O	2.30	0.78
21:E:101:LMU:H61	21:E:101:LMU:H11	1.65	0.78
21:K:105:LMU:O3'	21:K:105:LMU:C1B	2.28	0.78
2:2:42:ARG:HA	2:2:45:VAL:CB	2.14	0.78
2:2:55:ALA:HB3	2:2:56:MET:HE1	1.63	0.78
3:3:112:THR:O	3:3:114:PHE:N	2.17	0.78
5:A:80:SER:O	5:A:83:PHE:HB2	1.83	0.78
22:A:847:BCR:C23	22:A:847:BCR:H393	2.12	0.78
6:B:188:LEU:O	6:B:191:ALA:N	2.17	0.78
6:B:732:LYS:HB3	6:B:733:PHE:HA	0.79	0.78
6:B:654:HIS:CE1	20:B:849:CLA:NB	2.52	0.78
7:C:14:CYS:C	7:C:17:CYS:SG	2.61	0.78
20:A:826:CLA:C17	22:J:102:BCR:H15C	2.12	0.78
21:R:106:LMU:H21	21:R:106:LMU:O2'	1.84	0.78
1:1:185:TRP:HA	1:1:185:TRP:HE3	1.48	0.77
5:A:690:LEU:HD23	5:A:693:LEU:HD12	1.67	0.77
6:B:438:VAL:CG2	20:B:831:CLA:CMC	2.61	0.77
20:B:829:CLA:CBC	20:B:829:CLA:CHD	2.63	0.77
11:G:42:SER:CB	11:G:45:GLU:OE2	2.30	0.77
5:A:392:GLN:HA	5:A:395:LEU:HD23	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:464:ASN:HD22	5:A:464:ASN:N	1.81	0.77
20:A:820:CLA:CAD	20:A:821:CLA:HMA1	2.15	0.77
6:B:58:PHE:HB3	6:B:146:SER:HB3	1.65	0.77
7:C:12:ILE:HD12	7:C:12:ILE:N	1.98	0.77
11:G:47:GLY:N	11:G:48:ASP:CG	2.37	0.77
1:1:89:VAL:HG12	11:G:77:ILE:HG21	1.65	0.77
17:N:45:ASN:CB	17:N:57:LYS:HZ2	1.97	0.77
19:Q:2:FRU:C4	19:Q:2:FRU:O1	2.28	0.77
20:1:210:CLA:O1D	20:1:210:CLA:CAA	2.31	0.77
21:1:217:LMU:C1B	21:1:217:LMU:O6B	2.30	0.77
2:2:168:ARG:HH21	2:2:171:MET:CB	1.98	0.77
5:A:24:ARG:O	5:A:26:PRO:CB	2.32	0.77
5:A:443:ILE:HG21	5:A:558:LYS:HB2	1.66	0.77
5:A:680:LEU:HB3	20:A:851:CLA:O2A	1.84	0.77
5:A:78:VAL:HG11	20:A:805:CLA:HBC3	1.65	0.77
20:A:816:CLA:H2	20:A:816:CLA:CBA	2.14	0.77
20:A:841:CLA:H92	22:L:210:BCR:H321	1.64	0.77
6:B:127:ILE:CD1	6:B:198:ALA:HB2	2.13	0.77
9:E:48:ASN:ND2	9:E:71:LYS:NZ	2.32	0.77
19:T:1:GLC:O5	19:T:2:FRU:C1	2.30	0.77
3:3:194:ILE:CG1	20:3:304:CLA:CMC	2.60	0.77
20:3:313:CLA:HAA2	20:3:313:CLA:O2D	1.84	0.77
5:A:168:ALA:O	5:A:171:ALA:HB3	1.82	0.77
5:A:58:HIS:CE1	20:A:803:CLA:ND	2.52	0.77
5:A:723:ARG:HH11	5:A:723:ARG:HG2	1.50	0.77
5:A:737:HIS:HA	5:A:740:LEU:CD2	2.14	0.77
22:A:843:BCR:C23	22:A:843:BCR:C40	2.60	0.77
21:A:855:LMU:H91	21:A:855:LMU:C3	2.08	0.77
5:A:90:PHE:CE1	20:A:805:CLA:H91	2.20	0.77
6:B:334:LEU:HB2	20:B:805:CLA:HMD3	1.66	0.77
7:C:1:MET:N	7:C:4:SER:OG	2.17	0.77
16:L:124:LYS:HZ2	16:L:124:LYS:HB2	1.45	0.77
20:1:202:CLA:C10	20:1:202:CLA:H41	2.15	0.77
2:2:116:PRO:O	2:2:131:THR:CB	2.32	0.77
3:3:48:PHE:HD2	3:3:49:ILE:CG2	1.82	0.77
4:4:171:ASN:C	4:4:173:THR:N	2.38	0.77
20:4:316:CLA:CHD	20:4:316:CLA:HBC3	2.14	0.77
4:4:90:LEU:CD2	4:4:90:LEU:N	2.47	0.77
4:4:94:GLU:CB	4:4:95:PHE:HD1	1.97	0.77
5:A:281:LEU:HD13	20:A:816:CLA:H2A	1.65	0.77
5:A:411:ALA:HB2	22:A:846:BCR:C39	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:137:THR:HA	6:B:140:ILE:CG1	2.14	0.77
6:B:394:PHE:O	6:B:542:ARG:NE	2.18	0.77
20:B:807:CLA:HMC2	22:B:846:BCR:C28	2.14	0.77
20:B:832:CLA:HMD2	20:B:833:CLA:C2C	2.14	0.77
7:C:70:TRP:O	7:C:72:GLU:HB2	1.84	0.77
11:G:45:GLU:O	11:G:46:ALA:HB3	1.84	0.77
6:B:685:THR:OG1	20:L:202:CLA:H3A	1.84	0.77
17:N:45:ASN:HD21	17:N:54:LYS:CG	1.93	0.77
20:2:322:CLA:H41	20:2:322:CLA:C9	2.13	0.77
2:2:73:ILE:O	2:2:74:LEU:HG	1.84	0.77
5:A:454:GLY:H	5:A:457:SER:CB	1.96	0.77
20:A:808:CLA:H111	22:J:102:BCR:C11	2.13	0.77
6:B:664:LEU:O	6:B:667:TRP:CZ3	2.37	0.77
6:B:76:ALA:O	6:B:78:VAL:N	2.18	0.77
10:F:62:LEU:HG	10:F:72:ILE:CD1	2.13	0.77
15:K:27:ALA:CB	15:K:28:PRO:HD3	2.14	0.77
16:L:32:LEU:HD13	20:L:203:CLA:HED1	1.67	0.77
1:1:185:TRP:CE3	1:1:185:TRP:CA	2.67	0.77
4:4:99:HIS:ND1	4:4:103:ILE:HD11	1.99	0.77
20:A:816:CLA:HBA2	20:A:816:CLA:C2	2.13	0.77
5:A:442:ILE:CG2	20:A:829:CLA:HMC3	2.14	0.77
5:A:669:GLY:H	6:B:445:ALA:HA	1.49	0.77
6:B:503:GLU:HB3	6:B:507:SER:CB	2.15	0.77
7:C:20:ALA:O	7:C:21:CYS:HB2	1.83	0.77
9:E:90:VAL:HG12	9:E:90:VAL:O	1.85	0.77
11:G:42:SER:CB	11:G:45:GLU:OE1	2.29	0.77
17:N:65:LEU:CD2	17:N:66:ASP:O	2.32	0.77
21:R:104:LMU:H5'	21:R:104:LMU:O2'	1.84	0.77
18:R:37:UNK:O	18:R:42:UNK:C	2.33	0.77
20:B:821:CLA:H43	20:B:821:CLA:CAA	2.14	0.77
20:B:828:CLA:CAA	20:B:828:CLA:HED2	2.15	0.77
20:B:823:CLA:CMB	22:B:845:BCR:H352	2.14	0.77
7:C:7:ILE:HG22	7:C:65:VAL:HG23	1.67	0.77
10:F:23:LYS:CB	10:F:24:LYS:HZ3	1.98	0.77
17:N:50:GLN:HA	17:N:51:ASP:O	1.84	0.77
19:X:1:GLC:H62	19:X:1:GLC:O3	1.85	0.77
5:A:626:GLY:CA	5:A:636:HIS:HA	2.15	0.77
20:A:826:CLA:C10	22:A:847:BCR:H372	2.14	0.77
6:B:196:HIS:CE1	20:B:813:CLA:HED2	2.19	0.77
21:B:847:LMU:O6B	21:B:847:LMU:H3'	1.84	0.77
15:K:9:LEU:O	15:K:12:VAL:HB	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:64:TYR:CB	20:3:311:CLA:H42	2.15	0.77
4:4:34:PRO:HA	4:4:35:GLU:CD	2.06	0.77
6:B:347:LEU:HD22	6:B:351:HIS:CE1	2.20	0.77
6:B:493:TRP:HE1	20:B:814:CLA:HAC2	1.50	0.77
20:B:828:CLA:HAA1	20:B:828:CLA:HED2	1.67	0.77
8:D:78:ALA:CB	8:D:82:GLN:HE22	1.97	0.77
20:J:101:CLA:HBA2	20:J:101:CLA:HBD	0.81	0.77
17:N:57:LYS:O	17:N:60:PHE:CD1	2.37	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE2	2.38	0.77
20:2:302:CLA:O1A	20:2:302:CLA:C1A	2.33	0.76
2:2:42:ARG:HD3	2:2:45:VAL:CG2	2.06	0.76
5:A:316:MET:CG	5:A:317:TYR:HD1	1.91	0.76
6:B:507:SER:O	6:B:508:LEU:HB2	1.83	0.76
20:B:824:CLA:HED1	20:B:832:CLA:CBB	2.14	0.76
8:D:93:LYS:HB3	8:D:93:LYS:HZ3	1.47	0.76
15:K:17:LEU:HD22	15:K:17:LEU:C	2.06	0.76
16:L:163:LEU:CB	16:L:164:PRO:CA	2.62	0.76
17:N:5:GLU:OE2	17:N:6:TYR:CG	2.38	0.76
21:R:104:LMU:C6B	21:R:104:LMU:O3B	2.29	0.76
20:1:215:CLA:O1D	20:1:215:CLA:CBA	2.30	0.76
20:A:813:CLA:C2	20:A:813:CLA:HMA2	2.15	0.76
6:B:75:GLU:HB2	6:B:132:ASN:HB3	1.67	0.76
6:B:630:GLN:HE21	6:B:731:GLY:HA3	1.49	0.76
6:B:709:GLY:O	6:B:710:LEU:HB2	1.83	0.76
20:B:807:CLA:HBA1	20:B:825:CLA:OBD	1.86	0.76
11:G:44:PHE:H	11:G:45:GLU:HB2	1.49	0.76
20:2:316:CLA:H8	20:2:316:CLA:H151	1.67	0.76
5:A:107:GLU:CD	5:A:161:GLU:HG3	2.06	0.76
5:A:588:GLY:N	6:B:668:ARG:HD3	2.00	0.76
6:B:292:ARG:NH1	6:B:296:GLY:H	1.83	0.76
6:B:437:TYR:HB3	6:B:616:LEU:CD2	2.15	0.76
20:B:823:CLA:H72	20:B:837:CLA:C2D	2.16	0.76
5:A:586:ARG:HG3	7:C:49:VAL:HG21	1.67	0.76
10:F:20:GLN:O	10:F:21:ALA:CB	2.30	0.76
10:F:25:LEU:HD22	10:F:46:MET:HB3	1.66	0.76
21:H:106:LMU:H22	21:H:106:LMU:H6'2	1.65	0.76
12:H:65:LEU:HD23	20:H:109:CLA:C5	2.14	0.76
19:U:1:GLC:O5	19:U:2:FRU:C3	2.30	0.76
20:1:206:CLA:HBC2	20:1:206:CLA:HHD	1.67	0.76
20:1:215:CLA:HMA3	20:1:215:CLA:CED	2.14	0.76
2:2:79:TRP:CD1	2:2:81:THR:HG21	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:64:TYR:HB3	20:3:311:CLA:H43	1.65	0.76
4:4:100:TYR:HA	4:4:103:ILE:HG12	1.67	0.76
4:4:70:ILE:C	4:4:72:VAL:N	2.34	0.76
3:3:205:GLY:CA	5:A:252:ARG:HH22	1.99	0.76
5:A:56:ASN:O	5:A:57:LEU:HB3	1.85	0.76
5:A:132:LEU:HD11	5:A:674:ALA:HB2	1.65	0.76
20:A:825:CLA:CGD	20:A:825:CLA:HBA1	2.16	0.76
6:B:292:ARG:CZ	6:B:292:ARG:HA	2.14	0.76
8:D:78:ALA:O	8:D:79:ARG:HD3	1.84	0.76
10:F:93:ILE:HG21	22:F:202:BCR:C37	2.15	0.76
10:F:83:PHE:O	10:F:87:GLY:HA3	1.86	0.76
11:G:41:MET:O	11:G:42:SER:O	2.04	0.76
13:I:23:SER:O	13:I:26:LEU:HD23	1.86	0.76
15:K:58:ALA:HB1	20:K:108:CLA:HMD3	1.67	0.76
18:R:34:UNK:H	18:R:36:UNK:CB	1.99	0.76
4:4:99:HIS:O	4:4:103:ILE:HD13	1.85	0.76
5:A:591:GLN:HA	5:A:591:GLN:HE21	1.49	0.76
6:B:130:ARG:O	6:B:135:LEU:HD23	1.84	0.76
6:B:374:HIS:O	6:B:374:HIS:CG	2.38	0.76
20:A:837:CLA:HED1	20:B:803:CLA:H18	1.66	0.76
20:B:823:CLA:HMB3	22:B:845:BCR:H352	1.68	0.76
20:B:832:CLA:HBB2	22:B:845:BCR:H381	1.66	0.76
7:C:52:LYS:O	7:C:52:LYS:CG	2.34	0.76
17:N:45:ASN:HD22	17:N:57:LYS:HZ3	1.31	0.76
19:O:1:GLC:C2	19:O:2:FRU:O5	2.32	0.76
2:2:41:LEU:CG	2:2:42:ARG:H	1.81	0.76
4:4:75:TRP:HB2	20:4:311:CLA:HMD3	1.67	0.76
5:A:281:LEU:CD1	20:A:816:CLA:H2A	2.16	0.76
21:B:801:LMU:H4'	21:B:801:LMU:O2B	1.84	0.76
7:C:54:CYS:SG	24:C:102:SF4:S3	2.84	0.76
10:F:81:GLY:O	14:J:38:THR:HG23	1.85	0.76
20:J:101:CLA:CBD	20:J:101:CLA:CBA	2.48	0.76
17:N:70:GLU:CD	17:N:72:LYS:O	2.24	0.76
4:4:171:ASN:C	4:4:173:THR:H	1.86	0.76
4:4:81:GLU:O	4:4:82:GLU:HG2	1.85	0.76
5:A:233:LEU:O	5:A:235:ALA:N	2.19	0.76
5:A:246:HIS:O	5:A:248:PHE:CD2	2.36	0.76
20:A:824:CLA:HMA2	20:A:825:CLA:O1A	1.85	0.76
6:B:29:HIS:CG	20:B:805:CLA:HBB2	2.21	0.76
6:B:596:TRP:NE1	6:B:623:TYR:HB2	2.00	0.76
5:A:558:LYS:NZ	6:B:674:LEU:HB3	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:103:CLA:C15	20:J:103:CLA:O1A	2.33	0.76
17:N:59:PRO:HB3	17:N:75:TYR:CE1	2.20	0.76
2:2:205:PHE:CE1	2:2:206:ALA:HA	2.21	0.76
3:3:173:GLU:CG	3:3:174:LYS:H	1.98	0.76
4:4:121:PHE:O	4:4:122:LYS:CB	2.33	0.76
20:4:305:CLA:O2A	20:4:305:CLA:H2A	1.86	0.76
5:A:214:GLY:HA3	22:A:844:BCR:H15C	1.68	0.76
5:A:23:ASP:OD1	5:A:24:ARG:CD	2.30	0.76
5:A:353:SER:O	5:A:354:TRP:HB2	1.85	0.76
5:A:466:THR:HG21	20:B:808:CLA:CBB	2.16	0.76
5:A:491:TRP:HE1	20:A:834:CLA:H12	1.50	0.76
20:A:815:CLA:HBC3	20:A:815:CLA:HMC1	0.80	0.76
6:B:645:VAL:HG11	20:B:807:CLA:HAC1	1.68	0.76
20:J:103:CLA:C16	20:J:103:CLA:O1A	2.34	0.76
17:N:11:LYS:HG2	17:N:12:THR:H	1.51	0.76
17:N:65:LEU:HD23	17:N:66:ASP:C	2.06	0.76
4:4:126:LEU:HD23	4:4:127:PRO:CD	2.15	0.76
5:A:661:ALA:HA	5:A:664:VAL:HG13	1.67	0.76
6:B:325:THR:O	6:B:329:SER:HB2	1.86	0.76
21:K:106:LMU:C9	21:K:106:LMU:H41	2.15	0.76
21:R:109:LMU:C1B	21:R:109:LMU:O6B	2.31	0.76
20:1:202:CLA:HED3	20:1:202:CLA:CAA	2.15	0.76
2:2:129:LYS:O	2:2:132:GLY:CA	2.35	0.76
20:3:311:CLA:C2A	20:3:311:CLA:O1D	2.33	0.76
4:4:144:ALA:CB	4:4:147:LEU:O	2.28	0.76
5:A:32:GLU:OE2	20:A:811:CLA:HMA2	1.86	0.76
6:B:195:VAL:HA	6:B:199:ILE:HG13	1.67	0.76
5:A:668:TYR:OH	6:B:441:ASP:OD1	2.03	0.76
21:E:101:LMU:C6	21:E:101:LMU:H11	2.16	0.76
2:2:59:ALA:CB	2:2:172:LEU:HD22	2.16	0.75
4:4:106:TRP:CE3	20:4:314:CLA:HMA1	2.21	0.75
5:A:342:GLY:HA3	5:A:430:ASP:HB2	0.82	0.75
5:A:459:GLY:O	5:A:462:ILE:HG22	1.86	0.75
5:A:54:ILE:O	5:A:58:HIS:CD2	2.39	0.75
20:A:819:CLA:C2C	20:A:825:CLA:H171	2.16	0.75
8:D:28:ILE:HG12	8:D:67:ILE:HG13	1.69	0.75
9:E:39:LEU:O	9:E:40:ARG:HD3	1.85	0.75
11:G:44:PHE:H	11:G:45:GLU:CB	1.96	0.75
17:N:42:PHE:H	17:N:43:PRO:HD3	1.50	0.75
21:R:101:LMU:C1	21:R:101:LMU:H62	2.09	0.75
4:4:84:PHE:O	4:4:85:ALA:CB	2.28	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:822:CLA:HBB2	22:A:845:BCR:H351	1.68	0.75
6:B:693:TRP:HD1	20:B:838:CLA:C1D	1.99	0.75
20:B:816:CLA:CGA	20:B:816:CLA:H3A	2.16	0.75
20:B:821:CLA:H151	20:B:821:CLA:H102	0.80	0.75
11:G:46:ALA:H	11:G:49:THR:HG22	1.51	0.75
11:G:47:GLY:N	11:G:48:ASP:CA	2.40	0.75
16:L:63:LEU:HD22	16:L:64:LEU:N	2.00	0.75
17:N:4:GLU:OE2	17:N:5:GLU:HB2	1.86	0.75
20:2:312:CLA:CBC	20:2:312:CLA:HMC1	2.15	0.75
4:4:146:THR:O	20:4:306:CLA:HBA2	1.85	0.75
5:A:259:TYR:CE2	5:A:280:PHE:HA	2.21	0.75
5:A:555:ILE:HG22	6:B:670:TYR:CE2	2.21	0.75
5:A:636:HIS:C	5:A:638:THR:N	2.39	0.75
6:B:295:PHE:N	6:B:295:PHE:CD2	2.55	0.75
6:B:527:LEU:HD12	20:B:823:CLA:CHD	2.16	0.75
10:F:96:TRP:CZ3	10:F:134:PHE:HB2	2.20	0.75
11:G:7:VAL:CG2	11:G:8:ILE:N	2.48	0.75
15:K:17:LEU:C	15:K:17:LEU:HD23	1.97	0.75
1:1:63:LEU:HD22	1:1:64:GLY:N	2.01	0.75
5:A:735:VAL:O	5:A:739:LEU:HG	1.86	0.75
20:B:810:CLA:HAC1	20:B:811:CLA:HBB1	1.65	0.75
6:B:711:VAL:HG22	25:B:848:LMG:H391	1.68	0.75
7:C:1:MET:N	7:C:3:HIS:N	2.29	0.75
16:L:64:LEU:HA	16:L:67:PRO:CG	2.16	0.75
17:N:54:LYS:HG2	17:N:57:LYS:HZ3	1.49	0.75
18:R:35:UNK:O	18:R:36:UNK:C	2.34	0.75
4:4:30:LEU:O	4:4:30:LEU:CD1	2.30	0.75
5:A:375:HIS:CE1	20:A:825:CLA:NC	2.55	0.75
5:A:447:ASN:ND2	6:B:678:LEU:HD21	2.01	0.75
6:B:347:LEU:CD2	6:B:351:HIS:CE1	2.70	0.75
6:B:233:TYR:CD2	20:B:814:CLA:HED1	2.22	0.75
20:B:826:CLA:OBD	20:B:826:CLA:O1D	1.93	0.75
22:B:845:BCR:C23	22:B:845:BCR:H382	2.09	0.75
14:J:26:LEU:C	14:J:26:LEU:HD23	2.07	0.75
2:2:41:LEU:O	2:2:42:ARG:CG	2.33	0.75
6:B:315:LEU:HD13	6:B:315:LEU:O	1.87	0.75
6:B:531:THR:HG22	20:B:823:CLA:CMC	2.09	0.75
6:B:693:TRP:CD1	20:B:838:CLA:C1D	2.70	0.75
6:B:438:VAL:HG23	20:B:831:CLA:HAC1	1.67	0.75
20:B:839:CLA:H192	13:I:21:MET:HB3	1.68	0.75
21:H:104:LMU:H12	21:H:104:LMU:H52	1.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:103:CLA:HED3	20:J:103:CLA:C2A	2.16	0.75
15:K:11:MET:SD	15:K:11:MET:O	2.44	0.75
16:L:115:ALA:N	16:L:116:PRO:HD2	2.01	0.75
21:R:102:LMU:C6B	21:R:102:LMU:H6E	2.16	0.75
21:R:102:LMU:O5B	21:R:102:LMU:H6E	1.85	0.75
19:T:1:GLC:O5	19:T:2:FRU:H12	1.86	0.75
20:2:302:CLA:C4	20:2:302:CLA:O2A	2.30	0.75
20:2:308:CLA:HMD2	20:3:301:CLA:HMD3	1.66	0.75
4:4:104:ARG:NE	4:4:105:ARG:H	1.83	0.75
4:4:40:PHE:C	4:4:43:ALA:HB3	2.07	0.75
20:A:826:CLA:CBA	20:A:826:CLA:H43	2.16	0.75
6:B:122:GLN:HG3	6:B:361:ILE:HG12	1.69	0.75
9:E:39:LEU:C	9:E:40:ARG:HD3	2.06	0.75
10:F:7:PRO:HA	10:F:61:LEU:O	1.87	0.75
16:L:49:PRO:HB2	16:L:139:PHE:HB2	1.69	0.75
16:L:99:LEU:HD11	22:L:210:BCR:H313	1.69	0.75
17:N:72:LYS:HZ2	17:N:74:LYS:HG3	1.51	0.75
18:R:38:UNK:O	18:R:41:UNK:CB	2.34	0.75
1:1:24:PHE:CB	6:B:314:ARG:HH21	2.00	0.75
3:3:112:THR:OG1	3:3:113:LEU:HG	1.87	0.75
3:3:199:VAL:HG22	20:3:306:CLA:C3C	2.17	0.75
3:3:194:ILE:HD12	20:3:304:CLA:HMC2	1.65	0.75
20:4:318:CLA:CED	20:4:318:CLA:O1A	2.29	0.75
5:A:684:PHE:HD2	5:A:685:VAL:N	1.85	0.75
5:A:76:ARG:NH1	5:A:192:LYS:CG	2.44	0.75
20:A:805:CLA:C4	22:A:844:BCR:H313	2.16	0.75
5:A:747:TRP:CD2	22:A:847:BCR:H401	2.22	0.75
20:L:202:CLA:H52	20:L:203:CLA:CHB	2.16	0.75
21:R:103:LMU:O6'	21:R:103:LMU:C1	2.35	0.75
1:1:63:LEU:HD22	1:1:64:GLY:CA	2.17	0.75
2:2:169:LEU:HD22	20:2:305:CLA:CBB	2.05	0.75
20:A:830:CLA:C16	22:L:210:BCR:H362	2.15	0.75
6:B:124:TRP:CG	6:B:129:LEU:HD13	2.21	0.75
20:B:807:CLA:H42	20:B:807:CLA:C4C	2.17	0.75
11:G:47:GLY:H	11:G:48:ASP:HA	1.51	0.75
20:1:204:CLA:HMC3	20:1:209:CLA:CAC	2.17	0.74
1:1:24:PHE:HB3	6:B:314:ARG:NH2	2.01	0.74
2:2:167:GLY:O	2:2:169:LEU:N	2.20	0.74
4:4:38:ARG:HH11	4:4:38:ARG:HG2	1.50	0.74
4:4:81:GLU:O	4:4:82:GLU:CB	2.35	0.74
5:A:224:HIS:O	5:A:225:VAL:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:832:CLA:C3D	20:A:833:CLA:HAC1	2.16	0.74
20:A:839:CLA:CMA	20:A:839:CLA:CBA	2.30	0.74
20:B:814:CLA:HBA2	20:B:814:CLA:HED2	1.67	0.74
15:K:27:ALA:HB3	15:K:28:PRO:HD3	1.68	0.74
2:2:95:PHE:HA	2:2:98:GLU:HG2	1.70	0.74
5:A:393:LEU:HD11	5:A:750:PHE:CE1	2.21	0.74
5:A:648:THR:CG2	5:A:651:GLY:H	2.00	0.74
11:G:40:GLY:C	11:G:41:MET:SD	2.64	0.74
17:N:72:LYS:CG	17:N:74:LYS:H	1.96	0.74
4:4:150:LYS:HG3	4:4:150:LYS:O	1.87	0.74
5:A:284:ARG:HA	5:A:284:ARG:NH1	2.02	0.74
5:A:422:TYR:CD1	5:A:422:TYR:N	2.51	0.74
20:A:819:CLA:C8	22:A:845:BCR:H373	2.17	0.74
6:B:58:PHE:HB2	6:B:146:SER:HB2	1.70	0.74
5:A:458:PHE:CD2	20:B:850:CLA:HMB2	2.21	0.74
7:C:31:TRP:O	7:C:33:GLY:N	2.20	0.74
8:D:111:TYR:CD2	8:D:114:PRO:HB3	2.22	0.74
11:G:13:GLY:CA	11:G:16:LEU:HG	2.17	0.74
17:N:61:LEU:CG	17:N:62:SER:H	1.98	0.74
20:2:307:CLA:H51	20:2:307:CLA:HMA2	1.70	0.74
5:A:220:ARG:O	5:A:221:HIS:HB2	1.86	0.74
5:A:227:LEU:HD23	5:A:231:GLN:HE22	1.52	0.74
5:A:452:PHE:HE1	20:A:835:CLA:HBB2	1.44	0.74
21:H:107:LMU:H6E	21:H:107:LMU:O2B	1.88	0.74
16:L:36:TYR:CG	16:L:36:TYR:O	2.40	0.74
1:1:149:LYS:HB3	20:1:206:CLA:HMC2	1.68	0.74
1:1:185:TRP:CB	1:1:186:HIS:CG	2.69	0.74
22:A:846:BCR:HC8	22:A:846:BCR:H331	1.69	0.74
11:G:94:ASP:H	11:G:95:PRO:CD	1.99	0.74
12:H:23:VAL:HG12	12:H:23:VAL:O	1.87	0.74
14:J:11:ALA:HB1	14:J:12:PRO:CD	2.16	0.74
2:2:44:ASN:O	2:2:47:ALA:N	2.16	0.74
5:A:214:GLY:O	5:A:215:SER:HB3	1.86	0.74
5:A:488:PHE:CE2	5:A:533:PRO:HB3	2.23	0.74
5:A:707:ILE:O	5:A:711:HIS:CD2	2.41	0.74
20:A:822:CLA:CHD	22:A:845:BCR:C20	2.65	0.74
6:B:700:LEU:N	6:B:700:LEU:HD23	2.01	0.74
21:E:101:LMU:H12	21:E:101:LMU:C5	1.87	0.74
20:G:102:CLA:HHD	20:G:102:CLA:HBC3	0.77	0.74
22:B:842:BCR:H343	11:G:21:PHE:CD1	2.22	0.74
21:K:105:LMU:C2B	21:K:105:LMU:H3'	2.11	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:201:CLA:HBC2	20:L:201:CLA:CHD	2.09	0.74
1:1:39:TYR:CD2	20:1:209:CLA:OBD	2.40	0.74
20:2:307:CLA:HBA1	20:2:307:CLA:CBD	2.18	0.74
2:2:40:SER:O	2:2:41:LEU:HB3	1.88	0.74
20:4:305:CLA:CMC	20:4:305:CLA:HBC3	2.03	0.74
5:A:514:THR:O	5:A:531:PRO:O	2.05	0.74
5:A:691:MET:HE2	23:A:842:PQN:H2M2	1.70	0.74
6:B:91:ILE:HD12	6:B:104:PHE:CE2	2.22	0.74
6:B:304:ILE:HG22	20:B:820:CLA:CGD	2.18	0.74
10:F:30:LYS:O	10:F:31:LEU:CB	2.36	0.74
14:J:31:ARG:HA	14:J:34:PRO:HA	1.69	0.74
2:2:128:ASN:O	2:2:130:LEU:CD1	2.34	0.74
4:4:147:LEU:CD2	4:4:148:GLU:CB	2.66	0.74
5:A:755:ILE:O	5:A:756:ALA:HB3	1.85	0.74
6:B:290:MET:HA	20:B:819:CLA:HAC2	1.68	0.74
6:B:269:TRP:CB	6:B:497:TRP:HH2	2.00	0.74
6:B:323:TYR:CD1	20:B:822:CLA:HBC1	2.23	0.74
6:B:98:GLN:C	6:B:100:ALA:H	1.91	0.74
21:K:106:LMU:H5'	21:K:106:LMU:H32	0.75	0.74
2:2:42:ARG:HG3	2:2:45:VAL:HG11	1.68	0.74
5:A:364:MET:O	5:A:368:LEU:N	2.20	0.74
21:A:849:LMU:O6B	21:A:849:LMU:O1'	2.05	0.74
6:B:180:SER:HB2	6:B:288:GLY:HA3	1.68	0.74
7:C:12:ILE:HB	7:C:39:ILE:HA	1.68	0.74
9:E:44:TYR:CG	9:E:73:ASN:HB2	2.22	0.74
11:G:13:GLY:O	11:G:16:LEU:HG	1.88	0.74
15:K:17:LEU:HD22	15:K:18:MET:HA	1.69	0.74
2:2:171:MET:HE1	2:2:175:MET:HB2	1.68	0.74
3:3:181:LEU:HD13	3:3:182:LYS:HE2	1.68	0.74
5:A:103:PHE:N	5:A:103:PHE:CD2	2.56	0.74
5:A:553:VAL:H	5:A:556:LEU:HD12	1.53	0.74
20:A:815:CLA:HMC1	20:A:815:CLA:HBC2	1.67	0.74
20:B:806:CLA:H193	20:B:806:CLA:H91	1.70	0.74
20:H:101:CLA:O1A	20:H:101:CLA:C2	2.36	0.74
13:I:12:VAL:O	13:I:17:PRO:CD	2.35	0.74
16:L:27:VAL:O	20:L:202:CLA:O2A	2.05	0.74
17:N:67:LEU:CA	17:N:68:GLU:HG2	2.18	0.74
20:1:204:CLA:HMC1	20:1:204:CLA:CBC	2.17	0.73
21:1:217:LMU:C3'	21:1:217:LMU:C1	2.66	0.73
3:3:74:ALA:CA	20:3:307:CLA:C3D	2.59	0.73
4:4:126:LEU:HD23	4:4:127:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:171:ASN:O	4:4:172:VAL:C	2.25	0.73
4:4:98:SER:HB2	4:4:102:GLU:OE1	1.87	0.73
5:A:328:LYS:HE2	5:A:332:GLU:CD	2.08	0.73
5:A:479:ASP:HA	5:A:536:THR:HG23	1.70	0.73
5:A:54:ILE:O	5:A:58:HIS:HD2	1.70	0.73
20:A:809:CLA:CBB	20:B:831:CLA:CMD	2.64	0.73
5:A:691:MET:CE	23:A:842:PQN:H2M2	2.18	0.73
21:A:853:LMU:H1B	21:A:853:LMU:O3'	1.88	0.73
22:I:103:BCR:H382	22:I:103:BCR:H402	1.69	0.73
14:J:10:VAL:HG13	14:J:14:LEU:HG	1.69	0.73
16:L:124:LYS:O	16:L:126:GLN:N	2.21	0.73
2:2:164:ILE:O	2:2:167:GLY:CA	2.36	0.73
20:4:305:CLA:HED1	20:4:305:CLA:H2	1.69	0.73
20:4:316:CLA:HBA1	20:4:316:CLA:CBD	2.16	0.73
20:A:813:CLA:HBA1	20:A:823:CLA:C4	2.16	0.73
20:A:831:CLA:HBC3	20:A:831:CLA:HMC1	1.69	0.73
6:B:471:THR:HG23	6:B:502:ASN:ND2	2.02	0.73
7:C:44:ARG:HH21	8:D:127:ARG:CB	1.99	0.73
9:E:55:VAL:HG23	9:E:65:VAL:HB	1.70	0.73
9:E:88:GLU:O	9:E:90:VAL:HB	1.89	0.73
12:H:37:SER:HB3	16:L:51:LEU:HG	1.70	0.73
17:N:47:THR:CB	17:N:52:LEU:O	2.36	0.73
17:N:63:ASP:H	17:N:64:ASP:C	1.90	0.73
17:N:67:LEU:CB	17:N:68:GLU:CG	2.45	0.73
18:R:44:UNK:O	18:R:45:UNK:C	2.35	0.73
2:2:54:TRP:CD1	20:2:311:CLA:O1D	2.41	0.73
4:4:144:ALA:HB3	4:4:147:LEU:C	2.06	0.73
20:4:304:CLA:C2	20:4:304:CLA:O1A	2.29	0.73
20:A:814:CLA:CHC	22:A:843:BCR:C17	2.66	0.73
6:B:199:ILE:HG23	6:B:270:LEU:HD22	1.68	0.73
6:B:44:GLN:OE1	6:B:163:PRO:HB2	1.88	0.73
6:B:664:LEU:O	6:B:667:TRP:HZ3	1.71	0.73
20:B:824:CLA:H8	22:B:845:BCR:H12C	1.68	0.73
16:L:8:TYR:CE1	16:L:11:ILE:HG23	2.24	0.73
20:1:215:CLA:C4	20:1:215:CLA:H102	2.15	0.73
1:1:63:LEU:CD2	1:1:64:GLY:C	2.56	0.73
4:4:101:VAL:HG13	4:4:104:ARG:HH22	1.49	0.73
4:4:151:GLU:HA	4:4:154:ILE:HG23	1.67	0.73
4:4:193:ILE:H	4:4:193:ILE:HD12	1.52	0.73
4:4:58:MET:O	4:4:59:LEU:C	2.26	0.73
5:A:467:MET:HA	5:A:470:LEU:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:819:CLA:HMD2	20:A:821:CLA:HBB2	1.66	0.73
22:A:843:BCR:C12	22:A:843:BCR:H341	2.16	0.73
6:B:454:LEU:CD1	10:F:69:PRO:O	2.36	0.73
6:B:732:LYS:HG3	6:B:734:GLY:CA	2.19	0.73
20:B:820:CLA:CBB	20:B:820:CLA:H72	2.17	0.73
6:B:421:HIS:NE2	20:B:829:CLA:C4D	2.52	0.73
12:H:42:THR:HG22	12:H:45:ALA:HB2	1.69	0.73
20:L:209:CLA:HAA1	20:L:209:CLA:O1D	1.86	0.73
20:3:310:CLA:C2A	20:3:318:CLA:CAC	2.64	0.73
4:4:104:ARG:HE	4:4:105:ARG:N	1.85	0.73
5:A:217:SER:CB	22:A:843:BCR:H351	2.18	0.73
5:A:22:VAL:CG1	5:A:23:ASP:N	2.51	0.73
23:B:841:PQN:H192	22:B:846:BCR:C8	2.19	0.73
22:L:210:BCR:H403	22:L:210:BCR:C27	2.17	0.73
21:N:101:LMU:C3	21:N:101:LMU:O5'	2.30	0.73
20:4:319:CLA:HED3	20:4:319:CLA:O1A	1.89	0.73
4:4:72:VAL:CG1	4:4:72:VAL:O	2.30	0.73
5:A:370:ILE:HG22	5:A:400:MET:CA	2.17	0.73
5:A:457:SER:O	5:A:544:ILE:HD13	1.88	0.73
5:A:126:ILE:HG12	20:A:809:CLA:HMA3	1.71	0.73
21:A:854:LMU:C7	21:A:854:LMU:C11	2.66	0.73
6:B:533:ILE:HD11	6:B:575:ASP:O	1.88	0.73
7:C:29:ILE:HG23	8:D:126:GLY:HA2	1.71	0.73
21:D:201:LMU:H41	21:E:101:LMU:C12	2.17	0.73
9:E:58:ASP:OD2	9:E:60:LYS:NZ	2.18	0.73
9:E:86:GLU:HG3	9:E:87:VAL:H	0.71	0.73
21:H:106:LMU:H1B	21:H:106:LMU:H32	1.70	0.73
21:N:101:LMU:O2B	21:N:101:LMU:C5B	2.30	0.73
17:N:5:GLU:OE1	17:N:6:TYR:CZ	2.41	0.73
17:N:79:SER:CA	17:N:80:ASN:C	2.57	0.73
5:A:187:HIS:CD2	20:A:811:CLA:NC	2.38	0.73
20:A:804:CLA:H2A	20:A:804:CLA:CED	2.19	0.73
5:A:187:HIS:CE1	20:A:811:CLA:C4D	2.68	0.73
20:A:832:CLA:HBC2	20:A:832:CLA:HMC1	1.71	0.73
6:B:489:GLY:O	6:B:490:ARG:HG2	1.89	0.73
7:C:17:CYS:C	7:C:58:CYS:HB2	2.09	0.73
7:C:26:LEU:N	7:C:43:PRO:HG3	2.03	0.73
16:L:163:LEU:HB3	16:L:164:PRO:CA	2.11	0.73
2:2:100:VAL:CG2	2:2:101:PHE:N	2.52	0.73
21:2:317:LMU:C2'	21:2:317:LMU:H22	2.19	0.73
4:4:76:TYR:CD1	4:4:76:TYR:O	2.42	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:223:VAL:HG23	5:A:227:LEU:HD13	1.71	0.73
5:A:628:ILE:HG13	5:A:632:GLY:HA2	1.69	0.73
20:A:826:CLA:H172	22:J:102:BCR:H17C	1.70	0.73
20:A:833:CLA:O1A	20:A:833:CLA:H3A	1.86	0.73
6:B:190:TRP:HA	20:B:812:CLA:HBB2	1.70	0.73
6:B:655:LEU:HD21	20:B:839:CLA:CBB	2.18	0.73
21:L:205:LMU:H1'	21:L:205:LMU:O6'	1.85	0.73
21:1:213:LMU:C1'	21:1:213:LMU:O6'	2.30	0.73
1:1:45:ILE:HG22	1:1:48:ARG:HD2	1.71	0.73
2:2:205:PHE:CD1	2:2:206:ALA:CA	2.71	0.73
3:3:208:PRO:HB3	3:3:210:GLN:OE1	1.89	0.73
3:3:50:GLU:N	3:3:51:PRO:CD	2.52	0.73
3:3:52:LYS:O	3:3:56:TYR:HD2	1.63	0.73
3:3:92:TRP:HZ2	5:A:250:LEU:HD12	1.54	0.73
20:A:819:CLA:C4C	20:A:825:CLA:H172	2.18	0.73
20:A:824:CLA:H2	20:A:825:CLA:CED	2.18	0.73
17:N:5:GLU:CD	17:N:6:TYR:CG	2.62	0.73
20:2:302:CLA:H43	20:2:302:CLA:O2A	1.89	0.73
20:2:303:CLA:H93	20:2:303:CLA:H51	1.69	0.73
4:4:192:THR:CG2	4:4:193:ILE:O	2.28	0.73
5:A:684:PHE:C	5:A:684:PHE:HD2	1.91	0.73
5:A:714:LEU:HD13	22:F:203:BCR:H392	1.69	0.73
20:A:826:CLA:H102	22:A:847:BCR:H372	1.70	0.73
6:B:91:ILE:CD1	6:B:104:PHE:HE2	2.02	0.73
20:B:817:CLA:C3	20:B:822:CLA:H92	2.18	0.73
6:B:8:PHE:O	6:B:35:ASP:HB2	1.88	0.73
13:I:11:LEU:HG	22:I:103:BCR:HC7	1.67	0.73
20:A:831:CLA:C4	16:L:64:LEU:HD23	2.18	0.73
17:N:61:LEU:HD12	17:N:62:SER:CA	2.18	0.73
1:1:64:GLY:CA	1:1:66:GLY:O	2.37	0.72
2:2:98:GLU:HG3	2:2:99:LEU:CG	2.18	0.72
20:4:307:CLA:C2	20:4:307:CLA:O1A	2.29	0.72
5:A:218:TRP:O	5:A:222:GLN:HB2	1.88	0.72
5:A:387:THR:CG2	5:A:523:VAL:HG11	2.19	0.72
20:B:821:CLA:HMC1	20:B:821:CLA:HBC3	0.78	0.72
8:D:60:MET:SD	8:D:61:PRO:HD2	2.29	0.72
20:K:101:CLA:CMD	20:K:108:CLA:C1A	2.67	0.72
15:K:9:LEU:CD2	15:K:9:LEU:H	1.91	0.72
16:L:164:PRO:CA	16:L:165:TYR:CD2	2.71	0.72
16:L:40:LEU:HB3	16:L:41:PRO:HD3	1.70	0.72
17:N:62:SER:CB	17:N:66:ASP:CA	2.65	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:109:LMU:O5B	21:R:109:LMU:C5'	2.33	0.72
2:2:126:PRO:HD2	2:2:129:LYS:HB2	1.70	0.72
4:4:115:VAL:HG13	4:4:116:ASN:H	1.52	0.72
20:A:815:CLA:HBA1	20:A:815:CLA:CBD	2.19	0.72
20:A:824:CLA:H61	20:A:825:CLA:CED	2.19	0.72
20:A:841:CLA:C6	20:A:841:CLA:H112	2.16	0.72
6:B:329:SER:O	6:B:330:ILE:HG22	1.88	0.72
20:B:821:CLA:C4	20:B:821:CLA:HAA1	2.18	0.72
7:C:1:MET:H1	7:C:4:SER:CB	2.01	0.72
21:K:105:LMU:H1B	21:K:105:LMU:H3O2	1.51	0.72
20:L:202:CLA:HAC2	20:L:203:CLA:HMC3	1.71	0.72
21:N:101:LMU:H52	21:N:101:LMU:H92	0.73	0.72
17:N:35:VAL:HG12	17:N:37:PHE:CZ	2.25	0.72
17:N:41:LYS:HB2	17:N:42:PHE:HB3	0.80	0.72
17:N:60:PHE:HA	17:N:61:LEU:O	1.88	0.72
2:2:120:ASN:CG	14:J:5:LYS:HD2	2.10	0.72
2:2:211:LYS:HA	2:2:211:LYS:CE	2.17	0.72
5:A:79:PHE:HE2	5:A:185:HIS:CE1	2.06	0.72
5:A:29:THR:OG1	5:A:31:PHE:HB2	1.90	0.72
5:A:368:LEU:HD21	20:A:818:CLA:H91	1.63	0.72
5:A:41:SER:O	5:A:44:ILE:HA	1.88	0.72
20:A:825:CLA:C4	20:A:825:CLA:O2A	2.37	0.72
20:A:839:CLA:HBA1	20:A:839:CLA:HMA2	0.80	0.72
22:A:846:BCR:C8	22:A:846:BCR:H331	2.19	0.72
6:B:144:PHE:CD2	6:B:144:PHE:O	2.41	0.72
10:F:42:ILE:CG1	10:F:43:LYS:H	1.98	0.72
11:G:68:ILE:HG23	11:G:72:LEU:CD1	2.14	0.72
15:K:17:LEU:O	15:K:17:LEU:CD2	2.30	0.72
17:N:49:CYS:O	17:N:50:GLN:C	2.28	0.72
17:N:50:GLN:HA	17:N:51:ASP:C	2.09	0.72
2:2:120:ASN:HB3	2:2:121:THR:CB	2.15	0.72
20:2:316:CLA:H18	20:2:316:CLA:ND	2.03	0.72
4:4:144:ALA:CB	4:4:148:GLU:O	2.38	0.72
4:4:37:LEU:CA	4:4:39:TRP:HB2	2.11	0.72
5:A:27:ILE:O	5:A:27:ILE:CG2	2.30	0.72
5:A:281:LEU:HA	5:A:297:THR:O	1.89	0.72
5:A:542:HIS:HA	5:A:545:HIS:HD2	1.55	0.72
5:A:85:GLN:O	5:A:89:ILE:HG13	1.90	0.72
6:B:152:ALA:O	6:B:153:GLY:C	2.26	0.72
6:B:290:MET:HA	20:B:819:CLA:CAC	2.18	0.72
5:A:668:TYR:CD1	6:B:445:ALA:HB2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:555:ILE:HG22	6:B:670:TYR:HE2	1.54	0.72
20:B:823:CLA:HMB2	20:B:837:CLA:O1A	1.90	0.72
21:B:847:LMU:H111	21:B:847:LMU:C7	2.18	0.72
8:D:94:TYR:O	8:D:95:LYS:CG	2.37	0.72
10:F:63:CYS:HA	10:F:69:PRO:HA	1.72	0.72
12:H:44:ALA:HB3	16:L:145:PHE:HD1	1.53	0.72
20:A:841:CLA:HMB2	20:L:208:CLA:HBC1	1.70	0.72
16:L:36:TYR:O	16:L:36:TYR:CD1	2.41	0.72
17:N:48:GLY:HA3	17:N:49:CYS:HB2	1.70	0.72
17:N:61:LEU:HG	17:N:62:SER:H	1.54	0.72
17:N:75:TYR:C	17:N:76:LYS:O	2.26	0.72
20:2:322:CLA:H91	20:2:322:CLA:H151	1.70	0.72
3:3:106:TYR:CD2	3:3:107:TRP:CD1	2.78	0.72
3:3:84:ILE:CG1	20:3:302:CLA:O1A	2.37	0.72
4:4:192:THR:HG22	4:4:195:GLN:N	2.05	0.72
5:A:289:PRO:O	5:A:290:LEU:HB2	1.90	0.72
6:B:378:ILE:O	6:B:380:GLY:N	2.21	0.72
5:A:668:TYR:CE2	6:B:617:MET:SD	2.83	0.72
20:B:824:CLA:H122	22:B:845:BCR:C13	2.19	0.72
21:B:847:LMU:H5B	21:B:847:LMU:C4'	2.00	0.72
7:C:11:CYS:SG	7:C:12:ILE:N	2.62	0.72
16:L:48:ASN:HD22	16:L:115:ALA:HB2	1.54	0.72
16:L:164:PRO:CB	16:L:165:TYR:CD2	2.73	0.72
1:1:45:ILE:HA	1:1:48:ARG:HB2	1.71	0.72
5:A:281:LEU:HD12	20:A:816:CLA:CED	2.17	0.72
5:A:426:THR:HA	5:A:428:TYR:CE2	2.25	0.72
22:A:847:BCR:C32	22:J:102:BCR:H391	2.19	0.72
21:A:854:LMU:H81	21:A:854:LMU:H32	1.46	0.72
6:B:362:ALA:O	6:B:363:GLN:HG3	1.89	0.72
6:B:444:LEU:O	6:B:445:ALA:HB3	1.89	0.72
6:B:707:LEU:CD1	6:B:711:VAL:HG21	2.19	0.72
20:B:823:CLA:HED2	20:B:824:CLA:OBD	1.89	0.72
8:D:113:HIS:N	8:D:114:PRO:HD2	2.04	0.72
9:E:52:VAL:C	9:E:53:VAL:HG23	2.08	0.72
20:B:836:CLA:HBC1	10:F:83:PHE:HZ	1.49	0.72
11:G:33:LYS:CA	11:G:33:LYS:HE3	2.14	0.72
11:G:92:GLY:C	11:G:94:ASP:OD1	2.28	0.72
12:H:49:LYS:O	12:H:51:GLY:N	2.22	0.72
16:L:118:LEU:HD12	16:L:119:THR:N	2.03	0.72
6:B:25:ILE:HG22	22:L:210:BCR:C29	2.14	0.72
17:N:72:LYS:CB	17:N:74:LYS:HB2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:320:LMU:H12	21:4:320:LMU:O2'	1.88	0.72
6:B:38:THR:OG1	6:B:41:ARG:HB2	1.90	0.72
6:B:424:TRP:CZ2	20:B:829:CLA:HAC1	2.25	0.72
6:B:189:ALA:HB2	20:B:826:CLA:C20	2.19	0.72
6:B:390:GLY:HA3	22:B:845:BCR:HC22	1.71	0.72
20:A:841:CLA:HMD3	22:B:846:BCR:C3	2.20	0.72
23:B:841:PQN:H291	25:B:848:LMG:H201	1.70	0.72
22:B:852:BCR:HC8	20:L:208:CLA:HHC	1.71	0.72
7:C:6:LYS:HB3	7:C:63:LEU:HD21	1.72	0.72
11:G:13:GLY:O	11:G:16:LEU:CG	2.38	0.72
20:A:835:CLA:H192	20:L:202:CLA:CBB	2.20	0.72
19:X:1:GLC:C6	19:X:1:GLC:O3	2.30	0.72
3:3:52:LYS:HA	3:3:55:ALA:HB3	1.70	0.72
5:A:210:LEU:CD1	20:A:813:CLA:CMB	2.67	0.72
5:A:309:LEU:HD21	20:A:819:CLA:HMC3	1.72	0.72
5:A:334:HIS:HB3	20:A:820:CLA:CMA	2.19	0.72
20:A:824:CLA:HED3	20:A:825:CLA:CMD	2.10	0.72
20:A:837:CLA:C1C	20:B:803:CLA:HBC2	2.20	0.72
20:B:815:CLA:H52	20:B:824:CLA:CMB	2.20	0.72
10:F:125:LEU:O	10:F:126:ALA:CB	2.36	0.72
10:F:28:SER:O	10:F:29:LEU:C	2.27	0.72
10:F:93:ILE:O	10:F:96:TRP:CD1	2.40	0.72
12:H:21:TRP:H	12:H:22:ASP:HB3	1.55	0.72
16:L:107:PHE:HB2	16:L:109:GLU:OE1	1.89	0.72
16:L:5:LYS:HA	16:L:5:LYS:HE2	1.71	0.72
17:N:72:LYS:NZ	17:N:74:LYS:HG3	2.03	0.72
2:2:54:TRP:HZ2	2:2:109:ARG:CD	2.01	0.72
2:2:124:ILE:CG2	2:2:129:LYS:HB3	2.19	0.72
20:4:307:CLA:CMA	20:4:307:CLA:CGA	2.66	0.72
5:A:370:ILE:HD11	20:A:824:CLA:CAD	2.18	0.72
5:A:79:PHE:CE2	5:A:185:HIS:CE1	2.78	0.72
6:B:615:TYR:HD1	6:B:615:TYR:H	1.38	0.72
20:B:815:CLA:CBD	20:B:824:CLA:HBB2	2.20	0.72
11:G:28:ARG:CG	11:G:29:GLU:N	2.52	0.72
20:4:319:CLA:O1A	20:4:319:CLA:CED	2.38	0.72
5:A:76:ARG:O	5:A:186:TYR:HD2	1.72	0.72
5:A:331:LEU:CD2	5:A:331:LEU:O	2.29	0.72
9:E:53:VAL:HG12	9:E:54:ALA:H	1.55	0.72
11:G:42:SER:OG	11:G:45:GLU:CD	2.28	0.72
21:K:106:LMU:O5'	21:K:106:LMU:C3	2.37	0.72
16:L:66:GLY:N	16:L:67:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:1:GLC:O5	19:U:2:FRU:H3	1.90	0.72
4:4:152:LYS:CD	4:4:154:ILE:HD11	2.19	0.71
6:B:15:ASP:O	6:B:20:ARG:HG2	1.88	0.71
7:C:1:MET:H2	7:C:3:HIS:C	1.89	0.71
7:C:1:MET:CB	7:C:4:SER:HG	1.86	0.71
8:D:69:ARG:O	8:D:70:GLU:HB2	1.90	0.71
10:F:53:PHE:C	10:F:55:ASN:H	1.94	0.71
11:G:37:GLU:OE2	11:G:42:SER:HA	1.90	0.71
16:L:33:ILE:HG12	20:L:202:CLA:H42	1.71	0.71
17:N:74:LYS:O	17:N:76:LYS:N	2.23	0.71
19:O:1:GLC:O2	19:O:2:FRU:H5	1.88	0.71
2:2:42:ARG:HG3	2:2:45:VAL:CG1	2.20	0.71
2:2:91:THR:O	2:2:94:LEU:CB	2.35	0.71
5:A:340:GLY:O	5:A:343:HIS:N	2.22	0.71
20:A:818:CLA:O1A	20:A:827:CLA:H71	1.90	0.71
20:A:825:CLA:H42	20:A:825:CLA:O2A	1.90	0.71
22:A:847:BCR:HC31	22:F:202:BCR:H17C	1.72	0.71
1:1:25:ASP:N	6:B:314:ARG:NH2	2.26	0.71
20:B:813:CLA:O2D	20:B:813:CLA:OBD	2.06	0.71
7:C:74:THR:CB	7:C:80:ALA:HB2	2.20	0.71
10:F:17:ARG:HE	10:F:17:ARG:HA	1.54	0.71
20:B:836:CLA:H61	22:F:203:BCR:H323	1.71	0.71
21:K:105:LMU:H32	21:K:105:LMU:O5'	1.90	0.71
3:3:52:LYS:O	3:3:56:TYR:N	2.21	0.71
3:3:93:PHE:HD2	3:3:93:PHE:H	1.39	0.71
5:A:103:PHE:N	5:A:103:PHE:HD2	1.87	0.71
5:A:708:VAL:HA	5:A:711:HIS:HD2	1.54	0.71
5:A:121:GLN:NE2	20:A:809:CLA:HMD1	2.05	0.71
5:A:700:TRP:CZ2	23:A:842:PQN:H2M3	2.25	0.71
6:B:141:PHE:O	6:B:143:LEU:N	2.23	0.71
6:B:492:ILE:H	6:B:492:ILE:CD1	2.02	0.71
6:B:687:LEU:HD12	22:B:852:BCR:HC31	1.72	0.71
22:B:843:BCR:C33	22:B:843:BCR:HC8	2.20	0.71
21:B:847:LMU:H112	21:B:847:LMU:H72	1.64	0.71
10:F:83:PHE:O	10:F:87:GLY:CA	2.38	0.71
20:2:322:CLA:HMB1	20:J:103:CLA:H152	1.72	0.71
16:L:96:SER:OG	16:L:143:PHE:HD2	1.74	0.71
20:1:201:CLA:CBA	20:1:201:CLA:CMA	2.60	0.71
4:4:128:ALA:O	4:4:130:GLU:N	2.23	0.71
4:4:170:HIS:C	4:4:171:ASN:O	2.29	0.71
4:4:37:LEU:HA	4:4:39:TRP:CG	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:99:HIS:ND1	4:4:99:HIS:C	2.39	0.71
5:A:361:ASN:ND2	20:A:805:CLA:CED	2.53	0.71
6:B:463:ILE:O	6:B:464:GLN:HB3	1.91	0.71
20:B:824:CLA:H72	20:B:824:CLA:H41	1.71	0.71
20:B:836:CLA:H202	22:F:203:BCR:HC41	1.73	0.71
20:B:851:CLA:HMC1	20:B:851:CLA:CBC	2.20	0.71
9:E:52:VAL:CG1	9:E:53:VAL:H	1.93	0.71
10:F:93:ILE:CG2	22:F:202:BCR:C37	2.69	0.71
10:F:80:TRP:HE3	20:F:206:CLA:HMC2	1.55	0.71
11:G:21:PHE:O	11:G:23:PHE:CB	2.38	0.71
20:J:101:CLA:OBD	20:J:101:CLA:CED	2.38	0.71
20:1:202:CLA:HED3	20:1:202:CLA:CHA	2.18	0.71
3:3:84:ILE:N	20:3:302:CLA:C4	2.46	0.71
5:A:23:ASP:OD2	5:A:24:ARG:CD	2.36	0.71
5:A:249:ILE:O	5:A:251:ASN:N	2.23	0.71
22:A:845:BCR:C23	22:A:845:BCR:H382	2.09	0.71
6:B:145:LEU:HA	6:B:148:ILE:HD12	1.71	0.71
6:B:504:ASN:ND2	6:B:504:ASN:H	1.88	0.71
6:B:594:TRP:C	6:B:594:TRP:CD1	2.64	0.71
9:E:87:VAL:CG1	9:E:87:VAL:O	2.28	0.71
26:H:111:UNL:C2	26:H:111:UNL:C6	2.63	0.71
15:K:47:ILE:HG23	15:K:48:GLN:H	1.54	0.71
16:L:95:LEU:HA	16:L:98:CYS:HB2	1.71	0.71
17:N:74:LYS:O	17:N:75:TYR:C	2.29	0.71
2:2:129:LYS:C	2:2:131:THR:H	1.93	0.71
4:4:172:VAL:O	4:4:173:THR:HG22	1.90	0.71
4:4:36:ASN:C	4:4:39:TRP:CE3	2.64	0.71
5:A:462:ILE:CD1	20:B:850:CLA:H72	2.21	0.71
5:A:690:LEU:HD21	5:A:738:TYR:HE1	1.55	0.71
20:A:830:CLA:H152	22:L:210:BCR:C36	2.20	0.71
6:B:91:ILE:CD1	6:B:104:PHE:CE2	2.74	0.71
6:B:496:GLY:O	6:B:499:ASN:HB2	1.91	0.71
8:D:28:ILE:HG12	8:D:67:ILE:CG1	2.20	0.71
6:B:230:TRP:HH2	11:G:11:SER:HB2	1.55	0.71
20:K:101:CLA:HMD1	20:K:108:CLA:C1A	2.21	0.71
16:L:10:VAL:O	16:L:10:VAL:HG22	1.90	0.71
16:L:126:GLN:N	16:L:127:PRO:HD2	2.05	0.71
4:4:194:VAL:CG1	4:4:195:GLN:CA	2.64	0.71
5:A:491:TRP:NE1	20:A:834:CLA:H12	2.06	0.71
6:B:437:TYR:HB3	6:B:616:LEU:HD23	1.72	0.71
11:G:68:ILE:HG22	11:G:72:LEU:HD13	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:45:ASN:O	17:N:45:ASN:CG	2.29	0.71
5:A:119:SER:HB2	5:A:136:VAL:HG21	1.71	0.71
5:A:396:PHE:CE2	5:A:616:PHE:CG	2.79	0.71
5:A:466:THR:O	5:A:470:LEU:HG	1.90	0.71
5:A:618:TRP:CZ2	5:A:655:ASP:HB2	2.25	0.71
9:E:39:LEU:H	9:E:40:ARG:HH11	1.38	0.71
21:H:107:LMU:O2'	21:H:107:LMU:C1	2.33	0.71
1:1:63:LEU:CD1	1:1:63:LEU:H	2.01	0.71
4:4:192:THR:C	4:4:193:ILE:O	2.28	0.71
5:A:550:HIS:O	5:A:552:THR:O	2.07	0.71
5:A:443:ILE:HD11	5:A:557:LEU:HG	1.73	0.71
6:B:503:GLU:HB3	6:B:507:SER:HB2	1.71	0.71
6:B:595:HIS:HD2	6:B:623:TYR:OH	1.73	0.71
20:1:215:CLA:O1D	20:1:215:CLA:CGA	2.39	0.71
4:4:58:MET:O	4:4:61:PRO:CD	2.39	0.71
5:A:193:LEU:HA	5:A:196:PHE:CE2	2.26	0.71
5:A:387:THR:HG23	5:A:523:VAL:HG11	1.71	0.71
5:A:202:MET:HG3	20:A:813:CLA:HBC2	1.71	0.71
17:N:42:PHE:HD1	17:N:43:PRO:N	1.83	0.71
17:N:54:LYS:HG3	17:N:57:LYS:HZ3	1.53	0.71
17:N:54:LYS:HG2	17:N:57:LYS:NZ	2.05	0.71
21:1:217:LMU:C3'	21:1:217:LMU:H12	2.01	0.70
21:2:318:LMU:C6B	21:2:318:LMU:H2B	2.19	0.70
4:4:194:VAL:CB	4:4:195:GLN:CA	2.69	0.70
20:4:305:CLA:CMC	20:4:305:CLA:CBC	2.65	0.70
20:A:826:CLA:H111	22:J:102:BCR:H353	1.73	0.70
6:B:493:TRP:HB3	20:B:833:CLA:HED2	1.71	0.70
20:B:821:CLA:CBD	20:B:821:CLA:HAA2	2.20	0.70
9:E:68:ARG:NH2	9:E:69:PHE:HA	2.06	0.70
22:F:203:BCR:HC32	20:F:205:CLA:CMA	2.21	0.70
20:K:103:CLA:HBA1	20:K:103:CLA:O2D	1.91	0.70
17:N:63:ASP:H	17:N:65:LEU:N	1.87	0.70
17:N:65:LEU:O	17:N:66:ASP:C	2.29	0.70
20:2:308:CLA:H2A	20:2:308:CLA:O1D	1.91	0.70
2:2:40:SER:C	2:2:41:LEU:CD2	2.58	0.70
3:3:106:TYR:O	3:3:108:ALA:HB2	1.91	0.70
4:4:160:MET:HA	4:4:163:PHE:HB2	1.72	0.70
4:4:164:LEU:O	4:4:165:GLY:C	2.30	0.70
4:4:168:ILE:HD11	20:4:310:CLA:C3C	2.20	0.70
4:4:70:ILE:HG13	4:4:71:ASN:N	2.06	0.70
5:A:242:ILE:HG12	5:A:243:PRO:CD	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:HIS:CE1	5:A:442:ILE:HD11	2.25	0.70
7:C:5:VAL:HB	7:C:65:VAL:CA	2.13	0.70
10:F:24:LYS:C	10:F:26:GLN:H	1.93	0.70
16:L:52:ARG:O	16:L:56:VAL:HG23	1.90	0.70
21:N:101:LMU:H52	21:N:101:LMU:H91	1.65	0.70
1:1:25:ASP:HB3	1:1:26:PRO:CD	2.20	0.70
21:2:318:LMU:H6'1	21:2:318:LMU:H2B	1.73	0.70
4:4:124:TYR:HB3	4:4:143:PHE:CE1	2.25	0.70
5:A:207:LEU:HD12	5:A:310:PHE:CD1	2.25	0.70
5:A:211:LEU:O	5:A:214:GLY:O	2.09	0.70
5:A:397:THR:HB	5:A:613:ILE:HD11	1.73	0.70
5:A:431:LEU:O	5:A:435:VAL:HG12	1.90	0.70
5:A:445:HIS:O	5:A:446:LEU:CB	2.39	0.70
5:A:485:GLN:O	5:A:487:VAL:N	2.24	0.70
5:A:497:ALA:HB2	5:A:515:TRP:CB	2.20	0.70
20:A:804:CLA:H12	20:A:811:CLA:C6	2.14	0.70
5:A:368:LEU:HD22	20:A:818:CLA:H92	1.74	0.70
20:A:826:CLA:C7	22:A:847:BCR:H372	2.16	0.70
20:A:839:CLA:C3D	20:A:839:CLA:O1D	2.30	0.70
23:A:842:PQN:C13	22:F:202:BCR:H322	2.21	0.70
6:B:542:ARG:NH2	8:D:143:PRO:HG3	2.05	0.70
6:B:545:LYS:HG2	6:B:546:LEU:N	2.03	0.70
7:C:1:MET:SD	7:C:4:SER:CB	2.79	0.70
20:3:318:CLA:HMA2	20:3:318:CLA:C1	2.14	0.70
5:A:625:TRP:CB	5:A:637:ILE:HD11	2.20	0.70
6:B:174:ARG:NH1	20:B:822:CLA:CMD	2.54	0.70
8:D:48:ILE:CG2	8:D:83:CYS:HB2	2.21	0.70
11:G:46:ALA:C	11:G:48:ASP:OD1	2.29	0.70
12:H:21:TRP:H	12:H:22:ASP:CB	2.03	0.70
17:N:11:LYS:HD2	17:N:12:THR:O	1.92	0.70
17:N:18:ASP:HB3	17:N:22:LEU:HG	1.73	0.70
17:N:42:PHE:O	17:N:43:PRO:C	2.30	0.70
19:U:1:GLC:H3	19:U:2:FRU:C5	2.21	0.70
2:2:110:TRP:HA	2:2:113:ILE:CG2	2.21	0.70
3:3:157:ALA:C	3:3:158:TYR:CD2	2.64	0.70
5:A:423:ASP:HB3	5:A:424:PRO:CD	2.08	0.70
5:A:479:ASP:OD2	5:A:536:THR:HG23	1.90	0.70
5:A:663:GLN:HB3	5:A:752:ALA:O	1.90	0.70
20:A:841:CLA:HMC2	20:B:838:CLA:H11	1.74	0.70
5:A:216:LEU:HD12	22:A:843:BCR:H353	1.73	0.70
6:B:130:ARG:HG2	6:B:130:ARG:HH11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:295:PHE:N	6:B:295:PHE:HD2	1.85	0.70
6:B:375:HIS:HE1	20:B:826:CLA:NC	1.89	0.70
7:C:5:VAL:CB	7:C:65:VAL:HG22	2.22	0.70
8:D:91:ARG:HH12	8:D:119:TYR:HE1	1.38	0.70
8:D:47:VAL:HB	8:D:76:LYS:HA	1.73	0.70
9:E:44:TYR:CZ	9:E:73:ASN:HA	2.27	0.70
10:F:93:ILE:CG2	22:F:202:BCR:H371	2.22	0.70
17:N:4:GLU:OE2	17:N:4:GLU:C	2.30	0.70
17:N:70:GLU:C	17:N:72:LYS:N	2.34	0.70
19:P:1:GLC:HO2	19:P:2:FRU:H12	1.55	0.70
4:4:38:ARG:HH11	4:4:38:ARG:CG	2.02	0.70
4:4:75:TRP:CB	20:4:311:CLA:HMD3	2.22	0.70
5:A:396:PHE:HE2	5:A:616:PHE:CB	2.04	0.70
20:A:818:CLA:OBD	20:A:827:CLA:H43	1.91	0.70
6:B:172:GLU:HG3	6:B:301:ILE:HG13	1.72	0.70
20:B:823:CLA:H72	20:B:837:CLA:C3D	2.22	0.70
23:B:841:PQN:H142	23:B:841:PQN:H2M1	1.74	0.70
22:B:852:BCR:C33	22:B:852:BCR:HC8	2.22	0.70
12:H:45:ALA:O	12:H:47:PHE:N	2.25	0.70
2:2:113:ILE:HG13	2:2:114:LEU:N	2.06	0.70
20:4:306:CLA:CMC	20:4:306:CLA:CBC	2.33	0.70
4:4:97:LEU:C	4:4:99:HIS:N	2.36	0.70
5:A:225:VAL:O	5:A:229:ILE:HB	1.90	0.70
5:A:454:GLY:N	5:A:457:SER:HB3	2.00	0.70
5:A:545:HIS:CE1	5:A:612:VAL:HG22	2.27	0.70
5:A:59:ALA:O	5:A:61:ALA:N	2.23	0.70
20:A:822:CLA:HBB2	22:A:845:BCR:C35	2.17	0.70
21:A:854:LMU:O6'	21:A:854:LMU:H12	1.90	0.70
8:D:28:ILE:HG21	8:D:67:ILE:HG13	1.74	0.70
12:H:45:ALA:HB3	12:H:46:PRO:CD	2.21	0.70
20:K:101:CLA:HMD1	20:K:108:CLA:C4A	2.21	0.70
20:L:207:CLA:HAA2	20:L:207:CLA:HED2	1.74	0.70
18:R:37:UNK:O	18:R:43:UNK:N	2.24	0.70
1:1:57:ILE:O	1:1:59:VAL:C	2.30	0.70
3:3:163:PHE:O	3:3:164:PHE:HB2	1.91	0.70
20:A:825:CLA:HBA1	20:A:825:CLA:HBD	1.72	0.70
6:B:369:ALA:O	6:B:725:LEU:CD1	2.38	0.70
6:B:730:SER:C	6:B:731:GLY:O	2.29	0.70
6:B:174:ARG:NH1	20:B:822:CLA:HMD1	2.07	0.70
20:B:832:CLA:HMD2	20:B:833:CLA:C1C	2.21	0.70
5:A:470:LEU:HD13	6:B:95:HIS:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:42:GLU:HG2	9:E:43:SER:H	1.54	0.70
12:H:14:ILE:HG13	12:H:17:THR:OG1	1.92	0.70
1:1:179:THR:OG1	4:4:87:SER:OG	2.09	0.70
20:2:322:CLA:H72	20:2:322:CLA:H42	1.72	0.70
2:2:38:PRO:C	2:2:40:SER:OG	2.29	0.70
2:2:98:GLU:HG3	2:2:99:LEU:HG	1.73	0.70
20:4:304:CLA:CGD	20:4:304:CLA:CAA	2.70	0.70
4:4:31:ALA:O	4:4:32:GLU:C	2.30	0.70
5:A:385:LEU:O	5:A:386:ALA:CB	2.38	0.70
5:A:475:ASP:HB3	20:A:831:CLA:HED3	1.73	0.70
6:B:568:CYS:O	6:B:570:ILE:N	2.25	0.70
6:B:607:SER:HA	6:B:610:ASN:HD22	1.57	0.70
6:B:612:SER:HA	6:B:615:TYR:CE1	2.21	0.70
9:E:34:SER:O	9:E:35:LYS:HB3	1.91	0.70
10:F:116:GLN:C	10:F:118:GLU:H	1.92	0.70
12:H:10:ASP:HB3	12:H:13:ASP:HB2	1.72	0.70
19:P:1:GLC:C2	19:P:2:FRU:O5	2.35	0.70
1:1:142:GLU:OE1	20:1:201:CLA:C2D	2.40	0.70
2:2:195:ALA:HB1	2:2:197:LEU:HG	1.73	0.70
4:4:69:ILE:O	4:4:70:ILE:C	2.27	0.70
5:A:21:LEU:CD1	5:A:21:LEU:O	2.30	0.70
5:A:723:ARG:NH1	5:A:723:ARG:HG2	2.06	0.70
6:B:576:PHE:CE2	20:B:827:CLA:HAC1	2.26	0.70
20:B:827:CLA:HBC2	20:B:827:CLA:CMC	2.10	0.70
7:C:1:MET:CA	7:C:4:SER:OG	2.40	0.70
13:I:9:VAL:HG12	13:I:10:PRO:HD3	1.73	0.70
13:I:20:ALA:O	13:I:24:LEU:HB3	1.92	0.70
2:2:102:ILE:HG13	20:2:312:CLA:HMD2	1.74	0.69
2:2:113:ILE:HG13	2:2:114:LEU:H	1.57	0.69
5:A:141:ARG:HD3	10:F:39:ALA:HA	1.74	0.69
5:A:157:GLY:HA2	5:A:229:ILE:CG2	2.22	0.69
5:A:736:THR:HG21	20:A:828:CLA:H91	1.74	0.69
6:B:160:LYS:HZ3	6:B:160:LYS:HB2	1.56	0.69
6:B:293:THR:HG22	6:B:294:ASN:ND2	2.07	0.69
6:B:655:LEU:CD2	20:B:839:CLA:CBB	2.69	0.69
13:I:7:LEU:HD12	22:I:103:BCR:H333	0.89	0.69
22:3:314:BCR:H23C	22:3:314:BCR:H393	0.77	0.69
5:A:164:LEU:HA	5:A:167:THR:HG23	1.73	0.69
22:B:846:BCR:H17C	20:B:850:CLA:C10	2.18	0.69
21:H:107:LMU:O2B	21:H:107:LMU:H5'	1.92	0.69
16:L:163:LEU:HB3	16:L:164:PRO:CD	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:104:LMU:O2'	21:R:104:LMU:C5'	2.30	0.69
4:4:106:TRP:C	4:4:108:ASP:N	2.42	0.69
4:4:121:PHE:HD1	4:4:128:ALA:HB3	1.57	0.69
4:4:93:ILE:O	4:4:94:GLU:C	2.29	0.69
4:4:98:SER:C	4:4:102:GLU:OE1	2.30	0.69
5:A:308:ILE:HG13	20:A:816:CLA:HBB1	1.74	0.69
5:A:453:LEU:HD13	5:A:547:PHE:HA	1.74	0.69
5:A:685:VAL:HG12	5:A:741:GLY:HA2	1.74	0.69
20:A:819:CLA:H61	22:A:846:BCR:H19C	1.73	0.69
7:C:44:ARG:HH22	8:D:127:ARG:NE	1.90	0.69
8:D:111:TYR:HD2	8:D:114:PRO:CB	2.05	0.69
9:E:90:VAL:O	9:E:91:ALA:C	2.30	0.69
21:K:105:LMU:H41	21:K:105:LMU:O6'	1.91	0.69
16:L:43:TYR:O	16:L:44:ARG:HB2	1.91	0.69
17:N:76:LYS:HG3	17:N:77:CYS:N	2.00	0.69
21:R:109:LMU:C6'	21:R:109:LMU:O5B	2.39	0.69
5:A:370:ILE:HD12	20:A:824:CLA:O1D	1.92	0.69
20:A:851:CLA:CAD	20:A:851:CLA:CED	2.70	0.69
6:B:269:TRP:HE3	6:B:270:LEU:H	1.38	0.69
5:A:567:ARG:HH11	8:D:35:GLY:CA	2.02	0.69
20:H:102:CLA:C2C	22:I:103:BCR:HC21	2.22	0.69
12:H:53:LEU:CG	12:H:54:LEU:H	2.04	0.69
16:L:158:MET:CG	16:L:159:TYR:H	2.04	0.69
21:R:109:LMU:C1'	21:R:109:LMU:O6'	2.40	0.69
20:B:817:CLA:HBB2	20:B:822:CLA:H41	1.75	0.69
10:F:22:LEU:C	10:F:24:LYS:H	1.93	0.69
16:L:64:LEU:HA	16:L:67:PRO:HG2	1.73	0.69
18:R:34:UNK:C	18:R:38:UNK:CB	2.71	0.69
2:2:100:VAL:HG22	2:2:101:PHE:N	2.07	0.69
5:A:449:VAL:HG22	20:A:836:CLA:HMC3	1.75	0.69
20:A:838:CLA:H71	20:A:852:CLA:H171	1.72	0.69
6:B:124:TRP:HE1	6:B:129:LEU:HD22	1.57	0.69
6:B:409:ALA:C	6:B:411:MET:H	1.96	0.69
20:B:823:CLA:HHD	20:B:823:CLA:HBC3	1.74	0.69
7:C:31:TRP:HB2	7:C:39:ILE:HG21	1.75	0.69
10:F:15:ALA:O	10:F:18:GLU:HB2	1.92	0.69
10:F:47:GLU:HG3	10:F:51:LYS:CE	2.09	0.69
19:Z:1:GLC:O2	19:Z:1:GLC:H5	1.89	0.69
4:4:121:PHE:O	4:4:143:PHE:HD2	1.74	0.69
4:4:81:GLU:HA	4:4:81:GLU:OE2	1.92	0.69
5:A:263:ALA:O	5:A:264:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:808:CLA:C4	22:A:847:BCR:H383	2.23	0.69
6:B:25:ILE:HG21	22:L:210:BCR:H292	0.70	0.69
6:B:336:LEU:HD13	20:B:822:CLA:HBB1	1.75	0.69
7:C:78:GLY:O	7:C:81:TYR:CE1	2.42	0.69
22:F:203:BCR:H333	20:F:205:CLA:HHB	1.74	0.69
10:F:21:ALA:O	10:F:22:LEU:C	2.28	0.69
2:2:98:GLU:HG2	2:2:99:LEU:CD1	2.21	0.69
4:4:70:ILE:C	4:4:72:VAL:H	1.94	0.69
5:A:436:LEU:O	5:A:439:ARG:HB3	1.93	0.69
22:A:847:BCR:H311	20:A:852:CLA:H142	1.73	0.69
6:B:178:HIS:C	6:B:180:SER:H	1.94	0.69
6:B:404:ALA:C	6:B:406:ASN:N	2.45	0.69
6:B:438:VAL:O	6:B:441:ASP:N	2.26	0.69
23:B:841:PQN:H192	22:B:846:BCR:C10	2.09	0.69
20:B:850:CLA:H91	20:B:851:CLA:C9	2.22	0.69
21:E:101:LMU:C6	21:E:101:LMU:C1	2.71	0.69
11:G:62:ASP:HB2	11:G:63:PRO:HD3	1.73	0.69
16:L:25:THR:O	16:L:28:THR:HB	1.92	0.69
21:N:101:LMU:H6E	21:N:101:LMU:H51	0.72	0.69
19:Z:1:GLC:C5	19:Z:1:GLC:HO2	2.05	0.69
20:2:322:CLA:H152	20:2:322:CLA:C9	2.22	0.69
3:3:52:LYS:C	3:3:56:TYR:CD2	2.65	0.69
4:4:121:PHE:CD1	4:4:143:PHE:CE2	2.81	0.69
5:A:615:HIS:CE1	20:A:834:CLA:HBC3	2.28	0.69
6:B:124:TRP:HD1	6:B:124:TRP:O	1.76	0.69
6:B:242:HIS:O	6:B:243:LEU:HG	1.93	0.69
6:B:692:ARG:HH22	6:B:694:ARG:HG2	1.57	0.69
22:B:846:BCR:H382	22:B:846:BCR:C23	2.11	0.69
7:C:12:ILE:HB	7:C:38:GLN:O	1.93	0.69
7:C:2:SER:O	7:C:3:HIS:ND1	2.26	0.69
20:1:215:CLA:C2A	20:1:215:CLA:CGD	2.71	0.69
4:4:146:THR:O	4:4:146:THR:HG22	1.92	0.69
4:4:73:PRO:HB2	4:4:75:TRP:HB2	1.73	0.69
4:4:97:LEU:O	4:4:98:SER:C	2.31	0.69
5:A:259:TYR:CD2	5:A:280:PHE:HA	2.28	0.69
5:A:582:ASP:OD1	5:A:586:ARG:NH1	2.18	0.69
5:A:585:GLY:O	5:A:589:THR:OG1	2.11	0.69
6:B:292:ARG:NH2	6:B:297:ILE:HG13	2.07	0.69
7:C:55:GLU:C	7:C:57:ALA:H	1.96	0.69
8:D:102:ARG:NE	8:D:110:GLN:HB2	2.07	0.69
16:L:113:SER:O	16:L:116:PRO:HD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:100:VAL:HG22	2:2:101:PHE:H	1.56	0.69
3:3:182:LYS:O	3:3:186:ASN:N	2.23	0.69
3:3:97:PHE:CD2	3:3:97:PHE:N	2.59	0.69
5:A:390:ALA:HA	5:A:393:LEU:HD23	1.75	0.69
5:A:472:ARG:O	5:A:474:GLN:HG3	1.93	0.69
20:A:815:CLA:C2A	20:A:815:CLA:CED	2.70	0.69
20:A:850:CLA:HBC3	20:A:850:CLA:HHD	1.75	0.69
21:A:854:LMU:C7	21:A:854:LMU:C2	2.71	0.69
6:B:124:TRP:CD1	6:B:129:LEU:HD13	2.28	0.69
6:B:561:GLY:HA3	7:C:52:LYS:CG	2.21	0.69
20:B:830:CLA:H51	22:F:203:BCR:H401	1.75	0.69
20:B:807:CLA:CMC	22:B:846:BCR:H282	2.22	0.69
11:G:13:GLY:HA2	11:G:16:LEU:CG	2.23	0.69
21:H:104:LMU:H11	21:H:104:LMU:H3'	1.73	0.69
14:J:10:VAL:CG1	14:J:11:ALA:N	2.56	0.69
17:N:55:GLN:O	17:N:56:LYS:CG	2.41	0.69
18:R:51:UNK:O	18:R:52:UNK:CB	2.41	0.69
4:4:121:PHE:HZ	4:4:125:SER:O	1.76	0.68
20:A:808:CLA:HMB1	20:A:809:CLA:H11	1.75	0.68
6:B:468:GLY:O	6:B:470:THR:N	2.26	0.68
20:B:816:CLA:C3A	20:B:816:CLA:CGA	2.70	0.68
20:B:818:CLA:NB	20:B:818:CLA:H2	2.08	0.68
20:B:812:CLA:HMB3	22:B:844:BCR:H311	1.73	0.68
10:F:52:ARG:NH1	10:F:55:ASN:OD1	2.26	0.68
11:G:28:ARG:HD2	11:G:33:LYS:HE2	1.75	0.68
4:4:124:TYR:HB2	4:4:143:PHE:CD1	2.26	0.68
5:A:396:PHE:HE2	5:A:616:PHE:CG	2.10	0.68
6:B:347:LEU:HD13	6:B:351:HIS:HD1	1.58	0.68
7:C:65:VAL:HG12	7:C:66:ARG:H	1.57	0.68
12:H:32:TYR:OH	16:L:44:ARG:NE	2.18	0.68
20:3:308:CLA:HAC2	20:K:103:CLA:H91	1.75	0.68
17:N:67:LEU:CA	17:N:68:GLU:CG	2.70	0.68
20:R:108:CLA:H91	21:R:109:LMU:H4O1	1.58	0.68
21:2:318:LMU:O2'	21:2:318:LMU:C1	2.39	0.68
2:2:51:HIS:O	2:2:54:TRP:HB2	1.94	0.68
4:4:128:ALA:H	4:4:143:PHE:HZ	1.36	0.68
4:4:169:GLN:HG2	20:4:305:CLA:HAC2	1.75	0.68
4:4:192:THR:CG2	4:4:195:GLN:H	1.99	0.68
4:4:192:THR:HG21	4:4:195:GLN:CA	2.21	0.68
5:A:206:HIS:O	5:A:211:LEU:HD23	1.93	0.68
5:A:269:PHE:CE1	15:K:14:THR:CG2	2.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:ILE:HG23	5:A:403:GLY:CA	2.22	0.68
5:A:520:LEU:HD22	21:A:848:LMU:O2'	1.92	0.68
20:A:824:CLA:HBB2	20:A:836:CLA:H3A	1.75	0.68
6:B:188:LEU:HD11	20:B:813:CLA:CBB	2.23	0.68
6:B:299:HIS:CE1	20:B:820:CLA:HMD1	2.29	0.68
21:B:847:LMU:C10	21:B:847:LMU:H61	2.23	0.68
16:L:77:THR:HG21	16:L:82:ALA:HB1	1.74	0.68
16:L:69:VAL:HG11	16:L:84:GLY:H	1.58	0.68
20:2:322:CLA:H41	20:2:322:CLA:H93	1.75	0.68
3:3:197:TYR:OH	20:3:304:CLA:CHC	2.41	0.68
4:4:36:ASN:C	4:4:39:TRP:CG	2.67	0.68
4:4:71:ASN:O	4:4:72:VAL:C	2.30	0.68
4:4:97:LEU:C	4:4:99:HIS:H	1.94	0.68
5:A:206:HIS:C	5:A:211:LEU:HD23	2.14	0.68
5:A:408:VAL:HG11	5:A:602:LEU:HD23	1.75	0.68
5:A:464:ASN:HD22	5:A:464:ASN:H	1.39	0.68
5:A:472:ARG:HH22	16:L:74:LEU:HD21	1.58	0.68
5:A:51:THR:CG2	20:A:837:CLA:HBB2	2.18	0.68
6:B:711:VAL:O	6:B:711:VAL:CG1	2.42	0.68
21:B:847:LMU:C10	21:B:847:LMU:C6	2.66	0.68
7:C:20:ALA:O	7:C:21:CYS:CB	2.41	0.68
25:B:848:LMG:O3	7:C:70:TRP:NE1	2.26	0.68
13:I:10:PRO:HA	13:I:14:LEU:HB2	1.74	0.68
16:L:13:PRO:O	16:L:14:LEU:HB2	1.93	0.68
16:L:65:VAL:C	16:L:67:PRO:HD2	2.12	0.68
17:N:65:LEU:HD23	17:N:66:ASP:O	1.93	0.68
20:1:206:CLA:H61	20:1:206:CLA:H122	1.76	0.68
3:3:87:GLU:CB	22:3:314:BCR:H382	2.22	0.68
5:A:170:GLY:O	5:A:173:VAL:CG2	2.39	0.68
5:A:174:PHE:CE2	20:A:805:CLA:H152	2.27	0.68
5:A:22:VAL:C	5:A:23:ASP:O	2.29	0.68
5:A:475:ASP:OD2	16:L:74:LEU:HA	1.93	0.68
5:A:620:MET:HG3	5:A:625:TRP:CE2	2.28	0.68
5:A:720:THR:HG22	5:A:720:THR:O	1.93	0.68
20:A:830:CLA:O1A	20:A:841:CLA:C1	2.41	0.68
6:B:469:LYS:HE2	6:B:471:THR:OG1	1.93	0.68
10:F:95:GLY:O	10:F:99:TRP:HB2	1.93	0.68
17:N:40:CYS:N	17:N:41:LYS:HA	2.09	0.68
4:4:117:GLN:O	4:4:122:LYS:C	2.31	0.68
5:A:472:ARG:HH12	16:L:74:LEU:CG	1.96	0.68
20:A:807:CLA:C3B	22:J:102:BCR:H332	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:849:LMU:H5'	21:A:849:LMU:O5B	1.93	0.68
6:B:294:ASN:OD1	11:G:38:GLN:CA	2.37	0.68
6:B:696:LYS:HG2	7:C:80:ALA:HA	1.75	0.68
20:B:803:CLA:NC	20:B:803:CLA:H52	2.09	0.68
20:B:810:CLA:HAC1	20:B:811:CLA:CBB	2.16	0.68
17:N:61:LEU:HD12	17:N:63:ASP:HB2	1.74	0.68
2:2:39:GLU:HA	2:2:40:SER:HB2	1.73	0.68
3:3:181:LEU:CA	3:3:182:LYS:HG3	2.20	0.68
3:3:93:PHE:N	3:3:95:THR:H	1.89	0.68
5:A:374:GLN:O	5:A:377:TYR:HD2	1.77	0.68
5:A:425:THR:O	5:A:427:ARG:NE	2.26	0.68
5:A:603:PHE:HZ	5:A:693:LEU:HD21	1.59	0.68
20:A:824:CLA:H172	22:A:845:BCR:H332	1.75	0.68
20:A:825:CLA:H101	20:A:825:CLA:H143	1.74	0.68
20:A:851:CLA:HMB3	20:B:849:CLA:C18	2.22	0.68
21:A:854:LMU:H71	21:A:854:LMU:C11	2.23	0.68
6:B:269:TRP:CD1	6:B:497:TRP:CH2	2.82	0.68
20:B:830:CLA:HBB2	22:F:202:BCR:C27	2.24	0.68
13:I:14:LEU:C	13:I:17:PRO:HD2	2.14	0.68
1:1:57:ILE:CD1	1:1:57:ILE:O	2.39	0.68
3:3:88:THR:N	22:3:314:BCR:H383	2.09	0.68
3:3:63:ARG:CZ	3:3:185:LYS:HG2	2.24	0.68
4:4:40:PHE:O	4:4:43:ALA:CB	2.29	0.68
5:A:158:ILE:HG22	20:A:814:CLA:HED3	1.75	0.68
5:A:207:LEU:HA	5:A:211:LEU:CG	2.23	0.68
5:A:400:MET:O	5:A:609:ILE:HD12	1.94	0.68
5:A:88:ILE:HG22	5:A:89:ILE:N	2.09	0.68
6:B:273:VAL:O	6:B:277:HIS:HD2	1.75	0.68
6:B:388:ALA:C	6:B:391:PRO:CD	2.61	0.68
6:B:697:PRO:HB3	20:B:838:CLA:HBC3	1.76	0.68
7:C:70:TRP:O	7:C:72:GLU:CB	2.41	0.68
9:E:53:VAL:O	9:E:55:VAL:N	2.25	0.68
11:G:12:THR:HG22	11:G:72:LEU:CD1	2.24	0.68
15:K:4:GLY:HA2	15:K:7:THR:HB	1.75	0.68
20:3:313:CLA:H143	20:3:313:CLA:H102	1.76	0.68
3:3:93:PHE:H	3:3:95:THR:N	1.89	0.68
4:4:164:LEU:O	4:4:167:ILE:N	2.27	0.68
4:4:36:ASN:OD1	4:4:39:TRP:CD1	2.47	0.68
5:A:244:LEU:HB2	5:A:247:GLU:HB2	1.76	0.68
5:A:309:LEU:O	5:A:310:PHE:HB2	1.93	0.68
5:A:624:VAL:O	5:A:636:HIS:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:68:THR:C	5:A:70:ASP:H	1.97	0.68
20:A:815:CLA:HED2	20:A:815:CLA:CBA	2.24	0.68
6:B:160:LYS:HE3	6:B:161:TRP:CD2	2.28	0.68
6:B:178:HIS:O	6:B:180:SER:N	2.27	0.68
6:B:595:HIS:CD2	6:B:623:TYR:OH	2.47	0.68
6:B:689:ASN:O	6:B:691:ILE:N	2.26	0.68
20:B:823:CLA:HED2	20:B:824:CLA:HMD1	1.76	0.68
8:D:49:THR:HG22	8:D:99:GLN:HB3	1.75	0.68
10:F:25:LEU:HD23	10:F:46:MET:HB3	1.73	0.68
2:2:127:ASN:HB3	14:J:1:MET:O	1.94	0.68
17:N:33:TYR:O	17:N:34:THR:HG22	1.94	0.68
17:N:40:CYS:H	17:N:41:LYS:HA	1.58	0.68
3:3:92:TRP:CA	3:3:93:PHE:CG	2.74	0.68
4:4:193:ILE:O	4:4:194:VAL:C	2.29	0.68
20:A:819:CLA:H111	20:A:819:CLA:H162	1.76	0.68
6:B:187:SER:O	6:B:189:ALA:N	2.27	0.68
6:B:267:SER:HA	6:B:356:PRO:O	1.94	0.68
5:A:131:ILE:HD13	6:B:446:PHE:C	2.14	0.68
6:B:46:ILE:HG21	20:B:805:CLA:HBC3	1.74	0.68
20:B:826:CLA:H101	22:B:844:BCR:H343	1.76	0.68
22:B:852:BCR:C38	22:B:852:BCR:H23C	2.24	0.68
20:L:201:CLA:H2	20:L:201:CLA:H72	1.76	0.68
19:X:1:GLC:H2	19:X:2:FRU:O4	1.94	0.68
2:2:124:ILE:HB	2:2:129:LYS:HB3	1.74	0.67
4:4:147:LEU:HD22	4:4:148:GLU:CG	2.21	0.67
5:A:204:ASN:O	5:A:205:HIS:CB	2.36	0.67
5:A:618:TRP:O	5:A:622:SER:HB3	1.94	0.67
5:A:207:LEU:HB2	20:A:819:CLA:HBB2	1.75	0.67
20:A:838:CLA:H142	20:A:852:CLA:H143	1.76	0.67
6:B:174:ARG:O	6:B:175:LEU:HB3	1.95	0.67
20:A:851:CLA:C1	6:B:616:LEU:HG	2.22	0.67
6:B:633:ASN:ND2	6:B:636:THR:HB	2.09	0.67
12:H:74:GLN:OE1	12:H:74:GLN:O	2.12	0.67
20:B:851:CLA:H142	22:I:101:BCR:C4	2.24	0.67
14:J:22:LEU:O	14:J:25:LEU:N	2.27	0.67
21:K:104:LMU:C1B	21:K:104:LMU:O6B	2.42	0.67
3:3:50:GLU:O	3:3:53:TRP:N	2.27	0.67
20:A:828:CLA:H101	20:A:828:CLA:H152	1.76	0.67
20:A:851:CLA:C3B	6:B:589:TRP:CH2	2.77	0.67
6:B:140:ILE:H	6:B:140:ILE:HD13	1.59	0.67
6:B:141:PHE:HD2	6:B:144:PHE:CE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:347:LEU:HD21	6:B:351:HIS:HE1	1.59	0.67
20:B:821:CLA:H42	20:B:821:CLA:CHB	2.23	0.67
22:B:846:BCR:C20	20:B:850:CLA:H151	2.24	0.67
7:C:75:ARG:HH22	8:D:110:GLN:CD	1.96	0.67
7:C:73:THR:N	7:C:76:SER:OG	2.27	0.67
8:D:28:ILE:CG2	8:D:67:ILE:HG13	2.25	0.67
11:G:28:ARG:NH2	11:G:29:GLU:O	2.28	0.67
21:R:102:LMU:O2'	21:R:102:LMU:H5'	1.92	0.67
3:3:92:TRP:HZ2	5:A:250:LEU:HB2	1.60	0.67
4:4:37:LEU:CA	4:4:39:TRP:CG	2.77	0.67
4:4:70:ILE:O	4:4:72:VAL:N	2.27	0.67
5:A:118:PRO:HB3	5:A:150:PHE:CE2	2.29	0.67
5:A:154:ARG:HH21	5:A:233:LEU:HD13	1.58	0.67
5:A:390:ALA:HA	5:A:393:LEU:CD2	2.24	0.67
20:A:836:CLA:HBC3	20:A:836:CLA:CMC	2.21	0.67
20:A:841:CLA:H152	22:B:852:BCR:H352	1.76	0.67
23:A:842:PQN:H142	22:F:202:BCR:HC22	1.75	0.67
6:B:450:GLU:O	6:B:452:GLN:N	2.25	0.67
5:A:705:GLU:HB3	6:B:545:LYS:HZ1	1.58	0.67
6:B:598:HIS:HB3	6:B:602:TRP:CZ3	2.30	0.67
5:A:680:LEU:HD21	6:B:617:MET:CE	2.24	0.67
6:B:649:MET:O	6:B:653:GLY:N	2.26	0.67
6:B:552:ASP:HA	8:D:144:ILE:HG22	1.76	0.67
12:H:63:SER:O	12:H:67:TYR:HB2	1.94	0.67
17:N:18:ASP:HB2	17:N:22:LEU:CD1	2.23	0.67
17:N:44:GLU:O	17:N:46:PHE:N	2.27	0.67
17:N:62:SER:HB2	17:N:66:ASP:OD1	1.94	0.67
2:2:97:VAL:O	2:2:100:VAL:HG13	1.94	0.67
21:3:322:LMU:H71	21:3:322:LMU:H32	1.77	0.67
5:A:25:ASP:N	5:A:26:PRO:CD	2.56	0.67
20:A:833:CLA:C2A	20:A:839:CLA:HBB1	2.25	0.67
6:B:30:ASP:OD2	6:B:396:ARG:NH1	2.26	0.67
6:B:398:TYR:HD1	6:B:542:ARG:NH2	1.91	0.67
8:D:60:MET:HG3	8:D:61:PRO:O	1.94	0.67
12:H:54:LEU:HD13	12:H:55:LYS:HG3	1.76	0.67
20:L:201:CLA:HED3	20:L:201:CLA:O1A	1.94	0.67
21:R:104:LMU:O2'	21:R:104:LMU:H1B	1.95	0.67
20:1:215:CLA:HAA2	20:1:215:CLA:CBD	2.25	0.67
20:1:215:CLA:CED	20:1:215:CLA:CHA	2.72	0.67
1:1:64:GLY:C	1:1:66:GLY:O	2.33	0.67
20:A:825:CLA:CMC	20:A:825:CLA:HBC2	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:826:CLA:H202	22:J:102:BCR:C15	2.24	0.67
20:B:815:CLA:CAD	20:B:824:CLA:CBB	2.71	0.67
20:B:851:CLA:C4	20:B:851:CLA:HHB	2.23	0.67
8:D:39:LYS:CD	8:D:42:VAL:CG1	2.72	0.67
16:L:60:HIS:HD2	20:L:208:CLA:HED1	1.57	0.67
17:N:61:LEU:HD12	17:N:62:SER:O	1.92	0.67
21:R:103:LMU:O6'	21:R:103:LMU:H12	1.94	0.67
2:2:98:GLU:HG2	2:2:99:LEU:HD11	1.76	0.67
4:4:194:VAL:CA	4:4:195:GLN:C	2.61	0.67
20:B:832:CLA:HMB3	20:B:835:CLA:HED3	1.77	0.67
8:D:126:GLY:C	8:D:127:ARG:HG2	2.14	0.67
11:G:28:ARG:HG2	11:G:29:GLU:H	1.56	0.67
11:G:49:THR:OG1	11:G:50:ARG:N	2.28	0.67
20:1:202:CLA:CBA	20:1:202:CLA:O2D	2.38	0.67
2:2:127:ASN:OD1	14:J:2:ARG:HA	1.93	0.67
2:2:189:ILE:HD13	2:2:189:ILE:H	1.58	0.67
3:3:74:ALA:CA	20:3:307:CLA:C1D	2.70	0.67
4:4:118:ASP:N	4:4:118:ASP:OD1	2.27	0.67
4:4:88:SER:C	4:4:90:LEU:HD22	2.14	0.67
5:A:270:PHE:CZ	20:A:839:CLA:O2A	2.47	0.67
20:A:808:CLA:H43	22:A:847:BCR:H383	1.77	0.67
20:A:825:CLA:HBA1	20:A:825:CLA:CBD	2.25	0.67
20:A:835:CLA:H11	20:A:835:CLA:ND	2.10	0.67
6:B:349:ALA:HB2	6:B:375:HIS:HB3	1.77	0.67
6:B:426:SER:O	6:B:430:GLY:N	2.26	0.67
22:B:846:BCR:C33	22:B:846:BCR:HC8	2.24	0.67
10:F:140:ALA:O	10:F:144:LEU:HB3	1.95	0.67
12:H:67:TYR:O	12:H:70:ALA:O	2.13	0.67
20:H:102:CLA:CAC	22:I:103:BCR:C2	2.71	0.67
20:K:108:CLA:H43	20:K:108:CLA:O2A	1.94	0.67
15:K:31:ASN:H	15:K:32:ARG:HH11	1.39	0.67
16:L:108:LYS:O	16:L:132:SER:CB	2.40	0.67
21:N:101:LMU:H32	21:N:101:LMU:C5'	2.24	0.67
17:N:2:VAL:O	17:N:2:VAL:HG23	1.95	0.67
3:3:47:GLY:O	3:3:49:ILE:N	2.27	0.67
4:4:106:TRP:O	4:4:108:ASP:N	2.28	0.67
20:4:304:CLA:HAA2	20:4:304:CLA:HED3	0.72	0.67
4:4:34:PRO:CB	4:4:35:GLU:OE1	2.43	0.67
5:A:107:GLU:OE1	5:A:161:GLU:CG	2.43	0.67
5:A:203:LEU:H	5:A:203:LEU:HD12	1.59	0.67
5:A:618:TRP:CZ2	5:A:655:ASP:CB	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:127:ILE:CD1	6:B:193:HIS:CE1	2.78	0.67
20:B:810:CLA:HAC2	20:B:811:CLA:HBB2	0.67	0.67
22:B:846:BCR:H19C	20:B:850:CLA:C15	2.22	0.67
21:B:847:LMU:H111	21:B:847:LMU:H72	1.77	0.67
7:C:60:THR:CG2	7:C:63:LEU:O	2.43	0.67
10:F:123:VAL:HB	10:F:126:ALA:C	2.15	0.67
20:H:101:CLA:HMA2	20:H:101:CLA:C2	2.19	0.67
12:H:30:SER:O	12:H:31:PRO:O	2.11	0.67
2:2:189:ILE:O	2:2:190:ASP:HB3	1.95	0.67
2:2:102:ILE:HD11	20:2:312:CLA:HMD1	1.76	0.67
3:3:107:TRP:CD1	3:3:108:ALA:CA	2.77	0.67
3:3:63:ARG:NH1	3:3:185:LYS:O	2.28	0.67
4:4:101:VAL:O	4:4:104:ARG:HB3	1.94	0.67
4:4:121:PHE:CZ	4:4:125:SER:O	2.48	0.67
5:A:207:LEU:CD2	5:A:314:GLY:HA2	2.25	0.67
20:A:801:CLA:O1D	20:A:801:CLA:CBA	2.43	0.67
20:A:824:CLA:C2	20:A:824:CLA:O1A	2.41	0.67
6:B:98:GLN:O	6:B:100:ALA:N	2.28	0.67
6:B:646:TRP:CH2	6:B:726:ILE:HD13	2.29	0.67
7:C:66:ARG:NH2	7:C:66:ARG:HG2	1.95	0.67
22:I:103:BCR:C8	22:I:103:BCR:H311	2.22	0.67
3:3:173:GLU:CG	3:3:174:LYS:N	2.57	0.67
4:4:169:GLN:CD	20:4:305:CLA:HHD	2.14	0.67
5:A:217:SER:HA	22:A:843:BCR:C35	2.23	0.67
5:A:629:ASN:HD21	5:A:633:VAL:HG23	1.59	0.67
5:A:692:PHE:CZ	20:A:838:CLA:HBC3	2.29	0.67
20:A:828:CLA:C10	20:A:828:CLA:H152	2.25	0.67
20:F:206:CLA:CAD	20:F:206:CLA:CED	2.73	0.67
1:1:179:THR:HG21	4:4:87:SER:O	1.94	0.66
2:2:102:ILE:C	20:2:311:CLA:CBB	2.55	0.66
3:3:106:TYR:CG	3:3:107:TRP:CD1	2.84	0.66
3:3:97:PHE:O	3:3:98:ILE:HG23	1.95	0.66
4:4:36:ASN:CA	4:4:39:TRP:CE3	2.78	0.66
5:A:27:ILE:CD1	5:A:27:ILE:C	2.63	0.66
20:A:815:CLA:HBB1	22:A:843:BCR:H352	1.76	0.66
20:A:850:CLA:HBC3	20:A:850:CLA:CHD	2.25	0.66
20:B:823:CLA:CAD	20:B:835:CLA:HBB1	2.25	0.66
7:C:66:ARG:HH21	7:C:66:ARG:CG	2.03	0.66
9:E:87:VAL:O	9:E:89:GLU:N	2.27	0.66
10:F:130:LEU:HD12	10:F:131:PHE:CD1	2.30	0.66
10:F:130:LEU:HD12	10:F:131:PHE:HD1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:839:CLA:C19	13:I:21:MET:CB	2.72	0.66
20:K:108:CLA:C4	20:K:108:CLA:O2A	2.42	0.66
19:X:1:GLC:C2	19:X:2:FRU:O4	2.42	0.66
20:4:306:CLA:HBD	20:4:306:CLA:HAA2	1.77	0.66
5:A:114:THR:CG2	5:A:115:HIS:CE1	2.75	0.66
5:A:397:THR:HB	5:A:613:ILE:CD1	2.26	0.66
5:A:708:VAL:HA	5:A:711:HIS:CD2	2.30	0.66
20:A:815:CLA:O1A	20:A:815:CLA:NA	2.28	0.66
20:A:851:CLA:H122	20:A:851:CLA:H92	1.77	0.66
6:B:154:TRP:HD1	6:B:158:GLN:HG2	1.59	0.66
6:B:247:THR:CG2	6:B:250:ALA:HB3	2.25	0.66
6:B:292:ARG:NH2	6:B:297:ILE:H	1.93	0.66
6:B:418:ILE:O	6:B:422:LEU:HD12	1.94	0.66
6:B:576:PHE:HE2	20:B:827:CLA:HAC1	1.58	0.66
7:C:55:GLU:O	7:C:57:ALA:N	2.21	0.66
20:J:101:CLA:CMC	20:J:101:CLA:HBC2	2.23	0.66
1:1:25:ASP:HB3	1:1:26:PRO:HD2	1.77	0.66
5:A:160:SER:HB2	5:A:163:GLN:OE1	1.96	0.66
5:A:22:VAL:CG1	5:A:23:ASP:H	2.08	0.66
5:A:631:GLN:HG3	5:A:631:GLN:O	1.96	0.66
5:A:98:PHE:O	5:A:99:HIS:HB2	1.94	0.66
6:B:127:ILE:CD1	6:B:193:HIS:HE1	2.08	0.66
20:B:803:CLA:H191	10:F:104:TYR:CB	2.22	0.66
7:C:14:CYS:O	7:C:14:CYS:SG	2.53	0.66
9:E:89:GLU:HG2	9:E:92:ALA:H	1.60	0.66
10:F:104:TYR:O	10:F:104:TYR:CD2	2.47	0.66
16:L:99:LEU:HD11	22:L:210:BCR:C31	2.26	0.66
17:N:65:LEU:O	17:N:67:LEU:N	2.29	0.66
17:N:80:ASN:OD1	17:N:82:PHE:HA	1.95	0.66
19:V:1:GLC:O5	19:V:2:FRU:H12	1.94	0.66
4:4:108:ASP:C	4:4:108:ASP:OD2	2.30	0.66
4:4:34:PRO:CA	4:4:35:GLU:OE1	2.44	0.66
4:4:93:ILE:O	4:4:95:PHE:N	2.27	0.66
5:A:173:VAL:HG23	5:A:174:PHE:HD1	1.61	0.66
5:A:42:ARG:C	5:A:44:ILE:H	1.98	0.66
5:A:660:GLN:O	5:A:661:ALA:CB	2.42	0.66
20:A:851:CLA:H11	6:B:616:LEU:CG	2.23	0.66
6:B:141:PHE:HA	6:B:144:PHE:CD1	2.31	0.66
6:B:414:HIS:O	6:B:414:HIS:CG	2.49	0.66
20:B:814:CLA:CHD	20:B:814:CLA:CBC	2.74	0.66
6:B:81:PRO:HG2	6:B:360:PHE:CD1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:530:THR:HG22	20:B:823:CLA:HMC1	1.76	0.66
5:A:458:PHE:CD2	20:B:850:CLA:CMB	2.78	0.66
8:D:44:GLU:CB	8:D:46:TYR:HE2	2.04	0.66
10:F:80:TRP:HZ3	20:F:205:CLA:CMC	2.08	0.66
20:A:830:CLA:C15	22:L:210:BCR:C36	2.74	0.66
16:L:99:LEU:HD11	22:L:210:BCR:HC7	1.76	0.66
17:N:45:ASN:HD21	17:N:54:LYS:HB2	1.51	0.66
17:N:81:VAL:O	17:N:83:TRP:N	2.29	0.66
21:2:319:LMU:O2B	21:2:319:LMU:H4'	1.94	0.66
4:4:69:ILE:O	4:4:71:ASN:N	2.29	0.66
5:A:123:VAL:HG22	5:A:133:ASN:OD1	1.94	0.66
5:A:129:GLN:O	5:A:130:GLU:HB2	1.95	0.66
5:A:229:ILE:CG1	5:A:243:PRO:HB3	2.25	0.66
5:A:578:ARG:O	5:A:579:PHE:CD1	2.49	0.66
20:B:811:CLA:HMC1	20:B:811:CLA:CBC	2.22	0.66
20:B:804:CLA:HBC3	20:B:827:CLA:H51	1.77	0.66
13:I:14:LEU:O	13:I:17:PRO:HD2	1.95	0.66
5:A:269:PHE:HE1	15:K:14:THR:CG2	2.09	0.66
12:H:44:ALA:HB2	16:L:145:PHE:CE1	2.29	0.66
20:1:215:CLA:HAA2	20:1:215:CLA:HBD	1.76	0.66
1:1:27:LEU:HD21	6:B:314:ARG:HD3	1.75	0.66
5:A:432:LEU:HA	5:A:435:VAL:HG13	1.78	0.66
20:A:819:CLA:HMC1	20:A:819:CLA:CBC	2.24	0.66
20:A:820:CLA:H2A	20:A:820:CLA:O1D	1.95	0.66
5:A:711:HIS:CG	20:A:837:CLA:HBC1	2.30	0.66
21:A:854:LMU:H112	21:A:854:LMU:H71	1.78	0.66
20:A:851:CLA:HED1	20:B:849:CLA:H61	1.77	0.66
11:G:23:PHE:CD2	11:G:24:PHE:HB2	2.31	0.66
21:H:104:LMU:C4	21:H:104:LMU:C8	2.65	0.66
20:J:101:CLA:H2	20:J:101:CLA:HMA2	1.76	0.66
21:K:105:LMU:O6'	21:K:105:LMU:H32	1.91	0.66
17:N:82:PHE:O	17:N:84:LYS:N	2.29	0.66
2:2:171:MET:SD	2:2:172:LEU:HA	2.36	0.66
4:4:86:SER:O	4:4:88:SER:N	2.29	0.66
5:A:255:LEU:CD1	5:A:280:PHE:HZ	2.09	0.66
5:A:539:PHE:HD2	5:A:539:PHE:O	1.78	0.66
6:B:349:ALA:CB	6:B:375:HIS:HB3	2.26	0.66
20:B:808:CLA:HAA1	20:B:808:CLA:H12	1.76	0.66
6:B:510:LEU:HD21	20:B:835:CLA:HHD	1.77	0.66
7:C:74:THR:O	7:C:76:SER:N	2.29	0.66
8:D:39:LYS:NZ	8:D:43:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:89:GLU:O	9:E:90:VAL:HB	1.96	0.66
10:F:131:PHE:HE1	19:W:2:FRU:HO3	1.37	0.66
11:G:60:SER:HG	11:G:63:PRO:HB2	1.58	0.66
21:H:104:LMU:H52	21:H:104:LMU:C1	2.22	0.66
14:J:2:ARG:NH1	14:J:8:LEU:HD13	2.04	0.66
20:K:108:CLA:C3A	20:K:108:CLA:CGA	2.73	0.66
20:K:108:CLA:C3A	20:K:108:CLA:O1A	2.32	0.66
16:L:10:VAL:O	16:L:10:VAL:CG2	2.44	0.66
16:L:64:LEU:HD22	16:L:91:LEU:HD22	1.78	0.66
17:N:62:SER:HB3	17:N:66:ASP:OD1	1.89	0.66
19:U:2:FRU:H11	19:U:2:FRU:O6	1.91	0.66
20:1:215:CLA:HAA2	20:1:215:CLA:CGD	2.26	0.66
2:2:103:GLY:CA	20:2:311:CLA:CBB	2.72	0.66
4:4:145:PRO:O	4:4:147:LEU:N	2.29	0.66
5:A:606:TYR:O	5:A:610:SER:CB	2.43	0.66
20:A:804:CLA:HHD	20:A:804:CLA:HBC3	1.76	0.66
20:A:832:CLA:O1A	20:A:833:CLA:HBC3	1.96	0.66
6:B:124:TRP:O	6:B:124:TRP:CD1	2.48	0.66
6:B:247:THR:HG23	6:B:250:ALA:HB3	1.77	0.66
21:B:801:LMU:C6'	21:B:801:LMU:H1B	2.26	0.66
10:F:22:LEU:O	10:F:25:LEU:N	2.29	0.66
11:G:93:TYR:N	11:G:94:ASP:OD1	2.28	0.66
20:B:808:CLA:H91	22:I:101:BCR:H361	1.76	0.66
20:K:102:CLA:O1A	20:K:102:CLA:H2A	1.95	0.66
16:L:69:VAL:HG11	16:L:84:GLY:N	2.10	0.66
17:N:61:LEU:O	17:N:62:SER:HB2	1.93	0.66
2:2:42:ARG:CB	2:2:45:VAL:HG21	2.24	0.66
2:2:93:THR:O	2:2:97:VAL:HG22	1.95	0.66
4:4:144:ALA:C	4:4:145:PRO:O	2.29	0.66
4:4:151:GLU:C	4:4:154:ILE:N	2.38	0.66
20:4:318:CLA:HED1	20:4:318:CLA:C1	2.11	0.66
5:A:636:HIS:O	5:A:638:THR:N	2.29	0.66
5:A:58:HIS:HB3	20:A:804:CLA:HBC1	1.77	0.66
20:A:820:CLA:HBC3	20:A:822:CLA:HED1	1.77	0.66
20:A:824:CLA:C4B	22:A:846:BCR:C37	2.66	0.66
6:B:203:ARG:H	6:B:270:LEU:HD11	1.61	0.66
5:A:128:GLY:HA3	6:B:446:PHE:CD2	2.31	0.66
20:B:824:CLA:H71	22:B:845:BCR:H14C	1.77	0.66
20:B:824:CLA:HED1	20:B:832:CLA:HBB1	1.76	0.66
20:B:827:CLA:CBC	20:B:827:CLA:CMC	2.56	0.66
21:D:201:LMU:H32	21:E:101:LMU:H121	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:24:PHE:CE1	11:G:27:GLN:O	2.49	0.66
17:N:49:CYS:C	17:N:51:ASP:O	2.34	0.66
1:1:57:ILE:O	1:1:59:VAL:N	2.28	0.66
2:2:106:GLU:O	20:2:311:CLA:HMA3	1.95	0.66
20:2:322:CLA:HBA2	20:2:322:CLA:C4A	2.25	0.66
2:2:43:TRP:O	2:2:44:ASN:C	2.30	0.66
4:4:150:LYS:CG	4:4:150:LYS:O	2.41	0.66
5:A:101:ALA:O	5:A:104:SER:HA	1.96	0.66
6:B:55:ALA:HB1	6:B:150:LEU:CD1	2.26	0.66
7:C:74:THR:O	7:C:75:ARG:C	2.30	0.66
8:D:101:TYR:CD1	8:D:114:PRO:HD3	2.31	0.66
10:F:22:LEU:O	10:F:24:LYS:N	2.29	0.66
11:G:13:GLY:O	11:G:16:LEU:CB	2.44	0.66
11:G:28:ARG:HH21	11:G:29:GLU:H	1.44	0.66
17:N:70:GLU:HB3	17:N:72:LYS:CA	2.26	0.66
20:R:107:CLA:O1A	20:R:107:CLA:H2A	1.94	0.66
4:4:101:VAL:O	4:4:104:ARG:CZ	2.45	0.65
4:4:71:ASN:O	4:4:73:PRO:N	2.28	0.65
5:A:23:ASP:OD2	5:A:24:ARG:N	2.29	0.65
5:A:23:ASP:OD1	5:A:24:ARG:NE	2.29	0.65
5:A:25:ASP:O	5:A:26:PRO:C	2.29	0.65
5:A:353:SER:HB2	5:A:356:ALA:HB3	1.78	0.65
5:A:625:TRP:HB2	5:A:637:ILE:HD11	1.78	0.65
5:A:645:SER:HB3	6:B:637:PRO:HG3	1.77	0.65
20:A:819:CLA:H8	22:A:846:BCR:H19C	1.76	0.65
6:B:292:ARG:HH22	6:B:297:ILE:HG13	1.60	0.65
6:B:538:ALA:O	6:B:540:ASP:N	2.29	0.65
6:B:73:ASN:HB3	6:B:76:ALA:HB3	1.76	0.65
20:B:851:CLA:HED3	20:B:851:CLA:CBA	2.27	0.65
21:E:101:LMU:H61	21:E:101:LMU:C1	2.25	0.65
10:F:21:ALA:O	10:F:23:LYS:N	2.29	0.65
21:H:108:LMU:H92	21:H:108:LMU:C4	2.18	0.65
22:I:103:BCR:H403	22:I:103:BCR:C27	2.20	0.65
13:I:12:VAL:CG2	20:I:102:CLA:O1A	2.42	0.65
14:J:10:VAL:HG13	14:J:11:ALA:H	1.59	0.65
21:K:106:LMU:O5'	21:K:106:LMU:C2	2.30	0.65
17:N:58:VAL:O	17:N:60:PHE:N	2.29	0.65
18:R:36:UNK:O	18:R:38:UNK:N	2.29	0.65
2:2:143:PHE:HD1	2:2:144:ASP:N	1.95	0.65
20:2:302:CLA:NA	20:2:302:CLA:O1A	2.29	0.65
4:4:52:MET:HE1	4:4:156:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:36:ASN:C	4:4:39:TRP:CD2	2.69	0.65
4:4:69:ILE:CG1	4:4:175:LYS:HB2	2.26	0.65
4:4:91:PHE:CG	4:4:92:VAL:N	2.60	0.65
5:A:664:VAL:CG2	5:A:665:ILE:HG23	2.26	0.65
6:B:366:THR:HG23	6:B:729:THR:HG22	1.78	0.65
6:B:708:VAL:O	6:B:710:LEU:O	2.15	0.65
7:C:7:ILE:HG22	7:C:65:VAL:HG21	1.76	0.65
20:H:101:CLA:C6	20:H:101:CLA:CMA	2.69	0.65
14:J:2:ARG:HH12	14:J:8:LEU:CD1	2.04	0.65
16:L:63:LEU:CD2	16:L:64:LEU:H	2.08	0.65
17:N:54:LYS:O	17:N:57:LYS:N	2.29	0.65
17:N:69:CYS:O	17:N:72:LYS:CE	2.44	0.65
3:3:52:LYS:O	3:3:56:TYR:CG	2.50	0.65
3:3:93:PHE:HD2	3:3:95:THR:H	1.41	0.65
4:4:92:VAL:HG12	4:4:93:ILE:H	1.60	0.65
5:A:187:HIS:CD2	20:A:811:CLA:C4C	2.79	0.65
5:A:22:VAL:N	5:A:23:ASP:O	2.30	0.65
5:A:390:ALA:HB1	5:A:754:ILE:HD13	1.79	0.65
5:A:362:LEU:CB	5:A:410:ALA:HB2	2.26	0.65
7:C:79:LEU:CD2	7:C:81:TYR:C	2.65	0.65
15:K:59:ASP:OD1	15:K:59:ASP:C	2.34	0.65
16:L:128:ASP:OD2	16:L:129:GLN:N	2.28	0.65
17:N:80:ASN:OD1	17:N:82:PHE:N	2.30	0.65
2:2:41:LEU:O	2:2:42:ARG:NE	2.28	0.65
3:3:163:PHE:C	3:3:163:PHE:HD1	1.99	0.65
4:4:58:MET:SD	4:4:59:LEU:HA	2.36	0.65
5:A:697:ARG:HD3	6:B:566:GLY:O	1.97	0.65
20:A:808:CLA:HMC3	20:A:809:CLA:HHD	1.76	0.65
5:A:370:ILE:HD13	20:A:824:CLA:CAD	2.26	0.65
20:A:827:CLA:CHD	22:A:844:BCR:H333	2.27	0.65
20:A:824:CLA:C3B	22:A:846:BCR:H373	2.27	0.65
6:B:388:ALA:O	6:B:391:PRO:HD2	1.95	0.65
7:C:1:MET:CG	7:C:4:SER:HG	2.02	0.65
8:D:102:ARG:HE	8:D:110:GLN:CB	2.08	0.65
9:E:65:VAL:HG13	9:E:82:TYR:O	1.96	0.65
10:F:147:GLY:HA2	10:F:150:VAL:HB	1.79	0.65
11:G:16:LEU:HA	11:G:68:ILE:HG13	1.77	0.65
17:N:24:THR:O	17:N:26:GLY:N	2.29	0.65
19:Q:2:FRU:H4	19:Q:2:FRU:O1	1.95	0.65
20:1:210:CLA:OBD	20:1:210:CLA:HMD1	1.95	0.65
21:1:219:LMU:C3'	21:1:219:LMU:O6B	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:59:VAL:CG1	1:1:60:PRO:HD2	2.26	0.65
5:A:109:TRP:HA	5:A:116:ILE:HG13	1.78	0.65
5:A:328:LYS:O	5:A:330:ILE:N	2.30	0.65
5:A:732:ALA:HB1	20:A:838:CLA:HED2	1.79	0.65
20:A:819:CLA:HMD1	20:A:820:CLA:HHD	1.79	0.65
6:B:171:ALA:O	6:B:172:GLU:HB2	1.97	0.65
6:B:663:PHE:O	6:B:664:LEU:CB	2.34	0.65
10:F:123:VAL:HB	10:F:126:ALA:O	1.97	0.65
10:F:151:ASP:C	10:F:154:PHE:HB3	2.16	0.65
11:G:83:TYR:CG	11:G:83:TYR:O	2.48	0.65
15:K:27:ALA:HB3	15:K:28:PRO:CD	2.25	0.65
16:L:13:PRO:HG2	16:L:18:PRO:HB3	1.77	0.65
18:R:38:UNK:C	18:R:39:UNK:O	2.43	0.65
2:2:205:PHE:HD1	2:2:206:ALA:H	0.67	0.65
2:2:42:ARG:O	2:2:44:ASN:N	2.29	0.65
3:3:107:TRP:CD1	3:3:108:ALA:HA	2.32	0.65
4:4:30:LEU:HD13	21:4:317:LMU:C12	2.25	0.65
20:A:851:CLA:H152	20:A:851:CLA:H91	1.77	0.65
6:B:119:GLY:O	6:B:121:TYR:N	2.29	0.65
6:B:324:ASP:O	6:B:328:ASN:HB2	1.96	0.65
6:B:646:TRP:CH2	6:B:726:ILE:HG21	2.32	0.65
7:C:1:MET:N	7:C:4:SER:CB	2.60	0.65
10:F:62:LEU:CG	10:F:72:ILE:HD13	2.25	0.65
11:G:16:LEU:HD23	11:G:68:ILE:HG21	1.79	0.65
21:K:106:LMU:C9	21:K:106:LMU:C4	2.67	0.65
15:K:20:PHE:HD2	15:K:21:ALA:CA	2.08	0.65
1:1:161:PHE:N	20:1:203:CLA:HBB2	2.12	0.65
20:1:215:CLA:HED3	20:1:215:CLA:C4A	2.26	0.65
21:1:219:LMU:O5B	21:1:219:LMU:H3'	1.78	0.65
2:2:161:THR:HB	2:2:165:LYS:HD2	1.79	0.65
2:2:43:TRP:O	2:2:45:VAL:N	2.29	0.65
2:2:81:THR:O	2:2:83:GLY:N	2.30	0.65
20:3:307:CLA:HHC	20:3:311:CLA:H11	1.79	0.65
4:4:88:SER:C	4:4:89:THR:HG22	2.17	0.65
5:A:362:LEU:HD11	20:A:828:CLA:HBB2	1.78	0.65
5:A:618:TRP:CH2	5:A:655:ASP:HB2	2.32	0.65
5:A:679:PHE:CE2	5:A:683:HIS:HD2	2.14	0.65
20:A:815:CLA:CBB	22:A:843:BCR:H352	2.27	0.65
6:B:247:THR:C	6:B:250:ALA:HB2	2.16	0.65
6:B:62:SER:OG	6:B:63:GLY:N	2.29	0.65
9:E:40:ARG:HB2	9:E:42:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:203:BCR:H333	20:F:205:CLA:HMA1	1.78	0.65
10:F:42:ILE:C	10:F:43:LYS:HE3	2.17	0.65
12:H:63:SER:O	12:H:67:TYR:CB	2.45	0.65
14:J:10:VAL:HG13	14:J:11:ALA:N	2.12	0.65
14:J:4:PHE:O	14:J:5:LYS:HB2	1.95	0.65
16:L:40:LEU:HB3	16:L:41:PRO:CD	2.27	0.65
2:2:110:TRP:CA	2:2:113:ILE:HG23	2.25	0.65
2:2:203:THR:HG23	2:2:204:ILE:N	2.12	0.65
20:2:303:CLA:CHD	20:2:303:CLA:HBC2	2.22	0.65
4:4:136:GLY:O	4:4:137:ILE:HB	1.96	0.65
5:A:393:LEU:HD11	5:A:750:PHE:CD1	2.31	0.65
5:A:705:GLU:HA	5:A:708:VAL:HB	1.79	0.65
20:A:832:CLA:CAD	20:A:833:CLA:HAC1	2.26	0.65
20:B:803:CLA:CBC	22:F:202:BCR:H332	2.27	0.65
20:B:805:CLA:H121	20:B:811:CLA:OBD	1.95	0.65
20:B:823:CLA:HBB1	20:B:837:CLA:HHB	1.79	0.65
20:B:830:CLA:HBB2	22:F:202:BCR:C26	2.26	0.65
1:1:59:VAL:HG12	1:1:60:PRO:C	2.18	0.65
2:2:120:ASN:N	2:2:120:ASN:OD1	2.28	0.65
21:2:317:LMU:C5'	21:2:317:LMU:O5B	2.42	0.65
20:3:302:CLA:HMC3	20:A:814:CLA:CBA	2.25	0.65
3:3:114:PHE:CD1	20:3:309:CLA:CHA	2.80	0.65
5:A:197:GLN:NE2	5:A:351:THR:HB	2.11	0.65
5:A:514:THR:HB	5:A:532:ILE:HG23	1.79	0.65
5:A:691:MET:CE	23:A:842:PQN:C2M	2.74	0.65
20:A:801:CLA:CAA	20:A:801:CLA:O1D	2.45	0.65
20:A:824:CLA:C6	20:A:825:CLA:HED2	2.25	0.65
6:B:317:ARG:NE	6:B:317:ARG:CA	2.55	0.65
6:B:556:SER:C	6:B:558:PRO:CD	2.61	0.65
6:B:607:SER:HA	6:B:610:ASN:ND2	2.12	0.65
6:B:625:TRP:HE3	6:B:626:LEU:N	1.94	0.65
7:C:55:GLU:C	7:C:57:ALA:N	2.50	0.65
7:C:7:ILE:C	7:C:8:TYR:O	2.35	0.65
11:G:47:GLY:N	11:G:48:ASP:OD1	2.30	0.65
21:K:105:LMU:H71	21:K:105:LMU:C1	2.25	0.65
1:1:185:TRP:O	1:1:186:HIS:ND1	2.30	0.65
2:2:97:VAL:HG23	2:2:98:GLU:H	1.62	0.65
4:4:101:VAL:O	4:4:104:ARG:NH2	2.30	0.65
4:4:121:PHE:CD1	4:4:128:ALA:HB3	2.32	0.65
5:A:402:ILE:HD11	20:A:827:CLA:HBB2	1.78	0.65
6:B:131:THR:CB	6:B:134:ASP:HB2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:190:TRP:HE3	20:B:812:CLA:CBB	2.09	0.65
6:B:20:ARG:HH11	6:B:20:ARG:HB3	1.61	0.65
6:B:527:LEU:HD13	6:B:586:THR:HG21	1.78	0.65
6:B:188:LEU:HD11	20:B:813:CLA:HBB2	1.79	0.65
6:B:493:TRP:HH2	20:B:833:CLA:HMA2	1.61	0.65
11:G:28:ARG:NH2	11:G:29:GLU:H	1.94	0.65
11:G:60:SER:CA	11:G:63:PRO:HD2	2.26	0.65
21:K:105:LMU:C3	21:K:105:LMU:O5'	2.45	0.65
17:N:65:LEU:HD23	17:N:66:ASP:N	2.11	0.65
1:1:140:LEU:H	1:1:140:LEU:HD23	1.63	0.64
2:2:54:TRP:HZ2	2:2:109:ARG:HB3	1.62	0.64
2:2:55:ALA:CB	2:2:56:MET:HE1	2.24	0.64
4:4:101:VAL:CG1	4:4:104:ARG:HH22	2.07	0.64
4:4:93:ILE:O	4:4:96:ILE:N	2.29	0.64
5:A:361:ASN:HD22	5:A:362:LEU:N	1.95	0.64
5:A:40:PHE:CE1	5:A:53:TRP:CD1	2.75	0.64
20:A:804:CLA:HBB2	20:A:806:CLA:C4D	2.26	0.64
5:A:281:LEU:HD11	20:A:816:CLA:HED2	1.79	0.64
20:A:835:CLA:C19	20:L:202:CLA:HBB1	2.27	0.64
6:B:224:PRO:HA	6:B:227:THR:OG1	1.97	0.64
6:B:432:HIS:CE1	20:B:830:CLA:NB	2.62	0.64
6:B:666:SER:O	6:B:667:TRP:HB2	1.96	0.64
20:B:824:CLA:C7	20:B:824:CLA:H41	2.27	0.64
6:B:438:VAL:CG2	20:B:831:CLA:HAC1	2.27	0.64
10:F:12:LYS:HG2	10:F:13:GLN:H	1.59	0.64
16:L:36:TYR:O	16:L:37:LEU:HB3	1.95	0.64
17:N:54:LYS:O	17:N:56:LYS:N	2.29	0.64
2:2:42:ARG:CG	2:2:45:VAL:CB	2.70	0.64
4:4:192:THR:HG21	4:4:195:GLN:HA	1.79	0.64
4:4:103:ILE:HG13	20:4:303:CLA:HMD1	1.78	0.64
5:A:382:TYR:CE2	20:A:827:CLA:HED3	2.32	0.64
6:B:175:LEU:O	6:B:179:LEU:HG	1.97	0.64
6:B:545:LYS:HD3	6:B:546:LEU:H	1.61	0.64
6:B:558:PRO:HG2	6:B:703:VAL:CB	2.21	0.64
6:B:174:ARG:HH11	20:B:822:CLA:HMD1	1.61	0.64
11:G:33:LYS:NZ	11:G:33:LYS:HA	2.12	0.64
20:H:101:CLA:CMC	20:H:101:CLA:HBC2	2.13	0.64
2:2:45:VAL:O	2:2:45:VAL:HG13	1.97	0.64
3:3:74:ALA:N	20:3:307:CLA:C2D	2.60	0.64
20:4:319:CLA:CMC	20:4:319:CLA:CBC	2.73	0.64
4:4:40:PHE:CA	4:4:43:ALA:HB2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:819:CLA:CHD	20:B:819:CLA:CBC	2.64	0.64
6:B:451:LYS:HD2	20:B:831:CLA:O2D	1.98	0.64
8:D:93:LYS:CB	8:D:93:LYS:NZ	2.60	0.64
9:E:44:TYR:HB3	9:E:45:TRP:CE3	2.32	0.64
11:G:48:ASP:N	11:G:48:ASP:OD1	2.29	0.64
21:H:107:LMU:H1B	21:H:107:LMU:O3'	1.97	0.64
12:H:14:ILE:O	12:H:16:ASN:N	2.29	0.64
3:3:198:PHE:HA	3:3:201:ALA:CB	2.18	0.64
4:4:121:PHE:HB2	4:4:128:ALA:HB3	1.79	0.64
4:4:158:ARG:CA	4:4:161:LEU:HD12	2.22	0.64
4:4:44:GLU:O	4:4:46:VAL:N	2.30	0.64
5:A:216:LEU:HD12	22:A:843:BCR:C35	2.27	0.64
5:A:281:LEU:O	5:A:283:PHE:N	2.29	0.64
5:A:53:TRP:HA	5:A:56:ASN:CB	2.27	0.64
20:A:814:CLA:CHC	22:A:843:BCR:C18	2.75	0.64
21:A:853:LMU:C3'	21:A:853:LMU:C2B	2.75	0.64
6:B:387:PHE:O	6:B:391:PRO:HD3	1.97	0.64
8:D:79:ARG:O	8:D:82:GLN:HB2	1.97	0.64
12:H:16:ASN:HD22	12:H:19:GLY:HA2	1.63	0.64
20:J:103:CLA:H152	20:J:103:CLA:O1A	1.97	0.64
20:K:101:CLA:OBD	20:K:108:CLA:CHB	2.46	0.64
20:A:829:CLA:HMB2	20:L:202:CLA:C1D	2.27	0.64
20:1:202:CLA:HED2	20:1:202:CLA:H2	1.78	0.64
20:3:310:CLA:C2A	20:3:318:CLA:CBC	2.76	0.64
20:4:304:CLA:O2D	20:4:304:CLA:HAA1	1.96	0.64
4:4:39:TRP:CA	4:4:40:PHE:HD1	2.09	0.64
4:4:58:MET:SD	4:4:59:LEU:CA	2.85	0.64
20:A:815:CLA:CMC	20:A:815:CLA:HBC2	2.24	0.64
5:A:368:LEU:CD1	20:A:825:CLA:C6	2.76	0.64
20:A:824:CLA:H43	20:A:835:CLA:HBA1	1.80	0.64
6:B:42:LEU:O	6:B:43:TYR:C	2.35	0.64
6:B:67:HIS:O	6:B:68:VAL:HG23	1.97	0.64
20:B:836:CLA:HHB	20:B:837:CLA:OBD	1.97	0.64
20:B:823:CLA:HMB3	22:B:845:BCR:H351	1.78	0.64
8:D:118:VAL:CG1	8:D:119:TYR:N	2.60	0.64
8:D:113:HIS:CD2	8:D:118:VAL:HG21	2.32	0.64
10:F:151:ASP:O	10:F:154:PHE:CB	2.40	0.64
12:H:75:ASP:CG	12:H:77:LEU:HG	2.18	0.64
15:K:52:PRO:O	15:K:56:THR:CG2	2.45	0.64
12:H:50:ARG:HG2	16:L:137:ALA:HB1	1.78	0.64
16:L:30:SER:HG	16:L:32:LEU:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:68:GLY:O	4:4:71:ASN:CB	2.29	0.64
5:A:340:GLY:O	5:A:343:HIS:CB	2.43	0.64
5:A:514:THR:HB	5:A:532:ILE:CG2	2.28	0.64
20:A:822:CLA:NC	22:A:845:BCR:H17C	2.12	0.64
6:B:142:LEU:HD21	22:B:844:BCR:H333	1.77	0.64
20:B:850:CLA:CBB	20:B:851:CLA:CHB	2.73	0.64
8:D:32:SER:H	16:L:23:LEU:HG	1.61	0.64
9:E:35:LYS:CE	9:E:89:GLU:OE2	2.46	0.64
10:F:100:VAL:CA	10:F:103:SER:OG	2.44	0.64
21:F:201:LMU:H6E	21:F:201:LMU:O5B	1.95	0.64
12:H:69:SER:OG	20:H:109:CLA:H2	1.97	0.64
17:N:39:SER:OG	17:N:40:CYS:N	2.30	0.64
17:N:41:LYS:HB2	17:N:42:PHE:CA	2.26	0.64
1:1:161:PHE:CD1	20:1:203:CLA:HBB1	2.33	0.64
1:1:64:GLY:HA3	1:1:66:GLY:O	1.97	0.64
5:A:401:TRP:O	5:A:405:PHE:HB2	1.98	0.64
5:A:544:ILE:O	5:A:548:THR:OG1	2.09	0.64
20:A:838:CLA:NC	20:A:838:CLA:C4	2.61	0.64
6:B:211:ASN:HB2	6:B:214:ASP:HB3	1.79	0.64
6:B:37:ILE:HD12	6:B:37:ILE:O	1.97	0.64
6:B:49:SER:O	6:B:52:GLY:N	2.31	0.64
23:B:841:PQN:H162	22:B:846:BCR:H332	1.63	0.64
20:A:851:CLA:HED1	20:B:849:CLA:H2	1.79	0.64
22:B:846:BCR:C35	20:B:851:CLA:H111	2.27	0.64
9:E:45:TRP:CZ3	9:E:78:SER:OG	2.51	0.64
10:F:11:SER:OG	10:F:14:PHE:HB3	1.97	0.64
10:F:62:LEU:CD2	10:F:72:ILE:HD13	2.27	0.64
12:H:45:ALA:HB3	12:H:46:PRO:HD3	1.78	0.64
15:K:51:ASP:C	15:K:51:ASP:OD1	2.35	0.64
17:N:5:GLU:OE2	17:N:6:TYR:HB2	1.97	0.64
17:N:80:ASN:C	17:N:82:PHE:H	2.00	0.64
17:N:83:TRP:O	17:N:83:TRP:HE3	1.80	0.64
2:2:124:ILE:CB	2:2:129:LYS:HB3	2.27	0.64
4:4:128:ALA:HB3	4:4:143:PHE:HE2	1.61	0.64
4:4:163:PHE:O	4:4:167:ILE:N	2.28	0.64
5:A:418:MET:O	5:A:564:ARG:HD2	1.98	0.64
20:A:803:CLA:HBA2	20:A:803:CLA:O1D	1.97	0.64
20:A:832:CLA:HMC1	20:A:832:CLA:HBC3	1.80	0.64
6:B:282:PHE:O	6:B:286:ILE:HG13	1.97	0.64
6:B:334:LEU:O	6:B:334:LEU:CG	2.46	0.64
20:B:810:CLA:H61	20:B:810:CLA:H11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:839:CLA:HED1	25:B:848:LMG:C21	2.28	0.64
7:C:59:PRO:HB3	7:C:61:ASP:OD1	1.98	0.64
9:E:36:VAL:C	9:E:49:VAL:HG13	2.18	0.64
11:G:37:GLU:OE2	11:G:42:SER:N	2.31	0.64
16:L:48:ASN:HB3	16:L:49:PRO:CD	2.27	0.64
2:2:74:LEU:O	2:2:75:ASN:ND2	2.29	0.64
4:4:154:ILE:O	4:4:157:GLY:HA3	1.97	0.64
5:A:66:SER:O	5:A:67:HIS:HB2	1.98	0.64
5:A:370:ILE:CD1	20:A:824:CLA:O1D	2.44	0.64
5:A:691:MET:HE3	23:A:842:PQN:C2M	2.27	0.64
5:A:657:LEU:HD23	20:A:850:CLA:C1D	2.28	0.64
6:B:103:ALA:O	6:B:104:PHE:CB	2.34	0.64
6:B:475:ASP:CA	6:B:480:SER:HA	2.27	0.64
6:B:535:VAL:HG13	6:B:536:LYS:N	2.13	0.64
6:B:608:GLN:O	6:B:612:SER:HB3	1.97	0.64
20:B:811:CLA:C4	20:B:816:CLA:CBC	2.75	0.64
10:F:147:GLY:C	10:F:150:VAL:HB	2.18	0.64
11:G:68:ILE:O	11:G:72:LEU:HB2	1.96	0.64
17:N:11:LYS:HG2	17:N:12:THR:N	2.13	0.64
17:N:63:ASP:CA	17:N:64:ASP:O	2.41	0.64
19:T:1:GLC:C5	19:T:2:FRU:C1	2.75	0.64
3:3:163:PHE:CD1	3:3:163:PHE:C	2.72	0.64
5:A:113:PRO:C	5:A:115:HIS:H	2.01	0.64
5:A:281:LEU:HG	5:A:282:THR:H	1.62	0.64
5:A:558:LYS:HZ2	6:B:674:LEU:CB	2.11	0.64
5:A:744:ALA:CB	22:A:847:BCR:C39	2.36	0.64
5:A:733:VAL:HG11	20:A:838:CLA:C2D	2.28	0.64
6:B:494:LEU:HD12	20:B:833:CLA:HED1	1.80	0.64
6:B:555:TYR:CD2	6:B:573:TRP:HB2	2.32	0.64
20:B:803:CLA:HMD3	22:F:202:BCR:C4	2.13	0.64
8:D:31:GLY:HA2	16:L:13:PRO:HB3	1.80	0.64
8:D:90:LEU:O	8:D:90:LEU:HD13	1.98	0.64
10:F:153:ASN:ND2	10:F:153:ASN:C	2.48	0.64
20:J:103:CLA:C16	20:J:103:CLA:O2A	2.45	0.64
20:3:308:CLA:HAC2	20:K:103:CLA:C9	2.28	0.64
17:N:80:ASN:O	17:N:82:PHE:N	2.28	0.64
17:N:81:VAL:O	17:N:82:PHE:C	2.37	0.64
20:2:303:CLA:H42	20:2:303:CLA:C4C	2.28	0.63
20:2:307:CLA:O1D	20:2:307:CLA:HBA2	1.96	0.63
4:4:69:ILE:CD1	4:4:175:LYS:CD	2.75	0.63
5:A:132:LEU:HD11	5:A:674:ALA:CB	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:366:THR:HG23	6:B:729:THR:CG2	2.28	0.63
6:B:475:ASP:HA	6:B:480:SER:HA	1.78	0.63
8:D:36:LEU:HD12	8:D:78:ALA:H	1.62	0.63
10:F:125:LEU:O	10:F:126:ALA:HB2	1.98	0.63
11:G:28:ARG:HG3	11:G:29:GLU:CG	2.28	0.63
16:L:128:ASP:CG	16:L:129:GLN:H	2.01	0.63
17:N:57:LYS:HG3	17:N:58:VAL:H	0.61	0.63
2:2:40:SER:O	2:2:41:LEU:CB	2.47	0.63
3:3:106:TYR:HB3	3:3:107:TRP:CD1	2.32	0.63
3:3:181:LEU:HD12	3:3:182:LYS:HE2	1.79	0.63
4:4:91:PHE:CE2	20:4:312:CLA:C3C	2.81	0.63
5:A:492:ILE:HA	5:A:495:THR:HG23	1.78	0.63
5:A:612:VAL:O	5:A:615:HIS:HB3	1.98	0.63
5:A:377:TYR:CD1	5:A:616:PHE:HE1	2.16	0.63
5:A:346:LEU:HD11	20:A:822:CLA:CHD	2.28	0.63
6:B:77:TRP:CZ2	6:B:122:GLN:NE2	2.67	0.63
6:B:530:THR:CG2	20:B:823:CLA:HMC1	2.29	0.63
6:B:334:LEU:CA	20:B:805:CLA:HMD3	2.29	0.63
20:B:810:CLA:HMC1	22:B:843:BCR:H373	1.79	0.63
10:F:130:LEU:CD1	10:F:131:PHE:HD1	2.12	0.63
10:F:22:LEU:O	10:F:25:LEU:HD12	1.97	0.63
21:H:106:LMU:H12	21:H:106:LMU:H2O2	1.60	0.63
13:I:22:ALA:O	13:I:23:SER:C	2.35	0.63
17:N:59:PRO:C	17:N:66:ASP:OD1	2.37	0.63
17:N:77:CYS:O	17:N:79:SER:N	2.30	0.63
20:2:307:CLA:HBD	20:2:307:CLA:CBA	2.28	0.63
21:2:317:LMU:C2'	21:2:317:LMU:C2	2.77	0.63
4:4:123:GLN:HG2	4:4:124:TYR:N	2.13	0.63
5:A:114:THR:CG2	5:A:115:HIS:ND1	2.59	0.63
5:A:207:LEU:O	5:A:310:PHE:CB	2.46	0.63
5:A:302:HIS:HB2	20:A:817:CLA:C1B	2.28	0.63
5:A:360:ILE:O	5:A:361:ASN:CB	2.45	0.63
5:A:434:ARG:O	5:A:437:ARG:HB2	1.99	0.63
5:A:187:HIS:CE1	20:A:811:CLA:C1A	2.71	0.63
20:A:815:CLA:CGA	20:A:815:CLA:C1A	2.66	0.63
21:A:853:LMU:C1B	21:A:853:LMU:O3'	2.47	0.63
6:B:17:THR:HA	6:B:696:LYS:H	1.63	0.63
6:B:269:TRP:HD1	6:B:497:TRP:CH2	2.17	0.63
6:B:92:TRP:O	6:B:92:TRP:CD1	2.51	0.63
11:G:42:SER:OG	11:G:43:HIS:C	2.37	0.63
11:G:7:VAL:HG23	11:G:8:ILE:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:101:CLA:H2	20:J:101:CLA:CMA	2.28	0.63
16:L:99:LEU:O	16:L:102:TYR:N	2.29	0.63
17:N:66:ASP:N	17:N:66:ASP:OD2	2.29	0.63
20:1:207:CLA:H43	20:1:207:CLA:CGA	2.28	0.63
4:4:97:LEU:O	4:4:99:HIS:N	2.32	0.63
5:A:530:LEU:HB2	5:A:531:PRO:HD2	1.81	0.63
20:A:814:CLA:HED2	20:A:814:CLA:H2A	1.81	0.63
20:A:830:CLA:C14	20:A:830:CLA:H101	2.29	0.63
6:B:203:ARG:HG2	6:B:204:GLY:H	1.63	0.63
6:B:216:LEU:O	6:B:218:TYR:N	2.31	0.63
6:B:577:TYR:HE2	6:B:578:LEU:HD12	1.64	0.63
6:B:732:LYS:CG	6:B:733:PHE:O	2.41	0.63
20:B:810:CLA:CMC	22:B:843:BCR:H373	2.27	0.63
20:L:201:CLA:O2A	20:L:201:CLA:HED1	1.98	0.63
22:I:103:BCR:C39	22:L:210:BCR:H401	2.28	0.63
21:N:101:LMU:C6'	21:N:101:LMU:H32	2.29	0.63
19:P:1:GLC:HO2	19:P:2:FRU:C1	2.10	0.63
2:2:103:GLY:O	2:2:104:TRP:C	2.36	0.63
2:2:98:GLU:CG	2:2:99:LEU:HD12	2.27	0.63
4:4:194:VAL:HG12	4:4:195:GLN:N	2.07	0.63
5:A:229:ILE:HG12	5:A:243:PRO:HB3	1.81	0.63
5:A:284:ARG:HH12	5:A:507:ALA:HB1	1.63	0.63
5:A:520:LEU:O	5:A:522:ALA:N	2.27	0.63
20:A:818:CLA:H93	20:A:818:CLA:H193	1.79	0.63
20:A:824:CLA:HBB2	20:A:836:CLA:CMA	2.29	0.63
6:B:447:GLY:O	6:B:449:PRO:HD3	1.98	0.63
6:B:79:GLN:O	6:B:80:ASP:HB3	1.96	0.63
20:B:828:CLA:HMB2	20:B:829:CLA:CHB	2.28	0.63
22:B:846:BCR:C17	20:B:850:CLA:H101	2.22	0.63
6:B:551:LYS:CE	8:D:143:PRO:HA	2.28	0.63
8:D:46:TYR:HE1	8:D:80:LYS:CE	2.11	0.63
20:H:101:CLA:CMA	20:H:101:CLA:C2	2.76	0.63
20:J:101:CLA:CBC	20:J:101:CLA:HMC1	2.25	0.63
20:L:201:CLA:HAA1	20:L:201:CLA:CED	2.27	0.63
17:N:41:LYS:CB	17:N:42:PHE:CB	2.56	0.63
17:N:72:LYS:HD2	17:N:72:LYS:N	2.07	0.63
17:N:72:LYS:CB	17:N:73:ASP:C	2.56	0.63
20:1:206:CLA:HBC3	20:1:206:CLA:HHD	1.76	0.63
3:3:50:GLU:N	3:3:51:PRO:HD3	2.13	0.63
4:4:52:MET:HE3	4:4:156:ASN:CB	2.28	0.63
5:A:174:PHE:O	5:A:175:ALA:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:210:LEU:HD12	20:A:813:CLA:CMB	2.27	0.63
5:A:308:ILE:CG2	5:A:309:LEU:N	2.61	0.63
5:A:425:THR:OG1	5:A:428:TYR:HE1	1.73	0.63
5:A:224:HIS:CE1	20:A:815:CLA:C4C	2.82	0.63
6:B:224:PRO:CB	6:B:227:THR:HB	2.28	0.63
20:B:807:CLA:HMC1	22:B:846:BCR:H282	1.80	0.63
7:C:62:PHE:CE2	8:D:137:ILE:HB	2.33	0.63
20:B:836:CLA:C12	22:F:203:BCR:C31	2.76	0.63
17:N:29:PHE:CE1	17:N:32:ALA:HB3	2.33	0.63
1:1:179:THR:HG21	4:4:87:SER:C	2.19	0.63
4:4:76:TYR:O	4:4:77:ALA:HB3	1.96	0.63
5:A:664:VAL:HG23	5:A:665:ILE:HG23	1.80	0.63
5:A:690:LEU:CD2	6:B:661:PHE:HE1	2.12	0.63
5:A:701:GLN:O	5:A:704:ILE:N	2.32	0.63
20:A:826:CLA:H102	22:A:847:BCR:C37	2.29	0.63
5:A:87:SER:OG	5:A:179:LEU:HB2	1.98	0.63
6:B:247:THR:HG23	6:B:250:ALA:CB	2.28	0.63
6:B:655:LEU:HD21	20:B:839:CLA:HBB1	1.81	0.63
6:B:715:VAL:HG23	6:B:719:PHE:HD2	1.62	0.63
20:B:824:CLA:H8	22:B:845:BCR:H14C	1.80	0.63
10:F:20:GLN:CD	10:F:20:GLN:C	2.54	0.63
21:H:108:LMU:O1'	21:H:108:LMU:C4	2.30	0.63
20:J:103:CLA:CGA	20:J:103:CLA:C16	2.77	0.63
8:D:31:GLY:HA3	16:L:23:LEU:HD21	1.80	0.63
17:N:34:THR:C	17:N:36:GLU:H	2.01	0.63
20:1:202:CLA:CED	20:1:202:CLA:C2	2.62	0.63
20:1:215:CLA:HED3	20:1:215:CLA:C3A	2.29	0.63
2:2:63:PHE:HD2	2:2:172:LEU:HD21	1.63	0.63
4:4:70:ILE:CG1	4:4:71:ASN:N	2.62	0.63
5:A:249:ILE:C	5:A:251:ASN:H	2.01	0.63
5:A:254:LEU:C	5:A:256:ALA:H	2.02	0.63
5:A:472:ARG:N	5:A:473:PRO:HD2	2.12	0.63
5:A:508:THR:O	5:A:509:ALA:CB	2.47	0.63
5:A:439:ARG:NH1	5:A:565:SER:O	2.32	0.63
5:A:599:PHE:CD2	5:A:735:VAL:HG21	2.34	0.63
5:A:304:LEU:CD2	20:A:816:CLA:HBB2	2.24	0.63
20:A:824:CLA:HMA3	20:A:825:CLA:O1A	1.98	0.63
5:A:705:GLU:HB3	6:B:545:LYS:NZ	2.14	0.63
7:C:28:MET:HG2	7:C:38:GLN:HE21	1.64	0.63
7:C:77:MET:O	7:C:79:LEU:N	2.29	0.63
20:F:205:CLA:HBC2	20:F:205:CLA:CHD	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:92:GLY:O	11:G:93:TYR:C	2.36	0.63
11:G:93:TYR:CA	11:G:94:ASP:CG	2.59	0.63
21:H:105:LMU:C2'	21:H:105:LMU:C6'	2.63	0.63
13:I:11:LEU:HD11	22:I:103:BCR:C10	2.29	0.63
16:L:122:GLY:O	16:L:124:LYS:N	2.32	0.63
21:R:102:LMU:H92	21:R:102:LMU:C5	2.18	0.63
20:R:107:CLA:NA	20:R:107:CLA:HED3	2.12	0.63
2:2:72:GLY:O	2:2:74:LEU:N	2.28	0.63
4:4:40:PHE:HB3	4:4:43:ALA:HB3	1.70	0.63
4:4:99:HIS:O	4:4:99:HIS:ND1	2.30	0.63
5:A:27:ILE:HG23	5:A:28:LYS:HG3	1.81	0.63
5:A:455:PHE:HD1	20:A:830:CLA:CMA	2.12	0.63
5:A:707:ILE:C	5:A:711:HIS:CD2	2.73	0.63
20:A:824:CLA:C3B	22:A:846:BCR:C22	2.77	0.63
5:A:691:MET:O	23:A:842:PQN:O1	2.17	0.63
22:A:847:BCR:H353	20:A:851:CLA:H41	1.81	0.63
20:B:826:CLA:H142	22:B:844:BCR:C10	2.24	0.63
20:B:823:CLA:H52	20:B:837:CLA:CBD	2.28	0.63
7:C:12:ILE:CB	7:C:39:ILE:HA	2.29	0.63
13:I:8:PHE:CE1	20:I:102:CLA:H43	2.33	0.63
17:N:62:SER:CA	17:N:66:ASP:H	2.12	0.63
4:4:93:ILE:CG2	4:4:94:GLU:N	2.61	0.62
5:A:201:SER:O	5:A:204:ASN:HB2	1.99	0.62
5:A:665:ILE:HD12	5:A:665:ILE:C	2.19	0.62
5:A:711:HIS:HB3	5:A:717:ALA:CB	2.29	0.62
20:A:815:CLA:NA	20:A:815:CLA:CGA	2.62	0.62
6:B:378:ILE:HG22	6:B:379:ALA:H	1.63	0.62
6:B:464:GLN:HA	6:B:467:HIS:HB2	1.80	0.62
6:B:670:TYR:C	6:B:670:TYR:CD1	2.72	0.62
22:B:844:BCR:HC8	22:B:844:BCR:H331	1.79	0.62
22:B:852:BCR:C38	22:B:852:BCR:C23	2.76	0.62
22:B:852:BCR:HC8	20:L:208:CLA:CHC	2.28	0.62
9:E:61:THR:HG22	9:E:62:ARG:N	2.11	0.62
10:F:80:TRP:HB3	20:F:206:CLA:HHC	1.81	0.62
13:I:26:LEU:HD13	13:I:30:LYS:HB3	1.80	0.62
17:N:54:LYS:CB	17:N:57:LYS:HE2	2.12	0.62
5:A:109:TRP:CH2	5:A:154:ARG:HD3	2.34	0.62
5:A:210:LEU:HD13	20:A:813:CLA:CMB	2.23	0.62
5:A:281:LEU:O	5:A:282:THR:C	2.36	0.62
5:A:426:THR:HA	5:A:428:TYR:CZ	2.34	0.62
20:A:808:CLA:H142	22:J:102:BCR:H14C	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:822:CLA:C1B	22:A:845:BCR:C15	2.77	0.62
6:B:392:ILE:HD13	20:B:827:CLA:CED	2.30	0.62
6:B:704:GLN:O	6:B:708:VAL:HG23	1.99	0.62
20:B:815:CLA:CBD	20:B:824:CLA:CBB	2.77	0.62
7:C:60:THR:HG23	7:C:63:LEU:O	1.99	0.62
8:D:48:ILE:CB	8:D:100:PHE:HB3	2.28	0.62
21:L:205:LMU:H11	21:L:205:LMU:O2'	1.98	0.62
4:4:106:TRP:CE3	20:4:314:CLA:CMA	2.82	0.62
4:4:62:GLU:O	4:4:65:THR:HG22	1.99	0.62
4:4:89:THR:N	4:4:90:LEU:CD2	2.52	0.62
5:A:360:ILE:HD13	22:A:845:BCR:H371	1.79	0.62
5:A:398:HIS:CD2	20:A:826:CLA:ND	2.67	0.62
5:A:412:ALA:HA	5:A:598:VAL:HG21	1.80	0.62
5:A:604:TRP:O	5:A:607:ASN:N	2.27	0.62
5:A:406:LEU:HD11	20:A:806:CLA:HMB3	1.80	0.62
6:B:120:VAL:CA	6:B:123:TRP:HD1	2.08	0.62
6:B:221:GLY:C	6:B:223:GLY:H	2.03	0.62
6:B:493:TRP:NE1	20:B:814:CLA:HAC2	2.13	0.62
6:B:545:LYS:CG	6:B:546:LEU:N	2.61	0.62
6:B:689:ASN:OD1	6:B:689:ASN:N	2.31	0.62
6:B:732:LYS:CD	6:B:734:GLY:N	2.60	0.62
20:B:807:CLA:CMC	22:B:846:BCR:C28	2.76	0.62
7:C:73:THR:C	7:C:76:SER:OG	2.37	0.62
15:K:53:ALA:HA	15:K:56:THR:HG23	1.80	0.62
1:1:57:ILE:CG1	1:1:57:ILE:O	2.44	0.62
2:2:42:ARG:HA	2:2:45:VAL:HG23	0.72	0.62
5:A:224:HIS:HE1	20:A:815:CLA:CHD	2.11	0.62
5:A:697:ARG:C	5:A:699:TYR:H	2.02	0.62
20:A:809:CLA:H51	22:J:102:BCR:H10C	1.82	0.62
20:A:809:CLA:HBA2	20:A:809:CLA:HBD	1.80	0.62
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.80	0.62
6:B:53:GLN:C	6:B:55:ALA:N	2.53	0.62
5:A:555:ILE:HG23	20:B:851:CLA:OBD	1.99	0.62
21:F:201:LMU:H11	21:F:201:LMU:H92	1.80	0.62
10:F:22:LEU:CA	10:F:25:LEU:HD13	2.29	0.62
21:H:106:LMU:C1B	21:H:106:LMU:H32	2.25	0.62
12:H:41:GLU:OE2	12:H:42:THR:OG1	2.15	0.62
20:H:109:CLA:HBB2	13:I:13:GLY:C	2.18	0.62
13:I:24:LEU:C	13:I:26:LEU:N	2.51	0.62
20:J:103:CLA:C16	20:J:103:CLA:C2	2.75	0.62
18:R:31:UNK:C	18:R:32:UNK:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:59:ILE:O	3:3:63:ARG:HG3	1.99	0.62
20:4:304:CLA:CGD	20:4:304:CLA:H2A	2.18	0.62
5:A:158:ILE:CG2	20:A:814:CLA:HED3	2.30	0.62
5:A:330:ILE:O	5:A:330:ILE:HG22	1.99	0.62
5:A:348:GLU:O	5:A:350:LEU:N	2.33	0.62
5:A:401:TRP:HD1	20:A:826:CLA:CHC	2.12	0.62
5:A:79:PHE:HE2	5:A:185:HIS:CG	2.17	0.62
20:A:825:CLA:HMC1	20:A:825:CLA:HBC3	1.76	0.62
20:A:826:CLA:H72	22:A:847:BCR:C37	2.20	0.62
6:B:467:HIS:NE2	20:B:832:CLA:C1A	2.63	0.62
5:A:702:GLU:HA	6:B:545:LYS:HE2	1.81	0.62
20:B:824:CLA:C7	22:B:845:BCR:H14C	2.30	0.62
8:D:37:LEU:O	8:D:39:LYS:N	2.32	0.62
8:D:78:ALA:O	8:D:79:ARG:NH1	2.33	0.62
6:B:25:ILE:CB	22:L:210:BCR:H292	2.28	0.62
1:1:28:GLY:O	20:1:211:CLA:C3C	2.47	0.62
4:4:145:PRO:O	4:4:146:THR:C	2.31	0.62
4:4:69:ILE:HD11	4:4:175:LYS:CD	2.21	0.62
4:4:73:PRO:O	4:4:74:LYS:HB2	1.99	0.62
5:A:122:VAL:HA	5:A:133:ASN:HD21	1.65	0.62
5:A:553:VAL:O	5:A:557:LEU:N	2.29	0.62
5:A:553:VAL:HG22	22:A:846:BCR:H401	1.81	0.62
21:A:854:LMU:H31	21:A:854:LMU:H1'	1.81	0.62
6:B:284:PHE:O	6:B:288:GLY:N	2.28	0.62
6:B:40:GLY:HA2	6:B:165:VAL:HG23	1.80	0.62
6:B:456:GLU:HG2	10:F:70:HIS:HB3	1.80	0.62
6:B:661:PHE:HB3	20:B:851:CLA:HBC3	1.81	0.62
20:B:806:CLA:HBB2	20:B:826:CLA:HHC	1.79	0.62
20:B:814:CLA:HBA1	20:B:814:CLA:HED2	1.81	0.62
6:B:289:LEU:HD22	22:B:842:BCR:H352	1.80	0.62
8:D:94:TYR:O	8:D:95:LYS:CB	2.48	0.62
10:F:103:SER:C	10:F:105:LEU:N	2.53	0.62
12:H:21:TRP:N	12:H:22:ASP:CB	2.61	0.62
16:L:64:LEU:HA	16:L:67:PRO:HG3	1.80	0.62
17:N:4:GLU:CD	17:N:5:GLU:HB2	2.20	0.62
17:N:58:VAL:C	17:N:60:PHE:H	2.03	0.62
2:2:168:ARG:HH11	2:2:168:ARG:HG2	1.64	0.62
2:2:44:ASN:ND2	14:J:1:MET:CB	2.62	0.62
2:2:56:MET:O	2:2:57:LEU:C	2.36	0.62
2:2:72:GLY:C	2:2:74:LEU:H	2.03	0.62
5:A:308:ILE:HG22	5:A:309:LEU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:399:HIS:O	5:A:400:MET:HB2	1.97	0.62
5:A:669:GLY:N	6:B:445:ALA:HA	2.15	0.62
20:A:807:CLA:HBA1	20:A:807:CLA:NA	2.05	0.62
20:A:804:CLA:HBA2	20:A:811:CLA:H62	1.82	0.62
6:B:527:LEU:HB3	20:B:823:CLA:C4C	2.29	0.62
20:B:823:CLA:H11	20:B:837:CLA:CBD	2.29	0.62
6:B:697:PRO:CB	20:B:838:CLA:HBC3	2.30	0.62
8:D:87:GLY:N	8:D:90:LEU:HB3	2.15	0.62
10:F:40:LEU:HA	10:F:42:ILE:CG1	2.26	0.62
17:N:66:ASP:C	17:N:67:LEU:CG	2.68	0.62
1:1:57:ILE:C	1:1:59:VAL:N	2.51	0.62
2:2:54:TRP:CZ2	2:2:109:ARG:CG	2.82	0.62
4:4:74:LYS:H	4:4:75:TRP:CB	2.13	0.62
5:A:558:LYS:NZ	6:B:674:LEU:HD23	2.15	0.62
5:A:40:PHE:CZ	5:A:56:ASN:HB3	2.35	0.62
20:A:812:CLA:C3D	20:A:813:CLA:HMC3	2.30	0.62
20:A:838:CLA:H161	22:A:847:BCR:HC22	1.82	0.62
20:B:815:CLA:HBD	20:B:824:CLA:HBB2	1.80	0.62
10:F:151:ASP:HA	10:F:154:PHE:HB3	1.80	0.62
21:G:101:LMU:H5'	21:G:101:LMU:O2'	2.00	0.62
12:H:14:ILE:O	12:H:14:ILE:HD13	1.99	0.62
20:2:322:CLA:CED	20:J:101:CLA:HMA3	2.27	0.62
20:J:101:CLA:CGA	20:J:101:CLA:O1D	2.47	0.62
16:L:30:SER:O	16:L:32:LEU:N	2.33	0.62
20:1:201:CLA:HBC3	20:1:201:CLA:HMC1	0.70	0.62
3:3:173:GLU:HG2	3:3:174:LYS:N	2.08	0.62
6:B:213:LEU:HD12	6:B:214:ASP:N	2.15	0.62
6:B:216:LEU:HD21	6:B:221:GLY:CA	2.30	0.62
6:B:560:ASP:CG	6:B:561:GLY:N	2.53	0.62
6:B:622:ASP:HA	6:B:626:LEU:HB3	1.82	0.62
6:B:715:VAL:O	6:B:719:PHE:N	2.32	0.62
6:B:190:TRP:HE3	20:B:812:CLA:HBB2	1.64	0.62
20:A:850:CLA:CAA	20:B:849:CLA:HBB2	2.27	0.62
10:F:84:ILE:O	10:F:87:GLY:N	2.26	0.62
12:H:57:LEU:O	12:H:57:LEU:HD13	1.99	0.62
20:A:826:CLA:C18	22:J:102:BCR:H17C	2.29	0.62
15:K:27:ALA:CB	15:K:28:PRO:CD	2.78	0.62
16:L:158:MET:SD	16:L:159:TYR:N	2.69	0.62
2:2:196:HIS:HE1	19:O:1:GLC:O3	1.78	0.62
2:2:187:GLY:O	2:2:189:ILE:HG12	2.00	0.62
3:3:181:LEU:HD13	3:3:181:LEU:N	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:194:ILE:HG13	20:3:304:CLA:C2C	2.30	0.62
5:A:302:HIS:HE1	20:A:818:CLA:CHB	2.13	0.62
5:A:448:TRP:CD1	20:A:830:CLA:HED2	2.35	0.62
5:A:711:HIS:NE2	20:A:837:CLA:HBC1	2.11	0.62
6:B:91:ILE:HD11	6:B:104:PHE:CD2	2.34	0.62
6:B:31:PHE:HB2	6:B:42:LEU:CD1	2.28	0.62
6:B:347:LEU:CD2	6:B:351:HIS:HE1	2.11	0.62
6:B:439:HIS:CD2	6:B:453:ILE:HG22	2.35	0.62
6:B:664:LEU:C	6:B:667:TRP:CZ3	2.70	0.62
20:B:803:CLA:HBB1	10:F:101:GLY:HA3	1.81	0.62
6:B:334:LEU:CB	20:B:805:CLA:HMD3	2.29	0.62
20:B:807:CLA:H142	20:B:807:CLA:C10	2.29	0.62
6:B:462:TRP:HZ3	20:B:832:CLA:CBC	2.12	0.62
9:E:73:ASN:C	9:E:73:ASN:HD22	2.04	0.62
12:H:25:GLY:CA	12:H:27:ASP:HB2	2.28	0.62
12:H:26:SER:C	12:H:27:ASP:O	2.34	0.62
20:J:101:CLA:CGD	20:J:101:CLA:HBA2	2.29	0.62
16:L:30:SER:C	16:L:32:LEU:H	2.03	0.62
17:N:67:LEU:HB2	17:N:68:GLU:HB3	1.82	0.62
1:1:44:LEU:HD22	1:1:154:ALA:HB3	1.80	0.61
2:2:166:ASN:OD1	2:2:169:LEU:HD12	2.00	0.61
3:3:62:GLY:HA2	3:3:65:ALA:HB3	1.82	0.61
3:3:83:LEU:C	20:3:302:CLA:H43	2.20	0.61
4:4:129:GLY:C	4:4:131:VAL:H	2.02	0.61
5:A:27:ILE:C	5:A:27:ILE:HD13	2.19	0.61
5:A:445:HIS:O	5:A:446:LEU:HB2	1.99	0.61
5:A:578:ARG:HA	5:A:595:TRP:HB2	1.80	0.61
20:A:818:CLA:C20	20:A:825:CLA:H3A	2.30	0.61
20:A:826:CLA:H171	22:J:102:BCR:H351	1.81	0.61
6:B:633:ASN:ND2	6:B:636:THR:CB	2.63	0.61
20:B:836:CLA:CGA	20:B:836:CLA:C1A	2.78	0.61
6:B:654:HIS:HE1	20:B:849:CLA:NB	1.96	0.61
7:C:44:ARG:NH2	8:D:127:ARG:CB	2.60	0.61
8:D:118:VAL:HG12	8:D:119:TYR:N	2.15	0.61
20:L:208:CLA:HBC3	20:L:208:CLA:CMC	2.30	0.61
3:3:52:LYS:CA	3:3:55:ALA:HB3	2.30	0.61
4:4:194:VAL:N	4:4:195:GLN:O	2.29	0.61
5:A:307:ALA:O	5:A:308:ILE:C	2.39	0.61
20:A:830:CLA:HAA1	22:B:852:BCR:C13	2.30	0.61
20:A:851:CLA:CED	20:B:849:CLA:H2	2.30	0.61
6:B:458:ILE:HG23	20:B:836:CLA:CMD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:82:PHE:O	6:B:84:VAL:N	2.33	0.61
9:E:32:ARG:HH22	9:E:53:VAL:HA	1.64	0.61
21:R:109:LMU:H1'	21:R:109:LMU:H6'	1.65	0.61
2:2:208:PHE:CG	2:2:209:THR:N	2.68	0.61
5:A:662:SER:HA	5:A:665:ILE:HD11	1.81	0.61
5:A:451:ILE:HD11	20:A:830:CLA:HED1	1.81	0.61
6:B:166:SER:O	6:B:168:PHE:N	2.33	0.61
6:B:196:HIS:CE1	20:B:813:CLA:ND	2.68	0.61
21:B:802:LMU:H3O2	21:B:802:LMU:C1B	2.13	0.61
20:B:824:CLA:C10	22:B:845:BCR:H14C	2.30	0.61
18:R:41:UNK:CA	18:R:42:UNK:CB	2.76	0.61
1:1:161:PHE:CD1	20:1:203:CLA:CBB	2.84	0.61
20:2:305:CLA:H2	20:2:308:CLA:HMD3	1.81	0.61
3:3:194:ILE:HD11	20:3:304:CLA:CMC	2.16	0.61
4:4:147:LEU:HD22	4:4:148:GLU:CB	2.29	0.61
4:4:118:ASP:HB2	20:4:306:CLA:HMB3	1.82	0.61
4:4:99:HIS:HD1	4:4:99:HIS:C	2.03	0.61
5:A:143:ILE:HD12	5:A:144:GLN:H	1.66	0.61
5:A:308:ILE:HG13	20:A:816:CLA:CBB	2.29	0.61
5:A:472:ARG:O	5:A:474:GLN:CG	2.47	0.61
20:A:838:CLA:H101	20:A:852:CLA:H152	1.81	0.61
6:B:658:ALA:O	6:B:661:PHE:HD2	1.84	0.61
6:B:692:ARG:NH2	6:B:694:ARG:HG2	2.15	0.61
6:B:592:PHE:HA	6:B:721:TYR:OH	2.01	0.61
20:B:821:CLA:CMC	20:B:821:CLA:HBC2	2.30	0.61
20:B:823:CLA:CMB	22:B:845:BCR:C35	2.76	0.61
10:F:10:GLU:OE1	10:F:11:SER:N	2.33	0.61
10:F:17:ARG:HA	10:F:17:ARG:NE	2.14	0.61
4:4:104:ARG:HA	4:4:107:GLN:HB2	1.83	0.61
4:4:40:PHE:CA	4:4:43:ALA:CB	2.79	0.61
5:A:261:SER:O	5:A:262:PHE:CD2	2.54	0.61
5:A:337:PRO:CD	20:A:840:CLA:HHC	2.31	0.61
6:B:98:GLN:C	6:B:100:ALA:N	2.53	0.61
6:B:433:THR:O	6:B:436:LEU:O	2.17	0.61
20:B:829:CLA:HBC2	20:B:829:CLA:CHD	2.20	0.61
20:B:839:CLA:H191	13:I:21:MET:HB2	1.83	0.61
20:H:101:CLA:CED	20:H:101:CLA:CAD	2.75	0.61
21:H:108:LMU:H101	21:H:108:LMU:H32	1.39	0.61
4:4:143:PHE:CB	4:4:150:LYS:HE2	2.29	0.61
5:A:105:ASN:HB2	5:A:140:PHE:HZ	1.66	0.61
5:A:308:ILE:HG21	20:A:816:CLA:HMC2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:582:ASP:HB3	5:A:589:THR:HG22	1.81	0.61
5:A:207:LEU:HB3	20:A:819:CLA:HBB2	1.83	0.61
5:A:711:HIS:NE2	20:A:837:CLA:CBC	2.62	0.61
6:B:127:ILE:HG12	6:B:193:HIS:HE1	1.65	0.61
7:C:1:MET:H2	7:C:3:HIS:H	1.42	0.61
8:D:102:ARG:NH2	8:D:109:VAL:O	2.33	0.61
11:G:37:GLU:OE2	11:G:42:SER:CA	2.49	0.61
15:K:17:LEU:HG	15:K:56:THR:CB	2.30	0.61
17:N:57:LYS:O	17:N:60:PHE:N	2.33	0.61
18:R:35:UNK:C	18:R:38:UNK:CB	2.79	0.61
2:2:187:GLY:O	2:2:188:PRO:C	2.38	0.61
4:4:37:LEU:O	4:4:39:TRP:CG	2.53	0.61
20:A:815:CLA:HBB1	22:A:843:BCR:C13	2.31	0.61
20:A:838:CLA:NC	20:A:838:CLA:H43	2.15	0.61
6:B:310:PRO:HB2	6:B:311:PRO:CD	2.31	0.61
6:B:371:LEU:HD21	20:B:826:CLA:HED3	1.82	0.61
6:B:668:ARG:HG3	6:B:700:LEU:O	2.00	0.61
20:B:839:CLA:HMC3	20:B:851:CLA:HMB3	1.83	0.61
21:B:847:LMU:H5'	21:B:847:LMU:O5B	2.01	0.61
10:F:90:PHE:HA	22:F:202:BCR:C39	2.31	0.61
14:J:2:ARG:HB3	14:J:7:TYR:CZ	2.36	0.61
17:N:1:GLY:C	17:N:2:VAL:HG13	2.21	0.61
17:N:65:LEU:HD21	17:N:66:ASP:O	2.00	0.61
2:2:159:LEU:O	2:2:160:ARG:C	2.39	0.61
4:4:194:VAL:CG1	4:4:195:GLN:HB3	2.30	0.61
5:A:170:GLY:C	5:A:173:VAL:HG22	2.20	0.61
5:A:358:LEU:HD21	5:A:413:HIS:ND1	2.15	0.61
20:A:841:CLA:H61	20:A:841:CLA:H112	1.81	0.61
6:B:212:PHE:CZ	20:B:812:CLA:HAC1	2.35	0.61
20:B:815:CLA:HBD	20:B:824:CLA:CBB	2.30	0.61
20:B:830:CLA:H71	22:F:203:BCR:H402	1.83	0.61
10:F:20:GLN:O	10:F:21:ALA:HB2	2.01	0.61
22:I:103:BCR:H382	22:I:103:BCR:C40	2.31	0.61
21:K:106:LMU:H3'	21:K:106:LMU:H31	1.81	0.61
17:N:39:SER:O	17:N:40:CYS:CB	2.48	0.61
2:2:79:TRP:CD1	2:2:81:THR:CG2	2.84	0.61
5:A:229:ILE:CG2	5:A:229:ILE:O	2.48	0.61
5:A:281:LEU:HD22	20:A:816:CLA:HMA3	1.83	0.61
5:A:527:VAL:CG1	5:A:528:ALA:N	2.64	0.61
20:A:824:CLA:HAA2	20:A:825:CLA:CAD	2.31	0.61
20:A:824:CLA:HMA1	22:A:846:BCR:H16C	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:84:GLY:O	5:A:87:SER:O	2.18	0.61
6:B:124:TRP:C	6:B:124:TRP:CD1	2.73	0.61
6:B:130:ARG:CG	6:B:130:ARG:HH11	2.13	0.61
6:B:143:LEU:C	6:B:145:LEU:H	2.03	0.61
6:B:623:TYR:O	6:B:624:LEU:HB2	1.99	0.61
6:B:290:MET:HG3	20:B:819:CLA:C2C	2.31	0.61
8:D:84:LEU:HD12	8:D:100:PHE:HZ	1.65	0.61
9:E:73:ASN:ND2	9:E:75:ALA:H	1.99	0.61
6:B:456:GLU:OE1	10:F:70:HIS:ND1	2.33	0.61
14:J:20:GLY:O	14:J:21:SER:HB2	2.01	0.61
17:N:5:GLU:CD	17:N:6:TYR:CD2	2.74	0.61
17:N:73:ASP:N	17:N:73:ASP:OD1	2.32	0.61
17:N:72:LYS:HZ3	17:N:74:LYS:CG	2.02	0.61
18:R:4:UNK:O	18:R:5:UNK:CB	2.49	0.61
2:2:85:GLN:OE1	2:2:86:GLU:N	2.34	0.61
2:2:98:GLU:OE2	20:2:312:CLA:ND	2.33	0.61
2:2:37:ASP:OD2	3:3:41:ASP:CB	2.49	0.61
4:4:94:GLU:HG2	4:4:95:PHE:CG	2.35	0.61
5:A:249:ILE:CG1	5:A:250:LEU:N	2.49	0.61
5:A:581:CYS:CB	5:A:590:CYS:O	2.49	0.61
5:A:389:TYR:HE1	5:A:625:TRP:CD1	2.19	0.61
6:B:459:PHE:O	6:B:463:ILE:HD13	2.01	0.61
5:A:705:GLU:HG2	6:B:545:LYS:HZ2	1.66	0.61
6:B:707:LEU:HD12	6:B:711:VAL:HG21	1.81	0.61
6:B:289:LEU:HD21	20:B:818:CLA:NA	2.16	0.61
7:C:28:MET:HB3	8:D:122:LYS:O	2.00	0.61
8:D:46:TYR:CD2	8:D:46:TYR:N	2.69	0.61
6:B:231:ASN:OD1	11:G:5:SER:HB2	2.01	0.61
16:L:33:ILE:HG12	20:L:202:CLA:C4	2.30	0.61
1:1:183:ASP:OD1	4:4:89:THR:HB	2.01	0.60
2:2:128:ASN:ND2	14:J:4:PHE:H	1.97	0.60
3:3:106:TYR:CD1	3:3:107:TRP:N	2.68	0.60
20:4:302:CLA:CHD	20:4:302:CLA:HBC3	2.24	0.60
5:A:123:VAL:O	5:A:124:TRP:HB2	2.01	0.60
5:A:394:SER:HB2	20:A:826:CLA:CMA	2.20	0.60
5:A:39:HIS:O	5:A:40:PHE:HB3	2.01	0.60
6:B:534:LEU:HD21	6:B:579:ALA:CB	2.31	0.60
8:D:117:GLY:O	8:D:118:VAL:CG2	2.39	0.60
6:B:295:PHE:HE2	11:G:38:GLN:NE2	1.99	0.60
12:H:39:PHE:O	12:H:40:PHE:CD1	2.54	0.60
13:I:2:ILE:HG12	13:I:3:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:826:CLA:C17	22:J:102:BCR:H17C	2.30	0.60
20:K:102:CLA:CBC	20:K:102:CLA:HMC1	2.20	0.60
16:L:46:ALA:HB2	16:L:52:ARG:NH2	2.16	0.60
1:1:32:VAL:HG21	20:1:211:CLA:ND	2.16	0.60
2:2:128:ASN:CG	2:2:130:LEU:HB2	2.21	0.60
4:4:70:ILE:O	4:4:73:PRO:HD2	2.00	0.60
5:A:360:ILE:O	5:A:361:ASN:HB3	2.01	0.60
5:A:446:LEU:CD1	5:A:554:LEU:HA	2.30	0.60
6:B:275:HIS:HD1	20:B:815:CLA:HMB1	1.64	0.60
6:B:555:TYR:O	6:B:571:SER:HB2	2.01	0.60
6:B:632:ILE:C	6:B:634:GLY:H	2.04	0.60
20:B:821:CLA:C1	20:B:821:CLA:HAA1	2.31	0.60
20:B:826:CLA:C14	22:B:844:BCR:H10C	2.25	0.60
7:C:74:THR:C	7:C:76:SER:H	2.01	0.60
9:E:39:LEU:H	9:E:40:ARG:CZ	2.14	0.60
9:E:37:LYS:HB2	9:E:49:VAL:HG22	1.81	0.60
16:L:161:LEU:CD1	16:L:162:ASP:HA	2.16	0.60
1:1:185:TRP:HE3	1:1:185:TRP:CA	2.12	0.60
2:2:37:ASP:CG	2:2:38:PRO:HD3	2.21	0.60
2:2:68:LEU:O	2:2:70:LYS:N	2.35	0.60
3:3:64:TYR:CB	20:3:311:CLA:C4	2.73	0.60
20:A:822:CLA:HBC1	22:A:845:BCR:C39	2.31	0.60
21:A:854:LMU:H32	21:A:854:LMU:H92	1.77	0.60
6:B:348:VAL:HG12	6:B:349:ALA:N	2.16	0.60
11:G:71:VAL:O	11:G:73:ALA:O	2.19	0.60
20:J:101:CLA:O1D	20:J:101:CLA:C1	2.47	0.60
15:K:51:ASP:OD1	15:K:55:PHE:CD1	2.54	0.60
20:A:829:CLA:HMB2	20:L:202:CLA:C2D	2.30	0.60
1:1:160:GLY:CA	20:1:203:CLA:HBB2	2.31	0.60
3:3:181:LEU:N	3:3:182:LYS:CD	2.64	0.60
4:4:107:GLN:O	20:4:302:CLA:HMA3	1.82	0.60
4:4:36:ASN:O	4:4:38:ARG:NH1	2.35	0.60
5:A:154:ARG:NH2	5:A:233:LEU:HD13	2.16	0.60
5:A:346:LEU:O	5:A:347:TYR:HB2	2.02	0.60
5:A:466:THR:HG22	20:B:808:CLA:HHC	1.82	0.60
20:A:824:CLA:H61	20:A:825:CLA:HED2	1.83	0.60
21:A:855:LMU:H91	21:A:855:LMU:H21	0.65	0.60
6:B:500:ALA:HB2	6:B:508:LEU:HD22	1.83	0.60
23:A:842:PQN:H251	20:B:803:CLA:HMC1	1.81	0.60
16:L:124:LYS:C	16:L:126:GLN:N	2.54	0.60
18:R:39:UNK:CB	18:R:40:UNK:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:GLY:HA2	20:2:311:CLA:CBB	2.32	0.60
2:2:73:ILE:HD13	2:2:75:ASN:HA	1.82	0.60
22:3:314:BCR:C23	22:3:314:BCR:C39	2.37	0.60
5:A:295:TRP:HB2	5:A:298:ASP:OD2	2.01	0.60
20:A:824:CLA:CAA	20:A:824:CLA:HED2	2.31	0.60
6:B:392:ILE:HG12	6:B:555:TYR:CD1	2.36	0.60
6:B:493:TRP:CB	20:B:833:CLA:HED2	2.31	0.60
6:B:559:CYS:HB2	6:B:702:ILE:HD12	1.82	0.60
20:B:807:CLA:H102	20:B:807:CLA:C14	2.30	0.60
9:E:48:ASN:ND2	9:E:71:LYS:HZ2	1.99	0.60
10:F:151:ASP:OD2	10:F:154:PHE:CD1	2.54	0.60
13:I:10:PRO:O	13:I:15:LEU:N	2.34	0.60
20:A:826:CLA:H172	22:J:102:BCR:C17	2.31	0.60
15:K:17:LEU:HD23	15:K:21:ALA:HB2	1.84	0.60
20:A:809:CLA:HMC1	20:A:809:CLA:HBC3	1.82	0.60
20:A:822:CLA:NC	22:A:845:BCR:C19	2.56	0.60
5:A:452:PHE:CD1	20:A:835:CLA:HBB2	2.36	0.60
6:B:488:ALA:HB1	20:B:834:CLA:C1C	2.32	0.60
6:B:569:ASP:HB3	6:B:574:ASP:HB3	1.84	0.60
6:B:646:TRP:O	6:B:649:MET:HB2	2.01	0.60
6:B:212:PHE:HZ	20:B:812:CLA:HAC1	1.67	0.60
7:C:62:PHE:CE1	9:E:42:GLU:HB2	2.37	0.60
8:D:79:ARG:H	8:D:82:GLN:NE2	2.00	0.60
8:D:86:LEU:C	8:D:90:LEU:HB3	2.22	0.60
9:E:72:VAL:O	9:E:73:ASN:CB	2.39	0.60
11:G:34:GLN:O	11:G:35:VAL:C	2.39	0.60
11:G:42:SER:OG	11:G:44:PHE:N	2.35	0.60
11:G:45:GLU:O	11:G:46:ALA:CB	2.49	0.60
21:H:108:LMU:H6'2	21:H:108:LMU:O3'	2.00	0.60
16:L:33:ILE:CD1	16:L:36:TYR:HD1	2.14	0.60
22:3:314:BCR:H321	22:3:314:BCR:HC8	1.84	0.60
4:4:128:ALA:O	4:4:130:GLU:HG2	2.02	0.60
5:A:389:TYR:CE1	5:A:625:TRP:CD1	2.89	0.60
6:B:194:LEU:O	6:B:198:ALA:HB3	2.01	0.60
6:B:551:LYS:CG	6:B:552:ASP:H	2.14	0.60
6:B:593:TYR:O	6:B:596:TRP:O	2.18	0.60
6:B:661:PHE:CB	20:B:851:CLA:HMC1	2.31	0.60
20:B:836:CLA:C12	22:F:203:BCR:H312	2.32	0.60
16:L:9:GLN:C	16:L:11:ILE:H	2.04	0.60
2:2:124:ILE:HG22	2:2:129:LYS:HB3	1.83	0.60
2:2:203:THR:O	2:2:204:ILE:CB	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:209:THR:HG23	2:2:209:THR:O	2.02	0.60
20:2:322:CLA:HMB3	20:J:103:CLA:H141	1.83	0.60
4:4:109:ILE:HG22	4:4:120:ILE:HG23	1.84	0.60
4:4:94:GLU:CB	4:4:95:PHE:HE1	1.89	0.60
5:A:131:ILE:CG2	5:A:132:LEU:N	2.65	0.60
20:A:832:CLA:H2A	20:A:832:CLA:O1D	2.00	0.60
21:A:854:LMU:C7	21:A:854:LMU:C3	2.75	0.60
5:A:98:PHE:O	5:A:99:HIS:CB	2.49	0.60
6:B:154:TRP:CD1	6:B:158:GLN:CG	2.85	0.60
6:B:625:TRP:CE3	6:B:626:LEU:N	2.69	0.60
9:E:41:ARG:HG3	9:E:46:PHE:CZ	2.37	0.60
9:E:56:ASP:HB2	9:E:64:PRO:CB	2.28	0.60
2:2:128:ASN:HD21	14:J:4:PHE:H	1.50	0.60
15:K:1:ASP:CA	15:K:5:SER:HB3	2.25	0.60
20:L:202:CLA:H92	20:L:203:CLA:H2	1.82	0.60
17:N:28:ASN:HA	17:N:30:ALA:H	1.66	0.60
18:R:35:UNK:N	18:R:38:UNK:CB	2.65	0.60
20:1:206:CLA:CHD	20:1:206:CLA:CBC	2.76	0.60
21:1:219:LMU:C1B	21:1:219:LMU:C6'	2.73	0.60
1:1:89:VAL:O	11:G:77:ILE:HD11	1.98	0.60
2:2:129:LYS:HA	2:2:131:THR:HG23	1.84	0.60
2:2:205:PHE:CE1	2:2:206:ALA:CA	2.85	0.60
20:2:307:CLA:CBA	20:2:307:CLA:CBD	2.80	0.60
5:A:334:HIS:HB3	20:A:820:CLA:HMA1	1.83	0.60
5:A:631:GLN:O	21:A:848:LMU:H6E	2.02	0.60
20:A:823:CLA:H112	20:A:823:CLA:OBD	2.01	0.60
20:A:826:CLA:C4	20:A:826:CLA:HBA1	2.29	0.60
5:A:499:ALA:HB3	20:A:832:CLA:O2D	2.02	0.60
20:A:814:CLA:CMB	22:A:843:BCR:H382	2.19	0.60
6:B:353:TYR:C	6:B:355:LEU:H	2.05	0.60
6:B:357:ALA:O	6:B:358:TYR:CD1	2.54	0.60
6:B:8:PHE:O	6:B:35:ASP:CB	2.49	0.60
6:B:374:HIS:HB2	20:B:825:CLA:C4B	2.30	0.60
6:B:393:PHE:CD2	6:B:397:ASP:OD1	2.47	0.60
20:B:809:CLA:HBD	20:B:809:CLA:O2A	2.01	0.60
11:G:93:TYR:CA	11:G:94:ASP:OD1	2.49	0.60
11:G:94:ASP:H	11:G:95:PRO:HD2	1.66	0.60
16:L:163:LEU:HB2	16:L:164:PRO:HG3	1.77	0.60
2:2:61:GLY:O	2:2:65:PRO:CG	2.49	0.60
5:A:243:PRO:O	5:A:244:LEU:O	2.19	0.60
5:A:257:GLN:O	5:A:258:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:693:LEU:HD11	5:A:738:TYR:CD1	2.37	0.60
20:A:809:CLA:HBA2	20:A:809:CLA:CHA	2.31	0.60
6:B:657:TRP:O	6:B:660:GLY:N	2.25	0.60
6:B:666:SER:HB3	6:B:671:TRP:NE1	2.12	0.60
5:A:653:LEU:HD23	20:B:849:CLA:HBC2	1.84	0.60
10:F:23:LYS:HB3	10:F:24:LYS:HZ3	1.67	0.60
10:F:46:MET:O	10:F:48:LYS:N	2.35	0.60
11:G:30:ASN:HD22	11:G:30:ASN:C	2.04	0.60
21:H:107:LMU:H6D	21:H:108:LMU:H3'	1.84	0.60
16:L:58:LEU:HD21	16:L:153:TRP:CZ2	2.37	0.60
2:2:204:ILE:O	2:2:205:PHE:HB3	2.02	0.59
20:2:303:CLA:O1D	20:2:303:CLA:H2A	2.02	0.59
3:3:141:GLN:HG2	3:3:142:TYR:N	2.16	0.59
20:3:302:CLA:CMA	20:3:302:CLA:HBA2	2.19	0.59
4:4:169:GLN:CD	20:4:305:CLA:HAC2	2.22	0.59
5:A:109:TRP:HH2	5:A:154:ARG:HD3	1.66	0.59
5:A:110:LEU:O	5:A:113:PRO:HD3	2.02	0.59
5:A:174:PHE:O	5:A:175:ALA:CB	2.49	0.59
5:A:472:ARG:N	5:A:473:PRO:CD	2.64	0.59
5:A:535:GLY:O	5:A:539:PHE:HB2	2.01	0.59
5:A:636:HIS:C	5:A:638:THR:H	2.04	0.59
5:A:684:PHE:CD2	5:A:685:VAL:N	2.69	0.59
5:A:451:ILE:HD11	20:A:830:CLA:CED	2.32	0.59
20:A:830:CLA:CBC	20:A:835:CLA:HBC2	2.32	0.59
6:B:436:LEU:O	6:B:437:TYR:HB2	2.02	0.59
6:B:652:PHE:O	6:B:656:VAL:HG23	2.01	0.59
6:B:697:PRO:O	7:C:79:LEU:HD11	2.02	0.59
6:B:707:LEU:O	6:B:710:LEU:HB3	2.02	0.59
20:B:807:CLA:H42	20:B:807:CLA:CHD	2.32	0.59
20:B:817:CLA:OBD	20:B:820:CLA:CBC	2.48	0.59
7:C:74:THR:O	7:C:77:MET:N	2.30	0.59
11:G:26:PHE:HB2	11:G:27:GLN:NE2	2.16	0.59
16:L:14:LEU:HD21	16:L:20:ILE:HG22	1.84	0.59
17:N:58:VAL:C	17:N:60:PHE:N	2.51	0.59
2:2:41:LEU:O	2:2:42:ARG:HD3	2.01	0.59
4:4:103:ILE:O	4:4:107:GLN:HB2	2.02	0.59
20:4:318:CLA:C2	20:4:318:CLA:HED3	2.31	0.59
4:4:76:TYR:CD1	4:4:76:TYR:C	2.72	0.59
5:A:165:TYR:O	5:A:165:TYR:CD2	2.55	0.59
5:A:309:LEU:HA	5:A:312:ILE:O	2.01	0.59
5:A:42:ARG:C	5:A:44:ILE:N	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:TRP:HE1	20:B:851:CLA:C1D	2.15	0.59
5:A:737:HIS:HA	5:A:740:LEU:HD23	1.83	0.59
5:A:755:ILE:O	5:A:756:ALA:CB	2.50	0.59
5:A:491:TRP:HE1	20:A:834:CLA:C1	2.15	0.59
6:B:187:SER:O	6:B:188:LEU:C	2.39	0.59
20:B:851:CLA:HED3	20:B:851:CLA:HBA2	1.84	0.59
12:H:25:GLY:C	12:H:27:ASP:N	2.37	0.59
1:1:161:PHE:N	20:1:203:CLA:CBB	2.66	0.59
5:A:373:ALA:O	5:A:396:PHE:CD1	2.54	0.59
5:A:678:PHE:O	5:A:680:LEU:N	2.35	0.59
5:A:708:VAL:CA	5:A:711:HIS:HD2	2.16	0.59
5:A:218:TRP:CA	20:A:814:CLA:HBB2	2.31	0.59
22:A:847:BCR:H322	22:J:102:BCR:H391	1.84	0.59
20:A:852:CLA:H3A	20:A:852:CLA:CGA	2.32	0.59
6:B:400:PRO:HD2	8:D:143:PRO:HD3	1.85	0.59
6:B:482:ASN:OD1	6:B:485:ALA:HB2	2.01	0.59
20:B:806:CLA:C19	20:B:825:CLA:H141	2.32	0.59
8:D:58:PHE:HD2	8:D:59:GLU:H	1.47	0.59
21:H:105:LMU:H2'	21:H:105:LMU:H6E	1.82	0.59
21:H:106:LMU:C4B	21:H:106:LMU:H31	2.33	0.59
22:I:101:BCR:H392	20:I:102:CLA:C14	2.32	0.59
15:K:7:THR:HA	15:K:10:ILE:CG1	2.32	0.59
16:L:36:TYR:OH	20:L:208:CLA:HBA2	2.02	0.59
17:N:33:TYR:O	17:N:34:THR:CG2	2.50	0.59
17:N:39:SER:OG	17:N:41:LYS:HA	2.02	0.59
1:1:185:TRP:HB2	1:1:186:HIS:NE2	2.14	0.59
20:1:207:CLA:CGD	20:1:207:CLA:HAA2	2.32	0.59
5:A:230:ASN:HA	5:A:233:LEU:HB2	1.84	0.59
5:A:413:HIS:ND1	5:A:416:ILE:HD12	2.17	0.59
20:A:822:CLA:C1B	22:A:845:BCR:H15C	2.33	0.59
5:A:746:THR:OG1	20:A:850:CLA:O1D	2.20	0.59
6:B:498:LEU:O	6:B:498:LEU:HD12	2.02	0.59
6:B:53:GLN:HA	6:B:53:GLN:OE1	1.91	0.59
6:B:670:TYR:OH	20:B:851:CLA:CAD	2.50	0.59
21:R:103:LMU:C6'	21:R:103:LMU:C4	2.75	0.59
2:2:42:ARG:C	2:2:44:ASN:N	2.52	0.59
2:2:43:TRP:CZ3	2:2:125:PHE:HB2	2.37	0.59
2:2:97:VAL:HA	2:2:100:VAL:CG1	2.33	0.59
5:A:302:HIS:HB2	20:A:817:CLA:CHB	2.31	0.59
5:A:455:PHE:HD1	20:A:830:CLA:HMA2	1.67	0.59
5:A:478:SER:HB3	5:A:644:GLN:CD	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:412:LEU:O	6:B:415:LYS:HB3	2.03	0.59
6:B:557:PHE:CD1	6:B:571:SER:HB3	2.37	0.59
6:B:727:ALA:C	6:B:728:SER:OG	2.40	0.59
20:B:825:CLA:HMC1	20:B:825:CLA:HBC3	1.85	0.59
5:A:547:PHE:HE2	20:B:851:CLA:O1A	1.86	0.59
7:C:49:VAL:HG22	7:C:50:GLY:H	1.68	0.59
10:F:103:SER:O	10:F:105:LEU:N	2.34	0.59
11:G:64:VAL:HG12	11:G:64:VAL:O	2.02	0.59
14:J:32:PHE:HE2	14:J:33:PHE:CZ	2.21	0.59
16:L:135:GLY:O	16:L:138:LYS:HG2	2.02	0.59
1:1:115:GLU:HG3	1:1:116:LYS:H	1.67	0.59
2:2:127:ASN:O	2:2:128:ASN:HB2	2.02	0.59
2:2:198:ALA:O	2:2:199:ASP:CB	2.50	0.59
20:2:316:CLA:C19	20:2:316:CLA:H152	2.22	0.59
2:2:50:VAL:O	2:2:54:TRP:CD1	2.44	0.59
6:B:409:ALA:C	6:B:411:MET:N	2.55	0.59
6:B:594:TRP:C	6:B:594:TRP:HD1	2.06	0.59
6:B:707:LEU:HD11	6:B:711:VAL:HG21	1.84	0.59
6:B:715:VAL:O	6:B:716:GLY:C	2.40	0.59
6:B:282:PHE:HE2	20:B:814:CLA:H3A	1.66	0.59
6:B:661:PHE:CB	20:B:851:CLA:CMC	2.80	0.59
8:D:111:TYR:CD2	8:D:114:PRO:CB	2.84	0.59
6:B:295:PHE:CE2	11:G:38:GLN:NE2	2.71	0.59
14:J:26:LEU:HD23	14:J:26:LEU:O	2.02	0.59
20:K:101:CLA:HMD3	20:K:108:CLA:ND	2.17	0.59
17:N:62:SER:O	17:N:66:ASP:CG	2.40	0.59
1:1:34:ALA:HB3	1:1:137:PRO:HB3	1.85	0.59
20:2:308:CLA:H2	20:2:308:CLA:C1B	2.32	0.59
3:3:90:LEU:HD12	3:3:90:LEU:H	1.67	0.59
4:4:118:ASP:CA	4:4:123:GLN:N	2.60	0.59
4:4:36:ASN:O	4:4:39:TRP:CD2	2.56	0.59
5:A:259:TYR:HB3	5:A:260:PRO:CD	2.30	0.59
5:A:432:LEU:C	5:A:434:ARG:N	2.55	0.59
20:A:804:CLA:H12	20:A:811:CLA:H92	1.83	0.59
20:A:817:CLA:H52	20:A:832:CLA:HBA1	1.84	0.59
5:A:370:ILE:CD1	20:A:824:CLA:C3D	2.78	0.59
6:B:154:TRP:CD1	6:B:158:GLN:HG2	2.38	0.59
6:B:50:HIS:HA	6:B:53:GLN:HB2	1.85	0.59
20:B:807:CLA:C1A	20:B:807:CLA:CGA	2.81	0.59
20:B:851:CLA:HMC1	20:B:851:CLA:HBC3	1.85	0.59
22:B:852:BCR:C33	22:B:852:BCR:C8	2.73	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:557:PHE:HE2	7:C:66:ARG:HE	1.48	0.59
20:G:102:CLA:CED	20:G:102:CLA:CAD	2.79	0.59
19:Z:1:GLC:O2	19:Z:1:GLC:C5	2.48	0.59
2:2:45:VAL:O	2:2:45:VAL:HG12	2.01	0.59
2:2:50:VAL:CG1	2:2:50:VAL:O	2.50	0.59
3:3:86:GLN:HB2	3:3:88:THR:CB	2.30	0.59
4:4:116:ASN:O	4:4:123:GLN:HG3	2.03	0.59
5:A:122:VAL:HG22	5:A:142:GLY:HA2	1.84	0.59
5:A:22:VAL:HG12	5:A:23:ASP:H	1.65	0.59
5:A:23:ASP:CB	5:A:24:ARG:HD3	2.29	0.59
5:A:309:LEU:HD23	5:A:309:LEU:C	2.23	0.59
5:A:497:ALA:O	5:A:498:LEU:HB2	2.02	0.59
5:A:502:THR:H	5:A:504:ALA:HB3	1.68	0.59
5:A:592:VAL:HG23	5:A:593:SER:H	1.66	0.59
5:A:681:GLY:HA2	5:A:684:PHE:HB3	1.84	0.59
5:A:368:LEU:HD12	20:A:825:CLA:C6	2.33	0.59
22:A:844:BCR:C23	22:A:844:BCR:H403	2.14	0.59
6:B:261:PHE:CZ	6:B:500:ALA:HB2	2.38	0.59
6:B:278:LEU:O	6:B:281:ALA:N	2.36	0.59
6:B:36:ASP:O	6:B:41:ARG:NE	2.36	0.59
6:B:442:VAL:HG21	20:B:831:CLA:CAC	2.28	0.59
20:B:829:CLA:HHD	20:B:829:CLA:HBC3	1.80	0.59
21:E:101:LMU:C3	21:E:101:LMU:C7	2.30	0.59
10:F:90:PHE:CD1	22:F:202:BCR:H23C	2.38	0.59
10:F:83:PHE:O	10:F:87:GLY:N	2.36	0.59
11:G:63:PRO:HG2	20:G:102:CLA:HMC1	1.84	0.59
21:H:108:LMU:C10	21:H:108:LMU:H31	2.13	0.59
12:H:21:TRP:N	12:H:22:ASP:CA	2.61	0.59
15:K:17:LEU:CG	15:K:56:THR:OG1	2.38	0.59
18:R:37:UNK:C	18:R:42:UNK:O	2.50	0.59
21:1:219:LMU:H2O2	21:1:219:LMU:C6B	2.14	0.59
21:2:317:LMU:H3'	21:2:317:LMU:C5B	2.33	0.59
2:2:39:GLU:N	2:2:40:SER:CA	2.66	0.59
2:2:57:LEU:HD23	2:2:58:GLY:N	2.18	0.59
3:3:194:ILE:HG23	3:3:197:TYR:OH	2.02	0.59
20:3:311:CLA:O1D	20:3:311:CLA:HAA2	2.03	0.59
4:4:104:ARG:HE	4:4:105:ARG:CA	2.16	0.59
4:4:121:PHE:O	4:4:143:PHE:CD2	2.55	0.59
4:4:49:ARG:O	4:4:53:LEU:CD1	2.51	0.59
4:4:70:ILE:CG1	4:4:71:ASN:H	2.16	0.59
20:A:817:CLA:HBC3	20:A:817:CLA:HMC1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:310:PRO:CB	6:B:311:PRO:CD	2.81	0.59
6:B:454:LEU:N	6:B:454:LEU:HD12	2.18	0.59
6:B:732:LYS:CG	6:B:733:PHE:HA	2.22	0.59
8:D:61:PRO:HD3	8:D:86:LEU:HD21	1.85	0.59
5:A:567:ARG:NH2	8:D:82:GLN:OE1	2.34	0.59
20:B:836:CLA:CBC	10:F:83:PHE:CZ	2.84	0.59
17:N:53:ALA:O	17:N:54:LYS:CD	2.51	0.59
17:N:72:LYS:N	17:N:72:LYS:HD3	2.18	0.59
21:R:109:LMU:H1B	21:R:109:LMU:H6B	1.63	0.59
19:Y:1:GLC:O6	19:Y:2:FRU:C2	2.50	0.59
2:2:98:GLU:HG3	2:2:99:LEU:HD12	1.85	0.59
5:A:193:LEU:O	5:A:194:ALA:C	2.41	0.59
5:A:44:ILE:O	5:A:46:LYS:HA	2.03	0.59
5:A:500:PRO:HB3	5:A:506:GLY:HA2	1.85	0.59
5:A:210:LEU:HD13	20:A:813:CLA:HHB	1.85	0.59
20:A:826:CLA:H18	20:A:851:CLA:H18	1.85	0.59
5:A:98:PHE:HD1	5:A:99:HIS:HD2	1.50	0.59
20:B:806:CLA:H191	20:B:825:CLA:H141	1.85	0.59
5:A:555:ILE:CG2	20:B:851:CLA:OBD	2.50	0.59
9:E:40:ARG:HH22	9:E:87:VAL:HG22	1.68	0.59
11:G:93:TYR:C	11:G:95:PRO:HD3	2.22	0.59
20:H:102:CLA:CHD	22:I:103:BCR:HC22	2.33	0.59
14:J:26:LEU:HA	14:J:29:ILE:HG22	1.85	0.59
16:L:40:LEU:CB	16:L:41:PRO:CD	2.81	0.59
16:L:50:LEU:HG	16:L:51:LEU:HD23	1.85	0.59
2:2:38:PRO:O	2:2:40:SER:CB	2.44	0.58
4:4:192:THR:HG22	4:4:194:VAL:C	2.23	0.58
5:A:588:GLY:N	6:B:668:ARG:NH1	2.50	0.58
6:B:277:HIS:HE1	20:B:816:CLA:NC	2.01	0.58
6:B:551:LYS:O	6:B:553:PHE:CD2	2.56	0.58
20:B:806:CLA:H71	25:B:848:LMG:H381	1.84	0.58
21:E:101:LMU:C2	21:E:101:LMU:H61	2.33	0.58
10:F:40:LEU:CA	10:F:42:ILE:HG12	2.30	0.58
20:H:103:CLA:H41	20:H:103:CLA:C10	2.33	0.58
20:J:101:CLA:O1D	20:J:101:CLA:H2A	2.03	0.58
6:B:694:ARG:HE	16:L:105:ALA:HA	1.67	0.58
16:L:45:THR:HA	16:L:52:ARG:HH12	1.66	0.58
2:2:181:HIS:CE1	20:2:304:CLA:CHA	2.86	0.58
20:2:305:CLA:HBC2	20:2:305:CLA:HMC1	1.84	0.58
20:2:322:CLA:H93	20:2:322:CLA:C4	2.33	0.58
2:2:57:LEU:O	2:2:60:ALA:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:183:GLN:HG2	4:4:183:GLN:O	2.03	0.58
20:4:302:CLA:H2A	20:4:302:CLA:O1D	2.03	0.58
20:4:304:CLA:O1A	20:4:304:CLA:H2	2.01	0.58
4:4:38:ARG:CG	4:4:39:TRP:H	2.06	0.58
4:4:67:ILE:HG22	4:4:67:ILE:O	2.02	0.58
5:A:396:PHE:O	5:A:396:PHE:CG	2.55	0.58
5:A:625:TRP:HB3	5:A:637:ILE:HD11	1.84	0.58
5:A:651:GLY:O	5:A:655:ASP:N	2.36	0.58
5:A:308:ILE:HD12	20:A:816:CLA:C8	2.34	0.58
20:A:819:CLA:C3C	20:A:825:CLA:C17	2.75	0.58
20:A:825:CLA:HBA2	22:A:846:BCR:H12C	1.85	0.58
6:B:156:HIS:O	6:B:163:PRO:HB3	2.03	0.58
6:B:376:GLN:HA	6:B:376:GLN:OE1	2.03	0.58
6:B:70:TRP:NE1	6:B:71:GLN:OE1	2.36	0.58
20:B:836:CLA:C6	22:F:203:BCR:H323	2.32	0.58
14:J:13:VAL:HG12	14:J:15:SER:HB2	1.85	0.58
17:N:63:ASP:N	17:N:64:ASP:CA	2.54	0.58
21:1:218:LMU:H41	21:1:218:LMU:H1'	1.84	0.58
3:3:157:ALA:O	3:3:158:TYR:HB2	2.02	0.58
20:3:302:CLA:HBC3	20:A:814:CLA:C2D	2.33	0.58
4:4:75:TRP:CD1	20:4:311:CLA:C1D	2.86	0.58
4:4:49:ARG:O	4:4:53:LEU:HD12	2.02	0.58
4:4:81:GLU:O	4:4:82:GLU:HB3	2.03	0.58
5:A:163:GLN:O	5:A:166:CYS:N	2.36	0.58
22:A:847:BCR:H312	20:A:852:CLA:C14	2.17	0.58
6:B:415:LYS:CE	6:B:539:LEU:O	2.50	0.58
20:B:823:CLA:CHB	20:B:837:CLA:HAA2	2.33	0.58
7:C:7:ILE:O	7:C:60:THR:HA	2.03	0.58
8:D:31:GLY:O	8:D:32:SER:CB	2.52	0.58
9:E:36:VAL:CG2	9:E:52:VAL:HG22	2.33	0.58
10:F:151:ASP:CA	10:F:154:PHE:HB3	2.33	0.58
16:L:36:TYR:CE1	20:L:202:CLA:H93	2.37	0.58
2:2:51:HIS:C	2:2:54:TRP:HB2	2.24	0.58
4:4:62:GLU:C	4:4:65:THR:HG22	2.24	0.58
5:A:225:VAL:HG12	5:A:248:PHE:CD1	2.39	0.58
5:A:298:ASP:OD2	5:A:298:ASP:N	2.37	0.58
20:A:838:CLA:C10	20:A:852:CLA:H152	2.33	0.58
6:B:186:SER:C	6:B:187:SER:O	2.42	0.58
6:B:193:HIS:HB2	20:B:812:CLA:CHC	2.33	0.58
5:A:705:GLU:CB	6:B:545:LYS:NZ	2.66	0.58
6:B:551:LYS:CD	8:D:143:PRO:HA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:822:CLA:H61	20:B:822:CLA:HMA2	1.84	0.58
7:C:1:MET:SD	7:C:4:SER:HB2	2.43	0.58
9:E:51:SER:O	9:E:68:ARG:N	2.27	0.58
9:E:69:PHE:CD2	9:E:71:LYS:HG2	2.38	0.58
3:3:52:LYS:N	3:3:55:ALA:HB3	2.19	0.58
5:A:112:ASP:O	5:A:116:ILE:HG12	2.02	0.58
5:A:390:ALA:CB	5:A:754:ILE:HD13	2.33	0.58
5:A:473:PRO:O	5:A:475:ASP:N	2.36	0.58
5:A:284:ARG:HH22	5:A:507:ALA:C	2.06	0.58
5:A:40:PHE:CE1	5:A:53:TRP:HD1	2.16	0.58
5:A:704:ILE:HA	5:A:707:ILE:HG13	1.85	0.58
20:A:807:CLA:C1	20:A:809:CLA:HED1	2.31	0.58
5:A:184:PHE:CE2	20:A:810:CLA:C2D	2.87	0.58
6:B:481:THR:O	6:B:482:ASN:HB2	2.03	0.58
6:B:615:TYR:HD1	6:B:615:TYR:N	2.01	0.58
8:D:31:GLY:HA2	16:L:13:PRO:CB	2.34	0.58
8:D:45:PHE:C	8:D:46:TYR:HD2	2.06	0.58
11:G:33:LYS:CA	11:G:33:LYS:CE	2.61	0.58
20:J:101:CLA:CGD	20:J:101:CLA:CBA	2.81	0.58
20:A:838:CLA:H192	14:J:19:PHE:CD2	2.39	0.58
2:2:211:LYS:HG2	3:3:113:LEU:CD1	2.31	0.58
20:3:313:CLA:H142	20:3:313:CLA:H102	1.64	0.58
4:4:126:LEU:HD23	4:4:127:PRO:HG3	1.86	0.58
4:4:154:ILE:CG1	4:4:155:ALA:N	2.56	0.58
4:4:163:PHE:O	4:4:164:LEU:C	2.40	0.58
5:A:157:GLY:O	5:A:158:ILE:HB	2.04	0.58
5:A:22:VAL:HG13	5:A:23:ASP:N	2.19	0.58
5:A:239:PRO:CA	5:A:242:ILE:HD11	2.29	0.58
5:A:218:TRP:HA	20:A:814:CLA:HBB2	1.85	0.58
6:B:55:ALA:HB1	6:B:150:LEU:HD11	1.84	0.58
6:B:710:LEU:C	6:B:712:HIS:N	2.55	0.58
6:B:276:HIS:HB2	20:B:815:CLA:C1B	2.33	0.58
6:B:421:HIS:CE1	20:B:829:CLA:C4D	2.86	0.58
6:B:662:MET:HG2	23:B:841:PQN:O1	2.03	0.58
20:B:826:CLA:C17	22:B:843:BCR:H363	2.34	0.58
7:C:6:LYS:N	7:C:65:VAL:HG22	2.19	0.58
9:E:48:ASN:ND2	9:E:71:LYS:HZ1	2.02	0.58
10:F:78:ARG:O	10:F:80:TRP:HD1	1.86	0.58
13:I:28:VAL:O	13:I:29:GLU:CD	2.42	0.58
20:L:201:CLA:H12	20:L:201:CLA:HED1	1.78	0.58
1:1:34:ALA:HB3	1:1:137:PRO:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:ARG:HG3	2:2:45:VAL:HB	1.85	0.58
2:2:65:PRO:O	2:2:66:GLU:O	2.21	0.58
4:4:158:ARG:O	4:4:159:LEU:C	2.41	0.58
4:4:90:LEU:H	4:4:90:LEU:CD2	2.16	0.58
20:A:809:CLA:CBD	20:A:809:CLA:HBA2	2.33	0.58
23:A:842:PQN:H241	23:A:842:PQN:H272	1.86	0.58
6:B:144:PHE:HD2	6:B:144:PHE:O	1.85	0.58
6:B:390:GLY:N	6:B:391:PRO:CD	2.67	0.58
6:B:458:ILE:HG13	6:B:459:PHE:N	2.16	0.58
6:B:460:ALA:O	6:B:461:GLN:C	2.42	0.58
6:B:628:SER:O	6:B:631:LEU:HD23	2.03	0.58
6:B:189:ALA:HA	20:B:813:CLA:HBB1	1.86	0.58
20:B:817:CLA:HBD	20:B:817:CLA:HBA1	1.86	0.58
11:G:46:ALA:CA	11:G:48:ASP:HB3	2.33	0.58
12:H:27:ASP:C	12:H:29:PRO:HD3	2.23	0.58
17:N:61:LEU:HD13	17:N:63:ASP:CB	2.28	0.58
19:Q:2:FRU:H11	19:Q:2:FRU:C6	1.98	0.58
18:R:35:UNK:C	18:R:36:UNK:O	2.51	0.58
1:1:25:ASP:CB	1:1:26:PRO:CD	2.81	0.58
2:2:64:ILE:HD13	20:2:303:CLA:HMB1	1.86	0.58
2:2:43:TRP:C	2:2:45:VAL:N	2.50	0.58
4:4:115:VAL:O	4:4:117:GLN:HG3	2.04	0.58
4:4:115:VAL:HG13	4:4:116:ASN:N	2.19	0.58
4:4:165:GLY:O	4:4:169:GLN:CG	2.48	0.58
5:A:362:LEU:HB3	5:A:406:LEU:O	2.03	0.58
5:A:592:VAL:HG23	5:A:593:SER:N	2.19	0.58
5:A:59:ALA:C	5:A:61:ALA:H	2.07	0.58
20:A:807:CLA:CBA	20:A:807:CLA:NA	2.56	0.58
6:B:224:PRO:O	6:B:226:LEU:N	2.37	0.58
6:B:378:ILE:HA	6:B:381:PHE:HB2	1.84	0.58
6:B:336:LEU:CD1	20:B:822:CLA:HBB1	2.32	0.58
20:B:827:CLA:H201	20:B:839:CLA:HBA1	1.86	0.58
6:B:95:HIS:CE1	20:B:808:CLA:HMB3	2.39	0.58
20:A:837:CLA:OBD	10:F:105:LEU:HD11	2.03	0.58
20:K:101:CLA:HMD3	20:K:108:CLA:NA	2.18	0.58
16:L:125:LYS:C	16:L:127:PRO:HD2	2.24	0.58
5:A:195:TRP:CZ2	20:A:810:CLA:CMA	2.83	0.58
5:A:468:SER:HB2	5:A:476:MET:SD	2.44	0.58
5:A:701:GLN:NE2	5:A:701:GLN:HA	2.19	0.58
20:A:815:CLA:HBB1	22:A:843:BCR:C11	2.34	0.58
6:B:555:TYR:CE2	6:B:573:TRP:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.39	0.58
10:F:23:LYS:O	10:F:24:LYS:NZ	2.27	0.58
20:4:305:CLA:H2	20:4:305:CLA:CED	2.34	0.58
5:A:105:ASN:HB2	5:A:140:PHE:CZ	2.39	0.58
5:A:154:ARG:HG3	5:A:383:PRO:HB2	1.86	0.58
5:A:185:HIS:O	5:A:188:LYS:N	2.37	0.58
5:A:284:ARG:HG3	5:A:295:TRP:CG	2.39	0.58
5:A:470:LEU:HG	20:B:808:CLA:HMC3	1.85	0.58
5:A:51:THR:HG21	20:A:837:CLA:CBB	2.23	0.58
5:A:740:LEU:HD13	20:A:838:CLA:HMA1	1.86	0.58
6:B:178:HIS:HE1	20:B:811:CLA:NC	2.00	0.58
6:B:305:LEU:O	6:B:306:GLU:C	2.43	0.58
6:B:649:MET:CE	6:B:723:ALA:HB2	2.34	0.58
20:B:821:CLA:H2	20:B:821:CLA:H71	1.81	0.58
20:B:827:CLA:H93	25:B:848:LMG:H311	1.85	0.58
20:A:850:CLA:H192	20:B:850:CLA:C2B	2.34	0.58
9:E:69:PHE:CD2	9:E:70:ALA:N	2.71	0.58
21:H:107:LMU:O3'	21:H:107:LMU:C1B	2.51	0.58
20:H:109:CLA:HAC2	22:I:101:BCR:H342	1.85	0.58
20:B:851:CLA:H142	22:I:101:BCR:HC41	1.85	0.58
20:J:101:CLA:HBA2	20:J:101:CLA:CHA	2.28	0.58
14:J:18:TRP:CH2	14:J:22:LEU:HD22	2.39	0.58
18:R:52:UNK:CB	18:R:53:UNK:CB	2.82	0.58
2:2:210:PRO:O	2:2:211:LYS:HB2	2.04	0.57
20:2:303:CLA:HHD	20:2:303:CLA:CBC	2.26	0.57
20:2:322:CLA:C9	20:2:322:CLA:H151	2.32	0.57
20:4:318:CLA:HED3	20:4:318:CLA:H12	1.39	0.57
5:A:223:VAL:O	5:A:228:PRO:HD3	2.03	0.57
5:A:462:ILE:HD11	20:B:850:CLA:C5	2.29	0.57
5:A:146:THR:HG21	5:A:751:LEU:HD22	1.86	0.57
20:A:814:CLA:HMC2	22:A:843:BCR:C15	2.33	0.57
6:B:175:LEU:HA	6:B:178:HIS:HB2	1.86	0.57
6:B:5:ILE:CB	6:B:6:PRO:HD2	2.31	0.57
6:B:722:ALA:O	6:B:726:ILE:HD12	2.04	0.57
6:B:91:ILE:HG22	20:B:808:CLA:CAD	2.34	0.57
7:C:52:LYS:C	7:C:54:CYS:N	2.56	0.57
10:F:22:LEU:O	10:F:25:LEU:HD13	2.02	0.57
10:F:2:ILE:HG22	10:F:3:ALA:N	2.19	0.57
11:G:31:MET:O	11:G:34:GLN:N	2.35	0.57
17:N:80:ASN:C	17:N:82:PHE:N	2.58	0.57
1:1:185:TRP:CB	1:1:186:HIS:NE2	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:PRO:HG2	2:2:129:LYS:N	2.17	0.57
3:3:162:PRO:HG2	3:3:164:PHE:CD1	2.39	0.57
5:A:316:MET:CA	5:A:317:TYR:HD1	2.16	0.57
5:A:341:GLN:HB3	5:A:434:ARG:NH1	2.19	0.57
5:A:513:LEU:HB3	5:A:529:LEU:HD13	1.85	0.57
5:A:81:ALA:CB	20:A:804:CLA:HMA3	2.28	0.57
6:B:266:GLN:HE21	6:B:363:GLN:HG2	1.69	0.57
6:B:257:ILE:HA	6:B:272:ASP:OD2	2.04	0.57
6:B:321:GLY:O	6:B:325:THR:HG22	2.04	0.57
6:B:510:LEU:HD22	6:B:510:LEU:H	1.69	0.57
6:B:549:ASP:OD1	7:C:63:LEU:HB3	2.05	0.57
21:B:801:LMU:H61	21:B:801:LMU:C10	2.21	0.57
20:B:823:CLA:CHD	20:B:823:CLA:HBC3	2.33	0.57
7:C:79:LEU:HD22	7:C:81:TYR:C	2.24	0.57
8:D:101:TYR:CE1	8:D:114:PRO:HD3	2.39	0.57
21:D:201:LMU:H82	21:D:201:LMU:H31	1.84	0.57
16:L:97:MET:HA	16:L:100:THR:HG23	1.86	0.57
2:2:77:PRO:O	17:N:3:ILE:CD1	2.52	0.57
17:N:48:GLY:HA3	17:N:49:CYS:C	2.14	0.57
17:N:67:LEU:CB	17:N:68:GLU:CB	2.80	0.57
18:R:38:UNK:C	18:R:42:UNK:O	2.52	0.57
4:4:114:SER:O	4:4:117:GLN:HG3	2.04	0.57
5:A:158:ILE:O	5:A:243:PRO:HG2	2.03	0.57
5:A:464:ASN:ND2	5:A:464:ASN:H	2.01	0.57
5:A:583:GLY:O	5:A:585:GLY:N	2.37	0.57
5:A:595:TRP:HE3	5:A:596:ASP:OD2	1.87	0.57
5:A:699:TYR:HD1	5:A:700:TRP:CD1	2.22	0.57
20:A:832:CLA:C1B	22:A:846:BCR:H333	2.34	0.57
1:1:27:LEU:HD22	6:B:314:ARG:CG	2.14	0.57
6:B:391:PRO:HB3	6:B:538:ALA:CA	2.34	0.57
6:B:53:GLN:O	6:B:55:ALA:N	2.33	0.57
6:B:553:PHE:O	6:B:554:GLY:C	2.41	0.57
6:B:594:TRP:CD2	6:B:598:HIS:CE1	2.93	0.57
8:D:99:GLN:OE1	8:D:101:TYR:OH	2.21	0.57
10:F:50:LYS:O	10:F:52:ARG:C	2.43	0.57
10:F:7:PRO:HB3	10:F:60:GLY:O	2.04	0.57
13:I:12:VAL:HG21	20:I:102:CLA:CGA	2.35	0.57
14:J:9:SER:O	14:J:10:VAL:CB	2.52	0.57
17:N:72:LYS:CD	17:N:74:LYS:H	2.17	0.57
1:1:185:TRP:C	1:1:186:HIS:HD1	2.03	0.57
2:2:203:THR:HG23	2:2:204:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:313:CLA:HMC1	20:3:313:CLA:HBC3	0.67	0.57
21:3:322:LMU:C3	21:3:322:LMU:H71	2.34	0.57
5:A:328:LYS:CG	5:A:332:GLU:CB	2.59	0.57
5:A:146:THR:HA	5:A:391:THR:HG23	1.85	0.57
5:A:402:ILE:C	5:A:404:GLY:H	2.07	0.57
5:A:708:VAL:O	5:A:711:HIS:HB2	2.05	0.57
20:A:804:CLA:CBA	20:A:811:CLA:H62	2.34	0.57
20:A:852:CLA:HMA1	20:A:852:CLA:H2	1.86	0.57
6:B:351:HIS:NE2	20:B:824:CLA:NC	2.53	0.57
6:B:486:LEU:O	6:B:487:ASN:HB3	2.05	0.57
6:B:422:LEU:CD1	6:B:535:VAL:HG11	2.27	0.57
8:D:118:VAL:CG1	8:D:119:TYR:H	2.17	0.57
8:D:29:PHE:O	8:D:30:ALA:HB3	2.04	0.57
9:E:40:ARG:CB	9:E:42:GLU:OE2	2.52	0.57
15:K:5:SER:O	15:K:9:LEU:CD2	2.52	0.57
16:L:164:PRO:CB	16:L:165:TYR:HB3	2.19	0.57
16:L:95:LEU:HD11	16:L:143:PHE:CZ	2.39	0.57
17:N:52:LEU:HB3	17:N:53:ALA:CA	2.34	0.57
21:R:103:LMU:H3O1	21:R:103:LMU:C6B	2.14	0.57
21:R:103:LMU:H6D	21:R:103:LMU:C4	2.34	0.57
20:A:822:CLA:C4B	22:A:845:BCR:H15C	2.34	0.57
20:A:830:CLA:HAA1	22:B:852:BCR:C14	2.35	0.57
20:A:851:CLA:C3D	20:A:851:CLA:HED2	2.35	0.57
6:B:674:LEU:HD12	6:B:674:LEU:C	2.25	0.57
20:B:808:CLA:HBB2	20:B:850:CLA:C13	2.30	0.57
16:L:63:LEU:O	16:L:64:LEU:C	2.42	0.57
17:N:80:ASN:O	17:N:82:PHE:HD2	1.88	0.57
19:X:1:GLC:O5	19:X:2:FRU:H5	2.04	0.57
2:2:86:GLU:HA	2:2:86:GLU:OE2	2.03	0.57
20:3:302:CLA:HBC2	20:A:814:CLA:C4D	2.34	0.57
4:4:101:VAL:HG12	4:4:102:GLU:N	2.20	0.57
20:4:307:CLA:O1D	20:4:307:CLA:C2A	2.52	0.57
5:A:156:SER:O	5:A:158:ILE:N	2.37	0.57
5:A:232:PHE:CZ	5:A:242:ILE:HG22	2.38	0.57
5:A:679:PHE:HE1	5:A:749:PHE:HB2	1.69	0.57
5:A:401:TRP:HB3	20:A:826:CLA:HMC3	1.86	0.57
20:A:805:CLA:HMC3	20:A:828:CLA:HMA1	1.86	0.57
20:A:839:CLA:O2D	20:A:839:CLA:HAA2	2.05	0.57
6:B:378:ILE:CA	6:B:381:PHE:HB2	2.35	0.57
6:B:399:ASN:O	6:B:401:GLU:N	2.38	0.57
6:B:545:LYS:CD	6:B:546:LEU:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:551:LYS:HE2	8:D:143:PRO:HA	1.86	0.57
6:B:707:LEU:HD11	20:B:827:CLA:C9	2.34	0.57
6:B:651:LEU:HB3	20:B:850:CLA:O2A	2.05	0.57
20:B:850:CLA:NB	20:B:851:CLA:HBB2	2.18	0.57
7:C:29:ILE:CG2	8:D:126:GLY:HA2	2.34	0.57
8:D:49:THR:OG1	8:D:74:LEU:HD12	2.05	0.57
17:N:50:GLN:N	17:N:51:ASP:O	2.37	0.57
17:N:61:LEU:HD21	17:N:63:ASP:C	2.15	0.57
19:P:1:GLC:HO2	19:P:2:FRU:C2	2.16	0.57
1:1:185:TRP:O	1:1:186:HIS:CG	2.57	0.57
21:2:313:LMU:H41	21:2:313:LMU:H6D	1.87	0.57
20:3:318:CLA:H3A	20:3:318:CLA:CGA	2.34	0.57
5:A:265:GLY:CA	5:A:272:LEU:HD21	2.34	0.57
5:A:694:PHE:HZ	6:B:661:PHE:CD1	2.22	0.57
5:A:83:PHE:CE1	20:A:813:CLA:HED1	2.40	0.57
20:A:826:CLA:C11	22:J:102:BCR:H353	2.34	0.57
20:A:839:CLA:C4D	20:A:839:CLA:O1D	2.33	0.57
6:B:25:ILE:HG22	22:L:210:BCR:H291	1.81	0.57
20:B:815:CLA:H12	20:B:815:CLA:C1A	2.35	0.57
20:B:833:CLA:CBB	22:B:845:BCR:H281	2.34	0.57
8:D:125:PRO:HG2	8:D:127:ARG:HD3	1.86	0.57
11:G:32:ALA:O	11:G:33:LYS:C	2.42	0.57
16:L:14:LEU:CD2	16:L:21:GLY:O	2.53	0.57
1:1:141:GLU:O	1:1:143:LEU:O	2.23	0.57
20:1:202:CLA:CAA	20:1:202:CLA:O2D	2.53	0.57
20:1:207:CLA:HBC3	20:1:207:CLA:CMC	2.32	0.57
4:4:100:TYR:O	4:4:103:ILE:HG12	2.05	0.57
5:A:123:VAL:HB	5:A:129:GLN:OE1	2.04	0.57
5:A:532:ILE:N	5:A:533:PRO:HD3	2.19	0.57
5:A:56:ASN:O	5:A:57:LEU:CB	2.50	0.57
5:A:81:ALA:HB1	20:A:804:CLA:HMA3	1.81	0.57
6:B:127:ILE:HD13	6:B:193:HIS:CE1	2.40	0.57
5:A:587:GLY:HA3	6:B:668:ARG:CZ	2.33	0.57
20:B:813:CLA:H2A	20:B:813:CLA:O1D	2.05	0.57
9:E:32:ARG:NH2	9:E:53:VAL:HA	2.20	0.57
9:E:39:LEU:N	9:E:40:ARG:HH11	1.94	0.57
22:A:847:BCR:C3	22:F:202:BCR:H17C	2.34	0.57
16:L:17:ASP:OD1	16:L:17:ASP:O	2.23	0.57
20:L:202:CLA:H142	20:L:203:CLA:H43	1.86	0.57
2:2:205:PHE:O	2:2:206:ALA:CB	2.53	0.57
5:A:158:ILE:HG23	5:A:163:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:431:LEU:O	5:A:435:VAL:CG1	2.53	0.57
5:A:114:THR:HG1	5:A:525:ASN:HB2	1.65	0.57
5:A:354:TRP:CZ2	20:A:823:CLA:H171	2.40	0.57
6:B:428:PHE:HA	20:B:830:CLA:O1D	2.05	0.57
6:B:486:LEU:HB2	6:B:489:GLY:O	2.05	0.57
6:B:615:TYR:CD1	6:B:615:TYR:N	2.72	0.57
20:B:819:CLA:HMA3	20:B:820:CLA:C4D	2.34	0.57
20:B:824:CLA:H72	20:B:824:CLA:C4	2.35	0.57
25:B:848:LMG:HC91	25:B:848:LMG:H111	1.87	0.57
20:B:850:CLA:H91	20:B:851:CLA:H92	1.87	0.57
8:D:140:ASN:HA	8:D:142:SER:OG	2.05	0.57
21:D:201:LMU:O2'	21:D:201:LMU:H12	2.05	0.57
20:B:836:CLA:H203	22:F:203:BCR:HC41	1.87	0.57
17:N:50:GLN:OE1	17:N:51:ASP:HA	2.04	0.57
2:2:50:VAL:HG12	2:2:50:VAL:O	2.03	0.57
4:4:47:ASN:HB3	4:4:161:LEU:CD2	2.31	0.57
5:A:240:LYS:H	5:A:243:PRO:HD3	1.69	0.57
5:A:258:LEU:O	5:A:280:PHE:CE1	2.58	0.57
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.40	0.57
5:A:547:PHE:O	5:A:551:VAL:CG1	2.46	0.57
5:A:619:LYS:HG2	5:A:642:PHE:CE1	2.40	0.57
20:A:840:CLA:O2D	20:A:840:CLA:HBA2	2.04	0.57
6:B:262:HIS:O	6:B:265:THR:O	2.23	0.57
6:B:305:LEU:HD22	20:B:821:CLA:O1D	2.05	0.57
6:B:34:HIS:O	6:B:36:ASP:N	2.37	0.57
6:B:351:HIS:HB3	20:B:815:CLA:CED	2.30	0.57
8:D:91:ARG:NH1	8:D:119:TYR:HE1	2.03	0.57
10:F:72:ILE:HG22	10:F:73:VAL:N	2.19	0.57
15:K:43:ARG:NE	15:K:43:ARG:HA	2.20	0.57
16:L:65:VAL:H	16:L:67:PRO:HD2	1.69	0.57
16:L:65:VAL:N	16:L:67:PRO:HD2	2.20	0.57
16:L:88:ALA:O	16:L:90:GLY:N	2.37	0.57
17:N:80:ASN:OD1	17:N:82:PHE:CA	2.53	0.57
1:1:160:GLY:HA3	20:1:203:CLA:HBB2	1.86	0.56
1:1:28:GLY:HA2	20:1:211:CLA:C3C	2.35	0.56
2:2:182:ILE:CG2	2:2:205:PHE:HB2	2.35	0.56
3:3:197:TYR:OH	20:3:304:CLA:C4B	2.53	0.56
2:2:37:ASP:CG	3:3:41:ASP:HB2	2.25	0.56
5:A:369:THR:HG21	5:A:402:ILE:CG2	2.35	0.56
5:A:442:ILE:HG23	20:A:829:CLA:CMC	2.25	0.56
5:A:544:ILE:HD11	20:A:850:CLA:H193	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:733:VAL:HG11	20:A:838:CLA:C1D	2.35	0.56
20:A:815:CLA:HAA2	20:A:815:CLA:C4	2.29	0.56
6:B:48:ALA:CB	6:B:157:LEU:HD22	2.34	0.56
6:B:444:LEU:O	6:B:445:ALA:CB	2.53	0.56
6:B:630:GLN:HE21	6:B:731:GLY:CA	2.15	0.56
25:B:848:LMG:H111	25:B:848:LMG:C9	2.35	0.56
9:E:44:TYR:CD2	9:E:45:TRP:HE3	2.23	0.56
20:A:808:CLA:H142	22:J:102:BCR:C13	2.35	0.56
4:4:193:ILE:HG21	14:J:42:PHE:HD1	1.69	0.56
15:K:53:ALA:O	15:K:54:GLY:C	2.41	0.56
16:L:164:PRO:CG	16:L:165:TYR:CE1	2.84	0.56
17:N:25:THR:CG2	17:N:26:GLY:N	2.68	0.56
17:N:52:LEU:HB3	17:N:53:ALA:HA	1.86	0.56
17:N:76:LYS:CG	17:N:77:CYS:H	2.07	0.56
20:R:108:CLA:H92	21:R:109:LMU:C4B	2.35	0.56
3:3:181:LEU:HD12	3:3:182:LYS:CE	2.35	0.56
4:4:100:TYR:CA	4:4:103:ILE:HG12	2.34	0.56
5:A:205:HIS:CE1	20:A:813:CLA:HMC2	2.40	0.56
20:A:815:CLA:H42	20:A:815:CLA:HAA1	1.85	0.56
20:A:824:CLA:H162	20:A:824:CLA:C11	2.35	0.56
10:F:131:PHE:O	10:F:133:GLY:N	2.38	0.56
20:J:101:CLA:O2A	20:J:101:CLA:H2A	2.05	0.56
15:K:20:PHE:CE2	15:K:52:PRO:HA	2.40	0.56
16:L:30:SER:C	16:L:32:LEU:N	2.59	0.56
20:A:841:CLA:H201	16:L:64:LEU:CD2	2.31	0.56
17:N:45:ASN:HA	17:N:57:LYS:NZ	2.19	0.56
1:1:48:ARG:O	1:1:52:LEU:HB2	2.05	0.56
2:2:178:TRP:O	2:2:182:ILE:N	2.25	0.56
4:4:93:ILE:C	4:4:95:PHE:N	2.54	0.56
5:A:40:PHE:H	5:A:44:ILE:HG21	1.71	0.56
5:A:462:ILE:HD11	20:B:850:CLA:H72	1.85	0.56
20:A:819:CLA:C1C	20:A:825:CLA:C17	2.80	0.56
20:A:841:CLA:H202	16:L:64:LEU:HD21	1.86	0.56
6:B:455:ILE:HD12	6:B:517:PHE:CZ	2.40	0.56
20:B:836:CLA:CBC	10:F:83:PHE:HZ	2.17	0.56
7:C:31:TRP:CB	7:C:39:ILE:HG21	2.35	0.56
6:B:561:GLY:CA	7:C:52:LYS:HG2	2.29	0.56
11:G:78:GLY:O	11:G:79:HIS:ND1	2.38	0.56
12:H:36:GLN:O	12:H:36:GLN:HG2	2.05	0.56
17:N:66:ASP:CA	17:N:67:LEU:HD12	2.32	0.56
1:1:185:TRP:HE3	1:1:185:TRP:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:118:CYS:C	2:2:119:VAL:HG13	2.15	0.56
3:3:194:ILE:HA	3:3:197:TYR:CE1	2.40	0.56
3:3:87:GLU:C	22:3:314:BCR:H383	2.22	0.56
4:4:193:ILE:CG2	4:4:194:VAL:N	2.61	0.56
5:A:284:ARG:NH1	5:A:507:ALA:HB1	2.19	0.56
5:A:733:VAL:CG1	20:A:838:CLA:C3D	2.83	0.56
5:A:214:GLY:HA3	22:A:844:BCR:C15	2.36	0.56
20:A:805:CLA:H201	22:A:844:BCR:C18	2.35	0.56
6:B:247:THR:CG2	6:B:250:ALA:CB	2.82	0.56
6:B:500:ALA:CB	6:B:508:LEU:HD22	2.35	0.56
6:B:553:PHE:O	6:B:555:TYR:N	2.39	0.56
6:B:597:LYS:O	6:B:598:HIS:HB2	2.05	0.56
6:B:284:PHE:CE1	20:B:817:CLA:HHC	2.41	0.56
20:B:822:CLA:C8	20:B:824:CLA:H43	2.35	0.56
20:B:824:CLA:C4	20:B:824:CLA:C7	2.84	0.56
20:B:835:CLA:HBC3	20:B:835:CLA:CMC	2.25	0.56
25:B:848:LMG:C11	25:B:848:LMG:C9	2.83	0.56
9:E:41:ARG:HG3	9:E:46:PHE:CE1	2.41	0.56
10:F:76:ASP:O	10:F:78:ARG:N	2.39	0.56
21:K:106:LMU:C3'	21:K:106:LMU:C3	2.78	0.56
16:L:54:VAL:O	16:L:58:LEU:HB2	2.04	0.56
16:L:66:GLY:C	20:L:209:CLA:HMC3	2.25	0.56
1:1:57:ILE:O	1:1:57:ILE:HG12	2.04	0.56
5:A:372:VAL:O	5:A:374:GLN:N	2.38	0.56
5:A:374:GLN:O	5:A:376:MET:N	2.38	0.56
20:A:827:CLA:H51	22:A:844:BCR:H331	1.88	0.56
20:A:839:CLA:C5	20:A:839:CLA:H93	2.31	0.56
21:A:854:LMU:C3	21:A:854:LMU:C9	2.62	0.56
6:B:559:CYS:SG	6:B:560:ASP:N	2.79	0.56
11:G:69:VAL:O	11:G:73:ALA:HB3	2.05	0.56
20:2:322:CLA:HMB1	20:J:103:CLA:C15	2.36	0.56
14:J:13:VAL:CG1	14:J:15:SER:HB2	2.36	0.56
20:A:841:CLA:H141	16:L:95:LEU:HD22	1.87	0.56
1:1:54:VAL:C	1:1:56:GLY:H	2.09	0.56
4:4:123:GLN:HG2	4:4:124:TYR:H	1.70	0.56
21:4:301:LMU:H1B	21:4:301:LMU:C6'	2.34	0.56
4:4:58:MET:SD	4:4:59:LEU:N	2.78	0.56
5:A:207:LEU:HA	5:A:211:LEU:HB2	1.86	0.56
5:A:223:VAL:HA	5:A:227:LEU:HB2	1.88	0.56
5:A:157:GLY:O	5:A:248:PHE:HE1	1.88	0.56
5:A:316:MET:HA	5:A:317:TYR:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:824:CLA:HMA2	20:A:825:CLA:CGA	2.35	0.56
6:B:266:GLN:O	6:B:267:SER:CB	2.45	0.56
6:B:37:ILE:C	6:B:37:ILE:HD12	2.26	0.56
20:B:827:CLA:C20	20:B:839:CLA:HBA1	2.35	0.56
6:B:486:LEU:HD13	20:B:833:CLA:HMD3	1.88	0.56
10:F:24:LYS:N	10:F:26:GLN:H	2.04	0.56
17:N:70:GLU:CB	17:N:72:LYS:H	2.15	0.56
21:1:219:LMU:C2'	21:1:219:LMU:C6B	2.80	0.56
3:3:48:PHE:CD2	3:3:49:ILE:CG2	2.69	0.56
4:4:100:TYR:CA	4:4:103:ILE:HD11	2.31	0.56
20:4:311:CLA:HBA2	20:4:311:CLA:HBD	1.88	0.56
5:A:309:LEU:O	5:A:310:PHE:CB	2.52	0.56
20:A:804:CLA:HBB2	20:A:806:CLA:CAD	2.35	0.56
6:B:388:ALA:HA	6:B:391:PRO:CG	2.35	0.56
6:B:633:ASN:O	6:B:636:THR:HB	2.06	0.56
20:B:827:CLA:H62	25:B:848:LMG:C18	2.34	0.56
22:B:846:BCR:H351	20:B:851:CLA:H111	1.85	0.56
8:D:39:LYS:HG3	8:D:43:GLU:HG2	1.88	0.56
9:E:39:LEU:HA	9:E:46:PHE:CE1	2.40	0.56
10:F:102:ARG:CD	10:F:106:ILE:HD11	2.36	0.56
12:H:67:TYR:C	12:H:67:TYR:HD1	2.09	0.56
17:N:47:THR:HG21	17:N:54:LYS:CE	2.30	0.56
2:2:203:THR:C	2:2:204:ILE:HG13	2.23	0.56
4:4:67:ILE:CG2	4:4:67:ILE:O	2.52	0.56
5:A:131:ILE:HD13	6:B:447:GLY:N	2.20	0.56
5:A:42:ARG:HA	5:A:44:ILE:HG12	1.88	0.56
20:A:803:CLA:HMB1	20:A:811:CLA:H18	1.87	0.56
6:B:275:HIS:O	6:B:278:LEU:HB3	2.05	0.56
6:B:408:LEU:O	6:B:411:MET:HB3	2.05	0.56
6:B:479:SER:O	6:B:481:THR:N	2.28	0.56
6:B:560:ASP:OD1	7:C:52:LYS:NZ	2.36	0.56
20:B:828:CLA:HAA2	20:B:828:CLA:HED2	1.85	0.56
20:B:830:CLA:H51	22:F:203:BCR:C40	2.35	0.56
9:E:48:ASN:HD21	9:E:71:LYS:NZ	2.04	0.56
10:F:126:ALA:O	10:F:128:SER:N	2.38	0.56
16:L:62:PHE:HB2	16:L:154:ALA:HB2	1.86	0.56
16:L:25:THR:HB	16:L:26:PRO:HD2	1.88	0.56
4:4:152:LYS:HA	4:4:154:ILE:HG12	1.87	0.56
20:1:206:CLA:O1D	21:4:301:LMU:O2'	2.23	0.56
5:A:133:ASN:HD22	5:A:142:GLY:HA2	1.69	0.56
5:A:287:LEU:N	5:A:295:TRP:HE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:527:VAL:CG1	5:A:528:ALA:H	2.18	0.56
5:A:582:ASP:HB3	5:A:589:THR:CG2	2.36	0.56
6:B:291:TYR:O	6:B:292:ARG:O	2.24	0.56
6:B:340:SER:O	6:B:344:ILE:HG13	2.06	0.56
6:B:363:GLN:HA	6:B:365:PHE:CE1	2.40	0.56
6:B:574:ASP:OD2	6:B:706:ARG:NE	2.39	0.56
20:B:821:CLA:CGD	20:B:821:CLA:C2A	2.83	0.56
20:B:823:CLA:HED2	20:B:824:CLA:CAD	2.35	0.56
20:B:836:CLA:H121	22:F:203:BCR:H311	1.88	0.56
21:B:847:LMU:C5B	21:B:847:LMU:C4'	2.72	0.56
10:F:80:TRP:CE3	20:F:206:CLA:HMC2	2.37	0.56
11:G:46:ALA:CA	11:G:48:ASP:CB	2.81	0.56
21:K:106:LMU:C5'	21:K:106:LMU:C2	2.84	0.56
20:A:831:CLA:O1D	16:L:73:PRO:HA	2.06	0.56
17:N:62:SER:O	17:N:63:ASP:CG	2.44	0.56
2:2:60:ALA:HA	2:2:63:PHE:CE2	2.41	0.56
4:4:94:GLU:CA	4:4:95:PHE:HD1	2.18	0.56
6:B:132:ASN:C	6:B:132:ASN:OD1	2.45	0.56
6:B:197:VAL:O	6:B:198:ALA:HB2	2.06	0.56
6:B:398:TYR:CD1	6:B:542:ARG:NH2	2.73	0.56
6:B:661:PHE:HB2	20:B:851:CLA:HMC1	1.84	0.56
20:B:808:CLA:H193	20:B:839:CLA:C4	2.36	0.56
9:E:88:GLU:O	9:E:90:VAL:HG23	2.06	0.56
10:F:22:LEU:CB	10:F:23:LYS:HD3	2.35	0.56
15:K:69:ILE:HA	15:K:72:VAL:CG1	2.34	0.56
12:H:36:GLN:HE22	20:L:207:CLA:CAD	2.19	0.56
16:L:32:LEU:CD1	20:L:203:CLA:HED1	2.35	0.56
2:2:171:MET:SD	2:2:172:LEU:N	2.79	0.56
4:4:104:ARG:HA	4:4:107:GLN:HE21	1.70	0.56
4:4:118:ASP:HA	4:4:122:LYS:CA	2.36	0.56
5:A:157:GLY:O	5:A:248:PHE:CE1	2.59	0.56
5:A:578:ARG:NH1	5:A:578:ARG:HB2	2.20	0.56
5:A:603:PHE:HZ	5:A:693:LEU:CD2	2.19	0.56
5:A:75:SER:HB3	5:A:354:TRP:CZ2	2.41	0.56
20:A:852:CLA:HBC2	20:A:852:CLA:HMC1	1.88	0.56
6:B:352:MET:SD	20:B:826:CLA:OBD	2.64	0.56
6:B:42:LEU:O	6:B:45:ASN:N	2.39	0.56
6:B:542:ARG:NH2	8:D:141:VAL:O	2.39	0.56
6:B:646:TRP:CZ3	6:B:726:ILE:HD13	2.41	0.56
20:B:821:CLA:H72	20:B:821:CLA:C2	2.31	0.56
6:B:340:SER:CA	20:B:824:CLA:H51	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:843:BCR:C33	22:B:843:BCR:C8	2.84	0.56
7:C:51:CYS:N	24:C:102:SF4:S1	2.74	0.56
8:D:124:ASN:CB	8:D:125:PRO:CD	2.82	0.56
8:D:69:ARG:O	8:D:70:GLU:CB	2.54	0.56
9:E:73:ASN:C	9:E:73:ASN:ND2	2.60	0.56
11:G:27:GLN:O	11:G:28:ARG:HB3	2.05	0.56
20:H:102:CLA:HAC2	22:I:103:BCR:C3	2.12	0.56
13:I:19:VAL:O	13:I:23:SER:N	2.39	0.56
16:L:25:THR:HB	16:L:26:PRO:CD	2.36	0.56
1:1:112:ARG:HH11	20:1:209:CLA:CGD	2.08	0.55
3:3:202:LEU:HB3	3:3:204:THR:HG23	1.87	0.55
3:3:94:ARG:C	3:3:97:PHE:HE1	2.09	0.55
4:4:106:TRP:HE3	20:4:314:CLA:CMA	2.14	0.55
5:A:150:PHE:H	5:A:153:TRP:HE3	1.49	0.55
20:A:831:CLA:CMC	20:A:831:CLA:HBC3	2.35	0.55
20:A:824:CLA:CBA	20:A:836:CLA:HED1	2.19	0.55
22:A:847:BCR:H15C	20:A:851:CLA:H151	1.88	0.55
6:B:255:LEU:HD12	20:B:814:CLA:O2D	2.06	0.55
20:B:828:CLA:HMB2	20:B:829:CLA:C4A	2.37	0.55
22:B:846:BCR:C20	20:B:850:CLA:C15	2.84	0.55
8:D:75:LEU:HD21	16:L:19:PHE:CZ	2.40	0.55
2:2:42:ARG:HD2	2:2:45:VAL:CG2	2.19	0.55
3:3:49:ILE:HA	3:3:51:PRO:HD2	1.88	0.55
4:4:37:LEU:HA	4:4:39:TRP:CD1	2.41	0.55
5:A:249:ILE:HG23	5:A:251:ASN:OD1	2.06	0.55
5:A:358:LEU:O	5:A:361:ASN:HB3	2.05	0.55
5:A:409:GLY:C	5:A:411:ALA:H	2.10	0.55
5:A:425:THR:O	5:A:428:TYR:CE1	2.59	0.55
5:A:559:GLY:HA2	5:A:597:HIS:ND1	2.21	0.55
5:A:88:ILE:CG2	5:A:89:ILE:N	2.69	0.55
6:B:686:PRO:HG2	20:L:202:CLA:H12	1.86	0.55
21:B:801:LMU:C1B	21:B:801:LMU:H6'	2.18	0.55
21:K:106:LMU:C1	21:K:106:LMU:H51	2.33	0.55
21:K:106:LMU:H12	21:K:106:LMU:C5	2.15	0.55
21:N:101:LMU:H41	21:N:101:LMU:O6'	2.05	0.55
1:1:111:GLN:HE21	1:1:111:GLN:HA	1.72	0.55
1:1:63:LEU:HD23	1:1:64:GLY:O	2.05	0.55
3:3:158:TYR:OH	20:3:305:CLA:C3B	2.53	0.55
4:4:70:ILE:O	4:4:73:PRO:CD	2.53	0.55
5:A:177:LEU:C	5:A:179:LEU:H	2.10	0.55
5:A:447:ASN:ND2	6:B:678:LEU:CD2	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:813:CLA:C1	20:A:813:CLA:HMA2	2.36	0.55
20:A:816:CLA:CBC	20:A:816:CLA:CMC	2.81	0.55
20:A:819:CLA:H43	20:A:822:CLA:H2	1.88	0.55
20:A:824:CLA:HBB2	20:A:836:CLA:C3A	2.36	0.55
6:B:117:TYR:O	6:B:367:THR:HG23	2.07	0.55
6:B:343:VAL:CG1	20:B:824:CLA:H2	2.36	0.55
6:B:715:VAL:HA	6:B:718:ILE:HG22	1.88	0.55
20:B:823:CLA:C7	20:B:837:CLA:C3D	2.84	0.55
20:B:806:CLA:C4	25:B:848:LMG:H321	2.36	0.55
11:G:19:GLY:C	11:G:21:PHE:HA	2.26	0.55
16:L:66:GLY:HA2	16:L:69:VAL:HG22	1.89	0.55
1:1:167:ALA:C	1:1:169:PRO:HD3	2.26	0.55
2:2:143:PHE:CD1	2:2:144:ASP:N	2.75	0.55
2:2:182:ILE:HG23	2:2:205:PHE:HB2	1.89	0.55
3:3:201:ALA:C	3:3:202:LEU:HD22	2.27	0.55
3:3:50:GLU:H	3:3:51:PRO:HD3	1.71	0.55
4:4:126:LEU:HD23	4:4:127:PRO:CG	2.36	0.55
5:A:158:ILE:HG23	5:A:163:GLN:HE22	1.72	0.55
5:A:536:THR:HA	5:A:539:PHE:CB	2.37	0.55
20:A:824:CLA:C3B	22:A:846:BCR:C21	2.85	0.55
6:B:427:LEU:HB3	20:B:830:CLA:HED1	1.89	0.55
6:B:476:ILE:O	6:B:479:SER:OG	2.16	0.55
7:C:75:ARG:NH1	8:D:110:GLN:OE1	2.38	0.55
8:D:64:GLY:O	8:D:65:ALA:CB	2.55	0.55
8:D:75:LEU:HD22	8:D:76:LYS:H	1.72	0.55
1:1:89:VAL:CG1	11:G:77:ILE:HG21	2.37	0.55
21:H:105:LMU:C9	21:H:105:LMU:H51	2.14	0.55
20:H:109:CLA:CHD	22:I:101:BCR:H342	2.36	0.55
16:L:27:VAL:CA	20:L:203:CLA:HMA3	2.12	0.55
2:2:51:HIS:O	2:2:55:ALA:N	2.29	0.55
2:2:67:PHE:O	2:2:68:LEU:C	2.45	0.55
5:A:141:ARG:HH21	5:A:141:ARG:CG	2.14	0.55
5:A:361:ASN:HD22	5:A:361:ASN:C	2.10	0.55
5:A:472:ARG:O	5:A:474:GLN:N	2.40	0.55
20:A:809:CLA:H51	22:J:102:BCR:C10	2.35	0.55
20:A:820:CLA:C2D	20:A:821:CLA:HMB3	2.36	0.55
5:A:88:ILE:HG22	5:A:89:ILE:H	1.72	0.55
6:B:14:GLN:H	6:B:14:GLN:HE21	1.55	0.55
6:B:310:PRO:CB	6:B:311:PRO:HD2	2.35	0.55
6:B:594:TRP:HD1	6:B:595:HIS:HB2	1.72	0.55
6:B:596:TRP:CZ3	6:B:613:SER:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:649:MET:HE3	6:B:723:ALA:HB2	1.89	0.55
9:E:40:ARG:NH2	9:E:87:VAL:HG22	2.21	0.55
10:F:117:LYS:N	10:F:118:GLU:OE2	2.39	0.55
10:F:123:VAL:HG13	14:J:7:TYR:H	1.71	0.55
20:L:201:CLA:H2	20:L:201:CLA:O1A	2.05	0.55
17:N:63:ASP:H	17:N:64:ASP:HB2	1.65	0.55
1:1:129:ASP:OD2	1:1:133:TYR:HA	2.07	0.55
2:2:129:LYS:C	2:2:131:THR:N	2.60	0.55
2:2:129:LYS:O	2:2:132:GLY:HA3	2.05	0.55
20:2:302:CLA:HBC3	20:2:302:CLA:CMC	2.28	0.55
21:2:317:LMU:H3'	21:2:317:LMU:O6B	2.06	0.55
2:2:57:LEU:CD2	2:2:58:GLY:N	2.69	0.55
3:3:181:LEU:CD1	3:3:182:LYS:CE	2.84	0.55
3:3:56:TYR:HD1	3:3:185:LYS:HZ1	1.51	0.55
4:4:120:ILE:H	4:4:120:ILE:HD12	1.72	0.55
4:4:30:LEU:CD1	21:4:317:LMU:H121	2.32	0.55
21:4:321:LMU:H32	21:4:321:LMU:O2'	2.06	0.55
5:A:100:GLY:HA3	5:A:153:TRP:CZ3	2.42	0.55
5:A:397:THR:HB	5:A:613:ILE:HG12	1.86	0.55
5:A:412:ALA:O	5:A:415:ALA:HB3	2.07	0.55
5:A:438:HIS:HB2	5:A:441:ALA:HB3	1.89	0.55
5:A:46:LYS:HG3	5:A:48:PRO:HB2	1.87	0.55
5:A:471:GLY:O	5:A:472:ARG:HG2	2.07	0.55
5:A:678:PHE:O	5:A:681:GLY:O	2.25	0.55
5:A:711:HIS:O	5:A:716:VAL:HG22	2.06	0.55
21:A:855:LMU:C1B	21:A:855:LMU:O4'	2.53	0.55
6:B:102:GLU:O	6:B:103:ALA:C	2.45	0.55
6:B:15:ASP:O	6:B:20:ARG:CG	2.55	0.55
6:B:416:GLU:H	6:B:416:GLU:CD	2.09	0.55
6:B:586:THR:C	6:B:588:GLY:N	2.55	0.55
6:B:597:LYS:HG2	20:B:835:CLA:HBC1	1.89	0.55
10:F:46:MET:O	10:F:49:THR:N	2.38	0.55
20:1:202:CLA:C7	20:1:202:CLA:H41	2.20	0.55
20:1:204:CLA:CHA	20:1:204:CLA:HBA1	2.36	0.55
1:1:54:VAL:O	1:1:56:GLY:N	2.40	0.55
1:1:85:LEU:H	1:1:85:LEU:HD13	1.70	0.55
2:2:163:GLU:OE1	2:2:163:GLU:HA	2.07	0.55
2:2:192:LEU:HG	2:2:193:PHE:N	2.22	0.55
3:3:74:ALA:HA	20:3:307:CLA:ND	2.21	0.55
4:4:192:THR:HG23	4:4:193:ILE:C	2.24	0.55
21:4:320:LMU:H5B	21:4:320:LMU:H3O2	1.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:334:HIS:HB3	20:A:820:CLA:HMA3	1.88	0.55
5:A:650:ASN:O	5:A:653:LEU:N	2.30	0.55
20:A:806:CLA:HED2	20:A:806:CLA:HBA2	1.88	0.55
20:A:815:CLA:CGD	20:A:815:CLA:H2A	2.36	0.55
20:A:825:CLA:H101	20:A:825:CLA:C14	2.37	0.55
6:B:577:TYR:CE2	6:B:578:LEU:HD12	2.41	0.55
6:B:732:LYS:HG3	6:B:733:PHE:O	2.04	0.55
6:B:76:ALA:O	6:B:79:GLN:N	2.39	0.55
20:B:839:CLA:CHD	23:B:841:PQN:H18	2.36	0.55
20:B:806:CLA:H43	25:B:848:LMG:H321	1.89	0.55
10:F:23:LYS:CA	10:F:24:LYS:NZ	2.69	0.55
10:F:40:LEU:HD12	10:F:42:ILE:HD11	1.89	0.55
11:G:5:SER:O	11:G:7:VAL:HG13	2.05	0.55
20:2:322:CLA:CMB	20:J:103:CLA:H152	2.36	0.55
14:J:19:PHE:O	14:J:23:ALA:HB3	2.06	0.55
16:L:56:VAL:HA	20:L:208:CLA:HED1	1.89	0.55
17:N:46:PHE:O	17:N:47:THR:CB	2.53	0.55
1:1:50:ALA:O	1:1:54:VAL:HG23	2.07	0.55
20:2:316:CLA:C8	20:2:316:CLA:H151	2.35	0.55
2:2:63:PHE:HE2	2:2:168:ARG:CD	2.20	0.55
3:3:134:LYS:O	3:3:135:PRO:C	2.44	0.55
5:A:210:LEU:N	5:A:213:LEU:H	2.05	0.55
5:A:262:PHE:O	5:A:264:GLU:N	2.40	0.55
20:A:815:CLA:CED	20:A:815:CLA:H2A	2.32	0.55
6:B:361:ILE:C	6:B:362:ALA:O	2.44	0.55
6:B:493:TRP:CH2	20:B:815:CLA:H122	2.41	0.55
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.89	0.55
6:B:75:GLU:CB	6:B:132:ASN:HD22	2.19	0.55
20:B:824:CLA:C10	20:B:824:CLA:H142	2.35	0.55
20:B:851:CLA:H41	20:B:851:CLA:CMB	2.37	0.55
7:C:69:LEU:HD23	7:C:70:TRP:N	2.21	0.55
7:C:74:THR:OG1	7:C:75:ARG:N	2.33	0.55
16:L:14:LEU:HD22	16:L:21:GLY:O	2.07	0.55
22:L:210:BCR:H331	22:L:210:BCR:C8	2.36	0.55
16:L:33:ILE:HD11	16:L:36:TYR:HD1	1.72	0.55
16:L:41:PRO:HG3	16:L:52:ARG:HD3	1.88	0.55
17:N:59:PRO:C	17:N:61:LEU:O	2.45	0.55
20:1:207:CLA:HBA2	20:1:207:CLA:HMA3	1.88	0.55
4:4:36:ASN:C	4:4:36:ASN:OD1	2.45	0.55
3:3:92:TRP:CZ2	5:A:250:LEU:HB2	2.40	0.55
5:A:278:ALA:O	5:A:279:ASP:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:408:VAL:HG21	5:A:602:LEU:HG	1.88	0.55
5:A:451:ILE:HD12	20:A:830:CLA:CED	2.07	0.55
5:A:520:LEU:HD22	21:A:848:LMU:O1'	2.07	0.55
5:A:679:PHE:O	5:A:683:HIS:HB2	2.07	0.55
20:A:804:CLA:HBC3	20:A:804:CLA:CHD	2.36	0.55
20:A:808:CLA:H2A	20:A:808:CLA:O2D	2.06	0.55
20:A:806:CLA:O1A	20:A:828:CLA:HMB2	2.07	0.55
6:B:275:HIS:ND1	20:B:815:CLA:HMB1	2.21	0.55
6:B:330:ILE:HD12	6:B:330:ILE:O	2.05	0.55
7:C:1:MET:H1	7:C:4:SER:CA	2.20	0.55
20:H:102:CLA:O1D	20:H:102:CLA:H2A	2.06	0.55
16:L:111:GLU:OE1	21:L:211:LMU:O6B	2.18	0.55
16:L:33:ILE:HD13	20:L:203:CLA:HBA1	1.89	0.55
16:L:87:ALA:O	16:L:89:ALA:N	2.40	0.55
4:4:58:MET:SD	4:4:58:MET:C	2.85	0.55
5:A:211:LEU:HB3	5:A:310:PHE:CD2	2.43	0.55
5:A:478:SER:C	5:A:480:THR:H	2.11	0.55
5:A:697:ARG:C	5:A:699:TYR:N	2.60	0.55
20:A:830:CLA:H142	20:A:830:CLA:H101	1.88	0.55
5:A:82:HIS:O	5:A:84:GLY:N	2.40	0.55
21:A:854:LMU:H31	21:A:854:LMU:C1'	2.36	0.55
6:B:91:ILE:HD11	6:B:104:PHE:CE2	2.42	0.55
6:B:475:ASP:HA	6:B:480:SER:C	2.27	0.55
6:B:616:LEU:O	6:B:619:TRP:HB2	2.06	0.55
6:B:633:ASN:HD22	6:B:636:THR:HB	1.72	0.55
6:B:427:LEU:HD13	20:B:803:CLA:OBD	2.07	0.55
20:B:826:CLA:H62	22:B:844:BCR:H321	1.88	0.55
10:F:20:GLN:O	10:F:21:ALA:HB3	2.05	0.55
10:F:25:LEU:HD21	10:F:46:MET:HB3	1.84	0.55
12:H:25:GLY:HA3	12:H:27:ASP:CG	2.27	0.55
15:K:62:ALA:O	15:K:65:ALA:CB	2.55	0.55
15:K:72:VAL:HG13	15:K:73:GLY:N	2.22	0.55
16:L:121:THR:OG1	16:L:122:GLY:N	2.38	0.55
20:L:202:CLA:H141	20:L:203:CLA:H93	1.89	0.55
16:L:50:LEU:HG	16:L:51:LEU:CD2	2.37	0.55
17:N:82:PHE:H	17:N:82:PHE:HD2	1.55	0.55
20:1:201:CLA:HBA2	20:1:201:CLA:CMA	2.26	0.54
5:A:24:ARG:O	5:A:25:ASP:C	2.46	0.54
5:A:541:VAL:CG1	5:A:615:HIS:CD2	2.72	0.54
20:A:806:CLA:H51	20:A:828:CLA:C4C	2.37	0.54
20:A:838:CLA:H62	20:A:852:CLA:H193	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:841:CLA:HAA2	20:L:202:CLA:HMB1	1.88	0.54
6:B:154:TRP:O	6:B:157:LEU:N	2.30	0.54
6:B:197:VAL:O	6:B:197:VAL:HG12	2.06	0.54
6:B:476:ILE:HG22	6:B:479:SER:OG	2.08	0.54
6:B:575:ASP:O	6:B:579:ALA:N	2.37	0.54
20:B:807:CLA:H2	20:B:807:CLA:H71	1.89	0.54
7:C:75:ARG:NH2	8:D:110:GLN:OE1	2.36	0.54
8:D:30:ALA:O	16:L:18:PRO:CB	2.51	0.54
21:R:109:LMU:H5'	21:R:109:LMU:O5B	2.07	0.54
3:3:156:PRO:O	3:3:157:ALA:C	2.46	0.54
3:3:94:ARG:C	3:3:97:PHE:CE1	2.81	0.54
4:4:114:SER:O	4:4:117:GLN:N	2.40	0.54
4:4:41:VAL:CG1	4:4:41:VAL:O	2.48	0.54
4:4:89:THR:CA	4:4:90:LEU:HD22	2.37	0.54
5:A:160:SER:O	5:A:163:GLN:CG	2.36	0.54
5:A:338:PHE:CE1	20:A:840:CLA:HBB1	2.42	0.54
5:A:337:PRO:HD2	20:A:840:CLA:HHC	1.88	0.54
6:B:437:TYR:CG	6:B:616:LEU:HD22	2.41	0.54
6:B:596:TRP:O	6:B:597:LYS:CB	2.54	0.54
6:B:707:LEU:HD13	25:B:848:LMG:H301	1.88	0.54
6:B:299:HIS:HE1	20:B:820:CLA:HMD1	1.72	0.54
10:F:104:TYR:HD2	10:F:104:TYR:O	1.88	0.54
11:G:18:LEU:C	11:G:21:PHE:H	2.10	0.54
11:G:19:GLY:O	11:G:22:VAL:N	2.40	0.54
16:L:58:LEU:HA	16:L:146:GLY:O	2.07	0.54
17:N:63:ASP:N	17:N:64:ASP:HB2	2.22	0.54
17:N:63:ASP:N	17:N:64:ASP:HB3	2.10	0.54
20:R:107:CLA:HBA2	20:R:107:CLA:HBD	1.89	0.54
1:1:29:LEU:O	1:1:31:GLU:N	2.41	0.54
2:2:166:ASN:OD1	2:2:169:LEU:CD1	2.55	0.54
2:2:170:ALA:O	2:2:171:MET:C	2.45	0.54
2:2:182:ILE:C	2:2:204:ILE:O	2.46	0.54
4:4:104:ARG:HA	4:4:107:GLN:NE2	2.22	0.54
4:4:163:PHE:O	4:4:166:PHE:N	2.40	0.54
4:4:68:GLY:C	4:4:69:ILE:O	2.46	0.54
4:4:69:ILE:CG2	4:4:70:ILE:N	2.52	0.54
5:A:229:ILE:HG13	5:A:243:PRO:HB3	1.90	0.54
5:A:479:ASP:OD1	5:A:536:THR:O	2.26	0.54
5:A:668:TYR:CE1	6:B:445:ALA:HB2	2.41	0.54
5:A:700:TRP:CZ3	20:A:852:CLA:O1D	2.60	0.54
5:A:714:LEU:HA	10:F:149:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:216:LEU:CD1	22:A:843:BCR:H352	2.38	0.54
6:B:172:GLU:C	6:B:176:ASN:HB2	2.27	0.54
6:B:463:ILE:O	6:B:464:GLN:CB	2.55	0.54
6:B:625:TRP:CE3	6:B:625:TRP:C	2.81	0.54
6:B:732:LYS:HG3	6:B:734:GLY:HA2	1.87	0.54
20:B:822:CLA:H61	20:B:822:CLA:CMA	2.37	0.54
20:B:851:CLA:H41	20:B:851:CLA:HMB2	1.88	0.54
9:E:48:ASN:OD1	9:E:48:ASN:C	2.45	0.54
12:H:27:ASP:O	12:H:29:PRO:HD3	2.06	0.54
12:H:67:TYR:CD1	12:H:67:TYR:C	2.81	0.54
16:L:160:VAL:O	16:L:160:VAL:CG2	2.29	0.54
16:L:55:GLU:HG3	20:L:207:CLA:C1A	2.37	0.54
1:1:149:LYS:HB3	20:1:206:CLA:CMC	2.37	0.54
1:1:32:VAL:HG21	20:1:211:CLA:C1D	2.37	0.54
4:4:42:GLN:NE2	4:4:119:PRO:HB2	2.23	0.54
5:A:124:TRP:HA	5:A:124:TRP:CE3	2.41	0.54
5:A:137:GLY:C	5:A:139:GLY:H	2.10	0.54
5:A:308:ILE:CD1	20:A:816:CLA:C8	2.85	0.54
5:A:618:TRP:HB2	5:A:656:PHE:CE1	2.43	0.54
5:A:672:LEU:HD23	5:A:672:LEU:H	1.71	0.54
20:A:808:CLA:CMB	20:A:809:CLA:H11	2.38	0.54
20:A:826:CLA:H43	20:A:826:CLA:CGA	2.36	0.54
5:A:83:PHE:HA	5:A:86:LEU:HD23	1.90	0.54
6:B:462:TRP:CZ3	20:B:832:CLA:CBC	2.91	0.54
6:B:475:ASP:O	6:B:479:SER:OG	2.26	0.54
20:B:836:CLA:C12	22:F:203:BCR:H311	2.37	0.54
7:C:39:ILE:HG23	7:C:40:ALA:N	2.23	0.54
10:F:152:ASN:H	10:F:152:ASN:ND2	2.05	0.54
22:F:202:BCR:HC8	22:F:202:BCR:C33	2.36	0.54
20:K:101:CLA:HBC3	20:K:101:CLA:HHD	1.89	0.54
21:N:101:LMU:H32	21:N:101:LMU:O6'	2.07	0.54
17:N:41:LYS:CB	17:N:42:PHE:CA	2.83	0.54
19:Q:2:FRU:C5	19:Q:2:FRU:O1	2.54	0.54
2:2:137:TYR:CD1	2:2:138:PRO:CD	2.89	0.54
2:2:198:ALA:O	2:2:199:ASP:CG	2.46	0.54
3:3:106:TYR:HB3	3:3:107:TRP:HD1	1.71	0.54
4:4:99:HIS:HD1	4:4:103:ILE:CD1	2.21	0.54
4:4:99:HIS:O	4:4:103:ILE:HD11	2.02	0.54
4:4:119:PRO:HD2	4:4:120:ILE:HD12	1.89	0.54
4:4:36:ASN:O	4:4:39:TRP:CG	2.60	0.54
4:4:38:ARG:CG	4:4:38:ARG:NH1	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:803:CLA:C4	20:A:838:CLA:H8	2.37	0.54
20:A:806:CLA:C7	20:A:806:CLA:H2	2.36	0.54
6:B:124:TRP:CZ2	6:B:135:LEU:HD22	2.43	0.54
6:B:224:PRO:HB3	6:B:227:THR:HB	1.89	0.54
6:B:431:PHE:HE2	20:B:830:CLA:CED	2.20	0.54
5:A:705:GLU:CB	6:B:545:LYS:HZ2	2.20	0.54
20:B:806:CLA:HHB	20:B:827:CLA:HBB2	1.90	0.54
15:K:17:LEU:HD22	15:K:18:MET:CA	2.36	0.54
6:B:25:ILE:HG22	22:L:210:BCR:C28	2.28	0.54
18:R:32:UNK:CB	18:R:33:UNK:CA	2.76	0.54
1:1:183:ASP:HB3	1:1:184:PRO:HD2	1.90	0.54
21:1:218:LMU:H3O2	21:1:218:LMU:C1B	2.21	0.54
2:2:54:TRP:CD2	20:2:311:CLA:O1D	2.60	0.54
20:4:319:CLA:HED2	20:4:319:CLA:H2A	0.71	0.54
4:4:88:SER:HB3	4:4:89:THR:HG22	1.90	0.54
5:A:618:TRP:CD1	5:A:618:TRP:O	2.60	0.54
5:A:622:SER:OG	5:A:642:PHE:HB2	2.07	0.54
5:A:733:VAL:HG11	20:A:838:CLA:C3D	2.37	0.54
5:A:731:ARG:O	5:A:735:VAL:HG23	2.08	0.54
20:A:815:CLA:HBB1	22:A:843:BCR:C35	2.38	0.54
5:A:378:SER:OG	20:A:825:CLA:HBC2	2.08	0.54
20:A:826:CLA:H122	20:A:826:CLA:H171	1.89	0.54
21:A:853:LMU:C2B	21:A:853:LMU:H3'	2.34	0.54
6:B:120:VAL:HA	6:B:123:TRP:HE1	1.66	0.54
6:B:166:SER:C	6:B:168:PHE:H	2.09	0.54
6:B:544:SER:O	6:B:546:LEU:N	2.41	0.54
6:B:550:LYS:CG	6:B:550:LYS:O	2.54	0.54
20:B:803:CLA:C4C	20:B:803:CLA:H52	2.38	0.54
20:B:830:CLA:CBB	22:F:202:BCR:H272	2.36	0.54
20:B:838:CLA:HMC1	20:B:838:CLA:HBC2	1.90	0.54
20:B:839:CLA:HMC1	20:B:839:CLA:CBC	2.27	0.54
10:F:23:LYS:HD3	10:F:23:LYS:N	2.20	0.54
11:G:85:ILE:O	11:G:86:LEU:HB2	2.08	0.54
20:H:103:CLA:H42	20:H:103:CLA:HAA1	1.90	0.54
16:L:39:ASN:O	16:L:52:ARG:NH2	2.24	0.54
17:N:62:SER:C	17:N:66:ASP:H	2.10	0.54
17:N:65:LEU:CG	17:N:65:LEU:O	2.54	0.54
20:1:215:CLA:CED	20:1:215:CLA:CMA	2.86	0.54
2:2:171:MET:SD	2:2:172:LEU:CA	2.95	0.54
3:3:66:MET:HG2	3:3:195:LEU:HD11	1.88	0.54
22:3:314:BCR:C31	22:3:314:BCR:C8	2.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:53:TRP:HA	3:3:56:TYR:HD2	1.73	0.54
3:3:95:THR:HB	3:3:96:GLY:O	2.08	0.54
4:4:107:GLN:CA	20:4:302:CLA:HMA2	2.31	0.54
4:4:70:ILE:HG13	4:4:71:ASN:H	1.71	0.54
5:A:162:LEU:C	5:A:165:TYR:HB3	2.28	0.54
5:A:680:LEU:HD21	6:B:617:MET:HE3	1.89	0.54
6:B:596:TRP:O	6:B:597:LYS:HB3	2.07	0.54
6:B:304:ILE:HD11	20:B:817:CLA:HED2	1.86	0.54
20:B:828:CLA:HAA2	20:B:828:CLA:CED	2.37	0.54
8:D:46:TYR:CE1	8:D:80:LYS:HE2	2.34	0.54
9:E:61:THR:CG2	9:E:62:ARG:H	2.08	0.54
17:N:46:PHE:C	17:N:47:THR:HG23	2.17	0.54
20:1:202:CLA:O2A	20:1:202:CLA:HMA3	2.08	0.54
4:4:191:ASN:C	4:4:191:ASN:OD1	2.44	0.54
4:4:40:PHE:HB3	4:4:43:ALA:HB1	1.75	0.54
4:4:92:VAL:CG1	4:4:93:ILE:N	2.69	0.54
5:A:250:LEU:O	5:A:252:ARG:HG2	2.08	0.54
5:A:455:PHE:O	20:A:831:CLA:CBB	2.56	0.54
5:A:591:GLN:OE1	5:A:600:LEU:HD21	2.07	0.54
5:A:207:LEU:HD13	20:A:819:CLA:HBB2	1.88	0.54
20:A:830:CLA:H162	22:L:210:BCR:H362	1.88	0.54
20:A:822:CLA:ND	22:A:845:BCR:C19	2.71	0.54
21:A:855:LMU:H4O1	21:A:855:LMU:C1B	2.20	0.54
6:B:278:LEU:HD12	20:B:814:CLA:HMA1	1.87	0.54
6:B:373:THR:O	6:B:377:TYR:N	2.31	0.54
6:B:415:LYS:CG	6:B:416:GLU:OE2	2.55	0.54
6:B:462:TRP:HZ3	20:B:832:CLA:HBC1	1.72	0.54
6:B:545:LYS:HG2	9:E:74:TYR:CE2	2.43	0.54
20:B:803:CLA:H71	20:B:803:CLA:HMC2	1.90	0.54
20:B:808:CLA:H143	20:B:825:CLA:H18	1.90	0.54
20:B:811:CLA:C4	20:B:816:CLA:HBC1	2.37	0.54
8:D:87:GLY:H	8:D:90:LEU:H	1.56	0.54
12:H:14:ILE:HD11	12:H:17:THR:H	1.73	0.54
21:K:104:LMU:O4'	21:K:105:LMU:O1'	2.26	0.54
16:L:60:HIS:HD2	20:L:208:CLA:CED	2.20	0.54
1:1:185:TRP:CA	1:1:186:HIS:HD1	2.18	0.54
2:2:125:PHE:O	2:2:126:PRO:C	2.46	0.54
2:2:42:ARG:CB	2:2:45:VAL:HB	2.37	0.54
4:4:40:PHE:CD1	4:4:40:PHE:N	2.72	0.54
5:A:144:GLN:CG	5:A:145:ILE:H	2.20	0.54
5:A:629:ASN:HD21	5:A:633:VAL:CG2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:831:CLA:O1D	16:L:73:PRO:O	2.26	0.54
5:A:723:ARG:O	20:A:837:CLA:CBB	2.56	0.54
5:A:84:GLY:C	5:A:87:SER:O	2.46	0.54
6:B:301:ILE:O	6:B:301:ILE:CG2	2.56	0.54
6:B:308:HIS:HD1	6:B:309:ILE:N	2.05	0.54
20:B:815:CLA:H112	20:B:833:CLA:H3A	1.90	0.54
22:B:845:BCR:C8	22:B:845:BCR:H311	2.38	0.54
10:F:22:LEU:C	10:F:25:LEU:HD13	2.27	0.54
1:1:161:PHE:HD1	20:1:203:CLA:CBB	2.21	0.54
1:1:160:GLY:O	1:1:162:CYS:N	2.41	0.54
20:1:202:CLA:CED	20:1:202:CLA:CHA	2.84	0.54
20:2:308:CLA:HBA1	21:3:321:LMU:H51	1.89	0.54
5:A:118:PRO:HB3	5:A:150:PHE:CD2	2.43	0.54
5:A:242:ILE:HG12	5:A:243:PRO:HG3	1.90	0.54
5:A:255:LEU:HD11	5:A:280:PHE:HZ	1.72	0.54
5:A:328:LYS:CD	5:A:332:GLU:HG3	2.28	0.54
5:A:361:ASN:O	5:A:365:LEU:N	2.39	0.54
5:A:656:PHE:O	5:A:659:ALA:N	2.40	0.54
20:A:819:CLA:CAA	20:A:823:CLA:HBB2	2.37	0.54
20:A:824:CLA:HAA2	20:A:825:CLA:OBD	2.08	0.54
20:A:841:CLA:CGA	20:A:841:CLA:C1A	2.86	0.54
6:B:233:TYR:HB3	6:B:254:ILE:O	2.08	0.54
6:B:456:GLU:HA	6:B:514:PRO:HD3	1.90	0.54
6:B:513:GLY:O	6:B:515:GLY:N	2.41	0.54
6:B:546:LEU:HD12	6:B:570:ILE:HD13	1.89	0.54
6:B:681:ALA:O	6:B:684:ARG:N	2.33	0.54
20:B:803:CLA:H2A	20:B:803:CLA:CED	2.31	0.54
6:B:167:TRP:CZ2	20:B:809:CLA:HMA1	2.43	0.54
6:B:190:TRP:CA	20:B:812:CLA:HBB2	2.38	0.54
6:B:655:LEU:HD22	20:B:839:CLA:CBB	2.37	0.54
7:C:35:LYS:C	7:C:37:LYS:H	2.10	0.54
8:D:102:ARG:HH21	8:D:110:GLN:HB2	1.72	0.54
12:H:77:LEU:HB3	12:H:78:PRO:CD	2.36	0.54
4:4:193:ILE:HG21	14:J:42:PHE:CD1	2.42	0.54
16:L:58:LEU:HD11	16:L:153:TRP:HZ2	1.73	0.54
21:R:101:LMU:C1	21:R:101:LMU:C6	2.76	0.54
2:2:102:ILE:CG1	20:2:312:CLA:HMD2	2.36	0.53
2:2:116:PRO:HB2	2:2:136:GLY:CA	2.35	0.53
4:4:147:LEU:HD21	4:4:148:GLU:CB	2.30	0.53
4:4:154:ILE:HG22	20:4:309:CLA:CHA	2.38	0.53
20:A:804:CLA:C2A	20:A:804:CLA:O2D	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:302:CLA:CMC	20:A:814:CLA:HBA2	2.29	0.53
20:A:822:CLA:NB	22:A:845:BCR:H15C	2.22	0.53
6:B:580:VAL:CG1	6:B:710:LEU:HD21	2.37	0.53
6:B:626:LEU:O	6:B:627:ASN:HB2	2.08	0.53
7:C:5:VAL:C	7:C:65:VAL:CG2	2.68	0.53
21:G:101:LMU:H4'	21:G:101:LMU:H6B	1.71	0.53
13:I:2:ILE:HG13	13:I:3:ASN:OD1	2.08	0.53
18:R:36:UNK:C	18:R:38:UNK:N	2.65	0.53
1:1:136:ASP:HB2	1:1:140:LEU:HB3	1.88	0.53
2:2:56:MET:SD	2:2:169:LEU:HA	2.49	0.53
2:2:205:PHE:HE1	2:2:206:ALA:HA	1.71	0.53
4:4:42:GLN:O	4:4:43:ALA:C	2.47	0.53
5:A:163:GLN:O	5:A:166:CYS:SG	2.66	0.53
5:A:308:ILE:O	5:A:311:LEU:HB2	2.08	0.53
5:A:527:VAL:HG13	5:A:528:ALA:H	1.73	0.53
5:A:638:THR:OG1	5:A:641:ASN:ND2	2.41	0.53
5:A:78:VAL:O	5:A:82:HIS:CB	2.55	0.53
20:A:819:CLA:C9	22:A:845:BCR:H371	2.21	0.53
20:A:822:CLA:C1C	22:A:845:BCR:H17C	2.38	0.53
5:A:453:LEU:HD21	20:A:835:CLA:CBB	2.38	0.53
5:A:214:GLY:CA	22:A:844:BCR:H15C	2.38	0.53
20:A:850:CLA:HMB3	20:A:851:CLA:CAD	2.38	0.53
6:B:132:ASN:HA	6:B:135:LEU:HG	1.90	0.53
6:B:160:LYS:HE3	6:B:161:TRP:CE2	2.43	0.53
6:B:203:ARG:HB3	6:B:270:LEU:HD12	1.89	0.53
6:B:50:HIS:HA	6:B:53:GLN:H	1.73	0.53
6:B:174:ARG:HH12	20:B:822:CLA:CMD	2.20	0.53
20:B:807:CLA:C14	20:B:825:CLA:H91	2.35	0.53
9:E:40:ARG:H	9:E:46:PHE:HE1	1.55	0.53
10:F:123:VAL:HG21	10:F:128:SER:OG	2.08	0.53
20:G:102:CLA:O1D	20:G:102:CLA:CAA	2.56	0.53
11:G:47:GLY:N	11:G:48:ASP:HA	2.16	0.53
13:I:29:GLU:HA	13:I:29:GLU:OE2	2.08	0.53
16:L:56:VAL:HG13	20:L:208:CLA:HED3	1.88	0.53
2:2:137:TYR:O	2:2:143:PHE:CE2	2.61	0.53
2:2:181:HIS:CE1	20:2:304:CLA:ND	2.75	0.53
3:3:56:TYR:O	3:3:60:ILE:HD12	2.07	0.53
5:A:148:GLY:C	5:A:149:PHE:O	2.43	0.53
5:A:439:ARG:HG2	5:A:562:PHE:CE2	2.43	0.53
5:A:449:VAL:CG2	20:A:836:CLA:HMC3	2.38	0.53
5:A:723:ARG:HH11	5:A:723:ARG:HG3	1.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:807:CLA:HHB	20:A:808:CLA:HMB3	1.89	0.53
20:A:838:CLA:C4A	20:A:838:CLA:HBA2	2.32	0.53
6:B:20:ARG:CG	6:B:20:ARG:HH11	2.21	0.53
6:B:222:LEU:O	6:B:222:LEU:HD23	2.07	0.53
6:B:406:ASN:C	6:B:406:ASN:HD22	2.11	0.53
5:A:709:TRP:CH2	6:B:417:ALA:HB2	2.44	0.53
6:B:533:ILE:O	6:B:537:GLY:N	2.30	0.53
21:B:801:LMU:H62	21:B:801:LMU:C10	2.29	0.53
6:B:648:TRP:CZ2	20:B:850:CLA:H62	2.43	0.53
9:E:50:GLY:HA3	9:E:69:PHE:HB2	1.91	0.53
20:L:208:CLA:HAC2	22:L:210:BCR:HC42	1.89	0.53
1:1:105:ILE:O	1:1:108:VAL:HG12	2.08	0.53
1:1:161:PHE:H	20:1:203:CLA:HBB2	1.66	0.53
3:3:49:ILE:HG13	3:3:52:LYS:HB2	1.90	0.53
5:A:187:HIS:NE2	20:A:811:CLA:C4C	2.53	0.53
20:A:826:CLA:C20	22:J:102:BCR:C16	2.87	0.53
6:B:304:ILE:HD11	20:B:817:CLA:HED3	1.90	0.53
1:1:27:LEU:CD2	6:B:314:ARG:CD	2.69	0.53
6:B:503:GLU:HB3	6:B:507:SER:CA	2.39	0.53
6:B:573:TRP:O	6:B:577:TYR:N	2.31	0.53
22:B:846:BCR:C33	22:B:846:BCR:C8	2.85	0.53
7:C:31:TRP:HD1	7:C:32:GLY:N	2.06	0.53
21:D:201:LMU:H1B	21:D:201:LMU:O6B	2.06	0.53
10:F:2:ILE:HG22	10:F:3:ALA:H	1.73	0.53
10:F:44:ALA:HB1	10:F:48:LYS:HB3	1.91	0.53
22:I:103:BCR:C38	22:I:103:BCR:C40	2.73	0.53
21:K:105:LMU:O2B	21:K:105:LMU:C4'	2.52	0.53
17:N:61:LEU:HG	17:N:62:SER:N	2.12	0.53
19:Z:1:GLC:HO2	19:Z:2:FRU:H5	1.69	0.53
2:2:97:VAL:HA	2:2:100:VAL:HG13	1.89	0.53
2:2:148:TRP:HH2	21:2:313:LMU:H12	1.72	0.53
5:A:253:ASP:O	5:A:256:ALA:CB	2.57	0.53
5:A:389:TYR:CE1	5:A:625:TRP:CG	2.96	0.53
20:A:807:CLA:CHD	20:A:807:CLA:HBC2	2.38	0.53
20:A:826:CLA:H122	20:A:826:CLA:C17	2.37	0.53
5:A:448:TRP:CD1	20:A:830:CLA:CED	2.92	0.53
6:B:87:ILE:O	6:B:121:TYR:HE2	1.91	0.53
6:B:492:ILE:HD13	6:B:492:ILE:N	2.14	0.53
20:B:814:CLA:CHD	20:B:814:CLA:HBC2	2.27	0.53
5:A:586:ARG:CG	7:C:49:VAL:HG21	2.38	0.53
8:D:28:ILE:O	8:D:66:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:48:ASP:HB3	11:G:49:THR:HG21	1.86	0.53
21:H:108:LMU:O3'	21:H:108:LMU:C5B	2.57	0.53
12:H:34:SER:OG	12:H:36:GLN:NE2	2.41	0.53
14:J:31:ARG:HH21	20:J:103:CLA:C3B	2.21	0.53
16:L:123:ARG:O	16:L:124:LYS:HE3	2.09	0.53
16:L:96:SER:HG	16:L:143:PHE:HD2	1.48	0.53
16:L:48:ASN:HB2	16:L:50:LEU:HD22	1.91	0.53
20:2:302:CLA:CMC	20:2:302:CLA:HBC2	2.32	0.53
4:4:128:ALA:CA	4:4:143:PHE:CZ	2.91	0.53
5:A:291:THR:O	5:A:293:GLY:N	2.36	0.53
5:A:379:MET:SD	5:A:512:SER:HB2	2.49	0.53
5:A:467:MET:HE1	5:A:475:ASP:O	2.09	0.53
5:A:466:THR:O	5:A:470:LEU:CG	2.57	0.53
5:A:615:HIS:ND1	20:A:834:CLA:HBC3	2.22	0.53
5:A:650:ASN:O	5:A:653:LEU:HD13	2.08	0.53
5:A:707:ILE:C	5:A:711:HIS:HD2	2.12	0.53
5:A:308:ILE:HD13	20:A:816:CLA:H91	1.72	0.53
20:A:825:CLA:CMC	20:A:825:CLA:CBC	2.63	0.53
6:B:20:ARG:CB	6:B:20:ARG:HH11	2.20	0.53
6:B:529:THR:HA	6:B:532:LEU:HD23	1.89	0.53
6:B:551:LYS:O	6:B:553:PHE:CE2	2.61	0.53
6:B:668:ARG:HH12	6:B:672:GLN:HG2	1.71	0.53
6:B:75:GLU:HB2	6:B:132:ASN:HD22	1.73	0.53
20:B:823:CLA:CGA	20:B:837:CLA:HAA1	2.37	0.53
22:B:846:BCR:C19	20:B:850:CLA:H112	2.28	0.53
20:B:850:CLA:CBB	20:B:851:CLA:C1B	2.80	0.53
7:C:74:THR:OG1	7:C:80:ALA:HB3	2.07	0.53
8:D:31:GLY:O	8:D:32:SER:HB2	2.09	0.53
10:F:126:ALA:O	10:F:128:SER:OG	2.17	0.53
10:F:23:LYS:CA	10:F:24:LYS:HZ3	2.22	0.53
11:G:19:GLY:HA2	11:G:22:VAL:H	1.74	0.53
11:G:69:VAL:O	11:G:73:ALA:CB	2.57	0.53
20:B:851:CLA:H142	22:I:101:BCR:HC42	1.88	0.53
12:H:65:LEU:HD11	16:L:90:GLY:HA2	1.90	0.53
2:2:42:ARG:C	2:2:45:VAL:H	2.11	0.53
4:4:75:TRP:HD1	20:4:311:CLA:HMD3	1.63	0.53
20:4:318:CLA:CHD	20:4:318:CLA:CBC	2.80	0.53
4:4:68:GLY:C	4:4:71:ASN:HB2	2.20	0.53
4:4:94:GLU:HG2	4:4:95:PHE:CZ	2.38	0.53
5:A:22:VAL:HG12	5:A:23:ASP:N	2.22	0.53
5:A:253:ASP:O	5:A:256:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:420:ARG:HG2	5:A:421:ASP:N	2.23	0.53
5:A:55:TRP:CD2	5:A:729:GLN:NE2	2.77	0.53
5:A:64:PHE:HE2	20:A:805:CLA:HMC1	1.74	0.53
20:A:826:CLA:CGA	20:A:826:CLA:C1A	2.87	0.53
6:B:189:ALA:CB	20:B:826:CLA:C20	2.69	0.53
6:B:188:LEU:HG	6:B:189:ALA:N	2.24	0.53
6:B:330:ILE:O	6:B:330:ILE:CD1	2.57	0.53
6:B:174:ARG:CB	20:B:811:CLA:HBC2	2.27	0.53
6:B:431:PHE:HE2	20:B:830:CLA:HED3	1.73	0.53
7:C:28:MET:SD	8:D:122:LYS:C	2.87	0.53
10:F:144:LEU:HG	10:F:145:LEU:HD23	1.91	0.53
10:F:149:LEU:HD23	10:F:153:ASN:ND2	2.23	0.53
6:B:302:LYS:HD3	11:G:49:THR:HA	1.91	0.53
22:I:103:BCR:H291	22:L:210:BCR:H281	1.89	0.53
22:I:101:BCR:H272	22:I:103:BCR:H352	1.90	0.53
20:A:807:CLA:HMB2	22:J:102:BCR:HC7	1.88	0.53
16:L:162:ASP:HB2	16:L:163:LEU:HA	1.91	0.53
17:N:37:PHE:CD2	17:N:37:PHE:N	2.76	0.53
17:N:69:CYS:O	17:N:70:GLU:O	2.26	0.53
17:N:69:CYS:O	17:N:72:LYS:CD	2.57	0.53
20:1:206:CLA:CGD	21:4:301:LMU:O2'	2.57	0.53
2:2:51:HIS:HA	2:2:54:TRP:HB2	1.91	0.53
5:A:281:LEU:HB2	5:A:301:HIS:HD2	1.73	0.53
5:A:567:ARG:NH2	5:A:567:ARG:HB3	2.23	0.53
20:A:823:CLA:C9	20:A:823:CLA:OBD	2.42	0.53
6:B:271:THR:OG1	6:B:272:ASP:N	2.41	0.53
6:B:302:LYS:O	6:B:303:TYR:CB	2.35	0.53
6:B:606:VAL:C	6:B:608:GLN:H	2.12	0.53
20:B:823:CLA:C2B	22:B:845:BCR:C35	2.87	0.53
10:F:128:SER:O	10:F:130:LEU:HD23	2.09	0.53
10:F:58:LYS:O	10:F:60:GLY:N	2.42	0.53
11:G:14:LEU:HG	11:G:14:LEU:O	2.07	0.53
11:G:13:GLY:O	11:G:16:LEU:HB2	2.07	0.53
6:B:294:ASN:CB	11:G:36:PRO:HD2	2.35	0.53
12:H:23:VAL:O	12:H:24:TYR:C	2.47	0.53
15:K:51:ASP:O	15:K:52:PRO:C	2.46	0.53
17:N:42:PHE:H	17:N:43:PRO:HD2	1.71	0.53
17:N:44:GLU:C	17:N:46:PHE:H	2.11	0.53
5:A:438:HIS:HB2	5:A:441:ALA:CB	2.39	0.53
5:A:40:PHE:N	5:A:44:ILE:HG21	2.24	0.53
5:A:473:PRO:O	5:A:474:GLN:C	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:143:LEU:C	6:B:145:LEU:N	2.62	0.53
6:B:44:GLN:CD	6:B:163:PRO:HB2	2.28	0.53
6:B:390:GLY:CA	22:B:845:BCR:HC22	2.38	0.53
6:B:78:VAL:HG23	6:B:78:VAL:O	2.08	0.53
22:B:846:BCR:C19	20:B:850:CLA:C15	2.80	0.53
20:B:850:CLA:C12	20:B:850:CLA:H71	2.38	0.53
8:D:40:ALA:HA	8:D:44:GLU:O	2.08	0.53
10:F:61:LEU:CD2	10:F:69:PRO:HB2	2.31	0.53
12:H:25:GLY:CA	12:H:27:ASP:CB	2.75	0.53
16:L:108:LYS:C	16:L:108:LYS:HE2	2.29	0.53
20:1:207:CLA:HAA2	20:1:207:CLA:CBD	2.39	0.53
1:1:57:ILE:O	1:1:59:VAL:CA	2.56	0.53
2:2:79:TRP:CG	2:2:79:TRP:O	2.62	0.53
5:A:441:ALA:HA	5:A:444:SER:HB3	1.91	0.53
20:A:825:CLA:O1D	20:A:825:CLA:CBA	2.46	0.53
20:A:841:CLA:H92	22:L:210:BCR:C32	2.36	0.53
21:A:854:LMU:H61	21:A:854:LMU:H21	1.85	0.53
21:A:855:LMU:H91	21:A:855:LMU:C1	2.31	0.53
6:B:127:ILE:CG1	6:B:193:HIS:HE1	2.21	0.53
6:B:338:LEU:O	6:B:339:ALA:HB3	2.09	0.53
6:B:378:ILE:HG22	6:B:379:ALA:N	2.24	0.53
6:B:719:PHE:CZ	20:B:825:CLA:H71	2.44	0.53
6:B:22:TRP:CE2	20:B:838:CLA:HMB1	2.44	0.53
6:B:717:TYR:O	20:B:849:CLA:HED3	2.09	0.53
9:E:86:GLU:CG	9:E:87:VAL:N	2.30	0.53
6:B:295:PHE:O	11:G:33:LYS:HB2	2.09	0.53
21:H:105:LMU:H2'	21:H:105:LMU:C6'	2.39	0.53
15:K:31:ASN:H	15:K:32:ARG:NH1	2.07	0.53
17:N:45:ASN:CA	17:N:57:LYS:NZ	2.72	0.53
17:N:58:VAL:CG1	17:N:59:PRO:CD	2.87	0.53
2:2:181:HIS:NE2	20:2:304:CLA:C4D	2.72	0.52
2:2:64:ILE:CG2	2:2:65:PRO:HD3	2.39	0.52
3:3:132:TRP:CZ3	3:3:155:GLU:OE1	2.57	0.52
3:3:52:LYS:C	3:3:56:TYR:HD2	2.10	0.52
4:4:121:PHE:CD2	4:4:122:LYS:N	2.77	0.52
4:4:147:LEU:CD1	4:4:148:GLU:CB	2.85	0.52
4:4:152:LYS:CA	4:4:154:ILE:HG12	2.32	0.52
4:4:69:ILE:O	4:4:71:ASN:CB	2.56	0.52
5:A:197:GLN:OE1	5:A:351:THR:O	2.27	0.52
5:A:293:GLY:O	5:A:294:LEU:HB3	2.08	0.52
5:A:430:ASP:H	5:A:433:ASP:CG	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:44:ILE:O	5:A:45:ALA:C	2.47	0.52
5:A:114:THR:O	5:A:525:ASN:ND2	2.42	0.52
5:A:725:LEU:HD21	20:A:838:CLA:HMD3	1.91	0.52
22:A:847:BCR:H17C	20:A:851:CLA:H172	1.91	0.52
6:B:431:PHE:CE2	20:B:830:CLA:HED3	2.44	0.52
20:B:804:CLA:CHD	22:I:103:BCR:H401	2.40	0.52
6:B:193:HIS:HD2	20:B:812:CLA:NC	2.07	0.52
20:B:830:CLA:CBB	22:F:202:BCR:C23	2.87	0.52
8:D:86:LEU:HD13	8:D:90:LEU:HG	1.90	0.52
10:F:90:PHE:HA	22:F:202:BCR:H392	1.91	0.52
10:F:92:TYR:C	10:F:92:TYR:CD2	2.82	0.52
20:G:102:CLA:C1	20:G:102:CLA:H3A	2.38	0.52
11:G:43:HIS:O	11:G:45:GLU:CA	2.56	0.52
20:H:102:CLA:C4C	22:I:103:BCR:C2	2.66	0.52
20:2:302:CLA:C3A	20:2:302:CLA:CGA	2.85	0.52
2:2:64:ILE:HG22	2:2:65:PRO:HD3	1.91	0.52
3:3:208:PRO:HB3	3:3:210:GLN:CD	2.29	0.52
4:4:53:LEU:O	4:4:54:GLY:C	2.48	0.52
5:A:242:ILE:HG12	5:A:243:PRO:CG	2.39	0.52
20:A:841:CLA:C11	20:A:841:CLA:H61	2.38	0.52
20:A:824:CLA:CHC	22:A:846:BCR:H371	2.38	0.52
6:B:376:GLN:HB3	6:B:587:ILE:HD12	1.91	0.52
20:B:823:CLA:H52	20:B:837:CLA:HBD	1.90	0.52
6:B:707:LEU:HD11	20:B:827:CLA:H91	1.91	0.52
6:B:431:PHE:CE2	20:B:830:CLA:CED	2.92	0.52
6:B:458:ILE:HD11	20:F:205:CLA:CED	2.39	0.52
10:F:73:VAL:HG11	10:F:83:PHE:HB2	1.89	0.52
20:G:102:CLA:O1D	20:G:102:CLA:HAA2	2.09	0.52
20:J:103:CLA:CHD	20:J:103:CLA:CBC	2.83	0.52
14:J:25:LEU:HA	14:J:28:GLU:HB2	1.92	0.52
21:N:101:LMU:C3	21:N:101:LMU:O6'	2.56	0.52
20:R:107:CLA:HED3	20:R:107:CLA:C4D	2.34	0.52
18:R:39:UNK:CA	18:R:41:UNK:CB	2.88	0.52
2:2:148:TRP:CH2	21:2:313:LMU:H12	2.44	0.52
2:2:161:THR:HB	2:2:165:LYS:HB2	1.91	0.52
20:3:318:CLA:H172	20:3:318:CLA:C12	2.29	0.52
4:4:81:GLU:CA	4:4:81:GLU:OE2	2.50	0.52
5:A:214:GLY:O	5:A:215:SER:CB	2.56	0.52
5:A:265:GLY:HA2	5:A:272:LEU:HD21	1.92	0.52
5:A:40:PHE:H	5:A:44:ILE:CG2	2.22	0.52
5:A:91:LEU:O	20:A:807:CLA:HMC3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:368:LEU:HD12	20:A:825:CLA:H61	1.89	0.52
6:B:228:GLY:HA3	11:G:8:ILE:HB	1.90	0.52
20:B:811:CLA:H41	20:B:816:CLA:HBC1	1.85	0.52
20:B:821:CLA:HMD2	20:B:822:CLA:HBB2	1.88	0.52
6:B:185:VAL:CG2	22:B:843:BCR:H272	2.39	0.52
7:C:29:ILE:HG23	8:D:126:GLY:CA	2.39	0.52
8:D:122:LYS:NZ	8:D:124:ASN:OD1	2.43	0.52
8:D:43:GLU:HG3	8:D:44:GLU:H	1.74	0.52
21:F:201:LMU:H6E	21:F:201:LMU:C1B	2.39	0.52
21:K:105:LMU:C4	21:K:105:LMU:C6'	2.88	0.52
16:L:66:GLY:N	16:L:67:PRO:CD	2.72	0.52
17:N:42:PHE:CD1	17:N:43:PRO:CA	2.92	0.52
1:1:183:ASP:HB3	1:1:184:PRO:CD	2.40	0.52
1:1:183:ASP:OD1	4:4:89:THR:CB	2.57	0.52
21:2:318:LMU:C2B	21:2:318:LMU:C6B	2.88	0.52
2:2:97:VAL:CA	2:2:100:VAL:HG13	2.39	0.52
3:3:182:LYS:O	3:3:185:LYS:HB3	2.10	0.52
4:4:147:LEU:HD13	4:4:148:GLU:HB2	1.89	0.52
4:4:75:TRP:CD2	4:4:76:TYR:N	2.77	0.52
5:A:351:THR:HA	20:A:823:CLA:H191	1.92	0.52
5:A:536:THR:HA	5:A:539:PHE:HB3	1.91	0.52
5:A:641:ASN:H	5:A:641:ASN:HD22	1.57	0.52
5:A:690:LEU:HD21	6:B:661:PHE:HE1	1.75	0.52
5:A:716:VAL:O	20:A:837:CLA:HMD3	2.09	0.52
6:B:486:LEU:HD12	20:B:833:CLA:OBD	2.09	0.52
6:B:98:GLN:NE2	6:B:98:GLN:O	2.43	0.52
7:C:1:MET:SD	7:C:4:SER:OG	2.67	0.52
8:D:116:ASP:HB3	8:D:127:ARG:HH12	1.73	0.52
8:D:86:LEU:CD1	8:D:90:LEU:HG	2.39	0.52
10:F:91:LEU:O	10:F:94:ALA:O	2.26	0.52
21:H:108:LMU:H92	21:H:108:LMU:C3	2.23	0.52
12:H:70:ALA:O	12:H:71:ASN:HB2	2.09	0.52
20:A:830:CLA:H152	22:L:210:BCR:H363	1.90	0.52
20:3:302:CLA:O1D	5:A:246:HIS:CD2	2.62	0.52
3:3:47:GLY:C	3:3:49:ILE:H	2.10	0.52
4:4:73:PRO:CB	4:4:75:TRP:HB2	2.38	0.52
5:A:378:SER:OG	5:A:378:SER:O	2.28	0.52
5:A:545:HIS:ND1	20:A:834:CLA:CBB	2.68	0.52
5:A:603:PHE:CZ	5:A:735:VAL:HG22	2.45	0.52
20:A:808:CLA:HBB2	20:A:809:CLA:C4D	2.39	0.52
20:A:851:CLA:H152	20:A:851:CLA:H101	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:18:THR:O	6:B:21:ILE:N	2.29	0.52
6:B:274:ALA:O	6:B:278:LEU:HB2	2.08	0.52
20:B:821:CLA:H12	20:B:821:CLA:CAA	2.23	0.52
20:B:832:CLA:C1D	20:B:833:CLA:HBB2	2.39	0.52
20:B:832:CLA:HMC3	20:B:835:CLA:H2	1.91	0.52
7:C:11:CYS:C	7:C:13:GLY:H	2.12	0.52
9:E:80:ASN:HB3	9:E:82:TYR:CE2	2.44	0.52
11:G:28:ARG:HH21	11:G:29:GLU:N	2.06	0.52
11:G:44:PHE:H	11:G:45:GLU:HB3	1.73	0.52
11:G:45:GLU:CA	11:G:49:THR:CG2	2.77	0.52
20:A:830:CLA:C15	22:L:210:BCR:H361	2.38	0.52
17:N:62:SER:O	17:N:66:ASP:OD2	2.28	0.52
2:2:168:ARG:NE	2:2:168:ARG:HA	2.25	0.52
3:3:49:ILE:CG1	3:3:52:LYS:HB2	2.39	0.52
5:A:453:LEU:CB	5:A:547:PHE:HB2	2.34	0.52
20:A:826:CLA:HBD	20:A:826:CLA:HAA1	1.91	0.52
6:B:188:LEU:HG	6:B:189:ALA:H	1.75	0.52
6:B:207:VAL:O	6:B:208:ARG:O	2.27	0.52
6:B:273:VAL:O	6:B:277:HIS:CD2	2.61	0.52
6:B:387:PHE:O	6:B:391:PRO:HG3	2.09	0.52
6:B:464:GLN:OE1	6:B:469:LYS:CD	2.54	0.52
6:B:700:LEU:N	6:B:700:LEU:CD2	2.72	0.52
5:A:710:ALA:CB	20:B:803:CLA:HED2	2.40	0.52
20:B:830:CLA:CBB	22:F:202:BCR:H23C	2.39	0.52
7:C:12:ILE:O	7:C:38:GLN:HG2	2.09	0.52
7:C:39:ILE:CG1	7:C:40:ALA:N	2.65	0.52
21:F:201:LMU:C9	21:F:201:LMU:H22	2.38	0.52
17:N:34:THR:C	17:N:36:GLU:N	2.63	0.52
17:N:80:ASN:O	17:N:80:ASN:OD1	2.28	0.52
21:R:102:LMU:O6'	21:R:102:LMU:O1B	2.28	0.52
2:2:167:GLY:O	2:2:168:ARG:C	2.48	0.52
3:3:60:ILE:HA	3:3:63:ARG:HD2	1.92	0.52
20:4:304:CLA:HBC3	20:4:304:CLA:HMC1	1.91	0.52
4:4:36:ASN:OD1	4:4:39:TRP:CE2	2.56	0.52
4:4:58:MET:O	4:4:60:LEU:N	2.43	0.52
5:A:223:VAL:CG1	5:A:224:HIS:N	2.72	0.52
5:A:310:PHE:H	5:A:313:ALA:HB3	1.74	0.52
5:A:353:SER:O	5:A:354:TRP:CB	2.58	0.52
5:A:472:ARG:NE	5:A:474:GLN:HG3	2.14	0.52
5:A:62:HIS:O	20:A:828:CLA:HAA2	2.10	0.52
20:3:302:CLA:CMC	20:A:814:CLA:CBA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:160:LYS:HG3	6:B:161:TRP:N	2.20	0.52
6:B:326:ILE:O	6:B:326:ILE:HG12	2.09	0.52
6:B:8:PHE:O	6:B:35:ASP:CG	2.48	0.52
6:B:427:LEU:C	20:B:830:CLA:HED2	2.30	0.52
20:B:804:CLA:HBC2	20:B:804:CLA:HMC1	1.92	0.52
20:B:814:CLA:HMA2	20:B:814:CLA:O2A	2.09	0.52
8:D:113:HIS:HD2	8:D:118:VAL:HG21	1.72	0.52
8:D:33:THR:HG23	16:L:23:LEU:HD12	1.92	0.52
5:A:701:GLN:OE1	9:E:74:TYR:HE1	1.92	0.52
20:B:803:CLA:HBC1	22:F:202:BCR:C33	2.40	0.52
11:G:13:GLY:C	11:G:16:LEU:HG	2.30	0.52
16:L:162:ASP:N	16:L:162:ASP:OD2	2.35	0.52
16:L:56:VAL:CA	20:L:208:CLA:HED2	2.33	0.52
17:N:5:GLU:OE2	17:N:6:TYR:CA	2.57	0.52
17:N:65:LEU:C	17:N:66:ASP:OD2	2.48	0.52
21:R:104:LMU:O3B	21:R:104:LMU:O6B	2.28	0.52
2:2:98:GLU:OE2	20:2:312:CLA:C4D	2.57	0.52
4:4:118:ASP:CG	4:4:123:GLN:CB	2.75	0.52
4:4:123:GLN:CG	4:4:124:TYR:H	2.23	0.52
4:4:192:THR:HG23	4:4:193:ILE:CA	2.40	0.52
5:A:207:LEU:HA	5:A:211:LEU:CB	2.39	0.52
5:A:341:GLN:O	5:A:344:LYS:HB2	2.10	0.52
5:A:331:LEU:CD1	5:A:346:LEU:CB	2.60	0.52
5:A:691:MET:HB2	20:A:852:CLA:C1C	2.39	0.52
5:A:703:LEU:O	5:A:707:ILE:HG12	2.09	0.52
6:B:122:GLN:O	6:B:126:THR:CB	2.57	0.52
6:B:124:TRP:C	6:B:124:TRP:HD1	2.11	0.52
6:B:393:PHE:CE1	6:B:394:PHE:CE2	2.98	0.52
7:C:19:ARG:NE	8:D:121:GLU:OE2	2.43	0.52
8:D:36:LEU:HD21	8:D:45:PHE:CZ	2.44	0.52
9:E:90:VAL:O	9:E:91:ALA:O	2.28	0.52
20:B:803:CLA:H191	10:F:104:TYR:CG	2.45	0.52
10:F:23:LYS:O	10:F:24:LYS:HE2	2.07	0.52
6:B:454:LEU:HD22	10:F:70:HIS:CD2	2.45	0.52
10:F:96:TRP:CE3	10:F:134:PHE:N	2.78	0.52
11:G:28:ARG:CG	11:G:29:GLU:HB2	2.39	0.52
11:G:68:ILE:H	11:G:68:ILE:HD12	1.75	0.52
13:I:17:PRO:O	13:I:18:ALA:C	2.48	0.52
17:N:46:PHE:O	17:N:47:THR:OG1	2.28	0.52
17:N:53:ALA:HB3	17:N:55:GLN:NE2	2.24	0.52
2:2:119:VAL:O	2:2:120:ASN:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:302:CLA:O1A	20:2:302:CLA:C4A	2.57	0.52
3:3:106:TYR:CB	3:3:107:TRP:CD1	2.92	0.52
4:4:128:ALA:HB3	4:4:143:PHE:CE2	2.35	0.52
20:4:302:CLA:OBD	20:4:302:CLA:O2D	2.28	0.52
5:A:149:PHE:O	5:A:150:PHE:HB2	2.09	0.52
5:A:32:GLU:HG3	5:A:33:GLN:N	2.25	0.52
5:A:389:TYR:CD1	5:A:625:TRP:CG	2.97	0.52
5:A:393:LEU:O	5:A:397:THR:CG2	2.55	0.52
5:A:631:GLN:O	5:A:632:GLY:C	2.48	0.52
20:A:806:CLA:CED	20:A:806:CLA:HBA2	2.40	0.52
20:A:824:CLA:HBB2	20:A:836:CLA:HMA1	1.92	0.52
21:A:855:LMU:O4'	21:A:855:LMU:O1B	2.27	0.52
20:B:823:CLA:H11	20:B:837:CLA:HBD	1.92	0.52
7:C:31:TRP:CD1	7:C:32:GLY:N	2.78	0.52
7:C:72:GLU:O	7:C:73:THR:O	2.27	0.52
8:D:131:GLY:O	8:D:132:LEU:HB2	2.08	0.52
11:G:96:SER:C	11:G:98:PHE:H	2.13	0.52
16:L:8:TYR:HE1	16:L:11:ILE:CG2	2.20	0.52
17:N:42:PHE:N	17:N:43:PRO:HD3	2.22	0.52
17:N:67:LEU:CD1	17:N:67:LEU:N	2.53	0.52
17:N:76:LYS:O	17:N:77:CYS:O	2.27	0.52
5:A:216:LEU:O	5:A:219:ALA:N	2.43	0.52
5:A:598:VAL:HG12	5:A:598:VAL:O	2.10	0.52
5:A:630:ASP:C	5:A:632:GLY:N	2.60	0.52
20:A:819:CLA:HBC2	20:A:825:CLA:H18	1.90	0.52
20:A:824:CLA:HHB	22:A:846:BCR:H363	1.87	0.52
5:A:398:HIS:HD2	20:A:826:CLA:ND	2.07	0.52
20:A:839:CLA:HMA3	20:A:839:CLA:CBA	2.30	0.52
20:A:840:CLA:CBA	20:A:840:CLA:CED	2.88	0.52
5:A:553:VAL:CG2	22:A:846:BCR:H401	2.38	0.52
9:E:89:GLU:O	9:E:90:VAL:CB	2.58	0.52
10:F:124:PRO:C	10:F:126:ALA:H	2.13	0.52
12:H:54:LEU:CD1	12:H:55:LYS:HG3	2.40	0.52
15:K:32:ARG:HA	15:K:32:ARG:NE	2.25	0.52
15:K:55:PHE:N	15:K:55:PHE:HD1	2.07	0.52
20:B:838:CLA:HBA1	22:L:210:BCR:H362	1.91	0.52
19:Q:1:GLC:O6	19:Q:2:FRU:H5	2.09	0.52
19:U:2:FRU:O6	19:U:2:FRU:C3	2.55	0.52
1:1:115:GLU:O	1:1:116:LYS:HB2	2.10	0.51
1:1:136:ASP:O	1:1:138:LYS:N	2.43	0.51
2:2:198:ALA:O	2:2:199:ASP:OD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:TRP:HZ2	2:2:109:ARG:HD3	1.76	0.51
5:A:216:LEU:CD1	22:A:843:BCR:C35	2.88	0.51
5:A:301:HIS:NE2	20:A:816:CLA:CHA	2.73	0.51
5:A:38:GLY:O	5:A:39:HIS:HB3	2.10	0.51
5:A:473:PRO:C	5:A:475:ASP:N	2.61	0.51
5:A:654:ARG:HA	6:B:632:ILE:HD13	1.91	0.51
5:A:734:GLY:O	5:A:736:THR:N	2.43	0.51
20:A:803:CLA:CGA	20:A:838:CLA:H2	2.40	0.51
6:B:55:ALA:HB1	6:B:150:LEU:HD12	1.91	0.51
6:B:525:LEU:HD22	6:B:529:THR:OG1	2.10	0.51
6:B:556:SER:O	25:B:848:LMG:HC2	2.10	0.51
6:B:290:MET:HG3	20:B:819:CLA:HMC3	1.92	0.51
6:B:530:THR:HG22	20:B:823:CLA:CMC	2.39	0.51
21:D:201:LMU:C1	21:D:201:LMU:O2'	2.58	0.51
11:G:47:GLY:N	11:G:48:ASP:HB3	2.08	0.51
16:L:102:TYR:C	16:L:104:ILE:H	2.13	0.51
8:D:75:LEU:HD21	16:L:19:PHE:CE2	2.45	0.51
17:N:63:ASP:OD1	17:N:66:ASP:OD2	2.28	0.51
19:Q:1:GLC:O6	19:Q:2:FRU:C5	2.59	0.51
18:R:35:UNK:O	18:R:42:UNK:O	2.29	0.51
4:4:103:ILE:HG13	20:4:303:CLA:CMD	2.39	0.51
4:4:34:PRO:CB	4:4:35:GLU:CB	2.61	0.51
5:A:211:LEU:HB3	5:A:310:PHE:CE2	2.44	0.51
5:A:218:TRP:N	20:A:814:CLA:HBB2	2.25	0.51
5:A:366:GLY:O	5:A:403:GLY:HA2	2.10	0.51
5:A:435:VAL:O	5:A:438:HIS:ND1	2.40	0.51
5:A:635:THR:HG22	5:A:635:THR:O	2.10	0.51
5:A:393:LEU:HD13	5:A:750:PHE:CE1	2.43	0.51
20:A:807:CLA:HMB3	20:A:808:CLA:HHB	1.92	0.51
20:A:824:CLA:H162	20:A:824:CLA:H111	1.92	0.51
20:A:826:CLA:H92	22:A:847:BCR:H373	1.91	0.51
6:B:130:ARG:NH1	6:B:130:ARG:CG	2.72	0.51
6:B:292:ARG:NE	6:B:297:ILE:O	2.43	0.51
6:B:440:ASN:ND2	6:B:453:ILE:O	2.43	0.51
6:B:697:PRO:HB3	20:B:838:CLA:CBC	2.41	0.51
20:B:809:CLA:H12	20:B:809:CLA:HAA2	1.92	0.51
21:B:847:LMU:C5B	21:B:847:LMU:O3'	2.47	0.51
6:B:560:ASP:OD1	7:C:66:ARG:HB3	2.09	0.51
9:E:40:ARG:N	9:E:46:PHE:HE1	2.08	0.51
9:E:88:GLU:O	9:E:90:VAL:CG2	2.57	0.51
10:F:93:ILE:HG22	22:F:202:BCR:C37	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:58:LEU:O	11:G:60:SER:N	2.43	0.51
20:H:109:CLA:HMA2	20:H:109:CLA:C1	2.40	0.51
15:K:17:LEU:CD2	15:K:21:ALA:HB2	2.40	0.51
16:L:160:VAL:O	16:L:161:LEU:O	2.29	0.51
20:L:201:CLA:O1A	20:L:201:CLA:HED1	2.01	0.51
16:L:33:ILE:O	16:L:36:TYR:N	2.44	0.51
17:N:75:TYR:HH	21:N:101:LMU:H4O1	1.58	0.51
17:N:4:GLU:C	17:N:4:GLU:CD	2.69	0.51
17:N:62:SER:O	17:N:66:ASP:OD1	2.28	0.51
17:N:70:GLU:O	17:N:72:LYS:N	2.40	0.51
18:R:37:UNK:O	18:R:42:UNK:O	2.28	0.51
2:2:68:LEU:O	2:2:69:THR:C	2.48	0.51
3:3:157:ALA:O	3:3:158:TYR:CD2	2.63	0.51
4:4:127:PRO:HB2	4:4:143:PHE:CE1	2.46	0.51
4:4:149:ALA:CB	4:4:151:GLU:CD	2.48	0.51
5:A:227:LEU:HD23	5:A:231:GLN:NE2	2.24	0.51
5:A:361:ASN:ND2	20:A:805:CLA:HED1	2.23	0.51
5:A:450:CYS:O	5:A:453:LEU:O	2.27	0.51
5:A:519:ASP:C	5:A:520:LEU:HG	2.30	0.51
5:A:685:VAL:O	5:A:688:PHE:HB3	2.10	0.51
20:A:814:CLA:CAB	22:A:843:BCR:H19C	2.33	0.51
6:B:16:PRO:HG3	7:C:74:THR:CG2	2.39	0.51
6:B:563:GLY:C	6:B:564:ARG:O	2.46	0.51
6:B:599:ILE:O	6:B:734:GLY:C	2.48	0.51
6:B:289:LEU:HA	20:B:818:CLA:O1D	2.10	0.51
7:C:12:ILE:HG21	7:C:39:ILE:C	2.31	0.51
7:C:7:ILE:CG2	7:C:65:VAL:HG21	2.41	0.51
9:E:69:PHE:HD2	9:E:71:LYS:HG2	1.76	0.51
20:4:310:CLA:C4B	20:F:206:CLA:H43	2.39	0.51
11:G:16:LEU:CD2	11:G:68:ILE:HG21	2.40	0.51
12:H:50:ARG:NH1	12:H:53:LEU:C	2.61	0.51
16:L:5:LYS:N	16:L:6:PRO:CD	2.73	0.51
17:N:49:CYS:O	17:N:51:ASP:O	2.29	0.51
20:R:107:CLA:CED	20:R:107:CLA:C4D	2.89	0.51
18:R:39:UNK:CA	18:R:42:UNK:CB	2.85	0.51
20:1:215:CLA:O1A	20:1:215:CLA:O1D	2.28	0.51
3:3:63:ARG:NH2	3:3:189:LEU:HD23	2.19	0.51
4:4:191:ASN:O	4:4:192:THR:O	2.29	0.51
5:A:207:LEU:HB3	20:A:819:CLA:CBB	2.40	0.51
5:A:25:ASP:N	5:A:26:PRO:HD2	2.22	0.51
5:A:571:ASP:OD2	8:D:88:THR:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:73:GLU:HA	5:A:76:ARG:HD2	1.91	0.51
5:A:281:LEU:HD22	20:A:816:CLA:CMA	2.40	0.51
20:A:819:CLA:HMC1	20:A:819:CLA:HBC2	1.92	0.51
20:A:826:CLA:H2A	20:A:826:CLA:O1D	2.10	0.51
6:B:299:HIS:NE2	6:B:304:ILE:HG21	2.25	0.51
6:B:317:ARG:NH2	6:B:410:ARG:HG2	2.25	0.51
6:B:536:LYS:O	6:B:537:GLY:C	2.48	0.51
6:B:570:ILE:HG13	6:B:570:ILE:O	2.10	0.51
21:G:101:LMU:C5'	21:G:101:LMU:O2'	2.43	0.51
11:G:21:PHE:O	11:G:23:PHE:N	2.43	0.51
11:G:38:GLN:O	11:G:40:GLY:O	2.28	0.51
11:G:43:HIS:O	11:G:45:GLU:N	2.44	0.51
12:H:20:GLN:C	12:H:22:ASP:HB3	2.31	0.51
21:K:109:LMU:O4'	21:K:109:LMU:O6B	2.28	0.51
16:L:161:LEU:HD11	16:L:163:LEU:N	2.26	0.51
17:N:42:PHE:HD1	17:N:43:PRO:CA	2.23	0.51
3:3:153:SER:OG	3:3:154:GLY:N	2.43	0.51
4:4:169:GLN:NE2	20:4:305:CLA:CHD	2.69	0.51
5:A:183:TRP:O	5:A:185:HIS:N	2.44	0.51
5:A:209:GLY:C	5:A:213:LEU:HB2	2.31	0.51
5:A:334:HIS:CB	20:A:820:CLA:HMA3	2.40	0.51
5:A:401:TRP:CZ3	5:A:609:ILE:HB	2.44	0.51
5:A:661:ALA:O	5:A:665:ILE:HG13	2.10	0.51
5:A:741:GLY:O	5:A:743:ILE:N	2.44	0.51
5:A:744:ALA:HB2	22:A:847:BCR:H391	0.59	0.51
6:B:70:TRP:HB3	6:B:136:TYR:OH	2.09	0.51
6:B:362:ALA:C	6:B:364:ASP:H	2.14	0.51
6:B:353:TYR:HB2	6:B:594:TRP:HH2	1.76	0.51
6:B:606:VAL:C	6:B:608:GLN:N	2.62	0.51
20:B:836:CLA:C6	22:F:203:BCR:C32	2.87	0.51
20:B:851:CLA:HMC1	20:B:851:CLA:HBC2	1.92	0.51
7:C:5:VAL:HB	7:C:65:VAL:HG22	1.91	0.51
8:D:58:PHE:CD2	8:D:59:GLU:N	2.78	0.51
10:F:100:VAL:C	10:F:103:SER:HG	2.12	0.51
10:F:104:TYR:C	10:F:104:TYR:CD2	2.84	0.51
16:L:123:ARG:C	16:L:124:LYS:HE3	2.31	0.51
17:N:27:ALA:O	17:N:28:ASN:O	2.29	0.51
18:R:30:UNK:O	18:R:32:UNK:N	2.43	0.51
18:R:38:UNK:O	18:R:42:UNK:C	2.59	0.51
19:Y:1:GLC:O6	19:Y:2:FRU:O5	2.29	0.51
4:4:174:GLY:O	4:4:175:LYS:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:37:LEU:O	4:4:38:ARG:O	2.27	0.51
5:A:335:LYS:CG	5:A:336:GLY:N	2.60	0.51
5:A:619:LYS:O	5:A:621:GLN:N	2.43	0.51
5:A:361:ASN:OD1	20:A:805:CLA:OBD	2.29	0.51
20:A:817:CLA:H51	20:A:825:CLA:HMB1	1.93	0.51
20:A:839:CLA:H91	15:K:61:LEU:CD1	2.36	0.51
6:B:247:THR:O	6:B:248:GLN:O	2.27	0.51
6:B:337:ALA:O	6:B:339:ALA:O	2.29	0.51
6:B:729:THR:CG2	6:B:729:THR:O	2.30	0.51
20:B:823:CLA:HBD	20:B:835:CLA:HMB3	1.92	0.51
9:E:63:TYR:HA	9:E:83:ALA:HB2	1.92	0.51
10:F:104:TYR:HD2	10:F:104:TYR:C	2.13	0.51
11:G:43:HIS:O	11:G:45:GLU:OE1	2.28	0.51
21:H:104:LMU:O3'	21:H:104:LMU:C2B	2.57	0.51
22:J:102:BCR:C39	22:J:102:BCR:C23	2.65	0.51
20:J:103:CLA:NA	20:J:103:CLA:HED3	2.12	0.51
2:2:183:TYR:O	2:2:184:THR:C	2.49	0.51
2:2:98:GLU:HG2	2:2:99:LEU:HD12	1.91	0.51
3:3:116:PHE:O	3:3:120:LEU:HB2	2.10	0.51
4:4:128:ALA:CA	4:4:143:PHE:HZ	2.23	0.51
4:4:72:VAL:O	4:4:73:PRO:O	2.28	0.51
5:A:212:GLY:C	5:A:214:GLY:H	2.13	0.51
5:A:298:ASP:O	5:A:301:HIS:N	2.44	0.51
5:A:356:ALA:O	5:A:360:ILE:HG22	2.10	0.51
5:A:369:THR:HG21	5:A:402:ILE:HG22	1.90	0.51
5:A:40:PHE:HZ	5:A:56:ASN:HB3	1.72	0.51
5:A:527:VAL:HG12	5:A:528:ALA:N	2.26	0.51
5:A:701:GLN:OE1	9:E:74:TYR:CE1	2.64	0.51
5:A:746:THR:O	5:A:750:PHE:N	2.37	0.51
6:B:124:TRP:CE2	6:B:129:LEU:HD22	2.45	0.51
6:B:197:VAL:O	6:B:198:ALA:CB	2.59	0.51
6:B:440:ASN:CG	6:B:614:THR:O	2.49	0.51
5:A:654:ARG:HH21	6:B:637:PRO:HD2	1.75	0.51
6:B:662:MET:O	6:B:663:PHE:C	2.48	0.51
6:B:681:ALA:O	6:B:683:GLU:N	2.44	0.51
6:B:730:SER:O	6:B:731:GLY:O	2.29	0.51
20:B:825:CLA:H3A	20:B:825:CLA:CGA	2.35	0.51
8:D:72:PRO:HB2	8:D:74:LEU:HB2	1.93	0.51
10:F:104:TYR:OH	10:F:122:ASP:N	2.33	0.51
11:G:33:LYS:O	11:G:34:GLN:O	2.28	0.51
11:G:58:LEU:HD12	11:G:59:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:26:SER:O	12:H:27:ASP:O	2.29	0.51
12:H:40:PHE:O	12:H:43:PHE:N	2.44	0.51
12:H:77:LEU:HB3	12:H:78:PRO:HD2	1.93	0.51
16:L:128:ASP:CG	16:L:129:GLN:N	2.63	0.51
21:L:204:LMU:O3'	21:L:204:LMU:C1B	2.56	0.51
17:N:47:THR:O	17:N:48:GLY:O	2.29	0.51
1:1:183:ASP:CB	1:1:184:PRO:CD	2.87	0.51
20:3:311:CLA:CAA	20:3:311:CLA:O1D	2.58	0.51
5:A:575:LEU:CD1	5:A:576:GLY:H	2.24	0.51
5:A:725:LEU:HD12	5:A:725:LEU:N	2.26	0.51
20:A:816:CLA:C2	20:A:816:CLA:CBA	2.77	0.51
20:A:817:CLA:C4A	20:A:817:CLA:H12	2.41	0.51
6:B:86:PRO:C	6:B:115:ASN:HB3	2.31	0.51
6:B:202:SER:CB	6:B:270:LEU:HD21	2.41	0.51
6:B:510:LEU:CD2	6:B:510:LEU:H	2.23	0.51
6:B:710:LEU:C	6:B:712:HIS:H	2.12	0.51
7:C:9:ASP:CB	24:C:103:SF4:S3	2.99	0.51
8:D:113:HIS:N	8:D:114:PRO:CD	2.74	0.51
8:D:132:LEU:HD23	8:D:133:ASN:O	2.10	0.51
10:F:80:TRP:CH2	20:F:205:CLA:HAC2	2.46	0.51
10:F:26:GLN:O	10:F:28:SER:OG	2.28	0.51
15:K:10:ILE:O	15:K:13:THR:CG2	2.41	0.51
15:K:62:ALA:O	15:K:65:ALA:HB2	2.11	0.51
16:L:96:SER:OG	16:L:143:PHE:CD2	2.57	0.51
17:N:38:GLY:HA3	17:N:46:PHE:CD1	2.46	0.51
17:N:72:LYS:HZ3	17:N:74:LYS:HA	1.76	0.51
2:2:101:PHE:O	2:2:102:ILE:C	2.49	0.51
2:2:204:ILE:O	2:2:205:PHE:CB	2.59	0.51
4:4:98:SER:O	4:4:102:GLU:CD	2.49	0.51
4:4:191:ASN:O	4:4:191:ASN:OD1	2.29	0.51
4:4:31:ALA:O	4:4:32:GLU:O	2.29	0.51
5:A:574:ASN:OD1	5:A:574:ASN:N	2.43	0.51
20:A:825:CLA:HBD	20:A:825:CLA:CBA	2.41	0.51
21:A:855:LMU:H92	21:A:855:LMU:C4	2.03	0.51
6:B:467:HIS:NE2	20:B:832:CLA:CHA	2.74	0.51
6:B:665:ILE:HD12	20:B:851:CLA:HBC1	1.93	0.51
6:B:74:PHE:C	6:B:76:ALA:H	2.14	0.51
20:B:824:CLA:H101	22:B:845:BCR:H14C	1.92	0.51
7:C:73:THR:OG1	7:C:76:SER:OG	2.29	0.51
20:F:205:CLA:H2A	20:F:205:CLA:O1D	2.11	0.51
16:L:164:PRO:HD3	16:L:165:TYR:CZ	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:36:TYR:HE1	20:L:202:CLA:H93	1.76	0.51
17:N:35:VAL:HG12	17:N:37:PHE:CE1	2.45	0.51
2:2:121:THR:OG1	2:2:121:THR:O	2.28	0.51
20:2:322:CLA:O2D	20:2:322:CLA:OBD	2.28	0.51
4:4:98:SER:OG	4:4:102:GLU:OE1	2.29	0.51
4:4:177:PRO:HB2	4:4:178:PHE:CD1	2.46	0.51
4:4:46:VAL:HG21	4:4:105:ARG:NH1	2.26	0.51
4:4:88:SER:C	4:4:89:THR:CG2	2.79	0.51
4:4:90:LEU:H	4:4:90:LEU:HD23	1.75	0.51
4:4:98:SER:O	4:4:102:GLU:OE1	2.29	0.51
5:A:224:HIS:HE1	20:A:815:CLA:C4C	2.24	0.51
5:A:254:LEU:C	5:A:256:ALA:N	2.64	0.51
5:A:464:ASN:O	5:A:468:SER:N	2.39	0.51
5:A:509:ALA:O	5:A:510:SER:OG	2.17	0.51
5:A:592:VAL:O	5:A:597:HIS:CD2	2.64	0.51
5:A:655:ASP:O	5:A:660:GLN:NE2	2.44	0.51
20:A:814:CLA:C4B	22:A:843:BCR:C20	2.87	0.51
5:A:747:TRP:CD2	22:A:847:BCR:H403	2.46	0.51
21:A:854:LMU:H111	21:A:854:LMU:H71	1.92	0.51
6:B:228:GLY:HA3	11:G:8:ILE:HD13	1.92	0.51
6:B:309:ILE:HD12	6:B:312:GLY:HA3	1.93	0.51
6:B:414:HIS:NE2	20:B:828:CLA:NA	2.59	0.51
6:B:436:LEU:O	6:B:437:TYR:CB	2.59	0.51
6:B:535:VAL:HG13	6:B:536:LYS:H	1.76	0.51
6:B:77:TRP:CE2	6:B:81:PRO:HB3	2.45	0.51
20:B:836:CLA:C16	22:F:203:BCR:H311	2.37	0.51
23:B:841:PQN:C29	25:B:848:LMG:H201	2.40	0.51
8:D:48:ILE:HG12	8:D:49:THR:N	2.23	0.51
8:D:50:TRP:N	8:D:50:TRP:CD1	2.79	0.51
10:F:50:LYS:C	10:F:52:ARG:N	2.64	0.51
10:F:83:PHE:C	10:F:86:PRO:HD2	2.32	0.51
21:G:101:LMU:O6B	21:G:101:LMU:O3'	2.29	0.51
22:I:103:BCR:H403	22:I:103:BCR:H271	1.92	0.51
20:A:830:CLA:H152	22:L:210:BCR:H361	1.93	0.51
16:L:9:GLN:HG3	16:L:10:VAL:H	1.76	0.51
17:N:38:GLY:C	17:N:39:SER:O	2.47	0.51
17:N:49:CYS:O	17:N:50:GLN:O	2.29	0.51
17:N:59:PRO:O	17:N:61:LEU:O	2.28	0.51
18:R:35:UNK:O	18:R:36:UNK:O	2.29	0.51
1:1:29:LEU:O	1:1:33:PRO:HD3	2.11	0.50
3:3:74:ALA:CB	3:3:75:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:104:ARG:HD2	20:4:313:CLA:C3C	2.35	0.50
20:4:302:CLA:HAA1	20:4:302:CLA:HBD	1.92	0.50
4:4:68:GLY:O	4:4:69:ILE:O	2.29	0.50
4:4:83:TYR:O	4:4:87:SER:OG	2.30	0.50
4:4:95:PHE:O	4:4:98:SER:OG	2.29	0.50
5:A:185:HIS:O	5:A:188:LYS:HG3	2.11	0.50
5:A:25:ASP:O	5:A:26:PRO:O	2.29	0.50
5:A:379:MET:SD	5:A:511:THR:O	2.69	0.50
5:A:580:PRO:HB3	5:A:727:ILE:HG21	1.92	0.50
5:A:747:TRP:HB2	20:A:826:CLA:HBB1	1.92	0.50
20:A:827:CLA:H52	20:A:827:CLA:CMD	2.41	0.50
20:A:830:CLA:H11	20:A:841:CLA:H43	1.93	0.50
5:A:88:ILE:C	5:A:90:PHE:N	2.62	0.50
6:B:58:PHE:CE2	6:B:145:LEU:HD12	2.45	0.50
6:B:231:ASN:O	6:B:233:TYR:N	2.44	0.50
6:B:290:MET:HG2	6:B:290:MET:O	2.10	0.50
6:B:382:ILE:O	6:B:385:GLY:N	2.41	0.50
6:B:17:THR:HA	6:B:696:LYS:N	2.26	0.50
20:B:850:CLA:C14	20:H:109:CLA:HBC3	2.41	0.50
7:C:72:GLU:C	7:C:73:THR:O	2.45	0.50
8:D:46:TYR:HD1	8:D:80:LYS:HB3	1.75	0.50
10:F:28:SER:O	10:F:30:LYS:O	2.27	0.50
10:F:53:PHE:C	10:F:55:ASN:N	2.63	0.50
20:G:102:CLA:O2A	20:G:102:CLA:CMA	2.59	0.50
11:G:32:ALA:C	11:G:34:GLN:N	2.64	0.50
20:H:101:CLA:H2A	20:H:101:CLA:O1A	2.08	0.50
20:B:808:CLA:C9	22:I:101:BCR:H361	2.39	0.50
15:K:24:PHE:CG	15:K:52:PRO:HG2	2.43	0.50
20:L:201:CLA:H2	20:L:201:CLA:C7	2.41	0.50
17:N:51:ASP:N	17:N:51:ASP:OD2	2.30	0.50
17:N:47:THR:OG1	17:N:52:LEU:O	2.28	0.50
18:R:38:UNK:O	18:R:42:UNK:O	2.29	0.50
1:1:42:SER:HA	1:1:45:ILE:HG12	1.92	0.50
2:2:37:ASP:OD2	3:3:41:ASP:OD1	2.29	0.50
5:A:274:TRP:NE1	5:A:277:TYR:CE2	2.79	0.50
5:A:529:LEU:H	5:A:529:LEU:HD12	1.76	0.50
5:A:68:THR:O	5:A:70:ASP:N	2.42	0.50
20:A:801:CLA:HAA1	20:A:801:CLA:CGD	2.42	0.50
20:A:812:CLA:C4D	20:A:813:CLA:HMC3	2.41	0.50
5:A:375:HIS:HE1	20:A:825:CLA:NC	2.07	0.50
20:A:840:CLA:CED	20:A:840:CLA:HBA1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:90:PHE:HE2	5:A:178:MET:SD	2.33	0.50
6:B:305:LEU:O	6:B:308:HIS:N	2.25	0.50
6:B:311:PRO:HD3	20:B:840:CLA:C3C	2.41	0.50
6:B:420:SER:O	6:B:424:TRP:N	2.35	0.50
20:B:811:CLA:H11	22:B:843:BCR:C10	2.41	0.50
10:F:116:GLN:O	10:F:118:GLU:N	2.44	0.50
6:B:458:ILE:HD11	20:F:205:CLA:HED1	1.92	0.50
10:F:28:SER:O	10:F:29:LEU:O	2.29	0.50
21:K:105:LMU:H5'	21:K:105:LMU:C2B	2.40	0.50
15:K:44:GLU:O	15:K:45:SER:CB	2.59	0.50
17:N:62:SER:O	17:N:63:ASP:OD1	2.29	0.50
21:R:103:LMU:C6	21:R:103:LMU:C2	2.71	0.50
2:2:106:GLU:O	20:2:311:CLA:CMA	2.60	0.50
3:3:109:ASP:O	3:3:110:SER:O	2.28	0.50
3:3:157:ALA:O	3:3:158:TYR:CB	2.59	0.50
3:3:92:TRP:O	3:3:95:THR:HG23	2.11	0.50
4:4:75:TRP:CH2	4:4:76:TYR:HB3	2.46	0.50
5:A:141:ARG:HG3	5:A:141:ARG:NH2	2.15	0.50
5:A:329:ASP:O	5:A:332:GLU:O	2.29	0.50
5:A:72:GLU:HB3	5:A:76:ARG:NH2	2.26	0.50
5:A:750:PHE:O	5:A:752:ALA:N	2.45	0.50
20:A:809:CLA:CBA	20:A:809:CLA:CHA	2.88	0.50
20:A:824:CLA:HBD	20:A:824:CLA:HAA1	1.93	0.50
20:A:825:CLA:H143	20:A:825:CLA:C10	2.40	0.50
20:A:803:CLA:H42	20:A:838:CLA:H8	1.91	0.50
20:A:841:CLA:HMB2	20:L:208:CLA:CBC	2.38	0.50
6:B:136:TYR:O	6:B:140:ILE:HD11	2.12	0.50
6:B:626:LEU:HD12	6:B:627:ASN:N	2.26	0.50
6:B:726:ILE:C	6:B:728:SER:H	2.13	0.50
20:B:819:CLA:HMA3	20:B:820:CLA:C3D	2.41	0.50
20:B:821:CLA:H43	20:B:821:CLA:C2A	2.39	0.50
6:B:310:PRO:O	20:B:840:CLA:CHD	2.60	0.50
7:C:15:THR:N	7:C:17:CYS:SG	2.84	0.50
21:H:104:LMU:O3B	19:Y:2:FRU:C6	2.56	0.50
21:H:108:LMU:O5B	21:H:108:LMU:O3'	2.29	0.50
17:N:45:ASN:CA	17:N:57:LYS:HZ2	2.24	0.50
17:N:45:ASN:O	17:N:45:ASN:ND2	2.45	0.50
17:N:82:PHE:N	17:N:82:PHE:HD2	2.08	0.50
19:Y:1:GLC:O6	19:Y:2:FRU:O2	2.30	0.50
3:3:205:GLY:CA	5:A:252:ARG:HH12	2.24	0.50
4:4:118:ASP:C	4:4:122:LYS:HA	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:40:PHE:C	4:4:43:ALA:CB	2.79	0.50
5:A:176:GLY:O	5:A:180:PHE:HB2	2.12	0.50
5:A:242:ILE:HD13	5:A:242:ILE:N	2.27	0.50
5:A:283:PHE:O	5:A:284:ARG:NH1	2.44	0.50
5:A:27:ILE:C	5:A:28:LYS:HG3	2.25	0.50
5:A:327:ILE:HG13	5:A:328:LYS:H	1.76	0.50
5:A:365:LEU:CD2	20:A:805:CLA:CED	2.67	0.50
5:A:430:ASP:O	5:A:434:ARG:HB2	2.12	0.50
5:A:547:PHE:CE2	20:B:851:CLA:O1A	2.63	0.50
5:A:685:VAL:HG12	5:A:741:GLY:CA	2.40	0.50
20:A:808:CLA:HBC3	20:A:808:CLA:HHD	1.93	0.50
5:A:126:ILE:CG1	20:A:809:CLA:HMA3	2.40	0.50
20:A:819:CLA:H18	22:A:845:BCR:H383	1.94	0.50
21:A:854:LMU:H112	21:A:854:LMU:H72	1.90	0.50
6:B:29:HIS:CE1	20:B:827:CLA:H43	2.46	0.50
6:B:631:LEU:HG	6:B:632:ILE:HG23	1.94	0.50
21:B:847:LMU:O6B	21:B:847:LMU:O3'	2.30	0.50
7:C:73:THR:O	7:C:76:SER:OG	2.29	0.50
11:G:8:ILE:CG1	11:G:8:ILE:O	2.56	0.50
16:L:163:LEU:HD13	16:L:164:PRO:CG	2.41	0.50
18:R:44:UNK:O	18:R:45:UNK:O	2.30	0.50
19:U:2:FRU:O1	19:U:2:FRU:O6	2.30	0.50
20:1:210:CLA:OBD	20:1:210:CLA:CMD	2.53	0.50
2:2:54:TRP:HZ2	2:2:109:ARG:CB	2.24	0.50
3:3:106:TYR:CD2	3:3:107:TRP:CG	2.99	0.50
3:3:86:GLN:HB2	3:3:88:THR:N	2.26	0.50
20:4:319:CLA:HBD	20:4:319:CLA:HAA2	1.94	0.50
5:A:169:ILE:O	5:A:173:VAL:HG13	2.11	0.50
5:A:24:ARG:O	5:A:25:ASP:O	2.30	0.50
5:A:394:SER:OG	5:A:395:LEU:N	2.44	0.50
5:A:620:MET:SD	5:A:624:VAL:HG21	2.52	0.50
5:A:672:LEU:C	5:A:674:ALA:H	2.08	0.50
20:A:815:CLA:O1D	20:A:815:CLA:OBD	2.30	0.50
20:A:850:CLA:HBB2	20:A:851:CLA:HED1	1.94	0.50
5:A:93:LEU:O	5:A:97:TYR:HD2	1.94	0.50
6:B:124:TRP:HZ2	6:B:135:LEU:HB2	1.76	0.50
6:B:331:HIS:CE1	6:B:392:ILE:CG2	2.91	0.50
6:B:406:ASN:ND2	6:B:406:ASN:C	2.65	0.50
20:B:823:CLA:OBD	20:B:835:CLA:HBB1	2.12	0.50
22:B:843:BCR:C8	22:B:843:BCR:H331	2.41	0.50
20:B:827:CLA:C9	25:B:848:LMG:H311	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:850:CLA:H122	20:B:850:CLA:H71	1.94	0.50
6:B:551:LYS:HE2	8:D:143:PRO:CA	2.42	0.50
17:N:58:VAL:HG12	17:N:59:PRO:HD3	1.94	0.50
17:N:82:PHE:N	17:N:82:PHE:CD2	2.78	0.50
18:R:38:UNK:O	18:R:39:UNK:O	2.30	0.50
1:1:185:TRP:O	1:1:186:HIS:O	2.30	0.50
4:4:115:VAL:C	4:4:117:GLN:HG3	2.32	0.50
5:A:188:LYS:O	5:A:190:ALA:N	2.45	0.50
5:A:354:TRP:O	5:A:358:LEU:N	2.44	0.50
5:A:409:GLY:C	5:A:411:ALA:N	2.65	0.50
5:A:538:ASP:O	5:A:542:HIS:HB2	2.10	0.50
5:A:558:LYS:HZ1	6:B:674:LEU:HD23	1.77	0.50
5:A:618:TRP:CZ2	5:A:655:ASP:HB3	2.46	0.50
5:A:685:VAL:CG1	5:A:741:GLY:HA2	2.42	0.50
6:B:31:PHE:O	6:B:32:GLU:C	2.49	0.50
6:B:420:SER:H	6:B:422:LEU:H	1.60	0.50
20:B:809:CLA:HBD	20:B:809:CLA:C1	2.41	0.50
20:B:823:CLA:HED1	20:B:824:CLA:HMD2	1.87	0.50
6:B:521:HIS:CE1	20:B:836:CLA:C4A	2.91	0.50
9:E:85:ASP:OD1	9:E:85:ASP:O	2.30	0.50
11:G:16:LEU:CD1	11:G:17:PHE:CE2	2.91	0.50
11:G:92:GLY:O	11:G:93:TYR:O	2.30	0.50
20:H:101:CLA:C6	20:H:101:CLA:HMA1	2.42	0.50
20:K:102:CLA:CMC	20:K:102:CLA:HBC2	2.20	0.50
20:A:839:CLA:C9	15:K:61:LEU:HD13	2.35	0.50
16:L:101:MET:SD	16:L:104:ILE:HG12	2.52	0.50
16:L:56:VAL:HG22	20:L:208:CLA:HED2	1.94	0.50
17:N:52:LEU:CB	17:N:53:ALA:CA	2.90	0.50
17:N:5:GLU:OE2	17:N:6:TYR:N	2.45	0.50
18:R:34:UNK:O	18:R:36:UNK:O	2.30	0.50
18:R:38:UNK:C	18:R:42:UNK:C	2.89	0.50
4:4:33:ASP:O	4:4:34:PRO:O	2.29	0.50
6:B:447:GLY:O	6:B:449:PRO:CD	2.60	0.50
6:B:50:HIS:CA	6:B:53:GLN:HB2	2.41	0.50
6:B:429:LEU:HD11	20:B:836:CLA:CMB	2.42	0.50
7:C:31:TRP:CD1	7:C:31:TRP:C	2.85	0.50
8:D:120:PRO:O	8:D:121:GLU:HB3	2.11	0.50
9:E:69:PHE:CG	9:E:70:ALA:N	2.79	0.50
9:E:88:GLU:O	9:E:90:VAL:N	2.44	0.50
20:2:322:CLA:CED	20:J:101:CLA:H2	2.42	0.50
15:K:17:LEU:HD22	15:K:18:MET:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:55:PHE:N	15:K:55:PHE:CD1	2.77	0.50
17:N:38:GLY:O	17:N:39:SER:O	2.29	0.50
20:2:302:CLA:H43	20:2:302:CLA:CGA	2.34	0.50
3:3:80:LYS:HD3	3:3:105:ASN:HB3	1.91	0.50
3:3:84:ILE:O	3:3:84:ILE:HD13	2.12	0.50
4:4:144:ALA:O	4:4:147:LEU:O	2.29	0.50
4:4:34:PRO:CA	4:4:35:GLU:CD	2.78	0.50
4:4:38:ARG:O	4:4:39:TRP:O	2.30	0.50
5:A:208:ALA:HA	5:A:310:PHE:C	2.28	0.50
5:A:249:ILE:HD13	5:A:250:LEU:HB2	1.93	0.50
5:A:249:ILE:N	5:A:251:ASN:OD1	2.45	0.50
5:A:364:MET:O	5:A:368:LEU:HB2	2.11	0.50
20:A:824:CLA:HED2	20:A:824:CLA:HAA1	1.92	0.50
5:A:382:TYR:HE2	20:A:827:CLA:HED3	1.74	0.50
6:B:141:PHE:O	6:B:144:PHE:N	2.45	0.50
6:B:22:TRP:HA	6:B:25:ILE:HD11	1.92	0.50
6:B:320:LYS:O	6:B:322:LEU:N	2.44	0.50
6:B:346:SER:O	6:B:350:GLN:N	2.43	0.50
6:B:509:PHE:CD2	6:B:509:PHE:N	2.80	0.50
6:B:67:HIS:O	6:B:88:ALA:O	2.30	0.50
6:B:290:MET:HB2	20:B:819:CLA:HMC3	1.94	0.50
6:B:718:ILE:HD11	20:B:825:CLA:HHC	1.94	0.50
20:B:826:CLA:H171	22:B:843:BCR:H363	1.92	0.50
25:B:848:LMG:C11	25:B:848:LMG:HC91	2.40	0.50
7:C:34:CYS:SG	7:C:39:ILE:HD12	2.52	0.50
9:E:41:ARG:NE	9:E:46:PHE:CZ	2.80	0.50
2:2:128:ASN:ND2	14:J:3:ASP:HB3	2.27	0.50
21:K:106:LMU:O6B	21:K:106:LMU:O4'	2.29	0.50
12:H:47:PHE:CD2	16:L:141:GLY:HA2	2.46	0.50
20:L:207:CLA:HHD	20:L:207:CLA:HBC2	1.94	0.50
17:N:47:THR:O	17:N:52:LEU:O	2.30	0.50
17:N:61:LEU:O	17:N:66:ASP:OD1	2.28	0.50
19:U:2:FRU:O6	19:U:2:FRU:O3	2.29	0.50
20:2:303:CLA:CHD	20:2:303:CLA:CBC	2.88	0.50
3:3:114:PHE:CE1	20:3:309:CLA:C3D	2.94	0.50
5:A:546:ALA:HB1	20:A:835:CLA:HMB3	1.94	0.50
5:A:553:VAL:O	5:A:557:LEU:HB2	2.11	0.50
5:A:630:ASP:O	5:A:632:GLY:N	2.45	0.50
20:A:818:CLA:CBB	20:A:818:CLA:H8	2.42	0.50
5:A:89:ILE:O	5:A:93:LEU:HG	2.12	0.50
6:B:125:TYR:CE1	6:B:130:ARG:NH1	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:178:HIS:C	6:B:180:SER:N	2.64	0.50
6:B:503:GLU:CB	6:B:507:SER:HB2	2.41	0.50
6:B:586:THR:O	6:B:589:TRP:N	2.44	0.50
6:B:441:ASP:OD1	6:B:617:MET:HB3	2.11	0.50
6:B:707:LEU:HD12	6:B:711:VAL:CG2	2.42	0.50
20:B:823:CLA:O2D	20:B:824:CLA:OBD	2.29	0.50
20:B:827:CLA:CMC	20:B:827:CLA:HBC3	2.36	0.50
20:B:826:CLA:H62	22:B:844:BCR:C32	2.42	0.50
6:B:11:GLY:CA	7:C:71:HIS:CD2	2.86	0.50
21:F:201:LMU:O5B	21:F:201:LMU:O6'	2.29	0.50
21:H:106:LMU:O5B	21:H:106:LMU:O1'	2.29	0.50
20:K:101:CLA:H2A	20:K:101:CLA:O1D	2.12	0.50
15:K:40:LEU:O	15:K:41:GLU:HG3	2.12	0.50
15:K:59:ASP:O	15:K:59:ASP:OD1	2.30	0.50
16:L:136:TRP:O	16:L:140:THR:HG23	2.12	0.50
1:1:64:GLY:O	1:1:66:GLY:O	2.30	0.49
2:2:137:TYR:HD1	2:2:138:PRO:CD	2.25	0.49
3:3:87:GLU:CA	22:3:314:BCR:C38	2.90	0.49
3:3:87:GLU:CB	22:3:314:BCR:C38	2.90	0.49
4:4:163:PHE:O	4:4:166:PHE:CB	2.56	0.49
4:4:75:TRP:CE3	4:4:76:TYR:HB3	2.47	0.49
5:A:131:ILE:HG23	5:A:132:LEU:N	2.27	0.49
5:A:301:HIS:NE2	20:A:816:CLA:C1A	2.75	0.49
5:A:332:GLU:HA	5:A:344:LYS:HG2	1.93	0.49
5:A:347:TYR:HE1	5:A:417:PHE:HZ	1.59	0.49
5:A:218:TRP:CZ3	20:A:814:CLA:HMB3	2.47	0.49
20:A:850:CLA:HMB3	20:A:851:CLA:HMD1	1.94	0.49
6:B:160:LYS:O	6:B:162:LYS:N	2.44	0.49
6:B:492:ILE:O	6:B:493:TRP:HB2	2.12	0.49
6:B:595:HIS:CE1	6:B:599:ILE:HD11	2.46	0.49
6:B:667:TRP:O	6:B:669:GLY:N	2.45	0.49
6:B:681:ALA:O	6:B:682:HIS:C	2.50	0.49
6:B:141:PHE:CG	20:B:812:CLA:H12	2.47	0.49
20:B:805:CLA:HAC1	20:B:827:CLA:HMA1	1.92	0.49
6:B:11:GLY:CA	7:C:71:HIS:HD2	2.07	0.49
10:F:19:LYS:O	10:F:23:LYS:HB2	2.11	0.49
11:G:37:GLU:O	11:G:38:GLN:O	2.29	0.49
11:G:44:PHE:C	11:G:46:ALA:HB2	2.32	0.49
12:H:45:ALA:C	12:H:48:THR:H	2.08	0.49
12:H:70:ALA:O	12:H:71:ASN:CB	2.59	0.49
15:K:23:ARG:O	15:K:23:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:123:ARG:HB3	16:L:126:GLN:CG	2.41	0.49
19:Y:1:GLC:C1	19:Y:2:FRU:O3	2.60	0.49
21:1:218:LMU:O5B	21:1:218:LMU:O3'	2.29	0.49
1:1:32:VAL:CG2	20:1:211:CLA:C1D	2.90	0.49
2:2:188:PRO:O	2:2:189:ILE:C	2.50	0.49
2:2:60:ALA:HA	2:2:63:PHE:CD2	2.48	0.49
3:3:86:GLN:HB2	3:3:88:THR:H	1.76	0.49
5:A:29:THR:OG1	5:A:31:PHE:CB	2.57	0.49
5:A:44:ILE:O	5:A:46:LYS:CA	2.60	0.49
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.26	0.49
5:A:744:ALA:HA	5:A:747:TRP:HB3	1.93	0.49
6:B:183:PHE:CE1	20:B:811:CLA:H51	2.48	0.49
6:B:190:TRP:CD2	20:B:816:CLA:HMD3	2.47	0.49
6:B:232:LEU:HD21	6:B:235:GLN:OE1	2.12	0.49
7:C:9:ASP:HB3	24:C:103:SF4:S3	2.52	0.49
10:F:25:LEU:O	10:F:26:GLN:O	2.30	0.49
21:H:108:LMU:O6B	21:H:108:LMU:O3'	2.29	0.49
14:J:22:LEU:O	14:J:23:ALA:C	2.51	0.49
2:2:120:ASN:CB	14:J:5:LYS:HD2	2.43	0.49
16:L:115:ALA:N	16:L:116:PRO:CD	2.70	0.49
21:1:218:LMU:H22	21:1:218:LMU:O5'	2.11	0.49
2:2:165:LYS:C	2:2:167:GLY:N	2.65	0.49
3:3:157:ALA:O	3:3:158:TYR:HD2	1.95	0.49
4:4:191:ASN:C	4:4:192:THR:O	2.50	0.49
4:4:69:ILE:C	4:4:71:ASN:N	2.60	0.49
5:A:197:GLN:NE2	5:A:351:THR:O	2.45	0.49
5:A:648:THR:O	5:A:649:ILE:HG22	2.11	0.49
20:A:819:CLA:H101	20:A:822:CLA:H93	1.94	0.49
20:A:835:CLA:H171	20:L:203:CLA:CBB	2.42	0.49
20:B:819:CLA:HMD2	22:B:842:BCR:C32	2.42	0.49
20:G:102:CLA:H3A	20:G:102:CLA:CGA	2.39	0.49
11:G:34:GLN:O	11:G:36:PRO:HD3	2.11	0.49
11:G:7:VAL:HG23	11:G:8:ILE:H	1.65	0.49
16:L:112:PRO:O	16:L:113:SER:HB3	2.12	0.49
16:L:11:ILE:O	16:L:12:GLN:HG3	2.12	0.49
16:L:48:ASN:CB	16:L:49:PRO:HD2	2.35	0.49
16:L:95:LEU:O	16:L:99:LEU:HD13	2.11	0.49
17:N:42:PHE:O	17:N:43:PRO:O	2.29	0.49
17:N:60:PHE:N	17:N:61:LEU:O	2.45	0.49
19:O:1:GLC:O2	19:O:2:FRU:O4	2.30	0.49
21:R:104:LMU:H5'	21:R:104:LMU:H2O2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:202:CLA:CBB	20:1:206:CLA:CHC	2.90	0.49
2:2:179:PHE:O	2:2:183:TYR:CD2	2.66	0.49
2:2:96:ILE:O	2:2:100:VAL:CG1	2.60	0.49
4:4:191:ASN:OD1	4:4:192:THR:O	2.29	0.49
20:4:306:CLA:HED2	20:4:306:CLA:CAD	2.43	0.49
5:A:144:GLN:C	5:A:145:ILE:HG12	2.33	0.49
5:A:163:GLN:C	5:A:165:TYR:N	2.63	0.49
5:A:594:ALA:O	5:A:598:VAL:HG23	2.11	0.49
5:A:678:PHE:CZ	20:A:826:CLA:H142	2.46	0.49
5:A:733:VAL:CG1	20:A:838:CLA:C4D	2.90	0.49
6:B:339:ALA:O	6:B:340:SER:CB	2.60	0.49
6:B:377:TYR:O	6:B:378:ILE:HB	2.13	0.49
6:B:517:PHE:O	6:B:517:PHE:CG	2.61	0.49
6:B:577:TYR:CD1	6:B:706:ARG:HB3	2.47	0.49
6:B:580:VAL:HG11	6:B:710:LEU:HD21	1.94	0.49
21:B:801:LMU:C1B	21:B:801:LMU:C6'	2.90	0.49
20:B:823:CLA:C4A	20:B:837:CLA:HAA2	2.43	0.49
20:B:830:CLA:HMD2	20:B:830:CLA:H13	1.94	0.49
5:A:567:ARG:HH11	8:D:35:GLY:N	2.11	0.49
9:E:43:SER:CB	9:E:82:TYR:HE1	2.21	0.49
11:G:57:LEU:O	11:G:61:ASN:OD1	2.30	0.49
13:I:24:LEU:HD21	22:L:210:BCR:H271	1.95	0.49
17:N:59:PRO:O	17:N:66:ASP:OD1	2.30	0.49
1:1:18:ALA:N	1:1:19:PRO:HD2	2.26	0.49
4:4:104:ARG:HA	4:4:107:GLN:CB	2.41	0.49
4:4:147:LEU:O	4:4:148:GLU:O	2.29	0.49
5:A:23:ASP:CA	5:A:24:ARG:HD3	2.42	0.49
5:A:385:LEU:O	5:A:386:ALA:HB3	2.12	0.49
5:A:568:LEU:O	5:A:586:ARG:HD3	2.12	0.49
6:B:247:THR:HB	6:B:248:GLN:OE1	2.11	0.49
6:B:724:PHE:CD1	20:B:849:CLA:HMD1	2.48	0.49
20:B:803:CLA:C1C	20:B:803:CLA:H52	2.43	0.49
6:B:392:ILE:HD13	20:B:827:CLA:HED1	1.93	0.49
20:B:826:CLA:H172	22:B:843:BCR:H363	1.93	0.49
23:B:841:PQN:H141	22:B:846:BCR:H331	1.94	0.49
7:C:63:LEU:CG	7:C:64:SER:N	2.49	0.49
6:B:564:ARG:NE	7:C:64:SER:OG	2.46	0.49
8:D:124:ASN:HB3	8:D:125:PRO:CD	2.29	0.49
21:E:101:LMU:O1B	21:E:101:LMU:O2'	2.30	0.49
9:E:55:VAL:CG2	9:E:65:VAL:HB	2.40	0.49
22:F:203:BCR:C33	20:F:205:CLA:HMA1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:LEU:HB3	10:F:25:LEU:HD13	1.94	0.49
15:K:11:MET:O	15:K:15:THR:OG1	2.30	0.49
20:L:208:CLA:CAC	22:L:210:BCR:HC42	2.42	0.49
19:P:1:GLC:O2	19:P:2:FRU:O5	2.29	0.49
21:R:103:LMU:H6'1	21:R:103:LMU:O3B	2.10	0.49
2:2:36:SER:O	2:2:37:ASP:HB2	2.11	0.49
3:3:133:ALA:O	3:3:134:LYS:HB2	2.12	0.49
5:A:109:TRP:HA	5:A:116:ILE:CG1	2.41	0.49
5:A:104:SER:OG	5:A:161:GLU:OE1	2.31	0.49
5:A:79:PHE:HZ	5:A:185:HIS:HE2	1.57	0.49
5:A:589:THR:HG22	5:A:589:THR:O	2.13	0.49
20:A:806:CLA:HBD	20:A:806:CLA:HAA2	1.94	0.49
6:B:502:ASN:OD1	6:B:511:THR:HG21	2.12	0.49
6:B:686:PRO:HD3	20:L:202:CLA:O1A	2.12	0.49
6:B:646:TRP:CZ3	6:B:726:ILE:CD1	2.95	0.49
6:B:724:PHE:CE2	20:B:849:CLA:CMD	2.96	0.49
7:C:6:LYS:O	7:C:63:LEU:HD21	2.12	0.49
7:C:42:ALA:O	8:D:129:GLY:HA3	2.13	0.49
10:F:151:ASP:HA	10:F:154:PHE:CB	2.43	0.49
10:F:23:LYS:O	10:F:24:LYS:CE	2.60	0.49
12:H:57:LEU:C	12:H:57:LEU:HD13	2.33	0.49
19:Z:1:GLC:C5	19:Z:2:FRU:HO4	2.25	0.49
5:A:185:HIS:O	5:A:187:HIS:N	2.46	0.49
5:A:364:MET:CE	20:A:825:CLA:H2	2.43	0.49
5:A:435:VAL:HA	5:A:438:HIS:HE1	1.76	0.49
5:A:508:THR:O	5:A:509:ALA:HB3	2.12	0.49
5:A:549:ILE:O	5:A:552:THR:O	2.30	0.49
6:B:247:THR:O	6:B:248:GLN:C	2.51	0.49
6:B:323:TYR:CD1	20:B:822:CLA:CBC	2.95	0.49
6:B:317:ARG:HD3	6:B:410:ARG:HG2	1.95	0.49
6:B:419:ILE:C	6:B:420:SER:OG	2.47	0.49
6:B:475:ASP:HA	6:B:480:SER:CA	2.43	0.49
6:B:647:ALA:O	6:B:651:LEU:HD22	2.12	0.49
20:B:815:CLA:H8	20:B:833:CLA:HMA1	1.93	0.49
20:B:821:CLA:H43	20:B:821:CLA:CHA	2.38	0.49
7:C:7:ILE:HA	7:C:60:THR:OG1	2.13	0.49
10:F:123:VAL:O	10:F:126:ALA:N	2.45	0.49
10:F:17:ARG:O	10:F:18:GLU:C	2.51	0.49
11:G:17:PHE:O	11:G:20:ARG:CB	2.57	0.49
13:I:4:LEU:HG	13:I:4:LEU:O	2.13	0.49
21:K:106:LMU:H51	21:K:106:LMU:H11	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD21	17:N:64:ASP:N	2.28	0.49
17:N:77:CYS:O	17:N:79:SER:O	2.29	0.49
19:Y:2:FRU:O1	19:Y:2:FRU:O6	2.30	0.49
3:3:158:TYR:CB	3:3:159:PRO:HD2	2.22	0.49
20:3:310:CLA:C2A	20:3:318:CLA:HHD	2.43	0.49
4:4:60:LEU:HG	4:4:61:PRO:CD	2.34	0.49
4:4:70:ILE:O	4:4:71:ASN:C	2.47	0.49
4:4:73:PRO:CB	4:4:75:TRP:HA	2.43	0.49
5:A:258:LEU:HG	5:A:280:PHE:CD1	2.48	0.49
5:A:331:LEU:CD2	5:A:343:HIS:C	2.61	0.49
5:A:733:VAL:HG21	20:A:838:CLA:HMD3	1.95	0.49
20:A:806:CLA:H51	20:A:828:CLA:NC	2.28	0.49
20:A:805:CLA:C4	22:A:844:BCR:C31	2.90	0.49
20:A:822:CLA:NC	22:A:845:BCR:C17	2.75	0.49
20:A:824:CLA:C3B	22:A:846:BCR:C37	2.90	0.49
5:A:747:TRP:CE3	22:A:847:BCR:H402	2.44	0.49
22:A:847:BCR:C15	20:A:851:CLA:H151	2.43	0.49
21:A:854:LMU:H1'	21:A:854:LMU:O6'	1.88	0.49
6:B:48:ALA:HB3	6:B:157:LEU:HD22	1.93	0.49
1:1:27:LEU:H	6:B:314:ARG:NH1	2.09	0.49
6:B:396:ARG:HH11	20:B:827:CLA:HED2	1.78	0.49
7:C:12:ILE:N	7:C:12:ILE:CD1	2.71	0.49
8:D:101:TYR:CD1	8:D:114:PRO:CD	2.95	0.49
8:D:28:ILE:O	8:D:66:ALA:CB	2.61	0.49
11:G:16:LEU:HB2	11:G:17:PHE:CD2	2.48	0.49
11:G:42:SER:OG	11:G:43:HIS:O	2.30	0.49
20:K:108:CLA:HAA2	20:K:108:CLA:HBD	1.93	0.49
15:K:5:SER:O	15:K:9:LEU:HD21	2.12	0.49
8:D:41:GLN:HG3	16:L:125:LYS:HZ2	1.78	0.49
17:N:45:ASN:O	17:N:46:PHE:O	2.30	0.49
19:O:1:GLC:O2	19:O:2:FRU:O5	2.28	0.49
19:S:1:GLC:O2	19:S:2:FRU:O1	2.29	0.49
1:1:184:PRO:O	1:1:185:TRP:CZ3	2.64	0.49
2:2:51:HIS:CA	2:2:54:TRP:HB2	2.42	0.49
3:3:129:PHE:O	3:3:129:PHE:CD1	2.66	0.49
3:3:74:ALA:CB	20:3:307:CLA:C1D	2.91	0.49
4:4:94:GLU:C	4:4:95:PHE:HD1	2.15	0.49
5:A:158:ILE:HG21	20:A:814:CLA:O1D	2.13	0.49
5:A:452:PHE:CD2	5:A:456:HIS:CE1	3.00	0.49
5:A:473:PRO:C	5:A:475:ASP:H	2.16	0.49
5:A:484:LEU:N	5:A:485:GLN:OE1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:497:ALA:HA	5:A:510:SER:OG	2.13	0.49
5:A:53:TRP:CA	5:A:56:ASN:HB2	2.37	0.49
20:A:805:CLA:HMB3	20:A:806:CLA:HAA1	1.95	0.49
20:A:808:CLA:HAA2	20:A:826:CLA:HED3	1.94	0.49
20:A:824:CLA:CBA	20:A:836:CLA:CED	2.87	0.49
20:A:822:CLA:CAB	22:A:845:BCR:H353	2.33	0.49
6:B:110:LEU:CD1	6:B:111:GLY:H	2.18	0.49
6:B:238:SER:OG	6:B:239:SER:N	2.45	0.49
6:B:255:LEU:HD23	6:B:255:LEU:N	2.28	0.49
6:B:292:ARG:CZ	6:B:297:ILE:H	2.26	0.49
6:B:535:VAL:CG2	6:B:539:LEU:HD23	2.42	0.49
6:B:724:PHE:CE1	20:B:849:CLA:HMD1	2.47	0.49
20:B:806:CLA:H161	20:B:806:CLA:H91	1.94	0.49
20:B:827:CLA:HMD2	25:B:848:LMG:H341	1.95	0.49
6:B:488:ALA:HB2	20:B:834:CLA:C3C	2.43	0.49
10:F:113:LYS:NZ	10:F:115:THR:HG21	2.27	0.49
10:F:80:TRP:CH2	20:F:205:CLA:CAC	2.95	0.49
10:F:22:LEU:HB2	10:F:23:LYS:HD3	1.94	0.49
11:G:46:ALA:N	11:G:48:ASP:CG	2.60	0.49
12:H:42:THR:O	12:H:45:ALA:N	2.46	0.49
14:J:21:SER:O	14:J:22:LEU:C	2.51	0.49
16:L:162:ASP:HB2	16:L:163:LEU:CA	2.43	0.49
16:L:5:LYS:N	16:L:6:PRO:HD3	2.28	0.49
16:L:63:LEU:HD13	16:L:64:LEU:HG	1.94	0.49
16:L:78:GLU:O	16:L:78:GLU:HG3	2.13	0.49
17:N:81:VAL:C	17:N:83:TRP:N	2.66	0.49
20:1:202:CLA:HED1	20:1:202:CLA:CGA	2.41	0.49
1:1:89:VAL:HB	1:1:90:PRO:CD	2.33	0.49
2:2:54:TRP:O	2:2:55:ALA:C	2.49	0.49
5:A:396:PHE:O	5:A:396:PHE:CD1	2.65	0.49
5:A:40:PHE:N	5:A:44:ILE:CG2	2.76	0.49
5:A:462:ILE:HG21	20:A:831:CLA:HMC3	1.95	0.49
5:A:453:LEU:CD2	20:A:835:CLA:CBB	2.90	0.49
6:B:343:VAL:HG11	20:B:824:CLA:H2	1.95	0.49
6:B:50:HIS:HB2	6:B:53:GLN:HB2	1.95	0.49
6:B:556:SER:CA	6:B:558:PRO:HD2	2.43	0.49
20:B:806:CLA:C2A	20:B:806:CLA:O1D	2.53	0.49
8:D:132:LEU:O	8:D:135:ARG:O	2.31	0.49
21:H:105:LMU:C2'	21:H:105:LMU:H6E	2.36	0.49
20:K:101:CLA:OBD	20:K:108:CLA:C1B	2.61	0.49
20:K:108:CLA:CMC	20:K:108:CLA:HBC2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:691:ILE:HA	16:L:102:TYR:OH	2.11	0.49
17:N:61:LEU:O	17:N:62:SER:O	2.30	0.49
17:N:62:SER:OG	17:N:66:ASP:HB3	2.13	0.49
18:R:34:UNK:CB	18:R:35:UNK:CA	2.79	0.49
19:Z:1:GLC:O5	19:Z:2:FRU:O4	2.29	0.49
1:1:181:LEU:HD12	1:1:182:ALA:H	1.78	0.48
2:2:43:TRP:CD2	2:2:125:PHE:CD1	3.01	0.48
2:2:208:PHE:O	2:2:209:THR:HB	2.13	0.48
4:4:90:LEU:CA	4:4:91:PHE:HB3	2.42	0.48
5:A:172:LEU:O	5:A:175:ALA:O	2.31	0.48
5:A:411:ALA:O	5:A:412:ALA:C	2.52	0.48
5:A:126:ILE:CD1	20:A:809:CLA:HMA3	2.43	0.48
20:A:815:CLA:CGA	20:A:815:CLA:C4A	2.91	0.48
20:A:819:CLA:HMC2	20:A:825:CLA:H193	1.94	0.48
5:A:455:PHE:CD1	20:A:830:CLA:HMA2	2.47	0.48
22:A:847:BCR:C35	20:A:851:CLA:H41	2.43	0.48
6:B:304:ILE:HG22	20:B:820:CLA:O1D	2.11	0.48
6:B:577:TYR:CE1	6:B:706:ARG:HB3	2.48	0.48
20:B:832:CLA:O1D	20:B:832:CLA:H2A	2.13	0.48
9:E:43:SER:HB2	9:E:82:TYR:CE1	2.34	0.48
9:E:52:VAL:HA	9:E:67:VAL:HA	1.96	0.48
20:3:302:CLA:HMA3	5:A:246:HIS:CE1	2.48	0.48
5:A:151:GLN:HA	5:A:154:ARG:HG2	1.95	0.48
5:A:220:ARG:O	5:A:221:HIS:CB	2.60	0.48
5:A:229:ILE:O	5:A:229:ILE:HG22	2.13	0.48
5:A:720:THR:O	5:A:720:THR:CG2	2.61	0.48
20:A:818:CLA:H203	20:A:825:CLA:HAA1	1.95	0.48
5:A:86:LEU:H	5:A:86:LEU:HD22	1.79	0.48
20:B:830:CLA:C5	22:F:203:BCR:C40	2.91	0.48
9:E:41:ARG:CD	9:E:46:PHE:CZ	2.96	0.48
11:G:19:GLY:N	11:G:21:PHE:H	2.11	0.48
11:G:50:ARG:HB2	11:G:51:ALA:HB2	1.94	0.48
21:H:106:LMU:C4	21:H:106:LMU:H2B	2.43	0.48
15:K:74:ILE:CG2	15:K:75:VAL:HG22	2.35	0.48
19:O:1:GLC:H2	19:O:2:FRU:O5	2.13	0.48
18:R:46:UNK:CB	18:R:47:UNK:CA	2.90	0.48
1:1:59:VAL:CG1	1:1:60:PRO:CD	2.91	0.48
2:2:115:ASN:ND2	2:2:115:ASN:N	2.60	0.48
2:2:117:GLY:HA3	2:2:131:THR:HA	1.94	0.48
2:2:166:ASN:O	2:2:166:ASN:ND2	2.46	0.48
3:3:114:PHE:HE1	20:3:309:CLA:C3D	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:108:ASP:OD2	4:4:108:ASP:O	2.30	0.48
5:A:299:ILE:HD11	20:A:818:CLA:HMA3	1.94	0.48
5:A:312:ILE:O	5:A:313:ALA:HB2	2.13	0.48
5:A:382:TYR:HB2	5:A:385:LEU:HD11	1.95	0.48
5:A:392:GLN:O	5:A:392:GLN:CG	2.62	0.48
5:A:747:TRP:HB2	20:A:826:CLA:CBB	2.43	0.48
6:B:293:THR:C	6:B:294:ASN:ND2	2.50	0.48
6:B:356:PRO:HB2	6:B:361:ILE:CG2	2.43	0.48
6:B:531:THR:O	6:B:535:VAL:CG1	2.54	0.48
6:B:546:LEU:HD11	6:B:567:THR:CG2	2.37	0.48
6:B:568:CYS:O	6:B:570:ILE:HG23	2.12	0.48
5:A:694:PHE:CZ	6:B:661:PHE:CD1	3.01	0.48
20:B:803:CLA:CBC	22:F:202:BCR:C33	2.91	0.48
20:B:815:CLA:O1D	20:B:816:CLA:HMA1	2.13	0.48
6:B:96:PHE:HZ	6:B:104:PHE:CE2	2.31	0.48
8:D:67:ILE:O	8:D:68:MET:HG3	2.12	0.48
9:E:60:LYS:CG	9:E:61:THR:N	2.70	0.48
11:G:34:GLN:O	11:G:36:PRO:N	2.45	0.48
13:I:9:VAL:H	13:I:10:PRO:CD	2.26	0.48
14:J:36:ALA:O	14:J:37:LEU:HB2	2.12	0.48
16:L:126:GLN:O	16:L:127:PRO:O	2.31	0.48
16:L:57:GLY:HA3	16:L:146:GLY:HA3	1.96	0.48
17:N:80:ASN:OD1	17:N:80:ASN:C	2.52	0.48
19:Q:2:FRU:O6	19:Q:2:FRU:O1	2.29	0.48
21:R:102:LMU:O6'	21:R:102:LMU:O2B	2.31	0.48
19:U:1:GLC:C2	19:U:2:FRU:O5	2.56	0.48
20:3:317:CLA:HBD	20:3:317:CLA:HAA2	1.95	0.48
21:3:322:LMU:O3'	21:3:322:LMU:O2B	2.29	0.48
3:3:74:ALA:HB2	20:3:307:CLA:C1D	2.43	0.48
5:A:165:TYR:HD2	5:A:165:TYR:O	1.95	0.48
5:A:312:ILE:O	5:A:313:ALA:CB	2.61	0.48
5:A:338:PHE:O	5:A:339:THR:O	2.30	0.48
5:A:506:GLY:O	5:A:507:ALA:HB3	2.13	0.48
5:A:569:ILE:HB	5:A:572:LYS:HG3	1.95	0.48
5:A:681:GLY:C	5:A:683:HIS:H	2.16	0.48
5:A:693:LEU:HD23	5:A:734:GLY:HA3	1.96	0.48
20:A:818:CLA:HAC2	22:A:844:BCR:H352	1.96	0.48
6:B:145:LEU:HD22	6:B:148:ILE:HD12	1.94	0.48
6:B:154:TRP:O	6:B:155:LEU:C	2.51	0.48
6:B:21:ILE:HD12	6:B:21:ILE:N	2.29	0.48
6:B:415:LYS:HG2	6:B:416:GLU:OE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:662:MET:HE2	23:B:841:PQN:H2M3	1.96	0.48
21:B:802:LMU:O4'	21:B:802:LMU:O6B	2.29	0.48
20:B:804:CLA:HBC3	20:B:827:CLA:H41	1.95	0.48
20:B:839:CLA:H51	23:B:841:PQN:H251	1.94	0.48
5:A:462:ILE:HD13	20:B:850:CLA:H72	1.95	0.48
7:C:29:ILE:CG2	8:D:126:GLY:CA	2.91	0.48
7:C:81:TYR:CD1	7:C:81:TYR:N	2.81	0.48
8:D:118:VAL:HG13	8:D:119:TYR:H	1.76	0.48
9:E:38:ILE:HB	9:E:46:PHE:O	2.14	0.48
10:F:123:VAL:HG13	14:J:7:TYR:N	2.28	0.48
11:G:43:HIS:C	11:G:45:GLU:CB	2.61	0.48
11:G:80:ILE:O	11:G:81:VAL:O	2.30	0.48
16:L:164:PRO:CG	16:L:165:TYR:CD2	2.79	0.48
16:L:65:VAL:C	16:L:67:PRO:CD	2.82	0.48
16:L:99:LEU:O	16:L:136:TRP:HZ3	1.96	0.48
2:2:42:ARG:CB	2:2:45:VAL:CB	2.91	0.48
3:3:94:ARG:CB	3:3:97:PHE:HE1	2.26	0.48
4:4:128:ALA:C	4:4:130:GLU:H	2.14	0.48
5:A:159:THR:O	5:A:163:GLN:OE1	2.31	0.48
5:A:430:ASP:HA	5:A:434:ARG:HH21	1.78	0.48
5:A:499:ALA:N	5:A:500:PRO:CD	2.76	0.48
5:A:679:PHE:CE2	5:A:683:HIS:CD2	2.99	0.48
5:A:679:PHE:O	5:A:683:HIS:CB	2.62	0.48
20:A:825:CLA:OBD	20:A:825:CLA:O2D	2.31	0.48
20:A:839:CLA:HMA3	20:A:839:CLA:HBA1	1.74	0.48
6:B:279:ALA:HA	20:B:814:CLA:HMA1	1.94	0.48
6:B:292:ARG:NH1	6:B:293:THR:H	2.12	0.48
6:B:471:THR:HB	6:B:472:TYR:CE1	2.49	0.48
6:B:560:ASP:HB2	7:C:66:ARG:CZ	2.41	0.48
6:B:601:LEU:O	6:B:601:LEU:HD22	2.12	0.48
6:B:63:GLY:HA2	6:B:66:PHE:HB3	1.96	0.48
6:B:720:THR:O	6:B:724:PHE:N	2.46	0.48
5:A:710:ALA:HB1	20:B:803:CLA:HED2	1.93	0.48
20:B:808:CLA:HED1	20:I:102:CLA:HMA2	1.95	0.48
6:B:304:ILE:CD1	20:B:817:CLA:CED	2.89	0.48
6:B:354:SER:OG	20:B:824:CLA:HBC3	2.13	0.48
20:B:851:CLA:C3A	20:B:851:CLA:O2A	2.57	0.48
8:D:58:PHE:HE2	8:D:60:MET:HA	1.78	0.48
21:E:101:LMU:O4'	21:E:101:LMU:O6B	2.29	0.48
15:K:4:GLY:HA2	15:K:7:THR:CB	2.42	0.48
20:1:201:CLA:HBA1	20:1:201:CLA:CMA	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:62:ILE:HG13	2:2:66:GLU:OE2	2.13	0.48
4:4:123:GLN:O	4:4:124:TYR:CB	2.62	0.48
5:A:578:ARG:O	5:A:593:SER:OG	2.27	0.48
5:A:665:ILE:CD1	5:A:665:ILE:C	2.82	0.48
5:A:64:PHE:CE1	5:A:74:ILE:HG22	2.49	0.48
20:A:818:CLA:H8	20:A:818:CLA:HBB2	1.96	0.48
20:A:832:CLA:C2B	22:A:846:BCR:H333	2.44	0.48
6:B:190:TRP:HE3	20:B:812:CLA:CAB	2.26	0.48
6:B:224:PRO:HB3	6:B:227:THR:CB	2.43	0.48
6:B:272:ASP:C	6:B:274:ALA:H	2.17	0.48
6:B:461:GLN:N	6:B:512:ILE:HD12	2.29	0.48
20:B:807:CLA:CBB	20:B:807:CLA:C9	2.67	0.48
6:B:81:PRO:HG2	6:B:360:PHE:CE1	2.48	0.48
20:B:830:CLA:CBB	22:F:202:BCR:C26	2.92	0.48
25:B:848:LMG:H111	25:B:848:LMG:O8	2.13	0.48
11:G:20:ARG:NH1	11:G:64:VAL:C	2.67	0.48
12:H:19:GLY:O	12:H:20:GLN:HB2	2.14	0.48
15:K:9:LEU:HA	15:K:12:VAL:CG2	2.44	0.48
15:K:5:SER:O	15:K:9:LEU:HG	2.14	0.48
17:N:28:ASN:CA	17:N:30:ALA:H	2.26	0.48
17:N:84:LYS:HZ2	17:N:84:LYS:HG2	1.43	0.48
19:Z:1:GLC:C2	19:Z:2:FRU:H5	2.38	0.48
20:1:202:CLA:HAA2	20:1:202:CLA:O2D	2.14	0.48
20:1:204:CLA:CMC	20:1:209:CLA:CAC	2.91	0.48
1:1:40:LYS:O	1:1:44:LEU:HG	2.13	0.48
2:2:98:GLU:C	2:2:99:LEU:HG	2.33	0.48
20:3:313:CLA:OBD	20:3:313:CLA:O1D	2.30	0.48
5:A:154:ARG:O	5:A:155:ALA:C	2.52	0.48
5:A:284:ARG:HB2	5:A:298:ASP:OD1	2.12	0.48
5:A:539:PHE:HE2	5:A:543:HIS:CE1	2.31	0.48
5:A:415:ALA:HB2	5:A:560:VAL:HG12	1.95	0.48
5:A:705:GLU:O	5:A:708:VAL:N	2.46	0.48
22:A:847:BCR:H17C	20:A:851:CLA:C17	2.44	0.48
6:B:36:ASP:O	6:B:41:ARG:CZ	2.62	0.48
6:B:471:THR:CG2	6:B:502:ASN:ND2	2.76	0.48
20:B:807:CLA:H162	20:B:825:CLA:H192	1.95	0.48
6:B:196:HIS:CE1	20:B:813:CLA:C4D	2.96	0.48
22:B:843:BCR:H15C	22:B:843:BCR:H351	1.69	0.48
20:4:305:CLA:CBA	20:F:206:CLA:H42	2.44	0.48
11:G:80:ILE:HD12	11:G:80:ILE:O	2.14	0.48
15:K:9:LEU:O	15:K:13:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:TYR:CD2	2:2:184:THR:N	2.81	0.48
2:2:41:LEU:CD2	2:2:42:ARG:HD3	2.44	0.48
20:3:302:CLA:CBA	20:3:302:CLA:HMA2	2.39	0.48
3:3:86:GLN:CB	3:3:88:THR:HB	2.37	0.48
4:4:124:TYR:HD1	4:4:127:PRO:HG2	1.78	0.48
4:4:147:LEU:CD2	4:4:148:GLU:HG2	2.33	0.48
4:4:192:THR:HG23	4:4:193:ILE:HB	1.96	0.48
5:A:103:PHE:H	5:A:103:PHE:HD2	1.60	0.48
5:A:159:THR:O	5:A:160:SER:CB	2.62	0.48
5:A:417:PHE:C	5:A:417:PHE:CD1	2.87	0.48
20:A:818:CLA:H71	20:A:818:CLA:CAB	2.44	0.48
6:B:180:SER:CB	6:B:288:GLY:HA3	2.41	0.48
20:B:849:CLA:H193	20:B:849:CLA:H161	1.53	0.48
12:H:20:GLN:HB2	12:H:22:ASP:CB	2.39	0.48
16:L:163:LEU:CD2	16:L:165:TYR:HA	2.38	0.48
17:N:83:TRP:O	17:N:83:TRP:CE3	2.64	0.48
18:R:7:UNK:O	18:R:10:UNK:CB	2.62	0.48
2:2:189:ILE:HD13	2:2:189:ILE:N	2.28	0.48
2:2:57:LEU:O	2:2:60:ALA:HB2	2.14	0.48
3:3:195:LEU:HA	3:3:198:PHE:HB2	1.96	0.48
5:A:218:TRP:HZ3	20:A:814:CLA:HMB3	1.78	0.48
5:A:229:ILE:HG12	5:A:243:PRO:CB	2.42	0.48
5:A:22:VAL:CA	5:A:23:ASP:O	2.62	0.48
5:A:258:LEU:HG	5:A:280:PHE:CE1	2.48	0.48
5:A:330:ILE:O	5:A:330:ILE:CG2	2.62	0.48
5:A:434:ARG:O	5:A:437:ARG:N	2.46	0.48
5:A:740:LEU:CD1	20:A:838:CLA:HMA1	2.43	0.48
20:A:815:CLA:HBB1	22:A:843:BCR:C12	2.44	0.48
22:A:844:BCR:H311	22:A:844:BCR:C8	2.43	0.48
20:A:824:CLA:H93	22:A:846:BCR:C10	2.44	0.48
6:B:309:ILE:HG22	6:B:319:HIS:CD2	2.48	0.48
20:B:832:CLA:CMD	20:B:833:CLA:C1C	2.91	0.48
10:F:124:PRO:O	10:F:125:LEU:HB2	2.13	0.48
10:F:131:PHE:C	10:F:133:GLY:N	2.66	0.48
10:F:22:LEU:CD1	10:F:22:LEU:N	2.32	0.48
20:B:808:CLA:H192	22:I:101:BCR:H19C	1.96	0.48
15:K:16:THR:O	15:K:17:LEU:C	2.50	0.48
1:1:27:LEU:O	1:1:31:GLU:HB2	2.14	0.48
2:2:96:ILE:O	2:2:100:VAL:HG12	2.14	0.48
20:2:303:CLA:HAA2	20:2:308:CLA:HED2	1.94	0.48
4:4:161:LEU:O	4:4:162:ALA:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:307:CLA:CMA	20:4:307:CLA:O2A	2.62	0.48
5:A:313:ALA:C	5:A:315:HIS:H	2.17	0.48
5:A:462:ILE:CG2	20:A:831:CLA:HMC3	2.43	0.48
5:A:650:ASN:O	5:A:654:ARG:N	2.36	0.48
5:A:700:TRP:HZ3	20:A:852:CLA:O1D	1.97	0.48
5:A:73:GLU:HA	5:A:76:ARG:HB2	1.95	0.48
20:A:826:CLA:C10	22:A:847:BCR:C37	2.87	0.48
20:A:832:CLA:C3D	20:A:833:CLA:CAC	2.91	0.48
6:B:135:LEU:O	6:B:135:LEU:HD12	2.14	0.48
6:B:292:ARG:HH22	20:B:818:CLA:HED1	1.77	0.48
6:B:382:ILE:CG2	6:B:383:MET:N	2.51	0.48
6:B:593:TYR:CZ	20:B:835:CLA:HBC2	2.48	0.48
6:B:91:ILE:CG2	20:B:808:CLA:HMD1	2.36	0.48
7:C:25:VAL:HA	7:C:43:PRO:CD	2.44	0.48
7:C:28:MET:HA	7:C:38:GLN:HB2	1.95	0.48
8:D:34:GLY:HA3	8:D:62:THR:HB	1.95	0.48
11:G:20:ARG:NH2	11:G:61:ASN:CA	2.77	0.48
11:G:30:ASN:ND2	11:G:34:GLN:H	2.12	0.48
16:L:99:LEU:HD11	22:L:210:BCR:C7	2.42	0.48
2:2:159:LEU:HD12	2:2:160:ARG:HG3	1.95	0.47
2:2:171:MET:HE1	2:2:175:MET:CB	2.41	0.47
20:3:311:CLA:CHD	20:3:311:CLA:HBC2	2.43	0.47
4:4:37:LEU:O	4:4:38:ARG:C	2.52	0.47
4:4:89:THR:H	4:4:90:LEU:HD22	1.71	0.47
5:A:110:LEU:CD1	5:A:239:PRO:HG2	2.36	0.47
5:A:329:ASP:OD2	20:A:821:CLA:HED1	2.14	0.47
20:A:839:CLA:H93	20:A:839:CLA:H51	1.95	0.47
6:B:125:TYR:HE1	6:B:130:ARG:NH1	2.12	0.47
6:B:167:TRP:O	6:B:167:TRP:CG	2.66	0.47
6:B:464:GLN:CG	6:B:469:LYS:HD3	2.43	0.47
6:B:479:SER:C	6:B:481:THR:H	2.16	0.47
6:B:535:VAL:CG1	6:B:536:LYS:N	2.76	0.47
6:B:594:TRP:CD1	6:B:595:HIS:N	2.82	0.47
6:B:672:GLN:NE2	6:B:672:GLN:CA	2.59	0.47
6:B:50:HIS:HB3	20:B:805:CLA:CHB	2.44	0.47
20:B:823:CLA:CAD	20:B:835:CLA:CBB	2.91	0.47
20:B:838:CLA:H191	13:I:21:MET:CE	2.44	0.47
7:C:17:CYS:SG	7:C:18:VAL:N	2.87	0.47
8:D:138:GLY:O	8:D:140:ASN:N	2.47	0.47
22:F:202:BCR:C8	22:F:202:BCR:C33	2.91	0.47
11:G:66:PHE:O	11:G:69:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:23:VAL:O	12:H:23:VAL:HG13	2.13	0.47
20:K:101:CLA:CHD	20:K:101:CLA:HBC3	2.44	0.47
21:K:105:LMU:H121	21:K:105:LMU:H91	1.48	0.47
16:L:36:TYR:O	16:L:37:LEU:CB	2.59	0.47
17:N:61:LEU:HG	17:N:64:ASP:HB2	1.95	0.47
1:1:160:GLY:C	1:1:162:CYS:H	2.17	0.47
2:2:85:GLN:O	2:2:86:GLU:OE2	2.31	0.47
4:4:106:TRP:CZ3	20:4:304:CLA:HBC1	2.48	0.47
4:4:192:THR:CG2	4:4:193:ILE:CA	2.93	0.47
20:4:319:CLA:O1A	20:4:319:CLA:H2A	2.14	0.47
4:4:36:ASN:CB	4:4:39:TRP:CH2	2.88	0.47
5:A:21:LEU:CA	5:A:22:VAL:HB	2.39	0.47
5:A:374:GLN:O	5:A:377:TYR:CD2	2.62	0.47
5:A:377:TYR:HD1	5:A:616:PHE:HE1	1.58	0.47
5:A:678:PHE:HZ	20:A:826:CLA:H142	1.79	0.47
5:A:679:PHE:O	5:A:679:PHE:CD2	2.67	0.47
5:A:733:VAL:HG11	20:A:838:CLA:C4D	2.44	0.47
20:A:824:CLA:HMB3	22:A:846:BCR:C17	2.44	0.47
20:A:835:CLA:H71	20:A:835:CLA:H112	1.37	0.47
5:A:99:HIS:C	5:A:101:ALA:H	2.16	0.47
6:B:167:TRP:HD1	11:G:41:MET:HE1	1.80	0.47
6:B:255:LEU:HA	6:B:271:THR:HB	1.96	0.47
5:A:131:ILE:HD13	6:B:447:GLY:CA	2.44	0.47
6:B:527:LEU:O	20:B:837:CLA:HMA3	2.13	0.47
6:B:573:TRP:O	6:B:576:PHE:HB3	2.14	0.47
6:B:628:SER:O	6:B:629:SER:C	2.52	0.47
6:B:732:LYS:CD	6:B:734:GLY:CA	2.92	0.47
20:B:816:CLA:CGA	20:B:816:CLA:C4A	2.92	0.47
22:B:846:BCR:C8	22:B:846:BCR:H331	2.44	0.47
20:B:849:CLA:H3A	20:B:849:CLA:HBA2	1.40	0.47
21:D:201:LMU:H92	21:E:101:LMU:H102	1.43	0.47
9:E:37:LYS:N	9:E:49:VAL:HG13	2.28	0.47
9:E:36:VAL:HG23	9:E:52:VAL:HG22	1.96	0.47
9:E:83:ALA:O	9:E:85:ASP:N	2.46	0.47
9:E:88:GLU:O	9:E:89:GLU:C	2.52	0.47
22:F:203:BCR:HC8	22:F:203:BCR:H311	1.96	0.47
20:L:201:CLA:CAA	20:L:201:CLA:CED	2.91	0.47
19:P:1:GLC:O5	19:P:2:FRU:O5	2.30	0.47
2:2:110:TRP:CE3	20:2:311:CLA:HED1	2.49	0.47
21:2:318:LMU:H62	21:2:318:LMU:H31	1.60	0.47
20:3:307:CLA:C3A	20:3:311:CLA:HBB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:318:CLA:H52	20:3:318:CLA:H93	1.96	0.47
4:4:166:PHE:CD2	4:4:167:ILE:N	2.82	0.47
4:4:36:ASN:CG	4:4:39:TRP:CZ2	2.75	0.47
5:A:302:HIS:CD2	20:A:817:CLA:NB	2.81	0.47
5:A:385:LEU:O	5:A:386:ALA:HB2	2.12	0.47
5:A:502:THR:C	5:A:504:ALA:N	2.68	0.47
5:A:629:ASN:CG	5:A:630:ASP:N	2.67	0.47
5:A:63:ASP:HA	20:A:828:CLA:HED2	1.96	0.47
5:A:703:LEU:HD13	5:A:707:ILE:HD11	1.96	0.47
20:A:825:CLA:H151	20:A:825:CLA:H111	1.56	0.47
5:A:78:VAL:O	5:A:82:HIS:CD2	2.66	0.47
5:A:462:ILE:HG21	20:A:831:CLA:CMC	2.44	0.47
6:B:309:ILE:HD11	6:B:313:GLY:H	1.80	0.47
6:B:31:PHE:O	6:B:37:ILE:HG21	2.13	0.47
6:B:600:THR:O	6:B:605:ASN:O	2.33	0.47
20:B:830:CLA:HBB2	22:F:202:BCR:C25	2.44	0.47
21:G:101:LMU:O1B	21:G:101:LMU:O2'	2.29	0.47
12:H:75:ASP:CB	12:H:77:LEU:HG	2.43	0.47
20:B:838:CLA:H91	22:I:101:BCR:H333	1.95	0.47
21:K:106:LMU:H122	21:K:106:LMU:H92	1.44	0.47
19:X:2:FRU:O1	19:X:2:FRU:O3	2.30	0.47
2:2:102:ILE:O	2:2:103:GLY:O	2.33	0.47
2:2:137:TYR:O	2:2:143:PHE:HE2	1.96	0.47
5:A:327:ILE:HG13	5:A:328:LYS:N	2.29	0.47
5:A:400:MET:HE3	5:A:612:VAL:HG11	1.96	0.47
5:A:426:THR:HG23	5:A:428:TYR:OH	2.14	0.47
5:A:53:TRP:HA	5:A:56:ASN:CG	2.35	0.47
5:A:603:PHE:CZ	5:A:693:LEU:CD2	2.97	0.47
20:A:806:CLA:HED2	20:A:806:CLA:H12	1.95	0.47
5:A:302:HIS:HD2	20:A:817:CLA:NB	2.11	0.47
6:B:198:ALA:H	6:B:200:PRO:HG2	1.79	0.47
6:B:280:ILE:HD13	20:B:816:CLA:HBB2	1.95	0.47
23:A:842:PQN:H221	20:B:803:CLA:HAC2	1.96	0.47
20:B:812:CLA:H111	20:B:812:CLA:H71	1.41	0.47
10:F:136:TRP:HB2	10:F:139:ALA:CB	2.44	0.47
20:H:109:CLA:HHD	22:I:101:BCR:H342	1.95	0.47
20:B:839:CLA:H191	13:I:21:MET:CB	2.40	0.47
15:K:20:PHE:CD2	15:K:21:ALA:CA	2.93	0.47
17:N:72:LYS:HB2	17:N:73:ASP:HA	1.86	0.47
2:2:54:TRP:CE2	2:2:109:ARG:CD	2.86	0.47
4:4:106:TRP:CH2	20:4:304:CLA:HBC1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:197:GLN:HE22	5:A:351:THR:CB	2.22	0.47
5:A:452:PHE:O	5:A:456:HIS:ND1	2.28	0.47
6:B:211:ASN:ND2	6:B:214:ASP:OD1	2.48	0.47
6:B:244:PHE:CD2	6:B:244:PHE:C	2.87	0.47
20:B:839:CLA:H2	23:B:841:PQN:H251	1.96	0.47
7:C:30:PRO:HB3	7:C:37:LYS:O	2.14	0.47
8:D:96:ILE:O	8:D:97:LYS:HB2	2.13	0.47
10:F:96:TRP:HZ2	20:F:204:CLA:CAB	2.27	0.47
10:F:43:LYS:HE3	10:F:43:LYS:N	2.29	0.47
16:L:164:PRO:N	16:L:165:TYR:CD2	2.81	0.47
16:L:63:LEU:O	16:L:65:VAL:N	2.48	0.47
17:N:44:GLU:HB3	17:N:45:ASN:H	1.41	0.47
19:P:2:FRU:C6	19:P:2:FRU:C1	2.55	0.47
19:Q:1:GLC:O5	19:Q:2:FRU:O5	2.30	0.47
21:R:109:LMU:H102	21:R:109:LMU:H71	1.65	0.47
21:1:219:LMU:H2B	21:1:219:LMU:H6E	1.96	0.47
2:2:163:GLU:HG2	20:2:308:CLA:C3C	2.43	0.47
2:2:179:PHE:CE1	2:2:183:TYR:CZ	3.02	0.47
21:2:319:LMU:H3B	21:2:319:LMU:H4'	1.95	0.47
3:3:73:ILE:C	20:3:307:CLA:C2D	2.83	0.47
4:4:53:LEU:O	4:4:56:ALA:N	2.47	0.47
5:A:217:SER:CA	22:A:843:BCR:C35	2.84	0.47
5:A:350:LEU:HA	5:A:350:LEU:HD23	1.50	0.47
5:A:402:ILE:HD11	20:A:827:CLA:CBB	2.43	0.47
5:A:347:TYR:HE1	5:A:417:PHE:CZ	2.32	0.47
5:A:41:SER:O	5:A:44:ILE:CA	2.61	0.47
5:A:541:VAL:HG12	5:A:545:HIS:NE2	2.30	0.47
5:A:553:VAL:N	5:A:556:LEU:HD12	2.26	0.47
5:A:605:MET:O	5:A:608:SER:N	2.48	0.47
5:A:64:PHE:CD1	5:A:74:ILE:HG22	2.50	0.47
5:A:68:THR:C	5:A:70:ASP:N	2.67	0.47
5:A:302:HIS:HE1	20:A:818:CLA:C1B	2.27	0.47
6:B:216:LEU:O	6:B:218:TYR:O	2.33	0.47
6:B:269:TRP:CD1	6:B:497:TRP:HH2	2.32	0.47
6:B:335:GLY:HA2	6:B:338:LEU:HB2	1.96	0.47
6:B:387:PHE:HE2	20:B:823:CLA:HHC	1.78	0.47
6:B:421:HIS:O	20:B:837:CLA:HMC3	2.14	0.47
6:B:448:THR:O	6:B:448:THR:OG1	2.31	0.47
6:B:395:ILE:HG22	6:B:551:LYS:HG3	1.96	0.47
6:B:290:MET:HA	20:B:819:CLA:C3C	2.44	0.47
20:B:826:CLA:H62	22:B:844:BCR:HC7	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:824:CLA:CED	20:B:832:CLA:CBB	2.90	0.47
8:D:139:LYS:HZ3	9:E:41:ARG:NH1	2.12	0.47
10:F:130:LEU:CD1	19:W:2:FRU:O3	2.63	0.47
16:L:23:LEU:O	16:L:25:THR:N	2.48	0.47
16:L:63:LEU:CD2	16:L:64:LEU:N	2.73	0.47
17:N:53:ALA:O	17:N:54:LYS:CB	2.61	0.47
17:N:58:VAL:CG1	17:N:59:PRO:HD3	2.44	0.47
21:1:219:LMU:O6B	21:1:219:LMU:O3'	2.29	0.47
1:1:44:LEU:CD1	1:1:151:GLY:HA2	2.45	0.47
2:2:128:ASN:CG	14:J:3:ASP:HB3	2.35	0.47
2:2:188:PRO:C	2:2:190:ASP:H	2.17	0.47
2:2:85:GLN:CA	2:2:85:GLN:OE1	2.59	0.47
3:3:171:LYS:HE3	3:3:171:LYS:N	2.29	0.47
5:A:248:PHE:HD2	5:A:248:PHE:N	1.93	0.47
5:A:457:SER:OG	5:A:544:ILE:HA	2.15	0.47
5:A:660:GLN:HE21	5:A:660:GLN:H	1.62	0.47
5:A:599:PHE:CZ	5:A:731:ARG:HB3	2.47	0.47
20:A:811:CLA:H202	20:A:811:CLA:H152	1.96	0.47
20:A:819:CLA:HMC1	20:A:819:CLA:HBC3	1.94	0.47
5:A:692:PHE:HE2	20:A:838:CLA:HBC3	1.71	0.47
6:B:361:ILE:HG22	6:B:361:ILE:O	2.15	0.47
6:B:653:GLY:HA3	6:B:720:THR:OG1	2.13	0.47
20:B:816:CLA:C15	20:B:817:CLA:H71	2.45	0.47
20:B:823:CLA:O1A	20:B:837:CLA:HAA1	2.15	0.47
6:B:693:TRP:HE1	20:B:838:CLA:HHD	1.79	0.47
9:E:69:PHE:CE2	9:E:70:ALA:HB3	2.50	0.47
10:F:116:GLN:C	10:F:118:GLU:N	2.57	0.47
11:G:30:ASN:ND2	11:G:31:MET:O	2.48	0.47
11:G:64:VAL:HG13	11:G:67:ASN:HB2	1.94	0.47
14:J:15:SER:HA	14:J:18:TRP:HB3	1.96	0.47
2:2:127:ASN:OD1	14:J:2:ARG:CG	2.63	0.47
16:L:5:LYS:CA	16:L:5:LYS:HE2	2.36	0.47
17:N:59:PRO:CA	17:N:66:ASP:OD1	2.63	0.47
20:3:317:CLA:HBC2	20:3:317:CLA:HMC1	1.96	0.47
3:3:59:ILE:HB	3:3:63:ARG:HH21	1.79	0.47
4:4:119:PRO:C	4:4:121:PHE:H	2.17	0.47
4:4:154:ILE:O	4:4:157:GLY:CA	2.63	0.47
4:4:158:ARG:O	4:4:161:LEU:O	2.33	0.47
4:4:63:VAL:O	4:4:65:THR:HG23	2.14	0.47
5:A:241:GLU:O	5:A:241:GLU:OE1	2.32	0.47
5:A:347:TYR:CE1	5:A:417:PHE:HZ	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:420:ARG:HB3	5:A:420:ARG:CZ	2.45	0.47
5:A:628:ILE:HG13	5:A:632:GLY:CA	2.42	0.47
5:A:680:LEU:HD22	5:A:680:LEU:N	2.29	0.47
5:A:711:HIS:CB	5:A:717:ALA:HB2	2.38	0.47
5:A:603:PHE:CE1	5:A:735:VAL:HA	2.50	0.47
20:A:841:CLA:HMC3	20:B:838:CLA:ND	2.30	0.47
20:A:852:CLA:H2	20:A:852:CLA:CMA	2.44	0.47
21:A:853:LMU:C2B	21:A:853:LMU:O3'	2.63	0.47
6:B:334:LEU:HB2	20:B:805:CLA:CMD	2.41	0.47
6:B:396:ARG:NH1	20:B:827:CLA:HED2	2.30	0.47
6:B:652:PHE:CZ	6:B:656:VAL:HG21	2.50	0.47
20:B:810:CLA:C1	20:B:810:CLA:H61	2.44	0.47
20:B:817:CLA:CHA	20:B:817:CLA:HBA1	2.44	0.47
23:B:841:PQN:H143	22:B:846:BCR:H322	1.95	0.47
10:F:95:GLY:O	10:F:99:TRP:CB	2.62	0.47
11:G:28:ARG:HG2	11:G:29:GLU:HB2	1.96	0.47
21:H:108:LMU:O4'	21:H:108:LMU:O2B	2.29	0.47
15:K:13:THR:OG1	15:K:14:THR:N	2.48	0.47
8:D:36:LEU:HB2	16:L:19:PHE:O	2.15	0.47
20:A:829:CLA:HMB2	20:L:202:CLA:C3D	2.45	0.47
17:N:68:GLU:O	17:N:69:CYS:HB2	2.13	0.47
2:2:148:TRP:O	2:2:150:SER:N	2.48	0.47
20:2:308:CLA:CGA	20:2:308:CLA:C1A	2.93	0.47
3:3:127:ARG:C	3:3:129:PHE:H	2.18	0.47
3:3:166:PRO:HB2	3:3:167:LEU:H	1.54	0.47
5:A:83:PHE:CE2	5:A:185:HIS:CD2	3.03	0.47
5:A:21:LEU:HA	5:A:21:LEU:HD13	1.39	0.47
5:A:265:GLY:HA3	5:A:272:LEU:HD21	1.97	0.47
20:A:826:CLA:H191	20:A:851:CLA:H13	1.97	0.47
21:A:854:LMU:H31	21:A:854:LMU:O6'	2.13	0.47
6:B:29:HIS:HB2	20:B:827:CLA:HBA1	1.97	0.47
20:B:835:CLA:CBC	20:B:835:CLA:HMC1	2.24	0.47
7:C:66:ARG:NH2	7:C:66:ARG:CG	2.70	0.47
10:F:44:ALA:C	10:F:46:MET:N	2.68	0.47
11:G:43:HIS:CA	11:G:44:PHE:CB	2.60	0.47
17:N:2:VAL:CG2	17:N:2:VAL:O	2.62	0.47
17:N:59:PRO:HG2	17:N:73:ASP:O	2.15	0.47
19:Z:1:GLC:C5	19:Z:2:FRU:O4	2.63	0.47
21:2:317:LMU:H3'	21:2:317:LMU:H5B	1.95	0.47
3:3:141:GLN:O	3:3:142:TYR:HB2	2.14	0.47
3:3:189:LEU:C	3:3:191:MET:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:140:PRO:O	4:4:141:LEU:HB2	2.13	0.47
21:4:301:LMU:O5B	21:4:301:LMU:H5'	2.13	0.47
5:A:185:HIS:O	5:A:186:TYR:C	2.53	0.47
5:A:258:LEU:O	5:A:259:TYR:HB2	2.14	0.47
5:A:281:LEU:C	5:A:283:PHE:N	2.68	0.47
5:A:354:TRP:O	5:A:357:GLN:N	2.48	0.47
5:A:409:GLY:O	5:A:411:ALA:N	2.48	0.47
5:A:663:GLN:OE1	5:A:753:ARG:NE	2.48	0.47
5:A:701:GLN:O	5:A:703:LEU:N	2.48	0.47
5:A:709:TRP:CE3	5:A:710:ALA:N	2.83	0.47
5:A:70:ASP:O	5:A:71:LEU:O	2.33	0.47
20:A:803:CLA:HBC3	20:A:803:CLA:HHD	1.97	0.47
20:A:811:CLA:C4A	20:A:811:CLA:CBA	2.92	0.47
5:A:372:VAL:HG22	20:A:818:CLA:C4	2.45	0.47
6:B:353:TYR:C	6:B:355:LEU:N	2.68	0.47
6:B:31:PHE:HB2	6:B:42:LEU:HD12	1.96	0.47
6:B:552:ASP:OD1	6:B:553:PHE:HD2	1.98	0.47
20:B:821:CLA:OBD	20:B:821:CLA:O1D	2.31	0.47
20:B:823:CLA:C2B	22:B:845:BCR:H352	2.45	0.47
7:C:14:CYS:SG	7:C:17:CYS:SG	3.13	0.47
5:A:584:PRO:HG2	7:C:66:ARG:HB2	1.97	0.47
7:C:70:TRP:O	7:C:71:HIS:C	2.53	0.47
8:D:26:SER:N	8:D:27:PRO:HD3	2.29	0.47
8:D:89:ARG:O	8:D:92:SER:N	2.48	0.47
21:G:101:LMU:H6'2	21:G:101:LMU:H1B	1.41	0.47
21:G:101:LMU:O5'	21:G:101:LMU:O3'	2.29	0.47
11:G:34:GLN:O	11:G:36:PRO:CD	2.63	0.47
21:H:108:LMU:H6B	21:H:108:LMU:H3O2	1.63	0.47
20:A:826:CLA:H202	22:J:102:BCR:C16	2.45	0.47
16:L:154:ALA:O	16:L:155:CYS:C	2.53	0.47
20:L:202:CLA:C9	20:L:203:CLA:H2	2.44	0.47
16:L:46:ALA:CB	16:L:52:ARG:NH2	2.78	0.47
17:N:47:THR:O	17:N:48:GLY:C	2.52	0.47
21:1:213:LMU:O1B	21:1:213:LMU:O4'	2.30	0.47
2:2:96:ILE:O	2:2:100:VAL:N	2.47	0.47
20:2:307:CLA:HMA2	20:2:307:CLA:C5	2.43	0.47
3:3:164:PHE:O	3:3:165:ASN:C	2.53	0.47
4:4:175:LYS:O	4:4:175:LYS:HD2	2.15	0.47
5:A:434:ARG:O	5:A:435:VAL:C	2.53	0.47
5:A:581:CYS:HB3	5:A:590:CYS:O	2.14	0.47
5:A:733:VAL:HG13	20:A:838:CLA:C3D	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:841:CLA:HMC3	20:B:838:CLA:C1D	2.45	0.47
6:B:127:ILE:O	6:B:128:GLY:C	2.53	0.47
6:B:183:PHE:HB3	6:B:284:PHE:HD2	1.80	0.47
6:B:470:THR:OG1	6:B:501:ILE:HG23	2.15	0.47
5:A:705:GLU:CG	6:B:545:LYS:HZ2	2.26	0.47
6:B:558:PRO:HB3	6:B:706:ARG:HH21	1.79	0.47
6:B:212:PHE:CE1	20:B:812:CLA:HHD	2.34	0.47
20:B:817:CLA:H61	20:B:817:CLA:H41	1.66	0.47
20:B:823:CLA:H11	20:B:837:CLA:CAD	2.44	0.47
7:C:17:CYS:O	7:C:58:CYS:HB2	2.14	0.47
8:D:48:ILE:CG1	8:D:49:THR:N	2.77	0.47
9:E:44:TYR:HB3	9:E:45:TRP:CZ3	2.51	0.47
10:F:137:PRO:O	10:F:139:ALA:N	2.47	0.47
20:G:102:CLA:H3A	20:G:102:CLA:C2	2.44	0.47
11:G:16:LEU:CD1	11:G:17:PHE:CZ	2.98	0.47
11:G:79:HIS:NE2	11:G:82:ALA:HB2	2.30	0.47
21:H:107:LMU:H62	21:H:107:LMU:H92	1.51	0.47
12:H:76:VAL:O	12:H:76:VAL:HG22	2.15	0.47
13:I:8:PHE:CD1	20:I:102:CLA:H12	2.49	0.47
17:N:70:GLU:HB3	17:N:72:LYS:HA	1.95	0.47
19:P:2:FRU:H62	19:P:2:FRU:H12	1.82	0.47
3:3:63:ARG:NH1	3:3:189:LEU:H	2.13	0.46
5:A:132:LEU:O	5:A:143:ILE:HB	2.15	0.46
5:A:193:LEU:O	5:A:195:TRP:N	2.49	0.46
5:A:463:HIS:NE2	5:A:467:MET:SD	2.88	0.46
5:A:539:PHE:CD2	5:A:539:PHE:C	2.89	0.46
5:A:132:LEU:HD13	5:A:671:SER:O	2.15	0.46
5:A:709:TRP:O	5:A:712:ASN:N	2.48	0.46
5:A:733:VAL:HG12	5:A:737:HIS:CE1	2.50	0.46
5:A:210:LEU:CD1	20:A:813:CLA:HHB	2.45	0.46
6:B:120:VAL:HG22	6:B:123:TRP:HE1	1.80	0.46
6:B:230:TRP:O	6:B:231:ASN:C	2.52	0.46
6:B:289:LEU:O	20:B:819:CLA:HMC1	2.15	0.46
6:B:290:MET:SD	6:B:291:TYR:CE1	3.08	0.46
6:B:9:SER:HA	6:B:35:ASP:OD1	2.15	0.46
6:B:540:ASP:OD1	6:B:540:ASP:N	2.47	0.46
6:B:708:VAL:C	6:B:710:LEU:O	2.53	0.46
20:B:835:CLA:OBD	20:B:835:CLA:O2D	2.33	0.46
6:B:693:TRP:CD1	20:B:838:CLA:HMD3	2.49	0.46
20:B:849:CLA:HMB3	20:B:850:CLA:CAD	2.45	0.46
21:F:201:LMU:O5B	21:F:201:LMU:C5'	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:294:ASN:O	11:G:36:PRO:HG2	2.15	0.46
11:G:37:GLU:O	11:G:38:GLN:C	2.52	0.46
16:L:123:ARG:HB3	16:L:126:GLN:HG3	1.96	0.46
16:L:108:LYS:HD3	16:L:132:SER:HB3	1.97	0.46
16:L:162:ASP:O	16:L:162:ASP:OD2	2.33	0.46
21:L:204:LMU:H1B	21:L:204:LMU:H6'2	1.43	0.46
2:2:102:ILE:HG22	2:2:106:GLU:HG3	1.98	0.46
2:2:73:ILE:HG22	2:2:73:ILE:O	2.15	0.46
20:3:307:CLA:C3B	20:3:311:CLA:H11	2.46	0.46
4:4:93:ILE:C	4:4:95:PHE:H	2.17	0.46
5:A:355:HIS:ND1	5:A:416:ILE:HG22	2.24	0.46
5:A:400:MET:CE	5:A:612:VAL:HG11	2.46	0.46
5:A:476:MET:O	5:A:477:PHE:HB2	2.16	0.46
5:A:493:GLN:OE1	5:A:534:LEU:HD11	2.15	0.46
5:A:680:LEU:HB3	20:A:851:CLA:C2	2.45	0.46
20:A:812:CLA:O1D	20:A:813:CLA:HMC1	2.16	0.46
5:A:98:PHE:HD1	5:A:99:HIS:CD2	2.32	0.46
6:B:334:LEU:HA	20:B:805:CLA:HMD3	1.97	0.46
6:B:30:ASP:O	6:B:34:HIS:HD2	1.98	0.46
6:B:350:GLN:O	6:B:353:TYR:CD1	2.69	0.46
6:B:478:LEU:O	6:B:479:SER:HB3	2.15	0.46
6:B:494:LEU:HD12	20:B:833:CLA:CED	2.44	0.46
7:C:77:MET:C	7:C:79:LEU:H	2.13	0.46
7:C:81:TYR:HD1	7:C:81:TYR:N	2.14	0.46
11:G:39:ASN:HA	11:G:40:GLY:O	2.15	0.46
22:I:103:BCR:H341	22:I:103:BCR:H11C	1.71	0.46
16:L:40:LEU:H	16:L:40:LEU:HD12	1.80	0.46
17:N:6:TYR:HA	17:N:6:TYR:HD2	1.69	0.46
17:N:70:GLU:CA	17:N:72:LYS:H	2.26	0.46
18:R:1:UNK:O	18:R:2:UNK:O	2.34	0.46
1:1:160:GLY:HA3	20:1:203:CLA:CBB	2.45	0.46
4:4:99:HIS:HD1	4:4:103:ILE:HD13	1.81	0.46
4:4:104:ARG:CG	4:4:105:ARG:N	2.74	0.46
4:4:107:GLN:HA	20:4:302:CLA:C2A	2.45	0.46
4:4:88:SER:O	4:4:90:LEU:CA	2.53	0.46
5:A:298:ASP:O	5:A:300:ALA:N	2.49	0.46
5:A:458:PHE:C	5:A:458:PHE:CD1	2.89	0.46
5:A:514:THR:HA	5:A:530:LEU:O	2.15	0.46
5:A:550:HIS:C	5:A:552:THR:O	2.53	0.46
5:A:616:PHE:O	5:A:620:MET:HB2	2.16	0.46
5:A:73:GLU:O	5:A:76:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:823:CLA:HBC2	20:A:823:CLA:HMC1	1.96	0.46
20:A:824:CLA:CED	20:A:825:CLA:HMD2	2.37	0.46
20:A:832:CLA:HBA2	20:A:832:CLA:H3A	1.51	0.46
22:A:847:BCR:C8	20:A:852:CLA:H142	2.45	0.46
6:B:322:LEU:O	6:B:326:ILE:HG22	2.16	0.46
6:B:527:LEU:CD1	6:B:586:THR:HG21	2.43	0.46
6:B:596:TRP:HZ3	6:B:613:SER:CB	2.28	0.46
6:B:732:LYS:C	6:B:733:PHE:O	2.53	0.46
6:B:590:VAL:HG21	20:B:835:CLA:HBB2	1.98	0.46
20:B:824:CLA:H122	22:B:845:BCR:C12	2.46	0.46
6:B:589:TRP:CD1	20:B:849:CLA:H152	2.51	0.46
8:D:137:ILE:H	8:D:137:ILE:HG13	1.41	0.46
10:F:145:LEU:C	10:F:146:ASN:ND2	2.69	0.46
10:F:34:ASP:O	10:F:34:ASP:OD2	2.33	0.46
10:F:41:ALA:O	10:F:44:ALA:O	2.33	0.46
11:G:16:LEU:HD12	11:G:17:PHE:CZ	2.48	0.46
11:G:48:ASP:CB	11:G:49:THR:CB	2.91	0.46
12:H:29:PRO:O	12:H:30:SER:OG	2.28	0.46
2:2:120:ASN:ND2	14:J:5:LYS:HD2	2.30	0.46
16:L:62:PHE:HE2	20:L:209:CLA:H2A	1.81	0.46
16:L:40:LEU:CB	16:L:41:PRO:HD3	2.37	0.46
17:N:42:PHE:CG	17:N:43:PRO:N	2.79	0.46
21:R:102:LMU:C6'	21:R:102:LMU:C1B	2.93	0.46
21:R:104:LMU:H6'2	21:R:104:LMU:O3B	2.12	0.46
21:1:219:LMU:O2'	21:1:219:LMU:O6B	2.29	0.46
1:1:63:LEU:CD2	1:1:64:GLY:CA	2.84	0.46
2:2:102:ILE:HD13	2:2:102:ILE:N	2.31	0.46
3:3:205:GLY:HA3	5:A:252:ARG:HH12	1.79	0.46
4:4:129:GLY:C	4:4:131:VAL:N	2.68	0.46
5:A:107:GLU:O	5:A:110:LEU:HG	2.15	0.46
5:A:265:GLY:HA2	5:A:272:LEU:CD2	2.46	0.46
5:A:27:ILE:C	5:A:28:LYS:CG	2.83	0.46
5:A:684:PHE:HD2	5:A:685:VAL:CA	2.27	0.46
20:A:811:CLA:H141	20:A:811:CLA:H171	1.97	0.46
20:A:812:CLA:HAA1	20:A:812:CLA:HBD	1.95	0.46
20:A:822:CLA:CBB	22:A:845:BCR:H352	2.29	0.46
20:A:852:CLA:H93	6:B:431:PHE:CD1	2.51	0.46
6:B:176:ASN:ND2	6:B:293:THR:OG1	2.47	0.46
20:B:805:CLA:H92	20:B:822:CLA:O1A	2.16	0.46
6:B:431:PHE:CD2	20:B:830:CLA:HMA3	2.50	0.46
7:C:52:LYS:C	7:C:54:CYS:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:514:PRO:HG2	10:F:70:HIS:CE1	2.49	0.46
14:J:2:ARG:CG	14:J:2:ARG:HH11	2.29	0.46
2:2:120:ASN:HB3	14:J:5:LYS:HD2	1.97	0.46
20:K:101:CLA:HBD	20:K:101:CLA:HAA2	1.96	0.46
16:L:151:VAL:O	16:L:154:ALA:HB3	2.15	0.46
16:L:56:VAL:CG1	20:L:208:CLA:CED	2.87	0.46
17:N:59:PRO:CB	17:N:75:TYR:CE1	2.95	0.46
1:1:185:TRP:HB3	1:1:186:HIS:NE2	2.31	0.46
2:2:191:ASN:HD21	2:2:194:ALA:HA	1.80	0.46
20:2:307:CLA:H2A	20:2:307:CLA:H2	1.97	0.46
20:3:311:CLA:H162	20:3:311:CLA:H141	1.59	0.46
3:3:56:TYR:HD1	3:3:185:LYS:CE	2.29	0.46
4:4:72:VAL:O	4:4:72:VAL:HG22	2.15	0.46
4:4:83:TYR:HB3	4:4:84:PHE:H	1.72	0.46
5:A:223:VAL:HG12	5:A:224:HIS:H	1.80	0.46
5:A:249:ILE:CG2	5:A:251:ASN:OD1	2.64	0.46
5:A:425:THR:O	5:A:427:ARG:CD	2.64	0.46
5:A:499:ALA:HB3	20:A:832:CLA:CED	2.45	0.46
5:A:636:HIS:O	5:A:637:ILE:C	2.53	0.46
20:A:819:CLA:H43	20:A:822:CLA:C2	2.45	0.46
5:A:680:LEU:HD12	20:A:851:CLA:O2A	2.16	0.46
6:B:377:TYR:O	6:B:378:ILE:CB	2.62	0.46
6:B:454:LEU:H	6:B:454:LEU:HD12	1.80	0.46
6:B:461:GLN:HE21	6:B:461:GLN:HB3	1.61	0.46
6:B:500:ALA:C	6:B:501:ILE:HG12	2.36	0.46
9:E:83:ALA:O	9:E:86:GLU:CG	2.49	0.46
11:G:57:LEU:O	11:G:57:LEU:HD22	2.16	0.46
14:J:21:SER:O	14:J:23:ALA:N	2.48	0.46
16:L:163:LEU:CD1	16:L:164:PRO:CB	2.47	0.46
2:2:42:ARG:CA	2:2:45:VAL:CB	2.84	0.46
2:2:73:ILE:CD1	2:2:75:ASN:HB2	2.46	0.46
20:3:311:CLA:H71	20:3:311:CLA:H112	1.47	0.46
3:3:84:ILE:HG23	3:3:84:ILE:O	2.16	0.46
4:4:103:ILE:HB	20:4:303:CLA:HMD1	1.96	0.46
5:A:208:ALA:HB2	5:A:314:GLY:CA	2.38	0.46
5:A:361:ASN:ND2	5:A:361:ASN:C	2.69	0.46
20:A:803:CLA:HBC3	20:A:803:CLA:CHD	2.46	0.46
20:A:804:CLA:HBA2	20:A:811:CLA:C6	2.44	0.46
5:A:308:ILE:HD13	20:A:816:CLA:C9	2.38	0.46
20:A:824:CLA:CMA	20:A:825:CLA:CGA	2.93	0.46
20:A:835:CLA:H203	20:L:202:CLA:HBB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:843:BCR:C12	22:A:843:BCR:C34	2.86	0.46
6:B:172:GLU:O	6:B:173:SER:C	2.54	0.46
6:B:580:VAL:HG11	6:B:710:LEU:HD11	1.97	0.46
20:B:803:CLA:H71	20:B:803:CLA:C2C	2.45	0.46
6:B:53:GLN:NE2	20:B:804:CLA:HBB1	2.30	0.46
20:B:826:CLA:H101	22:B:844:BCR:C34	2.44	0.46
6:B:429:LEU:HD11	20:B:836:CLA:HMB3	1.96	0.46
21:H:108:LMU:C2	21:H:108:LMU:H81	2.40	0.46
16:L:126:GLN:N	16:L:127:PRO:CD	2.78	0.46
17:N:27:ALA:O	17:N:28:ASN:C	2.54	0.46
1:1:59:VAL:HG12	1:1:60:PRO:N	2.26	0.46
2:2:157:LYS:HA	2:2:159:LEU:CD2	2.46	0.46
21:2:319:LMU:H52	21:2:319:LMU:H21	1.68	0.46
4:4:191:ASN:CG	4:4:191:ASN:O	2.52	0.46
4:4:51:ALA:O	4:4:55:VAL:HG13	2.16	0.46
5:A:76:ARG:C	5:A:186:TYR:HD2	2.19	0.46
5:A:24:ARG:N	5:A:24:ARG:CD	2.76	0.46
5:A:334:HIS:HD2	20:A:820:CLA:NB	2.14	0.46
5:A:358:LEU:HD11	5:A:413:HIS:HB2	1.90	0.46
5:A:369:THR:O	5:A:372:VAL:HG23	2.16	0.46
5:A:397:THR:HB	5:A:613:ILE:HG13	1.96	0.46
5:A:613:ILE:HG22	5:A:614:PHE:N	2.29	0.46
5:A:334:HIS:CD2	20:A:820:CLA:NB	2.84	0.46
6:B:57:ILE:HG22	6:B:58:PHE:CD1	2.50	0.46
6:B:596:TRP:CZ3	6:B:613:SER:CB	2.98	0.46
6:B:629:SER:O	6:B:630:GLN:C	2.53	0.46
6:B:278:LEU:CD1	20:B:814:CLA:HMA2	2.39	0.46
6:B:292:ARG:NH2	20:B:818:CLA:HED1	2.31	0.46
20:B:832:CLA:H3A	20:B:832:CLA:HBA2	1.47	0.46
6:B:486:LEU:CD1	20:B:833:CLA:HMD3	2.45	0.46
22:B:843:BCR:H341	22:B:843:BCR:H11C	1.68	0.46
7:C:26:LEU:O	7:C:43:PRO:HB3	2.16	0.46
7:C:28:MET:SD	8:D:122:LYS:O	2.74	0.46
12:H:53:LEU:HG	12:H:54:LEU:N	2.22	0.46
21:K:106:LMU:O6'	21:K:106:LMU:O1B	2.30	0.46
21:R:103:LMU:H1'	21:R:103:LMU:C4	2.43	0.46
2:2:171:MET:SD	2:2:172:LEU:CG	3.00	0.46
2:2:196:HIS:HB3	2:2:197:LEU:H	1.50	0.46
20:2:316:CLA:H111	20:2:316:CLA:H71	1.58	0.46
4:4:72:VAL:N	4:4:73:PRO:CD	2.78	0.46
5:A:462:ILE:O	5:A:466:THR:OG1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:746:THR:HG1	20:A:850:CLA:CGD	2.24	0.46
5:A:73:GLU:O	5:A:74:ILE:C	2.54	0.46
20:A:806:CLA:C7	20:A:806:CLA:C2	2.94	0.46
20:A:824:CLA:H93	22:A:846:BCR:H10C	1.97	0.46
6:B:164:SER:HB2	6:B:167:TRP:CE3	2.51	0.46
6:B:167:TRP:HB2	11:G:41:MET:HE3	1.97	0.46
6:B:318:GLY:HA3	6:B:405:ASP:OD2	2.15	0.46
6:B:415:LYS:HG3	6:B:416:GLU:OE2	2.15	0.46
6:B:442:VAL:O	6:B:446:PHE:HB2	2.16	0.46
6:B:721:TYR:HA	6:B:724:PHE:HB3	1.97	0.46
9:E:58:ASP:N	9:E:58:ASP:OD1	2.29	0.46
22:F:203:BCR:H24C	22:F:203:BCR:H371	1.51	0.46
11:G:10:LEU:HD23	11:G:13:GLY:HA3	1.98	0.46
11:G:24:PHE:C	11:G:26:PHE:N	2.69	0.46
20:H:109:CLA:O1D	20:H:109:CLA:H2A	2.16	0.46
16:L:158:MET:CG	16:L:159:TYR:N	2.75	0.46
19:O:2:FRU:O2	19:O:2:FRU:O4	2.34	0.46
2:2:44:ASN:HD21	14:J:1:MET:CB	2.09	0.46
21:3:322:LMU:C7	21:3:322:LMU:H32	2.23	0.46
4:4:116:ASN:HB3	4:4:118:ASP:OD1	2.16	0.46
20:4:307:CLA:O2D	20:4:307:CLA:HAA2	2.14	0.46
5:A:531:PRO:O	5:A:532:ILE:HG23	2.16	0.46
5:A:457:SER:HG	5:A:544:ILE:HA	1.80	0.46
5:A:593:SER:O	5:A:594:ALA:HB2	2.15	0.46
5:A:656:PHE:O	5:A:658:TRP:N	2.49	0.46
5:A:660:GLN:O	5:A:661:ALA:HB2	2.14	0.46
20:A:806:CLA:H11	20:A:828:CLA:O2A	2.16	0.46
22:A:843:BCR:C8	22:A:843:BCR:C31	2.65	0.46
20:A:822:CLA:NB	22:A:845:BCR:C15	2.78	0.46
6:B:224:PRO:CA	6:B:227:THR:OG1	2.63	0.46
6:B:399:ASN:O	6:B:399:ASN:OD1	2.34	0.46
5:A:709:TRP:CZ3	6:B:417:ALA:HA	2.50	0.46
6:B:544:SER:O	6:B:547:MET:C	2.55	0.46
6:B:568:CYS:C	6:B:570:ILE:HG23	2.36	0.46
6:B:700:LEU:H	6:B:700:LEU:HD23	1.80	0.46
6:B:389:HIS:HE1	20:B:827:CLA:NC	2.14	0.46
10:F:149:LEU:CD2	10:F:153:ASN:HD21	2.28	0.46
10:F:72:ILE:O	10:F:73:VAL:HG12	2.16	0.46
20:G:102:CLA:H3A	20:G:102:CLA:H2	1.98	0.46
26:H:111:UNL:O3'	26:H:111:UNL:O1'	2.28	0.46
12:H:66:THR:N	12:H:69:SER:HB3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:61:GLY:O	16:L:63:LEU:N	2.49	0.46
17:N:45:ASN:CG	17:N:57:LYS:NZ	2.69	0.46
2:2:125:PHE:O	2:2:127:ASN:HA	2.15	0.46
2:2:191:ASN:O	2:2:191:ASN:CG	2.53	0.46
3:3:112:THR:C	3:3:114:PHE:N	2.69	0.46
3:3:162:PRO:HG2	3:3:164:PHE:CG	2.51	0.46
3:3:165:ASN:HA	3:3:165:ASN:HD22	1.59	0.46
3:3:56:TYR:HD1	3:3:185:LYS:NZ	2.12	0.46
3:3:66:MET:CE	3:3:69:ALA:HB3	2.46	0.46
4:4:101:VAL:O	4:4:104:ARG:HD3	2.15	0.46
4:4:103:ILE:CB	20:4:303:CLA:HMD1	2.46	0.46
4:4:142:ASN:C	4:4:143:PHE:CG	2.89	0.46
4:4:69:ILE:O	4:4:71:ASN:HB2	2.16	0.46
5:A:22:VAL:H	5:A:23:ASP:C	2.19	0.46
5:A:296:LEU:C	5:A:298:ASP:N	2.68	0.46
5:A:374:GLN:C	5:A:376:MET:N	2.68	0.46
5:A:405:PHE:O	20:A:828:CLA:HMC1	2.15	0.46
5:A:584:PRO:HG3	6:B:559:CYS:SG	2.56	0.46
5:A:645:SER:O	5:A:651:GLY:HA3	2.15	0.46
5:A:49:ASP:HB2	5:A:720:THR:HA	1.97	0.46
20:A:819:CLA:H121	22:A:846:BCR:H23C	1.97	0.46
20:A:818:CLA:ND	20:A:827:CLA:H72	2.31	0.46
6:B:256:THR:HG22	6:B:271:THR:OG1	2.16	0.46
6:B:275:HIS:HD2	20:B:814:CLA:HMA3	1.81	0.46
6:B:336:LEU:HD13	20:B:822:CLA:CBB	2.45	0.46
6:B:435:GLY:HA3	20:B:831:CLA:CBB	2.46	0.46
6:B:518:LEU:O	6:B:521:HIS:N	2.41	0.46
6:B:714:SER:O	6:B:718:ILE:HG22	2.16	0.46
20:B:813:CLA:HMA1	22:B:844:BCR:H372	1.98	0.46
20:4:305:CLA:HAA1	20:F:206:CLA:H12	1.97	0.46
10:F:22:LEU:CB	10:F:25:LEU:HD13	2.46	0.46
10:F:37:ALA:N	10:F:38:PRO:HD3	2.31	0.46
10:F:63:CYS:CA	10:F:69:PRO:HA	2.43	0.46
10:F:78:ARG:O	10:F:80:TRP:CD1	2.69	0.46
11:G:28:ARG:CG	11:G:29:GLU:CB	2.94	0.46
13:I:15:LEU:HD12	13:I:18:ALA:HB3	1.98	0.46
21:K:106:LMU:O6'	21:K:106:LMU:O2B	2.30	0.46
15:K:24:PHE:CG	15:K:52:PRO:CG	2.99	0.46
1:1:34:ALA:O	1:1:35:ASN:C	2.55	0.45
1:1:64:GLY:C	1:1:66:GLY:N	2.69	0.45
2:2:102:ILE:CG2	2:2:106:GLU:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:ASN:O	2:2:129:LYS:C	2.54	0.45
3:3:106:TYR:O	3:3:107:TRP:C	2.54	0.45
3:3:132:TRP:HZ3	3:3:155:GLU:CD	1.82	0.45
3:3:188:ARG:HA	3:3:191:MET:HB2	1.97	0.45
5:A:126:ILE:O	5:A:129:GLN:HB2	2.16	0.45
5:A:302:HIS:O	5:A:306:ILE:CG1	2.51	0.45
5:A:552:THR:O	5:A:553:VAL:HB	2.16	0.45
5:A:685:VAL:CG1	5:A:741:GLY:CA	2.94	0.45
5:A:707:ILE:H	5:A:707:ILE:HG12	1.54	0.45
5:A:708:VAL:N	5:A:711:HIS:HD2	2.14	0.45
5:A:72:GLU:HB2	5:A:73:GLU:H	1.55	0.45
22:A:844:BCR:C8	22:A:844:BCR:C31	2.94	0.45
6:B:260:GLY:HA2	6:B:497:TRP:CE2	2.51	0.45
6:B:556:SER:HA	6:B:558:PRO:HD3	1.98	0.45
6:B:60:TRP:CD1	20:B:806:CLA:HBC1	2.51	0.45
6:B:193:HIS:CD2	20:B:812:CLA:NB	2.84	0.45
6:B:354:SER:OG	20:B:824:CLA:CBC	2.64	0.45
22:B:843:BCR:HC8	22:B:843:BCR:H331	1.95	0.45
21:B:847:LMU:O6B	21:B:847:LMU:O2'	2.30	0.45
6:B:721:TYR:N	20:B:849:CLA:O1D	2.49	0.45
20:B:849:CLA:HMB3	20:B:850:CLA:OBD	2.16	0.45
8:D:102:ARG:NH2	8:D:110:GLN:HB2	2.30	0.45
8:D:146:VAL:HG21	8:D:152:GLN:HG3	1.98	0.45
10:F:115:THR:O	10:F:116:GLN:CB	2.63	0.45
10:F:116:GLN:HA	10:F:118:GLU:OE1	2.16	0.45
10:F:123:VAL:CB	10:F:126:ALA:O	2.64	0.45
12:H:77:LEU:HD23	12:H:78:PRO:CD	2.46	0.45
16:L:123:ARG:CA	16:L:123:ARG:NE	2.71	0.45
16:L:59:ALA:HB2	20:L:207:CLA:HMA1	1.97	0.45
20:L:209:CLA:HHD	20:L:209:CLA:HBC2	1.88	0.45
17:N:7:LEU:O	17:N:8:GLU:HB2	2.16	0.45
19:O:1:GLC:C2	19:O:1:GLC:C6	2.87	0.45
1:1:34:ALA:O	1:1:38:ARG:N	2.40	0.45
2:2:39:GLU:CA	2:2:40:SER:CB	2.71	0.45
3:3:114:PHE:HD1	20:3:309:CLA:CHA	2.27	0.45
5:A:122:VAL:HG22	5:A:142:GLY:CA	2.46	0.45
5:A:637:ILE:HG12	5:A:637:ILE:H	1.52	0.45
5:A:660:GLN:O	5:A:661:ALA:HB3	2.15	0.45
5:A:669:GLY:H	6:B:445:ALA:CA	2.24	0.45
20:A:805:CLA:H202	20:A:805:CLA:H161	1.61	0.45
5:A:368:LEU:HD12	20:A:825:CLA:H62	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:840:CLA:CED	20:A:840:CLA:HBA2	2.46	0.45
6:B:103:ALA:HA	6:B:105:THR:O	2.17	0.45
6:B:221:GLY:C	6:B:223:GLY:N	2.69	0.45
6:B:428:PHE:HE1	20:B:830:CLA:HMD3	1.80	0.45
6:B:439:HIS:NE2	6:B:443:MET:SD	2.89	0.45
23:B:841:PQN:H192	22:B:846:BCR:HC8	1.95	0.45
8:D:132:LEU:HD12	8:D:136:SER:OG	2.17	0.45
8:D:31:GLY:CA	16:L:13:PRO:HB3	2.44	0.45
10:F:102:ARG:NH1	10:F:106:ILE:HD12	2.31	0.45
10:F:26:GLN:O	10:F:28:SER:N	2.49	0.45
11:G:57:LEU:CD2	11:G:57:LEU:O	2.64	0.45
21:H:108:LMU:H6'2	21:H:108:LMU:H1B	1.08	0.45
21:H:108:LMU:H41	21:H:108:LMU:H71	1.78	0.45
14:J:31:ARG:O	14:J:34:PRO:HG3	2.17	0.45
16:L:50:LEU:HD23	16:L:51:LEU:H	1.81	0.45
17:N:42:PHE:N	17:N:43:PRO:CD	2.58	0.45
2:2:41:LEU:C	2:2:42:ARG:HD3	2.36	0.45
3:3:90:LEU:HD12	3:3:90:LEU:N	2.31	0.45
4:4:75:TRP:CD1	20:4:311:CLA:CHD	2.99	0.45
20:4:311:CLA:CBD	20:4:311:CLA:HBA2	2.47	0.45
21:4:320:LMU:H3'	21:4:320:LMU:O6B	2.17	0.45
5:A:128:GLY:HA3	6:B:446:PHE:HD2	1.79	0.45
5:A:284:ARG:HG3	5:A:295:TRP:CB	2.47	0.45
5:A:377:TYR:CD1	5:A:616:PHE:CE1	3.02	0.45
5:A:551:VAL:HG21	5:A:604:TRP:CZ2	2.51	0.45
5:A:606:TYR:OH	20:A:850:CLA:HED3	2.17	0.45
5:A:657:LEU:HD13	20:A:850:CLA:H93	1.99	0.45
6:B:138:GLY:H	6:B:140:ILE:HG12	1.80	0.45
6:B:15:ASP:OD2	6:B:15:ASP:C	2.55	0.45
6:B:319:HIS:O	6:B:320:LYS:O	2.34	0.45
6:B:551:LYS:HG2	6:B:552:ASP:H	1.79	0.45
6:B:561:GLY:HA3	7:C:52:LYS:CB	2.46	0.45
6:B:638:LEU:N	6:B:638:LEU:HD22	2.31	0.45
23:B:841:PQN:H111	23:B:841:PQN:H2M1	1.67	0.45
10:F:24:LYS:HE3	10:F:24:LYS:N	2.24	0.45
20:H:103:CLA:HBD	20:H:103:CLA:HAA2	1.97	0.45
12:H:24:TYR:HB3	12:H:25:GLY:H	1.60	0.45
20:3:311:CLA:OBD	20:3:311:CLA:O2D	2.29	0.45
4:4:169:GLN:HE22	20:4:305:CLA:HHD	1.73	0.45
5:A:207:LEU:HD11	5:A:313:ALA:HB1	1.98	0.45
5:A:260:PRO:HG3	5:A:277:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:57:LEU:HD22	5:A:58:HIS:CD2	2.51	0.45
5:A:707:ILE:HG22	5:A:711:HIS:CD2	2.50	0.45
5:A:73:GLU:O	5:A:76:ARG:CA	2.64	0.45
20:A:804:CLA:HMC3	20:A:806:CLA:CED	2.47	0.45
20:A:837:CLA:H3A	20:A:837:CLA:HBA1	1.66	0.45
6:B:180:SER:O	6:B:181:GLY:C	2.54	0.45
6:B:336:LEU:CD1	20:B:822:CLA:CBB	2.95	0.45
6:B:513:GLY:O	6:B:516:ASP:OD1	2.34	0.45
6:B:626:LEU:O	6:B:627:ASN:CB	2.64	0.45
6:B:290:MET:CA	20:B:819:CLA:HAC2	2.44	0.45
20:B:806:CLA:CBC	20:B:825:CLA:CMD	2.95	0.45
20:B:831:CLA:H3A	20:B:831:CLA:HBA1	1.66	0.45
20:B:839:CLA:HHD	23:B:841:PQN:H18	1.98	0.45
8:D:46:TYR:HD2	8:D:46:TYR:N	2.11	0.45
10:F:104:TYR:OH	10:F:121:ILE:HA	2.17	0.45
10:F:22:LEU:HA	10:F:25:LEU:CD1	2.47	0.45
14:J:32:PHE:HE2	14:J:33:PHE:CE1	2.35	0.45
16:L:161:LEU:CD1	16:L:162:ASP:O	2.63	0.45
8:D:75:LEU:HD21	16:L:19:PHE:CE1	2.51	0.45
21:R:109:LMU:H22	21:R:109:LMU:O2'	2.17	0.45
20:1:210:CLA:CBD	20:1:210:CLA:HAA2	2.44	0.45
21:1:217:LMU:H2O2	21:1:217:LMU:H11	1.74	0.45
1:1:57:ILE:C	1:1:57:ILE:CD1	2.29	0.45
2:2:108:ARG:HD3	2:2:108:ARG:HA	1.75	0.45
2:2:54:TRP:CZ2	2:2:109:ARG:CB	2.99	0.45
3:3:84:ILE:HG13	20:3:302:CLA:O1A	2.15	0.45
20:4:306:CLA:CBD	20:4:306:CLA:HAA2	2.46	0.45
5:A:257:GLN:O	5:A:258:LEU:CB	2.65	0.45
5:A:499:ALA:O	5:A:501:GLY:N	2.38	0.45
5:A:575:LEU:HD12	5:A:575:LEU:H	1.81	0.45
5:A:680:LEU:CD2	6:B:617:MET:HB2	2.46	0.45
5:A:693:LEU:HD11	5:A:738:TYR:HD1	1.78	0.45
5:A:705:GLU:O	5:A:706:SER:C	2.55	0.45
20:A:810:CLA:HBB2	20:A:813:CLA:HMA3	1.97	0.45
5:A:372:VAL:HG22	20:A:818:CLA:H41	1.96	0.45
5:A:351:THR:O	20:A:823:CLA:H201	2.17	0.45
20:A:808:CLA:ND	20:A:826:CLA:C4	2.79	0.45
22:A:845:BCR:C8	22:A:845:BCR:H321	2.47	0.45
6:B:353:TYR:CB	6:B:594:TRP:CH2	2.99	0.45
6:B:535:VAL:O	6:B:539:LEU:HB2	2.17	0.45
6:B:557:PHE:O	6:B:557:PHE:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:668:ARG:NH1	6:B:672:GLN:HG2	2.31	0.45
20:B:817:CLA:C2	20:B:822:CLA:H92	2.45	0.45
22:B:842:BCR:H15C	22:B:842:BCR:H351	1.77	0.45
8:D:99:GLN:HG2	8:D:101:TYR:CE2	2.52	0.45
8:D:113:HIS:O	8:D:113:HIS:HD2	2.00	0.45
10:F:99:TRP:CZ3	10:F:140:ALA:HB2	2.52	0.45
11:G:16:LEU:CA	11:G:68:ILE:HG13	2.45	0.45
22:I:103:BCR:C39	22:L:210:BCR:C40	2.94	0.45
20:A:808:CLA:H111	22:J:102:BCR:C10	2.46	0.45
22:L:210:BCR:H341	22:L:210:BCR:H11C	1.83	0.45
16:L:56:VAL:HG13	20:L:208:CLA:HED2	1.96	0.45
21:R:103:LMU:H12	21:R:103:LMU:H6'	1.80	0.45
2:2:209:THR:CG2	2:2:209:THR:O	2.64	0.45
20:2:303:CLA:O2D	20:2:303:CLA:OBD	2.35	0.45
20:2:322:CLA:C8	20:2:322:CLA:C4	2.75	0.45
3:3:164:PHE:HD1	3:3:164:PHE:HA	1.71	0.45
5:A:34:TRP:O	5:A:35:ALA:CB	2.65	0.45
5:A:347:TYR:CE1	5:A:417:PHE:CZ	3.04	0.45
5:A:555:ILE:HG12	5:A:555:ILE:H	1.46	0.45
5:A:672:LEU:HD23	5:A:673:SER:H	1.81	0.45
5:A:683:HIS:O	20:A:851:CLA:HAA2	2.17	0.45
5:A:401:TRP:CB	20:A:826:CLA:HMC3	2.47	0.45
5:A:499:ALA:CB	20:A:832:CLA:O2D	2.64	0.45
20:A:839:CLA:H62	20:A:839:CLA:H41	1.45	0.45
6:B:141:PHE:O	6:B:142:LEU:C	2.55	0.45
6:B:167:TRP:O	6:B:167:TRP:CD2	2.70	0.45
6:B:216:LEU:O	6:B:217:PRO:C	2.54	0.45
6:B:176:ASN:ND2	6:B:291:TYR:O	2.48	0.45
6:B:393:PHE:CE2	6:B:398:TYR:HB2	2.52	0.45
6:B:395:ILE:HG13	6:B:395:ILE:H	1.72	0.45
6:B:535:VAL:CG1	6:B:536:LYS:H	2.30	0.45
6:B:369:ALA:C	6:B:725:LEU:HD11	2.36	0.45
20:B:824:CLA:H162	20:B:824:CLA:H202	1.64	0.45
20:B:826:CLA:HBA2	20:B:826:CLA:H3A	1.54	0.45
6:B:424:TRP:CH2	20:B:829:CLA:HAC1	2.52	0.45
8:D:40:ALA:O	8:D:45:PHE:CD2	2.69	0.45
10:F:131:PHE:CE1	19:W:2:FRU:O3	2.66	0.45
12:H:42:THR:HG22	12:H:45:ALA:CB	2.43	0.45
16:L:162:ASP:C	16:L:162:ASP:OD2	2.54	0.45
17:N:40:CYS:N	17:N:41:LYS:CA	2.79	0.45
17:N:59:PRO:HA	17:N:66:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:101:VAL:O	4:4:104:ARG:CD	2.64	0.45
4:4:164:LEU:O	4:4:166:PHE:N	2.50	0.45
20:4:306:CLA:HMC1	20:4:306:CLA:HBC2	0.67	0.45
4:4:30:LEU:CD1	21:4:317:LMU:C12	2.94	0.45
5:A:430:ASP:C	5:A:432:LEU:H	2.19	0.45
5:A:472:ARG:O	5:A:474:GLN:CB	2.65	0.45
20:A:815:CLA:O1A	20:A:815:CLA:C1A	2.63	0.45
20:A:826:CLA:H18	20:A:826:CLA:H122	1.98	0.45
20:A:824:CLA:C4	20:A:835:CLA:HBA1	2.46	0.45
22:A:845:BCR:H11C	22:A:845:BCR:H341	1.71	0.45
6:B:199:ILE:N	6:B:200:PRO:HD2	2.31	0.45
6:B:347:LEU:HD21	6:B:351:HIS:CE1	2.40	0.45
6:B:57:ILE:HG12	20:B:806:CLA:HMC2	1.98	0.45
8:D:139:LYS:HG2	8:D:141:VAL:HG22	1.97	0.45
10:F:23:LYS:HB3	10:F:24:LYS:NZ	2.19	0.45
21:G:101:LMU:H1B	21:G:101:LMU:H4B	1.57	0.45
11:G:33:LYS:O	11:G:34:GLN:HG2	2.15	0.45
20:A:826:CLA:C20	22:J:102:BCR:C15	2.93	0.45
17:N:62:SER:HB3	17:N:66:ASP:N	2.31	0.45
17:N:78:GLY:O	17:N:82:PHE:CE2	2.70	0.45
19:Y:1:GLC:O4	19:Y:1:GLC:O2	2.28	0.45
1:1:24:PHE:CB	6:B:314:ARG:NH2	2.70	0.45
2:2:102:ILE:HG13	20:2:312:CLA:CMD	2.43	0.45
2:2:127:ASN:HD21	14:J:7:TYR:CA	2.18	0.45
2:2:169:LEU:HD11	20:2:305:CLA:C1C	2.47	0.45
3:3:94:ARG:HG2	3:3:97:PHE:CD1	2.52	0.45
4:4:169:GLN:CA	4:4:169:GLN:NE2	2.68	0.45
20:4:302:CLA:H41	20:4:302:CLA:H62	1.58	0.45
20:4:304:CLA:CMC	20:4:304:CLA:HBC3	2.46	0.45
20:4:319:CLA:CMC	20:4:319:CLA:HBC3	2.12	0.45
5:A:163:GLN:C	5:A:165:TYR:H	2.19	0.45
5:A:436:LEU:C	5:A:438:HIS:O	2.55	0.45
5:A:438:HIS:NE2	20:A:829:CLA:ND	2.65	0.45
5:A:461:TYR:CD2	5:A:649:ILE:HD12	2.51	0.45
5:A:70:ASP:O	5:A:71:LEU:C	2.54	0.45
20:A:801:CLA:O1D	20:A:801:CLA:HAA1	2.14	0.45
5:A:83:PHE:HA	5:A:86:LEU:CD2	2.47	0.45
6:B:603:ARG:HB3	6:B:734:GLY:H	1.81	0.45
20:B:815:CLA:NA	20:B:815:CLA:H12	2.31	0.45
6:B:77:TRP:O	6:B:81:PRO:HG3	2.17	0.45
6:B:355:LEU:CD2	20:B:824:CLA:HMC2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:828:CLA:CAA	20:B:828:CLA:CED	2.89	0.45
6:B:564:ARG:NH2	7:C:66:ARG:HH12	2.15	0.45
9:E:46:PHE:CD2	9:E:47:LYS:N	2.85	0.45
9:E:62:ARG:O	9:E:83:ALA:CB	2.65	0.45
10:F:51:LYS:O	10:F:53:PHE:N	2.45	0.45
10:F:84:ILE:HD13	10:F:84:ILE:N	2.32	0.45
15:K:52:PRO:HB2	15:K:53:ALA:H	1.52	0.45
12:H:58:ILE:CD1	16:L:97:MET:SD	2.89	0.45
17:N:38:GLY:HA3	17:N:46:PHE:HD1	1.80	0.45
20:1:202:CLA:H42	20:1:202:CLA:H8	1.70	0.45
1:1:25:ASP:O	1:1:26:PRO:C	2.54	0.45
2:2:103:GLY:O	2:2:104:TRP:O	2.35	0.45
4:4:103:ILE:HB	20:4:303:CLA:CMD	2.46	0.45
20:4:310:CLA:C2D	20:4:312:CLA:C2A	2.95	0.45
4:4:89:THR:OG1	4:4:92:VAL:HB	2.16	0.45
5:A:164:LEU:HA	5:A:167:THR:CG2	2.43	0.45
5:A:308:ILE:HG21	20:A:816:CLA:CMC	2.47	0.45
5:A:539:PHE:O	5:A:539:PHE:CD2	2.65	0.45
5:A:665:ILE:HD12	5:A:666:GLN:N	2.31	0.45
5:A:515:TRP:CZ2	20:A:825:CLA:HMC3	2.52	0.45
20:A:831:CLA:H61	20:A:831:CLA:H41	1.62	0.45
22:A:847:BCR:H11C	22:A:847:BCR:H341	1.71	0.45
6:B:218:TYR:HB3	6:B:219:PRO:HD2	1.99	0.45
6:B:323:TYR:O	6:B:327:ASN:HB2	2.17	0.45
6:B:42:LEU:O	6:B:43:TYR:O	2.35	0.45
6:B:460:ALA:O	6:B:463:ILE:N	2.50	0.45
20:B:811:CLA:CMC	20:B:811:CLA:HBC3	2.24	0.45
20:B:823:CLA:CAB	20:B:837:CLA:HMA1	2.47	0.45
6:B:700:LEU:N	23:B:841:PQN:O4	2.43	0.45
9:E:60:LYS:HG3	9:E:61:THR:OG1	2.17	0.45
10:F:152:ASN:N	10:F:152:ASN:HD22	2.12	0.45
14:J:26:LEU:H	14:J:28:GLU:H	1.65	0.45
20:K:102:CLA:C3A	20:K:102:CLA:CGA	2.93	0.45
15:K:51:ASP:OD1	15:K:55:PHE:CB	2.65	0.45
20:L:202:CLA:H72	20:L:203:CLA:CBA	2.47	0.45
21:L:211:LMU:H82	21:L:211:LMU:H52	1.78	0.45
21:L:211:LMU:O6'	21:L:211:LMU:H81	2.16	0.45
16:L:65:VAL:C	16:L:69:VAL:HG22	2.36	0.45
17:N:62:SER:OG	17:N:66:ASP:HA	2.17	0.45
2:2:115:ASN:HD22	2:2:115:ASN:N	2.13	0.45
2:2:153:PRO:HB2	2:2:157:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:72:GLY:C	2:2:74:LEU:N	2.67	0.45
20:3:318:CLA:H41	20:3:318:CLA:H62	1.72	0.45
4:4:93:ILE:HG22	4:4:94:GLU:CA	2.45	0.45
5:A:113:PRO:O	5:A:115:HIS:CD2	2.70	0.45
5:A:163:GLN:O	5:A:165:TYR:N	2.50	0.45
5:A:488:PHE:CZ	5:A:533:PRO:HB3	2.52	0.45
5:A:53:TRP:HA	5:A:56:ASN:ND2	2.32	0.45
5:A:584:PRO:CB	7:C:67:VAL:HB	2.47	0.45
20:A:808:CLA:HBB2	20:A:809:CLA:C3D	2.47	0.45
20:A:818:CLA:H3A	20:A:818:CLA:HBA2	1.70	0.45
21:A:853:LMU:H22	21:A:853:LMU:H51	1.40	0.45
5:A:98:PHE:O	5:A:99:HIS:CD2	2.70	0.45
6:B:199:ILE:HG22	6:B:203:ARG:CZ	2.47	0.45
6:B:462:TRP:CZ3	20:B:832:CLA:HBC1	2.51	0.45
6:B:509:PHE:N	6:B:509:PHE:HD2	2.15	0.45
6:B:47:PHE:CZ	6:B:51:PHE:HE1	2.35	0.45
6:B:679:ALA:O	6:B:683:GLU:OE2	2.35	0.45
6:B:710:LEU:O	6:B:712:HIS:N	2.50	0.45
6:B:80:ASP:HA	6:B:81:PRO:HD3	1.57	0.45
6:B:718:ILE:HD11	20:B:825:CLA:CHC	2.46	0.45
6:B:719:PHE:CE2	20:B:825:CLA:H72	2.52	0.45
20:B:806:CLA:CBC	20:B:825:CLA:HMD3	2.47	0.45
22:B:846:BCR:C23	22:B:846:BCR:C38	2.74	0.45
7:C:12:ILE:HD12	7:C:12:ILE:H	1.80	0.45
8:D:139:LYS:NZ	9:E:41:ARG:NH1	2.64	0.45
4:4:193:ILE:CG2	14:J:42:PHE:HD1	2.30	0.45
20:1:215:CLA:HBA2	20:1:215:CLA:H12	1.60	0.44
21:1:219:LMU:H31	21:1:219:LMU:H61	1.59	0.44
1:1:38:ARG:NH2	1:1:139:LYS:HB2	2.31	0.44
2:2:168:ARG:NH2	2:2:171:MET:CB	2.63	0.44
2:2:91:THR:C	2:2:94:LEU:CB	2.86	0.44
2:2:93:THR:HA	2:2:96:ILE:HG12	1.98	0.44
3:3:111:TYR:HB2	3:3:112:THR:H	1.68	0.44
3:3:194:ILE:HG13	20:3:304:CLA:HMC1	1.90	0.44
3:3:93:PHE:HD2	3:3:95:THR:N	2.12	0.44
20:4:307:CLA:CHD	20:4:307:CLA:HBC3	2.47	0.44
4:4:61:PRO:HA	4:4:65:THR:O	2.17	0.44
5:A:173:VAL:O	5:A:175:ALA:O	2.35	0.44
5:A:363:ALA:O	5:A:367:SER:CB	2.65	0.44
5:A:615:HIS:CE1	20:A:834:CLA:CBC	2.98	0.44
5:A:396:PHE:CE2	5:A:616:PHE:CB	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:365:LEU:HD22	20:A:805:CLA:HED3	1.93	0.44
20:A:821:CLA:HAA2	20:A:821:CLA:CGD	2.48	0.44
5:A:451:ILE:HD13	20:A:830:CLA:HED1	1.97	0.44
22:A:844:BCR:H351	22:A:844:BCR:H15C	1.78	0.44
6:B:17:THR:OG1	6:B:18:THR:N	2.50	0.44
6:B:288:GLY:O	6:B:289:LEU:HB2	2.17	0.44
6:B:326:ILE:HG23	20:B:822:CLA:HBC3	1.99	0.44
6:B:347:LEU:HD13	6:B:351:HIS:ND1	2.30	0.44
6:B:355:LEU:HD21	20:B:824:CLA:HMC2	1.99	0.44
6:B:544:SER:N	6:B:547:MET:O	2.47	0.44
20:B:804:CLA:O1D	20:B:804:CLA:H2A	2.17	0.44
20:B:806:CLA:HBA1	20:B:806:CLA:H3A	1.70	0.44
6:B:719:PHE:CE2	20:B:825:CLA:C7	3.01	0.44
20:B:839:CLA:C2	23:B:841:PQN:H251	2.47	0.44
20:B:851:CLA:H162	20:B:851:CLA:H202	1.71	0.44
7:C:5:VAL:CA	7:C:65:VAL:HG22	2.45	0.44
9:E:36:VAL:CG2	9:E:52:VAL:CG2	2.94	0.44
10:F:151:ASP:O	10:F:154:PHE:N	2.51	0.44
10:F:152:ASN:N	10:F:152:ASN:ND2	2.64	0.44
10:F:89:LEU:HD12	10:F:89:LEU:HA	1.87	0.44
15:K:8:ASN:C	15:K:9:LEU:HD23	2.30	0.44
16:L:107:PHE:CB	16:L:109:GLU:OE1	2.61	0.44
20:L:201:CLA:HED3	20:L:201:CLA:H72	1.98	0.44
17:N:53:ALA:O	17:N:54:LYS:CG	2.65	0.44
1:1:181:LEU:HD13	20:1:203:CLA:HAC1	1.99	0.44
20:1:202:CLA:HBC2	20:1:202:CLA:HHD	1.98	0.44
4:4:101:VAL:HG13	4:4:101:VAL:O	2.12	0.44
5:A:336:GLY:HA3	20:A:840:CLA:CMC	2.48	0.44
5:A:370:ILE:CG2	5:A:400:MET:CA	2.85	0.44
5:A:349:ILE:HD13	5:A:422:TYR:HB3	1.99	0.44
5:A:567:ARG:HH11	8:D:34:GLY:C	2.20	0.44
5:A:596:ASP:HA	5:A:599:PHE:CB	2.39	0.44
20:A:807:CLA:HHD	20:A:807:CLA:HBC2	1.98	0.44
5:A:187:HIS:CE1	20:A:811:CLA:CHA	2.97	0.44
20:A:824:CLA:HMB3	22:A:846:BCR:C19	2.47	0.44
20:A:830:CLA:HED1	20:A:841:CLA:O1A	2.16	0.44
20:A:850:CLA:H162	20:A:850:CLA:H122	1.68	0.44
6:B:414:HIS:O	6:B:414:HIS:CD2	2.69	0.44
6:B:467:HIS:CD2	20:B:832:CLA:CGD	3.00	0.44
6:B:672:GLN:HE22	6:B:698:VAL:HA	1.83	0.44
20:B:809:CLA:H8	20:B:809:CLA:H51	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:812:CLA:H143	20:B:812:CLA:H162	1.72	0.44
20:A:830:CLA:H192	20:B:838:CLA:HMB2	1.99	0.44
6:B:661:PHE:HB3	20:B:851:CLA:HMC1	1.97	0.44
7:C:9:ASP:HB2	24:C:103:SF4:S3	2.57	0.44
8:D:74:LEU:HG	8:D:74:LEU:O	2.16	0.44
11:G:62:ASP:CB	11:G:63:PRO:HD3	2.42	0.44
20:J:101:CLA:CGD	20:J:101:CLA:O1A	2.65	0.44
14:J:32:PHE:CE2	14:J:33:PHE:CZ	3.03	0.44
14:J:2:ARG:HB3	14:J:7:TYR:CE1	2.53	0.44
21:K:105:LMU:H61	21:K:105:LMU:H31	1.49	0.44
21:K:106:LMU:O6'	21:K:106:LMU:C2B	2.65	0.44
16:L:127:PRO:O	16:L:128:ASP:O	2.36	0.44
20:L:207:CLA:HBA2	20:L:207:CLA:H3A	1.54	0.44
21:N:101:LMU:H91	21:N:101:LMU:C5	2.33	0.44
17:N:45:ASN:O	17:N:46:PHE:C	2.50	0.44
1:1:54:VAL:C	1:1:56:GLY:N	2.71	0.44
20:2:303:CLA:H42	20:2:303:CLA:CHD	2.48	0.44
20:3:302:CLA:HMA3	5:A:246:HIS:HE1	1.80	0.44
20:3:311:CLA:H12	20:3:311:CLA:H51	1.75	0.44
3:3:49:ILE:CG1	3:3:52:LYS:CB	2.94	0.44
3:3:86:GLN:HB2	3:3:88:THR:CA	2.48	0.44
4:4:152:LYS:HA	4:4:154:ILE:CG1	2.48	0.44
5:A:144:GLN:HG3	5:A:145:ILE:H	1.81	0.44
5:A:202:MET:HB3	20:A:823:CLA:HMD3	1.99	0.44
5:A:479:ASP:HA	5:A:536:THR:CG2	2.45	0.44
5:A:550:HIS:CD2	20:A:836:CLA:HMA3	2.52	0.44
5:A:581:CYS:HB2	5:A:590:CYS:O	2.16	0.44
5:A:586:ARG:H	7:C:49:VAL:HG22	1.83	0.44
5:A:729:GLN:O	5:A:732:ALA:HB3	2.17	0.44
6:B:145:LEU:HA	6:B:145:LEU:HD22	1.82	0.44
6:B:179:LEU:O	6:B:284:PHE:O	2.35	0.44
6:B:190:TRP:O	6:B:191:ALA:C	2.56	0.44
6:B:353:TYR:CD1	6:B:594:TRP:HZ3	2.29	0.44
6:B:623:TYR:H	6:B:626:LEU:HB3	1.81	0.44
20:B:823:CLA:C2	20:B:836:CLA:HBA2	2.47	0.44
22:B:845:BCR:H351	22:B:845:BCR:H15C	1.80	0.44
8:D:41:GLN:CD	8:D:41:GLN:C	2.76	0.44
9:E:65:VAL:HG23	9:E:66:VAL:O	2.17	0.44
10:F:33:ALA:C	10:F:35:ASP:H	2.20	0.44
21:G:101:LMU:H112	21:G:101:LMU:H82	1.37	0.44
21:H:106:LMU:H81	21:H:106:LMU:H52	1.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:40:PHE:O	12:H:41:GLU:C	2.56	0.44
15:K:35:THR:HG23	15:K:36:ALA:H	1.82	0.44
17:N:22:LEU:HD23	17:N:22:LEU:O	2.17	0.44
1:1:183:ASP:CB	1:1:184:PRO:HD2	2.47	0.44
2:2:97:VAL:C	2:2:100:VAL:HG13	2.37	0.44
2:2:116:PRO:O	2:2:135:VAL:O	2.36	0.44
2:2:98:GLU:OE1	20:2:312:CLA:C4C	2.65	0.44
2:2:54:TRP:CZ2	2:2:109:ARG:HD3	2.44	0.44
3:3:50:GLU:OE1	3:3:54:LEU:HB2	2.17	0.44
4:4:104:ARG:HD2	20:4:313:CLA:C1C	2.36	0.44
4:4:139:ASN:HA	4:4:139:ASN:HD22	1.64	0.44
4:4:146:THR:HA	4:4:147:LEU:HA	1.62	0.44
5:A:500:PRO:HA	5:A:504:ALA:HB1	1.98	0.44
5:A:76:ARG:CZ	5:A:192:LYS:CG	2.71	0.44
20:A:823:CLA:HMD2	20:A:823:CLA:C14	2.34	0.44
6:B:158:GLN:O	6:B:159:PRO:O	2.36	0.44
6:B:194:LEU:O	6:B:199:ILE:HG13	2.17	0.44
6:B:290:MET:HG3	20:B:819:CLA:CMC	2.47	0.44
6:B:343:VAL:HG12	20:B:824:CLA:H2	2.00	0.44
5:A:665:ILE:HD13	6:B:621:ARG:HG3	1.99	0.44
6:B:662:MET:O	6:B:664:LEU:N	2.51	0.44
6:B:67:HIS:CD2	6:B:71:GLN:HE22	2.35	0.44
6:B:726:ILE:C	6:B:728:SER:N	2.70	0.44
20:B:807:CLA:HMB3	20:I:102:CLA:HMA1	1.98	0.44
20:B:806:CLA:CBB	20:B:826:CLA:HHC	2.47	0.44
7:C:18:VAL:HB	7:C:58:CYS:HB2	2.00	0.44
8:D:152:GLN:HA	8:D:153:PRO:HD2	1.72	0.44
9:E:65:VAL:CG2	9:E:66:VAL:O	2.65	0.44
5:A:130:GLU:HG3	10:F:45:THR:HG21	1.99	0.44
10:F:62:LEU:HG	10:F:72:ILE:HD11	1.96	0.44
21:H:105:LMU:H42	21:H:105:LMU:H11	1.76	0.44
21:H:106:LMU:C1	21:H:106:LMU:C1B	2.95	0.44
12:H:45:ALA:CB	12:H:46:PRO:CD	2.88	0.44
12:H:75:ASP:HB3	12:H:77:LEU:HG	2.00	0.44
14:J:2:ARG:HH22	14:J:8:LEU:HD22	1.81	0.44
15:K:51:ASP:OD1	15:K:55:PHE:HB2	2.17	0.44
20:A:841:CLA:H93	22:L:210:BCR:H321	1.98	0.44
21:R:101:LMU:H3'	21:R:101:LMU:H1B	1.30	0.44
18:R:34:UNK:C	18:R:36:UNK:O	2.66	0.44
2:2:188:PRO:HB2	2:2:189:ILE:HD13	1.98	0.44
5:A:105:ASN:HB3	5:A:150:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:251:ASN:O	5:A:253:ASP:HB3	2.17	0.44
5:A:363:ALA:N	5:A:410:ALA:CB	2.81	0.44
5:A:432:LEU:O	5:A:435:VAL:N	2.50	0.44
5:A:467:MET:HE1	5:A:475:ASP:C	2.38	0.44
5:A:631:GLN:HG2	5:A:633:VAL:HG13	1.98	0.44
5:A:655:ASP:O	5:A:659:ALA:HB3	2.17	0.44
5:A:681:GLY:O	5:A:682:ALA:HB3	2.17	0.44
5:A:664:VAL:HG11	5:A:749:PHE:HA	1.99	0.44
20:3:302:CLA:CBC	20:A:814:CLA:C1D	2.95	0.44
20:A:817:CLA:C4C	20:A:817:CLA:H62	2.47	0.44
20:A:835:CLA:C1B	20:A:836:CLA:HMD3	2.47	0.44
6:B:32:GLU:N	6:B:42:LEU:HD13	2.33	0.44
6:B:693:TRP:CZ2	6:B:697:PRO:HG3	2.52	0.44
21:B:801:LMU:O6'	21:B:801:LMU:O1B	2.30	0.44
20:B:804:CLA:HBA2	20:B:804:CLA:H3A	1.53	0.44
6:B:493:TRP:HH2	20:B:815:CLA:H122	1.82	0.44
23:B:841:PQN:H142	23:B:841:PQN:C2M	2.47	0.44
7:C:53:ARG:O	7:C:55:GLU:O	2.36	0.44
8:D:21:ASP:HB3	8:D:22:PRO:HD3	1.99	0.44
22:F:203:BCR:C5	20:F:205:CLA:HMA1	2.47	0.44
20:F:206:CLA:O2D	20:F:206:CLA:OBD	2.31	0.44
12:H:11:LEU:HD22	12:H:11:LEU:HA	1.86	0.44
12:H:63:SER:O	12:H:67:TYR:HB3	2.16	0.44
17:N:45:ASN:HD21	17:N:53:ALA:C	2.02	0.44
18:R:50:UNK:HA	18:R:51:UNK:HA	1.69	0.44
2:2:178:TRP:CD1	2:2:178:TRP:N	2.84	0.44
20:2:307:CLA:HHD	20:2:307:CLA:HAC2	1.82	0.44
2:2:63:PHE:CD1	2:2:64:ILE:N	2.86	0.44
2:2:95:PHE:O	2:2:99:LEU:HD12	2.17	0.44
20:3:311:CLA:HBA2	20:3:311:CLA:H3A	1.61	0.44
3:3:86:GLN:CB	3:3:88:THR:H	2.31	0.44
4:4:142:ASN:O	4:4:143:PHE:CD2	2.70	0.44
5:A:179:LEU:HD13	5:A:179:LEU:O	2.17	0.44
5:A:223:VAL:CG1	5:A:224:HIS:H	2.30	0.44
5:A:154:ARG:NH2	5:A:233:LEU:CD1	2.80	0.44
5:A:539:PHE:HE2	5:A:543:HIS:HE1	1.66	0.44
5:A:569:ILE:HG12	5:A:586:ARG:NH1	2.33	0.44
5:A:334:HIS:HD2	20:A:820:CLA:C1B	2.30	0.44
5:A:700:TRP:CE2	23:A:842:PQN:H2M3	2.52	0.44
6:B:182:LEU:HG	6:B:183:PHE:N	2.32	0.44
6:B:247:THR:HG22	6:B:250:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:309:ILE:HA	6:B:310:PRO:HD3	1.81	0.44
6:B:332:PHE:HE1	6:B:408:LEU:CD2	2.30	0.44
6:B:385:GLY:N	20:B:827:CLA:HBC3	2.33	0.44
20:B:835:CLA:HAA1	20:B:836:CLA:HAA2	1.99	0.44
20:B:836:CLA:HBB2	20:B:836:CLA:C8	2.42	0.44
6:B:707:LEU:CD1	25:B:848:LMG:H301	2.48	0.44
7:C:60:THR:HG21	7:C:64:SER:HB3	1.99	0.44
15:K:47:ILE:HG23	15:K:48:GLN:N	2.28	0.44
16:L:95:LEU:HA	16:L:98:CYS:CB	2.42	0.44
17:N:72:LYS:HA	17:N:72:LYS:HD2	1.57	0.44
18:R:38:UNK:O	18:R:39:UNK:C	2.61	0.44
18:R:5:UNK:O	18:R:6:UNK:CB	2.65	0.44
20:1:202:CLA:HBA2	20:1:202:CLA:C2	2.47	0.44
1:1:27:LEU:HD13	1:1:28:GLY:H	1.83	0.44
1:1:63:LEU:HB2	1:1:65:TYR:N	2.32	0.44
2:2:70:LYS:CG	2:2:73:ILE:HG13	2.33	0.44
3:3:111:TYR:HB2	3:3:112:THR:HG22	2.00	0.44
3:3:112:THR:HG1	3:3:113:LEU:H	1.57	0.44
3:3:84:ILE:N	20:3:302:CLA:C3	2.65	0.44
4:4:107:GLN:HA	20:4:302:CLA:C3A	2.40	0.44
4:4:122:LYS:HG2	4:4:150:LYS:HE2	1.36	0.44
4:4:94:GLU:C	4:4:95:PHE:CD1	2.91	0.44
5:A:79:PHE:CD2	5:A:185:HIS:CD2	2.98	0.44
5:A:306:ILE:O	5:A:309:LEU:N	2.51	0.44
5:A:541:VAL:O	5:A:544:ILE:HG22	2.17	0.44
5:A:570:PRO:C	5:A:572:LYS:H	2.21	0.44
5:A:400:MET:HG3	5:A:609:ILE:HG23	2.00	0.44
5:A:650:ASN:C	5:A:652:TRP:N	2.69	0.44
20:A:809:CLA:HBC3	20:A:809:CLA:CMC	2.48	0.44
20:A:829:CLA:HMB2	20:L:202:CLA:C4D	2.48	0.44
21:A:854:LMU:H72	21:A:854:LMU:H42	1.51	0.44
6:B:167:TRP:CD1	11:G:41:MET:CE	3.01	0.44
6:B:341:LEU:O	6:B:345:THR:OG1	2.17	0.44
6:B:378:ILE:H	6:B:381:PHE:HD1	1.66	0.44
6:B:447:GLY:C	6:B:449:PRO:HD3	2.37	0.44
8:D:94:TYR:O	8:D:95:LYS:NZ	2.33	0.44
9:E:69:PHE:HD2	9:E:71:LYS:H	1.61	0.44
9:E:73:ASN:ND2	9:E:78:SER:HB2	2.33	0.44
10:F:13:GLN:HG3	10:F:66:ASP:H	1.83	0.44
10:F:61:LEU:HD23	10:F:69:PRO:HB3	1.96	0.44
11:G:28:ARG:NH2	11:G:28:ARG:CG	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:167:TRP:CB	11:G:41:MET:CE	2.90	0.44
11:G:88:THR:HG23	11:G:91:ASN:O	2.17	0.44
14:J:10:VAL:CG2	14:J:14:LEU:HD12	2.48	0.44
15:K:27:ALA:HB1	15:K:28:PRO:HD3	1.96	0.44
16:L:66:GLY:HA3	20:L:209:CLA:C4B	2.45	0.44
17:N:84:LYS:HA	17:N:85:TRP:HA	1.46	0.44
4:4:149:ALA:C	4:4:151:GLU:HG3	2.38	0.44
4:4:151:GLU:CA	4:4:154:ILE:H	2.27	0.44
4:4:75:TRP:HB2	20:4:311:CLA:CMD	2.44	0.44
5:A:131:ILE:HG21	6:B:446:PHE:HA	1.99	0.44
5:A:212:GLY:O	5:A:214:GLY:N	2.51	0.44
5:A:316:MET:CA	5:A:317:TYR:CB	2.94	0.44
5:A:390:ALA:HA	5:A:393:LEU:HD21	1.97	0.44
5:A:547:PHE:C	5:A:547:PHE:CD1	2.88	0.44
5:A:591:GLN:HA	5:A:591:GLN:NE2	2.25	0.44
20:A:801:CLA:CMC	20:A:801:CLA:CBC	2.80	0.44
5:A:143:ILE:HG12	20:A:808:CLA:HBC2	2.00	0.44
22:A:846:BCR:H341	22:A:846:BCR:H11C	1.70	0.44
6:B:242:HIS:CE1	6:B:244:PHE:HA	2.53	0.44
6:B:590:VAL:O	6:B:593:TYR:HB3	2.18	0.44
6:B:594:TRP:HD1	6:B:595:HIS:N	2.15	0.44
6:B:680:TRP:O	6:B:681:ALA:O	2.36	0.44
6:B:5:ILE:CB	6:B:6:PRO:CD	2.85	0.44
6:B:375:HIS:CE1	20:B:826:CLA:NC	2.77	0.44
6:B:289:LEU:CD2	22:B:842:BCR:H352	2.45	0.44
7:C:58:CYS:HA	7:C:59:PRO:HD2	1.66	0.44
7:C:62:PHE:CE2	9:E:42:GLU:CD	2.83	0.44
7:C:77:MET:C	7:C:79:LEU:N	2.69	0.44
8:D:29:PHE:HA	8:D:66:ALA:HB2	1.99	0.44
20:B:810:CLA:O2D	11:G:39:ASN:ND2	2.50	0.44
20:L:201:CLA:C2A	20:L:201:CLA:CGD	2.86	0.44
21:N:101:LMU:C3	21:N:101:LMU:C6'	2.95	0.44
17:N:32:ALA:CB	17:N:35:VAL:HA	2.47	0.44
17:N:62:SER:CB	17:N:66:ASP:HA	2.48	0.44
2:2:168:ARG:HH21	2:2:171:MET:CG	2.31	0.44
20:3:317:CLA:CBD	20:3:317:CLA:HAA2	2.48	0.44
4:4:156:ASN:N	4:4:156:ASN:OD1	2.51	0.44
4:4:82:GLU:O	4:4:83:TYR:HD1	2.01	0.44
5:A:568:LEU:HD21	5:A:586:ARG:HB3	1.99	0.44
5:A:682:ALA:HA	5:A:685:VAL:HG12	1.99	0.44
5:A:714:LEU:HB2	5:A:716:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:819:CLA:HMB2	20:A:823:CLA:HMA3	1.99	0.44
20:A:808:CLA:H161	20:A:828:CLA:C20	2.48	0.44
5:A:86:LEU:HA	5:A:89:ILE:HD12	1.99	0.44
6:B:120:VAL:C	6:B:123:TRP:HD1	2.20	0.44
6:B:154:TRP:CD1	6:B:154:TRP:C	2.91	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ2	2.52	0.44
6:B:434:LEU:O	6:B:438:VAL:HG13	2.18	0.44
6:B:673:GLU:O	6:B:676:GLU:HB2	2.18	0.44
6:B:74:PHE:C	6:B:76:ALA:N	2.70	0.44
5:A:462:ILE:HD13	20:B:850:CLA:H93	2.00	0.44
8:D:113:HIS:CD2	8:D:113:HIS:O	2.70	0.44
8:D:126:GLY:C	8:D:127:ARG:CG	2.85	0.44
8:D:79:ARG:H	8:D:82:GLN:HE21	1.63	0.44
10:F:47:GLU:N	10:F:50:LYS:HB2	2.33	0.44
6:B:454:LEU:HD13	10:F:69:PRO:O	2.14	0.44
11:G:46:ALA:C	11:G:48:ASP:CB	2.80	0.44
11:G:60:SER:O	11:G:62:ASP:N	2.50	0.44
21:H:106:LMU:H22	21:H:106:LMU:C6B	2.43	0.44
16:L:159:TYR:O	16:L:159:TYR:CG	2.71	0.44
16:L:64:LEU:CD2	16:L:91:LEU:HD22	2.48	0.44
17:N:42:PHE:CD1	17:N:43:PRO:CD	3.01	0.44
19:U:1:GLC:O5	19:U:2:FRU:O5	2.30	0.44
2:2:186:THR:O	2:2:188:PRO:O	2.36	0.43
2:2:69:THR:O	2:2:70:LYS:CD	2.66	0.43
3:3:132:TRP:CE3	3:3:155:GLU:HG2	2.26	0.43
3:3:199:VAL:HG22	20:3:306:CLA:C4C	2.48	0.43
5:A:113:PRO:C	5:A:115:HIS:N	2.69	0.43
5:A:222:GLN:O	5:A:227:LEU:HD12	2.18	0.43
5:A:343:HIS:O	5:A:346:LEU:HB2	2.18	0.43
5:A:379:MET:HE3	20:A:817:CLA:HED2	2.00	0.43
5:A:42:ARG:O	5:A:44:ILE:HG13	2.18	0.43
5:A:458:PHE:C	5:A:460:LEU:N	2.71	0.43
20:A:838:CLA:H41	20:A:838:CLA:NC	2.33	0.43
6:B:289:LEU:CD2	20:B:818:CLA:C1A	2.96	0.43
6:B:583:MET:CE	6:B:583:MET:O	2.66	0.43
20:B:805:CLA:HMC3	20:B:827:CLA:H3A	1.99	0.43
20:B:836:CLA:HBD	20:B:836:CLA:HAA1	1.99	0.43
7:C:55:GLU:HG3	7:C:60:THR:HG22	2.00	0.43
8:D:48:ILE:HA	8:D:100:PHE:HB3	1.99	0.43
21:D:201:LMU:C1B	21:D:201:LMU:O6B	2.66	0.43
9:E:37:LYS:CB	9:E:49:VAL:HG22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:25:THR:HG22	17:N:26:GLY:N	2.33	0.43
17:N:69:CYS:O	17:N:72:LYS:HD2	2.17	0.43
1:1:168:TYR:N	1:1:169:PRO:HD3	2.33	0.43
4:4:169:GLN:CG	20:4:305:CLA:CAC	2.89	0.43
4:4:107:GLN:HA	20:4:302:CLA:H2A	2.00	0.43
5:A:203:LEU:O	5:A:207:LEU:HD23	2.17	0.43
5:A:219:ALA:O	5:A:222:GLN:N	2.47	0.43
5:A:310:PHE:H	5:A:313:ALA:CB	2.31	0.43
5:A:536:THR:HA	5:A:539:PHE:HB2	2.00	0.43
5:A:588:GLY:N	6:B:668:ARG:CD	2.77	0.43
5:A:412:ALA:CB	5:A:598:VAL:HG11	2.30	0.43
5:A:651:GLY:O	5:A:655:ASP:HB2	2.18	0.43
5:A:680:LEU:HB3	20:A:851:CLA:C1	2.48	0.43
20:A:817:CLA:H3A	20:A:817:CLA:HBA2	1.24	0.43
20:A:819:CLA:HBA1	20:A:823:CLA:CBB	2.48	0.43
6:B:269:TRP:HA	6:B:269:TRP:CE3	2.53	0.43
6:B:330:ILE:HA	6:B:333:GLN:NE2	2.33	0.43
6:B:457:PRO:O	6:B:460:ALA:HB3	2.19	0.43
6:B:473:GLY:O	6:B:474:PHE:HB3	2.19	0.43
5:A:588:GLY:HA3	6:B:668:ARG:HB3	2.00	0.43
6:B:693:TRP:NE1	20:B:838:CLA:CHD	2.81	0.43
20:B:812:CLA:H3A	20:B:812:CLA:HBA2	1.58	0.43
20:B:819:CLA:HBA2	20:B:820:CLA:O1A	2.17	0.43
8:D:133:ASN:C	8:D:134:MET:SD	2.92	0.43
8:D:151:LYS:HB3	8:D:151:LYS:NZ	2.32	0.43
21:E:101:LMU:H12	21:E:101:LMU:H41	1.44	0.43
9:E:44:TYR:HD2	9:E:45:TRP:HE3	1.65	0.43
11:G:50:ARG:HB2	11:G:51:ALA:CA	2.48	0.43
20:H:109:CLA:CHD	22:I:101:BCR:C34	2.95	0.43
13:I:25:PHE:CE2	13:I:28:VAL:HG21	2.53	0.43
15:K:24:PHE:CD1	15:K:52:PRO:CG	2.89	0.43
16:L:43:TYR:O	16:L:44:ARG:CB	2.62	0.43
17:N:25:THR:HG22	17:N:26:GLY:H	1.83	0.43
21:R:109:LMU:H32	21:R:109:LMU:H62	1.69	0.43
2:2:99:LEU:HB3	2:2:102:ILE:HB	1.99	0.43
2:2:120:ASN:OD1	14:J:5:LYS:HG3	2.18	0.43
2:2:69:THR:O	2:2:70:LYS:CB	2.66	0.43
2:2:90:ASP:HB3	2:2:94:LEU:HB2	1.99	0.43
3:3:121:MET:O	20:3:311:CLA:HED1	2.18	0.43
4:4:41:VAL:HG12	4:4:41:VAL:O	2.06	0.43
5:A:388:ASP:O	5:A:390:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:58:HIS:CE1	20:A:803:CLA:C4D	3.01	0.43
20:A:839:CLA:CAA	20:A:839:CLA:CGD	2.96	0.43
6:B:460:ALA:O	6:B:462:TRP:N	2.51	0.43
6:B:727:ALA:O	6:B:728:SER:OG	2.29	0.43
6:B:493:TRP:CZ2	20:B:815:CLA:H122	2.53	0.43
20:B:825:CLA:H193	20:B:825:CLA:H161	1.88	0.43
22:B:845:BCR:C23	22:B:845:BCR:C38	2.67	0.43
8:D:56:GLN:OE1	8:D:94:TYR:CE2	2.71	0.43
8:D:92:SER:O	8:D:93:LYS:HG3	2.19	0.43
9:E:80:ASN:OD1	9:E:81:ASN:N	2.49	0.43
11:G:48:ASP:HB3	11:G:49:THR:CB	2.43	0.43
11:G:60:SER:O	11:G:61:ASN:C	2.56	0.43
20:A:826:CLA:C11	22:J:102:BCR:C35	2.96	0.43
20:A:838:CLA:C19	14:J:19:PHE:CD2	3.01	0.43
16:L:92:VAL:HG11	16:L:147:GLY:CA	2.48	0.43
16:L:163:LEU:HD13	16:L:165:TYR:HB3	2.00	0.43
16:L:77:THR:OG1	16:L:82:ALA:HB3	2.19	0.43
17:N:47:THR:CG2	17:N:54:LYS:HZ2	2.15	0.43
17:N:4:GLU:OE2	17:N:5:GLU:N	2.51	0.43
1:1:134:SER:HB3	1:1:135:LYS:H	1.60	0.43
2:2:127:ASN:OD1	14:J:7:TYR:CD2	2.71	0.43
20:2:322:CLA:HED2	20:J:101:CLA:H2	1.99	0.43
3:3:74:ALA:CA	20:3:307:CLA:C4D	2.84	0.43
3:3:50:GLU:OE2	3:3:54:LEU:HD13	2.17	0.43
4:4:103:ILE:CG1	20:4:303:CLA:HMD1	2.45	0.43
4:4:118:ASP:O	4:4:122:LYS:HA	2.18	0.43
5:A:154:ARG:NE	5:A:154:ARG:HA	2.32	0.43
5:A:478:SER:HB2	5:A:481:ALA:H	1.84	0.43
5:A:656:PHE:O	5:A:657:LEU:C	2.57	0.43
5:A:394:SER:CB	20:A:826:CLA:HMA1	2.27	0.43
20:A:827:CLA:HMD2	20:A:827:CLA:H52	2.00	0.43
6:B:505:SER:O	6:B:506:ASN:HB3	2.18	0.43
20:B:813:CLA:C4B	22:B:842:BCR:H291	2.49	0.43
20:B:815:CLA:H3A	20:B:815:CLA:HBA2	1.33	0.43
6:B:60:TRP:HH2	20:B:826:CLA:CHB	2.31	0.43
10:F:44:ALA:O	10:F:46:MET:HG2	2.19	0.43
11:G:92:GLY:O	11:G:94:ASP:OD1	2.36	0.43
21:H:107:LMU:H1'	21:H:107:LMU:H4'	1.55	0.43
20:H:109:CLA:H41	16:L:87:ALA:HB1	2.00	0.43
12:H:53:LEU:CG	12:H:54:LEU:N	2.77	0.43
16:L:124:LYS:NZ	16:L:124:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:62:SER:HA	17:N:64:ASP:HB3	2.01	0.43
17:N:72:LYS:HZ2	17:N:74:LYS:HG2	1.58	0.43
20:R:107:CLA:H41	20:R:107:CLA:H62	1.87	0.43
1:1:142:GLU:OE1	20:1:201:CLA:CMD	2.67	0.43
1:1:179:THR:CB	4:4:87:SER:CB	2.64	0.43
1:1:181:LEU:CD1	20:1:203:CLA:HAC1	2.48	0.43
20:1:203:CLA:O1A	20:1:203:CLA:C2	2.65	0.43
1:1:149:LYS:CB	20:1:206:CLA:HMC2	2.44	0.43
20:2:302:CLA:CMC	20:2:302:CLA:CBC	2.63	0.43
2:2:169:LEU:HD22	20:2:305:CLA:C4B	2.48	0.43
3:3:182:LYS:C	3:3:185:LYS:H	2.21	0.43
20:4:311:CLA:H41	20:4:311:CLA:C8	2.49	0.43
21:4:321:LMU:H101	21:4:321:LMU:H72	1.65	0.43
5:A:315:HIS:HB2	20:A:821:CLA:HBC1	2.01	0.43
5:A:388:ASP:OD1	5:A:391:THR:HB	2.18	0.43
5:A:560:VAL:O	5:A:563:ALA:HB2	2.17	0.43
5:A:575:LEU:HD13	5:A:576:GLY:H	1.84	0.43
6:B:112:PRO:O	6:B:113:VAL:HG13	2.19	0.43
6:B:22:TRP:HA	6:B:25:ILE:CD1	2.49	0.43
6:B:377:TYR:OH	6:B:717:TYR:HE1	2.02	0.43
6:B:568:CYS:HB3	6:B:569:ASP:H	1.65	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CH2	2.53	0.43
6:B:715:VAL:O	6:B:719:PHE:HB2	2.18	0.43
20:B:810:CLA:C4C	20:B:811:CLA:CBB	2.92	0.43
20:B:833:CLA:CBB	22:B:845:BCR:C28	2.97	0.43
6:B:659:THR:OG1	20:B:851:CLA:C3B	2.67	0.43
6:B:564:ARG:CZ	7:C:64:SER:OG	2.66	0.43
8:D:41:GLN:HG3	16:L:125:LYS:NZ	2.33	0.43
10:F:44:ALA:O	10:F:46:MET:N	2.50	0.43
10:F:80:TRP:CE3	20:F:206:CLA:CHC	3.01	0.43
16:L:65:VAL:O	16:L:69:VAL:N	2.52	0.43
1:1:185:TRP:CA	1:1:186:HIS:CE1	2.93	0.43
2:2:171:MET:SD	2:2:171:MET:O	2.76	0.43
20:2:302:CLA:CGA	20:2:302:CLA:C4A	2.97	0.43
2:2:79:TRP:O	2:2:79:TRP:CD2	2.72	0.43
20:3:318:CLA:H142	20:3:318:CLA:H101	2.00	0.43
5:A:284:ARG:CA	5:A:284:ARG:CZ	2.91	0.43
5:A:208:ALA:CA	5:A:310:PHE:O	2.43	0.43
5:A:506:GLY:O	5:A:507:ALA:CB	2.66	0.43
20:A:807:CLA:HAA1	20:A:809:CLA:HED1	2.01	0.43
6:B:144:PHE:O	6:B:148:ILE:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:167:TRP:HD1	11:G:41:MET:CE	2.31	0.43
6:B:488:ALA:CB	20:B:834:CLA:C1C	2.96	0.43
6:B:583:MET:HA	20:B:823:CLA:HBC1	2.00	0.43
6:B:621:ARG:HB3	6:B:621:ARG:HE	1.57	0.43
6:B:632:ILE:C	6:B:634:GLY:N	2.71	0.43
6:B:674:LEU:O	6:B:678:LEU:HB2	2.18	0.43
20:B:818:CLA:HMA1	11:G:21:PHE:CG	2.54	0.43
20:B:818:CLA:NA	20:B:818:CLA:O2A	2.52	0.43
20:B:820:CLA:H72	20:B:820:CLA:HBB1	1.97	0.43
8:D:125:PRO:HG2	8:D:127:ARG:HH11	1.82	0.43
21:E:101:LMU:H1B	21:E:101:LMU:H4B	1.51	0.43
9:E:42:GLU:CG	9:E:43:SER:N	2.70	0.43
10:F:53:PHE:O	10:F:55:ASN:N	2.52	0.43
21:H:104:LMU:H4B	21:H:104:LMU:H1B	1.07	0.43
21:N:101:LMU:H112	21:N:101:LMU:H81	1.60	0.43
17:N:29:PHE:O	17:N:33:TYR:N	2.51	0.43
19:P:2:FRU:O1	19:P:2:FRU:O3	2.29	0.43
21:R:103:LMU:O6'	21:R:103:LMU:H22	2.13	0.43
19:U:1:GLC:H5	19:U:2:FRU:O4	2.19	0.43
2:2:112:ASP:C	2:2:114:LEU:N	2.70	0.43
2:2:153:PRO:HB2	2:2:157:LYS:HZ1	1.84	0.43
21:3:322:LMU:H81	21:3:322:LMU:H52	1.53	0.43
4:4:44:GLU:O	4:4:45:LEU:C	2.56	0.43
5:A:224:HIS:HE1	20:A:815:CLA:C1D	2.31	0.43
5:A:249:ILE:C	5:A:251:ASN:N	2.65	0.43
5:A:379:MET:HB2	5:A:379:MET:HE2	1.80	0.43
5:A:40:PHE:O	5:A:40:PHE:CD1	2.72	0.43
5:A:530:LEU:HD11	5:A:624:VAL:HA	2.01	0.43
5:A:561:LEU:HA	5:A:561:LEU:HD23	1.75	0.43
5:A:654:ARG:HG3	5:A:655:ASP:N	2.33	0.43
5:A:705:GLU:HG2	6:B:545:LYS:NZ	2.31	0.43
5:A:74:ILE:O	5:A:78:VAL:HG13	2.19	0.43
20:A:825:CLA:H91	20:A:825:CLA:H112	1.60	0.43
6:B:126:THR:HG21	6:B:358:TYR:HD1	1.84	0.43
6:B:475:ASP:CB	6:B:480:SER:HA	2.49	0.43
6:B:535:VAL:HG23	6:B:539:LEU:HD23	1.99	0.43
6:B:555:TYR:HE2	6:B:573:TRP:HD1	1.67	0.43
6:B:661:PHE:O	6:B:665:ILE:N	2.51	0.43
6:B:662:MET:HB3	6:B:663:PHE:H	1.55	0.43
6:B:707:LEU:HD13	25:B:848:LMG:H331	2.00	0.43
20:B:824:CLA:H201	20:B:837:CLA:C2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:83:CYS:O	8:D:83:CYS:SG	2.76	0.43
9:E:40:ARG:N	9:E:46:PHE:CE1	2.82	0.43
11:G:93:TYR:CG	11:G:94:ASP:HB2	2.54	0.43
21:H:105:LMU:H1'	21:H:105:LMU:H6D	1.18	0.43
21:K:106:LMU:H4B	21:K:106:LMU:H1B	1.56	0.43
16:L:127:PRO:C	16:L:128:ASP:O	2.57	0.43
16:L:99:LEU:HD12	22:L:210:BCR:HC7	2.00	0.43
17:N:6:TYR:H	17:N:8:GLU:HA	1.84	0.43
19:U:1:GLC:O5	19:U:2:FRU:C4	2.65	0.43
2:2:47:ALA:HB1	2:2:110:TRP:CZ2	2.54	0.43
2:2:150:SER:HB3	2:2:151:ALA:H	1.50	0.43
2:2:191:ASN:O	2:2:192:LEU:C	2.57	0.43
20:2:305:CLA:H2	20:2:308:CLA:CMD	2.49	0.43
4:4:167:ILE:C	4:4:169:GLN:H	2.22	0.43
5:A:277:TYR:CD2	5:A:278:ALA:N	2.87	0.43
5:A:413:HIS:CG	5:A:416:ILE:HD12	2.54	0.43
5:A:538:ASP:O	5:A:542:HIS:CD2	2.71	0.43
5:A:703:LEU:O	5:A:707:ILE:CG1	2.67	0.43
5:A:129:GLN:HE22	20:A:809:CLA:C1A	2.15	0.43
20:A:811:CLA:CMC	20:A:811:CLA:HBC3	2.38	0.43
22:A:847:BCR:C12	20:A:851:CLA:H122	2.48	0.43
21:A:854:LMU:O6'	21:A:854:LMU:H41	2.17	0.43
6:B:17:THR:HA	6:B:696:LYS:CB	2.48	0.43
6:B:393:PHE:CZ	6:B:398:TYR:CD2	3.07	0.43
5:A:706:SER:HB3	6:B:419:ILE:O	2.18	0.43
6:B:458:ILE:HG13	6:B:459:PHE:CD1	2.54	0.43
6:B:175:LEU:HD11	20:B:817:CLA:CMA	2.49	0.43
20:B:836:CLA:HBC1	10:F:83:PHE:CE1	2.52	0.43
6:B:655:LEU:CD2	20:B:839:CLA:CAB	2.97	0.43
11:G:75:GLY:O	11:G:80:ILE:HG23	2.19	0.43
12:H:54:LEU:O	12:H:54:LEU:HD22	2.19	0.43
20:K:102:CLA:HMD2	21:K:109:LMU:H52	2.01	0.43
16:L:107:PHE:HA	16:L:133:ALA:HB2	2.00	0.43
21:N:101:LMU:H21	21:N:101:LMU:H1'	1.66	0.43
21:2:317:LMU:H71	21:2:317:LMU:H41	1.80	0.43
20:3:318:CLA:H112	20:3:318:CLA:H71	1.54	0.43
4:4:30:LEU:O	4:4:32:GLU:OE1	2.36	0.43
5:A:163:GLN:HA	5:A:166:CYS:SG	2.59	0.43
5:A:422:TYR:N	5:A:422:TYR:HD1	2.11	0.43
5:A:620:MET:C	5:A:623:ASP:O	2.57	0.43
20:A:805:CLA:H122	22:A:843:BCR:C39	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:808:CLA:H161	20:A:808:CLA:H122	1.73	0.43
20:A:808:CLA:HBC3	20:A:808:CLA:CHD	2.48	0.43
20:A:819:CLA:H111	20:A:819:CLA:C16	2.47	0.43
20:A:827:CLA:C4C	22:A:844:BCR:H333	2.48	0.43
24:A:857:SF4:S1	6:B:560:ASP:O	2.77	0.43
6:B:114:ASN:O	6:B:115:ASN:OD1	2.37	0.43
6:B:175:LEU:O	6:B:179:LEU:CG	2.66	0.43
6:B:182:LEU:HG	6:B:183:PHE:H	1.84	0.43
6:B:183:PHE:HB3	6:B:284:PHE:CD2	2.54	0.43
6:B:361:ILE:O	6:B:362:ALA:O	2.36	0.43
6:B:556:SER:CA	6:B:558:PRO:CD	2.97	0.43
6:B:625:TRP:CD2	6:B:625:TRP:C	2.91	0.43
20:B:818:CLA:C1C	20:B:818:CLA:H43	2.49	0.43
20:B:851:CLA:C3A	20:B:851:CLA:CGA	2.92	0.43
7:C:27:GLU:OE1	7:C:40:ALA:HB3	2.18	0.43
8:D:112:LEU:N	8:D:114:PRO:HG2	2.34	0.43
8:D:94:TYR:O	8:D:95:LYS:HB3	2.19	0.43
10:F:104:TYR:N	10:F:129:LEU:HD13	2.34	0.43
10:F:149:LEU:HD23	10:F:153:ASN:HD21	1.83	0.43
13:I:8:PHE:HB3	20:I:102:CLA:OBD	2.16	0.43
14:J:38:THR:O	14:J:39:PHE:CB	2.67	0.43
16:L:49:PRO:HG3	16:L:131:GLN:NE2	2.34	0.43
16:L:161:LEU:HA	16:L:161:LEU:HD13	1.63	0.43
17:N:45:ASN:HA	17:N:57:LYS:HZ3	1.84	0.43
20:1:202:CLA:HMC1	20:1:202:CLA:HAC1	1.86	0.43
2:2:69:THR:O	2:2:70:LYS:CG	2.66	0.43
2:2:73:ILE:HD13	2:2:75:ASN:CB	2.49	0.43
4:4:158:ARG:HG2	4:4:159:LEU:N	2.31	0.43
20:4:316:CLA:C3D	20:4:316:CLA:O1D	2.57	0.43
5:A:141:ARG:HE	10:F:40:LEU:H	1.67	0.43
5:A:361:ASN:O	5:A:364:MET:N	2.52	0.43
5:A:575:LEU:HD13	5:A:579:PHE:HB3	2.00	0.43
5:A:370:ILE:HD11	20:A:824:CLA:O1D	2.17	0.43
5:A:78:VAL:O	5:A:82:HIS:CG	2.72	0.43
5:A:553:VAL:CG2	22:A:846:BCR:C40	2.97	0.43
6:B:274:ALA:HA	6:B:277:HIS:HB2	2.00	0.43
6:B:332:PHE:HE1	6:B:408:LEU:HD21	1.84	0.43
6:B:543:GLY:HA3	6:B:548:PRO:O	2.19	0.43
5:A:697:ARG:CD	6:B:566:GLY:O	2.66	0.43
6:B:693:TRP:CD1	20:B:838:CLA:CMD	3.02	0.43
6:B:190:TRP:CE3	20:B:812:CLA:HBB2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:826:CLA:H122	22:B:843:BCR:C14	2.49	0.43
6:B:91:ILE:HD12	20:B:808:CLA:HMD3	2.00	0.43
7:C:60:THR:HG21	7:C:63:LEU:O	2.16	0.43
8:D:149:THR:O	8:D:151:LYS:N	2.51	0.43
10:F:52:ARG:N	10:F:52:ARG:HD2	2.33	0.43
20:L:201:CLA:O2D	20:L:201:CLA:HBA2	2.17	0.43
20:L:209:CLA:CAA	20:L:209:CLA:O1D	2.63	0.43
16:L:33:ILE:HG23	16:L:34:ALA:N	2.34	0.43
19:T:1:GLC:C5	19:T:2:FRU:H12	2.46	0.43
3:3:114:PHE:CE1	20:3:309:CLA:C4D	3.02	0.42
3:3:127:ARG:HG2	3:3:131:ASP:OD1	2.18	0.42
20:3:313:CLA:O1A	20:3:313:CLA:H3A	2.19	0.42
3:3:49:ILE:O	3:3:49:ILE:HG23	2.18	0.42
4:4:147:LEU:HD22	4:4:148:GLU:HA	1.96	0.42
4:4:151:GLU:CA	4:4:154:ILE:HG23	2.45	0.42
4:4:99:HIS:ND1	4:4:103:ILE:HD13	2.29	0.42
5:A:249:ILE:CD1	5:A:250:LEU:HB2	2.48	0.42
5:A:299:ILE:HD12	5:A:299:ILE:HA	1.69	0.42
5:A:358:LEU:HD11	5:A:413:HIS:CD2	2.51	0.42
5:A:419:VAL:HG21	5:A:577:PHE:HB2	2.01	0.42
5:A:553:VAL:O	5:A:557:LEU:CB	2.67	0.42
5:A:680:LEU:HD21	6:B:617:MET:HB2	2.00	0.42
20:A:808:CLA:CGA	20:A:826:CLA:H11	2.49	0.42
20:A:831:CLA:HMD2	6:B:95:HIS:HD2	1.84	0.42
20:A:838:CLA:H13	20:A:838:CLA:H193	2.00	0.42
22:A:846:BCR:H15C	22:A:846:BCR:H351	1.86	0.42
6:B:192:GLY:HA2	20:B:813:CLA:CHC	2.49	0.42
6:B:8:PHE:CD2	6:B:34:HIS:ND1	2.87	0.42
6:B:440:ASN:OD1	6:B:452:GLN:NE2	2.52	0.42
6:B:493:TRP:HE1	20:B:814:CLA:CAC	2.28	0.42
6:B:668:ARG:CG	6:B:700:LEU:O	2.67	0.42
6:B:70:TRP:H	6:B:70:TRP:HD1	1.65	0.42
6:B:167:TRP:HZ2	20:B:811:CLA:HAC1	1.74	0.42
20:B:825:CLA:H41	20:B:825:CLA:H71	2.01	0.42
6:B:348:VAL:HG21	20:B:826:CLA:HHD	1.99	0.42
6:B:398:TYR:O	8:D:143:PRO:HG2	2.18	0.42
8:D:84:LEU:HD12	8:D:100:PHE:CZ	2.50	0.42
21:E:101:LMU:H3O2	21:E:101:LMU:C6'	2.20	0.42
10:F:26:GLN:HB3	10:F:27:ALA:H	1.68	0.42
22:I:101:BCR:H342	22:I:101:BCR:HC7	1.61	0.42
20:K:102:CLA:H43	20:K:102:CLA:HMA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:10:ILE:HA	15:K:13:THR:HG22	1.85	0.42
17:N:67:LEU:CB	17:N:68:GLU:HB3	2.46	0.42
2:2:154:GLN:OE1	2:2:154:GLN:HA	2.19	0.42
2:2:99:LEU:HD23	2:2:102:ILE:CG1	2.50	0.42
21:3:322:LMU:H61	21:3:322:LMU:H32	1.50	0.42
4:4:104:ARG:CZ	4:4:105:ARG:H	2.32	0.42
4:4:127:PRO:HB2	4:4:143:PHE:HE1	1.83	0.42
4:4:163:PHE:O	4:4:166:PHE:CA	2.68	0.42
5:A:108:ALA:CB	5:A:138:GLY:HA3	2.41	0.42
5:A:90:PHE:HB3	5:A:175:ALA:HB2	2.01	0.42
5:A:277:TYR:HD2	5:A:278:ALA:N	2.17	0.42
5:A:588:GLY:H	6:B:668:ARG:HH11	1.63	0.42
5:A:664:VAL:HG22	5:A:665:ILE:HG23	1.99	0.42
20:A:822:CLA:HBC1	22:A:845:BCR:H393	2.02	0.42
20:A:826:CLA:H162	20:A:826:CLA:H193	1.74	0.42
6:B:139:ALA:O	6:B:141:PHE:N	2.52	0.42
6:B:172:GLU:O	6:B:176:ASN:N	2.51	0.42
6:B:655:LEU:HD22	20:B:839:CLA:CAB	2.48	0.42
20:B:811:CLA:C1	22:B:843:BCR:C10	2.96	0.42
7:C:63:LEU:CD1	7:C:65:VAL:H	2.33	0.42
8:D:20:LEU:O	8:D:21:ASP:C	2.58	0.42
11:G:27:GLN:HG2	20:G:102:CLA:C4D	2.49	0.42
11:G:67:ASN:HA	11:G:70:ASP:CG	2.38	0.42
21:H:104:LMU:H82	21:H:104:LMU:C4	2.30	0.42
17:N:72:LYS:CA	17:N:73:ASP:C	2.88	0.42
1:1:38:ARG:CZ	1:1:139:LYS:CB	2.97	0.42
2:2:73:ILE:HD13	2:2:75:ASN:CA	2.48	0.42
4:4:149:ALA:CA	4:4:151:GLU:CG	2.96	0.42
4:4:179:ASP:H	4:4:184:HIS:CD2	2.37	0.42
21:4:322:LMU:H1B	21:4:322:LMU:H5'	1.48	0.42
5:A:149:PHE:C	5:A:151:GLN:N	2.71	0.42
5:A:159:THR:OG1	5:A:239:PRO:HB3	2.20	0.42
5:A:472:ARG:HG2	6:B:97:GLY:HA3	2.02	0.42
5:A:648:THR:HG23	5:A:650:ASN:H	1.83	0.42
5:A:67:HIS:O	5:A:68:THR:HB	2.20	0.42
5:A:693:LEU:CD2	5:A:734:GLY:HA3	2.49	0.42
6:B:58:PHE:HE2	6:B:145:LEU:HD12	1.85	0.42
6:B:160:LYS:HB2	6:B:160:LYS:NZ	2.30	0.42
6:B:203:ARG:CG	6:B:204:GLY:N	2.70	0.42
6:B:531:THR:HG21	20:B:823:CLA:CHC	2.49	0.42
20:B:827:CLA:HHD	25:B:848:LMG:H352	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:848:LMG:H292	25:B:848:LMG:H112	2.00	0.42
22:B:852:BCR:HC7	22:B:852:BCR:H342	1.53	0.42
7:C:44:ARG:NH2	8:D:127:ARG:NE	2.64	0.42
8:D:41:GLN:NE2	8:D:42:VAL:HA	2.34	0.42
9:E:69:PHE:CD2	9:E:71:LYS:N	2.82	0.42
9:E:88:GLU:O	9:E:90:VAL:HA	2.14	0.42
10:F:39:ALA:O	10:F:42:ILE:CG2	2.68	0.42
10:F:96:TRP:HZ3	10:F:134:PHE:CB	2.21	0.42
11:G:42:SER:HG	11:G:45:GLU:CB	2.32	0.42
12:H:27:ASP:O	12:H:29:PRO:CD	2.67	0.42
14:J:10:VAL:HG13	14:J:14:LEU:CG	2.43	0.42
21:K:105:LMU:H11	21:K:105:LMU:H71	1.99	0.42
20:L:203:CLA:H41	20:L:203:CLA:H62	1.62	0.42
16:L:99:LEU:HB3	16:L:140:THR:HG21	2.02	0.42
2:2:54:TRP:CZ2	2:2:109:ARG:HB3	2.49	0.42
2:2:197:LEU:O	2:2:198:ALA:HB2	2.20	0.42
20:2:303:CLA:H3A	20:2:303:CLA:HBA2	1.79	0.42
4:4:121:PHE:O	4:4:122:LYS:CG	2.66	0.42
4:4:38:ARG:O	4:4:39:TRP:C	2.56	0.42
5:A:173:VAL:HG23	5:A:174:PHE:N	2.34	0.42
5:A:254:LEU:HD13	5:A:254:LEU:HA	1.66	0.42
5:A:204:ASN:HA	5:A:314:GLY:O	2.20	0.42
5:A:374:GLN:C	5:A:376:MET:H	2.21	0.42
5:A:579:PHE:HA	5:A:580:PRO:HD2	1.64	0.42
5:A:64:PHE:HZ	5:A:77:LYS:CE	2.32	0.42
5:A:705:GLU:OE1	5:A:708:VAL:HG12	2.19	0.42
5:A:606:TYR:HB2	5:A:739:LEU:HD22	2.01	0.42
5:A:748:ALA:O	5:A:749:PHE:C	2.58	0.42
22:A:845:BCR:H351	22:A:845:BCR:H15C	1.83	0.42
21:A:854:LMU:H6'	21:A:854:LMU:H12	1.84	0.42
6:B:144:PHE:CD2	6:B:144:PHE:C	2.92	0.42
6:B:174:ARG:C	6:B:176:ASN:H	2.22	0.42
6:B:176:ASN:ND2	6:B:292:ARG:O	2.52	0.42
6:B:416:GLU:N	6:B:416:GLU:CD	2.73	0.42
6:B:674:LEU:CD1	6:B:674:LEU:C	2.88	0.42
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.74	0.42
20:B:815:CLA:HMC2	20:B:815:CLA:H141	2.02	0.42
20:B:817:CLA:HBB2	20:B:822:CLA:C4	2.47	0.42
20:B:849:CLA:HAA2	20:B:849:CLA:H11	2.02	0.42
10:F:123:VAL:O	10:F:126:ALA:CA	2.68	0.42
23:A:842:PQN:C15	22:F:202:BCR:H322	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:45:GLU:C	11:G:49:THR:CG2	2.62	0.42
11:G:93:TYR:CB	11:G:94:ASP:HB2	2.42	0.42
21:K:105:LMU:H1'	21:K:105:LMU:H4'	1.57	0.42
16:L:66:GLY:CA	16:L:69:VAL:HG22	2.48	0.42
19:U:1:GLC:C5	19:U:2:FRU:O4	2.67	0.42
19:Y:1:GLC:HO6	19:Y:2:FRU:C2	2.31	0.42
2:2:205:PHE:O	2:2:206:ALA:HB2	2.19	0.42
2:2:73:ILE:HD13	2:2:75:ASN:HB2	2.02	0.42
22:3:314:BCR:H11C	22:3:314:BCR:H341	1.57	0.42
4:4:108:ASP:O	4:4:111:ASN:C	2.57	0.42
4:4:121:PHE:HB2	4:4:128:ALA:CB	2.48	0.42
4:4:122:LYS:HB2	4:4:143:PHE:HD2	0.51	0.42
4:4:166:PHE:O	4:4:169:GLN:N	2.50	0.42
20:4:311:CLA:HED2	20:4:311:CLA:H2A	2.02	0.42
5:A:193:LEU:O	5:A:196:PHE:CD2	2.73	0.42
5:A:227:LEU:O	5:A:231:GLN:HB2	2.18	0.42
5:A:34:TRP:O	5:A:35:ALA:HB3	2.20	0.42
5:A:445:HIS:CE1	20:A:829:CLA:HMB1	2.53	0.42
5:A:620:MET:HG3	5:A:625:TRP:CD2	2.54	0.42
5:A:662:SER:HA	5:A:665:ILE:CD1	2.49	0.42
5:A:82:HIS:CE1	20:A:805:CLA:HAA1	2.54	0.42
20:A:851:CLA:C9	20:A:851:CLA:H122	2.47	0.42
5:A:96:MET:N	5:A:98:PHE:O	2.52	0.42
6:B:216:LEU:HD22	6:B:218:TYR:H	1.84	0.42
6:B:228:GLY:CA	11:G:8:ILE:HB	2.49	0.42
6:B:278:LEU:O	6:B:279:ALA:C	2.58	0.42
6:B:477:PRO:O	6:B:478:LEU:HD22	2.18	0.42
6:B:518:LEU:O	6:B:519:VAL:C	2.58	0.42
6:B:531:THR:O	6:B:535:VAL:N	2.50	0.42
6:B:685:THR:HA	6:B:686:PRO:HD3	1.92	0.42
6:B:17:THR:CA	6:B:696:LYS:H	2.31	0.42
20:B:836:CLA:C9	20:B:836:CLA:CBB	2.55	0.42
8:D:152:GLN:O	8:D:154:TYR:N	2.53	0.42
8:D:24:THR:OG1	8:D:24:THR:O	2.30	0.42
9:E:36:VAL:CG1	9:E:87:VAL:HG11	2.49	0.42
9:E:87:VAL:C	9:E:89:GLU:N	2.67	0.42
11:G:60:SER:C	11:G:62:ASP:N	2.71	0.42
11:G:80:ILE:O	11:G:81:VAL:C	2.58	0.42
12:H:45:ALA:HA	12:H:48:THR:OG1	2.19	0.42
13:I:8:PHE:HE1	22:I:103:BCR:C9	2.32	0.42
16:L:127:PRO:O	16:L:128:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:139:ASN:HA	4:4:140:PRO:HD3	1.84	0.42
5:A:193:LEU:HA	5:A:196:PHE:HE2	1.80	0.42
5:A:281:LEU:HB2	5:A:301:HIS:CD2	2.52	0.42
5:A:648:THR:C	5:A:650:ASN:H	2.23	0.42
5:A:672:LEU:CD2	5:A:672:LEU:H	2.32	0.42
20:A:818:CLA:HMB2	20:A:818:CLA:H2	2.02	0.42
20:A:819:CLA:H91	20:A:819:CLA:H112	1.82	0.42
20:A:820:CLA:OBD	20:A:820:CLA:O2D	2.37	0.42
5:A:351:THR:CA	20:A:823:CLA:H191	2.49	0.42
20:A:831:CLA:HBC2	20:H:109:CLA:HBC1	2.01	0.42
21:A:849:LMU:H41	21:A:849:LMU:H12	1.70	0.42
6:B:541:ALA:HB2	6:B:572:ALA:CB	2.49	0.42
20:B:809:CLA:HBD	20:B:809:CLA:CGA	2.50	0.42
20:B:821:CLA:H161	20:B:821:CLA:H141	1.65	0.42
20:B:832:CLA:ND	20:B:833:CLA:CBB	2.82	0.42
20:B:838:CLA:C19	13:I:21:MET:CE	2.98	0.42
5:A:584:PRO:HB2	7:C:67:VAL:HB	2.01	0.42
11:G:5:SER:O	11:G:7:VAL:CG1	2.68	0.42
12:H:45:ALA:N	12:H:46:PRO:HD2	2.34	0.42
17:N:14:LYS:HB2	17:N:17:ASN:OD1	2.20	0.42
17:N:4:GLU:OE2	17:N:5:GLU:CB	2.61	0.42
19:S:1:GLC:HO2	19:S:2:FRU:H11	1.80	0.42
1:1:109:GLU:HB3	20:1:209:CLA:HMA3	2.01	0.42
1:1:179:THR:HB	1:1:180:HIS:H	1.54	0.42
2:2:37:ASP:OD2	3:3:41:ASP:HB2	2.18	0.42
3:3:206:VAL:HB	3:3:207:GLY:H	1.69	0.42
3:3:96:GLY:C	3:3:97:PHE:CG	2.92	0.42
4:4:142:ASN:O	4:4:143:PHE:HB2	2.19	0.42
5:A:177:LEU:HA	5:A:177:LEU:HD22	1.89	0.42
5:A:207:LEU:HD11	5:A:313:ALA:CB	2.49	0.42
5:A:210:LEU:HD23	5:A:211:LEU:N	2.35	0.42
5:A:334:HIS:HB3	20:A:820:CLA:CHB	2.49	0.42
5:A:467:MET:HB3	5:A:467:MET:HE3	1.73	0.42
5:A:570:PRO:C	5:A:572:LYS:N	2.73	0.42
20:A:820:CLA:H52	20:A:820:CLA:C1C	2.49	0.42
20:A:820:CLA:HBA2	20:A:820:CLA:H3A	1.62	0.42
20:A:824:CLA:CBB	20:A:836:CLA:HMA1	2.49	0.42
6:B:260:GLY:O	6:B:262:HIS:NE2	2.52	0.42
6:B:350:GLN:HG3	6:B:372:TYR:HE1	1.84	0.42
6:B:439:HIS:HB2	20:B:831:CLA:C1C	2.49	0.42
6:B:503:GLU:CA	6:B:507:SER:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:707:LEU:HG	6:B:708:VAL:N	2.34	0.42
20:B:803:CLA:HHD	20:B:803:CLA:HBC3	2.01	0.42
6:B:167:TRP:CD1	20:B:810:CLA:HED1	2.55	0.42
6:B:326:ILE:CG2	20:B:822:CLA:HBC3	2.48	0.42
25:B:848:LMG:C11	25:B:848:LMG:O8	2.68	0.42
10:F:128:SER:C	10:F:130:LEU:HD23	2.40	0.42
10:F:131:PHE:O	10:F:132:ARG:C	2.56	0.42
10:F:96:TRP:CZ3	10:F:134:PHE:N	2.87	0.42
12:H:77:LEU:CD2	12:H:78:PRO:HD2	2.50	0.42
15:K:44:GLU:O	15:K:45:SER:HB2	2.19	0.42
16:L:63:LEU:CG	16:L:64:LEU:H	2.27	0.42
17:N:45:ASN:HA	17:N:57:LYS:HZ2	1.83	0.42
17:N:57:LYS:O	17:N:58:VAL:C	2.57	0.42
17:N:72:LYS:CB	17:N:74:LYS:H	2.21	0.42
2:2:208:PHE:CE1	2:2:209:THR:O	2.73	0.42
21:2:317:LMU:H3'	21:2:317:LMU:C6B	2.50	0.42
5:A:164:LEU:CA	5:A:167:THR:HG23	2.47	0.42
5:A:183:TRP:C	5:A:185:HIS:H	2.23	0.42
5:A:345:GLY:C	5:A:347:TYR:N	2.66	0.42
5:A:430:ASP:O	5:A:434:ARG:N	2.45	0.42
5:A:630:ASP:C	5:A:632:GLY:H	2.21	0.42
5:A:667:SER:OG	5:A:667:SER:O	2.37	0.42
5:A:79:PHE:CE2	5:A:185:HIS:CG	2.94	0.42
20:A:805:CLA:C4B	20:A:828:CLA:HMB2	2.50	0.42
6:B:262:HIS:ND1	6:B:265:THR:O	2.40	0.42
6:B:292:ARG:NE	6:B:292:ARG:CA	2.64	0.42
6:B:10:GLN:HB2	6:B:35:ASP:OD2	2.19	0.42
6:B:366:THR:C	6:B:368:GLN:N	2.73	0.42
6:B:429:LEU:HA	6:B:429:LEU:HD23	1.64	0.42
6:B:269:TRP:CG	6:B:497:TRP:HH2	2.38	0.42
6:B:661:PHE:O	6:B:662:MET:O	2.37	0.42
6:B:724:PHE:CZ	20:B:849:CLA:HMD1	2.55	0.42
8:D:49:THR:C	8:D:50:TRP:HD1	2.23	0.42
9:E:37:LYS:HD2	9:E:47:LYS:HE3	2.02	0.42
11:G:28:ARG:HG2	11:G:29:GLU:CB	2.50	0.42
11:G:62:ASP:HB2	11:G:63:PRO:CD	2.45	0.42
11:G:79:HIS:CG	11:G:79:HIS:O	2.72	0.42
21:H:106:LMU:H4B	21:H:106:LMU:H31	2.02	0.42
15:K:8:ASN:CB	15:K:9:LEU:HD23	2.50	0.42
16:L:33:ILE:HG13	16:L:37:LEU:HD21	2.02	0.42
16:L:56:VAL:CB	20:L:208:CLA:HED2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:38:UNK:C	18:R:42:UNK:CA	2.97	0.42
2:2:81:THR:O	2:2:82:ALA:C	2.56	0.42
3:3:106:TYR:CB	3:3:107:TRP:HD1	2.32	0.42
3:3:92:TRP:HZ2	5:A:250:LEU:CD1	2.28	0.42
4:4:88:SER:C	4:4:90:LEU:HD13	2.39	0.42
5:A:210:LEU:N	5:A:213:LEU:N	2.68	0.42
5:A:586:ARG:HG3	7:C:49:VAL:CG2	2.43	0.42
5:A:132:LEU:HD21	5:A:674:ALA:HB2	2.02	0.42
5:A:737:HIS:CE1	20:A:838:CLA:NA	2.88	0.42
20:A:839:CLA:H51	20:A:839:CLA:H102	2.02	0.42
20:A:841:CLA:CGA	20:A:841:CLA:CHA	2.98	0.42
6:B:213:LEU:HD12	6:B:214:ASP:H	1.83	0.42
6:B:470:THR:H	6:B:501:ILE:HG23	1.84	0.42
6:B:534:LEU:CD2	6:B:579:ALA:HB2	2.50	0.42
6:B:583:MET:O	6:B:587:ILE:HB	2.20	0.42
6:B:594:TRP:HD1	6:B:595:HIS:CB	2.33	0.42
5:A:680:LEU:HG	6:B:617:MET:HB2	2.02	0.42
6:B:190:TRP:CE2	20:B:816:CLA:CMD	3.03	0.42
22:B:842:BCR:H343	11:G:21:PHE:CE1	2.55	0.42
11:G:32:ALA:O	11:G:34:GLN:C	2.58	0.42
11:G:44:PHE:CA	11:G:46:ALA:HB2	2.49	0.42
12:H:36:GLN:O	12:H:36:GLN:CG	2.68	0.42
14:J:37:LEU:O	14:J:38:THR:OG1	2.35	0.42
16:L:135:GLY:HA2	16:L:138:LYS:HE2	2.02	0.42
16:L:149:SER:C	16:L:151:VAL:N	2.73	0.42
16:L:160:VAL:C	16:L:161:LEU:O	2.58	0.42
2:2:103:GLY:HA2	20:2:311:CLA:CAB	2.49	0.42
4:4:121:PHE:CD1	4:4:143:PHE:CZ	3.08	0.42
4:4:147:LEU:HD13	4:4:148:GLU:CA	2.43	0.42
20:4:311:CLA:CHD	20:4:311:CLA:HBC2	2.50	0.42
5:A:150:PHE:O	5:A:151:GLN:HG3	2.20	0.42
5:A:224:HIS:CE1	20:A:815:CLA:C1D	3.02	0.42
5:A:274:TRP:CZ2	5:A:278:ALA:HA	2.55	0.42
5:A:338:PHE:C	5:A:338:PHE:CD2	2.93	0.42
5:A:349:ILE:CD1	5:A:422:TYR:HB3	2.50	0.42
5:A:466:THR:HG21	20:B:808:CLA:HBB1	2.01	0.42
5:A:604:TRP:O	5:A:605:MET:C	2.59	0.42
5:A:621:GLN:HG2	5:A:637:ILE:CD1	2.40	0.42
5:A:680:LEU:HD21	6:B:617:MET:SD	2.60	0.42
6:B:230:TRP:CH2	11:G:11:SER:CB	2.94	0.42
6:B:25:ILE:H	6:B:25:ILE:HG13	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:310:PRO:CG	6:B:311:PRO:CD	2.88	0.42
6:B:381:PHE:HA	6:B:583:MET:SD	2.60	0.42
6:B:707:LEU:O	6:B:710:LEU:CB	2.68	0.42
7:C:63:LEU:CD1	7:C:64:SER:H	2.32	0.42
8:D:139:LYS:NZ	9:E:41:ARG:HH11	2.18	0.42
10:F:23:LYS:C	10:F:26:GLN:H	2.23	0.42
10:F:65:SER:C	10:F:67:GLY:H	2.23	0.42
11:G:24:PHE:HB3	11:G:28:ARG:HH11	1.85	0.42
11:G:43:HIS:C	11:G:45:GLU:CA	2.88	0.42
11:G:50:ARG:CB	11:G:51:ALA:CA	2.97	0.42
21:K:104:LMU:H4B	21:K:104:LMU:H1B	1.53	0.42
16:L:12:GLN:HA	16:L:13:PRO:HD3	1.82	0.42
20:L:207:CLA:H11	20:L:207:CLA:C4D	2.50	0.42
16:L:46:ALA:N	16:L:52:ARG:HH12	2.18	0.42
17:N:44:GLU:C	17:N:46:PHE:N	2.68	0.42
21:R:106:LMU:H52	21:R:106:LMU:H21	1.82	0.42
20:1:206:CLA:H121	20:1:206:CLA:HBC3	2.02	0.41
1:1:38:ARG:CZ	1:1:139:LYS:HB3	2.50	0.41
2:2:59:ALA:HB3	2:2:172:LEU:HD22	1.99	0.41
20:2:303:CLA:CHD	20:2:303:CLA:C4	2.97	0.41
2:2:181:HIS:HE1	20:2:304:CLA:CHA	2.32	0.41
2:2:66:GLU:HB3	2:2:67:PHE:H	1.54	0.41
3:3:207:GLY:O	3:3:208:PRO:C	2.58	0.41
3:3:52:LYS:O	3:3:56:TYR:CB	2.68	0.41
3:3:94:ARG:CA	3:3:97:PHE:HE1	2.33	0.41
4:4:36:ASN:OD1	4:4:37:LEU:N	2.52	0.41
4:4:86:SER:O	4:4:87:SER:C	2.56	0.41
5:A:183:TRP:C	5:A:185:HIS:N	2.73	0.41
5:A:216:LEU:CD1	22:A:843:BCR:H11C	2.50	0.41
5:A:527:VAL:HG12	5:A:528:ALA:O	2.20	0.41
5:A:536:THR:O	5:A:537:ALA:HB3	2.20	0.41
5:A:694:PHE:HZ	6:B:661:PHE:CE1	2.38	0.41
20:A:808:CLA:H3A	20:A:808:CLA:HBA2	1.39	0.41
20:A:815:CLA:CGD	20:A:815:CLA:C2A	2.95	0.41
5:A:207:LEU:CD1	20:A:819:CLA:HBB2	2.50	0.41
20:A:836:CLA:CBC	20:A:836:CLA:CMC	2.96	0.41
5:A:87:SER:O	5:A:88:ILE:HB	2.19	0.41
5:A:92:TRP:C	5:A:94:SER:H	2.22	0.41
6:B:16:PRO:HG3	7:C:74:THR:HG22	2.02	0.41
6:B:266:GLN:NE2	6:B:363:GLN:HG2	2.34	0.41
6:B:373:THR:C	6:B:376:GLN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:393:PHE:CZ	6:B:398:TYR:HD2	2.37	0.41
6:B:587:ILE:O	6:B:587:ILE:CG2	2.67	0.41
6:B:588:GLY:O	6:B:592:PHE:CB	2.52	0.41
5:A:680:LEU:CG	6:B:617:MET:HB2	2.50	0.41
6:B:304:ILE:CD1	20:B:817:CLA:HED3	2.50	0.41
20:B:806:CLA:H192	20:B:825:CLA:H141	2.02	0.41
21:D:201:LMU:H41	21:E:101:LMU:H121	2.00	0.41
9:E:34:SER:O	9:E:35:LYS:CB	2.64	0.41
21:F:201:LMU:H101	21:F:201:LMU:H72	1.66	0.41
10:F:75:GLY:O	20:F:205:CLA:HAC2	2.19	0.41
11:G:20:ARG:NH2	11:G:61:ASN:C	2.74	0.41
17:N:57:LYS:O	17:N:60:PHE:HD1	1.99	0.41
17:N:64:ASP:HB3	17:N:65:LEU:H	1.43	0.41
21:1:217:LMU:C1B	21:1:217:LMU:O3'	2.68	0.41
1:1:38:ARG:HH12	1:1:138:LYS:HD2	1.85	0.41
1:1:63:LEU:CG	1:1:63:LEU:O	2.67	0.41
21:2:317:LMU:H2'	21:2:317:LMU:C2	2.49	0.41
20:2:322:CLA:HED1	20:J:101:CLA:C2	2.50	0.41
2:2:51:HIS:HA	2:2:54:TRP:CD1	2.55	0.41
21:3:321:LMU:O2'	21:3:321:LMU:H22	2.20	0.41
4:4:103:ILE:HD13	4:4:103:ILE:H	1.84	0.41
4:4:148:GLU:HB3	4:4:149:ALA:H	1.78	0.41
5:A:163:GLN:CG	5:A:164:LEU:N	2.83	0.41
5:A:79:PHE:HZ	5:A:185:HIS:NE2	2.08	0.41
5:A:21:LEU:CD1	5:A:21:LEU:C	2.59	0.41
5:A:224:HIS:CE1	20:A:815:CLA:NC	2.88	0.41
5:A:244:LEU:H	5:A:244:LEU:HD12	1.85	0.41
5:A:357:GLN:NE2	5:A:360:ILE:HG23	2.35	0.41
5:A:408:VAL:O	5:A:411:ALA:HB3	2.20	0.41
5:A:127:VAL:CG2	20:A:809:CLA:HBB2	2.50	0.41
20:A:824:CLA:C5	20:A:825:CLA:CED	2.86	0.41
20:A:826:CLA:H202	22:J:102:BCR:H15C	1.99	0.41
22:A:844:BCR:HC8	22:A:844:BCR:C31	2.50	0.41
5:A:657:LEU:HD23	20:A:850:CLA:C2D	2.50	0.41
5:A:98:PHE:CD1	5:A:98:PHE:C	2.94	0.41
6:B:116:ALA:CB	6:B:121:TYR:CD2	3.04	0.41
6:B:348:VAL:HG22	20:B:826:CLA:HMD3	2.02	0.41
6:B:325:THR:HG21	6:B:403:ASN:HD21	1.86	0.41
6:B:486:LEU:HD12	20:B:833:CLA:CMD	2.49	0.41
6:B:387:PHE:CB	6:B:534:LEU:HD13	2.49	0.41
6:B:560:ASP:CG	7:C:66:ARG:CZ	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:534:LEU:HD21	6:B:579:ALA:HB2	2.01	0.41
5:A:650:ASN:HD22	6:B:635:ILE:CD1	2.33	0.41
6:B:431:PHE:CD2	20:B:830:CLA:CMA	3.03	0.41
8:D:93:LYS:CB	8:D:93:LYS:HZ2	2.30	0.41
9:E:60:LYS:CG	9:E:61:THR:H	2.19	0.41
10:F:126:ALA:HB1	10:F:129:LEU:HD12	2.02	0.41
10:F:144:LEU:CD1	10:F:149:LEU:HD13	2.50	0.41
10:F:24:LYS:HA	10:F:26:GLN:H	1.79	0.41
21:G:101:LMU:H92	21:G:101:LMU:H61	1.69	0.41
11:G:18:LEU:HD23	11:G:18:LEU:N	2.35	0.41
22:I:101:BCR:H371	22:I:101:BCR:H24C	1.01	0.41
10:F:125:LEU:HD11	14:J:18:TRP:CZ3	2.55	0.41
21:K:105:LMU:H52	21:K:105:LMU:H81	1.59	0.41
16:L:149:SER:C	16:L:151:VAL:H	2.23	0.41
16:L:68:PHE:CD1	16:L:68:PHE:N	2.88	0.41
18:R:41:UNK:N	18:R:42:UNK:CB	2.83	0.41
2:2:188:PRO:C	2:2:190:ASP:N	2.72	0.41
20:2:307:CLA:H42	20:2:307:CLA:H11	1.87	0.41
3:3:111:TYR:HB2	3:3:112:THR:CG2	2.51	0.41
3:3:153:SER:C	3:3:161:GLY:HA2	2.41	0.41
20:3:313:CLA:H12	20:3:313:CLA:H52	1.77	0.41
4:4:144:ALA:HB2	4:4:148:GLU:O	2.18	0.41
4:4:75:TRP:CG	20:4:311:CLA:CMD	2.93	0.41
5:A:378:SER:HG	5:A:512:SER:HG	1.68	0.41
5:A:663:GLN:OE1	5:A:753:ARG:CZ	2.69	0.41
5:A:66:SER:O	5:A:67:HIS:CB	2.67	0.41
20:A:816:CLA:H12	20:A:816:CLA:H43	1.90	0.41
5:A:334:HIS:CD2	20:A:820:CLA:C1B	3.03	0.41
20:A:821:CLA:HED2	20:A:821:CLA:CBA	2.50	0.41
21:A:854:LMU:H6D	21:A:854:LMU:H1'	1.44	0.41
6:B:152:ALA:O	6:B:153:GLY:O	2.37	0.41
6:B:175:LEU:HD11	20:B:817:CLA:HMA1	2.03	0.41
6:B:262:HIS:HA	6:B:263:PRO:HD2	1.93	0.41
6:B:332:PHE:CE1	6:B:408:LEU:HD21	2.55	0.41
6:B:347:LEU:O	6:B:351:HIS:HB2	2.20	0.41
6:B:557:PHE:HE2	7:C:66:ARG:NE	2.16	0.41
6:B:70:TRP:CD1	6:B:70:TRP:N	2.88	0.41
20:B:836:CLA:H161	20:B:836:CLA:H203	1.91	0.41
6:B:188:LEU:HD21	22:B:843:BCR:H281	2.03	0.41
22:B:846:BCR:H353	20:B:851:CLA:H122	2.02	0.41
20:B:851:CLA:H161	20:B:851:CLA:H141	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:43:SER:O	9:E:46:PHE:HB2	2.20	0.41
10:F:147:GLY:O	10:F:149:LEU:O	2.38	0.41
10:F:80:TRP:HZ3	20:F:205:CLA:HMC3	1.82	0.41
20:G:102:CLA:C1A	20:G:102:CLA:O1D	2.64	0.41
11:G:28:ARG:HG3	11:G:29:GLU:CB	2.50	0.41
11:G:83:TYR:CD1	11:G:83:TYR:O	2.72	0.41
21:H:106:LMU:H91	21:H:106:LMU:H121	1.84	0.41
12:H:77:LEU:HD23	12:H:78:PRO:HD2	2.02	0.41
13:I:10:PRO:O	13:I:11:LEU:C	2.58	0.41
15:K:46:GLY:O	15:K:47:ILE:HB	2.20	0.41
16:L:10:VAL:HG13	16:L:12:GLN:HE22	1.85	0.41
16:L:33:ILE:O	16:L:35:TRP:N	2.53	0.41
2:2:54:TRP:NE1	2:2:109:ARG:HD2	2.32	0.41
2:2:152:SER:C	2:2:154:GLN:H	2.24	0.41
2:2:57:LEU:C	2:2:57:LEU:HD23	2.40	0.41
20:3:313:CLA:HAA2	20:3:313:CLA:CBD	2.49	0.41
4:4:142:ASN:O	4:4:143:PHE:CB	2.67	0.41
4:4:35:GLU:HB3	4:4:36:ASN:CB	2.24	0.41
4:4:56:ALA:O	4:4:57:GLY:C	2.59	0.41
5:A:97:TYR:HA	5:A:153:TRP:HZ2	1.85	0.41
20:A:806:CLA:HBA2	20:A:806:CLA:H12	1.78	0.41
5:A:182:GLY:C	20:A:811:CLA:HAC1	2.40	0.41
5:A:224:HIS:CE1	20:A:815:CLA:CHD	2.99	0.41
5:A:376:MET:HE3	20:A:827:CLA:OBD	2.20	0.41
21:A:849:LMU:H21	21:A:849:LMU:H1'	1.59	0.41
5:A:88:ILE:O	5:A:92:TRP:N	2.44	0.41
5:A:87:SER:HA	5:A:90:PHE:HB2	2.02	0.41
5:A:693:LEU:HD13	6:B:665:ILE:HD13	2.02	0.41
6:B:674:LEU:HA	6:B:677:THR:HG23	2.03	0.41
6:B:68:VAL:O	6:B:69:ALA:CB	2.68	0.41
6:B:75:GLU:HB2	6:B:132:ASN:CB	2.42	0.41
20:B:804:CLA:HMC3	20:B:806:CLA:OBD	2.20	0.41
23:B:841:PQN:H161	23:B:841:PQN:H141	1.41	0.41
20:B:826:CLA:C19	22:B:844:BCR:H14C	2.51	0.41
7:C:6:LYS:O	7:C:63:LEU:CD2	2.68	0.41
7:C:74:THR:HB	7:C:80:ALA:HB2	1.97	0.41
8:D:100:PHE:O	8:D:113:HIS:HB2	2.21	0.41
11:G:17:PHE:N	11:G:17:PHE:CD2	2.87	0.41
13:I:11:LEU:O	13:I:11:LEU:HD13	2.21	0.41
16:L:64:LEU:CA	16:L:67:PRO:HG2	2.46	0.41
17:N:72:LYS:HB3	17:N:74:LYS:HB2	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:219:LMU:C2'	21:1:219:LMU:O6B	2.68	0.41
2:2:57:LEU:O	2:2:60:ALA:N	2.48	0.41
2:2:91:THR:N	2:2:94:LEU:HB2	2.35	0.41
3:3:158:TYR:C	3:3:160:GLY:N	2.70	0.41
20:3:318:CLA:H122	20:3:318:CLA:C17	2.31	0.41
4:4:115:VAL:O	4:4:116:ASN:C	2.57	0.41
4:4:160:MET:HA	4:4:163:PHE:CB	2.44	0.41
4:4:36:ASN:O	4:4:39:TRP:CA	2.68	0.41
5:A:126:ILE:H	5:A:126:ILE:HG13	1.58	0.41
5:A:75:SER:HB3	5:A:354:TRP:HZ2	1.83	0.41
5:A:490:GLN:C	5:A:490:GLN:HE21	2.24	0.41
5:A:599:PHE:CD1	5:A:600:LEU:HD23	2.36	0.41
5:A:690:LEU:O	5:A:694:PHE:N	2.42	0.41
5:A:81:ALA:CA	20:A:804:CLA:HMA1	2.44	0.41
20:3:302:CLA:HBC3	20:A:814:CLA:C1D	2.50	0.41
20:A:824:CLA:CED	20:A:824:CLA:HAA1	2.50	0.41
20:A:824:CLA:H11	20:A:836:CLA:CAD	2.51	0.41
20:A:841:CLA:H152	22:B:852:BCR:C35	2.47	0.41
20:A:850:CLA:HHD	20:A:850:CLA:CBC	2.43	0.41
5:A:684:PHE:HB2	20:A:851:CLA:HAA1	2.02	0.41
6:B:120:VAL:O	6:B:123:TRP:HD1	2.02	0.41
6:B:190:TRP:C	6:B:192:GLY:N	2.73	0.41
6:B:196:HIS:CE1	20:B:813:CLA:C1D	3.04	0.41
6:B:180:SER:OG	6:B:285:LEU:HA	2.20	0.41
6:B:293:THR:HG21	20:B:810:CLA:HMA3	2.02	0.41
6:B:362:ALA:HA	6:B:365:PHE:H	1.84	0.41
6:B:393:PHE:CE2	6:B:398:TYR:HD2	2.38	0.41
6:B:690:LEU:HD21	16:L:129:GLN:HA	2.01	0.41
20:B:828:CLA:H3A	20:B:828:CLA:HBA2	1.47	0.41
6:B:486:LEU:CD1	20:B:833:CLA:CMD	2.99	0.41
10:F:113:LYS:HA	10:F:114:PRO:HD3	1.63	0.41
10:F:151:ASP:OD2	10:F:154:PHE:CG	2.73	0.41
11:G:60:SER:C	11:G:63:PRO:HD2	2.41	0.41
16:L:33:ILE:HD12	16:L:36:TYR:HD1	1.85	0.41
17:N:53:ALA:C	17:N:54:LYS:HD2	2.41	0.41
20:1:215:CLA:H111	20:1:215:CLA:H143	1.56	0.41
2:2:202:ALA:O	2:2:203:THR:OG1	2.29	0.41
20:2:307:CLA:HED3	20:2:307:CLA:CAD	2.27	0.41
20:2:312:CLA:CBC	20:2:312:CLA:CMC	2.93	0.41
3:3:197:TYR:CE1	20:3:304:CLA:CAB	3.03	0.41
3:3:197:TYR:OH	20:3:304:CLA:C1C	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:87:GLU:CA	22:3:314:BCR:H382	2.50	0.41
4:4:30:LEU:O	4:4:30:LEU:CG	2.66	0.41
4:4:76:TYR:HD1	4:4:76:TYR:O	1.97	0.41
5:A:158:ILE:HA	5:A:243:PRO:O	2.20	0.41
5:A:35:ALA:O	5:A:36:LYS:HB2	2.21	0.41
5:A:509:ALA:O	5:A:510:SER:CB	2.68	0.41
20:A:805:CLA:H41	22:A:844:BCR:C31	2.51	0.41
20:A:839:CLA:H122	20:A:839:CLA:H72	1.88	0.41
6:B:174:ARG:HH12	20:B:822:CLA:HMD2	1.85	0.41
6:B:586:THR:O	6:B:590:VAL:HG12	2.21	0.41
20:B:815:CLA:H2	20:B:824:CLA:HBB1	2.02	0.41
20:B:823:CLA:H3A	20:B:823:CLA:HBA2	1.39	0.41
8:D:77:LEU:HD23	8:D:77:LEU:HA	1.66	0.41
10:F:23:LYS:O	10:F:26:GLN:CB	2.48	0.41
11:G:20:ARG:NH2	11:G:61:ASN:HA	2.36	0.41
12:H:37:SER:C	12:H:39:PHE:H	2.23	0.41
21:K:109:LMU:H122	21:K:109:LMU:H91	1.27	0.41
15:K:51:ASP:N	15:K:52:PRO:HD2	2.36	0.41
16:L:123:ARG:C	16:L:124:LYS:HD3	2.41	0.41
20:L:207:CLA:CAA	20:L:207:CLA:HED2	2.47	0.41
16:L:68:PHE:HD1	16:L:68:PHE:H	1.68	0.41
21:N:101:LMU:C4	21:N:101:LMU:C6'	2.92	0.41
4:4:160:MET:CA	4:4:163:PHE:HB2	2.47	0.41
20:4:318:CLA:H52	20:4:318:CLA:H11	1.86	0.41
4:4:80:LYS:O	4:4:81:GLU:HG2	2.21	0.41
5:A:76:ARG:NE	5:A:192:LYS:HA	2.35	0.41
5:A:205:HIS:CG	20:A:813:CLA:HMC2	2.55	0.41
5:A:445:HIS:CD2	20:A:829:CLA:HMB1	2.56	0.41
5:A:571:ASP:HB3	7:C:53:ARG:HH12	1.84	0.41
20:A:805:CLA:H141	20:A:805:CLA:H161	1.63	0.41
20:A:833:CLA:HBC1	22:A:846:BCR:C3	2.39	0.41
22:A:845:BCR:C8	22:A:845:BCR:C32	2.98	0.41
6:B:192:GLY:HA2	20:B:813:CLA:HMC3	2.03	0.41
6:B:448:THR:OG1	6:B:451:LYS:HB2	2.20	0.41
6:B:522:ALA:O	6:B:589:TRP:HE3	2.03	0.41
6:B:594:TRP:CD1	6:B:595:HIS:HB2	2.53	0.41
6:B:710:LEU:HA	6:B:710:LEU:HD22	1.94	0.41
6:B:603:ARG:HB2	6:B:732:LYS:HD3	2.03	0.41
21:B:801:LMU:H91	21:B:801:LMU:H62	1.94	0.41
20:B:820:CLA:HBA2	20:B:820:CLA:H3A	1.43	0.41
7:C:7:ILE:HG12	7:C:8:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:53:PRO:HB2	8:D:54:LYS:H	1.63	0.41
9:E:36:VAL:HG11	9:E:87:VAL:HG11	2.03	0.41
10:F:22:LEU:HA	10:F:25:LEU:HD13	2.03	0.41
21:K:106:LMU:O2B	21:K:106:LMU:H5B	2.21	0.41
16:L:15:ASN:N	16:L:24:GLU:OE1	2.53	0.41
16:L:95:LEU:HD13	22:L:210:BCR:H313	1.98	0.41
17:N:45:ASN:CG	17:N:57:LYS:HZ1	2.17	0.41
19:P:1:GLC:C1	19:P:1:GLC:HO6	2.33	0.41
19:Z:1:GLC:HO2	19:Z:2:FRU:C5	2.26	0.41
2:2:191:ASN:ND2	2:2:196:HIS:ND1	2.69	0.41
3:3:189:LEU:C	3:3:191:MET:N	2.74	0.41
20:3:311:CLA:H143	20:3:311:CLA:H111	1.60	0.41
3:3:49:ILE:CA	3:3:51:PRO:HD2	2.51	0.41
4:4:108:ASP:O	4:4:111:ASN:O	2.39	0.41
4:4:127:PRO:HB2	4:4:128:ALA:H	1.52	0.41
20:4:318:CLA:H41	20:4:318:CLA:H61	1.64	0.41
4:4:44:GLU:HB3	4:4:45:LEU:H	1.73	0.41
5:A:344:LYS:HE2	5:A:344:LYS:HB3	1.89	0.41
5:A:554:LEU:CD2	20:B:851:CLA:O2D	2.69	0.41
5:A:57:LEU:O	5:A:61:ALA:HB2	2.21	0.41
20:A:811:CLA:H72	20:A:811:CLA:H111	1.49	0.41
6:B:309:ILE:CD1	6:B:312:GLY:HA3	2.51	0.41
6:B:525:LEU:O	6:B:525:LEU:CD2	2.55	0.41
6:B:657:TRP:HB3	6:B:658:ALA:H	1.58	0.41
6:B:658:ALA:O	6:B:661:PHE:CD2	2.69	0.41
20:B:807:CLA:H193	20:B:825:CLA:H192	2.02	0.41
20:B:819:CLA:HBC3	22:B:842:BCR:HC7	2.01	0.41
20:B:824:CLA:H8	22:B:845:BCR:C12	2.45	0.41
7:C:5:VAL:HG23	7:C:65:VAL:HG21	1.23	0.41
7:C:69:LEU:O	7:C:71:HIS:N	2.53	0.41
8:D:111:TYR:CD2	8:D:114:PRO:CG	3.04	0.41
7:C:62:PHE:CZ	9:E:42:GLU:CB	3.04	0.41
16:L:90:GLY:O	16:L:94:ILE:N	2.49	0.41
17:N:35:VAL:HG12	17:N:35:VAL:O	2.20	0.41
17:N:65:LEU:O	17:N:67:LEU:CA	2.69	0.41
17:N:69:CYS:O	17:N:72:LYS:HE3	2.20	0.41
17:N:72:LYS:CD	17:N:74:LYS:HG3	2.44	0.41
21:3:321:LMU:H3B	19:S:2:FRU:O4	2.21	0.41
19:V:2:FRU:O1	19:V:2:FRU:O3	2.29	0.41
20:1:215:CLA:CAA	20:1:215:CLA:O2D	2.65	0.41
3:3:120:LEU:O	3:3:123:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:47:GLY:O	3:3:48:PHE:CD2	2.74	0.41
5:A:124:TRP:HA	5:A:124:TRP:HE3	1.84	0.41
5:A:177:LEU:C	5:A:179:LEU:N	2.74	0.41
5:A:277:TYR:HD2	5:A:279:ASP:H	1.68	0.41
5:A:432:LEU:O	5:A:434:ARG:N	2.53	0.41
5:A:436:LEU:O	5:A:438:HIS:O	2.37	0.41
5:A:44:ILE:HG13	5:A:44:ILE:H	1.57	0.41
5:A:76:ARG:HE	5:A:192:LYS:HA	1.86	0.41
20:A:803:CLA:HBB2	20:A:804:CLA:C1C	2.51	0.41
20:A:828:CLA:HBD	20:A:828:CLA:HAA1	2.02	0.41
22:A:844:BCR:H11C	22:A:844:BCR:H341	1.69	0.41
22:A:847:BCR:C39	22:A:847:BCR:C23	2.74	0.41
6:B:122:GLN:HG3	6:B:361:ILE:CG1	2.44	0.41
6:B:303:TYR:H	6:B:306:GLU:HB2	1.84	0.41
6:B:307:ALA:O	6:B:308:HIS:O	2.38	0.41
6:B:606:VAL:O	6:B:608:GLN:N	2.53	0.41
6:B:696:LYS:NZ	8:D:39:LYS:HE3	2.35	0.41
20:B:811:CLA:CMC	20:B:811:CLA:CBC	2.91	0.41
20:B:820:CLA:CBB	20:B:820:CLA:H51	2.50	0.41
20:B:819:CLA:CBA	20:B:820:CLA:O1A	2.68	0.41
6:B:431:PHE:HD2	20:B:830:CLA:HMA3	1.85	0.41
20:B:832:CLA:HMD2	20:B:833:CLA:CMC	2.51	0.41
20:B:834:CLA:H3A	20:B:834:CLA:HBA2	1.67	0.41
20:B:838:CLA:H191	13:I:21:MET:HE1	2.03	0.41
23:B:841:PQN:C17	22:B:846:BCR:C33	2.93	0.41
20:B:806:CLA:C7	25:B:848:LMG:H381	2.49	0.41
20:B:830:CLA:C7	22:F:203:BCR:H402	2.50	0.41
10:F:17:ARG:O	10:F:21:ALA:HB3	2.21	0.41
11:G:44:PHE:HA	11:G:46:ALA:HB2	2.03	0.41
14:J:19:PHE:C	14:J:19:PHE:CD2	2.94	0.41
16:L:6:PRO:HB2	16:L:9:GLN:O	2.20	0.41
21:R:102:LMU:H92	21:R:102:LMU:H62	1.26	0.41
21:R:109:LMU:O2'	21:R:109:LMU:C2	2.68	0.41
1:1:142:GLU:OE1	20:1:201:CLA:HMD3	2.20	0.41
20:1:202:CLA:H8	20:1:202:CLA:H41	0.50	0.41
1:1:36:LEU:O	1:1:40:LYS:N	2.54	0.41
3:3:158:TYR:CB	3:3:159:PRO:CD	2.82	0.41
5:A:227:LEU:HG	5:A:296:LEU:HB2	2.03	0.41
5:A:430:ASP:O	5:A:432:LEU:N	2.54	0.41
5:A:523:VAL:HG13	5:A:524:GLY:N	2.36	0.41
5:A:703:LEU:HA	5:A:703:LEU:HD22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:825:CLA:H62	20:A:825:CLA:H2	1.90	0.41
5:A:449:VAL:HG21	20:A:836:CLA:CHC	2.50	0.41
6:B:416:GLU:O	6:B:420:SER:OG	2.39	0.41
6:B:577:TYR:C	6:B:577:TYR:CD2	2.93	0.41
6:B:605:ASN:HD22	6:B:605:ASN:C	2.24	0.41
20:B:830:CLA:HBA1	20:B:830:CLA:HBD	2.01	0.41
20:B:832:CLA:ND	20:B:833:CLA:HBB2	2.36	0.41
8:D:70:GLU:OE1	8:D:71:GLY:O	2.39	0.41
8:D:86:LEU:HA	8:D:90:LEU:HB2	2.02	0.41
10:F:17:ARG:CA	10:F:17:ARG:NE	2.83	0.41
10:F:26:GLN:C	10:F:28:SER:H	2.24	0.41
11:G:23:PHE:CE2	11:G:24:PHE:HB2	2.56	0.41
6:B:694:ARG:HD2	13:I:28:VAL:CG1	2.51	0.41
20:J:103:CLA:CHA	20:J:103:CLA:HED2	2.45	0.41
16:L:14:LEU:HD21	16:L:21:GLY:O	2.20	0.41
17:N:57:LYS:CG	17:N:58:VAL:N	2.27	0.41
21:R:101:LMU:H1'	21:R:101:LMU:H4'	1.86	0.41
21:R:109:LMU:C5B	21:R:109:LMU:H6D	2.50	0.41
1:1:121:LYS:HB3	1:1:124:PRO:HG3	2.03	0.41
20:1:206:CLA:H62	20:1:206:CLA:H41	1.76	0.41
21:1:218:LMU:O3'	21:1:218:LMU:C1B	2.65	0.41
2:2:52:SER:C	2:2:54:TRP:N	2.75	0.41
3:3:84:ILE:N	3:3:85:PRO:HD3	2.36	0.41
3:3:92:TRP:O	3:3:95:THR:CG2	2.68	0.41
20:4:316:CLA:CHD	20:4:316:CLA:CBC	2.83	0.41
5:A:316:MET:HA	5:A:317:TYR:HA	1.69	0.41
5:A:370:ILE:CD1	20:A:824:CLA:CGD	2.99	0.41
5:A:554:LEU:HD21	20:B:851:CLA:O2D	2.20	0.41
20:A:818:CLA:H8	20:A:818:CLA:H152	2.02	0.41
5:A:376:MET:CE	20:A:827:CLA:OBD	2.69	0.41
20:A:831:CLA:HBA1	20:A:831:CLA:H3A	1.84	0.41
5:A:614:PHE:HE1	20:A:850:CLA:H62	1.86	0.41
6:B:301:ILE:O	6:B:301:ILE:HG23	2.21	0.41
6:B:334:LEU:HD22	20:B:805:CLA:CHD	2.51	0.41
6:B:696:LYS:HE2	6:B:696:LYS:HB2	1.83	0.41
20:B:823:CLA:H42	20:B:836:CLA:CBA	2.51	0.41
22:B:844:BCR:C33	22:B:844:BCR:C8	2.86	0.41
22:B:844:BCR:H351	22:B:844:BCR:H15C	1.78	0.41
21:B:847:LMU:H62	21:B:847:LMU:H91	1.67	0.41
8:D:96:ILE:O	8:D:97:LYS:CB	2.69	0.41
20:B:830:CLA:HAA1	22:F:202:BCR:H16C	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:141:ARG:CD	10:F:40:LEU:H	2.34	0.41
11:G:58:LEU:HB2	11:G:59:LYS:H	1.35	0.41
21:H:104:LMU:H81	21:H:104:LMU:C4	2.40	0.41
16:L:112:PRO:O	16:L:113:SER:CB	2.68	0.41
20:L:207:CLA:HBC2	20:L:207:CLA:CHD	2.51	0.41
17:N:45:ASN:ND2	17:N:54:LYS:CD	2.73	0.41
17:N:9:LYS:HB3	17:N:9:LYS:HE2	1.86	0.41
2:2:109:ARG:O	2:2:113:ILE:HG23	2.21	0.40
2:2:182:ILE:HG22	2:2:205:PHE:HB2	2.03	0.40
2:2:42:ARG:CG	2:2:45:VAL:HB	2.47	0.40
4:4:127:PRO:O	4:4:129:GLY:N	2.37	0.40
21:4:301:LMU:H6D	21:4:301:LMU:H1'	1.87	0.40
5:A:112:ASP:N	5:A:113:PRO:HD3	2.36	0.40
5:A:156:SER:HB2	5:A:159:THR:H	1.86	0.40
5:A:226:SER:O	5:A:230:ASN:OD1	2.39	0.40
5:A:392:GLN:O	5:A:392:GLN:CD	2.60	0.40
5:A:483:GLN:HA	5:A:483:GLN:OE1	2.21	0.40
5:A:541:VAL:HA	5:A:544:ILE:HG22	2.03	0.40
5:A:691:MET:HE3	23:A:842:PQN:H2M1	2.01	0.40
5:A:744:ALA:HB2	22:A:847:BCR:C30	2.36	0.40
20:A:805:CLA:HBA1	20:A:805:CLA:H3A	1.66	0.40
20:A:806:CLA:C2	20:A:806:CLA:H71	2.51	0.40
5:A:369:THR:HG22	20:A:827:CLA:HMC1	2.02	0.40
6:B:197:VAL:HG22	6:B:207:VAL:HG11	2.03	0.40
6:B:308:HIS:ND1	6:B:309:ILE:N	2.68	0.40
6:B:53:GLN:O	6:B:54:LEU:HB2	2.21	0.40
5:A:588:GLY:N	6:B:668:ARG:CZ	2.84	0.40
6:B:693:TRP:HE1	20:B:838:CLA:CHD	2.33	0.40
6:B:51:PHE:CD1	20:B:811:CLA:HED1	2.56	0.40
20:B:817:CLA:HMD3	20:B:819:CLA:C3B	2.51	0.40
6:B:593:TYR:CD1	20:B:835:CLA:HMC2	2.56	0.40
7:C:73:THR:HB	7:C:74:THR:H	1.17	0.40
10:F:23:LYS:HD2	10:F:23:LYS:HA	1.60	0.40
10:F:46:MET:C	10:F:50:LYS:HB2	2.41	0.40
10:F:68:LEU:HA	10:F:69:PRO:HD3	1.88	0.40
12:H:55:LYS:O	12:H:56:PHE:HB2	2.21	0.40
13:I:1:MET:O	13:I:2:ILE:CG2	2.59	0.40
13:I:20:ALA:O	13:I:24:LEU:N	2.54	0.40
22:J:102:BCR:C8	22:J:102:BCR:H311	2.51	0.40
16:L:104:ILE:HD12	16:L:104:ILE:C	2.42	0.40
20:L:202:CLA:H72	20:L:203:CLA:HBA1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:109:GLU:OE2	20:1:209:CLA:C1B	2.69	0.40
2:2:70:LYS:HE3	2:2:70:LYS:HB3	1.70	0.40
21:2:317:LMU:H6'1	21:3:321:LMU:H111	2.02	0.40
3:3:50:GLU:HG3	3:3:51:PRO:N	2.36	0.40
4:4:99:HIS:C	4:4:103:ILE:HD11	2.41	0.40
4:4:32:GLU:CD	4:4:32:GLU:H	2.23	0.40
5:A:225:VAL:C	5:A:228:PRO:HD2	2.42	0.40
5:A:414:ALA:O	5:A:417:PHE:HB3	2.21	0.40
5:A:583:GLY:O	5:A:589:THR:HB	2.21	0.40
5:A:639:ALA:O	5:A:640:GLY:C	2.59	0.40
5:A:753:ARG:HH11	5:A:753:ARG:HD3	1.73	0.40
5:A:281:LEU:CD2	20:A:816:CLA:CMA	3.00	0.40
5:A:364:MET:HG3	20:A:823:CLA:HMB2	2.01	0.40
5:A:382:TYR:CD2	20:A:827:CLA:HED3	2.56	0.40
5:A:445:HIS:CE1	20:A:829:CLA:CMB	3.04	0.40
20:A:831:CLA:C4	16:L:64:LEU:CD2	2.94	0.40
20:A:838:CLA:HBA2	20:A:838:CLA:H3A	1.66	0.40
6:B:256:THR:HG23	6:B:272:ASP:OD1	2.22	0.40
6:B:260:GLY:H	6:B:269:TRP:HE1	1.69	0.40
6:B:285:LEU:HD12	22:B:842:BCR:C17	2.51	0.40
6:B:288:GLY:O	6:B:289:LEU:HD12	2.21	0.40
6:B:691:ILE:O	6:B:691:ILE:HG22	2.21	0.40
20:B:803:CLA:C4A	20:B:803:CLA:HBA2	2.50	0.40
6:B:560:ASP:CG	7:C:52:LYS:HZ3	2.24	0.40
8:D:48:ILE:CA	8:D:100:PHE:HB3	2.51	0.40
8:D:109:VAL:O	8:D:110:GLN:HG3	2.21	0.40
10:F:142:ARG:NH1	10:F:142:ARG:HA	2.35	0.40
10:F:77:GLN:O	10:F:78:ARG:HG2	2.21	0.40
12:H:19:GLY:O	12:H:20:GLN:CB	2.69	0.40
16:L:125:LYS:C	16:L:127:PRO:CD	2.88	0.40
17:N:58:VAL:O	17:N:59:PRO:C	2.59	0.40
20:1:202:CLA:CBB	20:1:206:CLA:HHC	2.51	0.40
21:1:219:LMU:H1B	21:1:219:LMU:H5'	1.31	0.40
2:2:124:ILE:O	2:2:125:PHE:CG	2.74	0.40
3:3:192:LEU:C	3:3:194:ILE:H	2.23	0.40
4:4:187:ASP:HA	4:4:188:PRO:HD3	1.81	0.40
4:4:192:THR:CG2	4:4:193:ILE:N	2.84	0.40
5:A:46:LYS:HG2	5:A:46:LYS:H	1.80	0.40
5:A:567:ARG:HH21	5:A:567:ARG:CB	2.34	0.40
20:A:806:CLA:HAA2	20:A:806:CLA:CBD	2.52	0.40
20:A:808:CLA:H112	20:A:826:CLA:H91	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:451:ILE:HD13	20:A:830:CLA:CED	2.42	0.40
20:A:851:CLA:CED	20:A:851:CLA:C3D	2.98	0.40
6:B:22:TRP:CZ2	20:B:838:CLA:HMB1	2.57	0.40
6:B:353:TYR:HB2	6:B:594:TRP:CH2	2.56	0.40
20:A:837:CLA:NC	20:B:803:CLA:HBC2	2.36	0.40
6:B:299:HIS:NE2	20:B:819:CLA:CED	2.85	0.40
20:B:839:CLA:HBA2	20:B:839:CLA:H3A	1.76	0.40
7:C:51:CYS:HB2	7:C:53:ARG:H	1.85	0.40
7:C:3:HIS:ND1	7:C:69:LEU:HD12	2.37	0.40
10:F:116:GLN:HE21	10:F:116:GLN:HB2	1.61	0.40
10:F:29:LEU:HB3	10:F:30:LYS:H	1.72	0.40
10:F:51:LYS:C	10:F:53:PHE:N	2.74	0.40
10:F:6:THR:HB	10:F:7:PRO:HD2	2.02	0.40
11:G:71:VAL:O	11:G:76:SER:OG	2.39	0.40
12:H:62:GLY:O	13:I:15:LEU:HD22	2.20	0.40
15:K:5:SER:C	15:K:7:THR:N	2.75	0.40
16:L:77:THR:HG21	16:L:82:ALA:CB	2.47	0.40
16:L:9:GLN:HG3	16:L:10:VAL:N	2.36	0.40
19:Z:1:GLC:C2	19:Z:2:FRU:C5	2.97	0.40
2:2:95:PHE:O	2:2:99:LEU:N	2.44	0.40
3:3:56:TYR:CD1	3:3:185:LYS:NZ	2.84	0.40
4:4:147:LEU:HD22	4:4:148:GLU:HG2	2.02	0.40
4:4:166:PHE:O	4:4:169:GLN:CB	2.55	0.40
4:4:184:HIS:ND1	4:4:184:HIS:C	2.74	0.40
5:A:150:PHE:N	5:A:153:TRP:HE3	2.19	0.40
5:A:173:VAL:HG23	5:A:174:PHE:H	1.86	0.40
5:A:242:ILE:CG1	5:A:243:PRO:HD3	2.44	0.40
5:A:413:HIS:HA	5:A:416:ILE:HD12	2.03	0.40
5:A:416:ILE:O	5:A:420:ARG:O	2.38	0.40
5:A:606:TYR:HH	20:A:850:CLA:HED3	1.87	0.40
5:A:751:LEU:H	5:A:751:LEU:HG	1.69	0.40
22:A:847:BCR:H371	22:A:847:BCR:H24C	1.79	0.40
6:B:137:THR:HA	6:B:140:ILE:CD1	2.52	0.40
6:B:285:LEU:O	6:B:288:GLY:O	2.39	0.40
6:B:122:GLN:HB2	6:B:358:TYR:HB3	2.02	0.40
6:B:387:PHE:O	6:B:391:PRO:CD	2.67	0.40
6:B:500:ALA:HB3	6:B:507:SER:O	2.21	0.40
6:B:52:GLY:O	6:B:56:ILE:HG12	2.21	0.40
20:B:808:CLA:H93	20:B:808:CLA:H61	1.85	0.40
7:C:11:CYS:C	7:C:13:GLY:N	2.74	0.40
10:F:96:TRP:HE3	10:F:134:PHE:N	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:28:ARG:CD	11:G:33:LYS:HE2	2.48	0.40
11:G:58:LEU:HA	11:G:61:ASN:OD1	2.21	0.40
22:I:101:BCR:H321	22:I:101:BCR:HC7	1.92	0.40
13:I:12:VAL:HG23	13:I:13:GLY:H	1.87	0.40
16:L:21:GLY:C	16:L:23:LEU:H	2.24	0.40
16:L:33:ILE:HG13	16:L:37:LEU:CD2	2.52	0.40
19:U:2:FRU:O1	19:U:2:FRU:O3	2.29	0.40
21:2:319:LMU:C3B	21:2:319:LMU:H4'	2.47	0.40
20:1:206:CLA:CAA	21:4:301:LMU:O3'	2.62	0.40
20:4:304:CLA:HMB1	20:4:304:CLA:CBB	2.50	0.40
5:A:126:ILE:O	5:A:126:ILE:HD12	2.22	0.40
5:A:213:LEU:O	22:A:844:BCR:C17	2.70	0.40
5:A:396:PHE:CE2	5:A:616:PHE:CD1	3.09	0.40
5:A:40:PHE:O	5:A:40:PHE:CG	2.74	0.40
5:A:701:GLN:NE2	5:A:724:ALA:H	2.20	0.40
5:A:652:TRP:CE2	20:A:850:CLA:H142	2.56	0.40
6:B:174:ARG:O	6:B:175:LEU:CB	2.67	0.40
6:B:188:LEU:O	6:B:190:TRP:N	2.55	0.40
6:B:193:HIS:O	6:B:194:LEU:C	2.58	0.40
6:B:203:ARG:HB3	6:B:270:LEU:CD1	2.51	0.40
6:B:222:LEU:O	6:B:223:GLY:C	2.60	0.40
6:B:227:THR:O	6:B:229:GLN:N	2.54	0.40
6:B:300:SER:O	6:B:302:LYS:O	2.40	0.40
6:B:435:GLY:HA3	20:B:831:CLA:HBB1	2.02	0.40
6:B:471:THR:O	6:B:472:TYR:C	2.60	0.40
22:B:842:BCR:H341	22:B:842:BCR:H11C	1.73	0.40
23:A:842:PQN:H152	22:F:202:BCR:H322	2.02	0.40
12:H:53:LEU:O	12:H:54:LEU:HB3	2.22	0.40
20:B:804:CLA:C4C	22:I:103:BCR:H401	2.51	0.40
15:K:11:MET:SD	15:K:15:THR:OG1	2.79	0.40
20:L:208:CLA:HAC1	22:L:210:BCR:H322	2.03	0.40

All (69) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:314:BCR:C28	21:B:847:LMU:C5[2_556]	0.48	1.72
22:3:314:BCR:C40	21:B:847:LMU:C8[2_556]	0.57	1.63
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	0.69	1.51
3:3:181:LEU:CG	6:B:490:ARG:NH2[1_556]	0.72	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.72	1.48
22:3:314:BCR:C38	21:B:847:LMU:C12[2_556]	0.82	1.38
4:4:130:GLU:C	16:L:159:TYR:OH[1_655]	0.88	1.32
3:3:182:LYS:NZ	6:B:491:ASN:ND2[1_556]	0.89	1.31
11:G:31:MET:CE	17:N:85:TRP:CD1[2_546]	1.03	1.17
3:3:181:LEU:CD1	6:B:490:ARG:NH2[1_556]	1.08	1.12
22:3:314:BCR:C29	21:B:847:LMU:C7[2_556]	1.12	1.08
22:3:314:BCR:C26	21:B:847:LMU:C11[2_556]	1.15	1.05
22:3:314:BCR:C29	21:B:847:LMU:C6[2_556]	1.21	0.99
22:3:314:BCR:C28	21:B:847:LMU:C6[2_556]	1.26	0.94
11:G:31:MET:SD	17:N:85:TRP:CD2[2_546]	1.27	0.93
3:3:182:LYS:CE	6:B:491:ASN:ND2[1_556]	1.30	0.90
22:3:314:BCR:C25	21:B:847:LMU:C10[2_556]	1.30	0.90
22:3:314:BCR:C38	21:B:847:LMU:C11[2_556]	1.37	0.83
3:3:181:LEU:CD2	6:B:490:ARG:NH1[1_556]	1.39	0.81
22:3:314:BCR:C30	21:B:847:LMU:C6[2_556]	1.40	0.80
22:3:314:BCR:C30	21:B:847:LMU:C7[2_556]	1.42	0.78
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.43	0.77
22:3:314:BCR:C25	21:B:847:LMU:C9[2_556]	1.50	0.70
22:3:314:BCR:C25	21:B:847:LMU:C6[2_556]	1.52	0.68
22:3:314:BCR:C40	21:B:847:LMU:C9[2_556]	1.53	0.67
22:3:314:BCR:C24	21:B:847:LMU:C10[2_556]	1.53	0.67
21:4:320:LMU:C6B	21:R:109:LMU:C11[1_654]	1.58	0.62
3:3:181:LEU:CG	6:B:490:ARG:CZ[1_556]	1.58	0.62
22:3:314:BCR:C30	21:B:847:LMU:C8[2_556]	1.59	0.61
22:3:314:BCR:C29	21:B:847:LMU:C5[2_556]	1.62	0.58
22:3:314:BCR:C30	21:B:847:LMU:C9[2_556]	1.65	0.55
11:G:31:MET:SD	17:N:85:TRP:CG[2_546]	1.66	0.54
22:3:314:BCR:C27	21:B:847:LMU:C6[2_556]	1.68	0.52
4:4:130:GLU:O	16:L:159:TYR:CZ[1_655]	1.68	0.52
22:3:314:BCR:C26	21:B:847:LMU:C10[2_556]	1.69	0.51
22:3:314:BCR:C26	21:B:847:LMU:C6[2_556]	1.69	0.51
3:3:181:LEU:CD2	6:B:490:ARG:CZ[1_556]	1.70	0.50
11:G:31:MET:CE	17:N:85:TRP:CG[2_546]	1.71	0.49
11:G:34:GLN:NE2	21:2:320:LMU:C7[2_646]	1.71	0.49
22:3:314:BCR:C24	21:B:847:LMU:C9[2_556]	1.72	0.48
3:3:181:LEU:CD2	6:B:490:ARG:NH2[1_556]	1.73	0.47
20:1:207:CLA:O1A	20:K:101:CLA:O2A[1_654]	1.74	0.46
22:3:314:BCR:C40	21:B:847:LMU:C7[2_556]	1.78	0.42
22:3:314:BCR:C25	21:B:847:LMU:C11[2_556]	1.81	0.39
6:B:295:PHE:CE1	17:N:85:TRP:CH2[2_546]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:314:BCR:C28	21:B:847:LMU:C4[2_556]	1.85	0.35
22:3:314:BCR:C38	21:B:847:LMU:C10[2_556]	1.86	0.34
11:G:30:ASN:OD1	21:2:320:LMU:C9[2_646]	1.88	0.32
11:G:31:MET:CE	17:N:85:TRP:CD2[2_546]	1.89	0.31
22:3:314:BCR:C26	21:B:847:LMU:C12[2_556]	1.89	0.31
11:G:31:MET:SD	17:N:85:TRP:CE2[2_546]	1.89	0.31
3:3:182:LYS:NZ	6:B:491:ASN:CG[1_556]	1.91	0.29
6:B:3:LEU:CD2	10:F:34:ASP:OD2[2_546]	1.93	0.27
4:4:130:GLU:CA	16:L:159:TYR:OH[1_655]	1.94	0.26
4:4:126:LEU:CD2	16:L:74:LEU:O[1_655]	1.95	0.25
22:3:314:BCR:C27	21:B:847:LMU:C5[2_556]	1.96	0.24
21:4:320:LMU:C6B	21:R:109:LMU:C12[1_654]	1.97	0.23
21:4:320:LMU:C6B	21:R:109:LMU:C10[1_654]	2.02	0.18
11:G:31:MET:SD	17:N:85:TRP:CE3[2_546]	2.05	0.15
4:4:131:VAL:N	16:L:159:TYR:OH[1_655]	2.05	0.15
4:4:133:TYR:OH	16:L:156:PHE:O[1_655]	2.07	0.13
21:4:320:LMU:O3B	21:R:109:LMU:C10[1_654]	2.08	0.12
21:4:320:LMU:O6B	21:R:109:LMU:C12[1_654]	2.08	0.12
6:B:295:PHE:CE1	17:N:85:TRP:CZ3[2_546]	2.10	0.10
3:3:87:GLU:O	21:B:847:LMU:C12[2_556]	2.13	0.07
4:4:126:LEU:O	16:L:78:GLU:N[1_655]	2.14	0.06
3:3:181:LEU:CB	6:B:490:ARG:NH2[1_556]	2.14	0.06
21:2:313:LMU:O2B	20:A:833:CLA:CMB[1_655]	2.16	0.04
3:3:87:GLU:C	21:B:847:LMU:C12[2_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	160/241 (66%)	83 (52%)	47 (29%)	30 (19%)	0 2
2	2	174/269 (65%)	62 (36%)	48 (28%)	64 (37%)	0 0
3	3	154/276 (56%)	77 (50%)	42 (27%)	35 (23%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	164/251 (65%)	56 (34%)	47 (29%)	61 (37%)	0	0
5	A	726/758 (96%)	333 (46%)	198 (27%)	195 (27%)	0	0
6	B	731/734 (100%)	362 (50%)	186 (25%)	183 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	49 (36%)	41 (30%)	46 (34%)	0	0
9	E	63/143 (44%)	28 (44%)	15 (24%)	20 (32%)	0	0
10	F	152/231 (66%)	69 (45%)	41 (27%)	42 (28%)	0	0
11	G	93/167 (56%)	37 (40%)	25 (27%)	31 (33%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	54 (66%)	12 (15%)	16 (20%)	0	2
16	L	159/216 (74%)	65 (41%)	46 (29%)	48 (30%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3091/4108 (75%)	1377 (44%)	833 (27%)	881 (28%)	0	0

All (881) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	90	PRO
1	1	130	PRO
1	1	137	PRO
1	1	161	PHE
1	1	178	ALA
1	1	183	ASP
2	2	37	ASP
2	2	40	SER
2	2	41	LEU
2	2	42	ARG
2	2	45	VAL
2	2	66	GLU
2	2	70	LYS
2	2	74	LEU
2	2	75	ASN

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Mol	Chain	Res	Type
2	2	81	THR
2	2	104	TRP
2	2	120	ASN
2	2	125	PHE
2	2	128	ASN
2	2	129	LYS
2	2	130	LEU
2	2	149	GLY
2	2	154	GLN
2	2	159	LEU
2	2	160	ARG
2	2	188	PRO
2	2	189	ILE
2	2	190	ASP
2	2	197	LEU
2	2	200	PRO
2	2	204	ILE
2	2	207	ALA
2	2	209	THR
2	2	210	PRO
3	3	48	PHE
3	3	49	ILE
3	3	85	PRO
3	3	97	PHE
3	3	107	TRP
3	3	108	ALA
3	3	110	SER
3	3	111	TYR
3	3	113	LEU
3	3	134	LYS
3	3	135	PRO
3	3	142	TYR
3	3	158	TYR
3	3	159	PRO
3	3	164	PHE
3	3	166	PRO
3	3	167	LEU
3	3	172	ASP
3	3	206	VAL
3	3	210	GLN
4	4	32	GLU
4	4	34	PRO

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Mol	Chain	Res	Type
4	4	35	GLU
4	4	38	ARG
4	4	45	LEU
4	4	60	LEU
4	4	66	SER
4	4	69	ILE
4	4	73	PRO
4	4	74	LYS
4	4	82	GLU
4	4	84	PHE
4	4	87	SER
4	4	88	SER
4	4	107	GLN
4	4	115	VAL
4	4	121	PHE
4	4	122	LYS
4	4	125	SER
4	4	126	LEU
4	4	128	ALA
4	4	141	LEU
4	4	143	PHE
4	4	148	GLU
4	4	150	LYS
4	4	171	ASN
4	4	172	VAL
4	4	173	THR
4	4	175	LYS
4	4	178	PHE
4	4	192	THR
4	4	193	ILE
5	A	22	VAL
5	A	23	ASP
5	A	25	ASP
5	A	26	PRO
5	A	27	ILE
5	A	28	LYS
5	A	35	ALA
5	A	36	LYS
5	A	40	PHE
5	A	60	ASP
5	A	67	HIS
5	A	69	SER

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Mol	Chain	Res	Type
5	A	71	LEU
5	A	82	HIS
5	A	83	PHE
5	A	88	ILE
5	A	99	HIS
5	A	104	SER
5	A	155	ALA
5	A	156	SER
5	A	157	GLY
5	A	158	ILE
5	A	159	THR
5	A	160	SER
5	A	175	ALA
5	A	193	LEU
5	A	205	HIS
5	A	221	HIS
5	A	237	VAL
5	A	244	LEU
5	A	247	GLU
5	A	250	LEU
5	A	252	ARG
5	A	258	LEU
5	A	268	PRO
5	A	279	ASP
5	A	280	PHE
5	A	281	LEU
5	A	282	THR
5	A	283	PHE
5	A	286	GLY
5	A	299	ILE
5	A	307	ALA
5	A	310	PHE
5	A	328	LYS
5	A	329	ASP
5	A	333	ALA
5	A	339	THR
5	A	346	LEU
5	A	349	ILE
5	A	361	ASN
5	A	386	ALA
5	A	389	TYR
5	A	423	ASP

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Mol	Chain	Res	Type
5	A	427	ARG
5	A	428	TYR
5	A	429	ASN
5	A	433	ASP
5	A	473	PRO
5	A	474	GLN
5	A	477	PHE
5	A	486	PRO
5	A	489	ALA
5	A	498	LEU
5	A	507	ALA
5	A	508	THR
5	A	509	ALA
5	A	510	SER
5	A	521	VAL
5	A	523	VAL
5	A	553	VAL
5	A	578	ARG
5	A	579	PHE
5	A	594	ALA
5	A	643	ALA
5	A	657	LEU
5	A	673	SER
5	A	679	PHE
5	A	727	ILE
5	A	735	VAL
5	A	750	PHE
5	A	751	LEU
5	A	752	ALA
5	A	757	VAL
6	B	5	ILE
6	B	6	PRO
6	B	26	ALA
6	B	35	ASP
6	B	68	VAL
6	B	69	ALA
6	B	77	TRP
6	B	80	ASP
6	B	83	HIS
6	B	86	PRO
6	B	99	PRO
6	B	104	PHE

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Mol	Chain	Res	Type
6	B	120	VAL
6	B	129	LEU
6	B	136	TYR
6	B	140	ILE
6	B	142	LEU
6	B	159	PRO
6	B	160	LYS
6	B	167	TRP
6	B	182	LEU
6	B	187	SER
6	B	198	ALA
6	B	208	ARG
6	B	231	ASN
6	B	248	GLN
6	B	265	THR
6	B	292	ARG
6	B	293	THR
6	B	294	ASN
6	B	308	HIS
6	B	310	PRO
6	B	320	LYS
6	B	321	GLY
6	B	362	ALA
6	B	375	HIS
6	B	378	ILE
6	B	382	ILE
6	B	383	MET
6	B	405	ASP
6	B	420	SER
6	B	450	GLU
6	B	479	SER
6	B	480	SER
6	B	490	ARG
6	B	494	LEU
6	B	495	PRO
6	B	505	SER
6	B	506	ASN
6	B	512	ILE
6	B	528	HIS
6	B	539	LEU
6	B	545	LYS
6	B	555	TYR

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Mol	Chain	Res	Type
6	B	569	ASP
6	B	587	ILE
6	B	599	ILE
6	B	603	ARG
6	B	605	ASN
6	B	610	ASN
6	B	629	SER
6	B	636	THR
6	B	639	VAL
6	B	657	TRP
6	B	661	PHE
6	B	662	MET
6	B	668	ARG
6	B	681	ALA
6	B	682	HIS
6	B	691	ILE
6	B	707	LEU
6	B	710	LEU
6	B	731	GLY
7	C	8	TYR
7	C	21	CYS
7	C	32	GLY
7	C	49	VAL
7	C	56	SER
7	C	59	PRO
7	C	62	PHE
7	C	65	VAL
7	C	66	ARG
7	C	75	ARG
8	D	32	SER
8	D	36	LEU
8	D	38	ARG
8	D	65	ALA
8	D	70	GLU
8	D	78	ALA
8	D	94	TYR
8	D	95	LYS
8	D	97	LYS
8	D	109	VAL
8	D	114	PRO
8	D	115	LYS
8	D	119	TYR

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Mol	Chain	Res	Type
8	D	120	PRO
8	D	121	GLU
8	D	124	ASN
8	D	132	LEU
8	D	139	LYS
8	D	146	VAL
8	D	151	LYS
8	D	153	PRO
9	E	35	LYS
9	E	46	PHE
9	E	53	VAL
9	E	54	ALA
9	E	60	LYS
9	E	64	PRO
9	E	65	VAL
9	E	72	VAL
9	E	73	ASN
9	E	86	GLU
9	E	87	VAL
9	E	90	VAL
10	F	2	ILE
10	F	7	PRO
10	F	12	LYS
10	F	21	ALA
10	F	25	LEU
10	F	26	GLN
10	F	31	LEU
10	F	35	ASP
10	F	38	PRO
10	F	42	ILE
10	F	47	GLU
10	F	52	ARG
10	F	54	ASP
10	F	58	LYS
10	F	59	TYR
10	F	77	GLN
10	F	109	ARG
10	F	116	GLN
10	F	127	SER
10	F	130	LEU
10	F	152	ASN
10	F	153	ASN

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Mol	Chain	Res	Type
11	G	31	MET
11	G	33	LYS
11	G	34	GLN
11	G	38	GLN
11	G	42	SER
11	G	50	ARG
11	G	59	LYS
11	G	61	ASN
11	G	70	ASP
11	G	74	TRP
11	G	81	VAL
11	G	86	LEU
11	G	87	ALA
11	G	94	ASP
12	H	15	ALA
12	H	17	THR
12	H	20	GLN
12	H	24	TYR
12	H	31	PRO
12	H	41	GLU
12	H	46	PRO
12	H	50	ARG
12	H	52	LEU
12	H	56	PHE
12	H	71	ASN
12	H	77	LEU
13	I	22	ALA
13	I	23	SER
14	J	5	LYS
14	J	6	THR
14	J	10	VAL
14	J	22	LEU
14	J	39	PHE
15	K	41	GLU
15	K	44	GLU
15	K	47	ILE
15	K	52	PRO
15	K	75	VAL
16	L	6	PRO
16	L	8	TYR
16	L	10	VAL
16	L	37	LEU

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Mol	Chain	Res	Type
16	L	43	TYR
16	L	44	ARG
16	L	46	ALA
16	L	63	LEU
16	L	75	ARG
16	L	76	ASN
16	L	88	ALA
16	L	97	MET
16	L	121	THR
16	L	123	ARG
16	L	125	LYS
16	L	127	PRO
16	L	128	ASP
16	L	129	GLN
16	L	149	SER
16	L	154	ALA
16	L	158	MET
16	L	163	LEU
16	L	164	PRO
17	N	2	VAL
17	N	7	LEU
17	N	11	LYS
17	N	24	THR
17	N	27	ALA
17	N	28	ASN
17	N	40	CYS
17	N	43	PRO
17	N	45	ASN
17	N	47	THR
17	N	51	ASP
17	N	58	VAL
17	N	61	LEU
17	N	63	ASP
17	N	66	ASP
17	N	68	GLU
17	N	75	TYR
17	N	76	LYS
17	N	77	CYS
17	N	80	ASN
17	N	82	PHE
17	N	83	TRP
1	1	21	ASP

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Mol	Chain	Res	Type
1	1	27	LEU
1	1	28	GLY
1	1	29	LEU
1	1	61	GLU
2	2	69	THR
2	2	71	LEU
2	2	73	ILE
2	2	82	ALA
2	2	91	THR
2	2	103	GLY
2	2	113	ILE
2	2	136	GLY
2	2	163	GLU
2	2	168	ARG
2	2	192	LEU
2	2	194	ALA
2	2	205	PHE
2	2	206	ALA
2	2	208	PHE
3	3	52	LYS
3	3	77	ILE
3	3	95	THR
3	3	106	TYR
3	3	137	SER
3	3	162	PRO
3	3	208	PRO
4	4	36	ASN
4	4	59	LEU
4	4	70	ILE
4	4	71	ASN
4	4	85	ALA
4	4	91	PHE
4	4	106	TRP
4	4	127	PRO
4	4	129	GLY
4	4	154	ILE
4	4	162	ALA
4	4	167	ILE
4	4	186	SER
4	4	188	PRO
5	A	39	HIS
5	A	45	ALA

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Mol	Chain	Res	Type
5	A	57	LEU
5	A	74	ILE
5	A	96	MET
5	A	105	ASN
5	A	130	GLU
5	A	144	GLN
5	A	149	PHE
5	A	184	PHE
5	A	189	ALA
5	A	210	LEU
5	A	213	LEU
5	A	215	SER
5	A	234	ASN
5	A	242	ILE
5	A	243	PRO
5	A	263	ALA
5	A	266	ALA
5	A	278	ALA
5	A	290	LEU
5	A	292	GLY
5	A	308	ILE
5	A	313	ALA
5	A	337	PRO
5	A	347	TYR
5	A	373	ALA
5	A	400	MET
5	A	421	ASP
5	A	424	PRO
5	A	431	LEU
5	A	439	ARG
5	A	446	LEU
5	A	476	MET
5	A	479	ASP
5	A	505	PRO
5	A	511	THR
5	A	514	THR
5	A	516	GLY
5	A	518	GLY
5	A	538	ASP
5	A	574	ASN
5	A	592	VAL
5	A	624	VAL

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Mol	Chain	Res	Type
5	A	637	ILE
5	A	640	GLY
5	A	649	ILE
5	A	661	ALA
5	A	671	SER
5	A	701	GLN
5	A	742	GLY
6	B	20	ARG
6	B	42	LEU
6	B	103	ALA
6	B	105	THR
6	B	115	ASN
6	B	128	GLY
6	B	153	GLY
6	B	188	LEU
6	B	207	VAL
6	B	222	LEU
6	B	224	PRO
6	B	228	GLY
6	B	230	TRP
6	B	232	LEU
6	B	234	ALA
6	B	237	PRO
6	B	247	THR
6	B	267	SER
6	B	318	GLY
6	B	330	ILE
6	B	371	LEU
6	B	437	TYR
6	B	464	GLN
6	B	469	LYS
6	B	481	THR
6	B	503	GLU
6	B	514	PRO
6	B	554	GLY
6	B	592	PHE
6	B	664	LEU
6	B	690	LEU
6	B	716	GLY
6	B	733	PHE
7	C	10	THR
7	C	22	PRO

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Mol	Chain	Res	Type
7	C	43	PRO
7	C	61	ASP
7	C	64	SER
7	C	68	TYR
7	C	70	TRP
8	D	26	SER
8	D	31	GLY
8	D	35	GLY
8	D	53	PRO
8	D	63	GLY
8	D	110	GLN
8	D	129	GLY
8	D	130	VAL
8	D	138	GLY
8	D	150	GLY
9	E	30	PRO
9	E	42	GLU
9	E	89	GLU
9	E	91	ALA
10	F	46	MET
10	F	126	ALA
10	F	138	VAL
10	F	141	TYR
11	G	22	VAL
11	G	28	ARG
11	G	46	ALA
11	G	63	PRO
11	G	80	ILE
11	G	85	ILE
11	G	93	TYR
12	H	23	VAL
12	H	34	SER
12	H	37	SER
12	H	44	ALA
12	H	75	ASP
13	I	25	PHE
14	J	26	LEU
14	J	37	LEU
15	K	27	ALA
15	K	32	ARG
15	K	35	THR
15	K	40	LEU

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Mol	Chain	Res	Type
15	K	45	SER
15	K	73	GLY
15	K	79	LYS
16	L	11	ILE
16	L	24	GLU
16	L	27	VAL
16	L	36	TYR
16	L	64	LEU
16	L	89	ALA
16	L	108	LYS
16	L	120	LEU
16	L	161	LEU
17	N	35	VAL
17	N	42	PHE
17	N	48	GLY
17	N	54	LYS
17	N	69	CYS
17	N	71	GLY
17	N	74	LYS
17	N	78	GLY
1	1	55	PRO
1	1	78	PRO
1	1	79	GLY
1	1	118	PRO
1	1	122	LYS
1	1	133	TYR
1	1	184	PRO
2	2	53	ARG
2	2	94	LEU
2	2	96	ILE
2	2	114	LEU
3	3	88	THR
3	3	91	PRO
3	3	153	SER
3	3	157	ALA
4	4	93	ILE
4	4	119	PRO
4	4	145	PRO
5	A	41	SER
5	A	63	ASP
5	A	73	GLU
5	A	114	THR

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Mol	Chain	Res	Type
5	A	116	ILE
5	A	124	TRP
5	A	127	VAL
5	A	151	GLN
5	A	200	GLU
5	A	225	VAL
5	A	305	ALA
5	A	317	TYR
5	A	354	TRP
5	A	355	HIS
5	A	404	GLY
5	A	426	THR
5	A	485	GLN
5	A	537	ALA
5	A	659	ALA
5	A	717	ALA
6	B	8	PHE
6	B	41	ARG
6	B	43	TYR
6	B	71	GLN
6	B	161	TRP
6	B	173	SER
6	B	178	HIS
6	B	179	LEU
6	B	189	ALA
6	B	223	GLY
6	B	225	LEU
6	B	239	SER
6	B	240	SER
6	B	272	ASP
6	B	273	VAL
6	B	278	LEU
6	B	281	ALA
6	B	309	ILE
6	B	361	ILE
6	B	400	PRO
6	B	468	GLY
6	B	474	PHE
6	B	477	PRO
6	B	482	ASN
6	B	493	TRP
6	B	501	ILE

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Mol	Chain	Res	Type
6	B	558	PRO
6	B	732	LYS
7	C	37	LYS
8	D	55	GLU
8	D	93	LYS
8	D	128	GLN
10	F	11	SER
10	F	34	ASP
10	F	44	ALA
10	F	53	PHE
10	F	63	CYS
10	F	114	PRO
11	G	84	TYR
11	G	89	ALA
12	H	27	ASP
12	H	45	ALA
13	I	2	ILE
14	J	9	SER
14	J	23	ALA
14	J	38	THR
15	K	48	GLN
16	L	113	SER
16	L	147	GLY
17	N	9	LYS
17	N	21	ARG
17	N	56	LYS
17	N	81	VAL
1	1	124	PRO
1	1	140	LEU
1	1	177	LEU
2	2	57	LEU
2	2	109	ARG
2	2	150	SER
2	2	180	GLN
2	2	186	THR
2	2	198	ALA
3	3	75	PRO
3	3	141	GLN
3	3	156	PRO
3	3	169	PHE
4	4	57	GLY
4	4	72	VAL

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Mol	Chain	Res	Type
4	4	112	PRO
4	4	139	ASN
4	4	177	PRO
4	4	187	ASP
5	A	31	PHE
5	A	37	PRO
5	A	135	ASP
5	A	230	ASN
5	A	276	LYS
5	A	410	ALA
5	A	422	TYR
5	A	571	ASP
5	A	702	GLU
5	A	738	TYR
6	B	54	LEU
6	B	164	SER
6	B	170	ASN
6	B	217	PRO
6	B	227	THR
6	B	229	GLN
6	B	270	LEU
6	B	335	GLY
6	B	354	SER
6	B	379	ALA
6	B	451	LYS
6	B	475	ASP
6	B	476	ILE
6	B	478	LEU
6	B	540	ASP
6	B	595	HIS
6	B	596	TRP
6	B	623	TYR
6	B	627	ASN
6	B	687	LEU
6	B	730	SER
7	C	9	ASP
7	C	12	ILE
7	C	28	MET
8	D	46	TYR
8	D	60	MET
8	D	106	SER
8	D	143	PRO

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Mol	Chain	Res	Type
9	E	61	THR
9	E	84	LEU
10	F	39	ALA
10	F	83	PHE
10	F	117	LYS
10	F	128	SER
10	F	132	ARG
10	F	151	ASP
11	G	36	PRO
11	G	56	SER
11	G	96	SER
12	H	18	THR
13	I	9	VAL
15	K	29	SER
16	L	48	ASN
16	L	50	LEU
16	L	85	SER
16	L	86	LEU
16	L	112	PRO
17	N	17	ASN
17	N	25	THR
17	N	49	CYS
17	N	70	GLU
1	1	84	TYR
2	2	68	LEU
2	2	115	ASN
2	2	140	GLY
2	2	146	LEU
2	2	179	PHE
2	2	187	GLY
4	4	92	VAL
4	4	137	ILE
5	A	95	GLY
5	A	186	TYR
5	A	235	ALA
5	A	269	PHE
5	A	306	ILE
5	A	353	SER
5	A	375	HIS
5	A	472	ARG
5	A	503	THR
5	A	580	PRO

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Mol	Chain	Res	Type
5	A	709	TRP
5	A	720	THR
6	B	139	ALA
6	B	206	TYR
6	B	212	PHE
6	B	421	HIS
6	B	460	ALA
6	B	472	TYR
6	B	550	LYS
6	B	559	CYS
6	B	586	THR
6	B	593	TYR
6	B	598	HIS
6	B	704	GLN
6	B	708	VAL
7	C	30	PRO
7	C	35	LYS
7	C	52	LYS
7	C	58	CYS
7	C	73	THR
8	D	22	PRO
8	D	40	ALA
8	D	104	PHE
8	D	125	PRO
8	D	148	PHE
9	E	52	VAL
10	F	73	VAL
11	G	91	ASN
12	H	16	ASN
12	H	74	GLN
13	I	5	PRO
16	L	61	GLY
16	L	135	GLY
16	L	159	TYR
17	N	34	THR
17	N	50	GLN
17	N	62	SER
1	1	32	VAL
1	1	125	GLY
1	1	145	VAL
2	2	116	PRO
4	4	118	ASP

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Mol	Chain	Res	Type
5	A	29	THR
5	A	48	PRO
5	A	86	LEU
5	A	179	LEU
5	A	239	PRO
5	A	259	TYR
5	A	500	PRO
5	A	570	PRO
5	A	721	GLN
6	B	94	PRO
6	B	162	LYS
6	B	219	PRO
6	B	360	PHE
6	B	367	THR
6	B	391	PRO
6	B	498	LEU
6	B	564	ARG
6	B	630	GLN
7	C	55	GLU
8	D	34	GLY
10	F	37	ALA
10	F	61	LEU
10	F	102	ARG
11	G	67	ASN
12	H	72	ALA
15	K	34	ALA
15	K	51	ASP
16	L	69	VAL
16	L	157	LEU
4	4	168	ILE
5	A	223	VAL
5	A	229	ILE
5	A	531	PRO
5	A	584	PRO
5	A	696	GLY
5	A	754	ILE
6	B	557	PHE
6	B	711	VAL
4	4	165	GLY
5	A	190	ALA
5	A	716	VAL
6	B	606	VAL

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Mol	Chain	Res	Type
8	D	67	ILE
9	E	55	VAL
11	G	64	VAL
11	G	71	VAL
16	L	53	GLY
16	L	72	GLY
16	L	150	GLY
17	N	59	PRO
2	2	182	ILE
6	B	87	ILE
6	B	463	ILE
8	D	28	ILE
11	G	35	VAL
1	1	89	VAL
1	1	173	PRO
2	2	135	VAL
2	2	167	GLY
5	A	718	PRO
6	B	113	VAL
12	H	60	GLY
13	I	12	VAL
4	4	63	VAL
16	L	16	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	126/190 (66%)	99 (79%)	27 (21%)	1 5
2	2	141/216 (65%)	78 (55%)	63 (45%)	0 0
3	3	118/215 (55%)	78 (66%)	40 (34%)	0 1
4	4	139/201 (69%)	73 (52%)	66 (48%)	0 0
5	A	592/618 (96%)	395 (67%)	197 (33%)	0 1
6	B	598/600 (100%)	369 (62%)	229 (38%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	C	70/70 (100%)	40 (57%)	30 (43%)	0 0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0 1
9	E	56/114 (49%)	36 (64%)	20 (36%)	0 1
10	F	127/190 (67%)	74 (58%)	53 (42%)	0 0
11	G	79/144 (55%)	47 (60%)	32 (40%)	0 1
12	H	57/115 (50%)	26 (46%)	31 (54%)	0 0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0 2
14	J	36/39 (92%)	24 (67%)	12 (33%)	0 1
15	K	61/102 (60%)	39 (64%)	22 (36%)	0 1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0 1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0 0
All	All	2542/3331 (76%)	1585 (62%)	957 (38%)	0 1

All (957) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	SER
1	1	27	LEU
1	1	37	GLU
1	1	43	GLU
1	1	47	CYS
1	1	52	LEU
1	1	57	ILE
1	1	63	LEU
1	1	65	TYR
1	1	85	LEU
1	1	105	ILE
1	1	110	HIS
1	1	111	GLN
1	1	117	ASP
1	1	120	LYS
1	1	121	LYS
1	1	129	ASP
1	1	133	TYR
1	1	134	SER
1	1	136	ASP
1	1	139	LYS
1	1	140	LEU

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Mol	Chain	Res	Type
1	1	142	GLU
1	1	179	THR
1	1	181	LEU
1	1	183	ASP
1	1	185	TRP
2	2	37	ASP
2	2	41	LEU
2	2	42	ARG
2	2	53	ARG
2	2	57	LEU
2	2	63	PHE
2	2	64	ILE
2	2	66	GLU
2	2	67	PHE
2	2	69	THR
2	2	70	LYS
2	2	73	ILE
2	2	75	ASN
2	2	76	THR
2	2	78	SER
2	2	79	TRP
2	2	80	TYR
2	2	85	GLN
2	2	86	GLU
2	2	87	TYR
2	2	89	THR
2	2	92	THR
2	2	95	PHE
2	2	97	VAL
2	2	98	GLU
2	2	99	LEU
2	2	100	VAL
2	2	101	PHE
2	2	109	ARG
2	2	110	TRP
2	2	112	ASP
2	2	115	ASN
2	2	118	CYS
2	2	120	ASN
2	2	122	ASP
2	2	127	ASN
2	2	131	THR

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Mol	Chain	Res	Type
2	2	133	THR
2	2	137	TYR
2	2	143	PHE
2	2	144	ASP
2	2	146	LEU
2	2	150	SER
2	2	157	LYS
2	2	159	LEU
2	2	160	ARG
2	2	161	THR
2	2	162	LYS
2	2	164	ILE
2	2	171	MET
2	2	179	PHE
2	2	180	GLN
2	2	183	TYR
2	2	189	ILE
2	2	190	ASP
2	2	191	ASN
2	2	193	PHE
2	2	196	HIS
2	2	199	ASP
2	2	201	HIS
2	2	204	ILE
2	2	205	PHE
2	2	211	LYS
3	3	50	GLU
3	3	60	ILE
3	3	67	LEU
3	3	73	ILE
3	3	76	GLU
3	3	78	LEU
3	3	83	LEU
3	3	84	ILE
3	3	86	GLN
3	3	90	LEU
3	3	93	PHE
3	3	94	ARG
3	3	95	THR
3	3	97	PHE
3	3	106	TYR
3	3	107	TRP

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Mol	Chain	Res	Type
3	3	109	ASP
3	3	111	TYR
3	3	112	THR
3	3	128	ARG
3	3	131	ASP
3	3	141	GLN
3	3	146	LEU
3	3	150	LEU
3	3	163	PHE
3	3	164	PHE
3	3	165	ASN
3	3	171	LYS
3	3	181	LEU
3	3	182	LYS
3	3	185	LYS
3	3	188	ARG
3	3	191	MET
3	3	192	LEU
3	3	195	LEU
3	3	198	PHE
3	3	200	GLN
3	3	204	THR
3	3	209	TYR
3	3	210	GLN
4	4	32	GLU
4	4	35	GLU
4	4	38	ARG
4	4	45	LEU
4	4	49	ARG
4	4	50	TRP
4	4	52	MET
4	4	59	LEU
4	4	60	LEU
4	4	64	PHE
4	4	66	SER
4	4	67	ILE
4	4	75	TRP
4	4	76	TYR
4	4	82	GLU
4	4	83	TYR
4	4	84	PHE
4	4	87	SER

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Mol	Chain	Res	Type
4	4	90	LEU
4	4	91	PHE
4	4	92	VAL
4	4	93	ILE
4	4	94	GLU
4	4	95	PHE
4	4	97	LEU
4	4	99	HIS
4	4	101	VAL
4	4	103	ILE
4	4	104	ARG
4	4	105	ARG
4	4	107	GLN
4	4	109	ILE
4	4	118	ASP
4	4	120	ILE
4	4	121	PHE
4	4	122	LYS
4	4	125	SER
4	4	126	LEU
4	4	131	VAL
4	4	139	ASN
4	4	146	THR
4	4	147	LEU
4	4	150	LYS
4	4	151	GLU
4	4	152	LYS
4	4	154	ILE
4	4	156	ASN
4	4	158	ARG
4	4	159	LEU
4	4	160	MET
4	4	161	LEU
4	4	163	PHE
4	4	164	LEU
4	4	167	ILE
4	4	168	ILE
4	4	169	GLN
4	4	172	VAL
4	4	175	LYS
4	4	178	PHE
4	4	180	ASN

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Mol	Chain	Res	Type
4	4	184	HIS
4	4	186	SER
4	4	187	ASP
4	4	189	TRP
4	4	190	HIS
4	4	192	THR
5	A	21	LEU
5	A	24	ARG
5	A	27	ILE
5	A	31	PHE
5	A	34	TRP
5	A	40	PHE
5	A	44	ILE
5	A	46	LYS
5	A	50	THR
5	A	52	THR
5	A	60	ASP
5	A	62	HIS
5	A	63	ASP
5	A	68	THR
5	A	69	SER
5	A	71	LEU
5	A	72	GLU
5	A	78	VAL
5	A	82	HIS
5	A	83	PHE
5	A	86	LEU
5	A	88	ILE
5	A	94	SER
5	A	102	ARG
5	A	103	PHE
5	A	107	GLU
5	A	109	TRP
5	A	111	ASN
5	A	114	THR
5	A	124	TRP
5	A	130	GLU
5	A	131	ILE
5	A	133	ASN
5	A	135	ASP
5	A	141	ARG
5	A	144	GLN

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Mol	Chain	Res	Type
5	A	164	LEU
5	A	167	THR
5	A	172	LEU
5	A	177	LEU
5	A	180	PHE
5	A	188	LYS
5	A	193	LEU
5	A	197	GLN
5	A	203	LEU
5	A	207	LEU
5	A	213	LEU
5	A	223	VAL
5	A	224	HIS
5	A	227	LEU
5	A	230	ASN
5	A	231	GLN
5	A	232	PHE
5	A	238	ASP
5	A	242	ILE
5	A	248	PHE
5	A	249	ILE
5	A	251	ASN
5	A	253	ASP
5	A	254	LEU
5	A	255	LEU
5	A	261	SER
5	A	262	PHE
5	A	277	TYR
5	A	281	LEU
5	A	284	ARG
5	A	287	LEU
5	A	290	LEU
5	A	296	LEU
5	A	297	THR
5	A	298	ASP
5	A	299	ILE
5	A	304	LEU
5	A	308	ILE
5	A	309	LEU
5	A	316	MET
5	A	331	LEU
5	A	332	GLU

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Mol	Chain	Res	Type
5	A	334	HIS
5	A	339	THR
5	A	341	GLN
5	A	352	THR
5	A	353	SER
5	A	357	GLN
5	A	361	ASN
5	A	368	LEU
5	A	369	THR
5	A	375	HIS
5	A	376	MET
5	A	377	TYR
5	A	379	MET
5	A	384	TYR
5	A	387	THR
5	A	391	THR
5	A	392	GLN
5	A	393	LEU
5	A	397	THR
5	A	400	MET
5	A	402	ILE
5	A	405	PHE
5	A	420	ARG
5	A	422	TYR
5	A	426	THR
5	A	427	ARG
5	A	433	ASP
5	A	434	ARG
5	A	435	VAL
5	A	438	HIS
5	A	439	ARG
5	A	440	ASP
5	A	444	SER
5	A	446	LEU
5	A	458	PHE
5	A	462	ILE
5	A	464	ASN
5	A	466	THR
5	A	477	PHE
5	A	479	ASP
5	A	480	THR
5	A	488	PHE

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Mol	Chain	Res	Type
5	A	490	GLN
5	A	495	THR
5	A	498	LEU
5	A	503	THR
5	A	514	THR
5	A	520	LEU
5	A	521	VAL
5	A	529	LEU
5	A	530	LEU
5	A	532	ILE
5	A	536	THR
5	A	539	PHE
5	A	540	LEU
5	A	547	PHE
5	A	548	THR
5	A	553	VAL
5	A	554	LEU
5	A	555	ILE
5	A	557	LEU
5	A	558	LYS
5	A	561	LEU
5	A	564	ARG
5	A	567	ARG
5	A	568	LEU
5	A	569	ILE
5	A	572	LYS
5	A	575	LEU
5	A	577	PHE
5	A	578	ARG
5	A	590	CYS
5	A	591	GLN
5	A	600	LEU
5	A	605	MET
5	A	607	ASN
5	A	613	ILE
5	A	614	PHE
5	A	623	ASP
5	A	629	ASN
5	A	630	ASP
5	A	631	GLN
5	A	633	VAL
5	A	637	ILE

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Mol	Chain	Res	Type
5	A	638	THR
5	A	641	ASN
5	A	642	PHE
5	A	644	GLN
5	A	645	SER
5	A	646	SER
5	A	653	LEU
5	A	654	ARG
5	A	657	LEU
5	A	660	GLN
5	A	662	SER
5	A	663	GLN
5	A	664	VAL
5	A	673	SER
5	A	677	LEU
5	A	684	PHE
5	A	685	VAL
5	A	689	SER
5	A	691	MET
5	A	692	PHE
5	A	697	ARG
5	A	703	LEU
5	A	707	ILE
5	A	715	LYS
5	A	723	ARG
5	A	726	SER
5	A	727	ILE
5	A	728	VAL
5	A	733	VAL
5	A	735	VAL
5	A	736	THR
5	A	740	LEU
5	A	745	THR
5	A	751	LEU
5	A	754	ILE
6	B	3	LEU
6	B	4	ARG
6	B	5	ILE
6	B	6	PRO
6	B	9	SER
6	B	14	GLN
6	B	15	ASP

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Mol	Chain	Res	Type
6	B	17	THR
6	B	19	ARG
6	B	20	ARG
6	B	25	ILE
6	B	35	ASP
6	B	41	ARG
6	B	45	ASN
6	B	46	ILE
6	B	50	HIS
6	B	51	PHE
6	B	53	GLN
6	B	57	ILE
6	B	67	HIS
6	B	70	TRP
6	B	71	GLN
6	B	75	GLU
6	B	83	HIS
6	B	84	VAL
6	B	91	ILE
6	B	104	PHE
6	B	110	LEU
6	B	113	VAL
6	B	114	ASN
6	B	121	TYR
6	B	122	GLN
6	B	123	TRP
6	B	124	TRP
6	B	127	ILE
6	B	129	LEU
6	B	130	ARG
6	B	132	ASN
6	B	134	ASP
6	B	136	TYR
6	B	137	THR
6	B	140	ILE
6	B	142	LEU
6	B	143	LEU
6	B	144	PHE
6	B	145	LEU
6	B	151	LEU
6	B	154	TRP
6	B	157	LEU

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Mol	Chain	Res	Type
6	B	160	LYS
6	B	161	TRP
6	B	164	SER
6	B	175	LEU
6	B	177	HIS
6	B	178	HIS
6	B	180	SER
6	B	188	LEU
6	B	195	VAL
6	B	199	ILE
6	B	203	ARG
6	B	206	TYR
6	B	208	ARG
6	B	210	ASN
6	B	214	ASP
6	B	216	LEU
6	B	226	LEU
6	B	229	GLN
6	B	231	ASN
6	B	232	LEU
6	B	243	LEU
6	B	246	THR
6	B	248	GLN
6	B	257	ILE
6	B	258	LEU
6	B	262	HIS
6	B	265	THR
6	B	266	GLN
6	B	269	TRP
6	B	270	LEU
6	B	271	THR
6	B	272	ASP
6	B	278	LEU
6	B	285	LEU
6	B	292	ARG
6	B	294	ASN
6	B	295	PHE
6	B	297	ILE
6	B	299	HIS
6	B	300	SER
6	B	301	ILE
6	B	309	ILE

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Mol	Chain	Res	Type
6	B	315	LEU
6	B	317	ARG
6	B	325	THR
6	B	326	ILE
6	B	330	ILE
6	B	332	PHE
6	B	348	VAL
6	B	350	GLN
6	B	352	MET
6	B	353	TYR
6	B	355	LEU
6	B	361	ILE
6	B	363	GLN
6	B	364	ASP
6	B	365	PHE
6	B	372	TYR
6	B	374	HIS
6	B	382	ILE
6	B	383	MET
6	B	384	THR
6	B	387	PHE
6	B	393	PHE
6	B	396	ARG
6	B	403	ASN
6	B	406	ASN
6	B	407	VAL
6	B	410	ARG
6	B	412	LEU
6	B	418	ILE
6	B	419	ILE
6	B	420	SER
6	B	422	LEU
6	B	423	SER
6	B	427	LEU
6	B	428	PHE
6	B	431	PHE
6	B	436	LEU
6	B	437	TYR
6	B	438	VAL
6	B	440	ASN
6	B	443	MET
6	B	446	PHE

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Mol	Chain	Res	Type
6	B	448	THR
6	B	452	GLN
6	B	454	LEU
6	B	458	ILE
6	B	461	GLN
6	B	464	GLN
6	B	471	THR
6	B	472	TYR
6	B	478	LEU
6	B	481	THR
6	B	486	LEU
6	B	492	ILE
6	B	494	LEU
6	B	501	ILE
6	B	502	ASN
6	B	504	ASN
6	B	508	LEU
6	B	509	PHE
6	B	510	LEU
6	B	512	ILE
6	B	514	PRO
6	B	516	ASP
6	B	517	PHE
6	B	521	HIS
6	B	525	LEU
6	B	527	LEU
6	B	528	HIS
6	B	532	LEU
6	B	533	ILE
6	B	539	LEU
6	B	540	ASP
6	B	544	SER
6	B	545	LYS
6	B	551	LYS
6	B	555	TYR
6	B	560	ASP
6	B	564	ARG
6	B	569	ASP
6	B	577	TYR
6	B	578	LEU
6	B	580	VAL
6	B	583	MET

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Mol	Chain	Res	Type
6	B	584	LEU
6	B	587	ILE
6	B	592	PHE
6	B	594	TRP
6	B	596	TRP
6	B	601	LEU
6	B	603	ARG
6	B	605	ASN
6	B	606	VAL
6	B	607	SER
6	B	608	GLN
6	B	611	GLU
6	B	615	TYR
6	B	616	LEU
6	B	617	MET
6	B	620	LEU
6	B	621	ARG
6	B	622	ASP
6	B	629	SER
6	B	631	LEU
6	B	633	ASN
6	B	638	LEU
6	B	640	CYS
6	B	643	LEU
6	B	645	VAL
6	B	649	MET
6	B	651	LEU
6	B	659	THR
6	B	662	MET
6	B	664	LEU
6	B	665	ILE
6	B	670	TYR
6	B	672	GLN
6	B	674	LEU
6	B	676	GLU
6	B	677	THR
6	B	682	HIS
6	B	685	THR
6	B	689	ASN
6	B	690	LEU
6	B	691	ILE
6	B	692	ARG

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Mol	Chain	Res	Type
6	B	700	LEU
6	B	702	ILE
6	B	703	VAL
6	B	710	LEU
6	B	712	HIS
6	B	715	VAL
6	B	718	ILE
6	B	719	PHE
6	B	721	TYR
6	B	725	LEU
6	B	732	LYS
6	B	733	PHE
7	C	2	SER
7	C	4	SER
7	C	7	ILE
7	C	10	THR
7	C	12	ILE
7	C	15	THR
7	C	16	GLN
7	C	18	VAL
7	C	23	THR
7	C	24	ASP
7	C	28	MET
7	C	37	LYS
7	C	38	GLN
7	C	45	THR
7	C	48	CYS
7	C	52	LYS
7	C	58	CYS
7	C	59	PRO
7	C	62	PHE
7	C	63	LEU
7	C	66	ARG
7	C	67	VAL
7	C	68	TYR
7	C	69	LEU
7	C	70	TRP
7	C	73	THR
7	C	74	THR
7	C	77	MET
7	C	79	LEU
7	C	81	TYR

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Mol	Chain	Res	Type
8	D	26	SER
8	D	28	ILE
8	D	41	GLN
8	D	44	GLU
8	D	46	TYR
8	D	47	VAL
8	D	48	ILE
8	D	49	THR
8	D	50	TRP
8	D	56	GLN
8	D	57	ILE
8	D	58	PHE
8	D	69	ARG
8	D	70	GLU
8	D	73	ASN
8	D	75	LEU
8	D	79	ARG
8	D	81	GLU
8	D	82	GLN
8	D	83	CYS
8	D	86	LEU
8	D	89	ARG
8	D	92	SER
8	D	93	LYS
8	D	95	LYS
8	D	96	ILE
8	D	98	TYR
8	D	104	PHE
8	D	105	PRO
8	D	111	TYR
8	D	116	ASP
8	D	121	GLU
8	D	122	LYS
8	D	123	VAL
8	D	127	ARG
8	D	128	GLN
8	D	134	MET
8	D	135	ARG
8	D	137	ILE
8	D	139	LYS
8	D	144	ILE
8	D	147	LYS

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Mol	Chain	Res	Type
8	D	151	LYS
9	E	28	ILE
9	E	31	LYS
9	E	32	ARG
9	E	35	LYS
9	E	36	VAL
9	E	39	LEU
9	E	40	ARG
9	E	42	GLU
9	E	45	TRP
9	E	47	LYS
9	E	48	ASN
9	E	55	VAL
9	E	56	ASP
9	E	58	ASP
9	E	61	THR
9	E	68	ARG
9	E	73	ASN
9	E	76	ASN
9	E	79	THR
9	E	84	LEU
10	F	8	CYS
10	F	9	LYS
10	F	12	LYS
10	F	13	GLN
10	F	14	PHE
10	F	17	ARG
10	F	18	GLU
10	F	20	GLN
10	F	23	LYS
10	F	24	LYS
10	F	25	LEU
10	F	26	GLN
10	F	28	SER
10	F	29	LEU
10	F	31	LEU
10	F	43	LYS
10	F	48	LYS
10	F	51	LYS
10	F	52	ARG
10	F	53	PHE
10	F	61	LEU

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Mol	Chain	Res	Type
10	F	71	LEU
10	F	77	GLN
10	F	78	ARG
10	F	79	HIS
10	F	83	PHE
10	F	88	ILE
10	F	91	LEU
10	F	92	TYR
10	F	93	ILE
10	F	96	TRP
10	F	100	VAL
10	F	104	TYR
10	F	106	ILE
10	F	108	ILE
10	F	110	ASP
10	F	111	GLU
10	F	113	LYS
10	F	115	THR
10	F	116	GLN
10	F	119	ILE
10	F	121	ILE
10	F	123	VAL
10	F	135	SER
10	F	136	TRP
10	F	137	PRO
10	F	138	VAL
10	F	141	TYR
10	F	142	ARG
10	F	143	GLU
10	F	146	ASN
10	F	153	ASN
10	F	154	PHE
11	G	7	VAL
11	G	10	LEU
11	G	12	THR
11	G	15	SER
11	G	17	PHE
11	G	18	LEU
11	G	22	VAL
11	G	24	PHE
11	G	28	ARG
11	G	30	ASN

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Mol	Chain	Res	Type
11	G	31	MET
11	G	33	LYS
11	G	39	ASN
11	G	41	MET
11	G	42	SER
11	G	43	HIS
11	G	44	PHE
11	G	45	GLU
11	G	48	ASP
11	G	49	THR
11	G	50	ARG
11	G	55	VAL
11	G	57	LEU
11	G	58	LEU
11	G	62	ASP
11	G	71	VAL
11	G	76	SER
11	G	83	TYR
11	G	88	THR
11	G	91	ASN
11	G	93	TYR
11	G	97	PHE
12	H	11	LEU
12	H	14	ILE
12	H	17	THR
12	H	20	GLN
12	H	21	TRP
12	H	24	TYR
12	H	30	SER
12	H	32	TYR
12	H	33	ASN
12	H	35	LEU
12	H	36	GLN
12	H	37	SER
12	H	41	GLU
12	H	42	THR
12	H	43	PHE
12	H	47	PHE
12	H	48	THR
12	H	49	LYS
12	H	52	LEU
12	H	53	LEU

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Mol	Chain	Res	Type
12	H	54	LEU
12	H	55	LYS
12	H	56	PHE
12	H	57	LEU
12	H	59	LEU
12	H	64	LEU
12	H	66	THR
12	H	67	TYR
12	H	69	SER
12	H	75	ASP
12	H	77	LEU
13	I	3	ASN
13	I	7	LEU
13	I	9	VAL
13	I	11	LEU
13	I	12	VAL
13	I	16	PHE
13	I	26	LEU
13	I	30	LYS
14	J	2	ARG
14	J	3	ASP
14	J	4	PHE
14	J	5	LYS
14	J	9	SER
14	J	13	VAL
14	J	14	LEU
14	J	16	THR
14	J	19	PHE
14	J	35	ASP
14	J	37	LEU
14	J	41	PHE
15	K	3	ILE
15	K	9	LEU
15	K	10	ILE
15	K	11	MET
15	K	13	THR
15	K	15	THR
15	K	17	LEU
15	K	19	LEU
15	K	20	PHE
15	K	23	ARG
15	K	32	ARG

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Mol	Chain	Res	Type
15	K	40	LEU
15	K	41	GLU
15	K	43	ARG
15	K	44	GLU
15	K	45	SER
15	K	48	GLN
15	K	56	THR
15	K	59	ASP
15	K	63	CYS
15	K	69	ILE
15	K	72	VAL
16	L	5	LYS
16	L	8	TYR
16	L	9	GLN
16	L	10	VAL
16	L	14	LEU
16	L	15	ASN
16	L	20	ILE
16	L	30	SER
16	L	32	LEU
16	L	38	SER
16	L	39	ASN
16	L	40	LEU
16	L	44	ARG
16	L	52	ARG
16	L	54	VAL
16	L	58	LEU
16	L	63	LEU
16	L	68	PHE
16	L	70	LYS
16	L	74	LEU
16	L	76	ASN
16	L	77	THR
16	L	79	TYR
16	L	94	ILE
16	L	97	MET
16	L	107	PHE
16	L	108	LYS
16	L	111	GLU
16	L	118	LEU
16	L	120	LEU
16	L	123	ARG

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Mol	Chain	Res	Type
16	L	124	LYS
16	L	134	ASP
16	L	136	TRP
16	L	140	THR
16	L	145	PHE
16	L	149	SER
16	L	152	THR
16	L	158	MET
16	L	159	TYR
16	L	161	LEU
16	L	163	LEU
16	L	165	TYR
17	N	4	GLU
17	N	5	GLU
17	N	6	TYR
17	N	10	SER
17	N	11	LYS
17	N	16	LEU
17	N	25	THR
17	N	28	ASN
17	N	29	PHE
17	N	33	TYR
17	N	37	PHE
17	N	39	SER
17	N	40	CYS
17	N	41	LYS
17	N	46	PHE
17	N	49	CYS
17	N	50	GLN
17	N	51	ASP
17	N	52	LEU
17	N	54	LYS
17	N	55	GLN
17	N	57	LYS
17	N	58	VAL
17	N	60	PHE
17	N	61	LEU
17	N	62	SER
17	N	64	ASP
17	N	65	LEU
17	N	66	ASP
17	N	67	LEU

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Mol	Chain	Res	Type
17	N	68	GLU
17	N	69	CYS
17	N	70	GLU
17	N	72	LYS
17	N	73	ASP
17	N	75	TYR
17	N	79	SER
17	N	81	VAL
17	N	82	PHE
17	N	83	TRP
17	N	84	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	111	GLN
2	2	115	ASN
2	2	128	ASN
2	2	181	HIS
2	2	191	ASN
3	3	105	ASN
3	3	126	HIS
3	3	165	ASN
4	4	71	ASN
4	4	169	GLN
4	4	170	HIS
4	4	180	ASN
5	A	58	HIS
5	A	99	HIS
5	A	121	GLN
5	A	129	GLN
5	A	144	GLN
5	A	197	GLN
5	A	224	HIS
5	A	230	ASN
5	A	231	GLN
5	A	246	HIS
5	A	302	HIS
5	A	303	HIS
5	A	343	HIS
5	A	361	ASN
5	A	375	HIS

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Mol	Chain	Res	Type
5	A	398	HIS
5	A	447	ASN
5	A	464	ASN
5	A	474	GLN
5	A	490	GLN
5	A	542	HIS
5	A	545	HIS
5	A	591	GLN
5	A	607	ASN
5	A	629	ASN
5	A	636	HIS
5	A	641	ASN
5	A	660	GLN
5	A	683	HIS
5	A	701	GLN
5	A	711	HIS
6	B	14	GLN
6	B	29	HIS
6	B	34	HIS
6	B	50	HIS
6	B	67	HIS
6	B	71	GLN
6	B	95	HIS
6	B	122	GLN
6	B	158	GLN
6	B	178	HIS
6	B	193	HIS
6	B	220	GLN
6	B	266	GLN
6	B	277	HIS
6	B	328	ASN
6	B	333	GLN
6	B	375	HIS
6	B	399	ASN
6	B	403	ASN
6	B	406	ASN
6	B	432	HIS
6	B	461	GLN
6	B	502	ASN
6	B	504	ASN
6	B	506	ASN
6	B	521	HIS

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Mol	Chain	Res	Type
6	B	528	HIS
6	B	595	HIS
6	B	605	ASN
6	B	608	GLN
6	B	610	ASN
6	B	630	GLN
6	B	633	ASN
6	B	641	ASN
6	B	672	GLN
6	B	712	HIS
7	C	71	HIS
8	D	41	GLN
8	D	56	GLN
8	D	73	ASN
8	D	82	GLN
8	D	128	GLN
8	D	133	ASN
8	D	152	GLN
9	E	48	ASN
9	E	73	ASN
10	F	77	GLN
10	F	116	GLN
10	F	146	ASN
10	F	152	ASN
10	F	153	ASN
11	G	61	ASN
11	G	67	ASN
12	H	16	ASN
12	H	33	ASN
12	H	36	GLN
12	H	71	ASN
14	J	30	ASN
15	K	80	ASN
16	L	12	GLN
16	L	15	ASN
16	L	39	ASN
16	L	48	ASN
16	L	131	GLN
17	N	45	ASN
17	N	55	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	GLC	M	1	19	11,11,12	0.86	0	15,15,17	2.46	4 (26%)
19	FRU	M	2	19	11,12,12	1.15	2 (18%)	10,18,18	0.97	0
19	GLC	O	1	19	10,10,12	1.48	3 (30%)	14,14,17	3.32	9 (64%)
19	FRU	O	2	19	11,12,12	1.11	1 (9%)	10,18,18	2.31	3 (30%)
19	GLC	P	1	19	11,11,12	1.51	2 (18%)	15,15,17	2.88	10 (66%)
19	FRU	P	2	19	11,12,12	1.38	2 (18%)	10,18,18	2.17	2 (20%)
19	GLC	Q	1	19	11,11,12	1.02	0	15,15,17	3.55	8 (53%)
19	FRU	Q	2	19	11,12,12	1.29	1 (9%)	10,18,18	1.71	2 (20%)
19	GLC	S	1	19	11,11,12	1.19	1 (9%)	15,15,17	1.61	3 (20%)
19	FRU	S	2	19	11,12,12	2.16	4 (36%)	10,18,18	2.83	4 (40%)
19	GLC	T	1	19	11,11,12	1.36	2 (18%)	15,15,17	1.81	3 (20%)
19	FRU	T	2	19	11,12,12	1.74	2 (18%)	10,18,18	2.33	4 (40%)
19	GLC	U	1	19	11,11,12	1.37	1 (9%)	15,15,17	1.56	3 (20%)
19	FRU	U	2	19	11,12,12	1.25	1 (9%)	10,18,18	1.61	2 (20%)
19	GLC	V	1	19	11,11,12	1.15	1 (9%)	15,15,17	3.47	6 (40%)
19	FRU	V	2	19	11,12,12	1.16	0	10,18,18	2.27	4 (40%)
19	GLC	W	1	19	11,11,12	1.16	1 (9%)	15,15,17	1.60	3 (20%)
19	FRU	W	2	19	11,12,12	1.23	1 (9%)	10,18,18	2.21	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	GLC	X	1	19	11,11,12	1.29	1 (9%)	15,15,17	2.17	4 (26%)
19	FRU	X	2	19	11,12,12	1.17	1 (9%)	10,18,18	1.83	4 (40%)
19	GLC	Y	1	19	11,11,12	1.95	3 (27%)	15,15,17	4.48	8 (53%)
19	FRU	Y	2	19	11,12,12	1.17	2 (18%)	10,18,18	2.41	3 (30%)
19	GLC	Z	1	19	11,11,12	1.08	0	15,15,17	2.04	5 (33%)
19	FRU	Z	2	19	11,12,12	0.70	0	10,18,18	1.67	4 (40%)
19	GLC	a	1	19	11,11,12	1.73	2 (18%)	15,15,17	2.10	5 (33%)
19	FRU	a	2	19	11,12,12	1.06	0	10,18,18	2.02	5 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	M	1	19	-	2/2/19/22	0/1/1/1
19	FRU	M	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	O	1	19	-	-	0/1/1/1
19	FRU	O	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	P	1	19	-	1/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	1/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	4/5/24/24	0/1/1/1
19	GLC	S	1	19	-	2/2/19/22	0/1/1/1
19	FRU	S	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	5/5/24/24	0/1/1/1
19	GLC	V	1	19	-	2/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	W	1	19	-	2/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	3/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	Z	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Z	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	a	1	19	-	0/2/19/22	0/1/1/1
19	FRU	a	2	19	1/1/4/4	3/5/24/24	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	1	GLC	O5-C1	-4.80	1.36	1.43
19	S	2	FRU	O5-C2	-3.61	1.37	1.43
19	U	2	FRU	O5-C2	-3.34	1.38	1.43
19	Q	2	FRU	O5-C2	-3.19	1.38	1.43
19	T	2	FRU	O5-C2	-3.14	1.38	1.43
19	S	2	FRU	C1-C2	-3.12	1.47	1.52
19	T	2	FRU	O2-C2	-3.05	1.35	1.40
19	S	2	FRU	O2-C2	-2.96	1.35	1.40
19	a	1	GLC	O5-C5	-2.92	1.37	1.43
19	S	2	FRU	O3-C3	-2.82	1.37	1.42
19	a	1	GLC	O5-C1	-2.79	1.39	1.43
19	P	2	FRU	O5-C2	-2.76	1.39	1.43
19	P	1	GLC	O5-C1	-2.75	1.39	1.43
19	M	2	FRU	O2-C2	2.63	1.45	1.40
19	W	2	FRU	O3-C3	-2.46	1.37	1.42
19	O	1	GLC	O5-C5	-2.44	1.38	1.43
19	O	1	GLC	O5-C1	-2.41	1.39	1.43
19	T	1	GLC	O5-C1	-2.41	1.39	1.43
19	X	1	GLC	O5-C1	-2.40	1.39	1.43
19	X	2	FRU	O5-C2	-2.40	1.39	1.43
19	Y	2	FRU	O5-C2	-2.37	1.39	1.43
19	U	1	GLC	O5-C1	-2.35	1.40	1.43
19	O	2	FRU	O5-C5	-2.34	1.38	1.43
19	W	1	GLC	C2-C3	-2.31	1.49	1.52
19	Y	2	FRU	C1-C2	-2.28	1.48	1.52
19	P	2	FRU	O5-C5	-2.27	1.38	1.43
19	P	1	GLC	O5-C5	-2.26	1.38	1.43
19	O	1	GLC	O2-C2	-2.25	1.38	1.43
19	M	2	FRU	C1-C2	2.25	1.55	1.52
19	S	1	GLC	O5-C5	-2.11	1.39	1.43
19	Y	1	GLC	O5-C5	-2.10	1.39	1.43
19	Y	1	GLC	O3-C3	-2.10	1.38	1.43
19	T	1	GLC	C2-C3	-2.10	1.49	1.52
19	V	1	GLC	C4-C3	-2.05	1.47	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	1	GLC	C1-O5-C5	-11.22	97.00	112.19
19	M	1	GLC	C1-O5-C5	7.92	122.92	112.19
19	O	1	GLC	C1-C2-C3	7.69	119.11	109.67
19	V	1	GLC	C1-O5-C5	7.47	122.31	112.19
19	Y	1	GLC	O5-C1-C2	-7.39	99.37	110.77
19	Q	1	GLC	O3-C3-C2	6.94	123.28	109.99
19	S	2	FRU	O1-C1-C2	-6.91	97.18	111.86
19	V	1	GLC	O5-C5-C6	6.55	117.48	107.20
19	P	2	FRU	O1-C1-C2	-5.88	99.37	111.86
19	Q	1	GLC	C2-C3-C4	-5.82	100.83	110.89
19	Y	1	GLC	C6-C5-C4	5.77	126.52	113.00
19	Q	1	GLC	C3-C4-C5	-5.41	100.59	110.24
19	Q	1	GLC	O5-C1-C2	5.27	118.91	110.77
19	Y	1	GLC	C3-C4-C5	-5.20	100.97	110.24
19	Z	1	GLC	C1-C2-C3	-5.13	103.36	109.67
19	T	2	FRU	C6-C5-C4	-5.11	102.76	115.09
19	Y	2	FRU	O1-C1-C2	-5.09	101.05	111.86
19	O	1	GLC	O5-C5-C4	-5.06	100.44	109.52
19	P	1	GLC	O3-C3-C4	5.00	121.90	110.35
19	V	1	GLC	C3-C4-C5	-4.87	101.55	110.24
19	Y	1	GLC	O2-C2-C3	-4.86	100.40	110.14
19	a	1	GLC	C1-C2-C3	-4.84	103.72	109.67
19	V	1	GLC	C2-C3-C4	-4.83	102.54	110.89
19	X	1	GLC	C3-C4-C5	-4.66	101.93	110.24
19	Y	2	FRU	O2-C2-O5	4.50	118.20	109.50
19	O	2	FRU	O4-C4-C3	-4.50	98.69	112.15
19	P	1	GLC	C2-C3-C4	-4.38	103.32	110.89
19	X	1	GLC	C6-C5-C4	-4.32	102.88	113.00
19	V	1	GLC	O3-C3-C2	4.12	117.89	109.99
19	P	1	GLC	C1-C2-C3	-4.12	104.61	109.67
19	O	2	FRU	O2-C2-O5	-4.02	101.73	109.50
19	Y	1	GLC	C2-C3-C4	-3.92	104.12	110.89
19	Q	1	GLC	C1-O5-C5	3.87	117.43	112.19
19	W	2	FRU	O1-C1-C2	-3.85	103.69	111.86
19	W	2	FRU	O2-C2-O5	3.84	116.91	109.50
19	O	1	GLC	O2-C2-C1	-3.80	101.37	109.15
19	O	2	FRU	O1-C1-C2	3.68	119.68	111.86
19	a	1	GLC	O5-C5-C4	-3.65	101.95	110.83
19	T	1	GLC	O5-C1-C2	3.59	116.31	110.77
19	S	2	FRU	O3-C3-C4	-3.47	101.32	113.32
19	V	2	FRU	O3-C3-C4	-3.46	101.38	113.32
19	P	1	GLC	O6-C6-C5	-3.44	99.49	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	O	1	GLC	O3-C3-C2	3.43	116.55	109.99
19	T	2	FRU	O6-C6-C5	-3.42	99.56	111.29
19	P	1	GLC	C3-C4-C5	-3.41	104.16	110.24
19	V	2	FRU	O5-C5-C6	3.39	118.28	108.85
19	O	1	GLC	O5-C1-C2	3.35	115.95	110.77
19	U	2	FRU	O2-C2-O5	-3.31	103.12	109.50
19	W	2	FRU	O4-C4-C3	-3.30	102.26	112.15
19	T	1	GLC	C2-C3-C4	-3.30	105.19	110.89
19	X	2	FRU	O2-C2-O5	-3.29	103.15	109.50
19	Q	1	GLC	O4-C4-C5	3.26	117.39	109.30
19	S	1	GLC	O2-C2-C1	3.24	115.78	109.15
19	P	1	GLC	C6-C5-C4	-3.23	105.43	113.00
19	W	1	GLC	O5-C5-C6	3.23	112.26	107.20
19	Y	1	GLC	O5-C5-C4	-3.19	103.07	110.83
19	X	1	GLC	C2-C3-C4	-3.15	105.44	110.89
19	a	2	FRU	O4-C4-C5	3.12	120.06	111.05
19	Q	2	FRU	O2-C2-O5	3.08	115.44	109.50
19	U	2	FRU	C6-C5-C4	-3.06	107.70	115.09
19	Q	1	GLC	O2-C2-C3	3.05	116.25	110.14
19	a	1	GLC	O5-C5-C6	3.05	111.98	107.20
19	a	1	GLC	C1-O5-C5	-3.03	108.09	112.19
19	W	1	GLC	C2-C3-C4	-3.01	105.69	110.89
19	V	2	FRU	O1-C1-C2	-3.00	105.49	111.86
19	P	1	GLC	O2-C2-C3	2.98	116.12	110.14
19	W	1	GLC	O2-C2-C3	-2.87	104.39	110.14
19	V	2	FRU	O6-C6-C5	2.81	120.94	111.29
19	Z	2	FRU	O2-C2-O5	2.80	114.91	109.50
19	V	1	GLC	O3-C3-C4	-2.77	103.94	110.35
19	S	1	GLC	O5-C1-C2	2.77	115.05	110.77
19	U	1	GLC	C1-C2-C3	-2.74	106.29	109.67
19	S	2	FRU	O2-C2-O5	-2.69	104.31	109.50
19	X	2	FRU	O5-C5-C6	2.66	116.24	108.85
19	T	1	GLC	C1-O5-C5	2.65	115.78	112.19
19	P	2	FRU	O2-C2-O5	2.61	114.55	109.50
19	U	1	GLC	C1-O5-C5	2.61	115.73	112.19
19	X	2	FRU	O4-C4-C5	-2.59	103.56	111.05
19	a	2	FRU	O3-C3-C4	-2.57	104.45	113.32
19	O	1	GLC	C1-O5-C5	-2.55	106.99	112.78
19	P	1	GLC	O4-C4-C3	2.53	116.20	110.35
19	S	2	FRU	O4-C4-C3	-2.50	104.66	112.15
19	O	1	GLC	O4-C4-C5	-2.46	104.21	109.67
19	Z	2	FRU	O5-C5-C6	2.45	115.68	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	1	GLC	O3-C3-C2	-2.45	105.30	109.99
19	T	2	FRU	O5-C5-C6	2.41	115.57	108.85
19	T	2	FRU	O1-C1-C2	-2.41	106.74	111.86
19	Z	1	GLC	C2-C3-C4	-2.40	106.73	110.89
19	P	1	GLC	O5-C1-C2	-2.40	107.06	110.77
19	M	1	GLC	O5-C5-C4	2.40	116.67	110.83
19	M	1	GLC	O3-C3-C2	2.39	114.56	109.99
19	X	1	GLC	O3-C3-C4	-2.39	104.83	110.35
19	a	2	FRU	O1-C1-C2	-2.38	106.80	111.86
19	Z	1	GLC	C1-O5-C5	-2.37	108.98	112.19
19	a	1	GLC	O3-C3-C2	-2.36	105.48	109.99
19	Y	1	GLC	O4-C4-C3	-2.34	104.93	110.35
19	O	1	GLC	O3-C3-C4	2.34	115.76	110.35
19	Q	1	GLC	C6-C5-C4	2.34	118.48	113.00
19	S	1	GLC	C3-C4-C5	2.32	114.39	110.24
19	Q	2	FRU	O1-C1-C2	-2.29	106.99	111.86
19	Y	2	FRU	C6-C5-C4	-2.29	109.58	115.09
19	Z	2	FRU	O4-C4-C5	-2.26	104.52	111.05
19	a	2	FRU	O4-C4-C3	-2.22	105.52	112.15
19	Z	2	FRU	C6-C5-C4	-2.20	109.79	115.09
19	O	1	GLC	C2-C3-C4	-2.18	107.12	110.89
19	U	1	GLC	O5-C5-C6	2.18	110.62	107.20
19	M	1	GLC	C1-C2-C3	-2.16	107.01	109.67
19	X	2	FRU	C6-C5-C4	-2.15	109.90	115.09
19	a	2	FRU	C6-C5-C4	2.13	120.21	115.09
19	Z	1	GLC	O2-C2-C3	-2.12	105.88	110.14
19	P	1	GLC	O3-C3-C2	2.04	113.91	109.99

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	a	2	FRU	C2
19	S	2	FRU	C2
19	O	2	FRU	C2
19	Z	2	FRU	C2
19	U	2	FRU	C2
19	T	2	FRU	C2
19	P	2	FRU	C2
19	M	2	FRU	C2
19	X	2	FRU	C2
19	W	2	FRU	C2
19	Y	2	FRU	C2

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Mol	Chain	Res	Type	Atom
19	V	2	FRU	C2
19	Q	2	FRU	C2

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	C4-C5-C6-O6
19	X	2	FRU	O1-C1-C2-C3
19	X	2	FRU	O1-C1-C2-O2
19	X	2	FRU	O1-C1-C2-O5
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	U	1	GLC	O5-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	U	2	FRU	O5-C5-C6-O6
19	Y	2	FRU	C4-C5-C6-O6
19	S	1	GLC	O5-C5-C6-O6
19	W	1	GLC	O5-C5-C6-O6
19	X	1	GLC	O5-C5-C6-O6
19	U	1	GLC	C4-C5-C6-O6
19	X	1	GLC	C4-C5-C6-O6
19	Q	2	FRU	O5-C5-C6-O6
19	Z	1	GLC	O5-C5-C6-O6
19	Y	2	FRU	O5-C5-C6-O6
19	Z	1	GLC	C4-C5-C6-O6
19	M	1	GLC	C4-C5-C6-O6
19	M	1	GLC	O5-C5-C6-O6
19	S	1	GLC	C4-C5-C6-O6
19	a	2	FRU	O1-C1-C2-O5
19	Q	2	FRU	O1-C1-C2-O5
19	P	2	FRU	C4-C5-C6-O6
19	V	1	GLC	O5-C5-C6-O6
19	T	1	GLC	C4-C5-C6-O6
19	U	2	FRU	O1-C1-C2-O5
19	W	1	GLC	C4-C5-C6-O6
19	T	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	C4-C5-C6-O6
19	T	2	FRU	O1-C1-C2-O5
19	M	2	FRU	O5-C5-C6-O6
19	S	2	FRU	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
19	a	2	FRU	O1-C1-C2-O2
19	T	2	FRU	O1-C1-C2-O2
19	a	2	FRU	O1-C1-C2-C3
19	V	1	GLC	C4-C5-C6-O6
19	W	2	FRU	O5-C5-C6-O6
19	Z	2	FRU	C4-C5-C6-O6
19	M	2	FRU	O1-C1-C2-O5
19	V	2	FRU	O1-C1-C2-O5
19	S	2	FRU	O1-C1-C2-C3
19	T	2	FRU	O1-C1-C2-C3
19	Y	2	FRU	O1-C1-C2-C3
19	P	1	GLC	C4-C5-C6-O6
19	W	2	FRU	C4-C5-C6-O6
19	S	2	FRU	O5-C5-C6-O6

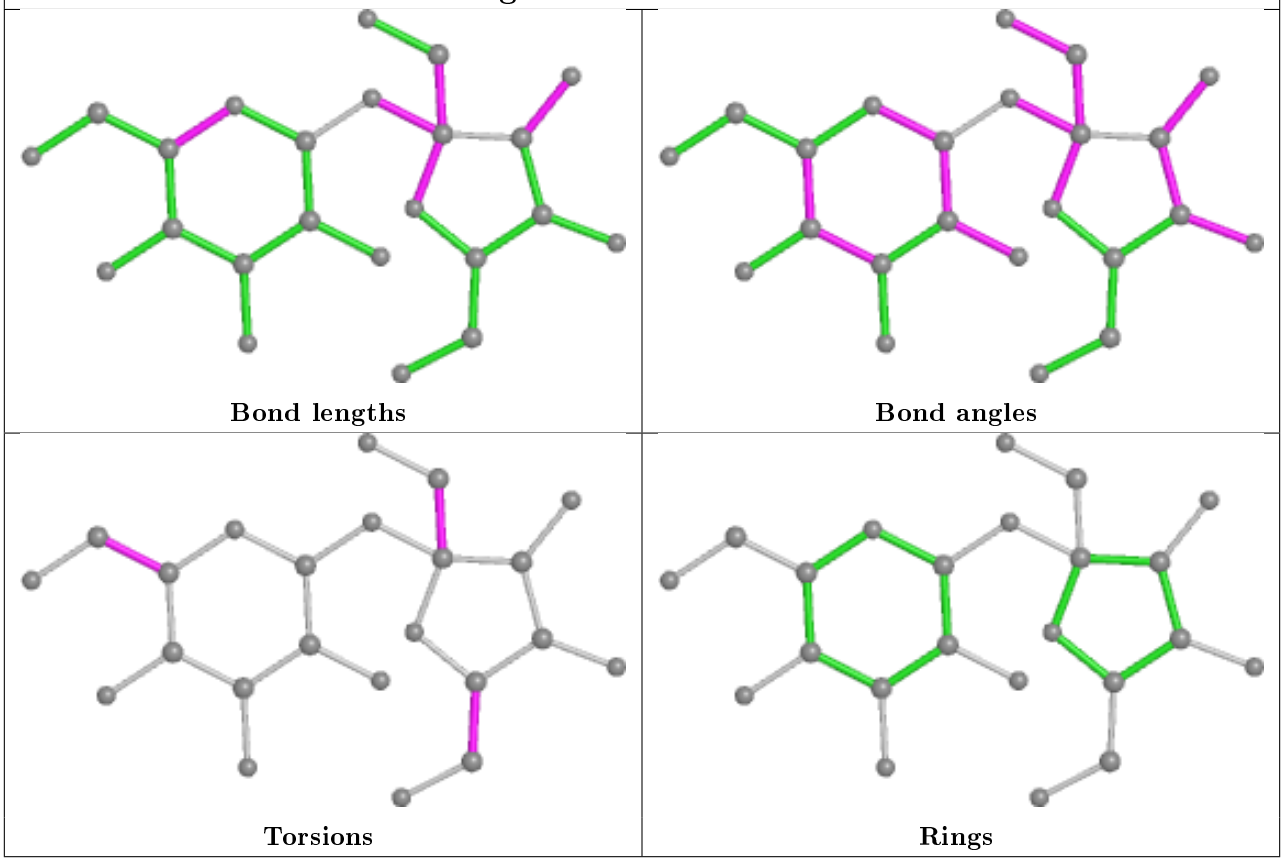
There are no ring outliers.

22 monomers are involved in 129 short contacts:

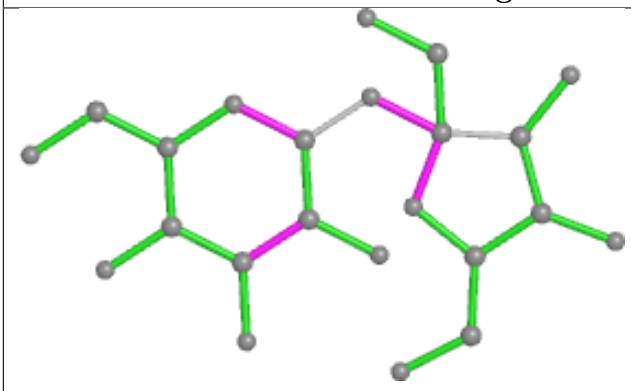
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S	2	FRU	7	0
19	O	2	FRU	7	0
19	S	1	GLC	6	0
19	Z	2	FRU	9	0
19	O	1	GLC	10	0
19	U	2	FRU	20	0
19	T	2	FRU	7	0
19	W	1	GLC	2	0
19	U	1	GLC	11	0
19	T	1	GLC	7	0
19	Z	1	GLC	13	0
19	P	1	GLC	13	0
19	P	2	FRU	17	0
19	X	1	GLC	9	0
19	Q	1	GLC	5	0
19	Y	1	GLC	7	0
19	X	2	FRU	8	0
19	V	1	GLC	1	0
19	W	2	FRU	3	0
19	Y	2	FRU	18	0
19	V	2	FRU	2	0
19	Q	2	FRU	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

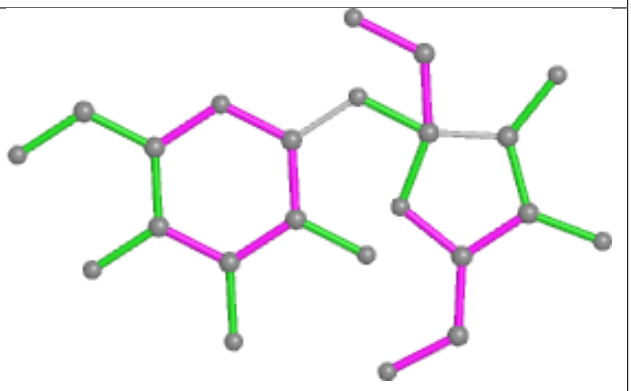
Oligosaccharide Chain S



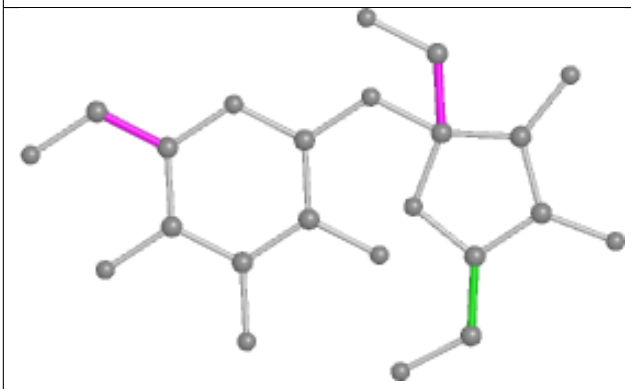
Oligosaccharide Chain T



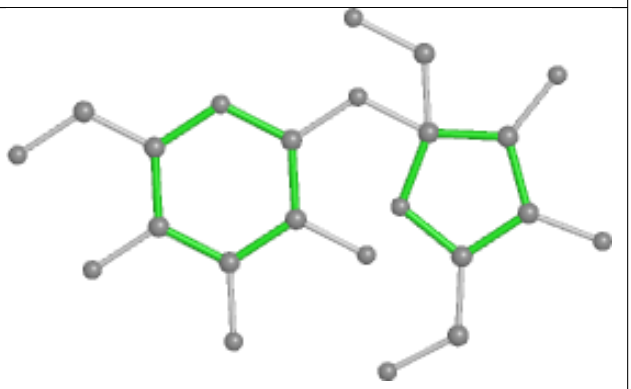
Bond lengths



Bond angles

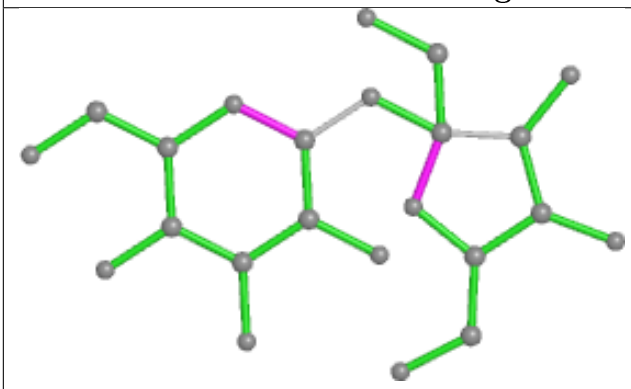


Torsions

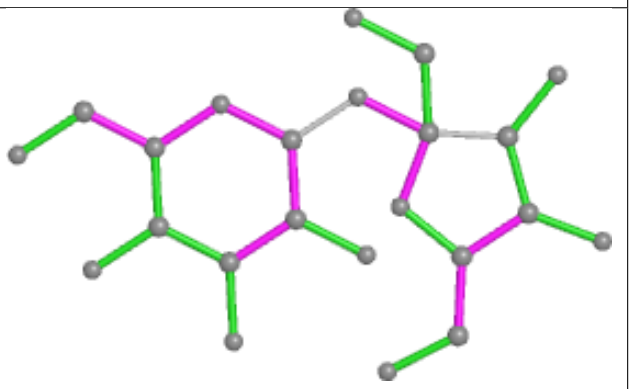


Rings

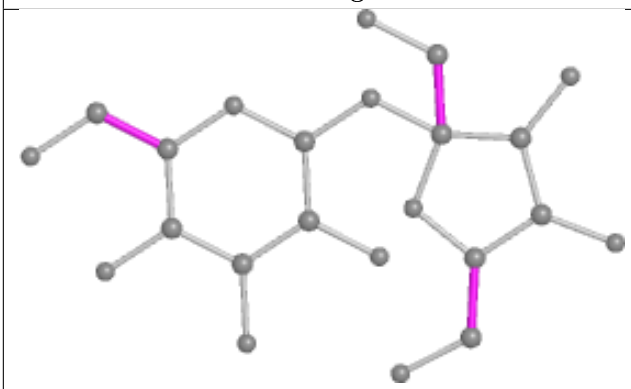
Oligosaccharide Chain U



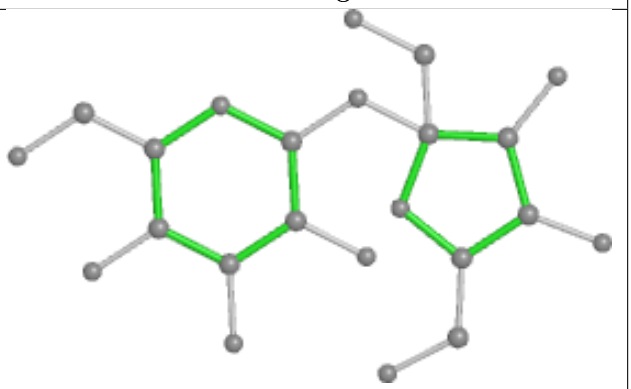
Bond lengths



Bond angles

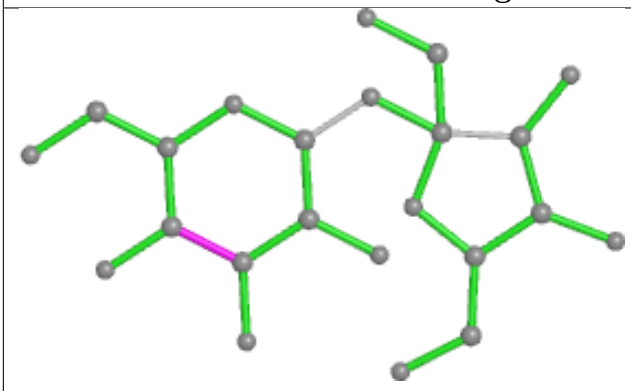


Torsions

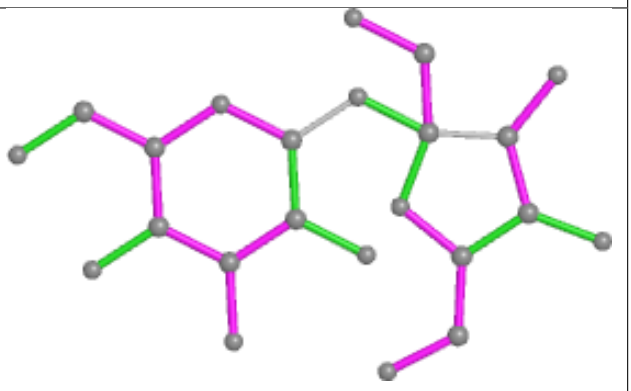


Rings

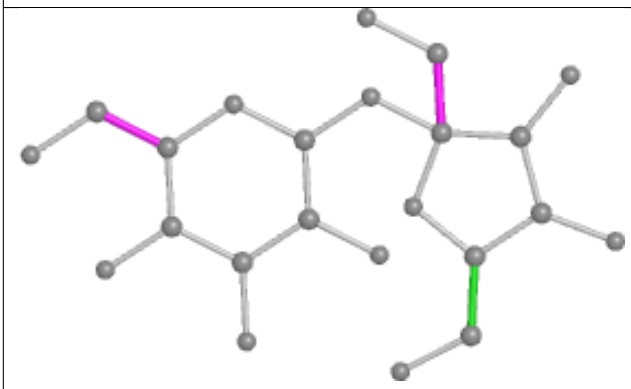
Oligosaccharide Chain V



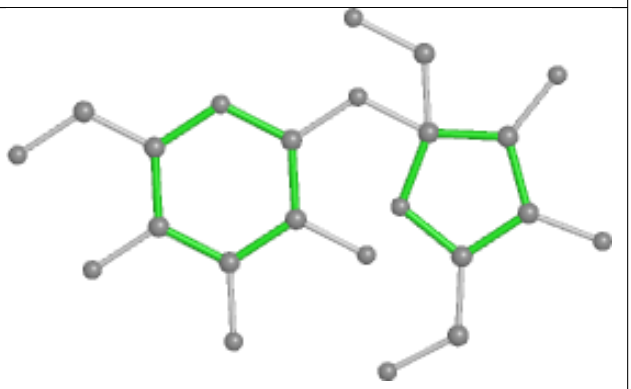
Bond lengths



Bond angles

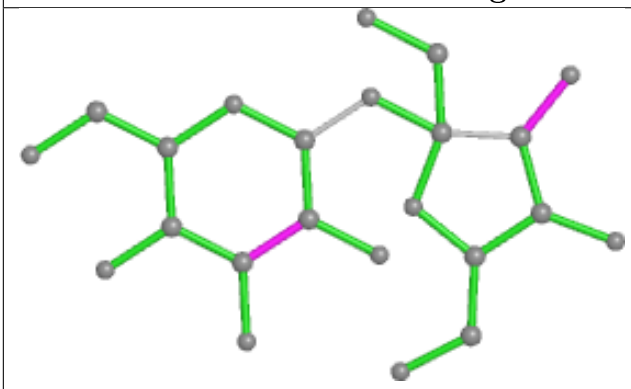


Torsions

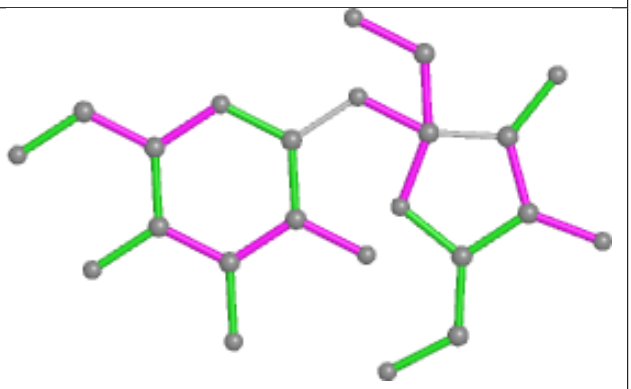


Rings

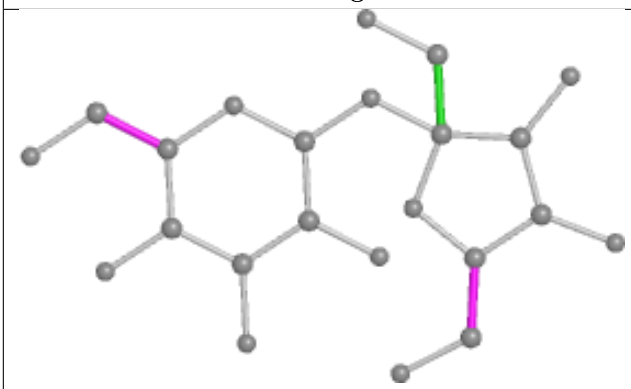
Oligosaccharide Chain W



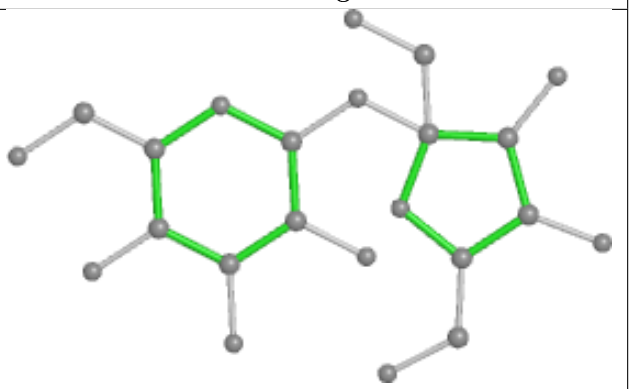
Bond lengths



Bond angles

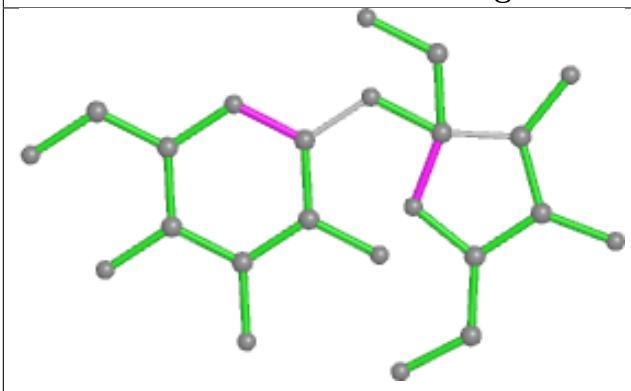


Torsions

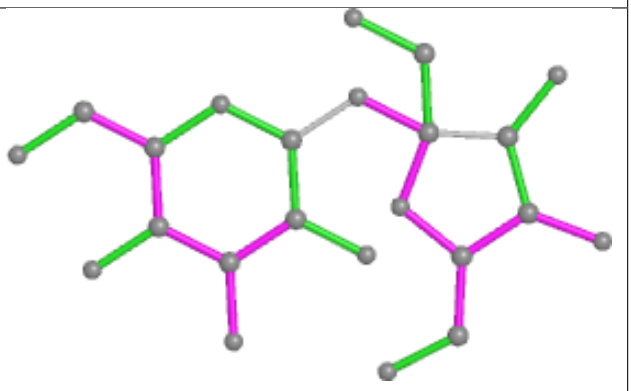


Rings

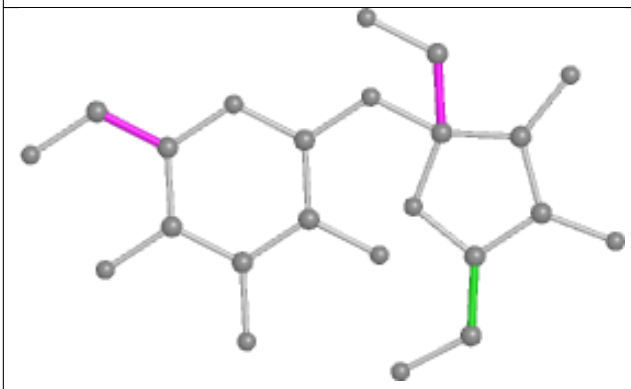
Oligosaccharide Chain X



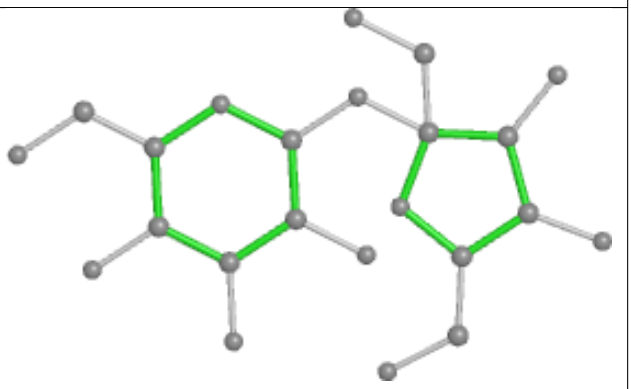
Bond lengths



Bond angles

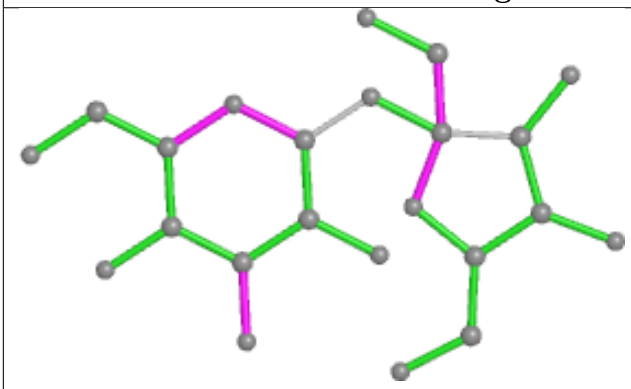


Torsions

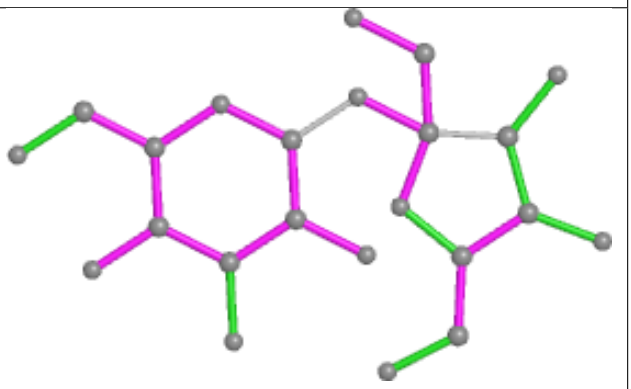


Rings

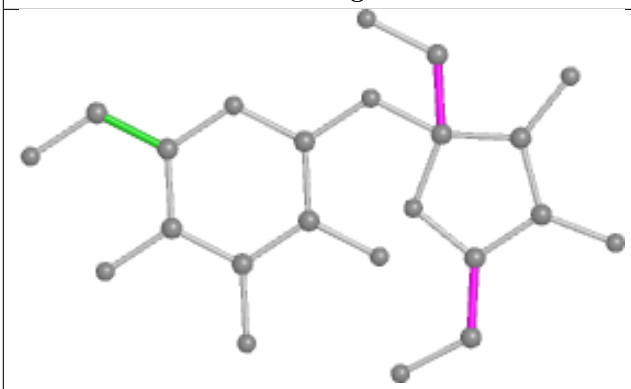
Oligosaccharide Chain Y



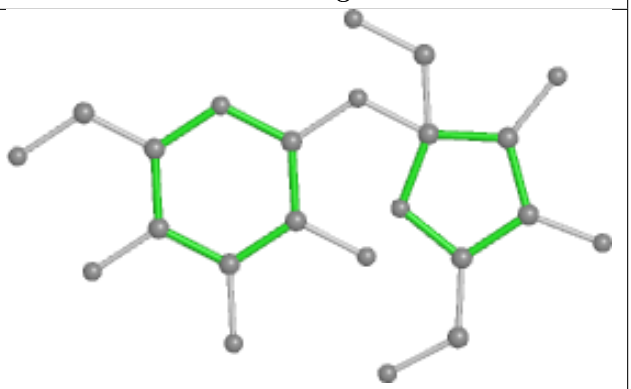
Bond lengths



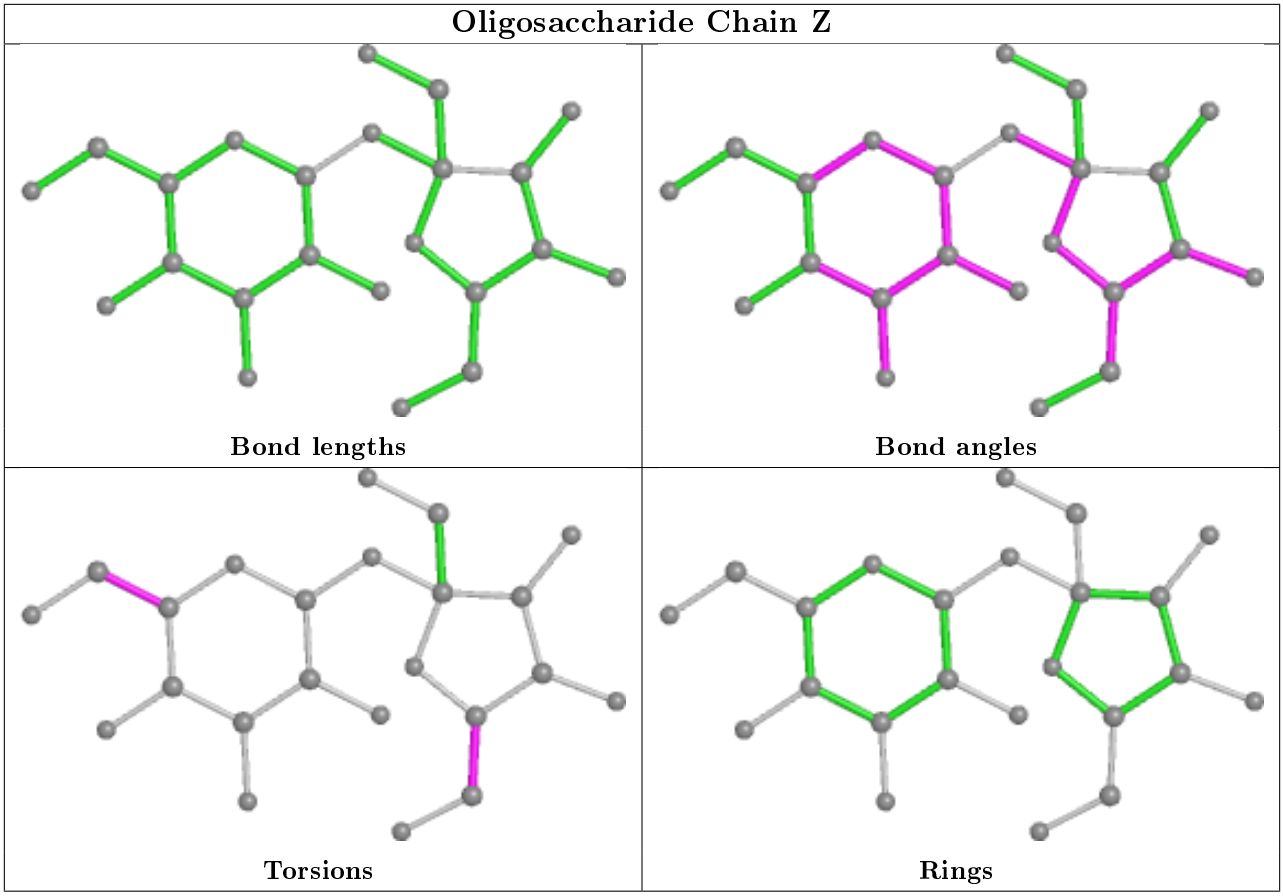
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 249 ligands modelled in this entry, 1 is unknown - leaving 248 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	J	103	-	55,69,73	2.11	12 (21%)	62,108,113	3.35	18 (29%)
22	BCR	B	852	-	41,41,41	3.47	21 (51%)	56,56,56	6.45	26 (46%)
20	CLA	4	316	-	40,54,73	2.83	17 (42%)	44,90,113	3.46	19 (43%)
20	CLA	A	809	-	46,60,73	2.20	14 (30%)	51,97,113	3.42	24 (47%)
20	CLA	3	303	-	22,32,73	2.82	11 (50%)	26,54,113	3.22	15 (57%)
20	CLA	B	825	-	59,73,73	2.13	12 (20%)	67,113,113	3.71	24 (35%)
20	CLA	B	806	-	59,73,73	2.12	14 (23%)	67,113,113	3.30	29 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	851	-	59,73,73	2.06	12 (20%)	67,113,113	3.02	23 (34%)
20	CLA	A	851	-	59,73,73	2.07	13 (22%)	67,113,113	3.09	21 (31%)
20	CLA	2	303	-	59,73,73	2.05	11 (18%)	67,113,113	2.94	25 (37%)
20	CLA	B	836	-	59,73,73	1.94	12 (20%)	67,113,113	2.87	17 (25%)
20	CLA	3	308	-	36,50,73	2.42	10 (27%)	39,85,113	4.23	20 (51%)
20	CLA	4	304	-	59,73,73	2.51	20 (33%)	67,113,113	4.08	29 (43%)
20	CLA	4	302	-	49,63,73	2.30	13 (26%)	55,101,113	3.57	18 (32%)
20	CLA	A	827	-	49,63,73	2.26	12 (24%)	55,101,113	3.43	20 (36%)
20	CLA	A	816	-	48,62,73	2.62	16 (33%)	53,99,113	3.83	22 (41%)
20	CLA	1	203	-	41,55,73	2.43	10 (24%)	45,91,113	4.23	19 (42%)
20	CLA	2	305	-	44,58,73	2.30	13 (29%)	49,95,113	3.73	20 (40%)
20	CLA	1	209	1	30,44,73	2.66	9 (30%)	35,78,113	3.98	13 (37%)
22	BCR	B	843	-	41,41,41	2.11	5 (12%)	56,56,56	5.92	21 (37%)
21	LMU	4	317	-	36,36,36	0.75	1 (2%)	47,47,47	1.15	3 (6%)
20	CLA	2	322	-	55,69,73	2.22	17 (30%)	62,108,113	3.53	28 (45%)
20	CLA	A	818	-	59,73,73	2.01	12 (20%)	67,113,113	3.11	25 (37%)
22	BCR	B	844	-	41,41,41	1.91	4 (9%)	56,56,56	5.05	24 (42%)
22	BCR	I	101	-	41,41,41	2.84	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	A	841	-	59,73,73	2.03	13 (22%)	67,113,113	3.61	21 (31%)
20	CLA	F	206	-	47,61,73	2.69	16 (34%)	52,98,113	3.57	21 (40%)
21	LMU	1	217	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
21	LMU	2	313	-	36,36,36	0.82	1 (2%)	47,47,47	0.91	2 (4%)
20	CLA	4	305	-	49,63,73	2.14	12 (24%)	55,101,113	3.23	20 (36%)
21	LMU	4	320	-	35,35,36	0.30	0	46,46,47	0.72	1 (2%)
20	CLA	B	811	-	52,66,73	2.67	18 (34%)	58,104,113	4.27	27 (46%)
20	CLA	3	310	-	22,32,73	2.27	9 (40%)	26,54,113	3.59	14 (53%)
20	CLA	B	814	-	40,54,73	2.46	11 (27%)	44,90,113	3.71	17 (38%)
22	BCR	A	847	-	41,41,41	2.06	5 (12%)	56,56,56	5.93	22 (39%)
21	LMU	N	101	-	36,36,36	0.55	1 (2%)	47,47,47	2.05	13 (27%)
20	CLA	2	310	-	22,32,73	1.89	5 (22%)	26,54,113	3.05	17 (65%)
20	CLA	4	306	-	44,58,73	2.71	15 (34%)	49,95,113	4.89	21 (42%)
21	LMU	4	322	-	36,36,36	0.75	1 (2%)	47,47,47	1.26	4 (8%)
22	BCR	F	203	-	41,41,41	3.03	14 (34%)	56,56,56	6.09	31 (55%)
22	BCR	A	845	-	41,41,41	2.00	5 (12%)	56,56,56	5.92	23 (41%)
20	CLA	A	812	-	48,62,73	2.16	10 (20%)	53,99,113	3.40	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LMU	L	205	-	36,36,36	0.80	2 (5%)	47,47,47	1.89	16 (34%)
21	LMU	H	107	-	36,36,36	0.77	0	47,47,47	2.24	14 (29%)
20	CLA	2	308	-	59,73,73	2.03	9 (15%)	67,113,113	3.04	23 (34%)
20	CLA	A	805	-	59,73,73	2.01	12 (20%)	67,113,113	3.04	21 (31%)
20	CLA	B	829	-	44,58,73	2.20	10 (22%)	49,95,113	3.44	20 (40%)
20	CLA	K	102	-	44,58,73	2.69	19 (43%)	49,95,113	4.06	22 (44%)
20	CLA	2	316	-	59,73,73	2.07	12 (20%)	67,113,113	3.89	21 (31%)
20	CLA	B	834	-	45,59,73	2.43	12 (26%)	50,96,113	3.88	19 (38%)
20	CLA	1	211	-	22,32,73	1.94	6 (27%)	26,54,113	3.28	17 (65%)
20	CLA	A	833	5	36,53,73	2.42	11 (30%)	39,89,113	4.73	21 (53%)
20	CLA	A	814	-	36,53,73	2.63	11 (30%)	39,89,113	3.80	16 (41%)
20	CLA	F	205	-	35,49,73	2.55	13 (37%)	38,84,113	4.05	18 (47%)
20	CLA	G	102	-	45,59,73	2.61	16 (35%)	50,96,113	4.15	20 (40%)
20	CLA	4	313	-	22,32,73	1.88	4 (18%)	26,54,113	3.18	18 (69%)
20	CLA	B	826	-	59,73,73	2.12	13 (22%)	67,113,113	3.29	22 (32%)
20	CLA	3	305	-	22,32,73	2.69	9 (40%)	26,54,113	3.50	16 (61%)
20	CLA	A	824	-	59,73,73	1.99	13 (22%)	67,113,113	3.22	19 (28%)
20	CLA	B	804	-	36,53,73	2.41	12 (33%)	39,89,113	3.81	16 (41%)
20	CLA	R	107	-	51,65,73	2.15	11 (21%)	57,103,113	3.85	22 (38%)
20	CLA	B	812	-	59,73,73	2.10	11 (18%)	67,113,113	2.67	21 (31%)
20	CLA	3	306	-	22,32,73	1.94	7 (31%)	26,54,113	3.27	16 (61%)
20	CLA	B	818	-	44,58,73	2.27	12 (27%)	49,95,113	3.68	18 (36%)
21	LMU	L	204	-	36,36,36	0.69	2 (5%)	47,47,47	2.38	14 (29%)
21	LMU	R	101	-	36,36,36	1.04	2 (5%)	47,47,47	2.44	13 (27%)
20	CLA	B	820	-	49,63,73	2.28	13 (26%)	55,101,113	3.51	18 (32%)
20	CLA	4	308	-	30,44,73	2.70	13 (43%)	35,78,113	4.37	14 (40%)
20	CLA	A	825	-	59,73,73	2.01	13 (22%)	67,113,113	3.22	18 (26%)
20	CLA	B	807	-	59,73,73	2.18	11 (18%)	67,113,113	3.17	23 (34%)
20	CLA	A	838	-	59,73,73	2.10	10 (16%)	67,113,113	3.31	23 (34%)
20	CLA	4	314	-	30,44,73	2.60	9 (30%)	35,78,113	4.59	18 (51%)
20	CLA	A	837	-	41,55,73	2.59	12 (29%)	45,91,113	3.92	20 (44%)
20	CLA	1	201	-	40,54,73	2.76	17 (42%)	44,90,113	4.80	27 (61%)
20	CLA	B	850	-	59,73,73	2.02	13 (22%)	67,113,113	3.32	24 (35%)
24	SF4	C	103	7	0,12,12	0.00	-	-		
20	CLA	1	208	-	22,32,73	3.08	11 (50%)	26,54,113	3.96	17 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	2	307	-	59,73,73	2.39	19 (32%)	67,113,113	3.74	22 (32%)
22	BCR	B	845	-	41,41,41	2.16	5 (12%)	56,56,56	5.93	23 (41%)
20	CLA	A	801	-	40,54,73	2.59	13 (32%)	48,90,113	5.54	29 (60%)
21	LMU	B	801	-	36,36,36	0.67	0	47,47,47	2.44	16 (34%)
20	CLA	3	309	-	22,32,73	2.00	7 (31%)	26,54,113	2.94	16 (61%)
20	CLA	B	816	-	54,68,73	2.01	11 (20%)	61,107,113	3.69	22 (36%)
20	CLA	B	830	-	59,73,73	2.10	13 (22%)	67,113,113	3.37	23 (34%)
20	CLA	1	207	-	45,59,73	2.43	14 (31%)	50,96,113	4.08	25 (50%)
20	CLA	3	313	-	59,73,73	2.55	18 (30%)	67,113,113	4.36	25 (37%)
22	BCR	A	844	-	41,41,41	2.03	4 (9%)	56,56,56	5.93	20 (35%)
20	CLA	3	311	-	59,73,73	2.29	18 (30%)	67,113,113	4.53	24 (35%)
20	CLA	3	316	-	22,32,73	2.01	6 (27%)	26,54,113	3.24	15 (57%)
20	CLA	A	811	-	59,73,73	2.09	11 (18%)	67,113,113	3.05	24 (35%)
21	LMU	H	108	-	36,36,36	1.03	3 (8%)	47,47,47	2.76	19 (40%)
20	CLA	2	315	-	22,32,73	1.92	6 (27%)	26,54,113	2.82	14 (53%)
21	LMU	E	101	-	36,36,36	0.93	2 (5%)	47,47,47	3.05	25 (53%)
20	CLA	H	102	-	49,63,73	2.27	10 (20%)	55,101,113	3.86	23 (41%)
21	LMU	R	105	-	36,36,36	0.86	1 (2%)	47,47,47	1.64	11 (23%)
21	LMU	A	848	-	36,36,36	0.87	0	47,47,47	1.41	6 (12%)
20	CLA	L	202	-	59,73,73	2.03	10 (16%)	67,113,113	2.66	21 (31%)
22	BCR	F	202	-	41,41,41	1.99	4 (9%)	56,56,56	5.89	20 (35%)
20	CLA	A	810	-	36,53,73	2.51	12 (33%)	39,89,113	4.25	19 (48%)
20	CLA	B	849	-	59,73,73	2.00	13 (22%)	67,113,113	3.37	25 (37%)
21	LMU	K	109	-	36,36,36	0.79	1 (2%)	47,47,47	2.27	12 (25%)
22	BCR	L	210	-	41,41,41	2.56	11 (26%)	56,56,56	5.71	20 (35%)
21	LMU	R	102	-	36,36,36	0.43	0	47,47,47	1.74	12 (25%)
21	LMU	K	104	-	36,36,36	0.67	1 (2%)	47,47,47	1.90	13 (27%)
20	CLA	3	302	-	44,58,73	3.14	14 (31%)	49,95,113	3.73	21 (42%)
20	CLA	4	311	-	49,63,73	2.26	9 (18%)	55,101,113	3.31	20 (36%)
20	CLA	B	805	-	54,68,73	2.11	10 (18%)	61,107,113	3.92	26 (42%)
21	LMU	1	219	-	36,36,36	1.02	2 (5%)	47,47,47	2.24	13 (27%)
21	LMU	B	802	-	36,36,36	1.02	4 (11%)	47,47,47	2.47	13 (27%)
22	BCR	J	102	-	41,41,41	1.93	4 (9%)	56,56,56	5.92	19 (33%)
20	CLA	A	850	-	59,73,73	2.12	12 (20%)	67,113,113	3.60	22 (32%)
20	CLA	K	103	-	59,73,73	2.05	10 (16%)	67,113,113	2.90	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LMU	H	106	-	36,36,36	1.05	4 (11%)	47,47,47	2.75	19 (40%)
20	CLA	J	101	-	42,56,73	2.44	13 (30%)	46,92,113	3.80	16 (34%)
21	LMU	3	322	-	36,36,36	0.71	0	47,47,47	1.91	11 (23%)
23	PQN	B	841	-	34,34,34	1.67	2 (5%)	42,45,45	1.60	6 (14%)
20	CLA	A	802	-	22,32,73	2.36	9 (40%)	26,54,113	3.99	14 (53%)
20	CLA	B	822	-	48,62,73	2.32	14 (29%)	53,99,113	2.87	24 (45%)
20	CLA	A	852	-	59,73,73	2.19	12 (20%)	67,113,113	3.33	21 (31%)
20	CLA	A	819	-	59,73,73	1.96	10 (16%)	67,113,113	3.28	21 (31%)
20	CLA	A	813	-	48,62,73	2.12	11 (22%)	53,99,113	3.49	22 (41%)
20	CLA	1	204	-	40,54,73	2.59	11 (27%)	44,90,113	2.67	18 (40%)
21	LMU	A	854	-	36,36,36	0.69	1 (2%)	47,47,47	1.89	11 (23%)
20	CLA	B	824	-	59,73,73	1.99	12 (20%)	67,113,113	3.15	18 (26%)
20	CLA	A	808	5	59,73,73	2.15	13 (22%)	67,113,113	3.35	25 (37%)
21	LMU	K	106	-	36,36,36	0.46	0	47,47,47	2.20	17 (36%)
20	CLA	A	803	-	44,58,73	2.38	13 (29%)	49,95,113	3.76	22 (44%)
20	CLA	B	821	-	59,73,73	2.92	21 (35%)	67,113,113	3.62	20 (29%)
20	CLA	B	833	20	36,53,73	2.52	10 (27%)	39,89,113	3.96	16 (41%)
20	CLA	3	318	-	59,73,73	1.92	11 (18%)	67,113,113	2.58	22 (32%)
21	LMU	H	104	-	36,36,36	1.13	4 (11%)	47,47,47	3.11	22 (46%)
21	LMU	R	103	-	36,36,36	0.78	0	47,47,47	2.05	14 (29%)
20	CLA	1	205	-	22,32,73	2.26	10 (45%)	26,54,113	4.03	16 (61%)
20	CLA	4	315	-	22,32,73	1.84	5 (22%)	26,54,113	2.61	15 (57%)
20	CLA	B	815	-	53,67,73	2.09	12 (22%)	59,105,113	2.60	18 (30%)
20	CLA	2	306	-	22,32,73	2.06	10 (45%)	26,54,113	3.48	15 (57%)
20	CLA	2	311	2	44,58,73	2.31	10 (22%)	49,95,113	3.67	19 (38%)
22	BCR	I	103	-	41,41,41	2.82	11 (26%)	56,56,56	6.56	29 (51%)
20	CLA	A	832	-	44,58,73	2.30	11 (25%)	49,95,113	3.50	19 (38%)
20	CLA	A	817	-	46,60,73	2.35	12 (26%)	51,97,113	3.83	19 (37%)
20	CLA	R	108	-	52,66,73	2.70	16 (30%)	58,104,113	3.51	25 (43%)
20	CLA	1	215	-	55,69,73	2.24	16 (29%)	62,108,113	3.57	27 (43%)
20	CLA	2	304	-	22,32,73	2.48	11 (50%)	26,54,113	3.56	17 (65%)
20	CLA	H	101	-	49,63,73	2.54	17 (34%)	55,101,113	4.84	26 (47%)
20	CLA	A	821	5	36,50,73	2.45	10 (27%)	39,85,113	4.26	17 (43%)
20	CLA	A	839	-	59,73,73	2.47	16 (27%)	67,113,113	3.86	27 (40%)
20	CLA	3	317	-	44,58,73	2.36	10 (22%)	49,95,113	2.88	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LMU	R	104	-	36,36,36	0.77	1 (2%)	47,47,47	2.17	18 (38%)
20	CLA	3	320	-	22,32,73	1.87	5 (22%)	26,54,113	2.79	11 (42%)
21	LMU	A	849	-	36,36,36	0.86	1 (2%)	47,47,47	1.67	10 (21%)
20	CLA	B	817	-	55,69,73	2.02	12 (21%)	62,108,113	3.60	23 (37%)
20	CLA	4	319	-	41,55,73	2.35	12 (29%)	45,91,113	3.75	16 (35%)
20	CLA	L	209	-	44,58,73	2.47	14 (31%)	49,95,113	4.24	20 (40%)
20	CLA	B	823	-	52,66,73	2.19	12 (23%)	58,104,113	3.45	18 (31%)
24	SF4	A	857	5,6	0,12,12	0.00	-	-		
20	CLA	B	827	-	59,73,73	2.02	13 (22%)	67,113,113	3.08	19 (28%)
24	SF4	C	102	7	0,12,12	0.00	-	-		
21	LMU	4	321	-	36,36,36	0.95	1 (2%)	47,47,47	1.40	8 (17%)
20	CLA	I	102	-	54,68,73	2.08	10 (18%)	61,107,113	3.74	19 (31%)
21	LMU	3	321	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
21	LMU	2	320	-	36,36,36	1.04	1 (2%)	47,47,47	1.37	3 (6%)
20	CLA	B	810	-	49,63,73	2.08	11 (22%)	55,101,113	3.52	21 (38%)
20	CLA	L	207	16	44,58,73	2.37	12 (27%)	49,95,113	3.74	20 (40%)
20	CLA	3	307	-	22,32,73	1.91	7 (31%)	26,54,113	3.27	17 (65%)
21	LMU	H	105	-	36,36,36	0.98	1 (2%)	47,47,47	2.33	16 (34%)
21	LMU	2	318	-	36,36,36	1.06	1 (2%)	47,47,47	1.93	15 (31%)
20	CLA	1	216	-	22,32,73	2.27	11 (50%)	26,54,113	2.91	16 (61%)
20	CLA	4	307	-	46,60,73	3.13	22 (47%)	51,97,113	5.12	36 (70%)
21	LMU	1	218	-	36,36,36	0.44	0	47,47,47	1.61	9 (19%)
20	CLA	4	310	-	22,32,73	2.75	11 (50%)	26,54,113	3.05	14 (53%)
21	LMU	D	201	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
21	LMU	1	213	-	36,36,36	0.81	0	47,47,47	2.10	16 (34%)
20	CLA	B	840	-	30,44,73	2.72	11 (36%)	35,78,113	4.39	19 (54%)
20	CLA	B	828	-	44,58,73	2.42	9 (20%)	49,95,113	3.42	23 (46%)
21	LMU	K	105	-	36,36,36	0.53	0	47,47,47	2.04	15 (31%)
20	CLA	A	804	-	49,63,73	2.34	11 (22%)	55,101,113	2.78	19 (34%)
20	CLA	A	836	-	41,55,73	2.34	11 (26%)	45,91,113	2.38	17 (37%)
20	CLA	A	822	-	49,63,73	2.24	11 (22%)	55,101,113	3.60	22 (40%)
20	CLA	1	210	-	45,59,73	3.09	19 (42%)	50,96,113	4.84	26 (52%)
20	CLA	K	108	-	44,58,73	2.31	13 (29%)	49,95,113	3.70	18 (36%)
21	LMU	L	211	-	36,36,36	0.87	1 (2%)	47,47,47	1.50	9 (19%)
21	LMU	B	847	-	36,36,36	1.00	1 (2%)	47,47,47	2.37	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	B	846	-	41,41,41	2.10	4 (9%)	56,56,56	5.93	21 (37%)
20	CLA	B	809	-	48,62,73	2.43	10 (20%)	58,100,113	3.39	24 (41%)
20	CLA	A	829	-	44,58,73	2.27	10 (22%)	49,95,113	3.80	23 (46%)
20	CLA	A	834	-	43,57,73	2.40	11 (25%)	46,93,113	3.83	19 (41%)
20	CLA	A	820	-	45,59,73	2.34	12 (26%)	50,96,113	3.55	20 (40%)
20	CLA	B	831	-	44,58,73	2.43	14 (31%)	49,95,113	4.01	22 (44%)
20	CLA	B	803	-	59,73,73	2.15	13 (22%)	67,113,113	2.62	25 (37%)
20	CLA	B	808	6	59,73,73	1.94	11 (18%)	67,113,113	3.43	20 (29%)
21	LMU	2	317	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
21	LMU	A	855	-	36,36,36	0.78	1 (2%)	47,47,47	1.95	17 (36%)
20	CLA	3	301	-	30,44,73	2.50	9 (30%)	35,78,113	4.52	19 (54%)
20	CLA	B	837	-	41,55,73	2.33	12 (29%)	45,91,113	3.65	18 (40%)
21	LMU	A	856	-	36,36,36	0.78	1 (2%)	47,47,47	1.59	8 (17%)
20	CLA	1	214	-	22,32,73	1.80	5 (22%)	26,54,113	3.10	17 (65%)
22	BCR	B	842	-	41,41,41	1.97	4 (9%)	56,56,56	5.89	20 (35%)
20	CLA	4	303	-	30,44,73	2.92	12 (40%)	35,78,113	4.79	18 (51%)
20	CLA	H	103	-	49,63,73	2.23	13 (26%)	55,101,113	3.63	20 (36%)
21	LMU	A	853	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
20	CLA	K	101	-	36,53,73	2.56	12 (33%)	39,89,113	4.10	15 (38%)
20	CLA	B	835	-	54,68,73	2.00	10 (18%)	61,107,113	3.57	16 (26%)
20	CLA	3	319	-	22,32,73	2.50	10 (45%)	26,54,113	3.64	16 (61%)
20	CLA	B	839	-	59,73,73	1.98	14 (23%)	67,113,113	2.96	21 (31%)
20	CLA	B	838	-	59,73,73	2.08	13 (22%)	67,113,113	3.00	24 (35%)
20	CLA	2	301	-	22,32,73	3.15	11 (50%)	26,54,113	3.74	17 (65%)
21	LMU	4	301	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)
20	CLA	1	202	-	51,65,73	2.46	18 (35%)	57,103,113	4.16	27 (47%)
25	LMG	B	848	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
21	LMU	G	101	-	36,36,36	1.02	2 (5%)	47,47,47	2.58	13 (27%)
20	CLA	1	206	-	55,69,73	2.15	11 (20%)	62,108,113	3.06	20 (32%)
20	CLA	A	807	-	40,54,73	2.92	19 (47%)	44,90,113	5.25	24 (54%)
20	CLA	B	832	20	36,53,73	2.72	11 (30%)	39,89,113	4.13	17 (43%)
20	CLA	B	813	-	54,68,73	2.10	12 (22%)	61,107,113	2.92	19 (31%)
21	LMU	C	101	-	36,36,36	0.85	1 (2%)	47,47,47	1.37	7 (14%)
20	CLA	A	830	-	59,73,73	2.05	13 (22%)	67,113,113	3.30	19 (28%)
20	CLA	3	304	-	30,44,73	2.55	9 (30%)	35,78,113	3.93	15 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PQN	A	842	-	34,34,34	1.73	3 (8%)	42,45,45	1.52	7 (16%)
20	CLA	A	831	-	49,63,73	2.14	11 (22%)	55,101,113	3.54	22 (40%)
20	CLA	A	815	-	44,58,73	3.02	21 (47%)	49,95,113	4.96	31 (63%)
20	CLA	A	840	-	44,58,73	2.30	10 (22%)	49,95,113	3.83	19 (38%)
20	CLA	2	309	-	22,32,73	1.98	6 (27%)	26,54,113	3.15	15 (57%)
20	CLA	4	309	-	22,32,73	3.09	13 (59%)	26,54,113	4.03	17 (65%)
20	CLA	A	826	-	59,73,73	2.00	11 (18%)	67,113,113	3.61	26 (38%)
22	BCR	A	846	-	41,41,41	2.08	4 (9%)	56,56,56	5.92	22 (39%)
21	LMU	R	106	-	36,36,36	0.88	1 (2%)	47,47,47	1.57	10 (21%)
20	CLA	4	312	-	22,32,73	1.93	6 (27%)	26,54,113	3.25	15 (57%)
22	BCR	3	314	-	41,41,41	2.06	5 (12%)	56,56,56	5.89	21 (37%)
20	CLA	F	204	-	30,44,73	2.56	8 (26%)	35,78,113	3.84	21 (60%)
20	CLA	3	312	-	22,32,73	2.86	9 (40%)	26,54,113	4.43	19 (73%)
21	LMU	1	220	-	36,36,36	0.59	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	H	109	-	54,68,73	2.09	12 (22%)	61,107,113	3.55	22 (36%)
20	CLA	1	212	-	22,32,73	2.44	9 (40%)	26,54,113	3.71	16 (61%)
20	CLA	L	203	-	49,63,73	2.32	10 (20%)	55,101,113	2.96	21 (38%)
21	LMU	R	109	-	36,36,36	0.37	0	47,47,47	0.70	1 (2%)
20	CLA	L	201	-	49,63,73	2.64	16 (32%)	55,101,113	4.50	24 (43%)
20	CLA	B	819	-	40,54,73	2.38	9 (22%)	44,90,113	4.14	18 (40%)
20	CLA	2	302	-	45,59,73	2.31	12 (26%)	50,96,113	3.64	17 (34%)
20	CLA	A	823	-	59,73,73	1.87	10 (16%)	67,113,113	2.59	21 (31%)
20	CLA	A	828	-	59,73,73	1.99	12 (20%)	67,113,113	3.50	24 (35%)
20	CLA	2	312	-	44,58,73	2.42	10 (22%)	49,95,113	4.29	19 (38%)
20	CLA	L	208	-	41,55,73	2.34	9 (21%)	45,91,113	4.05	25 (55%)
20	CLA	4	318	-	46,60,73	2.83	16 (34%)	51,97,113	4.57	25 (49%)
22	BCR	A	843	-	41,41,41	1.93	4 (9%)	56,56,56	5.89	19 (33%)
21	LMU	F	201	-	35,35,36	1.30	4 (11%)	46,46,47	2.37	15 (32%)
21	LMU	2	319	-	36,36,36	1.01	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	A	806	-	49,63,73	2.22	11 (22%)	55,101,113	3.61	21 (38%)
20	CLA	A	835	-	59,73,73	2.10	12 (20%)	67,113,113	3.29	24 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	J	103	-	4/4/19/25	24/33/131/135	-
22	BCR	B	852	-	-	12/29/63/63	0/2/2/2
20	CLA	4	316	-	3/3/16/25	10/15/113/135	-
20	CLA	A	809	-	3/3/17/25	10/22/120/135	-
20	CLA	3	303	-	3/3/7/25	-	-
20	CLA	B	825	-	4/4/20/25	16/37/135/135	-
20	CLA	B	806	-	4/4/20/25	17/37/135/135	-
20	CLA	B	851	-	4/4/20/25	18/37/135/135	-
20	CLA	A	851	-	4/4/20/25	18/37/135/135	-
20	CLA	2	303	-	4/4/20/25	17/37/135/135	-
20	CLA	B	836	-	4/4/20/25	17/37/135/135	-
20	CLA	3	308	-	3/3/15/25	5/10/108/135	-
20	CLA	4	304	-	5/5/20/25	20/37/135/135	-
20	CLA	4	302	-	4/4/18/25	14/25/123/135	-
20	CLA	A	827	-	4/4/18/25	11/25/123/135	-
20	CLA	A	816	-	3/3/17/25	11/24/122/135	-
20	CLA	1	203	-	3/3/16/25	8/16/114/135	-
20	CLA	2	305	-	3/3/17/25	9/19/117/135	-
20	CLA	1	209	1	3/3/14/25	-	-
22	BCR	B	843	-	-	7/29/63/63	0/2/2/2
21	LMU	4	317	-	-	13/21/61/61	0/2/2/2
20	CLA	2	322	-	4/4/19/25	21/33/131/135	-
20	CLA	A	818	-	4/4/20/25	18/37/135/135	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	A	841	-	4/4/20/25	16/37/135/135	-
20	CLA	F	206	-	6/6/17/25	9/23/121/135	-
21	LMU	1	217	-	-	14/21/61/61	0/2/2/2
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	4	305	-	4/4/18/25	12/25/123/135	-
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
20	CLA	B	811	-	4/4/18/25	17/29/127/135	-
20	CLA	3	310	-	3/3/7/25	-	-
21	LMU	A	848	-	-	16/21/61/61	0/2/2/2
20	CLA	B	814	-	3/3/16/25	9/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	847	-	-	10/29/63/63	0/2/2/2
21	LMU	N	101	-	-	15/21/61/61	0/2/2/2
20	CLA	2	310	-	3/3/7/25	-	-
20	CLA	4	306	-	3/3/17/25	9/19/117/135	-
21	LMU	4	322	-	-	14/21/61/61	0/2/2/2
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
22	BCR	A	845	-	-	14/29/63/63	0/2/2/2
20	CLA	A	812	-	3/3/17/25	13/24/122/135	-
21	LMU	L	205	-	-	14/21/61/61	0/2/2/2
21	LMU	H	107	-	-	12/21/61/61	0/2/2/2
20	CLA	2	308	-	4/4/20/25	15/37/135/135	-
20	CLA	A	805	-	4/4/20/25	23/37/135/135	-
20	CLA	B	829	-	3/3/17/25	12/19/117/135	-
20	CLA	K	102	-	3/3/17/25	9/19/117/135	-
21	LMU	L	204	-	-	14/21/61/61	0/2/2/2
20	CLA	2	316	-	4/4/20/25	17/37/135/135	-
20	CLA	B	834	-	3/3/17/25	9/21/119/135	-
20	CLA	1	211	-	3/3/7/25	-	-
20	CLA	A	833	5	3/3/16/25	5/11/111/135	-
20	CLA	A	814	-	3/3/16/25	7/11/111/135	-
20	CLA	F	205	-	3/3/15/25	5/8/106/135	-
20	CLA	G	102	-	3/3/17/25	8/21/119/135	-
20	CLA	4	313	-	3/3/7/25	-	-
20	CLA	B	826	-	4/4/20/25	17/37/135/135	-
20	CLA	3	305	-	3/3/7/25	-	-
20	CLA	A	824	-	4/4/20/25	17/37/135/135	-
20	CLA	B	804	-	3/3/16/25	6/11/111/135	-
20	CLA	R	107	-	4/4/18/25	13/28/126/135	-
20	CLA	B	812	-	4/4/20/25	24/37/135/135	-
20	CLA	3	306	-	3/3/7/25	-	-
20	CLA	B	818	-	3/3/17/25	6/19/117/135	-
20	CLA	2	306	-	3/3/7/25	-	-
21	LMU	R	101	-	1/1/10/10	11/21/61/61	0/2/2/2
21	LMU	K	105	-	-	18/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	820	-	4/4/18/25	9/25/123/135	-
20	CLA	4	308	-	3/3/14/25	-	-
20	CLA	A	825	-	4/4/20/25	22/37/135/135	-
20	CLA	B	807	-	4/4/20/25	9/37/135/135	-
20	CLA	A	838	-	4/4/20/25	19/37/135/135	-
20	CLA	4	314	-	3/3/14/25	-	-
21	LMU	A	853	-	-	19/21/61/61	0/2/2/2
20	CLA	A	837	-	3/3/16/25	11/16/114/135	-
20	CLA	1	201	-	3/3/16/25	10/15/113/135	-
20	CLA	B	850	-	4/4/20/25	15/37/135/135	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	1	208	-	3/3/7/25	-	-
20	CLA	2	307	-	4/4/20/25	20/37/135/135	-
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
20	CLA	A	801	-	5/5/16/25	12/16/112/135	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2
20	CLA	3	309	-	3/3/7/25	-	-
20	CLA	B	816	-	4/4/19/25	13/31/129/135	-
20	CLA	B	830	-	4/4/20/25	21/37/135/135	-
20	CLA	1	207	-	4/4/17/25	9/21/119/135	-
20	CLA	3	313	-	4/4/20/25	18/37/135/135	-
22	BCR	A	844	-	-	12/29/63/63	0/2/2/2
20	CLA	3	316	-	3/3/7/25	-	-
20	CLA	A	811	-	4/4/20/25	25/37/135/135	-
21	LMU	H	108	-	-	14/21/61/61	0/2/2/2
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
20	CLA	2	315	-	3/3/7/25	-	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
21	LMU	3	322	-	-	15/21/61/61	0/2/2/2
20	CLA	L	202	-	4/4/20/25	15/37/135/135	-
21	LMU	R	105	-	-	15/21/61/61	0/2/2/2
20	CLA	4	319	-	3/3/16/25	9/16/114/135	-
20	CLA	B	815	-	4/4/18/25	12/30/128/135	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	810	-	3/3/16/25	3/11/111/135	-
20	CLA	B	849	-	4/4/20/25	21/37/135/135	-
21	LMU	K	109	-	-	12/21/61/61	0/2/2/2
22	BCR	L	210	-	-	10/29/63/63	0/2/2/2
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
21	LMU	K	104	-	-	12/21/61/61	0/2/2/2
20	CLA	3	302	-	3/3/17/25	3/19/117/135	-
20	CLA	4	311	-	4/4/18/25	13/25/123/135	-
20	CLA	B	805	-	4/4/19/25	21/31/129/135	-
20	CLA	A	822	-	4/4/18/25	9/25/123/135	-
20	CLA	1	214	-	3/3/7/25	-	-
22	BCR	J	102	-	-	12/29/63/63	0/2/2/2
20	CLA	A	850	-	4/4/20/25	25/37/135/135	-
20	CLA	K	103	-	4/4/20/25	21/37/135/135	-
21	LMU	H	106	-	-	13/21/61/61	0/2/2/2
20	CLA	J	101	-	3/3/16/25	10/17/115/135	-
20	CLA	B	838	-	4/4/20/25	20/37/135/135	-
23	PQN	B	841	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	A	802	-	3/3/7/25	-	-
20	CLA	B	822	-	3/3/17/25	8/24/122/135	-
20	CLA	A	852	-	4/4/20/25	24/37/135/135	-
20	CLA	A	819	-	4/4/20/25	16/37/135/135	-
20	CLA	A	813	-	3/3/17/25	11/24/122/135	-
20	CLA	1	204	-	3/3/16/25	6/15/113/135	-
21	LMU	A	854	-	-	11/21/61/61	0/2/2/2
20	CLA	B	824	-	4/4/20/25	21/37/135/135	-
20	CLA	A	808	5	4/4/20/25	21/37/135/135	-
21	LMU	K	106	-	-	15/21/61/61	0/2/2/2
20	CLA	A	803	-	3/3/17/25	5/19/117/135	-
20	CLA	B	821	-	3/3/20/25	19/37/135/135	-
20	CLA	B	833	20	3/3/16/25	6/11/111/135	-
20	CLA	3	318	-	4/4/20/25	19/37/135/135	-
21	LMU	H	104	-	-	14/21/61/61	0/2/2/2
21	LMU	R	103	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	205	-	3/3/7/25	-	-
20	CLA	4	315	-	3/3/7/25	-	-
20	CLA	3	311	-	4/4/20/25	22/37/135/135	-
21	LMU	R	106	-	-	13/21/61/61	0/2/2/2
20	CLA	2	311	2	3/3/17/25	6/19/117/135	-
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	A	832	-	3/3/17/25	12/19/117/135	-
20	CLA	A	817	-	3/3/17/25	14/22/120/135	-
20	CLA	R	108	-	4/4/18/25	17/29/127/135	-
20	CLA	2	304	-	3/3/7/25	-	-
20	CLA	H	101	-	4/4/18/25	16/25/123/135	-
20	CLA	A	821	5	3/3/15/25	2/10/108/135	-
20	CLA	A	839	-	4/4/20/25	22/37/135/135	-
20	CLA	3	317	-	3/3/17/25	9/19/117/135	-
21	LMU	R	104	-	-	17/21/61/61	0/2/2/2
20	CLA	3	320	-	3/3/7/25	-	-
21	LMU	A	849	-	-	13/21/61/61	0/2/2/2
20	CLA	B	817	-	4/4/19/25	17/33/131/135	-
20	CLA	L	209	-	4/4/17/25	10/19/117/135	-
24	SF4	A	857	5,6	-	-	0/6/5/5
20	CLA	B	827	-	4/4/20/25	27/37/135/135	-
24	SF4	C	102	7	-	-	0/6/5/5
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	I	102	-	4/4/19/25	13/31/129/135	-
21	LMU	3	321	-	-	11/21/61/61	0/2/2/2
21	LMU	2	320	-	-	8/21/61/61	0/2/2/2
20	CLA	B	810	-	4/4/18/25	12/25/123/135	-
20	CLA	L	207	16	3/3/17/25	8/19/117/135	-
20	CLA	3	307	-	3/3/7/25	-	-
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	1	216	-	3/3/7/25	-	-
20	CLA	4	307	-	4/4/17/25	7/22/120/135	-
21	LMU	1	218	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	310	-	3/3/7/25	-	-
21	LMU	D	201	-	-	14/21/61/61	0/2/2/2
21	LMU	1	213	-	-	13/21/61/61	0/2/2/2
20	CLA	B	840	-	3/3/14/25	-	-
20	CLA	B	828	-	3/3/17/25	9/19/117/135	-
20	CLA	B	823	-	4/4/18/25	17/29/127/135	-
20	CLA	A	804	-	4/4/18/25	13/25/123/135	-
20	CLA	A	836	-	3/3/16/25	8/16/114/135	-
20	CLA	1	215	-	4/4/19/25	21/33/131/135	-
20	CLA	1	210	-	4/4/17/25	9/21/119/135	-
20	CLA	K	108	-	3/3/17/25	5/19/117/135	-
21	LMU	L	211	-	-	14/21/61/61	0/2/2/2
21	LMU	B	847	-	-	10/21/61/61	0/2/2/2
22	BCR	B	846	-	-	12/29/63/63	0/2/2/2
20	CLA	B	809	-	4/4/18/25	11/25/121/135	-
20	CLA	A	829	-	3/3/17/25	3/19/117/135	-
20	CLA	A	834	-	3/3/16/25	9/18/116/135	-
20	CLA	A	820	-	3/3/17/25	9/21/119/135	-
20	CLA	B	831	-	3/3/17/25	6/19/117/135	-
20	CLA	B	803	-	4/4/20/25	21/37/135/135	-
20	CLA	B	808	6	4/4/20/25	19/37/135/135	-
21	LMU	2	317	-	-	14/21/61/61	0/2/2/2
21	LMU	A	855	-	-	14/21/61/61	0/2/2/2
20	CLA	3	301	-	3/3/14/25	-	-
20	CLA	B	837	-	3/3/16/25	6/16/114/135	-
21	LMU	A	856	-	-	14/21/61/61	0/2/2/2
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
20	CLA	4	303	-	3/3/14/25	-	-
20	CLA	H	103	-	4/4/18/25	14/25/123/135	-
21	LMU	1	219	-	-	13/21/61/61	0/2/2/2
20	CLA	K	101	-	3/3/16/25	5/11/111/135	-
20	CLA	B	835	-	4/4/19/25	15/31/129/135	-
20	CLA	3	319	-	3/3/7/25	-	-
20	CLA	B	839	-	4/4/20/25	18/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	301	-	3/3/7/25	-	-
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
20	CLA	1	202	-	4/4/18/25	16/28/126/135	-
25	LMG	B	848	-	-	23/44/64/70	0/1/1/1
21	LMU	G	101	-	-	15/21/61/61	0/2/2/2
20	CLA	1	206	-	4/4/19/25	20/33/131/135	-
20	CLA	A	807	-	3/3/16/25	6/15/113/135	-
20	CLA	B	832	20	3/3/16/25	9/11/111/135	-
20	CLA	B	813	-	4/4/19/25	14/31/129/135	-
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	830	-	4/4/20/25	21/37/135/135	-
20	CLA	3	304	-	3/3/14/25	-	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	A	831	-	4/4/18/25	14/25/123/135	-
20	CLA	A	815	-	3/3/17/25	8/19/117/135	-
20	CLA	A	840	-	3/3/17/25	11/19/117/135	-
20	CLA	2	309	-	3/3/7/25	-	-
20	CLA	4	309	-	3/3/7/25	-	-
20	CLA	A	826	-	4/4/20/25	16/37/135/135	-
22	BCR	A	846	-	-	17/29/63/63	0/2/2/2
20	CLA	4	312	-	3/3/7/25	-	-
22	BCR	3	314	-	-	13/29/63/63	0/2/2/2
20	CLA	F	204	-	3/3/14/25	-	-
20	CLA	3	312	-	3/3/7/25	-	-
21	LMU	1	220	-	-	13/21/61/61	0/2/2/2
20	CLA	H	109	-	4/4/19/25	13/31/129/135	-
20	CLA	1	212	-	3/3/7/25	-	-
20	CLA	L	203	-	4/4/18/25	7/25/123/135	-
21	LMU	R	109	-	-	16/21/61/61	0/2/2/2
20	CLA	L	201	-	5/5/18/25	12/25/123/135	-
20	CLA	B	819	-	3/3/16/25	13/15/113/135	-
20	CLA	2	302	-	3/3/17/25	11/21/119/135	-
20	CLA	A	823	-	4/4/20/25	20/37/135/135	-
20	CLA	A	828	-	4/4/20/25	18/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	312	-	3/3/17/25	11/19/117/135	-
20	CLA	H	102	-	4/4/18/25	9/25/123/135	-
20	CLA	L	208	-	3/3/16/25	9/16/114/135	-
20	CLA	4	318	-	3/3/17/25	12/22/120/135	-
22	BCR	A	843	-	-	11/29/63/63	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2
20	CLA	A	806	-	4/4/18/25	7/25/123/135	-
20	CLA	A	835	-	4/4/20/25	17/37/135/135	-

All (2242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	BCR	C21-C22	-11.54	1.20	1.35
22	I	101	BCR	C21-C22	-10.73	1.21	1.35
22	F	203	BCR	C21-C22	-10.22	1.22	1.35
22	B	852	BCR	C20-C21	-10.12	1.12	1.43
20	F	206	CLA	C3B-CAB	-9.63	1.28	1.47
20	R	108	CLA	C3B-CAB	-9.56	1.28	1.47
22	I	103	BCR	C21-C22	-9.51	1.23	1.35
20	4	318	CLA	C3B-CAB	-9.30	1.29	1.47
20	1	210	CLA	C3B-CAB	-9.25	1.29	1.47
20	3	302	CLA	C4B-NB	-9.15	1.27	1.35
20	3	302	CLA	C1B-NB	-9.05	1.27	1.35
20	B	821	CLA	C3B-CAB	-9.01	1.29	1.47
20	A	815	CLA	C3B-CAB	-8.91	1.29	1.47
22	L	210	BCR	C20-C21	-8.88	1.15	1.43
20	B	821	CLA	C1B-NB	-8.84	1.27	1.35
22	L	210	BCR	C21-C22	-8.79	1.24	1.35
20	4	307	CLA	C1B-NB	-8.78	1.27	1.35
22	F	203	BCR	C20-C21	-8.68	1.16	1.43
20	2	301	CLA	CHB-C4A	-8.57	1.28	1.34
20	B	821	CLA	C4C-C3C	-8.54	1.30	1.45
20	B	807	CLA	C3B-CAB	-8.53	1.30	1.47
20	4	308	CLA	CAB-C3B	-8.52	1.33	1.51
20	2	307	CLA	C3B-CAB	-8.51	1.30	1.47
20	4	303	CLA	CAB-C3B	-8.48	1.34	1.51
22	I	101	BCR	C20-C21	-8.45	1.17	1.43
20	A	807	CLA	C3B-CAB	-8.45	1.30	1.47
22	B	845	BCR	C20-C21	-8.40	1.17	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	846	BCR	C20-C21	-8.38	1.17	1.43
22	B	843	BCR	C20-C21	-8.38	1.17	1.43
20	4	304	CLA	C3B-CAB	-8.35	1.30	1.47
20	B	809	CLA	CAB-C3B	-8.32	1.34	1.51
22	B	845	BCR	C21-C22	-8.32	1.24	1.35
22	A	846	BCR	C20-C21	-8.30	1.17	1.43
20	H	101	CLA	C3B-CAB	-8.22	1.31	1.47
22	A	844	BCR	C20-C21	-8.22	1.18	1.43
22	B	852	BCR	C17-C18	-8.18	1.24	1.35
20	4	306	CLA	C3B-CAB	-8.17	1.31	1.47
22	3	314	BCR	C20-C21	-8.17	1.18	1.43
22	A	847	BCR	C20-C21	-8.15	1.18	1.43
20	4	316	CLA	C3B-CAB	-8.12	1.31	1.47
20	2	311	CLA	C3B-CAB	-8.12	1.31	1.47
22	F	202	BCR	C20-C21	-8.10	1.18	1.43
22	B	843	BCR	C21-C22	-8.09	1.25	1.35
22	J	102	BCR	C20-C21	-8.09	1.18	1.43
22	B	842	BCR	C20-C21	-8.08	1.18	1.43
22	A	843	BCR	C20-C21	-8.07	1.18	1.43
22	A	845	BCR	C20-C21	-8.07	1.18	1.43
20	A	839	CLA	C3B-CAB	-8.07	1.31	1.47
20	B	806	CLA	C3B-CAB	-8.06	1.31	1.47
20	1	209	CLA	CAB-C3B	-8.04	1.34	1.51
20	B	840	CLA	CAB-C3B	-8.03	1.34	1.51
20	3	302	CLA	C3B-CAB	-8.00	1.31	1.47
20	B	811	CLA	C3B-CAB	-7.97	1.31	1.47
20	B	803	CLA	C3B-CAB	-7.96	1.31	1.47
20	4	314	CLA	CAB-C3B	-7.93	1.35	1.51
22	B	846	BCR	C21-C22	-7.93	1.25	1.35
20	A	852	CLA	C3B-CAB	-7.92	1.31	1.47
22	I	103	BCR	C20-C21	-7.88	1.19	1.43
20	A	808	CLA	C3B-CAB	-7.86	1.31	1.47
22	B	844	BCR	C20-C21	-7.85	1.19	1.43
22	A	846	BCR	C21-C22	-7.85	1.25	1.35
22	A	844	BCR	C21-C22	-7.84	1.25	1.35
20	3	311	CLA	C3B-CAB	-7.82	1.32	1.47
20	3	301	CLA	CAB-C3B	-7.82	1.35	1.51
20	3	304	CLA	CAB-C3B	-7.76	1.35	1.51
22	A	847	BCR	C21-C22	-7.76	1.25	1.35
20	A	826	CLA	C3B-CAB	-7.75	1.32	1.47
20	B	822	CLA	C3B-CAB	-7.74	1.32	1.47
22	3	314	BCR	C21-C22	-7.73	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	842	PQN	C3-C2	7.73	1.49	1.35
20	B	832	CLA	C3B-CAB	-7.70	1.32	1.47
20	A	801	CLA	CAB-C3B	-7.68	1.35	1.51
20	4	307	CLA	C4C-C3C	-7.65	1.31	1.45
20	A	835	CLA	C3B-CAB	-7.65	1.32	1.47
22	F	202	BCR	C21-C22	-7.63	1.25	1.35
23	B	841	PQN	C3-C2	7.62	1.49	1.35
20	B	851	CLA	C3B-CAB	-7.60	1.32	1.47
22	A	845	BCR	C21-C22	-7.59	1.25	1.35
20	A	827	CLA	C3B-CAB	-7.50	1.32	1.47
20	1	204	CLA	OBD-CAD	7.45	1.32	1.22
22	J	102	BCR	C21-C22	-7.45	1.25	1.35
22	A	843	BCR	C21-C22	-7.40	1.26	1.35
20	A	834	CLA	C3B-CAB	-7.37	1.32	1.47
20	2	302	CLA	C3B-CAB	-7.37	1.32	1.47
22	B	842	BCR	C21-C22	-7.35	1.26	1.35
20	B	839	CLA	C3B-CAB	-7.33	1.33	1.47
20	1	215	CLA	C3B-CAB	-7.31	1.33	1.47
20	B	826	CLA	C3B-CAB	-7.29	1.33	1.47
20	G	102	CLA	C3B-CAB	-7.28	1.33	1.47
20	F	204	CLA	CAB-C3B	-7.27	1.36	1.51
20	L	201	CLA	C3B-CAB	-7.27	1.33	1.47
20	3	313	CLA	C3B-CAB	-7.26	1.33	1.47
20	3	313	CLA	C4C-C3C	-7.26	1.32	1.45
20	K	102	CLA	C3B-CAB	-7.25	1.33	1.47
20	B	825	CLA	C3B-CAB	-7.24	1.33	1.47
20	B	820	CLA	C3B-CAB	-7.22	1.33	1.47
20	3	312	CLA	CHB-C4A	-7.19	1.29	1.34
22	I	103	BCR	C30-C25	-7.17	1.43	1.53
20	A	851	CLA	C3B-CAB	-7.16	1.33	1.47
20	B	836	CLA	C3B-CAB	-7.16	1.33	1.47
20	A	816	CLA	C3B-CAB	-7.15	1.33	1.47
20	2	305	CLA	CHC-C1C	7.12	1.53	1.35
20	B	830	CLA	C3B-CAB	-7.11	1.33	1.47
20	A	809	CLA	C3B-CAB	-7.08	1.33	1.47
20	2	322	CLA	C3B-CAB	-7.05	1.33	1.47
20	B	823	CLA	C3B-CAB	-7.05	1.33	1.47
20	L	208	CLA	C3B-CAB	-7.04	1.33	1.47
20	A	803	CLA	C3B-CAB	-7.04	1.33	1.47
20	1	208	CLA	CHB-C4A	-7.03	1.29	1.34
20	A	831	CLA	C3B-CAB	-7.01	1.33	1.47
20	1	202	CLA	C3B-CAB	-7.00	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	833	CLA	C3B-CAB	-6.98	1.33	1.47
20	A	811	CLA	C3B-CAB	-6.97	1.33	1.47
20	B	849	CLA	C3B-CAB	-6.97	1.33	1.47
20	A	810	CLA	CHC-C1C	6.96	1.52	1.35
20	B	835	CLA	C3B-CAB	-6.96	1.33	1.47
20	A	837	CLA	C3B-CAB	-6.96	1.33	1.47
20	B	834	CLA	CHC-C1C	6.95	1.52	1.35
20	B	828	CLA	C3B-CAB	-6.92	1.33	1.47
20	4	319	CLA	C3B-CAB	-6.92	1.33	1.47
20	B	837	CLA	CHC-C1C	6.91	1.52	1.35
20	J	101	CLA	C3B-CAB	-6.91	1.33	1.47
20	A	824	CLA	C3B-CAB	-6.91	1.33	1.47
20	K	101	CLA	C3B-CAB	-6.89	1.33	1.47
20	I	102	CLA	C3B-CAB	-6.88	1.33	1.47
20	A	805	CLA	C3B-CAB	-6.86	1.34	1.47
20	B	834	CLA	C3B-CAB	-6.86	1.34	1.47
20	B	850	CLA	C3B-CAB	-6.84	1.34	1.47
20	B	824	CLA	C3B-CAB	-6.84	1.34	1.47
20	A	830	CLA	C3B-CAB	-6.83	1.34	1.47
20	F	205	CLA	C3B-CAB	-6.83	1.34	1.47
20	K	108	CLA	C3B-CAB	-6.80	1.34	1.47
20	B	813	CLA	CHC-C1C	6.80	1.52	1.35
20	B	803	CLA	CHC-C1C	6.79	1.52	1.35
20	I	102	CLA	CHC-C1C	6.79	1.52	1.35
20	B	812	CLA	C3B-CAB	-6.78	1.34	1.47
20	1	207	CLA	CHC-C1C	6.78	1.52	1.35
20	A	841	CLA	C3B-CAB	-6.78	1.34	1.47
20	3	311	CLA	C4C-C3C	-6.77	1.33	1.45
20	A	838	CLA	C3B-CAB	-6.77	1.34	1.47
20	1	202	CLA	C1B-NB	-6.77	1.29	1.35
20	3	303	CLA	C1B-NB	-6.76	1.29	1.35
20	A	825	CLA	C3B-CAB	-6.76	1.34	1.47
20	A	836	CLA	C3B-CAB	-6.75	1.34	1.47
20	A	819	CLA	CHC-C1C	6.75	1.52	1.35
20	A	821	CLA	C3B-CAB	-6.74	1.34	1.47
20	1	210	CLA	C4C-C3C	-6.74	1.33	1.45
20	B	825	CLA	CHC-C1C	6.74	1.52	1.35
22	B	844	BCR	C21-C22	-6.74	1.26	1.35
20	3	317	CLA	CHC-C1C	6.74	1.52	1.35
20	J	103	CLA	C3B-CAB	-6.72	1.34	1.47
20	4	302	CLA	C3B-CAB	-6.72	1.34	1.47
20	A	808	CLA	CHC-C1C	6.72	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	811	CLA	C4C-C3C	-6.72	1.33	1.45
20	B	832	CLA	OBD-CAD	6.72	1.31	1.22
20	A	836	CLA	CHC-C1C	6.71	1.52	1.35
20	A	850	CLA	C3B-CAB	-6.71	1.34	1.47
20	B	808	CLA	C3B-CAB	-6.70	1.34	1.47
20	B	828	CLA	CHC-C1C	6.70	1.52	1.35
20	1	203	CLA	CHC-C1C	6.70	1.52	1.35
20	L	207	CLA	CHC-C1C	6.68	1.52	1.35
20	1	209	CLA	CHC-C1C	6.68	1.52	1.35
20	1	203	CLA	C3B-CAB	-6.67	1.34	1.47
20	A	832	CLA	C3B-CAB	-6.67	1.34	1.47
20	B	816	CLA	CHC-C1C	6.67	1.52	1.35
20	4	311	CLA	CHC-C1C	6.67	1.52	1.35
20	A	838	CLA	CHC-C1C	6.66	1.52	1.35
20	L	203	CLA	CHC-C1C	6.64	1.52	1.35
20	A	822	CLA	C3B-CAB	-6.62	1.34	1.47
20	L	202	CLA	C3B-CAB	-6.62	1.34	1.47
20	A	820	CLA	CHC-C1C	6.61	1.51	1.35
20	3	317	CLA	O2D-CGD	6.61	1.49	1.33
20	B	831	CLA	C3B-CAB	-6.61	1.34	1.47
20	2	312	CLA	CHC-C1C	6.60	1.51	1.35
20	L	203	CLA	OBD-CAD	6.60	1.31	1.22
20	L	203	CLA	C3B-CAB	-6.57	1.34	1.47
20	B	832	CLA	CHC-C1C	6.56	1.51	1.35
20	1	207	CLA	C3B-CAB	-6.56	1.34	1.47
20	K	103	CLA	CHC-C1C	6.55	1.51	1.35
20	1	206	CLA	OBD-CAD	6.54	1.31	1.22
20	4	306	CLA	CHC-C1C	6.52	1.51	1.35
20	A	814	CLA	CHC-C1C	6.52	1.51	1.35
20	4	305	CLA	C3B-CAB	-6.51	1.34	1.47
20	B	833	CLA	CHC-C1C	6.50	1.51	1.35
20	B	830	CLA	CHC-C1C	6.50	1.51	1.35
20	B	829	CLA	C3B-CAB	-6.48	1.34	1.47
20	H	102	CLA	CHC-C1C	6.48	1.51	1.35
20	A	814	CLA	OBD-CAD	6.47	1.31	1.22
20	L	209	CLA	C3B-CAB	-6.47	1.34	1.47
20	A	829	CLA	C3B-CAB	-6.47	1.34	1.47
20	4	310	CLA	C1B-NB	-6.46	1.29	1.35
20	L	201	CLA	CHC-C1C	6.45	1.51	1.35
20	A	804	CLA	CHC-C1C	6.44	1.51	1.35
20	A	813	CLA	CHC-C1C	6.44	1.51	1.35
20	A	817	CLA	C3B-CAB	-6.42	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	204	CLA	CHC-C1C	6.41	1.51	1.35
20	B	838	CLA	CHC-C1C	6.41	1.51	1.35
20	A	829	CLA	CHC-C1C	6.39	1.51	1.35
20	L	208	CLA	CHC-C1C	6.39	1.51	1.35
20	A	822	CLA	CHC-C1C	6.38	1.51	1.35
20	B	807	CLA	CHC-C1C	6.38	1.51	1.35
20	1	201	CLA	C3B-CAB	-6.38	1.34	1.47
20	1	206	CLA	C3B-CAB	-6.38	1.34	1.47
20	A	811	CLA	CHC-C1C	6.37	1.51	1.35
20	4	303	CLA	CHC-C1C	6.37	1.51	1.35
20	A	850	CLA	CHC-C1C	6.36	1.51	1.35
20	2	308	CLA	C3B-CAB	-6.36	1.35	1.47
20	2	308	CLA	CHC-C1C	6.36	1.51	1.35
20	B	809	CLA	CHC-C1C	6.36	1.51	1.35
20	B	817	CLA	CHC-C1C	6.36	1.51	1.35
20	H	102	CLA	C3B-CAB	-6.36	1.35	1.47
20	B	851	CLA	CHC-C1C	6.35	1.51	1.35
20	A	827	CLA	CHC-C1C	6.35	1.51	1.35
20	B	827	CLA	C3B-CAB	-6.34	1.35	1.47
20	A	818	CLA	CHC-C1C	6.34	1.51	1.35
20	4	302	CLA	CHC-C1C	6.34	1.51	1.35
20	2	312	CLA	C3B-CAB	-6.33	1.35	1.47
20	K	103	CLA	C3B-CAB	-6.32	1.35	1.47
20	H	103	CLA	CHC-C1C	6.32	1.51	1.35
20	L	207	CLA	C3B-CAB	-6.31	1.35	1.47
20	A	828	CLA	CHC-C1C	6.31	1.51	1.35
20	K	101	CLA	CHC-C1C	6.31	1.51	1.35
20	3	308	CLA	CHC-C1C	6.31	1.51	1.35
20	A	837	CLA	CHC-C1C	6.30	1.51	1.35
20	2	303	CLA	CHC-C1C	6.30	1.51	1.35
20	B	823	CLA	CHC-C1C	6.30	1.51	1.35
20	B	850	CLA	CHC-C1C	6.30	1.51	1.35
20	3	313	CLA	C1B-NB	-6.29	1.29	1.35
20	4	303	CLA	OBD-CAD	6.29	1.31	1.22
20	B	814	CLA	C3B-CAB	-6.29	1.35	1.47
20	3	318	CLA	C3B-CAB	-6.28	1.35	1.47
20	A	832	CLA	CHC-C1C	6.26	1.51	1.35
20	1	204	CLA	C3B-CAB	-6.26	1.35	1.47
20	A	817	CLA	CHC-C1C	6.25	1.51	1.35
20	B	814	CLA	OBD-CAD	6.25	1.31	1.22
20	A	840	CLA	C3B-CAB	-6.25	1.35	1.47
20	4	314	CLA	CHC-C1C	6.24	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	O2D-CGD	6.23	1.48	1.33
20	A	834	CLA	CHC-C1C	6.23	1.50	1.35
20	R	107	CLA	CHC-C1C	6.22	1.50	1.35
20	A	835	CLA	CHC-C1C	6.22	1.50	1.35
20	B	818	CLA	C3B-CAB	-6.22	1.35	1.47
20	A	823	CLA	CHC-C1C	6.22	1.50	1.35
20	A	818	CLA	C3B-CAB	-6.21	1.35	1.47
20	B	805	CLA	C3B-CAB	-6.21	1.35	1.47
20	4	319	CLA	CHC-C1C	6.20	1.50	1.35
20	A	807	CLA	C1B-NB	-6.20	1.29	1.35
20	A	851	CLA	CHC-C1C	6.20	1.50	1.35
20	1	206	CLA	CHC-C1C	6.20	1.50	1.35
20	3	308	CLA	O2D-CGD	6.20	1.48	1.33
20	J	101	CLA	CHC-C1C	6.19	1.50	1.35
20	3	308	CLA	C3B-CAB	-6.19	1.35	1.47
20	J	103	CLA	CHC-C1C	6.18	1.50	1.35
20	B	812	CLA	CHC-C1C	6.18	1.50	1.35
22	F	203	BCR	C30-C25	-6.18	1.45	1.53
20	H	102	CLA	O2D-CGD	6.18	1.48	1.33
20	A	806	CLA	CHC-C1C	6.18	1.50	1.35
20	3	301	CLA	CHC-C1C	6.18	1.50	1.35
20	4	309	CLA	C4B-NB	-6.17	1.29	1.35
20	A	823	CLA	C3B-CAB	-6.17	1.35	1.47
20	A	804	CLA	C3B-CAB	-6.17	1.35	1.47
20	2	316	CLA	CHC-C1C	6.16	1.50	1.35
20	A	816	CLA	CHC-C1C	6.16	1.50	1.35
20	4	316	CLA	CHC-C1C	6.15	1.50	1.35
20	A	841	CLA	CHC-C1C	6.15	1.50	1.35
20	L	209	CLA	CHC-C1C	6.14	1.50	1.35
20	B	820	CLA	CHC-C1C	6.14	1.50	1.35
20	H	103	CLA	O2D-CGD	6.14	1.48	1.33
20	4	311	CLA	O2D-CGD	6.14	1.48	1.33
20	A	850	CLA	O2D-CGD	6.13	1.48	1.33
20	B	840	CLA	OBD-CAD	6.13	1.30	1.22
20	A	801	CLA	O2D-CGD	6.12	1.48	1.33
20	A	801	CLA	CHC-C1C	6.12	1.50	1.35
20	B	818	CLA	CHC-C1C	6.12	1.50	1.35
20	4	307	CLA	C1C-C2C	-6.12	1.32	1.44
20	2	312	CLA	O2D-CGD	6.12	1.48	1.33
20	A	816	CLA	C1B-NB	-6.12	1.29	1.35
20	3	304	CLA	CHC-C1C	6.11	1.50	1.35
20	A	814	CLA	C3B-CAB	-6.11	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	810	CLA	C3B-CAB	-6.11	1.35	1.47
20	A	833	CLA	CHC-C1C	6.10	1.50	1.35
20	B	810	CLA	C3B-CAB	-6.10	1.35	1.47
20	B	819	CLA	CHC-C1C	6.10	1.50	1.35
20	B	813	CLA	C3B-CAB	-6.10	1.35	1.47
20	A	826	CLA	CHC-C1C	6.09	1.50	1.35
20	A	852	CLA	OBD-CAD	6.09	1.30	1.22
20	A	814	CLA	O2D-CGD	6.08	1.48	1.33
20	A	828	CLA	C3B-CAB	-6.07	1.35	1.47
20	B	804	CLA	CHC-C1C	6.07	1.50	1.35
20	3	318	CLA	CHC-C1C	6.07	1.50	1.35
20	4	305	CLA	CHC-C1C	6.06	1.50	1.35
20	A	803	CLA	CHC-C1C	6.05	1.50	1.35
20	B	838	CLA	C3B-CAB	-6.05	1.35	1.47
20	2	311	CLA	CHC-C1C	6.05	1.50	1.35
20	3	317	CLA	C3B-CAB	-6.05	1.35	1.47
20	A	817	CLA	O2D-CGD	6.04	1.47	1.33
20	A	812	CLA	CHC-C1C	6.04	1.50	1.35
20	B	849	CLA	CHC-C1C	6.04	1.50	1.35
20	B	834	CLA	OBD-CAD	6.04	1.30	1.22
20	B	840	CLA	CHC-C1C	6.03	1.50	1.35
20	A	821	CLA	O2D-CGD	6.03	1.47	1.33
20	2	302	CLA	CHC-C1C	6.03	1.50	1.35
20	4	311	CLA	C3B-CAB	-6.02	1.35	1.47
20	B	820	CLA	O2D-CGD	6.02	1.47	1.33
20	4	310	CLA	C4B-NB	-6.02	1.29	1.35
20	B	815	CLA	CHC-C1C	6.02	1.50	1.35
20	2	307	CLA	C1B-NB	-6.02	1.29	1.35
20	B	814	CLA	CHC-C1C	6.01	1.50	1.35
20	A	840	CLA	CHC-C1C	6.00	1.50	1.35
20	B	817	CLA	C3B-CAB	-6.00	1.35	1.47
20	2	316	CLA	C3B-CAB	-6.00	1.35	1.47
20	1	204	CLA	CHC-C1C	6.00	1.50	1.35
20	A	832	CLA	O2D-CGD	6.00	1.47	1.33
20	G	102	CLA	C4C-C3C	-5.99	1.34	1.45
20	F	205	CLA	CHC-C1C	5.98	1.50	1.35
20	2	305	CLA	C3B-CAB	-5.98	1.35	1.47
20	1	208	CLA	MG-NA	-5.97	1.92	2.06
20	B	808	CLA	CHC-C1C	5.96	1.50	1.35
20	B	835	CLA	CHC-C1C	5.96	1.50	1.35
20	B	810	CLA	CHC-C1C	5.96	1.50	1.35
20	A	833	CLA	C3B-CAB	-5.95	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	308	CLA	OBD-CAD	5.95	1.30	1.22
20	A	806	CLA	OBD-CAD	5.95	1.30	1.22
20	A	819	CLA	O2D-CGD	5.95	1.47	1.33
20	A	824	CLA	CHC-C1C	5.94	1.50	1.35
20	A	804	CLA	OBD-CAD	5.93	1.30	1.22
20	B	816	CLA	C3B-CAB	-5.93	1.35	1.47
20	B	804	CLA	OBD-CAD	5.93	1.30	1.22
20	A	839	CLA	O2D-CGD	5.92	1.47	1.33
20	A	806	CLA	C3B-CAB	-5.92	1.35	1.47
20	A	806	CLA	O2D-CGD	5.92	1.47	1.33
20	B	819	CLA	O2D-CGD	5.91	1.47	1.33
20	1	208	CLA	C1B-NB	-5.91	1.29	1.35
20	B	826	CLA	OBD-CAD	5.91	1.30	1.22
20	L	203	CLA	O2D-CGD	5.90	1.47	1.33
20	B	831	CLA	O2D-CGD	5.90	1.47	1.33
20	L	207	CLA	O2D-CGD	5.90	1.47	1.33
20	A	822	CLA	O2D-CGD	5.89	1.47	1.33
20	B	832	CLA	O2D-CGD	5.89	1.47	1.33
20	B	805	CLA	CHC-C1C	5.88	1.50	1.35
20	B	815	CLA	C3B-CAB	-5.87	1.36	1.47
20	B	811	CLA	CHC-C1C	5.86	1.50	1.35
20	B	821	CLA	C3B-C2B	-5.85	1.32	1.40
20	4	318	CLA	C1C-C2C	-5.85	1.33	1.44
20	4	307	CLA	CHC-C1C	5.85	1.50	1.35
20	B	812	CLA	O2D-CGD	5.85	1.47	1.33
20	1	206	CLA	O2D-CGD	5.84	1.47	1.33
20	B	807	CLA	O2D-CGD	5.83	1.47	1.33
20	L	202	CLA	O2D-CGD	5.83	1.47	1.33
20	2	308	CLA	O2D-CGD	5.82	1.47	1.33
20	2	322	CLA	CHC-C1C	5.82	1.49	1.35
20	B	822	CLA	CHC-C1C	5.82	1.49	1.35
20	B	836	CLA	CHC-C1C	5.82	1.49	1.35
20	B	826	CLA	CHC-C1C	5.82	1.49	1.35
20	3	312	CLA	MG-NA	-5.82	1.92	2.06
20	2	312	CLA	O2A-CGA	5.81	1.50	1.33
20	1	210	CLA	C3B-C2B	-5.80	1.32	1.40
20	B	827	CLA	CHC-C1C	5.80	1.49	1.35
20	B	804	CLA	C3B-CAB	-5.80	1.36	1.47
22	B	852	BCR	C20-C19	-5.80	1.19	1.34
20	L	202	CLA	CHC-C1C	5.79	1.49	1.35
20	H	103	CLA	C3B-CAB	-5.79	1.36	1.47
20	4	318	CLA	O2D-CGD	5.79	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	201	CLA	O2D-CGD	5.78	1.47	1.33
20	A	805	CLA	CHC-C1C	5.78	1.49	1.35
20	A	821	CLA	CHC-C1C	5.77	1.49	1.35
20	K	108	CLA	CHC-C1C	5.77	1.49	1.35
20	F	206	CLA	CHC-C1C	5.77	1.49	1.35
20	A	825	CLA	CHC-C1C	5.77	1.49	1.35
20	B	803	CLA	O2D-CGD	5.77	1.47	1.33
20	B	829	CLA	O2D-CGD	5.77	1.47	1.33
20	1	210	CLA	C3D-CAD	-5.76	1.31	1.46
20	B	812	CLA	OBD-CAD	5.76	1.30	1.22
20	3	319	CLA	MG-NA	-5.76	1.92	2.06
20	A	820	CLA	C3B-CAB	-5.76	1.36	1.47
20	H	109	CLA	C3B-CAB	-5.76	1.36	1.47
20	A	805	CLA	O2D-CGD	5.75	1.47	1.33
20	4	306	CLA	C1B-NB	-5.75	1.30	1.35
20	A	837	CLA	O2D-CGD	5.75	1.47	1.33
20	A	821	CLA	OBD-CAD	5.75	1.30	1.22
20	B	833	CLA	O2D-CGD	5.75	1.47	1.33
20	4	311	CLA	OBD-CAD	5.75	1.30	1.22
20	4	308	CLA	CHC-C1C	5.74	1.49	1.35
20	2	316	CLA	O2D-CGD	5.74	1.47	1.33
20	L	202	CLA	OBD-CAD	5.73	1.30	1.22
20	H	109	CLA	CHC-C1C	5.73	1.49	1.35
20	A	852	CLA	CHC-C1C	5.73	1.49	1.35
20	B	814	CLA	O2D-CGD	5.73	1.47	1.33
20	B	824	CLA	CHC-C1C	5.73	1.49	1.35
20	H	109	CLA	O2D-CGD	5.72	1.47	1.33
20	2	301	CLA	C4B-NB	-5.71	1.30	1.35
20	B	834	CLA	O2D-CGD	5.71	1.47	1.33
20	A	839	CLA	C1B-NB	-5.70	1.30	1.35
20	4	305	CLA	OBD-CAD	5.70	1.30	1.22
20	A	820	CLA	OBD-CAD	5.70	1.30	1.22
20	2	303	CLA	O2D-CGD	5.70	1.47	1.33
20	A	839	CLA	CHC-C1C	5.70	1.49	1.35
20	B	806	CLA	CHC-C1C	5.69	1.49	1.35
20	A	805	CLA	O2A-CGA	5.69	1.50	1.33
20	L	201	CLA	C4B-NB	-5.69	1.30	1.35
20	R	107	CLA	C3B-CAB	-5.68	1.36	1.47
20	B	809	CLA	O2A-CGA	5.68	1.49	1.33
20	A	804	CLA	O2A-CGA	5.67	1.49	1.33
20	2	303	CLA	OBD-CAD	5.66	1.30	1.22
20	H	102	CLA	OBD-CAD	5.66	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	822	CLA	O2D-CGD	5.65	1.47	1.33
20	2	322	CLA	O2D-CGD	5.64	1.47	1.33
20	B	812	CLA	O2A-CGA	5.64	1.49	1.33
20	B	815	CLA	O2D-CGD	5.63	1.46	1.33
20	A	820	CLA	O2D-CGD	5.63	1.46	1.33
20	A	810	CLA	O2D-CGD	5.63	1.46	1.33
20	4	304	CLA	CHC-C1C	5.63	1.49	1.35
20	L	209	CLA	O2D-CGD	5.62	1.46	1.33
20	R	107	CLA	O2A-CGA	5.61	1.49	1.33
20	B	813	CLA	O2D-CGD	5.60	1.46	1.33
20	B	822	CLA	OBD-CAD	5.60	1.30	1.22
20	B	819	CLA	OBD-CAD	5.59	1.30	1.22
20	A	830	CLA	CHC-C1C	5.59	1.49	1.35
20	3	308	CLA	OBD-CAD	5.58	1.30	1.22
20	A	831	CLA	O2D-CGD	5.58	1.46	1.33
20	R	107	CLA	O2D-CGD	5.57	1.46	1.33
20	B	816	CLA	O2D-CGD	5.57	1.46	1.33
20	1	204	CLA	O2D-CGD	5.56	1.46	1.33
20	4	314	CLA	OBD-CAD	5.56	1.30	1.22
20	A	840	CLA	OBD-CAD	5.56	1.30	1.22
20	B	839	CLA	CHC-C1C	5.56	1.49	1.35
20	B	805	CLA	O2D-CGD	5.54	1.46	1.33
20	A	813	CLA	C3B-CAB	-5.54	1.36	1.47
20	B	833	CLA	OBD-CAD	5.54	1.30	1.22
20	1	201	CLA	C1B-NB	-5.54	1.30	1.35
20	K	103	CLA	OBD-CAD	5.54	1.30	1.22
20	A	833	CLA	O2D-CGD	5.53	1.46	1.33
20	A	812	CLA	O2D-CGD	5.53	1.46	1.33
20	H	101	CLA	CHC-C1C	5.52	1.49	1.35
20	2	307	CLA	C4C-C3C	-5.52	1.35	1.45
20	A	838	CLA	O2D-CGD	5.52	1.46	1.33
20	1	201	CLA	OBD-CAD	5.52	1.30	1.22
20	R	108	CLA	C1B-NB	-5.51	1.30	1.35
20	B	837	CLA	C3B-CAB	-5.51	1.36	1.47
20	1	210	CLA	CHC-C1C	5.48	1.49	1.35
20	A	834	CLA	OBD-CAD	5.48	1.30	1.22
20	B	809	CLA	OBD-CAD	5.48	1.30	1.22
20	2	303	CLA	O2A-CGA	5.48	1.49	1.33
20	A	812	CLA	O2A-CGA	5.46	1.49	1.33
20	3	305	CLA	C1B-NB	-5.46	1.30	1.35
20	A	815	CLA	CHC-C1C	5.46	1.49	1.35
20	A	840	CLA	O2D-CGD	5.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	837	CLA	OBD-CAD	5.44	1.29	1.22
20	A	810	CLA	OBD-CAD	5.43	1.29	1.22
20	A	819	CLA	C3B-CAB	-5.43	1.36	1.47
20	K	103	CLA	O2D-CGD	5.43	1.46	1.33
20	K	102	CLA	C1C-C2C	-5.43	1.34	1.44
20	1	215	CLA	O2D-CGD	5.42	1.46	1.33
20	4	306	CLA	C4C-C3C	-5.41	1.35	1.45
20	K	102	CLA	C4C-C3C	-5.40	1.35	1.45
20	A	829	CLA	O2A-CGA	5.40	1.49	1.33
20	A	815	CLA	C1B-NB	-5.40	1.30	1.35
20	R	108	CLA	C3B-C2B	-5.40	1.32	1.40
20	A	827	CLA	O2A-CGA	5.39	1.49	1.33
20	A	815	CLA	C4C-C3C	-5.39	1.35	1.45
20	B	831	CLA	CHC-C1C	5.37	1.48	1.35
20	A	831	CLA	CHC-C1C	5.37	1.48	1.35
20	1	209	CLA	OBD-CAD	5.37	1.29	1.22
20	B	807	CLA	OBD-CAD	5.36	1.29	1.22
20	G	102	CLA	CHC-C1C	5.36	1.48	1.35
20	1	203	CLA	OBD-CAD	5.36	1.29	1.22
20	4	318	CLA	C1B-NB	-5.36	1.30	1.35
20	H	109	CLA	OBD-CAD	5.36	1.29	1.22
20	B	820	CLA	OBD-CAD	5.35	1.29	1.22
20	F	206	CLA	C3B-C2B	-5.35	1.33	1.40
20	A	803	CLA	OBD-CAD	5.34	1.29	1.22
20	A	841	CLA	OBD-CAD	5.34	1.29	1.22
20	A	812	CLA	C3B-CAB	-5.34	1.37	1.47
20	3	317	CLA	OBD-CAD	5.34	1.29	1.22
20	1	207	CLA	O2D-CGD	5.33	1.46	1.33
20	B	837	CLA	O2D-CGD	5.33	1.46	1.33
20	K	102	CLA	CHC-C1C	5.32	1.48	1.35
20	B	825	CLA	O2D-CGD	5.32	1.46	1.33
20	B	828	CLA	O2A-CGA	5.31	1.48	1.33
20	A	836	CLA	O2D-CGD	5.30	1.46	1.33
20	B	818	CLA	O2D-CGD	5.30	1.46	1.33
20	A	839	CLA	O2A-CGA	5.30	1.48	1.33
20	B	829	CLA	CHC-C1C	5.30	1.48	1.35
20	2	316	CLA	OBD-CAD	5.30	1.29	1.22
20	A	818	CLA	O2D-CGD	5.29	1.46	1.33
20	A	801	CLA	O2A-CGA	5.29	1.48	1.33
20	A	851	CLA	O2A-CGA	5.29	1.48	1.33
20	B	815	CLA	O2A-CGA	5.29	1.48	1.33
20	L	201	CLA	C1B-NB	-5.28	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	O2D-CGD	5.27	1.46	1.33
20	A	811	CLA	O2A-CGA	5.27	1.48	1.33
20	A	822	CLA	O2A-CGA	5.27	1.48	1.33
20	A	825	CLA	O2D-CGD	5.27	1.46	1.33
20	4	302	CLA	O2D-CGD	5.27	1.46	1.33
20	B	809	CLA	O2D-CGD	5.26	1.46	1.33
20	B	824	CLA	O2D-CGD	5.26	1.46	1.33
20	4	304	CLA	C3B-C2B	-5.25	1.33	1.40
20	3	318	CLA	O2D-CGD	5.25	1.46	1.33
20	B	826	CLA	O2D-CGD	5.24	1.46	1.33
20	B	821	CLA	CHC-C1C	5.23	1.48	1.35
20	K	108	CLA	O2D-CGD	5.22	1.45	1.33
20	A	803	CLA	O2D-CGD	5.22	1.45	1.33
20	2	316	CLA	O2A-CGA	5.22	1.48	1.33
20	L	208	CLA	O2D-CGD	5.22	1.45	1.33
20	B	805	CLA	O2A-CGA	5.21	1.48	1.33
20	I	102	CLA	O2A-CGA	5.20	1.48	1.33
20	A	828	CLA	O2D-CGD	5.20	1.45	1.33
20	3	302	CLA	CHC-C1C	5.19	1.48	1.35
20	3	305	CLA	CHB-C4A	-5.19	1.30	1.34
20	B	819	CLA	C3B-CAB	-5.19	1.37	1.47
20	2	301	CLA	C1B-NB	-5.18	1.30	1.35
20	2	304	CLA	CHB-C4A	-5.18	1.30	1.34
20	K	102	CLA	C1B-NB	-5.18	1.30	1.35
20	2	305	CLA	O2D-CGD	5.18	1.45	1.33
20	B	851	CLA	O2D-CGD	5.17	1.45	1.33
20	A	827	CLA	O2D-CGD	5.17	1.45	1.33
20	A	807	CLA	CHC-C1C	5.17	1.48	1.35
20	4	318	CLA	CHC-C1C	5.17	1.48	1.35
20	B	818	CLA	O2A-CGA	5.16	1.48	1.33
20	A	824	CLA	O2D-CGD	5.16	1.45	1.33
20	H	103	CLA	OBD-CAD	5.16	1.29	1.22
20	4	307	CLA	O2D-CGD	5.16	1.45	1.33
20	3	302	CLA	C3B-C2B	-5.15	1.33	1.40
20	A	841	CLA	O2D-CGD	5.15	1.45	1.33
20	1	215	CLA	C1B-NB	-5.15	1.30	1.35
20	4	315	CLA	CHC-C1C	5.15	1.52	1.39
20	F	205	CLA	O2D-CGD	5.15	1.45	1.33
20	2	309	CLA	CHC-C1C	5.15	1.52	1.39
20	B	849	CLA	OBD-CAD	5.14	1.29	1.22
20	F	206	CLA	OBD-CAD	5.14	1.29	1.22
20	H	109	CLA	O2A-CGA	5.14	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	852	CLA	O2D-CGD	5.13	1.45	1.33
20	1	203	CLA	O2D-CGD	5.13	1.45	1.33
20	3	318	CLA	OBD-CAD	5.12	1.29	1.22
20	F	204	CLA	OBD-CAD	5.12	1.29	1.22
20	3	313	CLA	CHC-C1C	5.12	1.48	1.35
20	4	305	CLA	O2D-CGD	5.12	1.45	1.33
20	A	811	CLA	O2D-CGD	5.11	1.45	1.33
20	4	303	CLA	C3A-C2A	-5.11	1.49	1.54
20	A	802	CLA	MG-NA	-5.11	1.94	2.06
20	B	830	CLA	O2A-CGA	5.11	1.48	1.33
20	A	816	CLA	C3B-C2B	-5.11	1.33	1.40
20	2	303	CLA	C3B-CAB	-5.11	1.37	1.47
20	B	803	CLA	OBD-CAD	5.11	1.29	1.22
20	B	838	CLA	O2D-CGD	5.11	1.45	1.33
20	4	316	CLA	C4C-C3C	-5.11	1.36	1.45
20	B	850	CLA	O2D-CGD	5.10	1.45	1.33
20	A	826	CLA	OBD-CAD	5.10	1.29	1.22
20	A	851	CLA	O2D-CGD	5.09	1.45	1.33
20	2	307	CLA	CHC-C1C	5.09	1.48	1.35
20	K	101	CLA	O2D-CGD	5.09	1.45	1.33
20	B	817	CLA	O2D-CGD	5.09	1.45	1.33
20	B	835	CLA	O2A-CGA	5.09	1.48	1.33
20	4	306	CLA	OBD-CAD	5.09	1.29	1.22
20	B	810	CLA	O2D-CGD	5.08	1.45	1.33
20	B	819	CLA	O2A-CGA	5.08	1.49	1.33
20	4	304	CLA	C1C-C2C	-5.07	1.34	1.44
20	J	103	CLA	O2D-CGD	5.07	1.45	1.33
20	2	312	CLA	OBD-CAD	5.07	1.29	1.22
20	B	817	CLA	O2A-CGA	5.06	1.48	1.33
20	2	302	CLA	O2D-CGD	5.06	1.45	1.33
20	L	207	CLA	OBD-CAD	5.05	1.29	1.22
20	K	103	CLA	O2A-CGA	5.05	1.48	1.33
22	I	103	BCR	C26-C25	-5.05	1.25	1.34
20	J	101	CLA	O2D-CGD	5.04	1.45	1.33
20	A	830	CLA	OBD-CAD	5.04	1.29	1.22
20	1	212	CLA	MG-NA	-5.04	1.94	2.06
20	A	838	CLA	OBD-CAD	5.02	1.29	1.22
20	A	834	CLA	O2D-CGD	5.02	1.45	1.33
20	B	811	CLA	C1C-C2C	-5.02	1.34	1.44
20	A	817	CLA	O2A-CGA	5.01	1.48	1.33
20	1	207	CLA	OBD-CAD	5.01	1.29	1.22
20	R	108	CLA	CHC-C1C	5.00	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	309	CLA	MG-NA	-5.00	1.94	2.06
20	B	808	CLA	O2D-CGD	5.00	1.45	1.33
20	B	815	CLA	OBD-CAD	4.99	1.29	1.22
20	4	304	CLA	C1B-NB	-4.99	1.30	1.35
20	4	307	CLA	C3B-CAB	-4.97	1.37	1.47
20	2	311	CLA	O2D-CGD	4.97	1.45	1.33
20	A	816	CLA	C4C-C3C	-4.96	1.36	1.45
20	A	832	CLA	O2A-CGA	4.96	1.47	1.33
20	3	313	CLA	O2D-CGD	4.95	1.45	1.33
20	4	313	CLA	CHC-C1C	4.94	1.51	1.39
20	1	207	CLA	O2A-CGA	4.94	1.47	1.33
20	A	817	CLA	OBD-CAD	4.94	1.29	1.22
20	4	302	CLA	OBD-CAD	4.94	1.29	1.22
20	3	311	CLA	O2D-CGD	4.93	1.45	1.33
20	A	809	CLA	CHC-C1C	4.93	1.47	1.35
20	A	818	CLA	O2A-CGA	4.93	1.47	1.33
20	A	822	CLA	OBD-CAD	4.93	1.29	1.22
20	A	834	CLA	O2A-CGA	4.92	1.47	1.33
20	A	828	CLA	OBD-CAD	4.92	1.29	1.22
20	L	207	CLA	O2A-CGA	4.92	1.47	1.33
20	R	108	CLA	C4C-C3C	-4.92	1.36	1.45
20	4	306	CLA	O2D-CGD	4.91	1.45	1.33
20	A	839	CLA	C4C-C3C	-4.91	1.36	1.45
20	B	823	CLA	O2D-CGD	4.91	1.45	1.33
20	B	821	CLA	MG-NA	-4.91	1.94	2.06
20	A	830	CLA	O2A-CGA	4.91	1.47	1.33
20	3	302	CLA	O2D-CGD	4.91	1.45	1.33
20	B	838	CLA	O2A-CGA	4.90	1.47	1.33
20	3	305	CLA	MG-NA	-4.89	1.94	2.06
20	L	209	CLA	OBD-CAD	4.89	1.29	1.22
20	B	851	CLA	O2A-CGA	4.89	1.47	1.33
20	4	309	CLA	C1B-NB	-4.89	1.30	1.35
20	A	802	CLA	CHC-C1C	4.89	1.51	1.39
20	F	205	CLA	OBD-CAD	4.88	1.29	1.22
20	A	838	CLA	O2A-CGA	4.87	1.47	1.33
20	B	849	CLA	O2D-CGD	4.87	1.45	1.33
20	A	809	CLA	OBD-CAD	4.86	1.29	1.22
20	4	307	CLA	MG-NA	-4.86	1.94	2.06
20	A	835	CLA	O2D-CGD	4.86	1.45	1.33
22	F	203	BCR	C1-C6	-4.85	1.47	1.53
20	B	813	CLA	OBD-CAD	4.85	1.29	1.22
20	A	816	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	307	CLA	C1C-C2C	-4.84	1.35	1.44
20	B	806	CLA	O2D-CGD	4.84	1.45	1.33
20	K	102	CLA	O2D-CGD	4.84	1.45	1.33
20	A	813	CLA	O2D-CGD	4.84	1.45	1.33
20	1	215	CLA	CHC-C1C	4.84	1.47	1.35
20	A	813	CLA	O2A-CGA	4.83	1.47	1.33
20	3	303	CLA	CHB-C4A	-4.83	1.31	1.34
20	B	850	CLA	OBD-CAD	4.83	1.29	1.22
20	3	316	CLA	CHC-C1C	4.82	1.51	1.39
20	B	834	CLA	O2A-CGA	4.81	1.47	1.33
20	4	318	CLA	C4C-C3C	-4.80	1.36	1.45
20	1	202	CLA	CHC-C1C	4.78	1.47	1.35
20	A	835	CLA	O2A-CGA	4.78	1.47	1.33
20	B	831	CLA	OBD-CAD	4.77	1.29	1.22
20	2	302	CLA	OBD-CAD	4.77	1.29	1.22
20	A	829	CLA	O2D-CGD	4.76	1.44	1.33
20	3	320	CLA	CHC-C1C	4.76	1.51	1.39
20	3	313	CLA	C1C-C2C	-4.75	1.35	1.44
20	A	831	CLA	O2A-CGA	4.75	1.47	1.33
20	2	308	CLA	O2A-CGA	4.75	1.47	1.33
20	1	210	CLA	C1B-NB	-4.75	1.31	1.35
20	1	211	CLA	CHC-C1C	4.74	1.51	1.39
22	B	852	BCR	C10-C9	-4.74	1.29	1.35
20	B	811	CLA	C1B-NB	-4.74	1.31	1.35
20	B	804	CLA	O2D-CGD	4.73	1.44	1.33
20	4	319	CLA	O2D-CGD	4.73	1.44	1.33
20	A	852	CLA	CHD-C4C	4.73	1.54	1.41
20	B	839	CLA	O2A-CGA	4.73	1.47	1.33
20	3	304	CLA	OBD-CAD	4.72	1.28	1.22
20	H	102	CLA	O2A-CGA	4.72	1.47	1.33
23	A	842	PQN	C10-C5	4.72	1.48	1.40
20	2	305	CLA	OBD-CAD	4.72	1.28	1.22
20	K	108	CLA	OBD-CAD	4.72	1.28	1.22
20	J	103	CLA	OBD-CAD	4.72	1.28	1.22
20	A	811	CLA	OBD-CAD	4.71	1.28	1.22
20	K	101	CLA	OBD-CAD	4.71	1.28	1.22
20	B	821	CLA	C4B-NB	-4.71	1.31	1.35
20	A	850	CLA	C4C-C3C	-4.71	1.36	1.45
20	L	203	CLA	O2A-CGA	4.71	1.47	1.33
20	3	311	CLA	C1C-C2C	-4.70	1.35	1.44
20	1	202	CLA	C1C-C2C	-4.70	1.35	1.44
20	B	836	CLA	O2A-CGA	4.70	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	212	CLA	C1B-NB	-4.70	1.31	1.35
20	B	850	CLA	O2A-CGA	4.70	1.47	1.33
20	1	203	CLA	O2A-CGA	4.70	1.47	1.33
20	4	304	CLA	C4C-C3C	-4.70	1.36	1.45
20	B	830	CLA	O2D-CGD	4.69	1.44	1.33
20	1	206	CLA	O2A-CGA	4.69	1.47	1.33
20	3	313	CLA	C4B-NB	-4.69	1.31	1.35
20	A	839	CLA	C1C-C2C	-4.68	1.35	1.44
20	A	819	CLA	O2A-CGA	4.67	1.47	1.33
20	A	825	CLA	OBD-CAD	4.67	1.28	1.22
20	A	808	CLA	OBD-CAD	4.67	1.28	1.22
23	B	841	PQN	C10-C5	4.67	1.48	1.40
20	H	101	CLA	C1C-C2C	-4.67	1.35	1.44
20	2	322	CLA	OBD-CAD	4.66	1.28	1.22
20	B	810	CLA	O2A-CGA	4.66	1.47	1.33
20	3	309	CLA	CHC-C1C	4.65	1.50	1.39
20	A	835	CLA	OBD-CAD	4.65	1.28	1.22
20	1	216	CLA	CHB-C4A	-4.65	1.31	1.34
20	L	202	CLA	O2A-CGA	4.65	1.46	1.33
20	4	309	CLA	C1C-NC	-4.65	1.28	1.38
20	A	804	CLA	O2D-CGD	4.64	1.44	1.33
20	B	813	CLA	O2A-CGA	4.64	1.46	1.33
20	1	210	CLA	C3D-C2D	-4.64	1.31	1.39
20	I	102	CLA	O2D-CGD	4.64	1.44	1.33
20	A	809	CLA	O2A-CGA	4.64	1.46	1.33
20	B	824	CLA	OBD-CAD	4.64	1.28	1.22
20	B	825	CLA	OBD-CAD	4.63	1.28	1.22
20	L	209	CLA	O2A-CGA	4.63	1.46	1.33
20	B	811	CLA	C3D-CAD	-4.63	1.34	1.46
20	A	827	CLA	OBD-CAD	4.63	1.28	1.22
20	2	311	CLA	O2A-CGA	4.63	1.46	1.33
20	H	103	CLA	O2A-CGA	4.63	1.46	1.33
20	L	208	CLA	OBD-CAD	4.63	1.28	1.22
20	A	830	CLA	O2D-CGD	4.63	1.44	1.33
20	A	807	CLA	C4C-C3C	-4.62	1.37	1.45
20	A	833	CLA	OBD-CAD	4.61	1.28	1.22
20	A	837	CLA	O2A-CGA	4.61	1.46	1.33
20	B	838	CLA	OBD-CAD	4.60	1.28	1.22
20	4	305	CLA	O2A-CGA	4.60	1.46	1.33
20	4	308	CLA	C3A-C2A	-4.59	1.50	1.54
20	B	839	CLA	O2D-CGD	4.59	1.44	1.33
20	B	811	CLA	C3B-C2B	-4.59	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	CHD-C4C	4.59	1.54	1.41
20	3	303	CLA	MG-NA	-4.59	1.95	2.06
20	1	210	CLA	O2D-CGD	4.58	1.44	1.33
20	B	805	CLA	OBD-CAD	4.56	1.28	1.22
20	L	201	CLA	O2D-CGD	4.56	1.44	1.33
20	2	315	CLA	CHC-C1C	4.56	1.50	1.39
20	A	815	CLA	C1C-NC	-4.56	1.31	1.37
20	1	210	CLA	C1C-C2C	-4.56	1.35	1.44
20	B	829	CLA	O2A-CGA	4.56	1.46	1.33
20	G	102	CLA	O2D-CGD	4.55	1.44	1.33
20	2	310	CLA	CHC-C1C	4.55	1.50	1.39
20	B	839	CLA	OBD-CAD	4.55	1.28	1.22
20	1	205	CLA	MG-NA	-4.55	1.95	2.06
20	B	823	CLA	OBD-CAD	4.54	1.28	1.22
20	A	810	CLA	CHD-C4C	4.53	1.54	1.41
22	L	210	BCR	C20-C19	-4.53	1.22	1.34
20	B	808	CLA	OBD-CAD	4.53	1.28	1.22
20	3	310	CLA	C1B-NB	-4.52	1.31	1.35
20	2	304	CLA	MG-NA	-4.52	1.95	2.06
20	A	820	CLA	O2A-CGA	4.52	1.46	1.33
20	J	101	CLA	OBD-CAD	4.50	1.28	1.22
20	A	815	CLA	C4B-NB	-4.50	1.31	1.35
20	A	840	CLA	CHD-C4C	4.50	1.54	1.41
20	2	305	CLA	O2A-CGA	4.50	1.46	1.33
20	A	840	CLA	O2A-CGA	4.50	1.46	1.33
20	G	102	CLA	OBD-CAD	4.50	1.28	1.22
20	A	815	CLA	MG-NA	-4.49	1.95	2.06
20	L	209	CLA	CMA-C3A	4.49	1.62	1.53
20	3	313	CLA	O2A-CGA	4.48	1.46	1.33
22	I	103	BCR	C1-C6	-4.48	1.47	1.53
20	3	318	CLA	O2A-CGA	4.47	1.46	1.33
20	H	101	CLA	MG-NA	-4.47	1.95	2.06
20	B	828	CLA	OBD-CAD	4.47	1.28	1.22
20	A	838	CLA	C4C-C3C	-4.47	1.37	1.45
20	A	823	CLA	O2D-CGD	4.47	1.44	1.33
20	B	820	CLA	O2A-CGA	4.46	1.46	1.33
20	4	316	CLA	C3B-C2B	-4.46	1.34	1.40
20	B	821	CLA	C1C-NC	-4.45	1.31	1.37
20	F	206	CLA	C4C-C3C	-4.44	1.37	1.45
20	A	808	CLA	O2A-CGA	4.42	1.46	1.33
20	3	306	CLA	CHC-C1C	4.42	1.50	1.39
22	F	203	BCR	C14-C13	-4.41	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	101	CLA	C4C-C3C	-4.41	1.37	1.45
20	B	831	CLA	O2A-CGA	4.41	1.46	1.33
20	A	826	CLA	CHD-C4C	4.41	1.53	1.41
20	R	108	CLA	C1C-C2C	-4.40	1.36	1.44
20	2	308	CLA	CHD-C4C	4.40	1.53	1.41
20	B	837	CLA	O2A-CGA	4.40	1.46	1.33
20	A	807	CLA	C1C-C2C	-4.39	1.36	1.44
20	B	822	CLA	O2A-CGA	4.39	1.46	1.33
20	B	827	CLA	OBD-CAD	4.39	1.28	1.22
20	A	803	CLA	O2A-CGA	4.39	1.46	1.33
20	R	108	CLA	O2A-CGA	4.38	1.46	1.33
20	B	836	CLA	O2D-CGD	4.38	1.43	1.33
20	A	828	CLA	O2A-CGA	4.37	1.46	1.33
20	1	203	CLA	C4B-CHC	4.37	1.53	1.41
20	4	311	CLA	O2A-CGA	4.37	1.46	1.33
20	A	806	CLA	O2A-CGA	4.36	1.46	1.33
20	L	208	CLA	O2A-CGA	4.36	1.46	1.33
20	4	319	CLA	O2A-CGA	4.36	1.46	1.33
20	F	204	CLA	CHD-C4C	4.36	1.53	1.41
20	R	108	CLA	O2D-CGD	4.35	1.43	1.33
20	A	812	CLA	OBD-CAD	4.35	1.28	1.22
20	4	312	CLA	CHC-C1C	4.35	1.50	1.39
20	B	828	CLA	CHD-C4C	4.35	1.53	1.41
20	1	214	CLA	CHC-C1C	4.34	1.50	1.39
20	A	823	CLA	O2A-CGA	4.33	1.46	1.33
20	B	829	CLA	OBD-CAD	4.33	1.28	1.22
20	A	809	CLA	C1C-C2C	-4.33	1.36	1.44
20	B	805	CLA	CHD-C4C	4.32	1.53	1.41
20	B	835	CLA	O2D-CGD	4.32	1.43	1.33
20	J	103	CLA	O2A-CGA	4.32	1.46	1.33
20	B	820	CLA	CHD-C4C	4.32	1.53	1.41
20	1	205	CLA	CHC-C1C	4.31	1.50	1.39
20	A	814	CLA	CHD-C4C	4.31	1.53	1.41
20	A	824	CLA	OBD-CAD	4.31	1.28	1.22
20	1	212	CLA	CHC-C1C	4.31	1.50	1.39
20	2	307	CLA	C3B-C2B	-4.30	1.34	1.40
20	B	824	CLA	O2A-CGA	4.30	1.45	1.33
20	A	814	CLA	C3B-C2B	-4.30	1.34	1.40
20	A	801	CLA	OBD-CAD	4.30	1.28	1.22
20	3	311	CLA	CHC-C1C	4.30	1.46	1.35
20	B	838	CLA	CHD-C4C	4.29	1.53	1.41
20	B	823	CLA	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	302	CLA	O2A-CGA	4.28	1.45	1.33
20	A	808	CLA	O2D-CGD	4.28	1.43	1.33
20	J	101	CLA	C4C-C3C	-4.27	1.37	1.45
20	A	824	CLA	O2A-CGA	4.26	1.45	1.33
20	K	103	CLA	C4B-CHC	4.26	1.52	1.41
20	L	208	CLA	CHD-C4C	4.26	1.53	1.41
20	2	307	CLA	MG-NA	-4.26	1.96	2.06
20	B	806	CLA	O2A-CGA	4.26	1.45	1.33
20	B	807	CLA	CHD-C4C	4.25	1.53	1.41
20	J	101	CLA	O2A-CGA	4.25	1.45	1.33
20	B	821	CLA	C1C-C2C	-4.25	1.36	1.44
20	B	809	CLA	CHD-C4C	4.25	1.53	1.41
20	4	302	CLA	O2A-CGA	4.25	1.45	1.33
20	L	201	CLA	C4C-C3C	-4.25	1.37	1.45
20	1	215	CLA	C4C-C3C	-4.25	1.37	1.45
20	A	819	CLA	OBD-CAD	4.25	1.28	1.22
20	F	206	CLA	O2D-CGD	4.24	1.43	1.33
22	F	203	BCR	C20-C19	-4.24	1.23	1.34
20	A	805	CLA	CHD-C4C	4.24	1.53	1.41
20	F	206	CLA	C1B-NB	-4.24	1.31	1.35
20	A	806	CLA	CHD-C4C	4.23	1.53	1.41
25	B	848	LMG	O8-C28	4.23	1.45	1.33
20	3	319	CLA	CHB-C4A	-4.22	1.31	1.34
20	A	807	CLA	CHD-C4C	4.22	1.53	1.41
20	B	827	CLA	O2A-CGA	4.21	1.45	1.33
20	3	307	CLA	CHC-C1C	4.21	1.49	1.39
20	A	815	CLA	O2D-CGD	4.20	1.43	1.33
20	1	204	CLA	O2A-CGA	4.20	1.46	1.33
20	A	818	CLA	OBD-CAD	4.20	1.28	1.22
20	3	301	CLA	OBD-CAD	4.19	1.28	1.22
20	A	835	CLA	CHD-C4C	4.19	1.53	1.41
20	2	311	CLA	OBD-CAD	4.19	1.28	1.22
20	2	301	CLA	MG-NA	-4.19	1.96	2.06
20	A	816	CLA	C3D-CAD	-4.19	1.35	1.46
20	K	102	CLA	MG-NA	-4.18	1.96	2.06
20	H	103	CLA	CHD-C4C	4.18	1.53	1.41
20	A	850	CLA	O2A-CGA	4.17	1.45	1.33
20	J	103	CLA	C4C-C3C	-4.17	1.37	1.45
20	3	317	CLA	CHD-C4C	4.17	1.53	1.41
20	3	317	CLA	C4B-CHC	4.17	1.52	1.41
20	4	309	CLA	C3C-C4C	-4.17	1.33	1.43
20	L	201	CLA	C3B-C2B	-4.17	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	850	CLA	OBD-CAD	4.17	1.28	1.22
20	K	101	CLA	C4C-C3C	-4.17	1.37	1.45
20	F	205	CLA	C3A-C2A	-4.17	1.50	1.54
20	4	308	CLA	OBD-CAD	4.16	1.28	1.22
20	H	102	CLA	CHD-C4C	4.16	1.53	1.41
20	4	309	CLA	CHB-C4A	-4.16	1.31	1.34
20	1	202	CLA	C4B-NB	-4.16	1.31	1.35
20	4	302	CLA	C4C-C3C	-4.16	1.37	1.45
20	1	210	CLA	O2A-CGA	4.15	1.45	1.33
20	A	812	CLA	CHD-C4C	4.15	1.53	1.41
20	G	102	CLA	O2A-CGA	4.15	1.45	1.33
20	A	839	CLA	C3B-C2B	-4.15	1.34	1.40
20	1	201	CLA	C4C-C3C	-4.14	1.37	1.45
20	B	830	CLA	OBD-CAD	4.14	1.28	1.22
20	A	826	CLA	O2D-CGD	4.14	1.43	1.33
20	B	812	CLA	CHD-C4C	4.14	1.53	1.41
20	4	311	CLA	C4C-C3C	-4.14	1.37	1.45
20	A	839	CLA	OBD-CAD	4.14	1.28	1.22
20	A	808	CLA	CHD-C4C	4.14	1.53	1.41
20	A	813	CLA	OBD-CAD	4.13	1.28	1.22
20	A	837	CLA	C4C-C3C	-4.13	1.37	1.45
20	1	209	CLA	C4B-CHC	4.13	1.52	1.41
20	A	836	CLA	OBD-CAD	4.12	1.28	1.22
20	L	201	CLA	O2A-CGA	4.12	1.45	1.33
25	B	848	LMG	O7-C10	4.12	1.45	1.34
20	B	836	CLA	CHD-C4C	4.12	1.53	1.41
20	3	316	CLA	CHD-C4C	4.12	1.53	1.41
20	A	837	CLA	C1C-C2C	-4.12	1.36	1.44
20	A	820	CLA	CHD-C4C	4.12	1.53	1.41
20	A	850	CLA	C4B-CHC	4.11	1.52	1.41
20	A	804	CLA	CHD-C4C	4.11	1.52	1.41
20	1	201	CLA	CHC-C1C	4.11	1.45	1.35
20	1	215	CLA	C1C-C2C	-4.11	1.36	1.44
20	3	317	CLA	O2A-CGA	4.11	1.45	1.33
22	I	101	BCR	C20-C19	-4.10	1.24	1.34
22	F	203	BCR	C17-C18	-4.10	1.30	1.35
20	A	818	CLA	C4C-C3C	-4.10	1.38	1.45
20	3	304	CLA	CHD-C4C	4.10	1.52	1.41
20	B	832	CLA	C4C-C3C	-4.10	1.38	1.45
20	A	811	CLA	CHD-C4C	4.09	1.52	1.41
20	A	823	CLA	OBD-CAD	4.08	1.28	1.22
20	2	322	CLA	C1B-NB	-4.08	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CHD-C4C	4.08	1.52	1.41
20	3	302	CLA	C1C-NC	-4.08	1.31	1.37
20	2	303	CLA	C4B-CHC	4.08	1.52	1.41
20	L	203	CLA	C4C-C3C	-4.08	1.38	1.45
20	A	831	CLA	OBD-CAD	4.08	1.28	1.22
22	L	210	BCR	C17-C18	-4.08	1.30	1.35
20	B	821	CLA	C3D-CAD	-4.07	1.35	1.46
20	A	832	CLA	OBD-CAD	4.07	1.28	1.22
20	A	809	CLA	CHD-C4C	4.07	1.52	1.41
20	R	108	CLA	C3D-CAD	-4.07	1.35	1.46
20	B	835	CLA	CHD-C4C	4.05	1.52	1.41
20	B	810	CLA	OBD-CAD	4.05	1.28	1.22
20	A	841	CLA	O2A-CGA	4.05	1.45	1.33
20	A	809	CLA	O2D-CGD	4.04	1.43	1.33
20	A	815	CLA	C1C-C2C	-4.04	1.36	1.44
20	B	822	CLA	CHD-C4C	4.03	1.52	1.41
20	B	825	CLA	O2A-CGA	4.03	1.45	1.33
20	A	823	CLA	CHD-C4C	4.03	1.52	1.41
20	A	825	CLA	O2A-CGA	4.03	1.45	1.33
20	A	832	CLA	CHD-C4C	4.02	1.52	1.41
20	B	806	CLA	C1C-C2C	-4.02	1.36	1.44
20	H	101	CLA	C3D-CAD	-4.02	1.35	1.46
20	R	107	CLA	CHD-C4C	4.02	1.52	1.41
20	A	807	CLA	C3B-C2B	-4.01	1.34	1.40
20	2	303	CLA	CHD-C4C	4.01	1.52	1.41
20	3	310	CLA	MG-NA	-4.00	1.96	2.06
20	3	313	CLA	MG-NA	-4.00	1.96	2.06
20	3	313	CLA	C1C-NC	-4.00	1.31	1.37
20	A	851	CLA	OBD-CAD	4.00	1.27	1.22
20	A	829	CLA	OBD-CAD	4.00	1.27	1.22
20	B	803	CLA	CHD-C4C	4.00	1.52	1.41
20	1	202	CLA	O2D-CGD	4.00	1.43	1.33
20	A	807	CLA	O2D-CGD	4.00	1.43	1.33
20	A	801	CLA	CHD-C4C	3.99	1.52	1.41
20	4	316	CLA	O2A-CGA	3.99	1.45	1.33
20	4	319	CLA	OBD-CAD	3.99	1.27	1.22
20	3	302	CLA	OBD-CAD	3.99	1.27	1.22
20	4	318	CLA	C3D-CAD	-3.99	1.36	1.46
20	B	849	CLA	O2A-CGA	3.98	1.45	1.33
20	B	813	CLA	C4B-CHC	3.98	1.52	1.41
20	B	817	CLA	OBD-CAD	3.98	1.27	1.22
20	B	850	CLA	CHD-C4C	3.98	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	311	CLA	CHD-C4C	3.98	1.52	1.41
20	1	201	CLA	C1C-C2C	-3.97	1.36	1.44
20	A	821	CLA	CHD-C4C	3.97	1.52	1.41
20	3	310	CLA	CHD-C4C	3.97	1.52	1.41
20	K	108	CLA	O2A-CGA	3.96	1.44	1.33
20	4	304	CLA	OBD-CAD	3.96	1.27	1.22
20	A	836	CLA	O2A-CGA	3.96	1.44	1.33
20	B	823	CLA	C4C-C3C	-3.96	1.38	1.45
20	4	312	CLA	MG-NA	-3.96	1.96	2.06
20	2	304	CLA	CHC-C1C	3.95	1.49	1.39
20	3	302	CLA	C4C-C3C	-3.95	1.38	1.45
20	1	208	CLA	C4B-NB	-3.95	1.31	1.35
20	4	316	CLA	C3D-CAD	-3.95	1.36	1.46
20	3	312	CLA	C4C-NC	-3.95	1.30	1.37
20	B	831	CLA	C1C-C2C	-3.94	1.36	1.44
20	B	807	CLA	O2A-CGA	3.94	1.44	1.33
20	3	313	CLA	C3D-CAD	-3.94	1.36	1.46
20	1	216	CLA	MG-NA	-3.94	1.96	2.06
20	4	304	CLA	O2D-CGD	3.94	1.42	1.33
20	A	852	CLA	O2A-CGA	3.93	1.44	1.33
20	A	833	CLA	CHD-C4C	3.93	1.52	1.41
20	3	316	CLA	C4B-CHC	3.93	1.51	1.43
20	B	834	CLA	CHD-C4C	3.93	1.52	1.41
20	1	211	CLA	CHD-C4C	3.93	1.52	1.41
20	A	828	CLA	CHD-C4C	3.93	1.52	1.41
20	A	819	CLA	CHD-C4C	3.92	1.52	1.41
20	A	803	CLA	CHD-C4C	3.92	1.52	1.41
20	B	804	CLA	CHD-C4C	3.92	1.52	1.41
20	4	310	CLA	MG-NA	-3.92	1.97	2.06
20	2	310	CLA	C4B-CHC	3.92	1.51	1.43
20	3	303	CLA	CHC-C1C	3.92	1.49	1.39
20	A	815	CLA	C3B-C2B	-3.92	1.34	1.40
20	L	202	CLA	CHD-C4C	3.91	1.52	1.41
20	A	831	CLA	CHD-C4C	3.91	1.52	1.41
20	A	807	CLA	C3D-CAD	-3.91	1.36	1.46
20	4	316	CLA	C4B-NB	-3.91	1.31	1.35
20	A	818	CLA	CHD-C4C	3.91	1.52	1.41
20	3	318	CLA	CHD-C4C	3.91	1.52	1.41
20	3	308	CLA	CHD-C4C	3.90	1.52	1.41
20	B	827	CLA	C4C-C3C	-3.90	1.38	1.45
20	B	826	CLA	O2A-CGA	3.90	1.44	1.33
20	B	851	CLA	OBD-CAD	3.90	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	836	CLA	OBD-CAD	3.90	1.27	1.22
20	4	314	CLA	C3A-C2A	-3.89	1.50	1.54
20	L	201	CLA	C3D-CAD	-3.89	1.36	1.46
20	B	809	CLA	C4B-CHC	3.89	1.51	1.41
20	A	841	CLA	CHD-C4C	3.89	1.52	1.41
20	1	203	CLA	CHD-C4C	3.89	1.52	1.41
20	3	320	CLA	CHD-C4C	3.88	1.52	1.41
20	4	307	CLA	C2A-C1A	-3.88	1.43	1.52
20	1	209	CLA	CHD-C4C	3.88	1.52	1.41
20	B	819	CLA	CHD-C4C	3.88	1.52	1.41
20	A	827	CLA	CHD-C4C	3.87	1.52	1.41
20	B	816	CLA	O2A-CGA	3.86	1.44	1.33
20	B	830	CLA	C4B-CHC	3.86	1.51	1.41
20	2	305	CLA	CHD-C4C	3.86	1.52	1.41
20	B	851	CLA	C4C-C3C	-3.86	1.38	1.45
20	A	822	CLA	CHD-C4C	3.86	1.52	1.41
20	B	814	CLA	CHD-C4C	3.86	1.52	1.41
20	1	201	CLA	C3D-CAD	-3.86	1.36	1.46
20	4	309	CLA	C2C-C1C	-3.85	1.34	1.43
20	B	818	CLA	OBD-CAD	3.84	1.27	1.22
20	4	316	CLA	C1C-C2C	-3.84	1.37	1.44
20	4	302	CLA	CHD-C4C	3.84	1.52	1.41
20	A	819	CLA	C4B-CHC	3.83	1.51	1.41
20	B	803	CLA	O2A-CGA	3.83	1.44	1.33
20	4	311	CLA	CHD-C4C	3.83	1.52	1.41
20	2	306	CLA	CHC-C1C	3.83	1.48	1.39
20	A	851	CLA	CHD-C4C	3.82	1.52	1.41
20	3	313	CLA	C3B-C2B	-3.82	1.35	1.40
20	4	304	CLA	MG-NA	-3.82	1.97	2.06
20	B	815	CLA	CHD-C4C	3.82	1.52	1.41
20	4	305	CLA	CHD-C4C	3.82	1.52	1.41
20	2	307	CLA	O2D-CGD	3.82	1.42	1.33
20	3	319	CLA	CHC-C1C	3.81	1.48	1.39
20	K	103	CLA	CHD-C4C	3.81	1.52	1.41
20	I	102	CLA	CHD-C4C	3.81	1.52	1.41
20	H	109	CLA	CHD-C4C	3.81	1.52	1.41
20	B	814	CLA	C4B-CHC	3.81	1.51	1.41
20	4	318	CLA	C3B-C2B	-3.81	1.35	1.40
20	B	838	CLA	C4B-NB	3.80	1.38	1.35
20	L	209	CLA	C4B-CHC	3.80	1.51	1.41
20	A	820	CLA	C4B-CHC	3.80	1.51	1.41
20	B	837	CLA	C4B-CHC	3.80	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	C4B-CHC	3.79	1.51	1.41
20	3	301	CLA	CHD-C4C	3.78	1.52	1.41
20	K	101	CLA	CHD-C4C	3.78	1.52	1.41
22	B	845	BCR	C20-C19	-3.78	1.24	1.34
20	R	108	CLA	C1C-NC	-3.78	1.32	1.37
20	B	818	CLA	C4B-CHC	3.78	1.51	1.41
20	3	312	CLA	C1B-NB	-3.77	1.31	1.35
20	B	814	CLA	O2A-CGA	3.77	1.45	1.33
20	B	823	CLA	CHD-C4C	3.77	1.52	1.41
20	B	824	CLA	C4C-C3C	-3.76	1.38	1.45
20	A	813	CLA	CHD-C4C	3.76	1.51	1.41
20	L	209	CLA	CHD-C4C	3.76	1.51	1.41
20	2	306	CLA	MG-NA	-3.76	1.97	2.06
20	H	101	CLA	C1B-NB	-3.76	1.31	1.35
20	B	806	CLA	CHD-C4C	3.76	1.51	1.41
20	B	837	CLA	OBD-CAD	3.75	1.27	1.22
20	1	207	CLA	CHD-C4C	3.75	1.51	1.41
20	B	831	CLA	CHD-C4C	3.75	1.51	1.41
20	A	803	CLA	C4C-C3C	-3.75	1.38	1.45
20	A	836	CLA	CHD-C4C	3.75	1.51	1.41
20	H	101	CLA	O2A-CGA	3.74	1.44	1.33
20	A	830	CLA	CHD-C4C	3.74	1.51	1.41
20	R	108	CLA	OBD-CAD	3.74	1.27	1.22
20	L	201	CLA	C1C-NC	-3.74	1.32	1.37
20	3	311	CLA	C3D-CAD	-3.74	1.36	1.46
22	B	843	BCR	C20-C19	-3.73	1.25	1.34
20	A	812	CLA	C4B-CHC	3.72	1.51	1.41
22	B	846	BCR	C20-C19	-3.72	1.25	1.34
20	2	316	CLA	CHD-C4C	3.72	1.51	1.41
20	1	201	CLA	O2A-CGA	3.72	1.44	1.33
20	B	833	CLA	C4B-CHC	3.71	1.51	1.41
20	1	204	CLA	CHD-C4C	3.71	1.51	1.41
20	1	215	CLA	OBD-CAD	3.71	1.27	1.22
22	I	101	BCR	C5-C6	-3.71	1.28	1.34
20	G	102	CLA	C1C-C2C	-3.71	1.37	1.44
20	4	303	CLA	CBD-CHA	-3.70	1.47	1.51
20	4	319	CLA	CHD-C4C	3.70	1.51	1.41
20	R	107	CLA	OBD-CAD	3.70	1.27	1.22
20	G	102	CLA	MG-NA	-3.70	1.97	2.06
20	1	202	CLA	C3D-CAD	-3.70	1.36	1.46
20	B	830	CLA	CHD-C4C	3.70	1.51	1.41
20	3	311	CLA	C1C-NC	-3.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	840	CLA	C3A-C2A	-3.69	1.51	1.54
20	4	319	CLA	C4C-C3C	-3.69	1.38	1.45
20	1	214	CLA	CHD-C4C	3.69	1.51	1.41
20	A	822	CLA	C4B-CHC	3.69	1.51	1.41
20	3	307	CLA	CHD-C4C	3.68	1.51	1.41
22	A	844	BCR	C20-C19	-3.68	1.25	1.34
20	A	810	CLA	C4B-CHC	3.68	1.51	1.41
20	A	815	CLA	O2A-CGA	3.68	1.44	1.33
20	2	315	CLA	CHD-C4C	3.68	1.51	1.41
20	I	102	CLA	C4C-C3C	-3.68	1.38	1.45
20	4	312	CLA	CHD-C4C	3.67	1.51	1.41
20	3	319	CLA	C4C-NC	-3.67	1.30	1.37
20	3	306	CLA	CHD-C4C	3.67	1.51	1.41
20	B	837	CLA	C4C-C3C	-3.67	1.38	1.45
20	B	807	CLA	C1C-C2C	-3.67	1.37	1.44
20	B	828	CLA	C4B-CHC	3.66	1.51	1.41
20	A	802	CLA	CHB-C4A	-3.66	1.32	1.34
20	1	210	CLA	C1C-NC	-3.66	1.32	1.37
20	L	207	CLA	CHD-C4C	3.66	1.51	1.41
20	B	832	CLA	C4B-CHC	3.66	1.51	1.41
20	A	825	CLA	C4C-C3C	-3.66	1.38	1.45
20	A	808	CLA	C4C-C3C	-3.66	1.38	1.45
20	B	826	CLA	C4B-CHC	3.66	1.51	1.41
20	2	304	CLA	C1B-NB	-3.66	1.31	1.35
20	A	839	CLA	MG-NA	-3.65	1.97	2.06
20	B	835	CLA	OBD-CAD	3.65	1.27	1.22
20	1	202	CLA	MG-NA	-3.65	1.97	2.06
20	4	307	CLA	MG-NC	-3.65	1.97	2.06
20	A	834	CLA	CHD-C4C	3.65	1.51	1.41
20	A	817	CLA	CHD-C4C	3.65	1.51	1.41
20	B	850	CLA	C4B-CHC	3.64	1.51	1.41
20	A	824	CLA	C4C-C3C	-3.64	1.38	1.45
20	4	302	CLA	C1C-C2C	-3.64	1.37	1.44
20	2	301	CLA	CHC-C1C	3.64	1.48	1.39
20	B	834	CLA	C4B-CHC	3.64	1.51	1.41
20	1	206	CLA	C4B-CHC	3.64	1.51	1.41
20	A	838	CLA	CHD-C4C	3.64	1.51	1.41
20	4	314	CLA	C4B-CHC	3.64	1.51	1.41
20	1	216	CLA	C1B-NB	-3.63	1.32	1.35
20	A	826	CLA	C4B-CHC	3.63	1.51	1.41
20	J	101	CLA	CHD-C4C	3.63	1.51	1.41
20	L	201	CLA	MG-NA	-3.63	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	CHD-C4C	3.63	1.51	1.41
20	1	207	CLA	C4B-CHC	3.63	1.51	1.41
20	1	212	CLA	CHD-C4C	3.63	1.51	1.41
20	G	102	CLA	C1C-NC	-3.63	1.32	1.37
20	A	824	CLA	CHD-C4C	3.63	1.51	1.41
21	2	320	LMU	O1'-C1'	3.63	1.46	1.40
20	4	309	CLA	C4C-NC	-3.63	1.31	1.37
20	B	808	CLA	C4B-CHC	3.62	1.51	1.41
20	A	826	CLA	O2A-CGA	3.62	1.43	1.33
20	B	840	CLA	CHD-C4C	3.62	1.51	1.41
20	H	101	CLA	O2D-CGD	3.62	1.42	1.33
20	A	852	CLA	C4B-CHC	3.62	1.51	1.41
20	R	108	CLA	C4B-NB	-3.62	1.32	1.35
20	4	318	CLA	CHD-C4C	3.62	1.51	1.41
20	B	805	CLA	C1C-C2C	-3.61	1.37	1.44
20	A	825	CLA	CHD-C4C	3.61	1.51	1.41
20	B	836	CLA	C4C-C3C	-3.61	1.38	1.45
20	L	201	CLA	C4B-CHC	3.61	1.51	1.41
20	A	829	CLA	CHD-C4C	3.61	1.51	1.41
20	4	311	CLA	C4B-CHC	3.60	1.51	1.41
20	A	817	CLA	C4B-CHC	3.60	1.51	1.41
20	2	312	CLA	CHD-C4C	3.60	1.51	1.41
20	B	833	CLA	CHD-C4C	3.59	1.51	1.41
20	B	849	CLA	C4B-CHC	3.59	1.51	1.41
20	I	102	CLA	C4B-CHC	3.59	1.51	1.41
20	3	301	CLA	C4B-CHC	3.59	1.51	1.41
20	F	205	CLA	C4C-C3C	-3.58	1.38	1.45
20	2	312	CLA	C4B-CHC	3.58	1.50	1.41
20	B	817	CLA	CHD-C4C	3.58	1.51	1.41
20	B	817	CLA	C4C-C3C	-3.58	1.38	1.45
20	2	302	CLA	CHD-C4C	3.58	1.51	1.41
20	2	302	CLA	C4C-C3C	-3.58	1.38	1.45
20	A	838	CLA	C4B-CHC	3.57	1.50	1.41
20	B	849	CLA	CHD-C4C	3.57	1.51	1.41
20	B	811	CLA	CBD-CGD	-3.57	1.41	1.52
20	H	102	CLA	C4B-CHC	3.57	1.50	1.41
20	J	103	CLA	CHD-C4C	3.57	1.51	1.41
20	F	205	CLA	CHD-C4C	3.56	1.51	1.41
20	3	304	CLA	C4B-CHC	3.56	1.50	1.41
20	A	833	CLA	C4C-C3C	-3.55	1.38	1.45
20	B	806	CLA	MG-NA	-3.55	1.97	2.06
20	L	207	CLA	C4C-C3C	-3.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	815	CLA	C4B-CHC	3.55	1.50	1.41
20	B	816	CLA	CHD-C4C	3.55	1.51	1.41
20	A	811	CLA	C1C-C2C	-3.54	1.37	1.44
20	4	316	CLA	MG-NA	-3.54	1.97	2.06
20	A	811	CLA	C4B-CHC	3.54	1.50	1.41
20	1	202	CLA	C4C-C3C	-3.53	1.39	1.45
22	A	846	BCR	C20-C19	-3.53	1.25	1.34
22	A	847	BCR	C20-C19	-3.53	1.25	1.34
20	B	826	CLA	C4C-C3C	-3.53	1.39	1.45
21	2	319	LMU	O1'-C1'	3.53	1.46	1.40
20	A	830	CLA	C4C-C3C	-3.53	1.39	1.45
20	A	837	CLA	CHD-C4C	3.53	1.51	1.41
20	4	307	CLA	C3D-CAD	-3.52	1.37	1.46
20	K	101	CLA	C1C-C2C	-3.52	1.37	1.44
20	B	819	CLA	C4B-CHC	3.52	1.50	1.41
20	K	108	CLA	C4C-C3C	-3.52	1.39	1.45
20	1	205	CLA	CHB-C4A	-3.52	1.32	1.34
20	1	208	CLA	CHC-C1C	3.52	1.48	1.39
20	L	208	CLA	C4B-CHC	3.52	1.50	1.41
20	B	806	CLA	C3B-C2B	-3.52	1.35	1.40
20	B	818	CLA	CHD-C4C	3.51	1.51	1.41
20	B	839	CLA	CHD-C4C	3.51	1.51	1.41
20	3	311	CLA	O2A-CGA	3.51	1.43	1.33
22	3	314	BCR	C20-C19	-3.50	1.25	1.34
20	L	207	CLA	C4B-CHC	3.50	1.50	1.41
20	L	203	CLA	C4B-CHC	3.50	1.50	1.41
20	H	101	CLA	CHD-C4C	3.50	1.51	1.41
20	B	816	CLA	C4C-C3C	-3.50	1.39	1.45
20	B	824	CLA	C4B-CHC	3.50	1.50	1.41
20	A	815	CLA	C3A-C2A	-3.50	1.44	1.54
20	B	851	CLA	CHD-C4C	3.49	1.51	1.41
20	K	108	CLA	CHD-C4C	3.49	1.51	1.41
20	A	830	CLA	C1C-C2C	-3.49	1.37	1.44
20	3	309	CLA	CHD-C4C	3.49	1.51	1.41
20	4	307	CLA	C3A-C2A	-3.49	1.44	1.54
20	2	322	CLA	C4C-C3C	-3.49	1.39	1.45
20	4	313	CLA	C4B-CHC	3.48	1.50	1.43
20	A	834	CLA	C4B-CHC	3.48	1.50	1.41
20	B	827	CLA	C3D-CAD	-3.48	1.37	1.46
20	3	302	CLA	MG-NA	-3.48	1.98	2.06
20	2	302	CLA	C4B-CHC	3.48	1.50	1.41
20	A	837	CLA	C1B-NB	-3.47	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	203	CLA	CHD-C4C	3.47	1.51	1.41
20	A	833	CLA	C1C-C2C	-3.47	1.37	1.44
20	G	102	CLA	C3B-C2B	-3.47	1.35	1.40
20	A	850	CLA	CHD-C4C	3.47	1.51	1.41
20	1	214	CLA	C4B-CHC	3.46	1.50	1.43
20	F	206	CLA	O2A-CGA	3.46	1.43	1.33
22	J	102	BCR	C20-C19	-3.46	1.25	1.34
20	2	309	CLA	MG-NA	-3.46	1.98	2.06
20	A	851	CLA	C4B-CHC	3.46	1.50	1.41
20	B	803	CLA	C4C-C3C	-3.46	1.39	1.45
20	1	216	CLA	CHC-C1C	3.45	1.48	1.39
20	A	820	CLA	C4C-C3C	-3.45	1.39	1.45
21	F	201	LMU	O1B-C4'	-3.45	1.34	1.43
20	F	205	CLA	C4B-CHC	3.45	1.50	1.41
20	A	837	CLA	MG-NA	-3.45	1.98	2.06
20	3	306	CLA	MG-NA	-3.45	1.98	2.06
22	F	202	BCR	C20-C19	-3.45	1.25	1.34
20	B	806	CLA	C4C-C3C	-3.44	1.39	1.45
22	B	842	BCR	C20-C19	-3.44	1.25	1.34
20	2	322	CLA	O2A-CGA	3.44	1.43	1.33
20	2	322	CLA	C4B-NB	-3.44	1.32	1.35
20	3	309	CLA	C1B-NB	-3.44	1.32	1.35
20	4	304	CLA	C3D-C2D	-3.44	1.33	1.39
20	4	308	CLA	CHD-C4C	3.44	1.51	1.41
20	3	318	CLA	C4B-CHC	3.44	1.50	1.41
20	3	307	CLA	MG-NA	-3.43	1.98	2.06
20	3	312	CLA	CHC-C1C	3.43	1.47	1.39
20	4	319	CLA	C4B-CHC	3.43	1.50	1.41
20	B	803	CLA	C4B-CHC	3.42	1.50	1.41
20	A	814	CLA	C4B-CHC	3.42	1.50	1.41
20	2	305	CLA	C4C-C3C	-3.42	1.39	1.45
20	F	206	CLA	C4B-CHC	3.42	1.50	1.41
20	4	308	CLA	C4B-CHC	3.42	1.50	1.41
20	L	201	CLA	OBD-CAD	3.42	1.27	1.22
22	A	845	BCR	C20-C19	-3.42	1.25	1.34
20	A	825	CLA	C1C-C2C	-3.41	1.38	1.44
20	4	307	CLA	C1C-NC	-3.41	1.32	1.37
20	A	829	CLA	C4B-CHC	3.41	1.50	1.41
20	3	303	CLA	C3C-C4C	-3.41	1.35	1.43
20	J	101	CLA	C1C-C2C	-3.41	1.38	1.44
20	B	840	CLA	C4B-CHC	3.41	1.50	1.41
20	B	833	CLA	C4C-C3C	-3.41	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	103	BCR	C20-C19	-3.40	1.25	1.34
20	4	315	CLA	CHD-C4C	3.40	1.50	1.41
20	B	813	CLA	CHD-C4C	3.40	1.50	1.41
20	B	831	CLA	C4B-CHC	3.40	1.50	1.41
20	G	102	CLA	C4B-NB	-3.40	1.32	1.35
20	2	309	CLA	CHD-C4C	3.40	1.50	1.41
20	A	840	CLA	C4B-CHC	3.40	1.50	1.41
20	B	803	CLA	C3B-C2B	-3.40	1.35	1.40
20	R	107	CLA	C4B-CHC	3.40	1.50	1.41
20	2	311	CLA	C4B-CHC	3.39	1.50	1.41
20	4	309	CLA	CHC-C1C	3.39	1.47	1.39
20	B	831	CLA	C4C-C3C	-3.39	1.39	1.45
20	B	832	CLA	CHD-C4C	3.39	1.50	1.41
20	L	202	CLA	C4B-CHC	3.39	1.50	1.41
22	F	203	BCR	C29-C30	-3.39	1.46	1.54
20	B	838	CLA	C4B-CHC	3.38	1.50	1.41
20	1	206	CLA	CHD-C4C	3.38	1.50	1.41
20	A	831	CLA	C1C-C2C	-3.38	1.38	1.44
20	4	303	CLA	CHD-C4C	3.38	1.50	1.41
22	I	103	BCR	C38-C26	-3.38	1.45	1.50
20	2	305	CLA	C4B-CHC	3.38	1.50	1.41
20	B	837	CLA	CHD-C4C	3.38	1.50	1.41
20	4	307	CLA	CAA-C2A	-3.37	1.47	1.54
20	B	820	CLA	C4B-CHC	3.37	1.50	1.41
20	B	829	CLA	CHD-C4C	3.37	1.50	1.41
20	K	102	CLA	O2A-CGA	3.37	1.43	1.33
20	1	201	CLA	MG-NA	-3.37	1.98	2.06
20	2	315	CLA	C4B-CHC	3.37	1.50	1.43
20	3	302	CLA	O2A-CGA	3.36	1.43	1.33
20	4	303	CLA	C4B-CHC	3.36	1.50	1.41
20	A	817	CLA	C4C-C3C	-3.36	1.39	1.45
20	2	307	CLA	C3D-CAD	-3.36	1.37	1.46
20	1	215	CLA	C3B-C2B	-3.36	1.35	1.40
22	A	843	BCR	C20-C19	-3.35	1.25	1.34
20	K	108	CLA	C1C-C2C	-3.35	1.38	1.44
20	A	852	CLA	C4C-C3C	-3.35	1.39	1.45
20	1	215	CLA	MG-NA	-3.35	1.98	2.06
20	B	810	CLA	C4B-CHC	3.34	1.50	1.41
20	4	310	CLA	CHC-C1C	3.34	1.47	1.39
20	A	816	CLA	C1C-C2C	-3.34	1.38	1.44
20	1	201	CLA	C3D-C2D	-3.33	1.33	1.39
20	F	204	CLA	C4B-CHC	3.33	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	302	CLA	C1C-C2C	-3.33	1.38	1.44
20	B	838	CLA	C1C-C2C	-3.33	1.38	1.44
20	G	102	CLA	CHD-C4C	3.33	1.50	1.41
20	1	212	CLA	C4B-NB	-3.32	1.32	1.35
20	B	808	CLA	C4C-C3C	-3.32	1.39	1.45
20	B	829	CLA	C4B-CHC	3.32	1.50	1.41
20	A	813	CLA	C1C-C2C	-3.31	1.38	1.44
20	B	823	CLA	C1C-C2C	-3.31	1.38	1.44
20	1	215	CLA	CHD-C4C	3.31	1.50	1.41
20	2	316	CLA	C4C-C3C	-3.31	1.39	1.45
20	A	806	CLA	C4B-CHC	3.31	1.50	1.41
20	B	824	CLA	CHD-C4C	3.31	1.50	1.41
20	4	313	CLA	MG-NA	-3.31	1.98	2.06
20	B	806	CLA	C4B-NB	-3.30	1.32	1.35
20	B	810	CLA	CHD-C4C	3.30	1.50	1.41
20	B	851	CLA	C4B-CHC	3.30	1.50	1.41
20	A	824	CLA	C4B-CHC	3.30	1.50	1.41
20	A	804	CLA	C4C-C3C	-3.30	1.39	1.45
20	4	304	CLA	C3D-CAD	-3.29	1.37	1.46
20	4	304	CLA	C1C-NC	-3.29	1.32	1.37
20	1	208	CLA	CHD-C4C	3.29	1.50	1.41
20	B	816	CLA	C4B-CHC	3.29	1.50	1.41
21	4	321	LMU	O1'-C1'	3.29	1.45	1.40
20	3	305	CLA	C4B-NB	-3.29	1.32	1.35
20	A	802	CLA	C3C-C4C	-3.28	1.35	1.43
20	1	210	CLA	C4B-NB	-3.28	1.32	1.35
20	A	836	CLA	C4B-CHC	3.28	1.50	1.41
20	K	102	CLA	OBD-CAD	3.28	1.26	1.22
20	2	308	CLA	C4B-CHC	3.27	1.50	1.41
20	R	108	CLA	MG-NA	-3.27	1.98	2.06
20	H	103	CLA	C4B-CHC	3.27	1.50	1.41
20	B	811	CLA	MG-NA	-3.26	1.98	2.06
20	B	805	CLA	C4C-C3C	-3.26	1.39	1.45
20	4	306	CLA	C1D-C2D	-3.26	1.35	1.42
20	4	315	CLA	C4B-CHC	3.25	1.50	1.43
20	A	804	CLA	C4B-CHC	3.25	1.50	1.41
20	F	206	CLA	C4B-NB	-3.25	1.32	1.35
20	2	322	CLA	C1C-C2C	-3.25	1.38	1.44
20	A	805	CLA	OBD-CAD	3.25	1.26	1.22
20	A	816	CLA	MG-NA	-3.24	1.98	2.06
20	B	822	CLA	C4B-CHC	3.24	1.50	1.41
22	I	101	BCR	C26-C25	-3.24	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	839	CLA	C3D-CAD	-3.24	1.37	1.46
20	A	841	CLA	C4C-C3C	-3.23	1.39	1.45
20	1	207	CLA	C2A-C1A	-3.23	1.44	1.52
20	K	108	CLA	C4B-CHC	3.23	1.50	1.41
20	A	818	CLA	C3B-C2B	-3.23	1.35	1.40
20	A	828	CLA	C4B-CHC	3.23	1.50	1.41
20	3	310	CLA	C2C-C1C	-3.23	1.35	1.43
20	B	814	CLA	C4C-C3C	-3.23	1.39	1.45
20	A	823	CLA	C4B-CHC	3.23	1.50	1.41
20	1	204	CLA	C3D-CAD	-3.22	1.37	1.46
20	B	811	CLA	C3D-C2D	-3.22	1.33	1.39
20	B	836	CLA	C1C-C2C	-3.22	1.38	1.44
22	B	852	BCR	C29-C30	-3.22	1.46	1.54
20	K	102	CLA	C4B-CHC	3.22	1.49	1.41
20	3	312	CLA	C2C-C1C	-3.21	1.35	1.43
21	H	108	LMU	O5B-C5B	-3.21	1.36	1.44
20	1	202	CLA	C3B-C2B	-3.21	1.35	1.40
20	3	305	CLA	CHC-C1C	3.21	1.47	1.39
20	J	103	CLA	C1C-C2C	-3.21	1.38	1.44
22	B	852	BCR	C30-C25	-3.21	1.49	1.53
20	G	102	CLA	C3D-CAD	-3.20	1.37	1.46
20	2	309	CLA	CHA-C1A	3.20	1.50	1.41
22	B	852	BCR	C40-C30	-3.20	1.47	1.53
20	1	204	CLA	C4B-CHC	3.20	1.49	1.41
20	A	816	CLA	C4B-CHC	3.20	1.49	1.41
20	L	209	CLA	C4C-C3C	-3.20	1.39	1.45
20	B	826	CLA	CHD-C4C	3.19	1.50	1.41
20	1	206	CLA	C4C-C3C	-3.19	1.39	1.45
20	B	851	CLA	C1C-C2C	-3.19	1.38	1.44
20	A	827	CLA	C4B-CHC	3.19	1.49	1.41
20	A	813	CLA	C4C-C3C	-3.19	1.39	1.45
20	B	834	CLA	C4C-C3C	-3.19	1.39	1.45
20	1	211	CLA	MG-NA	-3.18	1.98	2.06
20	B	821	CLA	O2A-CGA	3.18	1.42	1.33
20	2	310	CLA	CHD-C4C	3.18	1.50	1.41
20	K	102	CLA	C3D-CAD	-3.18	1.38	1.46
20	4	310	CLA	C2B-C1B	-3.18	1.34	1.39
20	H	101	CLA	CBD-CGD	-3.18	1.42	1.52
20	2	315	CLA	MG-NA	-3.18	1.98	2.06
21	F	201	LMU	C3'-C4'	-3.18	1.43	1.52
20	A	814	CLA	C1C-C2C	-3.17	1.38	1.44
20	A	832	CLA	C4B-CHC	3.17	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	C3D-CAD	-3.17	1.38	1.46
20	3	305	CLA	CHD-C4C	3.17	1.50	1.41
20	4	312	CLA	C4B-CHC	3.17	1.50	1.43
20	2	316	CLA	C1C-C2C	-3.17	1.38	1.44
22	B	852	BCR	C14-C13	-3.17	1.31	1.35
20	4	307	CLA	CHD-C4C	3.17	1.50	1.41
20	1	202	CLA	C1C-NC	-3.17	1.33	1.37
20	2	307	CLA	CHD-C4C	3.16	1.50	1.41
20	B	830	CLA	C4C-C3C	-3.16	1.39	1.45
20	B	823	CLA	C4B-CHC	3.16	1.49	1.41
20	B	811	CLA	C4B-CHC	3.16	1.49	1.41
20	K	101	CLA	MG-NA	-3.16	1.98	2.06
20	A	851	CLA	C4C-C3C	-3.16	1.39	1.45
20	4	306	CLA	O2A-CGA	3.16	1.42	1.33
20	4	307	CLA	O2A-CGA	3.16	1.42	1.33
21	G	101	LMU	O5B-C5B	-3.15	1.36	1.44
20	1	204	CLA	C1C-C2C	-3.15	1.38	1.44
20	1	204	CLA	C4C-C3C	-3.15	1.39	1.45
22	L	210	BCR	C30-C25	-3.15	1.49	1.53
20	B	804	CLA	C4B-CHC	3.15	1.49	1.41
20	B	825	CLA	C4C-C3C	-3.15	1.39	1.45
20	B	849	CLA	C4C-C3C	-3.15	1.39	1.45
21	F	201	LMU	C4'-C5'	-3.15	1.44	1.52
20	A	830	CLA	C1B-NB	-3.14	1.32	1.35
20	B	812	CLA	C4B-CHC	3.14	1.49	1.41
20	3	305	CLA	C1C-NC	-3.14	1.31	1.38
20	L	201	CLA	CHD-C4C	3.14	1.50	1.41
20	L	201	CLA	C3D-C2D	-3.14	1.33	1.39
20	B	807	CLA	C4C-C3C	-3.13	1.39	1.45
20	4	310	CLA	CHB-C4A	-3.13	1.32	1.34
20	4	316	CLA	O2D-CGD	3.13	1.40	1.33
20	A	824	CLA	C1C-C2C	-3.13	1.38	1.44
20	3	320	CLA	C4B-CHC	3.13	1.50	1.43
20	B	814	CLA	C1C-C2C	-3.13	1.38	1.44
22	B	852	BCR	C39-C30	-3.13	1.47	1.53
20	B	830	CLA	C3D-CAD	-3.13	1.38	1.46
20	B	819	CLA	C4C-C3C	-3.13	1.39	1.45
20	B	811	CLA	O2A-CGA	3.12	1.42	1.33
20	J	103	CLA	C4B-CHC	3.12	1.49	1.41
20	K	102	CLA	C1C-NC	-3.12	1.33	1.37
20	K	102	CLA	CHD-C4C	3.12	1.50	1.41
20	A	825	CLA	C4B-CHC	3.12	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	303	CLA	C2C-C1C	-3.12	1.35	1.43
20	H	109	CLA	C4B-CHC	3.11	1.49	1.41
20	A	821	CLA	C4B-CHC	3.11	1.49	1.41
20	1	202	CLA	O2A-CGA	3.11	1.42	1.33
20	A	850	CLA	C3B-C2B	-3.11	1.36	1.40
20	B	817	CLA	C4B-CHC	3.11	1.49	1.41
20	A	852	CLA	C1C-C2C	-3.11	1.38	1.44
20	3	316	CLA	CHA-C1A	3.11	1.50	1.41
20	4	314	CLA	CHD-C4C	3.11	1.50	1.41
20	A	815	CLA	MG-NC	-3.10	1.98	2.06
20	4	316	CLA	CBD-CGD	-3.10	1.42	1.52
20	3	309	CLA	MG-NA	-3.09	1.98	2.06
20	4	302	CLA	MG-NA	-3.09	1.98	2.06
20	B	850	CLA	C4C-C3C	-3.09	1.39	1.45
20	1	201	CLA	C4B-NB	-3.09	1.32	1.35
20	H	109	CLA	C4C-C3C	-3.09	1.39	1.45
20	4	306	CLA	C3B-C2B	-3.08	1.36	1.40
20	A	808	CLA	C3B-C2B	-3.07	1.36	1.40
20	2	306	CLA	C2C-C1C	-3.07	1.36	1.43
20	2	301	CLA	C2B-C1B	-3.07	1.34	1.39
20	A	812	CLA	C1C-C2C	-3.06	1.38	1.44
20	2	307	CLA	C4B-NB	-3.06	1.32	1.35
20	A	827	CLA	C3B-C2B	-3.06	1.36	1.40
20	1	207	CLA	C4C-C3C	-3.06	1.39	1.45
20	A	841	CLA	C4B-CHC	3.06	1.49	1.41
20	3	319	CLA	C1C-NC	-3.06	1.32	1.38
20	J	101	CLA	MG-NA	-3.06	1.99	2.06
20	2	312	CLA	C3D-CAD	-3.06	1.38	1.46
20	2	322	CLA	C4B-CHC	3.05	1.49	1.41
20	A	836	CLA	C4C-C3C	-3.05	1.39	1.45
20	A	833	CLA	C3D-CAD	-3.05	1.38	1.46
20	A	835	CLA	C4B-CHC	3.04	1.49	1.41
20	1	202	CLA	CHD-C4C	3.04	1.49	1.41
20	1	208	CLA	C2C-C1C	-3.04	1.36	1.43
20	A	834	CLA	C1C-C2C	-3.04	1.38	1.44
20	3	303	CLA	C1C-NC	-3.04	1.32	1.38
20	3	312	CLA	C4B-CHC	3.04	1.50	1.43
20	A	830	CLA	C4B-CHC	3.04	1.49	1.41
20	J	101	CLA	C4B-CHC	3.04	1.49	1.41
20	A	835	CLA	C1C-C2C	-3.04	1.38	1.44
20	A	807	CLA	O2A-CGA	3.03	1.42	1.33
20	A	825	CLA	C1B-NB	-3.03	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	810	CLA	C4C-C3C	-3.03	1.39	1.45
20	H	101	CLA	C1C-NC	-3.03	1.33	1.37
20	1	204	CLA	MG-NA	-3.03	1.99	2.06
20	A	806	CLA	C1C-C2C	-3.03	1.38	1.44
20	H	101	CLA	C3A-C2A	-3.03	1.46	1.54
20	A	801	CLA	C4B-CHC	3.02	1.49	1.41
20	A	801	CLA	C1C-C2C	-3.02	1.38	1.44
22	B	852	BCR	C31-C1	-3.02	1.47	1.53
20	B	838	CLA	C4C-C3C	-3.02	1.39	1.45
20	K	101	CLA	C4B-CHC	3.02	1.49	1.41
20	A	826	CLA	C1C-C2C	-3.02	1.38	1.44
20	L	201	CLA	C1C-C2C	-3.02	1.38	1.44
20	4	318	CLA	OBD-CAD	3.02	1.26	1.22
20	A	813	CLA	C4B-CHC	3.01	1.49	1.41
20	1	212	CLA	CHB-C4A	-3.01	1.32	1.34
20	A	803	CLA	C1C-C2C	-3.01	1.38	1.44
20	1	215	CLA	O2A-CGA	3.01	1.42	1.33
20	B	807	CLA	C4B-CHC	3.01	1.49	1.41
20	A	802	CLA	C4B-CHC	3.00	1.49	1.43
20	F	206	CLA	CHD-C4C	3.00	1.49	1.41
20	I	102	CLA	OBD-CAD	3.00	1.26	1.22
20	2	316	CLA	C4B-CHC	3.00	1.49	1.41
20	B	829	CLA	C4C-C3C	-3.00	1.39	1.45
20	3	310	CLA	CHA-C1A	3.00	1.49	1.41
20	B	835	CLA	C3D-CAD	-3.00	1.38	1.46
20	2	306	CLA	C3C-C4C	-3.00	1.36	1.43
20	3	311	CLA	OBD-CAD	3.00	1.26	1.22
20	B	826	CLA	C1B-NB	3.00	1.37	1.35
20	B	811	CLA	O2D-CGD	2.99	1.40	1.33
21	R	101	LMU	O2B-C2B	2.99	1.50	1.43
20	B	824	CLA	C1C-C2C	-2.99	1.38	1.44
20	A	815	CLA	CHD-C4C	2.99	1.49	1.41
20	A	835	CLA	C4C-C3C	-2.98	1.39	1.45
20	4	302	CLA	C4B-CHC	2.98	1.49	1.41
20	4	316	CLA	C4B-CHC	2.98	1.49	1.41
20	4	313	CLA	CHD-C4C	2.98	1.49	1.41
20	B	816	CLA	OBD-CAD	2.98	1.26	1.22
20	A	812	CLA	C4C-C3C	-2.98	1.39	1.45
21	H	104	LMU	O3B-C3B	2.98	1.50	1.43
20	A	805	CLA	C1C-C2C	-2.98	1.38	1.44
20	A	839	CLA	C4B-NB	-2.98	1.32	1.35
20	3	310	CLA	CHC-C1C	2.97	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	C1C-C2C	-2.97	1.38	1.44
20	G	102	CLA	C4B-CHC	2.97	1.49	1.41
20	B	821	CLA	C4B-CHC	2.97	1.49	1.41
20	4	305	CLA	C1C-C2C	-2.96	1.38	1.44
20	B	838	CLA	MG-NA	-2.96	1.99	2.06
20	B	804	CLA	C1B-NB	-2.96	1.32	1.35
20	3	306	CLA	CHA-C1A	2.96	1.49	1.41
20	4	306	CLA	C4B-CHC	2.96	1.49	1.41
20	K	103	CLA	C4C-C3C	-2.95	1.39	1.45
22	I	103	BCR	C10-C9	-2.95	1.31	1.35
20	1	203	CLA	C3D-CAD	-2.95	1.38	1.46
20	I	102	CLA	C3D-CAD	-2.95	1.38	1.46
20	F	204	CLA	C1C-C2C	-2.95	1.38	1.44
20	4	310	CLA	CHD-C4C	2.95	1.49	1.41
20	A	808	CLA	C4B-CHC	2.95	1.49	1.41
20	A	831	CLA	C4B-CHC	2.95	1.49	1.41
20	4	308	CLA	C1C-C2C	-2.94	1.38	1.44
20	4	311	CLA	C1B-CHB	2.94	1.49	1.41
20	B	808	CLA	C1C-C2C	-2.94	1.38	1.44
20	1	211	CLA	C4B-CHC	2.94	1.49	1.43
20	B	835	CLA	C1B-CHB	2.94	1.49	1.41
20	B	825	CLA	C3D-CAD	-2.94	1.38	1.46
20	3	307	CLA	CHA-C1A	2.93	1.49	1.41
20	B	821	CLA	C2A-C1A	-2.93	1.45	1.52
20	2	306	CLA	CHD-C4C	2.93	1.49	1.41
20	B	826	CLA	C1B-CHB	2.93	1.49	1.41
21	A	849	LMU	O1'-C1'	2.93	1.45	1.40
22	B	845	BCR	C30-C25	-2.93	1.49	1.53
20	J	103	CLA	MG-NA	-2.93	1.99	2.06
20	B	827	CLA	CHD-C4C	2.93	1.49	1.41
20	B	827	CLA	C1C-C2C	-2.92	1.38	1.44
20	B	823	CLA	MG-NA	-2.92	1.99	2.06
20	4	318	CLA	C1C-NC	-2.92	1.33	1.37
20	A	801	CLA	C3D-CAD	-2.92	1.38	1.46
20	F	205	CLA	C1C-C2C	-2.92	1.38	1.44
20	2	301	CLA	C1C-NC	-2.92	1.32	1.38
20	3	308	CLA	C4B-CHC	2.92	1.49	1.41
20	2	309	CLA	C4B-CHC	2.92	1.49	1.43
20	A	804	CLA	C1C-C2C	-2.92	1.38	1.44
20	B	808	CLA	O2A-CGA	2.92	1.41	1.33
20	A	819	CLA	C1C-C2C	-2.92	1.38	1.44
20	A	818	CLA	C4B-CHC	2.92	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	815	CLA	C3A-C4A	-2.92	1.42	1.51
22	F	203	BCR	C39-C30	-2.91	1.48	1.53
20	A	816	CLA	O2A-CGA	2.91	1.41	1.33
20	4	318	CLA	O2A-CGA	2.91	1.41	1.33
20	2	316	CLA	C3D-CAD	-2.91	1.38	1.46
20	A	816	CLA	C4B-NB	-2.90	1.32	1.35
20	A	815	CLA	C2A-C1A	-2.90	1.45	1.52
20	2	322	CLA	CHD-C4C	2.90	1.49	1.41
20	A	801	CLA	CMA-C3A	2.90	1.59	1.53
20	1	210	CLA	MG-NA	-2.90	1.99	2.06
20	2	301	CLA	CHD-C4C	2.90	1.49	1.41
20	4	319	CLA	C1C-C2C	-2.90	1.39	1.44
20	3	305	CLA	C2C-C1C	-2.90	1.36	1.43
20	L	203	CLA	C1B-CHB	2.90	1.49	1.41
20	A	805	CLA	C4B-CHC	2.90	1.49	1.41
22	I	101	BCR	C1-C6	-2.89	1.49	1.53
20	3	305	CLA	C3C-C4C	-2.89	1.36	1.43
20	1	206	CLA	C1B-CHB	2.89	1.49	1.41
20	3	307	CLA	C4B-CHC	2.88	1.49	1.43
20	B	813	CLA	C4C-C3C	-2.88	1.40	1.45
20	4	315	CLA	CHA-C1A	2.88	1.49	1.41
20	B	820	CLA	C1C-C2C	-2.88	1.39	1.44
20	3	319	CLA	C3C-C4C	-2.88	1.36	1.43
20	F	206	CLA	CAA-C2A	-2.88	1.48	1.54
20	B	831	CLA	C1B-NB	-2.88	1.32	1.35
20	B	815	CLA	C1C-C2C	-2.88	1.39	1.44
20	3	319	CLA	C4B-CHC	2.87	1.49	1.43
20	1	215	CLA	C3D-CAD	-2.87	1.38	1.46
22	I	101	BCR	C4-C5	-2.87	1.45	1.51
20	2	302	CLA	C1C-C2C	-2.87	1.39	1.44
20	1	214	CLA	CHA-C1A	2.87	1.49	1.41
20	3	311	CLA	C1B-CHB	2.87	1.49	1.41
20	B	827	CLA	C4B-CHC	2.87	1.49	1.41
20	A	835	CLA	MG-NA	-2.87	1.99	2.06
20	B	828	CLA	C1B-NB	-2.87	1.32	1.35
22	F	203	BCR	C40-C30	-2.87	1.48	1.53
20	2	304	CLA	C4C-NC	-2.87	1.32	1.37
20	B	830	CLA	C1C-C2C	-2.87	1.39	1.44
20	A	821	CLA	C1C-C2C	-2.86	1.39	1.44
20	3	303	CLA	C4C-NC	-2.86	1.32	1.37
21	H	104	LMU	O1'-C1'	2.86	1.45	1.40
20	B	805	CLA	C4B-CHC	2.86	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	318	LMU	O1'-C1'	2.86	1.45	1.40
20	B	819	CLA	C3D-CAD	-2.86	1.38	1.46
20	1	210	CLA	C1B-CHB	2.86	1.48	1.41
20	3	311	CLA	MG-NA	-2.85	1.99	2.06
20	4	308	CLA	C4C-C3C	-2.85	1.39	1.44
20	A	852	CLA	MG-NA	-2.85	1.99	2.06
20	A	803	CLA	C4B-CHC	2.85	1.48	1.41
20	A	807	CLA	OBD-CAD	2.85	1.26	1.22
20	3	311	CLA	C4B-NB	-2.85	1.32	1.35
20	A	816	CLA	C1C-NC	-2.85	1.33	1.37
20	4	305	CLA	C4B-CHC	2.85	1.48	1.41
20	A	815	CLA	CAA-C2A	-2.84	1.48	1.54
21	B	802	LMU	O5B-C5B	-2.84	1.37	1.44
20	K	108	CLA	C1B-NB	-2.84	1.32	1.35
20	3	309	CLA	CHB-C4A	-2.84	1.32	1.34
20	B	831	CLA	C3D-CAD	-2.84	1.38	1.46
20	A	821	CLA	C1B-CHB	2.84	1.48	1.41
20	H	109	CLA	C3D-CAD	-2.84	1.38	1.46
20	1	208	CLA	C2B-C1B	-2.84	1.35	1.39
20	2	310	CLA	MG-NA	-2.84	1.99	2.06
20	B	805	CLA	MG-NA	-2.83	1.99	2.06
20	B	806	CLA	OBD-CAD	2.83	1.26	1.22
20	4	307	CLA	CAC-C3C	-2.83	1.43	1.51
20	1	211	CLA	CHA-C1A	2.82	1.49	1.41
20	B	839	CLA	C3B-C2B	-2.82	1.36	1.40
22	3	314	BCR	C1-C6	-2.82	1.49	1.53
20	1	201	CLA	CHD-C4C	2.82	1.49	1.41
21	2	313	LMU	O1'-C1'	2.81	1.45	1.40
20	A	841	CLA	C3D-CAD	-2.81	1.38	1.46
20	A	810	CLA	C1C-C2C	-2.81	1.39	1.44
20	A	808	CLA	C3D-CAD	-2.81	1.38	1.46
20	B	831	CLA	C1C-NC	-2.81	1.33	1.37
20	1	208	CLA	C1C-NC	-2.80	1.32	1.38
20	2	301	CLA	C4B-CHC	2.80	1.49	1.43
20	1	212	CLA	C4B-CHC	2.80	1.49	1.43
22	B	843	BCR	C1-C6	-2.80	1.49	1.53
22	L	210	BCR	C40-C30	-2.80	1.48	1.53
20	A	816	CLA	CHD-C4C	2.80	1.49	1.41
20	A	833	CLA	C4B-CHC	2.80	1.48	1.41
20	B	835	CLA	C4B-CHC	2.80	1.48	1.41
20	3	316	CLA	MG-NA	-2.79	1.99	2.06
20	1	210	CLA	CHD-C4C	2.79	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	103	CLA	C3D-CAD	-2.79	1.39	1.46
20	B	828	CLA	C1C-C2C	-2.79	1.39	1.44
20	3	319	CLA	C2C-C1C	-2.79	1.36	1.43
20	A	807	CLA	MG-NA	-2.78	1.99	2.06
20	4	304	CLA	C4B-NB	-2.78	1.32	1.35
20	B	839	CLA	MG-NA	-2.78	1.99	2.06
20	A	826	CLA	C4C-C3C	-2.78	1.40	1.45
20	H	101	CLA	C4B-CHC	2.78	1.48	1.41
20	A	818	CLA	C1C-C2C	-2.78	1.39	1.44
22	B	852	BCR	C2-C1	-2.77	1.47	1.54
22	B	846	BCR	C1-C6	-2.77	1.50	1.53
22	I	101	BCR	C29-C30	-2.77	1.47	1.54
22	A	847	BCR	C1-C6	-2.77	1.50	1.53
20	4	306	CLA	C3D-CAD	-2.77	1.39	1.46
22	I	101	BCR	C32-C1	-2.77	1.48	1.53
20	A	814	CLA	C1B-NB	-2.76	1.32	1.35
20	1	209	CLA	C4C-C3C	-2.76	1.39	1.44
20	2	304	CLA	C2C-C1C	-2.76	1.36	1.43
20	K	103	CLA	C1B-CHB	2.76	1.48	1.41
20	B	839	CLA	C4B-CHC	2.76	1.48	1.41
20	F	206	CLA	C1C-C2C	-2.76	1.39	1.44
21	H	106	LMU	O5'-C5'	-2.76	1.37	1.44
20	B	818	CLA	C3D-CAD	-2.76	1.39	1.46
20	1	201	CLA	C1C-NC	-2.75	1.33	1.37
20	2	316	CLA	C1B-NB	-2.75	1.32	1.35
20	R	108	CLA	CHD-C4C	2.75	1.49	1.41
20	A	829	CLA	C3D-CAD	-2.75	1.39	1.46
20	J	101	CLA	C3D-CAD	-2.75	1.39	1.46
20	1	205	CLA	C1B-NB	-2.75	1.32	1.35
20	1	205	CLA	C4B-NB	-2.75	1.32	1.35
20	B	821	CLA	O2D-CGD	2.75	1.39	1.33
20	3	306	CLA	C4B-CHC	2.75	1.49	1.43
20	A	823	CLA	C3D-CAD	-2.74	1.39	1.46
20	R	107	CLA	C3D-CAD	-2.74	1.39	1.46
20	1	210	CLA	OBD-CAD	2.74	1.26	1.22
20	1	205	CLA	CHD-C4C	2.74	1.49	1.41
20	A	811	CLA	C4C-C3C	-2.74	1.40	1.45
20	2	312	CLA	C4C-C3C	-2.74	1.40	1.45
21	B	802	LMU	C4B-C5B	-2.74	1.47	1.53
20	3	320	CLA	CHA-C1A	2.73	1.49	1.41
20	1	201	CLA	C1D-C2D	-2.73	1.36	1.42
20	L	207	CLA	C1B-CHB	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	806	CLA	C4B-CHC	2.73	1.48	1.41
20	A	808	CLA	MG-NA	-2.73	1.99	2.06
20	2	303	CLA	C1C-C2C	-2.73	1.39	1.44
20	3	308	CLA	C1C-C2C	-2.73	1.39	1.44
20	A	839	CLA	C4B-CHC	2.72	1.48	1.41
20	B	810	CLA	C4C-C3C	-2.72	1.40	1.45
20	B	827	CLA	MG-NA	-2.72	1.99	2.06
20	K	101	CLA	C3D-CAD	-2.72	1.39	1.46
20	A	834	CLA	C1B-CHB	2.72	1.48	1.41
20	3	309	CLA	C4B-CHC	2.72	1.49	1.43
20	4	318	CLA	C3A-C2A	-2.72	1.46	1.54
22	B	844	BCR	C20-C19	-2.72	1.27	1.34
20	2	304	CLA	CHD-C4C	2.71	1.48	1.41
20	3	308	CLA	C1B-CHB	2.71	1.48	1.41
20	4	304	CLA	O2A-CGA	2.71	1.41	1.33
20	A	817	CLA	C3D-CAD	-2.71	1.39	1.46
20	F	206	CLA	C1C-NC	-2.71	1.33	1.37
20	A	834	CLA	C4C-C3C	-2.71	1.40	1.45
20	A	828	CLA	C3B-C2B	-2.71	1.36	1.40
20	3	301	CLA	C1B-CHB	2.71	1.48	1.41
20	1	215	CLA	C4B-NB	-2.71	1.32	1.35
20	B	833	CLA	C3D-CAD	-2.71	1.39	1.46
20	4	302	CLA	C3D-CAD	-2.71	1.39	1.46
20	1	216	CLA	CHD-C4C	2.71	1.48	1.41
22	B	852	BCR	C4-C5	-2.71	1.45	1.51
20	B	837	CLA	C1C-C2C	-2.69	1.39	1.44
20	1	216	CLA	C1C-NC	-2.69	1.32	1.38
21	C	101	LMU	O1'-C1'	2.69	1.44	1.40
20	3	303	CLA	C4B-NB	-2.69	1.32	1.35
20	B	806	CLA	C1C-NC	-2.69	1.33	1.37
20	B	851	CLA	C1C-NC	-2.68	1.33	1.37
20	A	806	CLA	C4C-C3C	-2.68	1.40	1.45
20	2	311	CLA	C1C-C2C	-2.68	1.39	1.44
20	4	304	CLA	CBD-CHA	-2.68	1.39	1.52
20	3	312	CLA	C3C-C4C	-2.68	1.36	1.43
20	H	103	CLA	C4C-C3C	-2.67	1.40	1.45
22	A	846	BCR	C30-C25	-2.67	1.50	1.53
21	R	105	LMU	O1'-C1'	2.67	1.44	1.40
20	A	817	CLA	C1C-C2C	-2.67	1.39	1.44
20	B	840	CLA	C1C-C2C	-2.67	1.39	1.44
20	R	107	CLA	C1B-CHB	2.67	1.48	1.41
20	A	804	CLA	C3B-C2B	-2.67	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	H	108	LMU	C4'-C5'	-2.67	1.45	1.52
21	L	205	LMU	C4B-C5B	-2.66	1.47	1.53
20	A	825	CLA	MG-NA	-2.66	1.99	2.06
20	B	818	CLA	C4C-C3C	-2.66	1.40	1.45
20	2	308	CLA	C1C-C2C	-2.66	1.39	1.44
20	2	304	CLA	C1C-NC	-2.66	1.32	1.38
20	H	101	CLA	C3B-C2B	-2.66	1.36	1.40
20	A	822	CLA	C4C-C3C	-2.66	1.40	1.45
20	A	805	CLA	C1B-CHB	2.66	1.48	1.41
22	B	852	BCR	C34-C9	-2.66	1.45	1.50
20	A	803	CLA	C3B-C2B	-2.66	1.36	1.40
20	3	312	CLA	CHD-C4C	2.66	1.48	1.41
20	B	836	CLA	C4B-CHC	2.66	1.48	1.41
20	2	306	CLA	C1B-NB	-2.65	1.32	1.35
20	2	306	CLA	C4C-NC	-2.65	1.32	1.37
20	B	818	CLA	C1B-CHB	2.65	1.48	1.41
20	3	309	CLA	CHA-C1A	2.65	1.48	1.41
20	A	807	CLA	C4B-NB	-2.65	1.32	1.35
20	2	310	CLA	CHA-C1A	2.65	1.48	1.41
20	4	318	CLA	MG-NA	-2.65	2.00	2.06
20	A	807	CLA	C3A-C2A	-2.65	1.47	1.54
20	A	840	CLA	C1C-C2C	-2.65	1.39	1.44
20	A	830	CLA	MG-NA	-2.64	2.00	2.06
20	B	816	CLA	C1B-CHB	2.64	1.48	1.41
20	B	823	CLA	C3D-CAD	-2.64	1.39	1.46
20	A	822	CLA	C3D-CAD	-2.63	1.39	1.46
20	4	316	CLA	C1C-NC	-2.63	1.33	1.37
20	R	108	CLA	C3D-C2D	-2.63	1.34	1.39
20	B	837	CLA	C1B-CHB	2.62	1.48	1.41
20	A	839	CLA	CHD-C4C	2.62	1.48	1.41
20	B	809	CLA	C4C-C3C	-2.62	1.40	1.45
20	A	833	CLA	MG-NA	-2.62	2.00	2.06
20	B	824	CLA	C3D-CAD	-2.62	1.39	1.46
20	B	804	CLA	C4C-C3C	-2.62	1.40	1.45
20	4	316	CLA	C1B-NB	-2.62	1.32	1.35
20	3	302	CLA	CHD-C4C	2.62	1.48	1.41
20	4	318	CLA	C4B-CHC	2.61	1.48	1.41
22	L	210	BCR	C31-C1	-2.61	1.48	1.53
20	1	205	CLA	C4B-CHC	2.61	1.49	1.43
20	H	101	CLA	C3D-C2D	-2.61	1.34	1.39
20	2	307	CLA	O2A-CGA	2.61	1.41	1.33
20	A	841	CLA	C1B-CHB	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	215	CLA	C4B-CHC	2.60	1.48	1.41
20	A	850	CLA	C3D-CAD	-2.60	1.39	1.46
20	B	850	CLA	C3B-C2B	-2.60	1.36	1.40
20	A	807	CLA	C2A-C1A	-2.60	1.46	1.52
20	B	809	CLA	C1C-C2C	-2.60	1.39	1.44
20	4	307	CLA	OBD-CAD	2.59	1.25	1.22
20	F	204	CLA	C3A-C2A	-2.59	1.52	1.54
20	3	311	CLA	CHD-C4C	2.59	1.48	1.41
20	B	821	CLA	CAC-C3C	-2.59	1.44	1.51
20	A	815	CLA	C3D-CAD	-2.59	1.39	1.46
20	4	310	CLA	C1C-NC	-2.59	1.32	1.38
20	A	839	CLA	C1C-NC	-2.59	1.33	1.37
20	A	802	CLA	C1C-NC	-2.58	1.32	1.38
22	F	203	BCR	C32-C1	-2.58	1.48	1.53
20	1	203	CLA	C1B-CHB	2.58	1.48	1.41
20	B	804	CLA	C3B-C2B	-2.58	1.36	1.40
20	A	839	CLA	C3D-C2D	-2.58	1.34	1.39
20	I	102	CLA	C1C-C2C	-2.57	1.39	1.44
20	A	813	CLA	MG-NA	-2.57	2.00	2.06
20	2	306	CLA	C4B-CHC	2.57	1.49	1.43
20	K	102	CLA	C3B-C2B	-2.57	1.36	1.40
20	4	306	CLA	MG-NA	-2.57	2.00	2.06
20	B	811	CLA	C1C-NC	-2.57	1.34	1.37
20	3	304	CLA	C4C-C3C	-2.57	1.39	1.44
20	3	319	CLA	MG-NC	-2.57	2.00	2.06
20	L	209	CLA	C3D-CAD	-2.57	1.39	1.46
20	A	836	CLA	C3B-C2B	-2.57	1.36	1.40
20	B	821	CLA	CHD-C4C	2.57	1.48	1.41
20	B	817	CLA	C3D-CAD	-2.56	1.39	1.46
20	4	307	CLA	C3D-C2D	-2.56	1.34	1.39
21	E	101	LMU	C4'-C5'	-2.56	1.46	1.52
20	B	804	CLA	MG-NA	-2.56	2.00	2.06
20	2	311	CLA	C1B-CHB	2.56	1.48	1.41
20	A	808	CLA	C2A-C1A	-2.56	1.46	1.52
20	2	315	CLA	CHA-C1A	2.56	1.48	1.41
20	B	832	CLA	C3D-CAD	-2.56	1.39	1.46
20	1	208	CLA	C3C-C4C	-2.56	1.37	1.43
20	3	304	CLA	C1B-CHB	2.55	1.48	1.41
21	H	105	LMU	C4B-C5B	-2.55	1.47	1.53
20	B	826	CLA	C3D-CAD	-2.55	1.39	1.46
20	B	836	CLA	C1B-CHB	2.55	1.48	1.41
20	B	851	CLA	MG-NA	-2.55	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	BCR	C37-C22	-2.55	1.45	1.50
20	B	811	CLA	C3A-C2A	-2.54	1.47	1.54
20	R	108	CLA	C1B-CHB	2.54	1.48	1.41
21	E	101	LMU	C4B-C3B	-2.54	1.45	1.52
20	4	309	CLA	MG-NC	-2.53	2.00	2.06
20	2	304	CLA	C3C-C4C	-2.53	1.37	1.43
20	B	808	CLA	C1B-NB	-2.53	1.32	1.35
20	A	831	CLA	C3A-C2A	-2.53	1.47	1.54
20	K	108	CLA	MG-NA	-2.53	2.00	2.06
20	B	817	CLA	C1B-CHB	2.53	1.48	1.41
20	H	103	CLA	C1C-C2C	-2.53	1.39	1.44
20	B	831	CLA	MG-NA	-2.53	2.00	2.06
20	1	202	CLA	C3D-C2D	-2.53	1.34	1.39
20	A	852	CLA	C1C-NC	-2.53	1.34	1.37
20	B	821	CLA	C3C-C2C	-2.53	1.31	1.36
20	A	807	CLA	C4B-CHC	2.53	1.48	1.41
22	B	842	BCR	C30-C25	-2.53	1.50	1.53
20	1	208	CLA	C4B-CHC	2.52	1.48	1.43
20	4	316	CLA	CHD-C4C	2.52	1.48	1.41
20	B	807	CLA	C3B-C2B	-2.52	1.36	1.40
20	1	207	CLA	C1B-CHB	2.51	1.48	1.41
20	A	837	CLA	C3B-C2B	-2.51	1.36	1.40
20	B	830	CLA	C3B-C2B	-2.51	1.36	1.40
20	A	815	CLA	C4B-CHC	2.51	1.48	1.41
20	A	801	CLA	C1B-CHB	2.51	1.48	1.41
20	A	802	CLA	CHD-C4C	2.51	1.48	1.41
20	A	816	CLA	OBD-CAD	2.51	1.25	1.22
21	G	101	LMU	C4B-C3B	2.51	1.58	1.52
20	A	829	CLA	C1C-C2C	-2.51	1.39	1.44
20	A	824	CLA	MG-NA	-2.50	2.00	2.06
20	B	821	CLA	O2D-CED	-2.50	1.39	1.45
20	1	202	CLA	C3A-C2A	-2.50	1.47	1.54
20	A	820	CLA	C3D-CAD	-2.50	1.39	1.46
20	A	809	CLA	C1B-CHB	2.50	1.47	1.41
20	B	816	CLA	C1C-C2C	-2.50	1.39	1.44
20	R	107	CLA	C4C-C3C	-2.50	1.40	1.45
20	4	318	CLA	C3D-C2D	-2.50	1.34	1.39
20	A	837	CLA	C4B-CHC	2.50	1.47	1.41
20	2	303	CLA	C3D-CAD	-2.50	1.39	1.46
20	3	301	CLA	C3D-CAD	-2.50	1.39	1.46
22	3	314	BCR	C30-C25	-2.50	1.50	1.53
20	4	304	CLA	MG-NC	-2.49	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	833	CLA	C1B-CHB	2.49	1.47	1.41
20	B	840	CLA	C1B-CHB	2.49	1.47	1.41
20	2	304	CLA	C4B-CHC	2.49	1.48	1.43
22	A	845	BCR	C1-C6	-2.49	1.50	1.53
20	4	306	CLA	C1C-C2C	-2.49	1.39	1.44
20	B	849	CLA	C1C-C2C	-2.49	1.39	1.44
20	2	322	CLA	C3B-C2B	-2.49	1.36	1.40
20	A	809	CLA	C3D-CAD	-2.48	1.39	1.46
20	1	216	CLA	C2C-C1C	-2.48	1.37	1.43
20	K	101	CLA	C3B-C2B	-2.48	1.36	1.40
20	B	811	CLA	OBD-CAD	2.48	1.25	1.22
20	2	308	CLA	C1B-CHB	2.48	1.47	1.41
20	B	817	CLA	MG-NA	-2.48	2.00	2.06
20	F	204	CLA	C4C-C3C	-2.48	1.39	1.44
20	3	317	CLA	C1B-CHB	2.48	1.47	1.41
21	4	322	LMU	O1'-C1'	2.48	1.44	1.40
20	1	205	CLA	C3C-C4C	-2.47	1.37	1.43
20	1	205	CLA	C2C-C1C	-2.47	1.37	1.43
20	A	830	CLA	C3D-CAD	-2.47	1.39	1.46
20	L	202	CLA	C4C-C3C	-2.47	1.40	1.45
20	A	852	CLA	C1B-NB	-2.47	1.33	1.35
20	2	303	CLA	C4C-C3C	-2.47	1.40	1.45
20	A	828	CLA	C1B-CHB	2.47	1.47	1.41
20	B	811	CLA	CAA-C2A	-2.47	1.49	1.54
20	B	834	CLA	C3D-CAD	-2.47	1.39	1.46
20	4	303	CLA	C4C-C3C	-2.47	1.39	1.44
20	F	206	CLA	C3D-CAD	-2.47	1.39	1.46
20	4	315	CLA	C1B-CHB	2.47	1.48	1.43
22	F	203	BCR	C10-C9	-2.46	1.32	1.35
20	3	310	CLA	C4B-NB	-2.46	1.33	1.35
20	2	316	CLA	C1B-CHB	2.46	1.47	1.41
20	3	313	CLA	MG-NC	-2.46	2.00	2.06
20	L	208	CLA	C3D-CAD	-2.46	1.39	1.46
20	A	829	CLA	C1B-CHB	2.46	1.47	1.41
20	2	307	CLA	C1B-CHB	2.46	1.47	1.41
20	1	207	CLA	C3D-CAD	-2.46	1.39	1.46
20	B	815	CLA	C1B-NB	-2.46	1.33	1.35
20	B	832	CLA	C1C-NC	-2.46	1.34	1.37
20	B	839	CLA	C3D-CAD	-2.46	1.39	1.46
20	4	309	CLA	CHD-C4C	2.46	1.48	1.41
20	A	809	CLA	C4B-CHC	2.46	1.47	1.41
20	A	828	CLA	C4C-C3C	-2.46	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	CHA-C1A	2.46	1.48	1.41
22	B	845	BCR	C1-C6	-2.46	1.50	1.53
20	B	814	CLA	C1B-CHB	2.45	1.47	1.41
20	A	816	CLA	C3D-C2D	-2.45	1.35	1.39
21	A	855	LMU	C4B-C5B	-2.45	1.47	1.53
20	H	103	CLA	C3D-CAD	-2.45	1.39	1.46
20	4	307	CLA	C3B-C2B	-2.45	1.37	1.40
20	H	109	CLA	C1C-C2C	-2.45	1.39	1.44
22	A	847	BCR	C30-C25	-2.45	1.50	1.53
20	2	322	CLA	C3A-C2A	-2.45	1.47	1.54
22	B	852	BCR	C32-C1	-2.45	1.48	1.53
20	A	831	CLA	C3D-CAD	-2.45	1.39	1.46
20	A	827	CLA	C1C-C2C	-2.45	1.39	1.44
22	I	101	BCR	C30-C25	-2.45	1.50	1.53
20	2	311	CLA	C3D-CAD	-2.45	1.39	1.46
20	A	831	CLA	C1B-CHB	2.45	1.47	1.41
20	F	206	CLA	C1B-CHB	2.45	1.47	1.41
20	A	802	CLA	C2C-C1C	-2.45	1.37	1.43
20	3	306	CLA	C2C-C1C	-2.44	1.37	1.43
20	A	841	CLA	C1C-C2C	-2.44	1.39	1.44
20	3	311	CLA	C1B-NB	-2.44	1.33	1.35
20	2	322	CLA	MG-NA	-2.44	2.00	2.06
20	A	851	CLA	C1C-C2C	-2.44	1.39	1.44
20	B	829	CLA	C3D-CAD	-2.43	1.39	1.46
22	B	852	BCR	C36-C18	-2.43	1.45	1.50
20	B	816	CLA	C3D-CAD	-2.43	1.39	1.46
20	B	839	CLA	C1C-C2C	-2.43	1.39	1.44
20	2	302	CLA	C3D-CAD	-2.43	1.39	1.46
20	4	314	CLA	C1C-C2C	-2.43	1.39	1.44
20	1	216	CLA	C4C-NC	-2.43	1.33	1.37
21	H	106	LMU	C1B-C2B	-2.43	1.45	1.52
20	A	803	CLA	C3D-CAD	-2.43	1.39	1.46
20	G	102	CLA	C1B-NB	-2.43	1.33	1.35
20	A	824	CLA	C3D-CAD	-2.43	1.39	1.46
20	4	319	CLA	C3D-CAD	-2.43	1.39	1.46
20	A	813	CLA	C3D-CAD	-2.42	1.39	1.46
20	A	820	CLA	C1C-C2C	-2.42	1.39	1.44
20	B	812	CLA	C4C-C3C	-2.42	1.40	1.45
20	A	832	CLA	MG-NA	-2.42	2.00	2.06
20	B	827	CLA	C1B-CHB	2.42	1.47	1.41
21	H	104	LMU	O5'-C1'	2.42	1.48	1.41
20	4	308	CLA	C3D-CAD	-2.42	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	MG-NA	-2.42	2.00	2.06
20	A	807	CLA	C1C-NC	-2.42	1.34	1.37
20	B	822	CLA	C1C-C2C	-2.41	1.39	1.44
20	2	312	CLA	C1B-NB	-2.41	1.33	1.35
20	4	303	CLA	C1C-C2C	-2.41	1.39	1.44
22	F	202	BCR	C30-C25	-2.41	1.50	1.53
20	A	851	CLA	MG-NA	-2.41	2.00	2.06
20	2	305	CLA	C1C-C2C	-2.41	1.39	1.44
20	B	806	CLA	C3D-CAD	-2.40	1.40	1.46
20	A	823	CLA	C1C-C2C	-2.40	1.39	1.44
20	B	809	CLA	C1B-CHB	2.40	1.47	1.41
20	H	102	CLA	C1C-C2C	-2.40	1.39	1.44
20	3	311	CLA	C3D-C2D	-2.40	1.35	1.39
20	1	203	CLA	C4C-C3C	-2.40	1.40	1.45
20	L	209	CLA	CBD-CGD	-2.40	1.44	1.52
20	B	832	CLA	C1C-C2C	-2.40	1.39	1.44
20	B	825	CLA	MG-NA	-2.40	2.00	2.06
20	A	827	CLA	C4C-C3C	-2.40	1.40	1.45
22	L	210	BCR	C1-C6	-2.40	1.50	1.53
20	4	302	CLA	C3B-C2B	-2.39	1.37	1.40
20	A	801	CLA	C3A-C2A	-2.39	1.47	1.54
20	A	828	CLA	C3D-CAD	-2.39	1.40	1.46
20	A	838	CLA	MG-NA	-2.39	2.00	2.06
20	1	209	CLA	C1B-CHB	2.39	1.47	1.41
20	A	841	CLA	MG-NA	-2.39	2.00	2.06
20	A	808	CLA	C1C-C2C	-2.39	1.39	1.44
22	I	101	BCR	C40-C30	-2.39	1.49	1.53
20	A	805	CLA	C3B-C2B	-2.39	1.37	1.40
20	B	810	CLA	C1B-CHB	2.39	1.47	1.41
20	B	810	CLA	C1C-C2C	-2.39	1.39	1.44
20	2	315	CLA	C1B-CHB	2.39	1.48	1.43
20	A	801	CLA	C2A-C1A	-2.39	1.46	1.52
22	B	852	BCR	C16-C15	-2.38	1.29	1.36
20	L	202	CLA	C1B-CHB	2.38	1.47	1.41
20	A	850	CLA	MG-NA	-2.38	2.00	2.06
20	1	212	CLA	C2B-C1B	-2.38	1.35	1.39
21	A	854	LMU	O5'-C5'	-2.38	1.38	1.44
20	B	831	CLA	C1B-CHB	2.38	1.47	1.41
20	3	301	CLA	C3A-C2A	-2.38	1.52	1.54
20	K	108	CLA	C3D-CAD	-2.38	1.40	1.46
20	2	307	CLA	C4B-CHC	2.38	1.47	1.41
20	4	314	CLA	C3D-CAD	-2.38	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	C3D-CAD	-2.38	1.40	1.46
20	4	302	CLA	C1B-NB	-2.38	1.33	1.35
20	4	310	CLA	C2C-C1C	-2.38	1.37	1.43
21	F	201	LMU	C4B-C3B	-2.37	1.46	1.52
20	B	810	CLA	C3D-CAD	-2.37	1.40	1.46
20	4	308	CLA	CBD-CHA	-2.37	1.48	1.51
20	A	832	CLA	C3D-CAD	-2.37	1.40	1.46
20	A	821	CLA	C4C-C3C	-2.37	1.41	1.45
20	B	836	CLA	C3D-CAD	-2.37	1.40	1.46
20	4	308	CLA	MG-NA	-2.37	2.00	2.06
20	4	319	CLA	MG-NA	-2.36	2.00	2.06
20	A	826	CLA	C1B-CHB	2.36	1.47	1.41
20	A	851	CLA	C3D-CAD	-2.36	1.40	1.46
20	1	216	CLA	C3C-C4C	-2.36	1.37	1.43
20	3	304	CLA	C1C-C2C	-2.36	1.40	1.44
20	F	205	CLA	C3D-CAD	-2.36	1.40	1.46
20	B	811	CLA	CHD-C4C	2.36	1.47	1.41
20	1	210	CLA	CBD-CGD	-2.36	1.45	1.52
20	K	103	CLA	C4B-NB	2.36	1.37	1.35
20	A	806	CLA	MG-NA	-2.35	2.00	2.06
20	3	302	CLA	C3D-CAD	-2.35	1.40	1.46
20	3	307	CLA	C2C-C1C	-2.35	1.37	1.43
20	B	822	CLA	C3B-C2B	-2.35	1.37	1.40
20	4	304	CLA	CBD-CGD	-2.35	1.45	1.52
20	B	835	CLA	C4C-C3C	-2.34	1.41	1.45
20	B	840	CLA	MG-NA	-2.34	2.00	2.06
20	B	813	CLA	C3D-CAD	-2.34	1.40	1.46
20	A	820	CLA	MG-NA	-2.34	2.00	2.06
20	4	316	CLA	OBD-CAD	2.34	1.25	1.22
22	I	101	BCR	C10-C9	-2.34	1.32	1.35
20	A	811	CLA	C3B-C2B	-2.34	1.37	1.40
20	4	307	CLA	C3A-C4A	-2.34	1.44	1.51
20	1	209	CLA	C3A-C2A	-2.33	1.52	1.54
20	B	821	CLA	CBD-CHA	-2.33	1.41	1.52
20	A	824	CLA	C1B-CHB	2.33	1.47	1.41
20	B	830	CLA	C1B-CHB	2.33	1.47	1.41
20	B	803	CLA	C2A-C1A	-2.33	1.47	1.52
22	I	101	BCR	C34-C9	-2.33	1.46	1.50
20	J	101	CLA	C3B-C2B	-2.33	1.37	1.40
20	A	827	CLA	C1B-CHB	2.33	1.47	1.41
20	A	824	CLA	C1B-NB	-2.33	1.33	1.35
20	L	209	CLA	C3A-C2A	-2.32	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	205	CLA	C1B-CHB	2.32	1.47	1.41
20	B	815	CLA	C1B-CHB	2.32	1.47	1.41
20	2	302	CLA	C1B-CHB	2.32	1.47	1.41
20	1	201	CLA	C3C-C2C	-2.32	1.31	1.36
20	1	215	CLA	C1C-NC	-2.32	1.34	1.37
22	B	852	BCR	C5-C6	-2.31	1.30	1.34
20	4	306	CLA	C4B-NB	-2.31	1.33	1.35
20	B	824	CLA	MG-NA	-2.31	2.00	2.06
20	H	103	CLA	C1B-CHB	2.31	1.47	1.41
20	L	207	CLA	C1C-C2C	-2.31	1.40	1.44
20	4	305	CLA	C1B-CHB	2.31	1.47	1.41
20	4	303	CLA	C3D-CAD	-2.31	1.40	1.46
20	B	803	CLA	C1B-CHB	2.31	1.47	1.41
20	1	207	CLA	CAA-C2A	-2.31	1.49	1.54
20	A	803	CLA	C1C-NC	-2.30	1.34	1.37
20	F	205	CLA	MG-NA	-2.30	2.00	2.06
20	4	308	CLA	C1B-CHB	2.30	1.47	1.41
21	L	204	LMU	C4B-C5B	-2.30	1.48	1.53
20	A	811	CLA	C3D-CAD	-2.30	1.40	1.46
20	3	313	CLA	CHD-C4C	2.30	1.47	1.41
21	L	204	LMU	O1'-C1'	2.29	1.44	1.40
20	3	303	CLA	CHD-C4C	2.29	1.47	1.41
20	2	302	CLA	MG-NA	-2.29	2.00	2.06
20	A	825	CLA	C1B-CHB	2.29	1.47	1.41
20	K	108	CLA	C1B-CHB	2.29	1.47	1.41
20	B	834	CLA	C1B-CHB	2.29	1.47	1.41
20	A	828	CLA	C1C-C2C	-2.29	1.40	1.44
20	G	102	CLA	CBD-CGD	-2.28	1.45	1.52
21	1	220	LMU	O1'-C1'	2.28	1.44	1.40
21	K	109	LMU	C4B-C5B	-2.28	1.48	1.53
20	1	210	CLA	C4B-CHC	2.28	1.47	1.41
20	3	320	CLA	MG-NA	-2.28	2.00	2.06
20	H	102	CLA	C4C-C3C	-2.28	1.41	1.45
20	2	305	CLA	MG-NA	-2.28	2.00	2.06
21	H	106	LMU	C3B-C2B	-2.28	1.46	1.52
20	A	819	CLA	C1B-CHB	2.28	1.47	1.41
21	A	856	LMU	O1'-C1'	2.28	1.44	1.40
20	2	303	CLA	MG-NA	-2.27	2.00	2.06
20	2	301	CLA	CHA-C1A	2.27	1.47	1.41
20	3	307	CLA	C3C-C4C	-2.27	1.37	1.43
20	4	304	CLA	C3A-C2A	-2.27	1.48	1.54
20	3	318	CLA	C4C-C3C	-2.27	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	812	CLA	C3B-C2B	-2.27	1.37	1.40
20	J	101	CLA	C1B-NB	-2.27	1.33	1.35
20	A	838	CLA	C3B-C2B	-2.27	1.37	1.40
20	1	206	CLA	C1C-C2C	-2.26	1.40	1.44
20	4	306	CLA	CHD-C4C	2.26	1.47	1.41
20	3	306	CLA	C3C-C4C	-2.26	1.37	1.43
20	B	849	CLA	C3B-C2B	-2.26	1.37	1.40
20	B	822	CLA	C1B-NB	-2.26	1.33	1.35
21	B	847	LMU	O1'-C1'	2.26	1.44	1.40
22	A	845	BCR	C30-C25	-2.26	1.50	1.53
20	B	824	CLA	C1B-CHB	2.25	1.47	1.41
22	F	203	BCR	C37-C22	-2.25	1.46	1.50
22	I	101	BCR	C23-C22	-2.25	1.41	1.45
20	H	109	CLA	C1B-NB	-2.25	1.33	1.35
20	B	812	CLA	C1C-C2C	-2.25	1.40	1.44
20	1	202	CLA	OBD-CAD	2.25	1.25	1.22
20	A	818	CLA	C1B-CHB	2.25	1.47	1.41
20	1	201	CLA	CMD-C2D	-2.25	1.46	1.51
20	3	316	CLA	C1B-CHB	2.25	1.48	1.43
20	H	109	CLA	C1B-CHB	2.24	1.47	1.41
20	4	319	CLA	C1B-CHB	2.24	1.47	1.41
20	B	812	CLA	C1B-CHB	2.24	1.47	1.41
21	L	211	LMU	O5B-C1B	2.24	1.47	1.41
20	3	304	CLA	C3A-C2A	-2.24	1.52	1.54
20	B	823	CLA	C3B-C2B	-2.23	1.37	1.40
20	4	305	CLA	C3D-CAD	-2.23	1.40	1.46
20	A	825	CLA	C3D-CAD	-2.23	1.40	1.46
20	A	836	CLA	C1B-CHB	2.23	1.47	1.41
20	3	318	CLA	C1C-C2C	-2.23	1.40	1.44
20	A	822	CLA	C1C-C2C	-2.23	1.40	1.44
21	K	104	LMU	C4B-C5B	-2.23	1.48	1.53
20	2	304	CLA	CHA-C1A	2.22	1.47	1.41
20	B	829	CLA	C1B-CHB	2.22	1.47	1.41
20	1	210	CLA	CBA-CGA	2.22	1.57	1.50
20	B	827	CLA	C3A-C2A	-2.22	1.48	1.54
20	A	810	CLA	MG-NA	-2.22	2.01	2.06
20	B	837	CLA	C3D-CAD	-2.22	1.40	1.46
20	3	301	CLA	C4C-C3C	-2.22	1.40	1.44
20	L	209	CLA	C1B-CHB	2.22	1.47	1.41
20	1	207	CLA	C3A-C2A	-2.22	1.48	1.54
20	A	803	CLA	C1B-CHB	2.22	1.47	1.41
20	B	850	CLA	C1C-C2C	-2.21	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	817	CLA	C1C-C2C	-2.21	1.40	1.44
21	1	219	LMU	O1B-C4'	-2.21	1.38	1.43
20	B	820	CLA	C1B-NB	-2.21	1.33	1.35
20	B	833	CLA	C1B-CHB	2.21	1.47	1.41
20	3	317	CLA	C4B-NB	2.21	1.37	1.35
20	B	804	CLA	C1C-C2C	-2.21	1.40	1.44
20	A	851	CLA	C3B-C2B	-2.21	1.37	1.40
20	A	817	CLA	C1B-CHB	2.21	1.47	1.41
20	2	322	CLA	C1C-NC	-2.20	1.34	1.37
20	K	102	CLA	O2A-C1	-2.20	1.40	1.46
20	B	826	CLA	C3B-C2B	-2.20	1.37	1.40
20	A	850	CLA	C1C-C2C	-2.20	1.40	1.44
20	L	208	CLA	C1C-C2C	-2.20	1.40	1.44
20	B	840	CLA	C4C-C3C	-2.19	1.40	1.44
20	A	835	CLA	C3B-C2B	-2.19	1.37	1.40
20	A	826	CLA	C3D-CAD	-2.19	1.40	1.46
20	A	818	CLA	MG-NA	-2.19	2.01	2.06
20	A	841	CLA	C3B-C2B	-2.19	1.37	1.40
20	3	303	CLA	C4B-CHC	2.19	1.48	1.43
20	B	814	CLA	C3D-CAD	-2.19	1.40	1.46
20	1	216	CLA	C4B-NB	-2.19	1.33	1.35
20	A	836	CLA	C1C-C2C	-2.19	1.40	1.44
20	2	307	CLA	O2A-C1	-2.19	1.40	1.46
20	B	820	CLA	C3D-CAD	-2.18	1.40	1.46
20	4	307	CLA	C3C-C2C	-2.18	1.32	1.36
20	B	849	CLA	C3D-CAD	-2.18	1.40	1.46
20	B	820	CLA	C1B-CHB	2.18	1.47	1.41
20	B	818	CLA	C1C-C2C	-2.18	1.40	1.44
20	A	804	CLA	MG-NA	-2.18	2.01	2.06
20	4	309	CLA	CHA-C1A	2.18	1.47	1.41
20	A	832	CLA	C1C-C2C	-2.18	1.40	1.44
20	2	322	CLA	C3A-C4A	-2.18	1.44	1.51
20	A	805	CLA	C3D-CAD	-2.17	1.40	1.46
20	B	833	CLA	C1C-C2C	-2.17	1.40	1.44
20	B	822	CLA	C3D-CAD	-2.17	1.40	1.46
20	4	310	CLA	C3C-C4C	-2.17	1.38	1.43
22	I	101	BCR	C2-C1	-2.17	1.49	1.54
20	B	849	CLA	C1B-CHB	2.17	1.47	1.41
20	4	303	CLA	C1B-CHB	2.17	1.47	1.41
20	4	307	CLA	C4B-NB	-2.17	1.33	1.35
20	B	815	CLA	C3D-CAD	-2.17	1.40	1.46
20	2	305	CLA	C1B-CHB	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	209	CLA	C1C-C2C	-2.17	1.40	1.44
20	L	207	CLA	C3D-CAD	-2.16	1.40	1.46
20	B	815	CLA	C4C-C3C	-2.16	1.41	1.45
20	2	306	CLA	CHA-C1A	2.16	1.47	1.41
21	1	219	LMU	O1'-C1'	2.16	1.43	1.40
20	B	836	CLA	C1C-NC	-2.16	1.34	1.37
20	2	306	CLA	C1C-NC	-2.16	1.33	1.38
20	B	826	CLA	C1C-C2C	-2.15	1.40	1.44
22	L	210	BCR	C2-C1	-2.15	1.49	1.54
20	2	307	CLA	OBD-CAD	2.15	1.25	1.22
22	A	843	BCR	C1-C6	-2.15	1.50	1.53
20	A	812	CLA	C1B-CHB	2.15	1.47	1.41
20	L	209	CLA	C3B-C2B	-2.15	1.37	1.40
20	2	307	CLA	CBD-CGD	-2.15	1.45	1.52
20	4	305	CLA	C4C-C3C	-2.15	1.41	1.45
20	1	214	CLA	MG-NA	-2.15	2.01	2.06
20	A	851	CLA	CBD-CGD	-2.15	1.45	1.52
20	B	849	CLA	MG-NA	-2.15	2.01	2.06
20	R	107	CLA	C1C-C2C	-2.14	1.40	1.44
20	3	313	CLA	C3C-C2C	-2.14	1.32	1.36
20	3	318	CLA	C1B-NB	-2.14	1.33	1.35
20	1	215	CLA	C1B-CHB	2.14	1.46	1.41
22	L	210	BCR	C26-C25	-2.14	1.30	1.34
20	2	305	CLA	C3D-CAD	-2.14	1.40	1.46
20	4	312	CLA	C3C-C4C	-2.13	1.38	1.43
20	J	103	CLA	C3B-C2B	-2.13	1.37	1.40
22	I	101	BCR	C37-C22	-2.13	1.46	1.50
20	4	303	CLA	C4B-NB	-2.13	1.33	1.35
20	B	838	CLA	C3D-CAD	-2.13	1.40	1.46
20	B	804	CLA	C3D-CAD	-2.13	1.40	1.46
20	B	832	CLA	C1B-CHB	2.13	1.46	1.41
21	B	802	LMU	C3B-C2B	-2.12	1.46	1.52
20	2	322	CLA	C3D-CAD	-2.12	1.40	1.46
20	2	307	CLA	C1D-C2D	-2.12	1.37	1.42
20	B	813	CLA	C1B-CHB	2.12	1.46	1.41
22	I	101	BCR	C33-C5	-2.12	1.47	1.50
20	2	309	CLA	C1B-NB	-2.12	1.33	1.35
20	4	310	CLA	C3B-C4B	-2.12	1.36	1.39
20	3	313	CLA	C4B-CHC	2.12	1.46	1.41
20	2	307	CLA	C1C-NC	-2.12	1.34	1.37
20	B	839	CLA	C4C-C3C	-2.11	1.41	1.45
20	B	834	CLA	MG-NA	-2.11	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	205	CLA	C1B-NB	-2.11	1.33	1.35
20	B	838	CLA	C1B-NB	-2.11	1.33	1.35
20	A	809	CLA	MG-NA	-2.11	2.01	2.06
20	4	316	CLA	C1B-CHB	2.11	1.46	1.41
20	2	301	CLA	C3C-C4C	-2.11	1.38	1.43
20	3	308	CLA	C3D-CAD	-2.11	1.40	1.46
20	B	818	CLA	C3A-C2A	-2.11	1.48	1.54
20	A	806	CLA	C1B-CHB	2.11	1.46	1.41
20	4	314	CLA	MG-NA	-2.11	2.01	2.06
20	B	840	CLA	C1B-NB	-2.11	1.33	1.35
20	B	837	CLA	C4B-NB	2.11	1.37	1.35
21	R	106	LMU	O1'-C1'	2.10	1.43	1.40
20	3	308	CLA	C4C-C3C	-2.10	1.41	1.45
20	A	809	CLA	C1C-NC	-2.10	1.34	1.37
20	B	803	CLA	C1C-C2C	-2.10	1.40	1.44
20	B	839	CLA	C1B-NB	-2.10	1.33	1.35
20	A	814	CLA	C4C-C3C	-2.10	1.41	1.45
23	A	842	PQN	O1-C1	2.10	1.27	1.23
22	B	844	BCR	C23-C22	2.10	1.50	1.45
20	B	822	CLA	C1A-CHA	2.10	1.51	1.43
20	B	822	CLA	C4C-C3C	-2.10	1.41	1.45
20	3	318	CLA	C3D-CAD	-2.10	1.40	1.46
20	A	809	CLA	C4B-NB	-2.10	1.33	1.35
20	A	835	CLA	C3D-CAD	-2.09	1.40	1.46
20	K	102	CLA	CMC-C2C	-2.09	1.46	1.50
20	3	310	CLA	C3C-C4C	-2.09	1.38	1.43
20	1	202	CLA	O2A-C1	-2.09	1.40	1.46
21	L	205	LMU	O5'-C5'	-2.09	1.39	1.44
21	R	101	LMU	O1'-C1'	2.09	1.43	1.40
22	J	102	BCR	C1-C6	-2.09	1.50	1.53
20	K	101	CLA	C1B-NB	-2.09	1.33	1.35
20	A	815	CLA	O2A-C1	-2.09	1.40	1.46
20	1	202	CLA	CAA-C2A	-2.08	1.50	1.54
20	A	830	CLA	C1B-CHB	2.08	1.46	1.41
20	H	102	CLA	MG-NA	-2.08	2.01	2.06
20	B	839	CLA	C1B-CHB	2.08	1.46	1.41
22	B	843	BCR	C30-C25	-2.08	1.50	1.53
20	A	821	CLA	C3B-C2B	-2.08	1.37	1.40
20	1	211	CLA	C1B-CHB	2.08	1.48	1.43
20	B	821	CLA	C3D-C2D	-2.08	1.35	1.39
20	1	212	CLA	C1C-NC	-2.08	1.33	1.38
20	B	821	CLA	CMB-C2B	-2.08	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	103	BCR	C32-C1	-2.07	1.49	1.53
20	L	202	CLA	C1C-C2C	-2.07	1.40	1.44
20	3	317	CLA	C4C-C3C	-2.07	1.41	1.45
20	A	817	CLA	MG-NA	-2.07	2.01	2.06
20	K	102	CLA	C3A-C2A	-2.07	1.48	1.54
20	H	103	CLA	C3B-C2B	-2.07	1.37	1.40
20	B	850	CLA	C1A-CHA	2.07	1.51	1.43
20	A	832	CLA	C4C-C3C	-2.07	1.41	1.45
20	3	319	CLA	C1B-NB	-2.07	1.33	1.35
20	A	823	CLA	MG-NA	-2.07	2.01	2.06
20	3	313	CLA	CAC-C3C	-2.07	1.45	1.51
21	H	106	LMU	C4B-C5B	-2.07	1.48	1.53
22	I	103	BCR	C37-C22	-2.07	1.46	1.50
20	A	834	CLA	MG-NA	-2.07	2.01	2.06
20	A	810	CLA	C3A-C2A	-2.06	1.48	1.54
20	L	203	CLA	C3D-CAD	-2.06	1.40	1.46
20	B	820	CLA	C4C-C3C	-2.06	1.41	1.45
20	A	810	CLA	C1B-CHB	2.06	1.46	1.41
20	B	803	CLA	MG-NA	-2.06	2.01	2.06
20	B	825	CLA	C1B-CHB	2.06	1.46	1.41
20	4	304	CLA	O2A-C1	-2.06	1.40	1.46
20	A	840	CLA	C3D-CAD	-2.06	1.40	1.46
22	B	852	BCR	C35-C13	-2.06	1.46	1.50
20	L	207	CLA	MG-NA	-2.06	2.01	2.06
20	B	851	CLA	C1B-CHB	2.06	1.46	1.41
20	4	308	CLA	C1B-NB	-2.06	1.33	1.35
20	2	305	CLA	C1A-CHA	2.06	1.51	1.43
21	N	101	LMU	O1'-C1'	2.05	1.43	1.40
20	B	813	CLA	C1C-C2C	-2.05	1.40	1.44
20	A	814	CLA	MG-NA	-2.05	2.01	2.06
20	B	820	CLA	MG-NA	-2.05	2.01	2.06
20	A	805	CLA	C1A-CHA	2.05	1.51	1.43
20	3	311	CLA	C3C-C2C	-2.05	1.32	1.36
20	3	311	CLA	C3B-C2B	-2.05	1.37	1.40
22	A	844	BCR	C1-C6	-2.05	1.51	1.53
20	3	311	CLA	C4B-CHC	2.05	1.46	1.41
20	H	103	CLA	MG-NA	-2.04	2.01	2.06
20	A	809	CLA	C4C-C3C	-2.04	1.41	1.45
20	K	102	CLA	C4B-NB	-2.04	1.33	1.35
20	B	830	CLA	C1A-CHA	2.04	1.51	1.43
20	B	822	CLA	C2-C3	2.03	1.37	1.33
20	1	216	CLA	C4B-CHC	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	R	104	LMU	C4B-C3B	-2.03	1.47	1.52
20	B	807	CLA	MG-NA	-2.03	2.01	2.06
21	B	802	LMU	O1'-C1'	2.03	1.43	1.40
20	A	807	CLA	C1B-CHB	2.03	1.46	1.41
20	A	810	CLA	C3D-CAD	-2.03	1.40	1.46
20	3	310	CLA	C4C-NC	-2.03	1.33	1.37
20	A	802	CLA	C1B-NB	-2.03	1.33	1.35
20	1	206	CLA	MG-NA	-2.02	2.01	2.06
20	3	313	CLA	OBD-CAD	2.02	1.25	1.22
20	A	815	CLA	C3D-C2D	-2.02	1.35	1.39
22	I	103	BCR	C7-C6	2.02	1.52	1.45
20	K	102	CLA	C3A-C4A	-2.02	1.45	1.51
20	A	807	CLA	CBD-CGD	-2.02	1.46	1.52
20	A	819	CLA	C4C-C3C	-2.02	1.41	1.45
20	A	822	CLA	C1B-CHB	2.02	1.46	1.41
22	F	203	BCR	C26-C25	-2.01	1.30	1.34
22	L	210	BCR	C36-C18	-2.01	1.46	1.50
20	1	205	CLA	C1C-NC	-2.01	1.34	1.38
20	A	840	CLA	MG-NA	-2.01	2.01	2.06
20	1	207	CLA	C1C-C2C	-2.01	1.40	1.44
20	A	820	CLA	C1B-CHB	2.01	1.46	1.41
20	B	834	CLA	C3B-C2B	-2.01	1.37	1.40
21	4	317	LMU	O1'-C1'	2.01	1.43	1.40
21	H	108	LMU	O1B-C4'	-2.01	1.38	1.43
21	H	104	LMU	O5'-C5'	2.01	1.49	1.44
20	4	309	CLA	C2B-C1B	-2.01	1.36	1.39
20	4	305	CLA	MG-NA	-2.01	2.01	2.06
20	B	813	CLA	MG-NA	-2.00	2.01	2.06
20	H	101	CLA	CBD-CHA	-2.00	1.42	1.52
20	A	827	CLA	MG-NA	-2.00	2.01	2.06
22	B	852	BCR	C19-C18	-2.00	1.41	1.45

All (4484) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	102	BCR	C20-C21-C22	36.89	179.96	127.31
22	A	846	BCR	C20-C21-C22	36.89	179.96	127.31
22	B	846	BCR	C20-C21-C22	36.87	179.93	127.31
22	A	845	BCR	C20-C21-C22	36.86	179.91	127.31
22	A	844	BCR	C20-C21-C22	36.84	179.89	127.31
22	A	847	BCR	C20-C21-C22	36.84	179.88	127.31
22	B	845	BCR	C20-C21-C22	36.83	179.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	202	BCR	C20-C21-C22	36.83	179.87	127.31
22	B	843	BCR	C20-C21-C22	36.81	179.84	127.31
22	B	842	BCR	C20-C21-C22	36.79	179.82	127.31
22	A	843	BCR	C20-C21-C22	36.79	179.82	127.31
22	3	314	BCR	C20-C21-C22	35.66	178.21	127.31
22	B	852	BCR	C20-C21-C22	35.19	177.53	127.31
22	L	210	BCR	C20-C21-C22	34.99	177.24	127.31
22	F	203	BCR	C20-C21-C22	34.75	176.91	127.31
22	I	103	BCR	C20-C21-C22	34.12	176.00	127.31
22	B	844	BCR	C20-C21-C22	30.04	170.18	127.31
22	I	101	BCR	C20-C21-C22	24.77	162.66	127.31
20	A	807	CLA	OBD-CAD-CBD	-23.21	92.73	125.89
20	H	101	CLA	OBD-CAD-CBD	-22.92	93.14	125.89
20	3	311	CLA	OBD-CAD-CBD	-22.21	94.17	125.89
20	4	306	CLA	OBD-CAD-CBD	-21.88	94.63	125.89
20	3	311	CLA	OBD-CAD-C3D	-19.62	95.40	127.98
20	1	210	CLA	OBD-CAD-C3D	-19.03	96.38	127.98
20	3	313	CLA	OBD-CAD-CBD	-18.72	99.15	125.89
20	A	815	CLA	OBD-CAD-CBD	-18.59	99.33	125.89
20	2	316	CLA	OBD-CAD-C3D	-18.53	97.22	127.98
20	A	833	CLA	OBD-CAD-C3D	-18.33	97.54	127.98
22	A	846	BCR	C21-C20-C19	18.19	179.99	123.22
22	F	202	BCR	C21-C20-C19	18.18	179.94	123.22
22	B	845	BCR	C21-C20-C19	18.17	179.93	123.22
22	B	846	BCR	C21-C20-C19	18.17	179.92	123.22
22	A	845	BCR	C21-C20-C19	18.17	179.91	123.22
22	B	842	BCR	C21-C20-C19	18.17	179.91	123.22
22	A	847	BCR	C21-C20-C19	18.16	179.89	123.22
22	B	843	BCR	C21-C20-C19	18.15	179.87	123.22
22	J	102	BCR	C21-C20-C19	18.15	179.86	123.22
22	A	844	BCR	C21-C20-C19	18.15	179.84	123.22
22	A	843	BCR	C21-C20-C19	18.14	179.82	123.22
20	B	816	CLA	OBD-CAD-CBD	-17.84	100.40	125.89
22	3	314	BCR	C21-C20-C19	17.67	178.36	123.22
22	L	210	BCR	C21-C20-C19	17.61	178.18	123.22
20	2	316	CLA	OBD-CAD-CBD	-17.61	100.73	125.89
20	4	307	CLA	OBD-CAD-CBD	-17.37	101.08	125.89
20	3	313	CLA	OBD-CAD-C3D	-17.29	99.27	127.98
22	F	203	BCR	C21-C20-C19	17.24	177.03	123.22
20	A	801	CLA	C4D-C3D-CAD	17.19	118.06	108.47
22	I	103	BCR	C21-C20-C19	17.08	176.51	123.22
20	A	840	CLA	OBD-CAD-CBD	-16.92	101.72	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	852	BCR	C21-C20-C19	16.89	175.92	123.22
20	2	312	CLA	OBD-CAD-CBD	-16.63	102.14	125.89
20	A	850	CLA	OBD-CAD-CBD	-16.58	102.21	125.89
20	B	835	CLA	OBD-CAD-C3D	-16.55	100.51	127.98
20	A	801	CLA	OBD-CAD-C3D	-16.53	100.53	127.98
20	B	825	CLA	OBD-CAD-CBD	-16.49	102.34	125.89
20	A	807	CLA	OBD-CAD-C3D	-16.36	100.81	127.98
20	A	841	CLA	OBD-CAD-CBD	-16.28	102.63	125.89
20	H	102	CLA	OBD-CAD-CBD	-16.22	102.72	125.89
20	4	306	CLA	OBD-CAD-C3D	-16.18	101.11	127.98
20	4	318	CLA	OBD-CAD-C3D	-16.17	101.13	127.98
20	A	826	CLA	OBD-CAD-CBD	-16.15	102.82	125.89
20	B	805	CLA	OBD-CAD-CBD	-16.05	102.96	125.89
20	B	808	CLA	OBD-CAD-C3D	-16.05	101.33	127.98
20	4	318	CLA	C4D-C3D-CAD	16.03	117.41	108.47
20	A	839	CLA	C4D-C3D-CAD	16.01	117.39	108.47
20	2	305	CLA	OBD-CAD-CBD	-15.96	103.09	125.89
20	I	102	CLA	OBD-CAD-CBD	-15.70	103.47	125.89
20	H	109	CLA	OBD-CAD-C3D	-15.64	102.01	127.98
20	A	834	CLA	OBD-CAD-CBD	-15.62	103.58	125.89
20	B	825	CLA	OBD-CAD-C3D	-15.52	102.22	127.98
20	B	821	CLA	OBD-CAD-CBD	-15.50	103.75	125.89
20	I	102	CLA	OBD-CAD-C3D	-15.48	102.29	127.98
20	L	209	CLA	OBD-CAD-C3D	-15.43	102.36	127.98
20	B	811	CLA	OBD-CAD-C3D	-15.41	102.39	127.98
20	A	816	CLA	OBD-CAD-C3D	-15.41	102.40	127.98
20	A	808	CLA	OBD-CAD-C3D	-15.28	102.62	127.98
20	B	819	CLA	OBD-CAD-C3D	-15.22	102.72	127.98
20	R	107	CLA	OBD-CAD-CBD	-15.17	104.22	125.89
20	L	201	CLA	OBD-CAD-C3D	-15.09	102.93	127.98
20	2	307	CLA	OBD-CAD-CBD	-15.08	104.35	125.89
20	1	202	CLA	C4D-C3D-CAD	15.07	116.88	108.47
20	2	312	CLA	OBD-CAD-C3D	-15.03	103.02	127.98
20	4	307	CLA	OBD-CAD-C3D	-14.81	103.40	127.98
22	B	844	BCR	C21-C20-C19	14.81	169.42	123.22
20	A	838	CLA	OBD-CAD-CBD	-14.79	104.76	125.89
20	1	201	CLA	OBD-CAD-C3D	-14.74	103.51	127.98
20	A	828	CLA	OBD-CAD-CBD	-14.66	104.95	125.89
20	A	841	CLA	OBD-CAD-C3D	-14.65	103.66	127.98
20	4	303	CLA	CAB-C3B-C4B	-14.65	105.95	128.46
20	A	822	CLA	OBD-CAD-C3D	-14.64	103.68	127.98
20	3	308	CLA	OBD-CAD-CBD	-14.61	105.03	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	810	CLA	OBD-CAD-CBD	-14.53	105.14	125.89
20	B	821	CLA	OBD-CAD-C3D	-14.44	104.00	127.98
20	A	829	CLA	OBD-CAD-C3D	-14.42	104.05	127.98
20	B	834	CLA	OBD-CAD-C3D	-14.33	104.18	127.98
20	H	101	CLA	OBD-CAD-C3D	-14.32	104.21	127.98
20	1	210	CLA	C4D-C3D-CAD	14.27	116.43	108.47
20	B	834	CLA	OBD-CAD-CBD	-14.26	105.52	125.89
20	A	826	CLA	OBD-CAD-C3D	-14.22	104.37	127.98
22	I	101	BCR	C24-C23-C22	-14.15	104.86	126.23
20	4	304	CLA	OBD-CAD-C3D	-14.01	104.71	127.98
20	A	852	CLA	OBD-CAD-C3D	-14.01	104.72	127.98
20	1	203	CLA	C4D-C3D-CAD	13.95	116.25	108.47
20	B	849	CLA	OBD-CAD-C3D	-13.93	104.84	127.98
20	L	209	CLA	OBD-CAD-CBD	-13.93	105.99	125.89
20	B	840	CLA	CAB-C3B-C4B	-13.92	107.08	128.46
20	B	832	CLA	OBD-CAD-C3D	-13.89	104.92	127.98
20	A	819	CLA	OBD-CAD-C3D	-13.88	104.94	127.98
20	G	102	CLA	OBD-CAD-CBD	-13.84	106.13	125.89
20	B	817	CLA	OBD-CAD-CBD	-13.82	106.15	125.89
20	L	207	CLA	OBD-CAD-CBD	-13.80	106.18	125.89
20	2	307	CLA	OBD-CAD-C3D	-13.68	105.27	127.98
20	K	102	CLA	OBD-CAD-CBD	-13.67	106.37	125.89
20	B	831	CLA	OBD-CAD-C3D	-13.66	105.30	127.98
20	B	833	CLA	OBD-CAD-C3D	-13.63	105.36	127.98
20	A	828	CLA	OBD-CAD-C3D	-13.62	105.36	127.98
20	A	812	CLA	OBD-CAD-CBD	-13.57	106.50	125.89
20	A	817	CLA	OBD-CAD-C3D	-13.57	105.46	127.98
20	1	201	CLA	C4D-C3D-CAD	13.53	116.02	108.47
20	4	314	CLA	CAB-C3B-C4B	-13.49	107.73	128.46
20	A	806	CLA	OBD-CAD-C3D	-13.48	105.60	127.98
20	A	830	CLA	OBD-CAD-C3D	-13.44	105.67	127.98
22	I	101	BCR	C21-C20-C19	13.44	165.15	123.22
20	A	801	CLA	CAB-C3B-C4B	-13.41	107.86	128.46
20	H	102	CLA	OBD-CAD-C3D	-13.40	105.73	127.98
20	B	811	CLA	C4D-C3D-CAD	13.40	115.94	108.47
20	B	820	CLA	OBD-CAD-CBD	-13.39	106.76	125.89
20	1	203	CLA	OBD-CAD-C3D	-13.37	105.78	127.98
20	B	849	CLA	OBD-CAD-CBD	-13.36	106.80	125.89
20	A	827	CLA	OBD-CAD-CBD	-13.33	106.85	125.89
20	R	107	CLA	C4D-C3D-CAD	13.21	115.84	108.47
20	B	827	CLA	C4D-C3D-CAD	13.18	115.82	108.47
20	A	814	CLA	OBD-CAD-CBD	-13.15	107.10	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	810	CLA	OBD-CAD-C3D	-13.15	106.14	127.98
20	A	810	CLA	OBD-CAD-C3D	-13.14	106.17	127.98
22	B	852	BCR	C7-C8-C9	-13.11	106.42	126.23
20	4	308	CLA	CAB-C3B-C4B	-13.11	108.32	128.46
20	3	301	CLA	CAB-C3B-C4B	-13.09	108.35	128.46
20	L	201	CLA	OBD-CAD-CBD	-13.03	107.27	125.89
20	B	818	CLA	C4D-C3D-CAD	13.00	115.72	108.47
22	I	103	BCR	C30-C25-C26	-13.00	104.31	122.61
20	A	824	CLA	OBD-CAD-CBD	-12.99	107.34	125.89
20	A	806	CLA	OBD-CAD-CBD	-12.99	107.34	125.89
20	A	805	CLA	OBD-CAD-C3D	-12.97	106.44	127.98
20	G	102	CLA	OBD-CAD-C3D	-12.97	106.44	127.98
20	2	311	CLA	OBD-CAD-C3D	-12.97	106.44	127.98
20	1	207	CLA	C4D-C3D-CAD	12.81	115.61	108.47
20	F	206	CLA	OBD-CAD-CBD	-12.80	107.61	125.89
20	B	817	CLA	OBD-CAD-C3D	-12.80	106.73	127.98
20	K	108	CLA	OBD-CAD-CBD	-12.75	107.68	125.89
20	H	109	CLA	OBD-CAD-CBD	-12.74	107.69	125.89
20	R	107	CLA	OBD-CAD-C3D	-12.73	106.85	127.98
20	B	824	CLA	OBD-CAD-CBD	-12.72	107.72	125.89
20	A	829	CLA	OBD-CAD-CBD	-12.70	107.74	125.89
20	B	837	CLA	OBD-CAD-CBD	-12.70	107.75	125.89
20	A	803	CLA	OBD-CAD-C3D	-12.67	106.94	127.98
20	L	208	CLA	OBD-CAD-C3D	-12.67	106.95	127.98
20	A	820	CLA	OBD-CAD-C3D	-12.63	107.01	127.98
20	A	825	CLA	OBD-CAD-CBD	-12.61	107.87	125.89
20	4	302	CLA	OBD-CAD-CBD	-12.61	107.88	125.89
20	B	811	CLA	OBD-CAD-CBD	-12.60	107.89	125.89
20	A	837	CLA	OBD-CAD-C3D	-12.60	107.06	127.98
20	H	103	CLA	C4D-C3D-CAD	12.58	115.49	108.47
20	B	839	CLA	C4D-C3D-CAD	12.57	115.48	108.47
20	A	817	CLA	OBD-CAD-CBD	-12.57	107.94	125.89
20	4	319	CLA	OBD-CAD-CBD	-12.56	107.95	125.89
20	A	819	CLA	OBD-CAD-CBD	-12.54	107.98	125.89
20	A	830	CLA	OBD-CAD-CBD	-12.51	108.03	125.89
20	4	314	CLA	OBD-CAD-C3D	-12.49	107.25	127.98
20	A	818	CLA	OBD-CAD-CBD	-12.44	108.12	125.89
20	B	810	CLA	OBD-CAD-CBD	-12.43	108.14	125.89
20	2	302	CLA	OBD-CAD-CBD	-12.42	108.15	125.89
20	K	102	CLA	OBD-CAD-C3D	-12.41	107.38	127.98
20	A	822	CLA	C4D-C3D-CAD	12.41	115.39	108.47
20	A	816	CLA	OBD-CAD-CBD	-12.39	108.19	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	821	CLA	OBD-CAD-CBD	-12.37	108.22	125.89
20	B	831	CLA	C4D-C3D-CAD	12.36	115.36	108.47
20	J	103	CLA	OBD-CAD-CBD	-12.35	108.25	125.89
20	F	205	CLA	OBD-CAD-CBD	-12.34	108.26	125.89
20	B	830	CLA	C4D-C3D-CAD	12.32	115.34	108.47
20	J	103	CLA	OBD-CAD-C3D	-12.31	107.54	127.98
20	1	209	CLA	CAB-C3B-C4B	-12.31	109.54	128.46
20	B	823	CLA	OBD-CAD-CBD	-12.31	108.31	125.89
20	4	311	CLA	C4D-C3D-CAD	12.29	115.32	108.47
20	1	203	CLA	OBD-CAD-CBD	-12.28	108.35	125.89
20	B	823	CLA	OBD-CAD-C3D	-12.28	107.60	127.98
20	B	850	CLA	OBD-CAD-CBD	-12.26	108.37	125.89
20	J	101	CLA	OBD-CAD-CBD	-12.26	108.38	125.89
20	4	319	CLA	OBD-CAD-C3D	-12.25	107.65	127.98
20	K	101	CLA	OBD-CAD-CBD	-12.24	108.41	125.89
20	R	108	CLA	C4D-C3D-CAD	12.23	115.29	108.47
20	A	850	CLA	C4D-C3D-CAD	12.21	115.28	108.47
20	B	824	CLA	OBD-CAD-C3D	-12.20	107.72	127.98
20	B	828	CLA	OBD-CAD-CBD	-12.19	108.47	125.89
20	B	808	CLA	OBD-CAD-CBD	-12.19	108.47	125.89
20	B	804	CLA	C4D-C3D-CAD	12.19	115.27	108.47
20	L	201	CLA	C4D-C3D-CAD	12.17	115.25	108.47
20	B	832	CLA	C4D-C3D-CAD	12.16	115.25	108.47
20	A	839	CLA	OBD-CAD-C3D	-12.15	107.80	127.98
20	B	805	CLA	OBD-CAD-C3D	-12.13	107.84	127.98
20	H	101	CLA	C4D-C3D-CAD	12.13	115.23	108.47
20	4	308	CLA	OBD-CAD-C3D	-12.13	107.84	127.98
20	J	101	CLA	OBD-CAD-C3D	-12.12	107.86	127.98
20	A	837	CLA	C4D-C3D-CAD	12.10	115.22	108.47
20	A	821	CLA	C4D-C3D-CAD	12.09	115.21	108.47
20	K	101	CLA	OBD-CAD-C3D	-12.08	107.93	127.98
20	B	850	CLA	OBD-CAD-C3D	-12.07	107.94	127.98
20	K	108	CLA	OBD-CAD-C3D	-12.02	108.02	127.98
20	A	813	CLA	OBD-CAD-CBD	-12.00	108.76	125.89
20	4	303	CLA	OBD-CAD-C3D	-12.00	108.06	127.98
20	3	304	CLA	OBD-CAD-C3D	-11.98	108.08	127.98
22	B	852	BCR	C15-C16-C17	-11.98	98.94	123.47
20	A	815	CLA	OBD-CAD-C3D	-11.98	108.10	127.98
20	2	302	CLA	OBD-CAD-C3D	-11.96	108.12	127.98
20	A	825	CLA	OBD-CAD-C3D	-11.95	108.14	127.98
20	3	313	CLA	C1D-CHD-C4C	-11.94	106.80	122.56
20	A	830	CLA	C4D-C3D-CAD	11.93	115.12	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	205	CLA	OBD-CAD-C3D	-11.90	108.22	127.98
20	4	302	CLA	OBD-CAD-C3D	-11.88	108.25	127.98
20	A	824	CLA	OBD-CAD-C3D	-11.86	108.29	127.98
20	2	322	CLA	C4D-C3D-CAD	11.85	115.08	108.47
20	1	215	CLA	OBD-CAD-C3D	-11.84	108.33	127.98
20	B	830	CLA	OBD-CAD-C3D	-11.80	108.38	127.98
20	3	301	CLA	OBD-CAD-C3D	-11.75	108.47	127.98
20	H	103	CLA	OBD-CAD-CBD	-11.75	109.11	125.89
20	A	811	CLA	C4D-C3D-CAD	11.74	115.02	108.47
20	B	816	CLA	OBD-CAD-C3D	-11.74	108.50	127.98
20	2	311	CLA	C4D-C3D-CAD	11.73	115.01	108.47
20	B	818	CLA	OBD-CAD-C3D	-11.71	108.54	127.98
20	3	302	CLA	C4D-C3D-CAD	11.70	114.99	108.47
20	B	838	CLA	C4D-C3D-CAD	11.70	114.99	108.47
20	A	851	CLA	OBD-CAD-CBD	-11.69	109.19	125.89
20	B	835	CLA	C4D-C3D-CAD	11.68	114.98	108.47
20	B	829	CLA	OBD-CAD-C3D	-11.68	108.59	127.98
20	A	801	CLA	OBD-CAD-CBD	-11.67	109.22	125.89
20	1	202	CLA	OBD-CAD-CBD	-11.66	109.24	125.89
20	B	806	CLA	OBD-CAD-C3D	-11.61	108.71	127.98
20	B	819	CLA	C4D-C3D-CAD	11.60	114.94	108.47
20	4	303	CLA	C4D-C3D-CAD	11.60	114.94	108.47
20	F	206	CLA	OBD-CAD-C3D	-11.59	108.73	127.98
20	4	305	CLA	C4D-C3D-CAD	11.47	114.87	108.47
20	B	805	CLA	C4D-C3D-CAD	11.45	114.85	108.47
20	B	813	CLA	OBD-CAD-C3D	-11.42	109.02	127.98
20	B	812	CLA	C4D-C3D-CAD	11.42	114.84	108.47
20	B	826	CLA	C4D-C3D-CAD	11.39	114.82	108.47
20	B	831	CLA	OBD-CAD-CBD	-11.38	109.64	125.89
20	B	817	CLA	C4D-C3D-CAD	11.37	114.81	108.47
20	A	852	CLA	OBD-CAD-CBD	-11.35	109.68	125.89
20	H	103	CLA	OBD-CAD-C3D	-11.35	109.14	127.98
20	A	832	CLA	OBD-CAD-CBD	-11.31	109.73	125.89
20	3	301	CLA	C4D-C3D-CAD	11.30	114.77	108.47
20	B	820	CLA	C4D-C3D-CAD	11.28	114.76	108.47
20	A	851	CLA	OBD-CAD-C3D	-11.28	109.25	127.98
20	R	108	CLA	OBD-CAD-C3D	-11.26	109.28	127.98
20	A	808	CLA	C4D-C3D-CAD	11.25	114.75	108.47
20	A	815	CLA	C4D-C3D-CAD	11.24	114.74	108.47
20	4	302	CLA	C4D-C3D-CAD	11.22	114.73	108.47
20	2	322	CLA	OBD-CAD-C3D	-11.22	109.35	127.98
20	3	302	CLA	OBD-CAD-CBD	-11.22	109.87	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	832	CLA	OBD-CAD-C3D	-11.21	109.37	127.98
20	3	308	CLA	C4D-C3D-CAD	11.19	114.71	108.47
20	2	307	CLA	C4D-C3D-CAD	11.19	114.71	108.47
20	L	207	CLA	C4D-C3D-CAD	11.18	114.70	108.47
20	A	817	CLA	C4D-C3D-CAD	11.18	114.70	108.47
20	B	820	CLA	OBD-CAD-C3D	-11.16	109.45	127.98
20	A	852	CLA	C4D-C3D-CAD	11.14	114.68	108.47
20	B	807	CLA	C4D-C3D-CAD	11.13	114.68	108.47
20	A	834	CLA	C4D-C3D-CAD	11.11	114.67	108.47
20	L	208	CLA	OBD-CAD-CBD	-11.08	110.06	125.89
20	F	204	CLA	C4D-C3D-CAD	11.06	114.64	108.47
20	4	314	CLA	C4D-C3D-CAD	11.04	114.63	108.47
20	B	814	CLA	OBD-CAD-CBD	-11.02	110.15	125.89
20	A	825	CLA	C4D-C3D-CAD	10.98	114.59	108.47
20	4	304	CLA	C4D-C3D-CAD	10.97	114.59	108.47
20	3	308	CLA	OBD-CAD-C3D	-10.95	109.81	127.98
20	A	835	CLA	C4D-C3D-CAD	10.95	114.57	108.47
20	A	826	CLA	C4D-C3D-CAD	10.91	114.56	108.47
20	1	206	CLA	C4D-C3D-CAD	10.91	114.55	108.47
20	2	305	CLA	C4D-C3D-CAD	10.90	114.55	108.47
22	I	101	BCR	C7-C8-C9	-10.87	109.81	126.23
20	2	308	CLA	OBD-CAD-C3D	-10.87	109.94	127.98
20	B	851	CLA	C4D-C3D-CAD	10.85	114.52	108.47
20	A	835	CLA	OBD-CAD-CBD	-10.85	110.40	125.89
20	J	101	CLA	C4D-C3D-CAD	10.83	114.51	108.47
20	A	824	CLA	C4D-C3D-CAD	10.81	114.50	108.47
20	K	101	CLA	C4D-C3D-CAD	10.80	114.49	108.47
20	A	820	CLA	OBD-CAD-CBD	-10.79	110.48	125.89
20	K	108	CLA	C4D-C3D-CAD	10.79	114.48	108.47
20	A	818	CLA	C4D-C3D-CAD	10.76	114.47	108.47
20	A	831	CLA	OBD-CAD-CBD	-10.74	110.55	125.89
20	4	307	CLA	C4D-C3D-CAD	10.73	114.45	108.47
20	A	833	CLA	C4D-C3D-CAD	10.71	114.44	108.47
20	H	109	CLA	C4D-C3D-CAD	10.68	114.43	108.47
20	A	833	CLA	OBD-CAD-CBD	-10.67	110.65	125.89
20	B	823	CLA	C4D-C3D-CAD	10.67	114.42	108.47
20	A	831	CLA	C4D-C3D-CAD	10.66	114.41	108.47
20	B	827	CLA	OBD-CAD-C3D	-10.58	110.41	127.98
20	A	832	CLA	C4D-C3D-CAD	10.58	114.37	108.47
20	B	810	CLA	C4D-C3D-CAD	10.57	114.36	108.47
20	K	102	CLA	C4D-C3D-CAD	10.57	114.36	108.47
20	K	103	CLA	OBD-CAD-CBD	-10.55	110.82	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	840	CLA	C4D-C3D-CAD	10.53	114.34	108.47
20	B	833	CLA	C4D-C3D-CAD	10.52	114.34	108.47
20	1	202	CLA	OBD-CAD-C3D	-10.50	110.54	127.98
20	1	215	CLA	C4D-C3D-CAD	10.48	114.31	108.47
20	2	303	CLA	C4D-C3D-CAD	10.47	114.31	108.47
20	B	851	CLA	OBD-CAD-C3D	-10.47	110.60	127.98
20	2	322	CLA	OBD-CAD-CBD	-10.47	110.94	125.89
20	A	806	CLA	C4D-C3D-CAD	10.45	114.30	108.47
20	1	201	CLA	C4A-NA-C1A	10.45	111.41	106.71
20	B	834	CLA	C4D-C3D-CAD	10.45	114.30	108.47
20	A	821	CLA	OBD-CAD-C3D	-10.44	110.65	127.98
22	I	103	BCR	C24-C23-C22	-10.43	110.48	126.23
20	B	807	CLA	OBD-CAD-CBD	-10.41	111.02	125.89
20	3	313	CLA	C4D-C3D-CAD	10.41	114.28	108.47
20	A	820	CLA	C4D-C3D-CAD	10.40	114.27	108.47
20	A	827	CLA	OBD-CAD-C3D	-10.40	110.72	127.98
20	A	831	CLA	OBD-CAD-C3D	-10.37	110.77	127.98
20	A	828	CLA	C4D-C3D-CAD	10.36	114.25	108.47
20	A	814	CLA	C4D-C3D-CAD	10.34	114.24	108.47
20	A	812	CLA	OBD-CAD-C3D	-10.32	110.84	127.98
20	A	803	CLA	C4D-C3D-CAD	10.32	114.22	108.47
20	B	829	CLA	OBD-CAD-CBD	-10.30	111.17	125.89
20	K	103	CLA	C4D-C3D-CAD	10.30	114.22	108.47
20	B	814	CLA	OBD-CAD-C3D	-10.29	110.90	127.98
20	F	205	CLA	C4D-C3D-CAD	10.27	114.20	108.47
20	A	801	CLA	C3D-CAD-CBD	-10.27	94.08	107.61
20	J	103	CLA	C4D-C3D-CAD	10.27	114.20	108.47
20	B	826	CLA	OBD-CAD-C3D	-10.27	110.94	127.98
20	A	840	CLA	OBD-CAD-C3D	-10.25	110.96	127.98
20	B	809	CLA	C4D-C3D-CAD	10.23	114.18	108.47
20	B	828	CLA	OBD-CAD-C3D	-10.23	111.00	127.98
20	L	201	CLA	C1D-CHD-C4C	-10.23	109.06	122.56
20	B	809	CLA	CAB-C3B-C4B	-10.22	112.76	128.46
20	B	814	CLA	C4D-C3D-CAD	10.20	114.16	108.47
20	4	308	CLA	C4D-C3D-CAD	10.20	114.16	108.47
20	2	305	CLA	OBD-CAD-C3D	-10.17	111.10	127.98
20	L	201	CLA	C1-C2-C3	-10.16	108.47	126.04
20	B	849	CLA	C4D-C3D-CAD	10.16	114.14	108.47
20	B	828	CLA	C4D-C3D-CAD	10.14	114.12	108.47
20	2	302	CLA	C4D-C3D-CAD	10.13	114.12	108.47
20	L	208	CLA	C4D-C3D-CAD	10.10	114.10	108.47
20	L	207	CLA	OBD-CAD-C3D	-10.10	111.22	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	308	CLA	OBD-CAD-CBD	-10.09	111.48	125.89
20	B	837	CLA	OBD-CAD-C3D	-10.07	111.26	127.98
20	A	835	CLA	OBD-CAD-C3D	-10.04	111.31	127.98
20	1	207	CLA	OBD-CAD-CBD	-10.04	111.55	125.89
20	A	807	CLA	C4D-C3D-CAD	9.99	114.04	108.47
20	A	822	CLA	OBD-CAD-CBD	-9.99	111.63	125.89
20	A	841	CLA	C4D-C3D-CAD	9.98	114.03	108.47
20	1	209	CLA	C4D-C3D-CAD	9.98	114.03	108.47
20	A	823	CLA	C4D-C3D-CAD	9.97	114.03	108.47
20	A	840	CLA	C4D-C3D-CAD	9.95	114.02	108.47
20	4	305	CLA	OBD-CAD-C3D	-9.94	111.47	127.98
20	G	102	CLA	C1D-CHD-C4C	-9.94	109.45	122.56
20	A	812	CLA	C4D-C3D-CAD	9.93	114.01	108.47
20	A	838	CLA	OBD-CAD-C3D	-9.93	111.50	127.98
20	A	850	CLA	OBD-CAD-C3D	-9.90	111.54	127.98
20	4	319	CLA	C4D-C3D-CAD	9.90	113.99	108.47
20	2	303	CLA	OBD-CAD-C3D	-9.88	111.58	127.98
20	2	312	CLA	C4D-C3D-CAD	9.86	113.97	108.47
20	2	307	CLA	C1D-CHD-C4C	-9.85	109.56	122.56
20	B	819	CLA	OBD-CAD-CBD	-9.85	111.82	125.89
20	2	316	CLA	C4D-C3D-CAD	9.78	113.93	108.47
20	2	308	CLA	C4D-C3D-CAD	9.77	113.92	108.47
20	B	808	CLA	C4D-C3D-CAD	9.76	113.91	108.47
20	B	824	CLA	C4D-C3D-CAD	9.75	113.91	108.47
20	B	806	CLA	OBD-CAD-CBD	-9.74	111.97	125.89
20	A	809	CLA	OBD-CAD-C3D	-9.74	111.81	127.98
20	A	813	CLA	C4D-C3D-CAD	9.73	113.90	108.47
20	3	304	CLA	CAB-C3B-C4B	-9.73	113.51	128.46
20	4	304	CLA	C3D-CAD-CBD	-9.73	94.80	107.61
20	4	311	CLA	OBD-CAD-C3D	-9.70	111.87	127.98
20	A	819	CLA	C4D-C3D-CAD	9.69	113.87	108.47
20	B	813	CLA	OBD-CAD-CBD	-9.65	112.11	125.89
22	F	203	BCR	C15-C14-C13	-9.63	113.57	127.31
20	2	311	CLA	OBD-CAD-CBD	-9.63	112.14	125.89
20	B	840	CLA	OBD-CAD-C3D	-9.61	112.03	127.98
20	B	836	CLA	C4D-C3D-CAD	9.60	113.83	108.47
20	A	805	CLA	C4D-C3D-CAD	9.59	113.82	108.47
20	3	318	CLA	OBD-CAD-C3D	-9.57	112.09	127.98
20	1	207	CLA	OBD-CAD-C3D	-9.56	112.11	127.98
20	B	816	CLA	C4D-C3D-CAD	9.56	113.80	108.47
20	H	102	CLA	C4D-C3D-CAD	9.56	113.80	108.47
20	L	202	CLA	OBD-CAD-C3D	-9.55	112.13	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	833	CLA	OBD-CAD-CBD	-9.53	112.28	125.89
20	B	818	CLA	OBD-CAD-CBD	-9.53	112.28	125.89
22	I	103	BCR	C1-C6-C5	-9.50	109.23	122.61
20	B	804	CLA	OBD-CAD-C3D	-9.43	112.32	127.98
20	A	838	CLA	C4D-C3D-CAD	9.43	113.73	108.47
20	1	209	CLA	CAB-C3B-C2B	-9.43	106.22	124.69
20	3	302	CLA	OBD-CAD-C3D	-9.40	112.38	127.98
20	B	830	CLA	OBD-CAD-CBD	-9.36	112.52	125.89
20	B	826	CLA	OBD-CAD-CBD	-9.36	112.52	125.89
20	A	837	CLA	OBD-CAD-CBD	-9.35	112.53	125.89
20	B	825	CLA	C4D-C3D-CAD	9.33	113.67	108.47
20	4	304	CLA	C1D-CHD-C4C	-9.32	110.25	122.56
20	L	203	CLA	C4D-C3D-CAD	9.32	113.67	108.47
20	I	102	CLA	C4D-C3D-CAD	9.32	113.67	108.47
20	G	102	CLA	C4D-C3D-CAD	9.30	113.65	108.47
20	A	809	CLA	C4D-C3D-CAD	9.25	113.63	108.47
22	I	101	BCR	C23-C22-C21	9.24	133.12	118.94
20	1	206	CLA	OBD-CAD-C3D	-9.23	112.66	127.98
20	A	815	CLA	CMA-C3A-C4A	-9.20	87.06	111.77
20	L	209	CLA	O2D-CGD-CBD	9.13	127.49	111.27
20	4	304	CLA	CGD-CBD-CAD	9.10	140.22	110.73
20	A	803	CLA	O2D-CGD-CBD	9.10	127.43	111.27
20	L	203	CLA	OBD-CAD-C3D	-9.09	112.88	127.98
20	A	813	CLA	OBD-CAD-C3D	-9.09	112.89	127.98
20	A	818	CLA	OBD-CAD-C3D	-9.08	112.90	127.98
20	4	303	CLA	C1D-CHD-C4C	-9.06	110.59	122.56
20	A	801	CLA	CAB-C3B-C2B	-9.06	106.94	124.69
22	3	314	BCR	C16-C17-C18	-9.04	114.41	127.31
20	B	830	CLA	CAA-C2A-C3A	-9.04	88.04	112.78
20	1	208	CLA	C2B-C1B-NB	9.04	118.03	110.11
20	A	816	CLA	C4D-C3D-CAD	9.03	113.50	108.47
20	A	851	CLA	C4D-C3D-CAD	8.99	113.48	108.47
20	B	811	CLA	C1D-CHD-C4C	-8.96	110.74	122.56
20	A	823	CLA	OBD-CAD-C3D	-8.95	113.12	127.98
20	A	815	CLA	C1D-CHD-C4C	-8.93	110.77	122.56
20	B	839	CLA	OBD-CAD-C3D	-8.93	113.16	127.98
20	A	805	CLA	OBD-CAD-CBD	-8.91	113.17	125.89
20	B	838	CLA	OBD-CAD-C3D	-8.90	113.21	127.98
20	4	304	CLA	OBD-CAD-CBD	-8.88	113.20	125.89
20	A	809	CLA	OBD-CAD-CBD	-8.88	113.21	125.89
20	B	836	CLA	OBD-CAD-C3D	-8.85	113.29	127.98
20	4	306	CLA	C1D-CHD-C4C	-8.84	110.89	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	318	CLA	CAA-C2A-C3A	-8.83	88.59	112.78
20	4	307	CLA	C1D-CHD-C4C	-8.79	110.96	122.56
20	A	814	CLA	OBD-CAD-C3D	-8.79	113.39	127.98
20	1	206	CLA	OBD-CAD-CBD	-8.78	113.34	125.89
20	3	304	CLA	C4D-C3D-CAD	8.77	113.36	108.47
20	B	836	CLA	OBD-CAD-CBD	-8.77	113.37	125.89
20	B	822	CLA	C4D-C3D-CAD	8.74	113.35	108.47
21	H	105	LMU	C3B-C4B-C5B	-8.74	94.64	110.24
20	B	806	CLA	C4D-C3D-CAD	8.74	113.34	108.47
20	A	810	CLA	C4D-C3D-CAD	8.71	113.33	108.47
20	K	103	CLA	OBD-CAD-C3D	-8.68	113.57	127.98
20	1	210	CLA	C1D-CHD-C4C	-8.64	111.15	122.56
20	B	832	CLA	OBD-CAD-CBD	-8.61	113.59	125.89
20	4	309	CLA	C2B-C1B-NB	8.59	117.63	110.11
20	4	316	CLA	OBD-CAD-C3D	-8.57	113.76	127.98
20	B	835	CLA	OBD-CAD-CBD	-8.56	113.66	125.89
21	1	219	LMU	C1B-O1B-C4'	-8.56	96.79	117.96
20	L	209	CLA	C4D-C3D-CAD	8.55	113.24	108.47
20	4	308	CLA	CAB-C3B-C2B	-8.54	107.96	124.69
20	3	301	CLA	CAB-C3B-C2B	-8.50	108.03	124.69
20	3	318	CLA	C4D-C3D-CAD	8.48	113.20	108.47
21	L	204	LMU	C1B-O1B-C4'	-8.46	97.02	117.96
20	4	318	CLA	OBD-CAD-CBD	-8.44	113.84	125.89
20	A	835	CLA	O2D-CGD-CBD	8.43	126.24	111.27
20	3	311	CLA	C4D-C3D-CAD	8.35	113.12	108.47
20	A	804	CLA	C4D-C3D-CAD	8.34	113.12	108.47
20	B	837	CLA	C4D-C3D-CAD	8.34	113.12	108.47
20	1	201	CLA	OBD-CAD-CBD	-8.32	114.00	125.89
20	A	827	CLA	C4D-C3D-CAD	8.31	113.10	108.47
20	1	207	CLA	C3A-C2A-C1A	8.27	113.73	101.34
20	B	813	CLA	C4D-C3D-CAD	8.26	113.08	108.47
20	1	215	CLA	O2D-CGD-CBD	8.25	125.94	111.27
20	A	839	CLA	O2D-CGD-CBD	8.23	125.89	111.27
20	3	313	CLA	CHD-C4C-NC	8.23	137.16	124.20
20	L	209	CLA	C1D-CHD-C4C	-8.20	111.73	122.56
20	A	808	CLA	OBD-CAD-CBD	-8.20	114.18	125.89
21	B	847	LMU	C1B-O5B-C5B	-8.20	97.60	113.69
20	4	316	CLA	C1D-CHD-C4C	-8.19	111.75	122.56
20	B	850	CLA	C4D-C3D-CAD	8.19	113.04	108.47
20	3	312	CLA	C2D-C3D-C4D	-8.15	99.28	106.30
22	I	101	BCR	C3-C4-C5	-8.14	99.55	114.08
20	2	322	CLA	C1D-CHD-C4C	-8.13	111.83	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	317	CLA	C4D-C3D-CAD	8.11	112.99	108.47
21	H	106	LMU	C1B-C2B-C3B	-8.11	93.12	110.00
20	A	811	CLA	OBD-CAD-C3D	-8.10	114.53	127.98
20	3	302	CLA	C1D-CHD-C4C	-8.10	111.87	122.56
20	B	838	CLA	OBD-CAD-CBD	-8.10	114.32	125.89
20	A	803	CLA	OBD-CAD-CBD	-8.07	114.36	125.89
20	B	851	CLA	OBD-CAD-CBD	-8.03	114.42	125.89
20	A	834	CLA	OBD-CAD-C3D	-8.02	114.66	127.98
20	H	101	CLA	C3D-CAD-CBD	-8.02	97.05	107.61
20	B	803	CLA	OBD-CAD-CBD	-7.99	114.48	125.89
20	B	840	CLA	CAB-C3B-C2B	-7.99	109.04	124.69
20	B	815	CLA	C4D-C3D-CAD	7.98	112.92	108.47
20	3	311	CLA	O2D-CGD-CBD	7.98	125.44	111.27
20	A	802	CLA	C2B-C1B-NB	7.95	117.07	110.11
22	F	203	BCR	C30-C25-C26	-7.93	111.45	122.61
20	1	212	CLA	C2B-C1B-NB	7.92	117.05	110.11
20	B	809	CLA	OBD-CAD-C3D	-7.91	114.84	127.98
22	I	103	BCR	C16-C15-C14	-7.91	107.27	123.47
20	3	312	CLA	C2B-C1B-NB	7.90	117.03	110.11
20	A	829	CLA	C4D-C3D-CAD	7.87	112.86	108.47
20	B	826	CLA	O2D-CGD-CBD	7.86	125.24	111.27
20	B	807	CLA	O2D-CGD-CBD	7.85	125.23	111.27
20	B	803	CLA	C4D-C3D-CAD	7.85	112.85	108.47
20	4	307	CLA	CHD-C4C-NC	7.83	136.54	124.20
20	H	101	CLA	C1D-CHD-C4C	-7.82	112.24	122.56
20	3	312	CLA	C3A-C4A-CHB	-7.81	114.35	123.91
20	B	819	CLA	C1D-CHD-C4C	-7.76	112.32	122.56
20	3	317	CLA	OBD-CAD-C3D	-7.75	115.11	127.98
21	H	104	LMU	C3B-C4B-C5B	-7.72	96.46	110.24
22	I	103	BCR	C34-C9-C10	-7.72	112.11	122.92
20	A	850	CLA	C3D-CAD-CBD	-7.72	97.45	107.61
20	B	808	CLA	C1D-CHD-C4C	-7.71	112.39	122.56
20	B	832	CLA	C1D-CHD-C4C	-7.70	112.40	122.56
22	B	852	BCR	C15-C14-C13	-7.69	116.34	127.31
20	B	827	CLA	O2D-CGD-CBD	7.67	124.90	111.27
20	A	829	CLA	O2D-CGD-CBD	7.66	124.88	111.27
20	B	815	CLA	OBD-CAD-C3D	-7.65	115.28	127.98
20	A	839	CLA	C1D-CHD-C4C	-7.63	112.48	122.56
20	A	816	CLA	C1D-CHD-C4C	-7.63	112.48	122.56
20	2	301	CLA	C3A-C4A-CHB	-7.61	114.59	123.91
20	A	827	CLA	O2D-CGD-CBD	7.60	124.77	111.27
20	A	804	CLA	OBD-CAD-CBD	-7.59	115.05	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	305	CLA	C4A-NA-C1A	7.57	110.11	106.71
20	B	804	CLA	O2D-CGD-CBD	7.57	124.72	111.27
20	F	204	CLA	C1B-C2B-C3B	-7.55	99.90	106.92
20	B	811	CLA	CHD-C4C-NC	7.54	136.08	124.20
21	E	101	LMU	C1B-O5B-C5B	-7.53	98.90	113.69
20	1	202	CLA	C1D-CHD-C4C	-7.52	112.64	122.56
20	R	108	CLA	C1D-CHD-C4C	-7.49	112.67	122.56
20	B	821	CLA	C4D-C3D-CAD	7.49	112.65	108.47
20	4	316	CLA	C4D-C3D-CAD	7.49	112.64	108.47
20	L	208	CLA	CAA-C2A-C3A	-7.47	92.32	112.78
20	B	827	CLA	C1D-CHD-C4C	-7.46	112.71	122.56
20	I	102	CLA	C1D-CHD-C4C	-7.46	112.72	122.56
21	E	101	LMU	C4B-C3B-C2B	-7.45	97.82	110.82
20	B	815	CLA	OBD-CAD-CBD	-7.45	115.26	125.89
20	4	311	CLA	C1D-CHD-C4C	-7.44	112.74	122.56
20	4	316	CLA	O2D-CGD-CBD	7.43	124.47	111.27
20	2	308	CLA	O2D-CGD-CBD	7.42	124.45	111.27
20	1	206	CLA	C1D-CHD-C4C	-7.41	112.78	122.56
20	B	836	CLA	O2D-CGD-CBD	7.40	124.42	111.27
20	1	215	CLA	C1D-CHD-C4C	-7.40	112.79	122.56
20	1	210	CLA	CHD-C4C-NC	7.38	135.83	124.20
20	1	208	CLA	C3B-C2B-C1B	-7.38	99.97	106.29
20	2	301	CLA	C3B-C2B-C1B	-7.38	99.98	106.29
21	B	802	LMU	O5B-C5B-C4B	-7.37	96.32	109.69
20	B	817	CLA	O2D-CGD-CBD	7.36	124.34	111.27
20	1	205	CLA	C2B-C1B-NB	7.36	116.56	110.11
20	1	210	CLA	C4A-NA-C1A	7.35	110.01	106.71
20	B	839	CLA	OBD-CAD-CBD	-7.33	115.42	125.89
20	L	202	CLA	OBD-CAD-CBD	-7.30	115.47	125.89
20	4	311	CLA	OBD-CAD-CBD	-7.29	115.47	125.89
20	F	206	CLA	C4D-C3D-CAD	7.28	112.53	108.47
20	G	102	CLA	CHD-C4C-NC	7.27	135.66	124.20
22	B	852	BCR	C3-C4-C5	-7.26	101.11	114.08
20	A	811	CLA	C1D-CHD-C4C	-7.26	112.97	122.56
20	4	304	CLA	CHD-C4C-NC	7.26	135.63	124.20
20	B	806	CLA	C1D-CHD-C4C	-7.23	113.02	122.56
20	3	317	CLA	OBD-CAD-CBD	-7.22	115.57	125.89
20	2	301	CLA	C2B-C1B-NB	7.19	116.41	110.11
20	A	851	CLA	C1D-CHD-C4C	-7.19	113.08	122.56
21	H	104	LMU	C1B-C2B-C3B	-7.18	95.04	110.00
20	3	312	CLA	C3D-C4D-ND	7.16	116.36	110.14
20	3	311	CLA	C1D-CHD-C4C	-7.16	113.11	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	305	CLA	O2D-CGD-CBD	7.15	123.98	111.27
20	1	210	CLA	CHD-C4C-C3C	-7.15	114.33	124.84
20	L	202	CLA	C4D-C3D-CAD	7.14	112.45	108.47
20	1	209	CLA	OBD-CAD-C3D	-7.13	116.14	127.98
20	2	312	CLA	C1D-CHD-C4C	-7.13	113.15	122.56
20	B	837	CLA	C1D-CHD-C4C	-7.11	113.18	122.56
20	1	201	CLA	C1D-CHD-C4C	-7.10	113.19	122.56
20	B	829	CLA	C4D-C3D-CAD	7.10	112.43	108.47
21	B	801	LMU	C3'-C4'-C5'	-7.09	94.66	110.93
20	F	206	CLA	C1D-CHD-C4C	-7.09	113.20	122.56
21	G	101	LMU	C1B-O5B-C5B	-7.09	99.77	113.69
20	3	310	CLA	C2B-C1B-NB	7.09	116.32	110.11
20	B	805	CLA	CAA-C2A-C3A	-7.09	93.38	112.78
20	1	210	CLA	O2A-CGA-O1A	-7.08	105.72	123.59
20	J	103	CLA	C1D-CHD-C4C	-7.08	113.22	122.56
21	F	201	LMU	C2'-C3'-C4'	-7.06	93.57	109.68
20	4	316	CLA	OBD-CAD-CBD	-7.05	115.82	125.89
20	A	811	CLA	OBD-CAD-CBD	-7.04	115.83	125.89
20	1	204	CLA	O2D-CGD-CBD	7.00	123.70	111.27
20	2	302	CLA	C1D-CHD-C4C	-6.98	113.34	122.56
20	B	822	CLA	C1D-CHD-C4C	-6.98	113.34	122.56
21	K	109	LMU	C3B-C4B-C5B	-6.97	97.81	110.24
20	B	804	CLA	OBD-CAD-CBD	-6.96	115.95	125.89
20	F	204	CLA	OBD-CAD-C3D	-6.96	116.43	127.98
21	H	107	LMU	C4B-C3B-C2B	-6.96	98.68	110.82
20	B	823	CLA	C1D-CHD-C4C	-6.95	113.39	122.56
20	B	837	CLA	O2D-CGD-CBD	6.94	123.61	111.27
20	A	813	CLA	C1D-CHD-C4C	-6.94	113.40	122.56
20	2	301	CLA	C1C-NC-C4C	-6.94	103.58	106.71
20	1	207	CLA	O2D-CGD-CBD	6.93	123.59	111.27
20	B	831	CLA	C1D-CHD-C4C	-6.93	113.41	122.56
22	B	852	BCR	C8-C9-C10	6.93	129.57	118.94
20	B	809	CLA	CAB-C3B-C2B	-6.92	111.14	124.69
20	4	319	CLA	C1D-CHD-C4C	-6.91	113.43	122.56
20	4	314	CLA	C1D-CHD-C4C	-6.91	113.44	122.56
20	K	101	CLA	C1D-CHD-C4C	-6.91	113.44	122.56
20	A	821	CLA	O2D-CGD-CBD	6.90	123.52	111.27
20	J	101	CLA	C1D-CHD-C4C	-6.89	113.47	122.56
20	4	305	CLA	OBD-CAD-CBD	-6.89	116.06	125.89
20	H	102	CLA	C1D-CHD-C4C	-6.87	113.49	122.56
20	1	209	CLA	C1D-CHD-C4C	-6.87	113.49	122.56
20	B	824	CLA	C1D-CHD-C4C	-6.87	113.50	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	104	LMU	C3'-C4'-C5'	-6.87	95.18	110.93
20	B	826	CLA	C1D-CHD-C4C	-6.86	113.50	122.56
21	R	101	LMU	O2B-C2B-C3B	6.86	126.21	110.35
20	A	817	CLA	C1D-CHD-C4C	-6.86	113.51	122.56
22	3	314	BCR	C11-C10-C9	-6.85	117.54	127.31
20	4	302	CLA	C1D-CHD-C4C	-6.83	113.54	122.56
20	4	309	CLA	C3B-C2B-C1B	-6.83	100.44	106.29
20	A	831	CLA	O2D-CGD-CBD	6.82	123.39	111.27
20	B	816	CLA	C1D-CHD-C4C	-6.82	113.56	122.56
21	H	108	LMU	O5'-C5'-C4'	-6.81	95.40	109.75
20	1	205	CLA	C2D-C3D-C4D	-6.80	100.44	106.30
20	A	802	CLA	C4A-NA-C1A	6.80	109.76	106.71
20	4	307	CLA	CMB-C2B-C1B	-6.79	118.03	128.46
20	4	304	CLA	CHC-C1C-NC	6.79	134.50	124.20
20	B	835	CLA	O2D-CGD-CBD	6.79	123.33	111.27
20	3	313	CLA	CHD-C4C-C3C	-6.78	114.87	124.84
20	4	303	CLA	CAB-C3B-C2B	-6.75	111.45	124.69
20	H	102	CLA	O2D-CGD-CBD	6.75	123.27	111.27
20	4	308	CLA	C1D-CHD-C4C	-6.75	113.65	122.56
20	4	307	CLA	CHC-C1C-NC	6.75	134.44	124.20
20	3	304	CLA	C1D-CHD-C4C	-6.74	113.67	122.56
20	A	833	CLA	C1D-CHD-C4C	-6.73	113.67	122.56
20	F	205	CLA	C1D-CHD-C4C	-6.73	113.67	122.56
20	A	807	CLA	O2D-CGD-CBD	6.72	123.22	111.27
20	A	801	CLA	O2D-CGD-CBD	6.72	123.21	111.27
20	1	208	CLA	C3A-C4A-CHB	-6.72	115.68	123.91
20	B	812	CLA	OBD-CAD-C3D	-6.70	116.85	127.98
20	A	828	CLA	O2D-CGD-CBD	6.70	123.18	111.27
20	B	809	CLA	OBD-CAD-CBD	-6.70	116.32	125.89
20	B	835	CLA	C1D-CHD-C4C	-6.68	113.74	122.56
21	H	107	LMU	C3B-C4B-C5B	-6.68	98.33	110.24
20	G	102	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
21	E	101	LMU	O2'-C2'-C1'	-6.67	93.85	110.05
20	A	839	CLA	CHC-C1C-NC	6.66	134.31	124.20
21	R	101	LMU	C4B-C3B-C2B	-6.65	99.21	110.82
20	L	207	CLA	C1D-CHD-C4C	-6.64	113.79	122.56
20	K	102	CLA	O2D-CGD-CBD	6.64	123.07	111.27
20	F	204	CLA	C1D-CHD-C4C	-6.63	113.80	122.56
20	L	207	CLA	O2D-CGD-CBD	6.63	123.04	111.27
20	B	822	CLA	O2D-CGD-CBD	6.62	123.03	111.27
20	A	838	CLA	C1D-CHD-C4C	-6.62	113.82	122.56
20	2	307	CLA	C1-C2-C3	-6.61	114.61	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	810	CLA	O2D-CGD-CBD	6.61	123.02	111.27
20	A	805	CLA	C1D-CHD-C4C	-6.61	113.83	122.56
20	L	203	CLA	C1D-CHD-C4C	-6.61	113.83	122.56
20	L	201	CLA	O2D-CGD-CBD	6.61	123.01	111.27
20	B	825	CLA	C1D-CHD-C4C	-6.60	113.84	122.56
20	3	311	CLA	CHD-C4C-NC	6.60	134.60	124.20
20	B	812	CLA	OBD-CAD-CBD	-6.60	116.47	125.89
20	B	807	CLA	O1D-CGD-CBD	-6.59	111.00	124.48
21	H	106	LMU	C1B-O5B-C5B	6.59	126.62	113.69
20	L	209	CLA	C3D-CAD-CBD	-6.57	98.96	107.61
20	2	322	CLA	O2D-CGD-CBD	6.57	122.94	111.27
20	3	319	CLA	C3A-C4A-CHB	-6.56	115.87	123.91
20	2	303	CLA	OBD-CAD-CBD	-6.56	116.52	125.89
20	B	851	CLA	C1D-CHD-C4C	-6.56	113.90	122.56
20	B	818	CLA	C1D-CHD-C4C	-6.56	113.90	122.56
20	B	821	CLA	CHD-C4C-C3C	-6.56	115.20	124.84
20	B	820	CLA	C1D-CHD-C4C	-6.54	113.92	122.56
20	B	825	CLA	O2D-CGD-CBD	6.54	122.89	111.27
21	R	101	LMU	O1B-C1B-C2B	6.54	125.05	108.10
20	A	850	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
20	1	204	CLA	C1D-CHD-C4C	-6.53	113.94	122.56
20	K	108	CLA	C1D-CHD-C4C	-6.53	113.94	122.56
20	B	850	CLA	C4-C3-C5	6.52	126.25	115.27
20	2	304	CLA	C2B-C1B-NB	6.52	115.82	110.11
20	3	319	CLA	C2B-C1B-NB	6.52	115.82	110.11
20	A	839	CLA	O1D-CGD-CBD	-6.52	111.15	124.48
20	B	809	CLA	O2D-CGD-CBD	6.51	122.84	111.27
20	B	839	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	A	824	CLA	C1D-CHD-C4C	-6.50	113.97	122.56
21	H	108	LMU	O5B-C1B-C2B	-6.50	96.59	110.35
22	F	203	BCR	C24-C23-C22	-6.50	116.41	126.23
20	3	310	CLA	C4A-NA-C1A	6.49	109.62	106.71
20	2	322	CLA	CAA-C2A-C3A	-6.49	95.01	112.78
20	A	826	CLA	C1D-CHD-C4C	-6.48	114.01	122.56
20	A	812	CLA	C1D-CHD-C4C	-6.47	114.01	122.56
20	4	312	CLA	C2B-C1B-NB	6.47	115.78	110.11
20	B	813	CLA	C1D-CHD-C4C	-6.47	114.02	122.56
20	R	108	CLA	OBD-CAD-CBD	-6.46	116.66	125.89
20	A	815	CLA	CHD-C4C-NC	6.46	134.38	124.20
20	A	818	CLA	C1D-CHD-C4C	-6.44	114.06	122.56
20	B	805	CLA	C1D-CHD-C4C	-6.43	114.07	122.56
20	A	803	CLA	C1D-CHD-C4C	-6.43	114.08	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	852	BCR	C4-C5-C6	-6.42	113.41	122.73
20	4	306	CLA	O2D-CGD-CBD	6.42	122.68	111.27
20	A	825	CLA	C1D-CHD-C4C	-6.41	114.09	122.56
20	3	301	CLA	C1D-CHD-C4C	-6.41	114.10	122.56
20	4	309	CLA	CHD-C4C-NC	6.41	134.09	124.21
20	2	304	CLA	C2D-C3D-C4D	-6.41	100.78	106.30
20	2	307	CLA	CHD-C4C-NC	6.40	134.29	124.20
20	2	306	CLA	C2D-C3D-C4D	-6.39	100.79	106.30
20	4	304	CLA	CAA-C2A-C3A	-6.38	95.31	112.78
20	B	850	CLA	C1D-CHD-C4C	-6.37	114.16	122.56
20	1	202	CLA	C1-C2-C3	-6.36	115.04	126.04
22	I	103	BCR	C8-C9-C10	6.36	128.70	118.94
20	1	211	CLA	C2B-C1B-NB	6.36	115.68	110.11
20	A	831	CLA	C1D-CHD-C4C	-6.35	114.17	122.56
20	B	809	CLA	C1D-CHD-C4C	-6.35	114.17	122.56
22	F	203	BCR	C3-C4-C5	-6.35	102.74	114.08
20	3	305	CLA	C2B-C1B-NB	6.35	115.67	110.11
20	A	836	CLA	C1D-CHD-C4C	-6.34	114.19	122.56
20	B	830	CLA	C1D-CHD-C4C	-6.34	114.19	122.56
20	4	318	CLA	C3D-CAD-CBD	-6.34	99.26	107.61
20	B	829	CLA	O2D-CGD-CBD	6.33	122.52	111.27
20	2	316	CLA	C1D-CHD-C4C	-6.33	114.21	122.56
20	B	819	CLA	CHD-C4C-NC	6.31	134.15	124.20
20	B	814	CLA	C1D-CHD-C4C	-6.30	114.25	122.56
20	B	806	CLA	O2D-CGD-CBD	6.30	122.46	111.27
20	I	102	CLA	O2D-CGD-CBD	6.29	122.45	111.27
20	B	811	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
20	A	820	CLA	C1D-CHD-C4C	-6.29	114.26	122.56
20	L	203	CLA	O2D-CGD-CBD	6.29	122.44	111.27
20	B	819	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
20	A	809	CLA	C1D-CHD-C4C	-6.28	114.27	122.56
20	4	306	CLA	C4D-C3D-CAD	6.27	111.97	108.47
20	A	815	CLA	C1-C2-C3	-6.25	116.64	126.75
22	B	852	BCR	C34-C9-C10	-6.24	114.18	122.92
20	A	807	CLA	CGD-CBD-CAD	-6.24	90.52	110.73
20	A	802	CLA	CHD-C4C-NC	6.24	133.84	124.21
20	B	804	CLA	C1D-CHD-C4C	-6.24	114.32	122.56
20	B	826	CLA	C4A-NA-C1A	6.24	109.51	106.71
21	H	108	LMU	C1B-C2B-C3B	-6.24	97.01	110.00
20	2	310	CLA	C2B-C1B-NB	6.24	115.57	110.11
20	1	202	CLA	C3D-CAD-CBD	-6.23	99.40	107.61
20	H	103	CLA	C1D-CHD-C4C	-6.23	114.34	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	318	CLA	CHC-C1C-NC	6.22	133.65	124.20
20	B	817	CLA	C1D-CHD-C4C	-6.22	114.35	122.56
20	1	205	CLA	C1D-CHD-C4C	-6.21	110.72	126.10
20	A	822	CLA	C1D-CHD-C4C	-6.20	114.37	122.56
20	A	836	CLA	O2D-CGD-CBD	6.19	122.27	111.27
22	I	103	BCR	C38-C26-C25	-6.19	117.58	124.53
20	A	801	CLA	CAA-C2A-C3A	6.19	129.72	112.78
20	K	103	CLA	C1D-CHD-C4C	-6.18	114.40	122.56
20	3	318	CLA	OBD-CAD-CBD	-6.18	117.06	125.89
20	G	102	CLA	O2D-CGD-CBD	6.18	122.24	111.27
20	A	828	CLA	C1D-CHD-C4C	-6.17	114.41	122.56
20	4	309	CLA	C4A-NA-C1A	6.17	109.48	106.71
20	1	203	CLA	O2D-CGD-CBD	6.15	122.20	111.27
20	A	823	CLA	C1D-CHD-C4C	-6.15	114.44	122.56
20	A	839	CLA	CMD-C2D-C3D	-6.15	113.18	124.68
20	B	807	CLA	OBD-CAD-C3D	-6.15	117.78	127.98
20	B	850	CLA	O2D-CGD-CBD	6.14	122.18	111.27
20	1	207	CLA	CBA-CAA-C2A	-6.13	95.75	113.86
20	1	214	CLA	C2B-C1B-NB	6.13	115.48	110.11
20	A	835	CLA	C1D-CHD-C4C	-6.13	114.46	122.56
20	B	833	CLA	C1D-CHD-C4C	-6.13	114.47	122.56
20	4	314	CLA	CAB-C3B-C2B	-6.12	112.69	124.69
21	K	106	LMU	C1-O1'-C1'	-6.11	103.70	113.84
20	A	819	CLA	C1D-CHD-C4C	-6.11	114.49	122.56
20	A	832	CLA	C1D-CHD-C4C	-6.11	114.50	122.56
20	B	838	CLA	O2D-CGD-CBD	6.10	122.11	111.27
20	B	831	CLA	O2D-CGD-CBD	6.10	122.11	111.27
20	R	108	CLA	C4A-NA-C1A	6.10	109.45	106.71
20	B	814	CLA	O2D-CGD-CBD	6.10	122.10	111.27
20	2	312	CLA	C4A-NA-C1A	6.09	109.45	106.71
20	A	802	CLA	C1D-CHD-C4C	-6.09	111.02	126.10
21	H	108	LMU	O5B-C5B-C4B	-6.09	98.63	109.69
20	A	852	CLA	O2D-CGD-CBD	6.09	122.08	111.27
20	3	317	CLA	C1D-CHD-C4C	-6.09	114.53	122.56
20	1	205	CLA	C3D-C2D-C1D	6.08	111.54	106.30
20	3	303	CLA	C2B-C1B-NB	6.07	115.43	110.11
20	3	311	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
20	2	303	CLA	C1D-CHD-C4C	-6.06	114.56	122.56
20	F	206	CLA	C1-C2-C3	-6.06	115.56	126.04
20	L	201	CLA	C4-C3-C5	6.06	125.46	115.27
20	4	311	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
20	A	840	CLA	C1D-CHD-C4C	-6.05	114.57	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	830	CLA	O2D-CGD-CBD	6.03	121.99	111.27
20	K	102	CLA	C1D-CHD-C4C	-6.03	114.60	122.56
20	L	208	CLA	C1D-CHD-C4C	-6.03	114.60	122.56
20	3	312	CLA	C3B-C2B-C1B	-6.02	101.13	106.29
20	4	307	CLA	CAA-C2A-C1A	6.01	131.69	111.97
20	A	830	CLA	C1D-CHD-C4C	-6.01	114.63	122.56
20	4	313	CLA	C2B-C1B-NB	6.01	115.37	110.11
20	1	208	CLA	C3D-C4D-ND	6.00	115.36	110.14
20	1	211	CLA	C3A-C4A-CHB	-6.00	116.56	123.91
21	H	108	LMU	C1B-O1B-C4'	-6.00	103.12	117.96
20	B	807	CLA	C4A-NA-C1A	5.99	109.40	106.71
20	L	202	CLA	O2D-CGD-CBD	5.98	121.90	111.27
20	3	304	CLA	CAB-C3B-C2B	-5.98	112.97	124.69
20	B	811	CLA	CMD-C2D-C3D	-5.98	113.50	124.68
21	G	101	LMU	O5B-C5B-C6B	-5.97	91.58	106.44
20	A	804	CLA	C1D-CHD-C4C	-5.97	114.67	122.56
20	A	821	CLA	C3D-CAD-CBD	-5.97	99.74	107.61
20	B	821	CLA	CBC-CAC-C3C	-5.96	96.00	112.43
20	B	839	CLA	C3D-CAD-CBD	-5.96	99.76	107.61
20	2	303	CLA	O2D-CGD-CBD	5.96	121.85	111.27
20	B	806	CLA	C4A-NA-C1A	5.95	109.38	106.71
20	3	312	CLA	C3D-C2D-C1D	5.95	111.43	106.30
20	1	210	CLA	CMD-C2D-C3D	-5.95	113.55	124.68
22	I	103	BCR	C38-C26-C27	5.95	125.04	113.62
20	2	316	CLA	O2D-CGD-CBD	5.94	121.82	111.27
20	A	802	CLA	C3B-C2B-C1B	-5.92	101.22	106.29
20	3	305	CLA	CHC-C1C-NC	5.91	132.96	124.23
20	B	805	CLA	O2D-CGD-CBD	5.91	121.77	111.27
20	B	807	CLA	C1D-CHD-C4C	-5.91	114.76	122.56
20	A	809	CLA	CHC-C1C-NC	5.91	133.17	124.20
20	4	311	CLA	CHD-C4C-NC	5.91	133.51	124.20
22	I	103	BCR	C29-C30-C25	-5.90	101.39	110.48
22	F	203	BCR	C35-C13-C14	-5.90	114.65	122.92
21	H	106	LMU	C3B-C4B-C5B	-5.90	99.71	110.24
20	A	837	CLA	C3D-CAD-CBD	-5.90	99.84	107.61
20	1	202	CLA	CHC-C1C-NC	5.89	133.15	124.20
20	A	839	CLA	C3D-CAD-CBD	-5.89	99.85	107.61
20	1	212	CLA	C3B-C2B-C1B	-5.89	101.25	106.29
20	B	829	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
21	B	802	LMU	C1B-O1B-C4'	-5.88	103.41	117.96
20	B	835	CLA	O2D-CGD-O1D	-5.86	112.38	123.84
20	A	827	CLA	C1D-CHD-C4C	-5.86	114.82	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	103	BCR	C11-C10-C9	-5.86	118.95	127.31
20	4	307	CLA	CBA-CAA-C2A	-5.86	96.58	113.86
20	B	834	CLA	C1D-CHD-C4C	-5.85	114.83	122.56
20	4	306	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
20	A	801	CLA	C1D-CHD-C4C	-5.85	114.84	122.56
20	2	306	CLA	C3D-C4D-ND	5.84	115.22	110.14
20	B	807	CLA	C3D-CAD-CBD	-5.84	99.92	107.61
20	K	103	CLA	O2D-CGD-CBD	5.84	121.64	111.27
20	B	811	CLA	CHC-C1C-NC	5.84	133.06	124.20
20	A	829	CLA	C1D-CHD-C4C	-5.83	114.86	122.56
20	A	821	CLA	C1D-CHD-C4C	-5.83	114.87	122.56
20	L	208	CLA	O2D-CGD-CBD	5.82	121.61	111.27
20	4	316	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
20	H	109	CLA	C1D-CHD-C4C	-5.81	114.88	122.56
20	1	203	CLA	C1D-CHD-C4C	-5.81	114.89	122.56
20	3	310	CLA	C3D-C4D-ND	5.81	115.19	110.14
20	1	215	CLA	CHD-C4C-NC	5.80	133.34	124.20
20	2	311	CLA	O2D-CGD-CBD	5.80	121.58	111.27
21	B	802	LMU	C3B-C4B-C5B	-5.79	99.90	110.24
20	R	108	CLA	CHD-C4C-NC	5.79	133.33	124.20
20	3	303	CLA	C2A-C1A-CHA	-5.79	112.76	122.63
20	B	829	CLA	C1D-CHD-C4C	-5.79	114.92	122.56
20	4	310	CLA	C1D-CHD-C4C	-5.79	111.78	126.10
20	1	207	CLA	CGD-CBD-CAD	-5.78	92.00	110.73
20	3	311	CLA	O1D-CGD-CBD	-5.78	112.65	124.48
20	1	201	CLA	CAC-C3C-C4C	5.78	132.31	124.81
20	A	850	CLA	CHD-C4C-NC	5.78	133.31	124.20
21	H	104	LMU	C1'-C2'-C3'	-5.78	97.96	110.00
20	B	821	CLA	CHD-C4C-NC	5.78	133.31	124.20
20	4	310	CLA	C2B-C1B-NB	5.78	115.17	110.11
20	1	212	CLA	C4A-NA-C1A	5.77	109.30	106.71
20	4	318	CLA	C1D-CHD-C4C	-5.77	114.95	122.56
20	3	316	CLA	C2B-C1B-NB	5.76	115.16	110.11
20	A	850	CLA	C1D-CHD-C4C	-5.76	114.96	122.56
20	A	833	CLA	O2D-CGD-CBD	5.76	121.50	111.27
20	1	206	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
20	1	210	CLA	CGD-CBD-CAD	-5.75	92.10	110.73
20	B	818	CLA	C3D-CAD-CBD	-5.75	100.03	107.61
20	1	207	CLA	C1D-CHD-C4C	-5.75	114.97	122.56
20	1	201	CLA	O2D-CGD-CBD	5.75	121.48	111.27
20	A	802	CLA	C3A-C4A-CHB	-5.74	116.88	123.91
20	B	803	CLA	OBD-CAD-C3D	-5.74	118.45	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	205	CLA	C3A-C4A-CHB	-5.74	116.88	123.91
20	B	833	CLA	O2D-CGD-CBD	5.74	121.46	111.27
20	A	837	CLA	C1D-CHD-C4C	-5.73	115.00	122.56
20	R	107	CLA	C1D-CHD-C4C	-5.73	115.00	122.56
20	A	814	CLA	O2D-CGD-CBD	5.72	121.44	111.27
21	H	104	LMU	C1'-O5'-C5'	5.70	124.87	113.69
22	I	103	BCR	C16-C17-C18	-5.69	119.19	127.31
20	B	829	CLA	CHD-C4C-NC	5.69	133.17	124.20
20	1	205	CLA	CHD-C4C-NC	5.69	132.98	124.21
20	A	838	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
21	K	104	LMU	C6B-C5B-C4B	-5.67	99.73	113.00
20	3	318	CLA	C1D-CHD-C4C	-5.67	115.08	122.56
20	A	808	CLA	C1D-CHD-C4C	-5.66	115.08	122.56
20	3	313	CLA	C1-C2-C3	-5.66	116.25	126.04
21	A	854	LMU	C1'-O5'-C5'	-5.66	102.58	113.69
20	1	208	CLA	C2D-C3D-C4D	-5.66	101.43	106.30
20	3	316	CLA	C3A-C4A-CHB	-5.65	116.99	123.91
20	B	836	CLA	C1D-CHD-C4C	-5.65	115.10	122.56
21	G	101	LMU	O4'-C4B-C3B	5.65	123.40	110.35
20	L	202	CLA	C1D-CHD-C4C	-5.65	115.11	122.56
20	A	815	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
20	2	305	CLA	C1D-CHD-C4C	-5.64	115.11	122.56
20	1	215	CLA	O2D-CGD-O1D	-5.63	112.82	123.84
20	A	816	CLA	C1-C2-C3	-5.63	116.30	126.04
20	B	821	CLA	C6-C5-C3	-5.63	98.70	113.45
20	1	202	CLA	CAC-C3C-C4C	5.62	132.11	124.81
20	1	210	CLA	O2A-CGA-CBA	5.62	129.54	111.91
20	L	209	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
20	3	306	CLA	CHD-C4C-NC	5.61	132.87	124.21
20	4	309	CLA	C1D-CHD-C4C	-5.61	112.22	126.10
20	A	809	CLA	O2D-CGD-CBD	5.61	121.23	111.27
20	A	841	CLA	C1D-CHD-C4C	-5.61	115.16	122.56
20	2	304	CLA	C3D-C4D-ND	5.61	115.01	110.14
22	I	103	BCR	C15-C16-C17	5.60	134.96	123.47
20	A	838	CLA	CHD-C4C-NC	5.60	133.03	124.20
20	3	305	CLA	CHD-C4C-NC	5.60	132.85	124.21
20	4	307	CLA	C4A-NA-C1A	5.60	109.22	106.71
22	I	101	BCR	C4-C5-C6	-5.59	114.61	122.73
20	L	209	CLA	CHD-C4C-NC	5.59	133.01	124.20
20	2	304	CLA	C3A-C4A-CHB	-5.59	117.07	123.91
20	A	822	CLA	C3D-CAD-CBD	-5.58	100.26	107.61
20	4	318	CLA	C1-C2-C3	-5.57	116.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	101	BCR	C30-C25-C24	5.57	131.53	115.78
20	A	834	CLA	C1D-CHD-C4C	-5.56	115.21	122.56
20	3	307	CLA	CHD-C4C-NC	5.56	132.79	124.21
21	B	802	LMU	O3B-C3B-C2B	-5.56	97.50	110.35
20	2	306	CLA	C2B-C1B-NB	5.56	114.98	110.11
20	2	312	CLA	O2D-CGD-CBD	5.55	121.14	111.27
20	2	315	CLA	C2B-C1B-NB	5.55	114.97	110.11
20	A	833	CLA	CHD-C4C-NC	5.55	132.94	124.20
20	2	306	CLA	C2A-C1A-CHA	-5.54	113.18	122.63
20	B	810	CLA	C1D-CHD-C4C	-5.54	115.24	122.56
20	3	309	CLA	C2B-C1B-NB	5.54	114.96	110.11
20	1	212	CLA	C3A-C4A-CHB	-5.54	117.12	123.91
20	4	306	CLA	O2A-CGA-CBA	5.54	129.29	111.91
20	1	212	CLA	C2A-C1A-CHA	-5.53	113.19	122.63
20	3	320	CLA	CHD-C4C-NC	5.53	132.74	124.21
20	B	851	CLA	C3D-CAD-CBD	-5.53	100.32	107.61
22	F	203	BCR	C10-C11-C12	-5.53	105.96	123.22
21	K	109	LMU	O1'-C1'-C2'	5.53	116.94	108.30
20	2	311	CLA	C1D-CHD-C4C	-5.53	115.26	122.56
22	B	852	BCR	C36-C18-C19	5.53	126.79	118.08
22	L	210	BCR	C27-C26-C25	-5.53	114.71	122.73
20	A	806	CLA	C1D-CHD-C4C	-5.53	115.27	122.56
20	3	306	CLA	C3A-C4A-CHB	-5.52	117.14	123.91
20	A	804	CLA	CHD-C4C-NC	5.52	132.91	124.20
20	4	316	CLA	O1D-CGD-CBD	-5.52	113.19	124.48
20	3	310	CLA	C2D-C3D-C4D	-5.52	101.55	106.30
21	L	204	LMU	O4'-C4B-C5B	-5.52	95.60	109.30
22	I	103	BCR	C7-C8-C9	5.52	134.57	126.23
20	B	805	CLA	CHC-C1C-NC	5.51	132.56	124.20
20	1	207	CLA	C3D-CAD-CBD	-5.50	100.36	107.61
20	L	201	CLA	CMD-C2D-C3D	-5.50	114.38	124.68
21	E	101	LMU	C3B-C4B-C5B	-5.50	100.42	110.24
20	1	205	CLA	C3B-C2B-C1B	-5.50	101.58	106.29
20	4	307	CLA	C3A-C2A-C1A	5.50	109.58	101.34
20	R	108	CLA	CHC-C1C-NC	5.49	132.54	124.20
20	A	834	CLA	O2D-CGD-CBD	5.49	121.02	111.27
20	2	306	CLA	CHC-C1C-NC	5.48	132.33	124.23
20	R	108	CLA	O2A-CGA-CBA	5.48	129.12	111.91
22	A	847	BCR	C16-C17-C18	-5.48	119.49	127.31
20	3	307	CLA	C3A-C4A-CHB	-5.46	117.22	123.91
20	H	101	CLA	CHD-C4C-NC	5.46	132.81	124.20
22	B	846	BCR	C16-C17-C18	-5.46	119.52	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	813	CLA	CHC-C1C-NC	5.46	132.49	124.20
20	1	205	CLA	C3D-C4D-ND	5.46	114.88	110.14
22	A	844	BCR	C15-C14-C13	-5.46	119.52	127.31
20	2	309	CLA	C2B-C1B-NB	5.45	114.89	110.11
20	B	806	CLA	CHC-C1C-NC	5.45	132.47	124.20
20	1	202	CLA	O2D-CGD-CBD	5.44	120.94	111.27
20	B	840	CLA	C1D-CHD-C4C	-5.44	115.38	122.56
20	F	204	CLA	CHD-C4C-NC	5.43	132.76	124.20
20	K	101	CLA	CHD-C4C-NC	5.43	132.76	124.20
22	L	210	BCR	C30-C25-C26	-5.43	114.97	122.61
22	A	844	BCR	C16-C17-C18	-5.43	119.57	127.31
20	A	805	CLA	CHC-C1C-NC	5.42	132.43	124.20
20	4	302	CLA	CHD-C4C-NC	5.41	132.73	124.20
20	3	317	CLA	O2D-CGD-CBD	5.41	120.88	111.27
20	B	839	CLA	C1D-CHD-C4C	-5.41	115.42	122.56
22	B	843	BCR	C11-C10-C9	-5.41	119.59	127.31
22	A	844	BCR	C11-C10-C9	-5.41	119.59	127.31
22	A	847	BCR	C15-C14-C13	-5.40	119.60	127.31
20	A	801	CLA	CMD-C2D-C3D	-5.40	114.57	124.68
20	G	102	CLA	C3D-CAD-CBD	-5.40	100.49	107.61
20	4	303	CLA	CHD-C4C-NC	5.40	132.71	124.20
20	A	817	CLA	O2D-CGD-CBD	5.39	120.84	111.27
20	3	302	CLA	CBA-CAA-C2A	-5.38	97.97	113.86
20	4	307	CLA	C3D-CAD-CBD	-5.38	100.52	107.61
20	L	203	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
20	B	832	CLA	C3D-CAD-CBD	-5.38	100.53	107.61
20	3	304	CLA	CHD-C4C-NC	5.37	132.67	124.20
20	J	101	CLA	CHD-C4C-NC	5.37	132.66	124.20
22	B	846	BCR	C11-C10-C9	-5.37	119.65	127.31
20	J	103	CLA	CHD-C4C-NC	5.37	132.66	124.20
20	B	815	CLA	O2D-CGD-CBD	5.36	120.80	111.27
20	4	309	CLA	C3A-C4A-CHB	-5.36	117.34	123.91
20	4	316	CLA	CHD-C4C-NC	5.36	132.64	124.20
20	B	823	CLA	CHD-C4C-NC	5.35	132.64	124.20
20	4	313	CLA	C3B-C2B-C1B	-5.35	101.71	106.29
20	4	312	CLA	C1D-CHD-C4C	-5.35	112.86	126.10
22	J	102	BCR	C15-C14-C13	-5.35	119.67	127.31
20	L	201	CLA	O2D-CGD-O1D	-5.35	113.38	123.84
20	A	802	CLA	CHC-C1C-NC	5.35	132.13	124.23
20	A	835	CLA	CHC-C1C-NC	5.35	132.31	124.20
20	A	837	CLA	O2D-CGD-CBD	5.34	120.76	111.27
20	A	803	CLA	CHD-C4C-NC	5.34	132.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	831	CLA	C3D-CAD-CBD	-5.34	100.58	107.61
20	A	818	CLA	CHD-C4C-NC	5.34	132.61	124.20
22	B	843	BCR	C15-C14-C13	-5.34	119.69	127.31
20	1	202	CLA	C4-C3-C5	5.34	124.25	115.27
21	F	201	LMU	C1B-O1B-C4'	-5.33	104.77	117.96
20	3	307	CLA	C2B-C1B-NB	5.33	114.78	110.11
20	H	101	CLA	CHC-C1C-NC	5.33	132.28	124.20
21	A	856	LMU	O1B-C4'-C3'	5.33	121.45	107.28
22	J	102	BCR	C11-C10-C9	-5.33	119.71	127.31
22	A	843	BCR	C11-C10-C9	-5.32	119.72	127.31
20	B	804	CLA	O2D-CGD-O1D	-5.32	113.44	123.84
22	B	846	BCR	C15-C14-C13	-5.32	119.72	127.31
20	A	839	CLA	CHD-C4C-NC	5.32	132.58	124.20
20	A	841	CLA	O2D-CGD-CBD	5.32	120.71	111.27
20	A	839	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
20	4	311	CLA	C3D-CAD-CBD	-5.31	100.61	107.61
20	R	108	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
21	1	213	LMU	C3'-C4'-C5'	-5.30	98.77	110.93
21	G	101	LMU	C1B-C2B-C3B	-5.30	98.95	110.00
20	A	833	CLA	CHC-C1C-NC	5.30	132.24	124.20
22	J	102	BCR	C16-C17-C18	-5.30	119.75	127.31
20	A	811	CLA	CHC-C1C-NC	5.30	132.24	124.20
20	A	808	CLA	O2D-CGD-CBD	5.30	120.68	111.27
20	3	313	CLA	CHC-C1C-NC	5.29	132.23	124.20
20	B	826	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
20	2	302	CLA	O2D-CGD-CBD	5.29	120.67	111.27
22	B	843	BCR	C16-C17-C18	-5.28	119.77	127.31
20	3	319	CLA	C2A-C1A-CHA	-5.28	113.62	122.63
20	A	816	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
20	1	208	CLA	C2A-C1A-CHA	-5.28	113.63	122.63
20	H	103	CLA	C3D-CAD-CBD	-5.28	100.66	107.61
21	H	105	LMU	C4B-C3B-C2B	-5.28	101.61	110.82
21	R	103	LMU	O3B-C3B-C4B	-5.28	98.15	110.35
20	B	818	CLA	CHD-C4C-NC	5.28	132.52	124.20
20	A	819	CLA	O2D-CGD-CBD	5.27	120.64	111.27
20	A	839	CLA	OBD-CAD-CBD	-5.27	118.37	125.89
20	B	803	CLA	CHD-C4C-NC	5.27	132.50	124.20
20	A	820	CLA	O2D-CGD-CBD	5.27	120.63	111.27
20	3	319	CLA	C3D-C4D-ND	5.26	114.72	110.14
20	R	107	CLA	C3D-CAD-CBD	-5.26	100.68	107.61
22	B	852	BCR	C10-C11-C12	-5.25	106.82	123.22
20	1	205	CLA	C2A-C1A-CHA	-5.25	113.67	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	309	CLA	CHC-C1C-NC	5.25	131.98	124.23
20	A	835	CLA	CHD-C4C-NC	5.25	132.48	124.20
20	4	312	CLA	CHD-C4C-NC	5.25	132.30	124.21
20	3	308	CLA	C1D-CHD-C4C	-5.24	115.64	122.56
20	A	852	CLA	C1D-CHD-C4C	-5.24	115.64	122.56
20	B	838	CLA	CHC-C1C-NC	5.24	132.16	124.20
20	3	313	CLA	C3D-CAD-CBD	-5.24	100.70	107.61
20	1	215	CLA	CGD-CBD-CAD	5.24	127.70	110.73
20	B	817	CLA	CHD-C4C-C3C	-5.23	117.14	124.84
21	G	101	LMU	O5B-C1B-C2B	-5.23	99.27	110.35
23	B	841	PQN	C11-C12-C13	-5.23	118.08	126.79
20	F	205	CLA	O2D-CGD-CBD	5.23	120.56	111.27
20	A	805	CLA	CHD-C4C-NC	5.23	132.44	124.20
20	B	830	CLA	C3D-CAD-CBD	-5.22	100.73	107.61
20	A	814	CLA	C1D-CHD-C4C	-5.22	115.67	122.56
20	2	309	CLA	C4A-NA-C1A	5.22	109.05	106.71
20	3	306	CLA	C2B-C1B-NB	5.21	114.68	110.11
20	3	308	CLA	O2D-CGD-CBD	5.21	120.53	111.27
20	1	203	CLA	C3D-CAD-CBD	-5.21	100.74	107.61
20	L	201	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
20	4	304	CLA	O2A-CGA-O1A	-5.21	110.45	123.59
22	F	202	BCR	C11-C10-C9	-5.21	119.88	127.31
22	A	843	BCR	C16-C17-C18	-5.20	119.89	127.31
20	A	810	CLA	C1D-CHD-C4C	-5.20	115.69	122.56
22	B	845	BCR	C11-C10-C9	-5.20	119.89	127.31
20	B	815	CLA	C1D-CHD-C4C	-5.19	115.70	122.56
20	J	103	CLA	O2D-CGD-CBD	5.19	120.49	111.27
20	4	312	CLA	C3A-C4A-CHB	-5.18	117.56	123.91
21	H	104	LMU	O5B-C5B-C4B	-5.18	100.28	109.69
20	1	212	CLA	C3D-C4D-ND	5.18	114.64	110.14
20	2	308	CLA	C1D-CHD-C4C	-5.18	115.72	122.56
22	F	202	BCR	C15-C14-C13	-5.18	119.92	127.31
20	1	210	CLA	CHC-C1C-NC	5.17	132.05	124.20
20	B	805	CLA	CHD-C4C-NC	5.17	132.36	124.20
21	R	101	LMU	C1'-C2'-C3'	-5.17	99.22	110.00
20	3	307	CLA	C1D-CHD-C4C	-5.17	113.31	126.10
20	A	825	CLA	O2D-CGD-CBD	5.17	120.45	111.27
21	G	101	LMU	O1B-C1B-C2B	5.16	121.48	108.10
20	A	809	CLA	CAC-C3C-C4C	5.16	131.51	124.81
20	A	841	CLA	C4A-NA-C1A	5.16	109.03	106.71
20	B	833	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
20	A	813	CLA	CHD-C4C-NC	5.16	132.33	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	306	CLA	C1D-CHD-C4C	-5.16	113.34	126.10
20	B	819	CLA	C3D-CAD-CBD	-5.15	100.82	107.61
20	3	320	CLA	C1D-CHD-C4C	-5.15	113.35	126.10
20	3	307	CLA	CHC-C1C-NC	5.15	131.83	124.23
22	A	843	BCR	C15-C14-C13	-5.14	119.97	127.31
20	3	305	CLA	C2A-C1A-CHA	-5.14	113.86	122.63
20	4	307	CLA	CMB-C2B-C3B	5.14	134.30	124.68
21	K	104	LMU	C4B-C3B-C2B	-5.14	101.85	110.82
20	3	302	CLA	O2D-CGD-CBD	5.13	120.39	111.27
22	A	845	BCR	C11-C10-C9	-5.13	119.98	127.31
20	3	319	CLA	C1D-CHD-C4C	-5.13	113.40	126.10
22	F	202	BCR	C16-C17-C18	-5.13	119.99	127.31
20	A	821	CLA	O1D-CGD-CBD	-5.13	113.99	124.48
22	B	844	BCR	C24-C23-C22	-5.13	118.49	126.23
20	A	813	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	B	845	BCR	C15-C14-C13	-5.12	120.00	127.31
20	B	850	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	B	842	BCR	C15-C14-C13	-5.12	120.00	127.31
20	F	206	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
20	3	312	CLA	C2A-C1A-CHA	-5.11	113.92	122.63
20	1	216	CLA	C3A-C4A-CHB	-5.10	117.66	123.91
20	1	215	CLA	CMD-C2D-C3D	-5.10	115.13	124.68
20	B	816	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
22	A	845	BCR	C16-C17-C18	-5.10	120.03	127.31
20	1	201	CLA	CAC-C3C-C2C	-5.10	118.81	127.53
20	1	201	CLA	CMD-C2D-C3D	-5.10	115.14	124.68
20	A	811	CLA	CMD-C2D-C3D	-5.09	115.15	124.68
20	4	306	CLA	CHD-C4C-NC	5.09	132.23	124.20
20	B	832	CLA	CHD-C4C-C3C	-5.09	117.35	124.84
20	1	210	CLA	C3D-CAD-CBD	-5.09	100.90	107.61
20	A	829	CLA	O2D-CGD-O1D	-5.09	113.88	123.84
20	4	304	CLA	O2D-CGD-CBD	5.09	120.31	111.27
22	B	845	BCR	C16-C17-C18	-5.09	120.05	127.31
20	A	833	CLA	C4A-NA-C1A	5.08	108.99	106.71
20	4	307	CLA	CBC-CAC-C3C	-5.08	98.43	112.43
20	A	815	CLA	C3D-CAD-CBD	-5.08	100.92	107.61
20	3	320	CLA	C2B-C1B-NB	5.08	114.56	110.11
20	3	306	CLA	CHC-C1C-NC	5.08	131.72	124.23
20	B	812	CLA	C3D-CAD-CBD	-5.08	100.92	107.61
22	B	842	BCR	C11-C10-C9	-5.07	120.07	127.31
20	A	830	CLA	C3D-CAD-CBD	-5.07	100.93	107.61
20	B	837	CLA	CHD-C4C-NC	5.07	132.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	215	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
20	A	851	CLA	CHD-C4C-NC	5.06	132.17	124.20
20	4	319	CLA	CHD-C4C-NC	5.05	132.17	124.20
22	I	101	BCR	C37-C22-C21	-5.05	115.85	122.92
22	A	845	BCR	C15-C14-C13	-5.05	120.10	127.31
20	2	302	CLA	CHD-C4C-NC	5.05	132.16	124.20
20	K	108	CLA	O2D-CGD-CBD	5.05	120.24	111.27
20	3	310	CLA	CHC-C1C-NC	5.05	131.68	124.23
20	L	202	CLA	C4-C3-C5	5.04	123.75	115.27
20	1	215	CLA	CED-O2D-CGD	5.04	127.34	115.94
20	A	837	CLA	CHC-C1C-NC	5.04	131.85	124.20
21	R	104	LMU	O1B-C1B-C2B	5.04	121.15	108.10
20	A	837	CLA	CHD-C4C-NC	5.03	132.14	124.20
20	B	803	CLA	C1D-CHD-C4C	-5.03	115.91	122.56
20	1	201	CLA	CHB-C4A-NA	5.03	131.47	124.51
21	E	101	LMU	O4'-C4B-C5B	5.03	121.79	109.30
20	4	308	CLA	CHD-C4C-NC	5.03	132.13	124.20
20	B	824	CLA	O2D-CGD-CBD	5.03	120.20	111.27
20	L	201	CLA	C4-C3-C2	-5.02	110.79	123.68
21	R	104	LMU	O3B-C3B-C4B	-5.02	98.74	110.35
20	L	207	CLA	CHD-C4C-NC	5.02	132.11	124.20
20	F	205	CLA	CHD-C4C-NC	5.02	132.11	124.20
20	3	308	CLA	C3D-CAD-CBD	-5.02	101.00	107.61
20	B	814	CLA	C3D-CAD-CBD	-5.02	101.00	107.61
20	1	206	CLA	C3D-CAD-CBD	-5.02	101.00	107.61
20	4	310	CLA	C3B-C2B-C1B	-5.02	102.00	106.29
20	B	808	CLA	C3D-CAD-CBD	-5.01	101.00	107.61
20	4	305	CLA	CHC-C1C-NC	5.01	131.80	124.20
20	A	806	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	4	304	CLA	CMD-C2D-C3D	-5.01	115.31	124.68
20	A	851	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
20	A	824	CLA	O2D-CGD-CBD	5.01	120.16	111.27
20	2	309	CLA	CHD-C4C-NC	5.01	131.93	124.21
20	A	813	CLA	C4A-NA-C1A	5.00	108.96	106.71
20	A	825	CLA	CHD-C4C-NC	5.00	132.09	124.20
20	A	824	CLA	CHD-C4C-NC	5.00	132.08	124.20
20	4	302	CLA	O2D-CGD-CBD	5.00	120.16	111.27
20	B	817	CLA	CHD-C4C-NC	5.00	132.08	124.20
20	A	811	CLA	C3D-CAD-CBD	-5.00	101.02	107.61
22	B	844	BCR	C16-C17-C18	-4.99	120.18	127.31
22	B	842	BCR	C16-C17-C18	-4.99	120.19	127.31
20	4	318	CLA	CHD-C4C-NC	4.99	132.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	206	CLA	CHD-C4C-NC	4.98	132.05	124.20
22	F	203	BCR	C16-C17-C18	-4.98	120.20	127.31
20	A	840	CLA	C3D-CAD-CBD	-4.98	101.05	107.61
20	B	838	CLA	CHD-C4C-NC	4.97	132.04	124.20
20	B	833	CLA	CHD-C4C-NC	4.97	132.04	124.20
20	2	304	CLA	C1D-CHD-C4C	-4.97	113.80	126.10
21	G	101	LMU	O3B-C3B-C4B	4.97	121.83	110.35
20	A	817	CLA	C3D-CAD-CBD	-4.96	101.07	107.61
20	1	211	CLA	C3B-C2B-C1B	-4.96	102.04	106.29
20	1	202	CLA	CMD-C2D-C3D	-4.96	115.40	124.68
20	B	805	CLA	C4A-NA-C1A	4.96	108.94	106.71
20	4	305	CLA	C4A-NA-C1A	4.95	108.93	106.71
20	1	210	CLA	CBA-CAA-C2A	4.95	128.47	113.86
20	4	304	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
20	1	202	CLA	CAA-C2A-C1A	4.95	128.19	111.97
22	I	103	BCR	C15-C14-C13	4.95	134.37	127.31
20	1	207	CLA	C4A-NA-C1A	4.94	108.93	106.71
20	A	835	CLA	CMD-C2D-C3D	-4.94	115.43	124.68
20	B	833	CLA	C3D-CAD-CBD	-4.94	101.10	107.61
20	B	840	CLA	C4A-NA-C1A	4.94	108.93	106.71
20	B	834	CLA	O2D-CGD-CBD	4.94	120.05	111.27
20	B	850	CLA	CHD-C4C-NC	4.94	131.99	124.20
20	4	306	CLA	O2A-CGA-O1A	-4.94	111.12	123.59
20	A	816	CLA	CHD-C4C-NC	4.94	131.99	124.20
20	I	102	CLA	CHD-C4C-NC	4.94	131.99	124.20
20	3	312	CLA	C4A-NA-C1A	4.94	108.93	106.71
20	A	801	CLA	CAC-C3C-C4C	4.94	131.22	124.81
20	B	811	CLA	CGD-CBD-CAD	-4.94	94.75	110.73
20	B	836	CLA	O2D-CGD-O1D	-4.94	114.19	123.84
20	1	207	CLA	CAA-C2A-C3A	4.93	126.29	112.78
20	B	821	CLA	C2A-C1A-CHA	-4.93	115.23	123.86
20	K	108	CLA	CHD-C4C-NC	4.93	131.97	124.20
20	2	307	CLA	CHC-C1C-NC	4.93	131.69	124.20
20	2	309	CLA	CHC-C1C-NC	4.93	131.51	124.23
20	A	808	CLA	CHD-C4C-NC	4.93	131.97	124.20
20	L	203	CLA	CHD-C4C-NC	4.93	131.97	124.20
20	R	108	CLA	C3D-CAD-CBD	-4.93	101.12	107.61
20	3	310	CLA	C2A-C1A-CHA	-4.92	114.24	122.63
20	H	103	CLA	C4A-NA-C1A	4.92	108.92	106.71
20	3	313	CLA	CBC-CAC-C3C	-4.92	98.87	112.43
20	K	101	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	B	825	CLA	CHD-C4C-NC	4.92	131.95	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	803	CLA	C3D-CAD-CBD	-4.92	101.13	107.61
20	A	802	CLA	C3D-C4D-ND	4.92	114.41	110.14
20	2	306	CLA	C3D-C2D-C1D	4.91	110.54	106.30
20	3	306	CLA	C4A-NA-C1A	4.91	108.92	106.71
21	H	105	LMU	O5'-C1'-C2'	-4.91	99.95	110.35
20	1	203	CLA	CMD-C2D-C3D	-4.91	115.49	124.68
20	B	824	CLA	CHD-C4C-NC	4.91	131.93	124.20
22	A	846	BCR	C11-C10-C9	-4.90	120.31	127.31
20	B	814	CLA	C4A-NA-C1A	4.90	108.91	106.71
20	2	306	CLA	CHD-C4C-NC	4.90	131.77	124.21
20	4	310	CLA	C3A-C4A-CHB	-4.90	117.92	123.91
20	1	207	CLA	C2A-C3A-C4A	-4.89	93.96	101.87
22	A	846	BCR	C16-C17-C18	-4.89	120.33	127.31
20	2	315	CLA	C1D-CHD-C4C	-4.89	114.00	126.10
22	L	210	BCR	C33-C5-C6	-4.89	119.04	124.53
20	K	102	CLA	CMB-C2B-C3B	4.89	133.82	124.68
20	B	831	CLA	CHD-C4C-C3C	-4.89	117.66	124.84
20	K	102	CLA	CHC-C1C-NC	4.88	131.61	124.20
20	1	214	CLA	C3A-C4A-CHB	-4.88	117.93	123.91
20	3	309	CLA	C3A-C4A-CHB	-4.88	117.93	123.91
20	B	821	CLA	O2D-CGD-O1D	-4.88	114.30	123.84
20	A	803	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
20	B	803	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
20	B	822	CLA	OBD-CAD-CBD	-4.87	118.93	125.89
20	B	838	CLA	CMD-C2D-C3D	-4.87	115.56	124.68
22	I	101	BCR	C28-C27-C26	-4.87	105.38	114.08
22	A	846	BCR	C15-C14-C13	-4.87	120.36	127.31
20	4	309	CLA	C3D-C4D-ND	4.87	114.37	110.14
20	B	803	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	B	801	LMU	O2'-C2'-C3'	4.87	121.60	110.35
20	A	826	CLA	C3D-CAD-CBD	-4.87	101.20	107.61
20	1	215	CLA	CHC-C1C-NC	4.86	131.58	124.20
20	3	303	CLA	CHC-C1C-NC	4.86	131.41	124.23
22	3	314	BCR	C33-C5-C6	-4.86	119.07	124.53
20	B	826	CLA	C3D-CAD-CBD	-4.86	101.21	107.61
20	A	815	CLA	CMA-C3A-C2A	-4.86	94.24	113.83
20	2	307	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
20	4	319	CLA	O2D-CGD-CBD	4.85	119.89	111.27
20	B	849	CLA	C1D-CHD-C4C	-4.85	116.16	122.56
20	2	310	CLA	C3A-C4A-CHB	-4.85	117.97	123.91
20	1	211	CLA	C1D-CHD-C4C	-4.85	114.11	126.10
20	A	817	CLA	CHD-C4C-C3C	-4.85	117.71	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	316	CLA	C1D-CHD-C4C	-4.84	114.12	126.10
20	3	318	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	A	812	CLA	CHD-C4C-NC	4.84	131.83	124.20
20	2	309	CLA	C1D-CHD-C4C	-4.84	114.12	126.10
20	B	818	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	4	303	CLA	C1B-C2B-C3B	-4.84	102.42	106.92
20	1	216	CLA	C2B-C1B-NB	4.84	114.35	110.11
20	J	101	CLA	O2D-CGD-CBD	4.84	119.86	111.27
20	B	811	CLA	C3D-CAD-CBD	-4.84	101.24	107.61
22	B	852	BCR	C16-C17-C18	-4.83	120.41	127.31
20	1	204	CLA	C4D-C3D-CAD	4.83	111.16	108.47
20	B	832	CLA	CHD-C4C-NC	4.83	131.81	124.20
21	N	101	LMU	O1'-C1'-C2'	4.83	115.84	108.30
20	B	814	CLA	CHD-C4C-NC	4.83	131.81	124.20
20	A	815	CLA	CAA-C2A-C3A	-4.83	99.56	112.78
20	1	212	CLA	C2D-C3D-C4D	-4.83	102.14	106.30
21	R	103	LMU	C1B-O1B-C4'	4.82	129.89	117.96
20	4	314	CLA	C1B-C2B-C3B	-4.81	102.44	106.92
20	2	304	CLA	CHD-C4C-NC	4.81	131.63	124.21
20	3	310	CLA	C3B-C2B-C1B	-4.81	102.17	106.29
20	A	831	CLA	CMD-C2D-C3D	-4.81	115.68	124.68
20	4	318	CLA	CMD-C2D-C3D	-4.81	115.68	124.68
20	3	305	CLA	C3A-C4A-CHB	-4.81	118.02	123.91
20	3	303	CLA	CHD-C4C-NC	4.80	131.62	124.21
20	B	806	CLA	CHD-C4C-NC	4.80	131.77	124.20
20	4	313	CLA	C2A-C1A-CHA	-4.80	114.45	122.63
22	A	847	BCR	C11-C10-C9	-4.80	120.46	127.31
20	3	319	CLA	C3B-C2B-C1B	-4.80	102.18	106.29
21	R	103	LMU	O1B-C4'-C3'	4.79	120.03	107.28
20	B	808	CLA	CHD-C4C-NC	4.79	131.75	124.20
20	4	318	CLA	O2D-CGD-CBD	4.79	119.78	111.27
20	L	207	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
20	B	816	CLA	CHD-C4C-NC	4.78	131.74	124.20
20	B	823	CLA	O2D-CGD-CBD	4.78	119.76	111.27
20	4	307	CLA	CHD-C4C-C3C	-4.78	117.82	124.84
21	2	318	LMU	C1B-O1B-C4'	-4.78	106.14	117.96
23	B	841	PQN	C2M-C2-C3	-4.77	116.61	124.40
20	4	309	CLA	C2A-C1A-CHA	-4.77	114.49	122.63
20	3	307	CLA	C4A-NA-C1A	4.77	108.85	106.71
21	B	801	LMU	C6B-C5B-C4B	-4.77	101.83	113.00
20	3	319	CLA	CHD-C4C-NC	4.77	131.57	124.21
20	B	804	CLA	CHD-C4C-NC	4.77	131.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	109	LMU	O5B-C5B-C4B	-4.77	101.04	109.69
20	F	206	CLA	C4-C3-C5	4.76	123.28	115.27
20	B	812	CLA	C1D-CHD-C4C	-4.76	116.28	122.56
20	3	319	CLA	C4A-NA-C1A	4.76	108.84	106.71
20	1	214	CLA	C1D-CHD-C4C	-4.75	114.33	126.10
20	A	841	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
22	3	314	BCR	C7-C8-C9	-4.75	119.06	126.23
20	3	304	CLA	CHD-C4C-C3C	-4.75	117.56	124.98
20	B	821	CLA	C1D-CHD-C4C	-4.75	116.29	122.56
20	3	302	CLA	C3D-CAD-CBD	-4.75	101.35	107.61
20	A	804	CLA	C1-O2A-CGA	4.74	128.89	116.44
20	A	826	CLA	C1-C2-C3	-4.74	117.84	126.04
20	H	101	CLA	C1-C2-C3	-4.74	117.84	126.04
20	4	307	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
20	B	818	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
20	B	811	CLA	O2D-CGD-CBD	4.74	119.69	111.27
21	B	847	LMU	O2B-C2B-C3B	-4.73	99.40	110.35
20	B	834	CLA	C4-C3-C5	4.73	121.39	115.98
20	4	302	CLA	C3D-CAD-CBD	-4.73	101.37	107.61
21	H	104	LMU	O3B-C3B-C4B	4.73	121.29	110.35
20	F	204	CLA	CHC-C1C-NC	4.73	131.38	124.20
20	A	852	CLA	CHD-C4C-NC	4.73	131.65	124.20
21	B	801	LMU	O5'-C5'-C6'	4.73	118.19	106.44
20	B	812	CLA	CMD-C2D-C3D	-4.73	115.84	124.68
20	B	837	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
20	1	205	CLA	CHC-C1C-NC	4.72	131.20	124.23
22	F	203	BCR	C34-C9-C8	4.72	125.51	118.08
20	A	811	CLA	CHD-C4C-NC	4.72	131.64	124.20
20	B	836	CLA	CHD-C4C-NC	4.71	131.63	124.20
20	A	831	CLA	O1D-CGD-CBD	-4.71	114.84	124.48
20	A	804	CLA	CHC-C1C-NC	4.71	131.35	124.20
21	K	105	LMU	O1B-C4'-C5'	4.71	122.35	109.45
21	L	204	LMU	O5B-C5B-C4B	-4.71	101.14	109.69
20	1	208	CLA	C4A-NA-C1A	4.70	108.82	106.71
20	A	801	CLA	CHC-C1C-NC	4.70	131.34	124.20
20	K	101	CLA	C3D-CAD-CBD	-4.70	101.41	107.61
20	K	102	CLA	CMA-C3A-C4A	-4.70	99.14	111.77
20	B	830	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
22	L	210	BCR	C7-C8-C9	-4.70	119.14	126.23
20	B	816	CLA	CHC-C1C-NC	4.69	131.32	124.20
20	B	830	CLA	CHD-C4C-NC	4.69	131.59	124.20
20	G	102	CLA	O1D-CGD-CBD	-4.69	114.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	201	LMU	C6B-C5B-C4B	-4.69	102.03	113.00
20	B	806	CLA	C6-C5-C3	-4.68	101.17	113.45
20	A	832	CLA	O2D-CGD-CBD	4.68	119.58	111.27
20	A	839	CLA	CMC-C2C-C1C	-4.68	117.91	125.04
20	1	212	CLA	C1D-CHD-C4C	-4.68	114.52	126.10
20	B	835	CLA	CHD-C4C-NC	4.68	131.57	124.20
20	A	826	CLA	CHD-C4C-NC	4.68	131.57	124.20
20	2	303	CLA	CHD-C4C-NC	4.68	131.57	124.20
21	E	101	LMU	O1'-C1'-C2'	-4.68	101.00	108.30
20	J	103	CLA	CHD-C4C-C3C	-4.67	117.97	124.84
20	K	103	CLA	CHD-C4C-NC	4.67	131.57	124.20
20	A	852	CLA	C1-C2-C3	4.67	134.13	126.04
20	A	828	CLA	CHD-C4C-NC	4.67	131.56	124.20
21	K	106	LMU	C4B-C3B-C2B	-4.67	102.67	110.82
20	H	103	CLA	C4-C3-C5	4.67	123.12	115.27
20	2	310	CLA	C3B-C2B-C1B	-4.67	102.29	106.29
20	3	319	CLA	C2D-C3D-C4D	-4.67	102.28	106.30
20	A	835	CLA	O2D-CGD-O1D	-4.67	114.72	123.84
20	4	305	CLA	C3D-CAD-CBD	-4.66	101.46	107.61
20	B	838	CLA	C1D-CHD-C4C	-4.66	116.40	122.56
20	J	101	CLA	C3D-CAD-CBD	-4.66	101.47	107.61
20	2	308	CLA	CHC-C1C-NC	4.66	131.28	124.20
20	L	208	CLA	CHD-C4C-NC	4.65	131.53	124.20
20	B	821	CLA	C3D-CAD-CBD	-4.65	101.48	107.61
22	L	210	BCR	C36-C18-C19	4.65	125.40	118.08
21	N	101	LMU	O5B-C5B-C4B	4.65	118.13	109.69
20	B	851	CLA	CHC-C1C-NC	4.64	131.25	124.20
20	3	303	CLA	C2D-C3D-C4D	-4.64	102.30	106.30
20	2	310	CLA	C1D-CHD-C4C	-4.64	114.61	126.10
20	K	103	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
21	2	318	LMU	O1'-C1'-C2'	4.64	115.55	108.30
20	B	806	CLA	CHB-C4A-NA	4.64	130.93	124.51
20	B	849	CLA	C3D-CAD-CBD	-4.64	101.50	107.61
20	2	304	CLA	CHC-C1C-NC	4.64	131.08	124.23
21	B	802	LMU	O3'-C3'-C2'	-4.64	99.63	110.35
20	1	209	CLA	CHD-C4C-NC	4.64	131.51	124.20
20	A	814	CLA	C3D-CAD-CBD	-4.63	101.50	107.61
20	3	316	CLA	C4A-NA-C1A	4.63	108.79	106.71
20	H	103	CLA	CHD-C4C-NC	4.63	131.50	124.20
20	K	102	CLA	C1-C2-C3	-4.63	119.26	126.75
20	4	312	CLA	CHC-C1C-NC	4.63	131.06	124.23
20	H	103	CLA	CMD-C2D-C3D	-4.62	116.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	813	CLA	C3D-CAD-CBD	-4.62	101.52	107.61
20	3	303	CLA	C1D-CHD-C4C	-4.62	114.67	126.10
22	3	314	BCR	C16-C15-C14	-4.62	114.01	123.47
20	1	201	CLA	CHD-C4C-NC	4.62	131.48	124.20
20	3	312	CLA	CHC-C1C-NC	4.62	131.05	124.23
20	2	315	CLA	C3A-C4A-CHB	-4.62	118.26	123.91
20	A	839	CLA	O2A-CGA-CBA	4.62	126.40	111.91
21	L	204	LMU	C1'-O5'-C5'	4.61	122.74	113.69
20	A	818	CLA	C3D-CAD-CBD	-4.61	101.53	107.61
20	A	828	CLA	C4A-NA-C1A	4.61	108.78	106.71
20	B	831	CLA	CHD-C4C-NC	4.61	131.47	124.20
20	A	811	CLA	C1-C2-C3	-4.61	118.07	126.04
20	B	828	CLA	C1D-CHD-C4C	-4.61	116.48	122.56
20	2	303	CLA	C3D-CAD-CBD	-4.61	101.54	107.61
20	A	831	CLA	CHC-C1C-NC	4.61	131.19	124.20
20	4	313	CLA	C1D-CHD-C4C	-4.61	114.70	126.10
21	3	322	LMU	O3B-C3B-C2B	-4.60	99.71	110.35
20	F	204	CLA	CAB-C3B-C4B	-4.60	121.39	128.46
20	1	212	CLA	CHC-C1C-NC	4.60	131.03	124.23
20	F	204	CLA	C4B-C3B-C2B	4.60	111.20	106.92
21	B	801	LMU	O1B-C4'-C3'	4.60	119.51	107.28
20	4	303	CLA	CHD-C4C-C3C	-4.60	117.80	124.98
20	A	802	CLA	C2A-C1A-CHA	-4.60	114.80	122.63
21	H	104	LMU	O4'-C4B-C5B	4.59	120.71	109.30
20	A	836	CLA	CHD-C4C-NC	4.59	131.44	124.20
20	A	838	CLA	O2D-CGD-CBD	4.59	119.43	111.27
20	L	201	CLA	CHD-C4C-NC	4.59	131.44	124.20
20	B	835	CLA	C3D-CAD-CBD	-4.59	101.56	107.61
20	A	835	CLA	C3D-CAD-CBD	-4.59	101.56	107.61
21	1	213	LMU	C1'-C2'-C3'	4.59	119.55	110.00
21	H	108	LMU	O5'-C5'-C6'	4.59	117.84	106.44
20	A	801	CLA	O2D-CGD-O1D	-4.58	114.87	123.84
21	H	104	LMU	O3B-C3B-C2B	4.58	120.94	110.35
20	1	216	CLA	C2A-C1A-CHA	-4.58	114.82	122.63
20	2	311	CLA	CAC-C3C-C4C	4.58	130.75	124.81
20	1	214	CLA	C3B-C2B-C1B	-4.58	102.37	106.29
22	B	844	BCR	C37-C22-C21	-4.58	116.51	122.92
20	A	827	CLA	C3D-CAD-CBD	-4.58	101.58	107.61
20	2	306	CLA	C4A-NA-C1A	4.58	108.76	106.71
20	A	804	CLA	O2A-CGA-CBA	4.57	126.26	111.91
20	1	206	CLA	O2D-CGD-CBD	4.57	119.39	111.27
20	H	109	CLA	O2D-CGD-CBD	4.57	119.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	202	CLA	CMB-C2B-C3B	4.57	133.22	124.68
20	B	809	CLA	C3D-CAD-CBD	-4.57	101.59	107.61
20	2	307	CLA	C3D-CAD-CBD	-4.56	101.59	107.61
22	B	844	BCR	C27-C26-C25	-4.56	116.11	122.73
20	A	815	CLA	CHC-C1C-NC	4.56	131.12	124.20
20	B	805	CLA	CHB-C4A-NA	4.56	130.82	124.51
20	B	823	CLA	C3D-CAD-CBD	-4.56	101.60	107.61
20	A	840	CLA	CMD-C2D-C3D	-4.56	116.15	124.68
21	K	109	LMU	C1B-C2B-C3B	4.56	119.49	110.00
20	B	824	CLA	CHD-C4C-C3C	-4.55	118.14	124.84
20	A	821	CLA	C4A-NA-C1A	4.55	108.75	106.71
20	B	817	CLA	C3D-CAD-CBD	-4.55	101.61	107.61
20	B	814	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
20	3	302	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
20	B	823	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
21	R	101	LMU	O1'-C1'-C2'	4.54	115.40	108.30
20	2	301	CLA	C2B-C3B-C4B	4.54	110.17	106.29
20	3	308	CLA	C4A-NA-C1A	4.54	108.75	106.71
20	B	821	CLA	CAA-C2A-C1A	-4.54	97.10	111.97
20	1	204	CLA	CHD-C4C-C3C	-4.54	118.17	124.84
20	B	834	CLA	CHD-C4C-NC	4.54	131.35	124.20
22	B	844	BCR	C34-C9-C10	-4.53	116.57	122.92
20	4	319	CLA	CHD-C4C-C3C	-4.53	118.17	124.84
20	4	312	CLA	C4A-NA-C1A	4.53	108.74	106.71
20	2	312	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
20	B	837	CLA	CHC-C1C-NC	4.53	131.08	124.20
21	A	849	LMU	C3B-C4B-C5B	-4.53	102.16	110.24
21	K	106	LMU	C3'-C4'-C5'	-4.53	100.55	110.93
20	2	308	CLA	O2D-CGD-O1D	-4.53	114.99	123.84
20	B	808	CLA	CHD-C4C-C3C	-4.53	118.19	124.84
20	A	834	CLA	CHD-C4C-NC	4.52	131.33	124.20
20	4	309	CLA	C2D-C3D-C4D	-4.52	102.40	106.30
20	3	312	CLA	CHD-C4C-NC	4.52	131.19	124.21
20	B	851	CLA	CHB-C4A-NA	4.52	130.77	124.51
20	B	835	CLA	CMD-C2D-C3D	-4.52	116.22	124.68
20	3	316	CLA	CHD-C4C-NC	4.52	131.18	124.21
20	3	301	CLA	CHD-C4C-NC	4.52	131.32	124.20
20	3	302	CLA	CAA-C2A-C1A	4.52	126.78	111.97
20	B	840	CLA	CAA-C2A-C3A	-4.51	105.57	116.10
20	3	319	CLA	CHC-C1C-NC	4.51	130.89	124.23
20	1	207	CLA	CHD-C4C-NC	4.51	131.30	124.20
20	2	302	CLA	CHD-C4C-C3C	-4.51	118.22	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	309	CLA	C3A-C4A-CHB	-4.50	118.39	123.91
20	B	851	CLA	CHD-C4C-NC	4.50	131.30	124.20
22	I	101	BCR	C37-C22-C23	-4.50	110.98	118.08
20	B	804	CLA	CMD-C2D-C3D	-4.50	116.25	124.68
20	A	820	CLA	CHD-C4C-NC	4.50	131.29	124.20
20	A	827	CLA	CHD-C4C-NC	4.50	131.29	124.20
20	A	812	CLA	O2D-CGD-CBD	4.50	119.26	111.27
20	B	813	CLA	CHD-C4C-C3C	-4.50	118.23	124.84
20	1	211	CLA	C4A-NA-C1A	4.49	108.73	106.71
20	3	316	CLA	C3D-C2D-C1D	4.49	110.17	106.30
21	2	320	LMU	O1'-C1'-C2'	4.49	115.31	108.30
20	A	837	CLA	CAA-CBA-CGA	-4.49	100.14	113.25
20	A	817	CLA	CHD-C4C-NC	4.49	131.27	124.20
21	4	322	LMU	O1'-C1'-C2'	4.49	115.31	108.30
22	B	844	BCR	C30-C25-C26	-4.49	116.30	122.61
20	J	103	CLA	C3D-CAD-CBD	-4.48	101.70	107.61
20	2	311	CLA	C3D-CAD-CBD	-4.48	101.70	107.61
22	A	843	BCR	C24-C23-C22	-4.48	119.46	126.23
22	B	852	BCR	C33-C5-C4	4.48	122.22	113.62
22	F	203	BCR	C8-C7-C6	-4.48	114.63	127.20
22	A	847	BCR	C33-C5-C6	-4.48	119.50	124.53
20	B	836	CLA	CHC-C1C-NC	4.48	130.99	124.20
20	A	804	CLA	OBD-CAD-C3D	-4.47	120.55	127.98
20	A	836	CLA	O2D-CGD-O1D	-4.47	115.09	123.84
20	B	839	CLA	O2A-CGA-CBA	4.47	125.94	111.91
20	4	313	CLA	C3A-C4A-CHB	-4.47	118.44	123.91
20	A	841	CLA	C1-C2-C3	-4.47	118.31	126.04
20	F	204	CLA	C4A-NA-C1A	4.47	108.72	106.71
20	2	310	CLA	CHD-C4C-NC	4.47	131.10	124.21
20	L	207	CLA	C3D-CAD-CBD	-4.47	101.72	107.61
20	1	212	CLA	CHD-C4C-NC	4.47	131.10	124.21
20	4	312	CLA	C3B-C2B-C1B	-4.47	102.47	106.29
20	K	101	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
20	A	851	CLA	C3D-CAD-CBD	-4.46	101.73	107.61
21	K	105	LMU	O1'-C1'-C2'	4.46	115.27	108.30
20	3	311	CLA	C4-C3-C5	4.46	122.78	115.27
20	1	207	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
20	B	827	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
20	2	315	CLA	CHD-C4C-NC	4.46	131.08	124.21
20	1	201	CLA	CHC-C1C-NC	4.45	130.96	124.20
20	A	831	CLA	C4-C3-C5	4.45	122.76	115.27
20	1	209	CLA	CHD-C4C-C3C	-4.45	118.02	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	838	CLA	C3D-CAD-CBD	-4.45	101.75	107.61
20	A	806	CLA	CHD-C4C-NC	4.45	131.22	124.20
20	A	825	CLA	C3D-CAD-CBD	-4.45	101.75	107.61
20	B	804	CLA	CHC-C1C-NC	4.44	130.94	124.20
20	1	201	CLA	CBC-CAC-C3C	-4.44	100.18	112.43
20	L	202	CLA	CHD-C4C-NC	4.44	131.20	124.20
20	B	809	CLA	CHD-C4C-NC	4.44	131.20	124.20
20	2	301	CLA	C2A-C3A-C4A	-4.44	97.21	104.18
21	K	105	LMU	C1'-O5'-C5'	-4.44	104.97	113.69
20	A	809	CLA	O2D-CGD-O1D	-4.44	115.16	123.84
20	B	804	CLA	C3D-CAD-CBD	-4.44	101.76	107.61
20	K	103	CLA	C3D-CAD-CBD	-4.44	101.76	107.61
20	A	832	CLA	C3D-CAD-CBD	-4.44	101.76	107.61
20	4	316	CLA	C4A-NA-C1A	4.44	108.70	106.71
20	4	314	CLA	CAC-C3C-C4C	4.44	131.80	125.04
22	A	845	BCR	C38-C26-C25	-4.44	119.54	124.53
20	R	107	CLA	O2A-CGA-CBA	4.44	125.83	111.91
20	F	205	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
20	3	308	CLA	CHC-C1C-NC	4.43	130.93	124.20
20	J	101	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
20	A	830	CLA	CHD-C4C-NC	4.43	131.18	124.20
20	A	807	CLA	CAA-C2A-C3A	-4.43	100.66	112.78
22	B	844	BCR	C8-C9-C10	4.43	125.73	118.94
22	J	102	BCR	C24-C23-C22	-4.43	119.55	126.23
22	I	103	BCR	C7-C6-C5	4.43	132.18	121.46
20	1	201	CLA	CED-O2D-CGD	4.42	125.94	115.94
20	4	302	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
20	2	309	CLA	C2A-C1A-CHA	-4.42	115.09	122.63
22	A	844	BCR	C7-C8-C9	-4.42	119.55	126.23
20	B	851	CLA	CGD-CBD-CAD	4.42	125.06	110.73
20	I	102	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
20	4	315	CLA	C1D-CHD-C4C	-4.42	115.17	126.10
20	B	820	CLA	C3D-CAD-CBD	-4.42	101.79	107.61
21	1	213	LMU	O1B-C4'-C5'	4.42	121.55	109.45
20	B	827	CLA	CHD-C4C-NC	4.42	131.16	124.20
21	K	105	LMU	C4B-C3B-C2B	-4.41	103.12	110.82
20	3	316	CLA	C2A-C1A-CHA	-4.41	115.11	122.63
20	B	812	CLA	CHD-C4C-NC	4.41	131.15	124.20
22	B	845	BCR	C33-C5-C6	-4.41	119.58	124.53
20	K	101	CLA	CHC-C1C-NC	4.41	130.89	124.20
20	1	204	CLA	O2D-CGD-O1D	-4.41	115.22	123.84
20	3	320	CLA	C3A-C4A-CHB	-4.41	118.51	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	301	CLA	CHD-C4C-C3C	-4.41	118.09	124.98
20	A	815	CLA	CHB-C4A-NA	4.41	130.61	124.51
21	C	101	LMU	O1'-C1'-C2'	4.41	115.18	108.30
20	2	322	CLA	C3D-CAD-CBD	-4.41	101.81	107.61
20	B	830	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
20	A	852	CLA	C3D-CAD-CBD	-4.40	101.81	107.61
20	4	307	CLA	C3C-C4C-NC	-4.40	105.63	110.57
20	A	808	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	A	801	CLA	C4A-NA-C1A	4.40	108.68	106.71
21	A	856	LMU	C3'-C4'-C5'	-4.40	100.84	110.93
20	R	107	CLA	CMD-C2D-C3D	-4.40	116.45	124.68
20	A	818	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	B	825	CLA	O1D-CGD-CBD	-4.40	115.49	124.48
21	1	213	LMU	C2'-C3'-C4'	4.39	119.71	109.68
22	L	210	BCR	C38-C26-C27	4.39	122.06	113.62
21	B	847	LMU	C3B-C4B-C5B	-4.39	102.40	110.24
20	1	203	CLA	CGD-CBD-CAD	-4.39	96.50	110.73
22	J	102	BCR	C7-C8-C9	-4.39	119.60	126.23
20	A	822	CLA	CHD-C4C-NC	4.39	131.12	124.20
20	4	310	CLA	CHD-C4C-NC	4.39	130.98	124.21
20	B	827	CLA	CMD-C2D-C3D	-4.39	116.47	124.68
20	2	311	CLA	O2D-CGD-O1D	-4.39	115.26	123.84
20	A	810	CLA	CHD-C4C-NC	4.38	131.11	124.20
20	1	204	CLA	CHD-C4C-NC	4.38	131.11	124.20
20	H	103	CLA	CHC-C1C-NC	4.38	130.85	124.20
20	B	840	CLA	CHD-C4C-NC	4.38	131.11	124.20
22	A	844	BCR	C24-C23-C22	-4.38	119.61	126.23
20	B	809	CLA	CMD-C2D-C3D	-4.38	116.48	124.68
20	B	810	CLA	C3D-CAD-CBD	-4.38	101.84	107.61
20	H	109	CLA	CHD-C4C-NC	4.38	131.10	124.20
20	B	836	CLA	C3D-CAD-CBD	-4.38	101.84	107.61
20	J	101	CLA	CHC-C1C-NC	4.38	130.84	124.20
22	B	846	BCR	C7-C8-C9	-4.38	119.62	126.23
20	A	851	CLA	CAA-C2A-C1A	4.38	126.32	111.97
20	L	201	CLA	C3D-CAD-CBD	-4.37	101.84	107.61
20	A	837	CLA	C4A-NA-C1A	4.37	108.67	106.71
20	B	850	CLA	CHB-C4A-NA	4.37	130.56	124.51
20	B	826	CLA	CHD-C4C-NC	4.37	131.09	124.20
20	4	302	CLA	CHC-C1C-NC	4.37	130.83	124.20
20	B	823	CLA	CHC-C1C-NC	4.37	130.83	124.20
20	A	834	CLA	CMD-C2D-C3D	-4.36	116.51	124.68
20	B	850	CLA	CHD-C4C-C3C	-4.36	118.42	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	203	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
20	B	807	CLA	CHC-C1C-NC	4.36	130.82	124.20
22	A	847	BCR	C38-C26-C25	-4.36	119.63	124.53
20	B	832	CLA	C4A-NA-C1A	4.36	108.67	106.71
20	3	305	CLA	C1D-CHD-C4C	-4.36	115.32	126.10
20	4	316	CLA	CGD-CBD-CAD	-4.36	96.63	110.73
20	I	102	CLA	C4A-NA-C1A	4.36	108.66	106.71
20	B	813	CLA	CHD-C4C-NC	4.36	131.06	124.20
20	A	811	CLA	C4A-NA-C1A	4.35	108.66	106.71
20	1	203	CLA	CHD-C4C-NC	4.35	131.05	124.20
20	3	310	CLA	C3D-C2D-C1D	4.34	110.04	106.30
20	A	819	CLA	C3D-CAD-CBD	-4.34	101.89	107.61
20	1	216	CLA	C4A-NA-C1A	4.34	108.66	106.71
22	A	846	BCR	C38-C26-C25	-4.33	119.66	124.53
20	A	820	CLA	C3D-CAD-CBD	-4.33	101.90	107.61
21	L	211	LMU	C3B-C4B-C5B	4.33	117.97	110.24
20	1	211	CLA	CHD-C4C-NC	4.33	130.89	124.21
22	B	843	BCR	C24-C23-C22	-4.33	119.70	126.23
22	B	845	BCR	C38-C26-C25	-4.33	119.67	124.53
20	L	208	CLA	C3D-CAD-CBD	-4.33	101.91	107.61
20	3	309	CLA	C1D-CHD-C4C	-4.33	115.39	126.10
20	H	101	CLA	CMA-C3A-C4A	-4.33	100.15	111.77
20	4	312	CLA	C2A-C1A-CHA	-4.32	115.26	122.63
20	A	802	CLA	C3C-C4C-CHD	-4.32	115.75	125.22
22	L	210	BCR	C3-C4-C5	-4.32	106.36	114.08
20	3	301	CLA	CBD-CHA-C1A	4.32	134.35	127.43
21	R	104	LMU	C6B-C5B-C4B	-4.32	102.89	113.00
20	3	309	CLA	CHC-C1C-NC	4.32	130.61	124.23
20	A	809	CLA	CHC-C1C-C2C	-4.32	114.77	126.72
20	1	203	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
20	K	102	CLA	O2D-CGD-O1D	-4.32	115.40	123.84
20	A	820	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	A	845	BCR	C33-C5-C6	-4.31	119.69	124.53
20	A	829	CLA	CHC-C1C-NC	4.31	130.75	124.20
20	A	841	CLA	CHD-C4C-NC	4.31	130.99	124.20
20	A	825	CLA	CHC-C1C-NC	4.30	130.73	124.20
20	A	808	CLA	O2D-CGD-O1D	-4.30	115.43	123.84
22	B	852	BCR	C37-C22-C21	-4.30	116.90	122.92
22	I	101	BCR	C30-C25-C26	-4.30	116.56	122.61
20	A	801	CLA	O2A-CGA-CBA	4.30	125.39	111.91
20	B	831	CLA	O1D-CGD-CBD	-4.29	115.70	124.48
20	3	311	CLA	CHC-C1C-NC	4.29	130.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	201	CLA	C1B-CHB-C4A	-4.29	121.61	130.12
20	A	814	CLA	CHC-C1C-NC	4.29	130.71	124.20
20	B	834	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
20	A	808	CLA	C4A-NA-C1A	4.29	108.63	106.71
20	A	809	CLA	C3D-CAD-CBD	-4.29	101.96	107.61
21	H	106	LMU	C4B-C3B-C2B	-4.29	103.34	110.82
20	1	216	CLA	C1D-CHD-C4C	-4.29	115.49	126.10
20	3	309	CLA	C2A-C1A-CHA	-4.28	115.33	122.63
21	H	106	LMU	O2B-C2B-C3B	-4.28	100.47	110.35
21	A	854	LMU	O1'-C1'-C2'	4.27	114.98	108.30
20	2	301	CLA	C1D-CHD-C4C	-4.27	115.53	126.10
20	A	805	CLA	C4A-NA-C1A	4.27	108.63	106.71
20	B	827	CLA	C3D-CAD-CBD	-4.27	101.98	107.61
20	2	303	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
20	4	305	CLA	C1D-CHD-C4C	-4.27	116.92	122.56
20	A	818	CLA	CHC-C1C-NC	4.27	130.68	124.20
22	A	843	BCR	C7-C8-C9	-4.27	119.79	126.23
21	H	106	LMU	C2'-C3'-C4'	4.27	119.42	109.68
20	A	824	CLA	C3D-CAD-CBD	-4.26	101.99	107.61
20	2	307	CLA	C4A-NA-C1A	4.26	108.62	106.71
20	4	310	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
20	1	214	CLA	CHD-C4C-NC	4.26	130.78	124.21
20	B	820	CLA	CHD-C4C-NC	4.26	130.91	124.20
20	A	807	CLA	CAA-C2A-C1A	-4.26	98.03	111.97
20	F	204	CLA	CMB-C2B-C3B	4.26	133.02	124.69
20	A	804	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
21	H	106	LMU	O5B-C5B-C4B	-4.25	101.97	109.69
20	B	849	CLA	CHC-C1C-NC	4.25	130.66	124.20
20	B	803	CLA	CMB-C2B-C3B	4.25	132.64	124.68
22	B	843	BCR	C7-C8-C9	-4.25	119.81	126.23
21	N	101	LMU	C4B-C3B-C2B	-4.25	103.41	110.82
20	A	808	CLA	CAA-C2A-C1A	-4.25	98.06	111.97
20	A	810	CLA	CHC-C1C-NC	4.25	130.64	124.20
21	H	104	LMU	O4'-C4B-C3B	4.25	120.16	110.35
20	B	828	CLA	C1-O2A-CGA	4.24	127.58	116.44
22	B	846	BCR	C24-C23-C22	-4.24	119.82	126.23
20	A	821	CLA	CHC-C1C-NC	4.24	130.64	124.20
20	B	851	CLA	CHD-C4C-C3C	-4.24	118.60	124.84
20	2	316	CLA	CHD-C4C-NC	4.24	130.88	124.20
20	B	820	CLA	CHC-C1C-NC	4.24	130.63	124.20
21	1	220	LMU	C1B-C2B-C3B	4.23	118.81	110.00
20	A	827	CLA	CHC-C1C-NC	4.23	130.63	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	803	CLA	O2D-CGD-O1D	-4.23	115.56	123.84
20	4	305	CLA	CAC-C3C-C4C	4.23	130.30	124.81
20	B	815	CLA	CHC-C1C-NC	4.23	130.62	124.20
20	K	108	CLA	C3D-CAD-CBD	-4.23	102.04	107.61
20	4	308	CLA	CHD-C4C-C3C	-4.22	118.38	124.98
22	A	845	BCR	C7-C8-C9	-4.22	119.86	126.23
20	B	807	CLA	C1-C2-C3	-4.22	118.75	126.04
20	A	813	CLA	CHD-C4C-C3C	-4.22	118.64	124.84
20	3	310	CLA	CHD-C4C-NC	4.21	130.71	124.21
22	B	845	BCR	C7-C8-C9	-4.21	119.87	126.23
20	4	314	CLA	CBD-CHA-C1A	4.21	134.17	127.43
20	B	805	CLA	CMD-C2D-C3D	-4.21	116.81	124.68
20	4	311	CLA	C4A-NA-C1A	4.21	108.60	106.71
20	2	304	CLA	C4A-NA-C1A	4.21	108.60	106.71
21	1	213	LMU	C1B-O5B-C5B	-4.21	105.43	113.69
20	1	215	CLA	C6-C5-C3	-4.21	102.43	113.45
20	R	107	CLA	CHD-C4C-NC	4.20	130.83	124.20
21	F	201	LMU	C4B-C3B-C2B	-4.20	103.48	110.82
21	R	105	LMU	O5B-C1B-C2B	4.20	119.25	110.35
21	1	218	LMU	C4B-C3B-C2B	-4.20	103.48	110.82
20	4	307	CLA	O2A-CGA-CBA	4.20	125.10	111.91
20	R	107	CLA	O2D-CGD-CBD	4.20	118.73	111.27
20	3	302	CLA	CHD-C4C-NC	4.20	130.82	124.20
20	L	203	CLA	C3D-CAD-CBD	-4.20	102.07	107.61
20	A	806	CLA	C3D-CAD-CBD	-4.20	102.08	107.61
20	H	101	CLA	CMD-C2D-C3D	-4.20	116.83	124.68
20	1	207	CLA	CMD-C2D-C3D	-4.20	116.83	124.68
22	A	846	BCR	C33-C5-C6	-4.19	119.82	124.53
22	3	314	BCR	C38-C26-C25	-4.19	119.82	124.53
20	B	828	CLA	C3D-CAD-CBD	-4.19	102.09	107.61
20	A	824	CLA	CHC-C1C-NC	4.19	130.56	124.20
21	H	108	LMU	O1B-C4'-C3'	4.19	118.43	107.28
20	K	102	CLA	CHD-C4C-NC	4.19	130.80	124.20
21	A	854	LMU	C1-O1'-C1'	-4.19	106.89	113.84
20	A	821	CLA	CAA-C2A-C1A	4.19	121.41	112.14
20	B	825	CLA	O2A-CGA-CBA	4.19	125.05	111.91
23	A	842	PQN	C14-C13-C15	4.19	122.31	115.27
20	K	108	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
20	3	309	CLA	CHD-C4C-NC	4.19	130.67	124.21
20	A	813	CLA	C1-C2-C3	-4.19	118.80	126.04
21	E	101	LMU	O3B-C3B-C2B	4.18	120.02	110.35
25	B	848	LMG	O7-C10-C11	4.18	120.51	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	103	CLA	CHC-C1C-NC	4.18	130.55	124.20
20	A	824	CLA	CHD-C4C-C3C	-4.18	118.70	124.84
22	B	842	BCR	C33-C5-C6	-4.18	119.84	124.53
20	B	803	CLA	C3D-CAD-CBD	-4.18	102.11	107.61
20	L	209	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
21	1	219	LMU	O1B-C4'-C5'	-4.17	98.02	109.45
20	F	206	CLA	CHD-C4C-NC	4.17	130.78	124.20
20	2	303	CLA	CMD-C2D-C3D	-4.16	116.89	124.68
20	A	832	CLA	CHD-C4C-NC	4.16	130.76	124.20
20	B	839	CLA	CHD-C4C-C3C	-4.16	118.72	124.84
21	L	204	LMU	C1B-O5B-C5B	-4.16	105.52	113.69
20	B	840	CLA	CMA-C3A-C2A	-4.16	106.39	116.10
20	4	315	CLA	C2B-C1B-NB	4.16	113.75	110.11
20	B	827	CLA	C4A-NA-C1A	4.15	108.57	106.71
21	B	802	LMU	O2'-C2'-C3'	-4.15	100.75	110.35
20	B	822	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
20	L	208	CLA	CHB-C4A-NA	4.15	130.25	124.51
22	A	846	BCR	C24-C23-C22	-4.15	119.96	126.23
22	I	101	BCR	C38-C26-C27	4.15	121.59	113.62
20	4	314	CLA	C4A-NA-C1A	4.15	108.57	106.71
20	A	823	CLA	C4-C3-C5	4.15	122.25	115.27
20	1	211	CLA	CHC-C1C-NC	4.15	130.35	124.23
20	F	205	CLA	CHC-C1C-NC	4.15	130.49	124.20
20	A	831	CLA	CAC-C3C-C4C	4.14	130.19	124.81
21	4	321	LMU	C2'-C3'-C4'	4.14	119.14	109.68
20	B	826	CLA	O2D-CGD-O1D	-4.14	115.74	123.84
20	4	304	CLA	C1-O2A-CGA	-4.14	105.58	116.44
21	2	318	LMU	C6B-C5B-C4B	4.14	122.70	113.00
20	2	316	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
20	2	305	CLA	O2D-CGD-CBD	4.14	118.62	111.27
20	F	205	CLA	C3D-CAD-CBD	-4.14	102.16	107.61
22	3	314	BCR	C11-C12-C13	-4.14	114.80	126.42
20	L	208	CLA	CHC-C1C-NC	4.14	130.48	124.20
20	3	316	CLA	C2D-C3D-C4D	-4.14	102.74	106.30
20	A	811	CLA	C11-C12-C13	-4.13	102.56	115.92
20	B	804	CLA	CHD-C4C-C3C	-4.13	118.76	124.84
20	4	304	CLA	C11-C10-C8	-4.13	102.56	115.92
20	G	102	CLA	C4A-NA-C1A	4.13	108.56	106.71
20	2	302	CLA	C3D-CAD-CBD	-4.13	102.17	107.61
20	4	305	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
20	4	319	CLA	C3D-CAD-CBD	-4.13	102.17	107.61
21	H	106	LMU	O1'-C1'-C2'	-4.13	101.86	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	833	CLA	C3D-CAD-CBD	-4.12	102.18	107.61
20	3	310	CLA	C3A-C4A-CHB	-4.12	118.86	123.91
20	A	814	CLA	CHD-C4C-NC	4.12	130.70	124.20
22	B	845	BCR	C24-C23-C22	-4.12	120.01	126.23
20	F	204	CLA	CMD-C2D-C3D	-4.12	116.97	124.68
21	B	802	LMU	O1'-C1'-C2'	4.12	114.73	108.30
20	B	810	CLA	O2D-CGD-CBD	4.12	118.58	111.27
20	A	821	CLA	CHD-C4C-NC	4.12	130.69	124.20
20	1	202	CLA	CHD-C4C-NC	4.12	130.69	124.20
20	A	839	CLA	C6-C5-C3	-4.11	102.67	113.45
20	2	315	CLA	CHC-C1C-NC	4.11	130.30	124.23
22	B	842	BCR	C7-C8-C9	-4.11	120.02	126.23
21	N	101	LMU	C2'-C3'-C4'	-4.11	100.30	109.68
20	3	301	CLA	C4A-NA-C1A	4.11	108.55	106.71
22	A	844	BCR	C38-C26-C25	-4.11	119.92	124.53
22	A	847	BCR	C24-C23-C22	-4.11	120.03	126.23
20	2	305	CLA	CHD-C4C-NC	4.11	130.67	124.20
20	A	839	CLA	CHC-C1C-C2C	-4.11	115.36	126.72
20	A	804	CLA	CMD-C2D-C3D	-4.10	117.00	124.68
21	B	801	LMU	C2'-C3'-C4'	-4.10	100.31	109.68
22	F	202	BCR	C7-C8-C9	-4.10	120.04	126.23
20	K	108	CLA	CHC-C1C-NC	4.10	130.43	124.20
20	A	816	CLA	O2D-CGD-CBD	4.10	118.55	111.27
20	1	211	CLA	C2A-C1A-CHA	-4.10	115.64	122.63
20	A	811	CLA	CAA-C2A-C3A	-4.10	101.56	112.78
20	B	829	CLA	O2A-C1-C2	4.10	119.40	108.64
20	A	819	CLA	CHD-C4C-NC	4.10	130.66	124.20
20	2	322	CLA	CAC-C3C-C4C	4.09	130.12	124.81
21	2	320	LMU	O1B-C4'-C5'	4.09	120.66	109.45
20	A	806	CLA	CHC-C1C-NC	4.09	130.41	124.20
20	B	825	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
22	B	843	BCR	C33-C5-C6	-4.09	119.94	124.53
21	B	801	LMU	O5B-C5B-C4B	4.09	117.12	109.69
20	A	806	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
21	L	205	LMU	O5'-C1'-C2'	-4.09	101.70	110.35
20	B	835	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
20	B	838	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
20	B	850	CLA	CAC-C3C-C4C	4.08	130.11	124.81
20	A	840	CLA	CHD-C4C-NC	4.08	130.64	124.20
20	4	308	CLA	CHC-C1C-NC	4.08	130.40	124.20
21	E	101	LMU	O1B-C1B-C2B	4.08	118.67	108.10
20	A	837	CLA	CHD-C4C-C3C	-4.08	118.84	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	805	CLA	C3D-CAD-CBD	-4.08	102.24	107.61
20	A	825	CLA	CHD-C4C-C3C	-4.08	118.85	124.84
20	A	810	CLA	CMD-C2D-C3D	-4.07	117.05	124.68
20	B	834	CLA	C3D-CAD-CBD	-4.07	102.24	107.61
20	H	101	CLA	O2A-CGA-CBA	4.07	124.68	111.91
20	4	319	CLA	CHC-C1C-NC	4.07	130.38	124.20
20	2	309	CLA	C2D-C3D-C4D	-4.07	102.80	106.30
20	4	314	CLA	CHD-C4C-NC	4.07	130.61	124.20
20	A	802	CLA	C2D-C3D-C4D	-4.07	102.80	106.30
20	2	302	CLA	CHC-C1C-NC	4.07	130.37	124.20
21	1	213	LMU	O3'-C3'-C4'	-4.07	99.17	109.94
22	B	846	BCR	C33-C5-C6	-4.07	119.96	124.53
20	4	318	CLA	C4A-NA-C1A	4.06	108.53	106.71
21	A	855	LMU	O3'-C3'-C2'	-4.06	100.95	110.35
20	2	312	CLA	CHD-C4C-NC	4.06	130.60	124.20
20	3	303	CLA	C3A-C4A-CHB	-4.06	118.94	123.91
20	2	304	CLA	C3D-C2D-C1D	4.06	109.80	106.30
20	1	201	CLA	CGD-CBD-CAD	-4.05	97.60	110.73
21	F	201	LMU	O3B-C3B-C4B	-4.05	100.98	110.35
20	B	810	CLA	CHD-C4C-NC	4.05	130.59	124.20
20	4	313	CLA	C3D-C2D-C1D	4.05	109.79	106.30
20	1	202	CLA	O2A-CGA-O1A	-4.05	113.37	123.59
20	A	819	CLA	CHC-C1C-NC	4.05	130.34	124.20
20	A	812	CLA	CHC-C1C-NC	4.05	130.34	124.20
20	A	823	CLA	OBD-CAD-CBD	-4.04	120.12	125.89
20	F	206	CLA	O2D-CGD-O1D	-4.04	115.93	123.84
20	1	205	CLA	C4A-NA-C1A	4.04	108.52	106.71
22	A	844	BCR	C33-C5-C6	-4.04	119.99	124.53
20	2	309	CLA	C3D-C4D-ND	4.04	113.65	110.14
21	B	847	LMU	O5B-C5B-C6B	4.04	116.48	106.44
20	A	841	CLA	C3D-CAD-CBD	-4.04	102.29	107.61
21	K	105	LMU	C1B-O1B-C4'	-4.04	107.98	117.96
20	B	828	CLA	O2D-CGD-CBD	4.03	118.44	111.27
20	3	306	CLA	C2A-C1A-CHA	-4.03	115.76	122.63
20	2	308	CLA	C6-C5-C3	-4.03	102.88	113.45
20	A	812	CLA	CHD-C4C-C3C	-4.03	118.91	124.84
22	I	101	BCR	C24-C25-C26	-4.03	111.70	121.46
22	A	846	BCR	C7-C8-C9	-4.03	120.14	126.23
21	K	106	LMU	C3B-C4B-C5B	-4.03	103.05	110.24
20	A	804	CLA	C3D-CAD-CBD	-4.03	102.30	107.61
20	4	306	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
20	B	814	CLA	CHC-C1C-NC	4.03	130.31	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	812	CLA	C3D-CAD-CBD	-4.03	102.30	107.61
20	2	316	CLA	CHC-C1C-NC	4.02	130.31	124.20
20	B	809	CLA	C1B-C2B-C3B	-4.02	103.18	106.92
20	2	304	CLA	C2A-C1A-CHA	-4.02	115.77	122.63
20	3	316	CLA	C3B-C2B-C1B	-4.02	102.85	106.29
20	4	309	CLA	C3C-C4C-CHD	-4.02	116.41	125.22
20	A	850	CLA	CED-O2D-CGD	4.02	125.03	115.94
20	3	307	CLA	C2A-C1A-CHA	-4.02	115.78	122.63
22	B	842	BCR	C38-C26-C25	-4.02	120.01	124.53
20	A	830	CLA	CHC-C1C-NC	4.02	130.30	124.20
20	H	102	CLA	C4-C3-C5	4.02	122.03	115.27
20	A	815	CLA	O2A-CGA-CBA	4.01	124.50	111.91
20	1	208	CLA	CHC-C1C-NC	4.01	130.16	124.23
22	F	202	BCR	C33-C5-C6	-4.01	120.02	124.53
20	L	203	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
20	1	210	CLA	CAA-C2A-C1A	-4.01	98.83	111.97
21	H	104	LMU	O5B-C5B-C6B	4.01	116.41	106.44
20	B	813	CLA	C3D-CAD-CBD	-4.01	102.33	107.61
20	A	830	CLA	O2D-CGD-CBD	4.01	118.39	111.27
20	H	102	CLA	CHC-C1C-NC	4.01	130.28	124.20
20	2	315	CLA	C2A-C1A-CHA	-4.01	115.80	122.63
21	F	201	LMU	C3'-C4'-C5'	-4.01	101.74	110.93
21	A	855	LMU	C2'-C3'-C4'	4.01	118.83	109.68
20	2	322	CLA	CHD-C4C-NC	4.01	130.51	124.20
20	A	838	CLA	C4A-NA-C1A	4.00	108.50	106.71
21	B	802	LMU	O1B-C1B-C2B	4.00	118.47	108.10
20	3	317	CLA	CHD-C4C-NC	4.00	130.51	124.20
22	I	103	BCR	C30-C25-C24	4.00	127.09	115.78
20	A	805	CLA	C3D-CAD-CBD	-4.00	102.34	107.61
20	K	102	CLA	O2A-CGA-CBA	4.00	124.45	111.91
20	L	203	CLA	OBD-CAD-CBD	-4.00	120.19	125.89
20	1	208	CLA	CHD-C4C-NC	3.99	130.37	124.21
20	A	832	CLA	C1-C2-C3	-3.99	120.29	126.75
20	A	840	CLA	CHC-C1C-NC	3.99	130.26	124.20
20	1	201	CLA	C3D-CAD-CBD	-3.99	102.35	107.61
20	A	852	CLA	CMD-C2D-C3D	-3.99	117.21	124.68
20	2	306	CLA	C1D-CHD-C4C	-3.99	116.23	126.10
20	4	302	CLA	C4A-NA-C1A	3.99	108.50	106.71
20	H	103	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
21	E	101	LMU	C1B-O1B-C4'	-3.99	108.09	117.96
20	A	851	CLA	CHC-C1C-NC	3.99	130.25	124.20
20	B	850	CLA	O2D-CGD-O1D	-3.99	116.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	812	CLA	O2D-CGD-CBD	3.98	118.35	111.27
20	B	832	CLA	O2D-CGD-CBD	3.98	118.35	111.27
20	4	315	CLA	C3A-C4A-CHB	-3.98	119.03	123.91
20	A	808	CLA	C3D-CAD-CBD	-3.98	102.36	107.61
20	1	216	CLA	CHD-C4C-NC	3.98	130.35	124.21
20	B	816	CLA	C3D-CAD-CBD	-3.98	102.36	107.61
20	A	834	CLA	C3D-CAD-CBD	-3.98	102.37	107.61
20	2	303	CLA	CHC-C1C-NC	3.98	130.24	124.20
20	2	305	CLA	CHC-C1C-NC	3.98	130.24	124.20
20	4	304	CLA	C1-C2-C3	-3.98	119.17	126.04
22	J	102	BCR	C38-C26-C25	-3.97	120.06	124.53
20	A	805	CLA	CHD-C4C-C3C	-3.97	119.00	124.84
20	2	303	CLA	C1-O2A-CGA	3.97	126.86	116.44
20	2	303	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
20	B	815	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
20	B	824	CLA	CHC-C1C-NC	3.97	130.22	124.20
21	4	317	LMU	C1B-O5B-C5B	3.97	121.47	113.69
20	B	811	CLA	CAA-CBA-CGA	-3.97	101.66	113.25
20	B	803	CLA	CHC-C1C-NC	3.97	130.22	124.20
20	1	214	CLA	C2D-C3D-C4D	-3.97	102.89	106.30
20	2	311	CLA	C4A-NA-C1A	3.96	108.49	106.71
20	3	318	CLA	CHD-C4C-NC	3.96	130.44	124.20
20	A	803	CLA	CHC-C1C-NC	3.96	130.21	124.20
21	B	801	LMU	C1B-O5B-C5B	3.96	121.45	113.69
20	K	101	CLA	C4A-NA-C1A	3.95	108.48	106.71
20	B	809	CLA	CHC-C1C-NC	3.95	130.20	124.20
20	A	836	CLA	CHC-C1C-NC	3.95	130.20	124.20
20	4	310	CLA	C1C-NC-C4C	-3.95	104.93	106.71
20	K	103	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
20	H	102	CLA	CHB-C4A-NA	3.95	129.97	124.51
20	3	317	CLA	CED-O2D-CGD	3.94	124.86	115.94
20	B	850	CLA	CHC-C1C-NC	3.94	130.19	124.20
20	3	304	CLA	CHC-C1C-NC	3.94	130.19	124.20
20	B	827	CLA	CHC-C1C-NC	3.94	130.19	124.20
20	A	823	CLA	CHC-C1C-NC	3.94	130.18	124.20
20	4	306	CLA	CAC-C3C-C4C	3.94	129.92	124.81
21	R	101	LMU	C1B-O1B-C4'	-3.94	108.22	117.96
20	A	832	CLA	CMD-C2D-C3D	-3.94	117.31	124.68
20	A	815	CLA	O2D-CGD-CBD	3.93	118.26	111.27
20	2	308	CLA	C3D-CAD-CBD	-3.93	102.43	107.61
20	B	822	CLA	C3D-CAD-CBD	-3.93	102.43	107.61
20	B	806	CLA	C3D-CAD-CBD	-3.93	102.43	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	105	LMU	C3B-C4B-C5B	-3.93	103.23	110.24
20	B	849	CLA	CHD-C4C-NC	3.93	130.39	124.20
20	H	102	CLA	CHD-C4C-NC	3.93	130.39	124.20
21	E	101	LMU	O5'-C1'-C2'	-3.93	102.04	110.35
21	R	104	LMU	O2'-C2'-C3'	-3.92	101.28	110.35
22	L	210	BCR	C11-C10-C9	-3.92	121.72	127.31
20	2	322	CLA	CHC-C1C-NC	3.92	130.15	124.20
22	I	101	BCR	C31-C1-C6	3.92	116.65	110.30
20	3	308	CLA	CAC-C3C-C4C	3.92	129.89	124.81
21	R	103	LMU	C1B-O5B-C5B	3.92	121.38	113.69
20	1	214	CLA	C3D-C2D-C1D	3.91	109.67	106.30
22	A	847	BCR	C7-C8-C9	-3.91	120.32	126.23
20	L	208	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
20	B	840	CLA	CBD-CHA-C1A	3.91	133.69	127.43
20	A	828	CLA	CHC-C1C-NC	3.91	130.13	124.20
22	B	843	BCR	C38-C26-C25	-3.91	120.14	124.53
20	L	203	CLA	C4A-NA-C1A	3.91	108.46	106.71
20	3	316	CLA	CHC-C1C-NC	3.91	130.00	124.23
20	L	209	CLA	O1D-CGD-CBD	-3.91	116.49	124.48
20	1	215	CLA	CAA-C2A-C3A	3.90	123.47	112.78
20	B	822	CLA	CAC-C3C-C4C	3.90	129.87	124.81
21	R	104	LMU	O2'-C2'-C1'	-3.90	100.57	110.05
20	A	852	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
20	B	810	CLA	CHC-C1C-NC	3.90	130.12	124.20
20	B	822	CLA	OBD-CAD-C3D	-3.90	121.51	127.98
20	R	107	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
20	1	214	CLA	CHC-C1C-NC	3.90	129.99	124.23
20	A	841	CLA	C6-C5-C3	-3.89	103.24	113.45
20	A	838	CLA	O2D-CGD-O1D	-3.89	116.22	123.84
20	A	809	CLA	CMD-C2D-C3D	-3.89	117.39	124.68
20	I	102	CLA	CHC-C1C-NC	3.89	130.11	124.20
20	2	310	CLA	C2A-C1A-CHA	-3.89	116.00	122.63
20	2	310	CLA	CHC-C1C-NC	3.89	129.98	124.23
20	4	307	CLA	CMD-C2D-C3D	-3.89	117.40	124.68
20	A	817	CLA	O2A-CGA-CBA	3.89	124.12	111.91
20	K	102	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
20	B	808	CLA	CMB-C2B-C3B	3.89	131.96	124.68
20	B	808	CLA	O2A-CGA-O1A	-3.89	113.78	123.59
21	R	103	LMU	C6B-C5B-C4B	-3.89	103.90	113.00
20	1	215	CLA	C2A-C1A-CHA	-3.89	117.06	123.86
20	B	816	CLA	C1-C2-C3	-3.89	119.32	126.04
22	I	103	BCR	C27-C26-C25	-3.89	117.09	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	824	CLA	C3D-CAD-CBD	-3.89	102.49	107.61
20	B	829	CLA	C4A-NA-C1A	3.89	108.45	106.71
20	A	831	CLA	CHC-C1C-C2C	-3.88	115.99	126.72
20	L	207	CLA	CHC-C1C-NC	3.88	130.09	124.20
20	A	828	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
20	A	807	CLA	CHC-C1C-NC	3.88	130.08	124.20
21	2	319	LMU	O1'-C1'-C2'	3.88	114.35	108.30
20	F	204	CLA	CHD-C4C-C3C	-3.87	118.93	124.98
20	1	207	CLA	CHC-C1C-NC	3.87	130.08	124.20
20	2	305	CLA	C3D-CAD-CBD	-3.87	102.51	107.61
22	F	202	BCR	C24-C23-C22	-3.87	120.39	126.23
20	1	201	CLA	CAA-C2A-C3A	-3.87	102.18	112.78
20	3	304	CLA	C1B-C2B-C3B	-3.87	103.32	106.92
20	3	305	CLA	C3B-C2B-C1B	-3.87	102.98	106.29
20	A	801	CLA	CED-O2D-CGD	3.87	124.68	115.94
21	K	109	LMU	O3'-C3'-C2'	-3.87	101.41	110.35
20	A	838	CLA	CMC-C2C-C1C	3.86	130.92	125.04
20	A	826	CLA	CMD-C2D-C3D	-3.86	117.45	124.68
20	4	318	CLA	CHD-C4C-C3C	-3.86	119.16	124.84
20	3	303	CLA	C3D-C4D-ND	3.86	113.49	110.14
20	B	839	CLA	CHD-C4C-NC	3.86	130.28	124.20
21	A	848	LMU	O5'-C5'-C4'	3.86	117.88	109.75
20	3	320	CLA	C4A-NA-C1A	3.85	108.44	106.71
20	A	815	CLA	CMB-C2B-C3B	3.85	131.89	124.68
20	3	312	CLA	C1D-CHD-C4C	-3.85	116.56	126.10
20	A	807	CLA	CHD-C4C-NC	3.85	130.27	124.20
20	B	825	CLA	CHC-C1C-NC	3.85	130.05	124.20
20	A	823	CLA	CHD-C4C-NC	3.85	130.27	124.20
20	A	810	CLA	CMB-C2B-C3B	3.85	131.88	124.68
20	A	836	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
20	A	834	CLA	CHC-C1C-NC	3.85	130.04	124.20
20	2	311	CLA	CMD-C2D-C3D	-3.85	117.47	124.68
20	4	307	CLA	C2A-C3A-C4A	-3.85	95.65	101.87
20	B	840	CLA	CHD-C4C-C3C	-3.85	118.97	124.98
20	B	820	CLA	CMD-C2D-C3D	-3.85	117.48	124.68
23	A	842	PQN	C2M-C2-C3	-3.85	118.12	124.40
20	B	819	CLA	CHB-C4A-NA	3.84	129.83	124.51
21	K	109	LMU	O5B-C5B-C6B	3.84	115.99	106.44
20	G	102	CLA	CHC-C1C-NC	3.84	130.03	124.20
20	H	102	CLA	C3D-CAD-CBD	-3.84	102.54	107.61
20	B	827	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
20	1	215	CLA	CMA-C3A-C2A	-3.84	98.33	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	322	LMU	C3'-C4'-C5'	-3.84	102.12	110.93
20	A	819	CLA	CHD-C4C-C3C	-3.84	119.19	124.84
20	B	831	CLA	CHC-C1C-NC	3.84	130.03	124.20
20	4	303	CLA	CAA-C2A-C3A	-3.84	107.14	116.10
20	B	810	CLA	CHD-C4C-C3C	-3.84	119.20	124.84
20	B	814	CLA	O1D-CGD-CBD	-3.83	116.65	124.48
20	4	304	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
22	A	845	BCR	C24-C23-C22	-3.83	120.45	126.23
21	N	101	LMU	C3'-C4'-C5'	-3.83	102.15	110.93
20	A	806	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
20	A	809	CLA	O2A-CGA-CBA	3.83	123.92	111.91
20	3	308	CLA	CHD-C4C-NC	3.83	130.23	124.20
20	2	310	CLA	C2D-C3D-C4D	-3.83	103.01	106.30
20	2	312	CLA	C3D-CAD-CBD	-3.82	102.57	107.61
20	3	301	CLA	C1B-C2B-C3B	-3.82	103.36	106.92
21	R	106	LMU	O3B-C3B-C4B	3.82	119.19	110.35
20	A	811	CLA	CMB-C2B-C1B	3.82	134.34	128.46
20	3	320	CLA	CHC-C1C-NC	3.82	129.87	124.23
20	3	309	CLA	C4A-NA-C1A	3.82	108.42	106.71
21	H	106	LMU	C1'-C2'-C3'	-3.82	102.05	110.00
21	R	102	LMU	C3'-C4'-C5'	-3.82	102.17	110.93
20	B	822	CLA	CHD-C4C-NC	3.82	130.22	124.20
21	H	107	LMU	O5'-C5'-C4'	-3.81	101.71	109.75
20	2	304	CLA	C3B-C2B-C1B	-3.81	103.03	106.29
20	4	307	CLA	CGD-CBD-CAD	3.81	123.08	110.73
20	A	823	CLA	C3D-CAD-CBD	-3.81	102.59	107.61
20	A	833	CLA	CMD-C2D-C3D	-3.81	117.56	124.68
22	B	846	BCR	C38-C26-C25	-3.81	120.25	124.53
20	A	813	CLA	CHB-C4A-NA	3.80	129.77	124.51
20	2	305	CLA	CHD-C4C-C3C	-3.80	119.25	124.84
20	3	320	CLA	C3B-C2B-C1B	-3.80	103.03	106.29
20	1	215	CLA	O2A-CGA-O1A	-3.80	114.00	123.59
20	B	815	CLA	CHD-C4C-NC	3.80	130.19	124.20
22	B	842	BCR	C24-C23-C22	-3.80	120.49	126.23
20	B	830	CLA	CHC-C1C-NC	3.80	129.97	124.20
20	A	817	CLA	CHC-C1C-NC	3.80	129.97	124.20
20	4	304	CLA	O2A-CGA-CBA	3.80	123.83	111.91
21	K	104	LMU	O6B-C6B-C5B	-3.80	98.26	111.29
22	J	102	BCR	C33-C5-C6	-3.80	120.26	124.53
20	A	828	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
20	A	852	CLA	CHD-C4C-C3C	-3.80	119.26	124.84
20	4	318	CLA	C4-C3-C5	3.79	121.65	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	202	CLA	O1D-CGD-CBD	-3.79	116.72	124.48
20	H	109	CLA	CHC-C1C-NC	3.79	129.96	124.20
20	3	307	CLA	C3B-C2B-C1B	-3.79	103.04	106.29
20	B	826	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	B	841	PQN	C2M-C2-C1	3.79	122.55	116.27
20	B	839	CLA	CHC-C1C-NC	3.79	129.95	124.20
20	2	308	CLA	CHD-C4C-NC	3.79	130.17	124.20
20	2	302	CLA	C4-C3-C5	3.78	120.31	115.98
20	B	807	CLA	CHB-C4A-NA	3.78	129.74	124.51
20	A	808	CLA	C6-C5-C3	-3.78	103.54	113.45
20	A	851	CLA	O2A-CGA-CBA	3.78	123.77	111.91
20	B	803	CLA	C4A-NA-C1A	3.78	108.41	106.71
20	R	107	CLA	CHC-C1C-NC	3.78	129.94	124.20
20	B	820	CLA	C4-C3-C5	3.78	121.63	115.27
20	B	812	CLA	CHC-C1C-NC	3.78	129.93	124.20
20	A	815	CLA	C2A-C1A-CHA	-3.77	117.26	123.86
20	B	828	CLA	CHC-C1C-NC	3.77	129.93	124.20
20	B	816	CLA	O2A-C1-C2	3.77	118.54	108.64
20	3	317	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
21	R	106	LMU	C1B-O1B-C4'	-3.77	108.65	117.96
20	A	831	CLA	C3D-CAD-CBD	-3.76	102.65	107.61
20	B	806	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
21	B	847	LMU	C3'-C4'-C5'	-3.76	102.30	110.93
20	B	838	CLA	O2A-CGA-CBA	3.76	123.72	111.91
20	A	818	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	1	219	LMU	C3'-C4'-C5'	-3.76	102.30	110.93
20	A	828	CLA	C4-C3-C5	3.76	121.60	115.27
20	4	315	CLA	C2A-C1A-CHA	-3.76	116.22	122.63
20	B	813	CLA	O2D-CGD-CBD	3.76	117.95	111.27
20	B	829	CLA	C1-C2-C3	-3.76	120.67	126.75
21	H	107	LMU	C1B-O5B-C5B	3.76	121.07	113.69
20	B	816	CLA	C4A-NA-C1A	3.76	108.40	106.71
20	B	808	CLA	CGD-CBD-CAD	3.76	122.91	110.73
20	2	316	CLA	C3D-CAD-CBD	-3.76	102.66	107.61
20	A	824	CLA	CMD-C2D-C3D	-3.76	117.65	124.68
20	B	849	CLA	CAA-C2A-C3A	-3.75	102.50	112.78
20	4	315	CLA	CHD-C4C-NC	3.75	130.00	124.21
20	J	101	CLA	C4A-NA-C1A	3.75	108.39	106.71
20	F	206	CLA	C4-C3-C2	-3.75	114.06	123.68
20	A	808	CLA	CHB-C4A-NA	3.75	129.70	124.51
20	K	108	CLA	C1-C2-C3	-3.75	120.68	126.75
20	L	202	CLA	CHD-C4C-C3C	-3.75	119.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	825	CLA	CMD-C2D-C3D	-3.75	117.66	124.68
20	A	808	CLA	CHC-C1C-NC	3.75	129.89	124.20
20	4	313	CLA	C2D-C3D-C4D	-3.75	103.07	106.30
22	F	203	BCR	C40-C30-C25	-3.75	104.22	110.30
20	B	850	CLA	C5-C3-C2	-3.75	113.54	121.12
20	B	828	CLA	CAC-C3C-C4C	3.74	129.67	124.81
20	B	822	CLA	CAA-CBA-CGA	-3.74	102.32	113.25
20	3	303	CLA	C4A-NA-C1A	3.74	108.39	106.71
20	B	807	CLA	CHD-C4C-NC	3.74	130.10	124.20
22	F	202	BCR	C38-C26-C25	-3.74	120.33	124.53
20	3	312	CLA	C2A-C3A-C4A	-3.74	98.31	104.18
21	A	854	LMU	C1B-C2B-C3B	3.74	117.78	110.00
21	1	219	LMU	C3B-C4B-C5B	3.74	116.91	110.24
20	3	312	CLA	C2C-C1C-CHC	-3.74	116.72	125.67
20	2	306	CLA	C3B-C2B-C1B	-3.74	103.09	106.29
20	1	202	CLA	CBA-CAA-C2A	-3.73	102.84	113.86
20	2	301	CLA	C2A-C1A-CHA	-3.73	116.26	122.63
21	N	101	LMU	O2B-C2B-C3B	-3.73	101.72	110.35
20	A	831	CLA	CMA-C3A-C2A	-3.73	98.77	113.83
20	L	208	CLA	CGD-CBD-CAD	-3.73	98.64	110.73
20	B	821	CLA	O2D-CGD-CBD	3.73	117.90	111.27
20	B	820	CLA	CED-O2D-CGD	3.73	124.38	115.94
20	3	318	CLA	CHB-C4A-NA	3.73	129.67	124.51
20	B	836	CLA	CMD-C2D-C3D	-3.73	117.70	124.68
21	R	103	LMU	O2B-C2B-C1B	3.73	119.10	110.05
20	3	311	CLA	CED-O2D-CGD	3.73	124.37	115.94
20	R	108	CLA	O2D-CGD-CBD	3.73	117.89	111.27
21	L	205	LMU	O5B-C5B-C4B	-3.73	102.93	109.69
20	B	819	CLA	CHC-C1C-NC	3.72	129.85	124.20
20	H	109	CLA	C3D-CAD-CBD	-3.72	102.70	107.61
21	1	220	LMU	C6B-C5B-C4B	-3.72	104.28	113.00
20	H	109	CLA	CHD-C4C-C3C	-3.72	119.37	124.84
20	4	318	CLA	CHC-C1C-C2C	-3.72	116.43	126.72
20	4	303	CLA	CMB-C2B-C3B	3.72	131.97	124.69
20	A	816	CLA	C4-C3-C5	3.72	121.52	115.27
20	L	208	CLA	CHD-C4C-C3C	-3.72	119.38	124.84
20	2	312	CLA	CGD-CBD-CAD	-3.72	98.70	110.73
20	K	108	CLA	CMD-C2D-C3D	-3.71	117.73	124.68
20	B	811	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
20	B	818	CLA	CMD-C2D-C3D	-3.71	117.73	124.68
21	R	104	LMU	C3B-C4B-C5B	-3.71	103.62	110.24
22	F	203	BCR	C27-C26-C25	-3.71	117.34	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	311	CLA	CHC-C1C-NC	3.71	129.84	124.20
20	A	807	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
20	1	201	CLA	CMC-C2C-C1C	3.71	130.69	125.04
20	1	207	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
21	R	102	LMU	C1-O1'-C1'	-3.70	107.70	113.84
20	3	318	CLA	C3D-CAD-CBD	-3.70	102.73	107.61
20	1	215	CLA	CAA-C2A-C1A	3.70	124.11	111.97
20	3	320	CLA	C3D-C4D-ND	3.70	113.36	110.14
20	1	204	CLA	OBD-CAD-C3D	-3.70	121.84	127.98
20	2	312	CLA	CHC-C1C-NC	3.70	129.82	124.20
20	H	101	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
20	3	306	CLA	C2D-C3D-C4D	-3.70	103.12	106.30
20	4	318	CLA	CHB-C4A-NA	3.70	129.62	124.51
20	1	216	CLA	CHC-C1C-NC	3.69	129.69	124.23
20	A	839	CLA	C6-C7-C8	-3.69	103.98	115.92
20	3	312	CLA	CHB-C4A-NA	3.69	129.99	124.34
20	B	819	CLA	O2D-CGD-CBD	3.69	117.83	111.27
20	4	306	CLA	CBC-CAC-C3C	-3.69	102.25	112.43
21	1	219	LMU	O5'-C1'-C2'	3.69	118.16	110.35
20	B	811	CLA	C6-C7-C8	-3.68	104.01	115.92
20	F	206	CLA	O2D-CGD-CBD	3.68	117.81	111.27
21	B	801	LMU	O5B-C5B-C6B	3.68	115.59	106.44
20	1	215	CLA	C7-C6-C5	-3.68	103.36	113.36
20	B	849	CLA	CBA-CAA-C2A	-3.68	103.00	113.86
22	A	843	BCR	C38-C26-C25	-3.68	120.39	124.53
20	1	210	CLA	C1-C2-C3	-3.68	119.68	126.04
20	3	319	CLA	CHB-C4A-NA	3.68	129.97	124.34
20	B	826	CLA	CHB-C4A-NA	3.68	129.60	124.51
20	4	310	CLA	C2A-C3A-C4A	-3.68	98.41	104.18
21	K	109	LMU	O2'-C2'-C1'	3.67	118.97	110.05
20	4	303	CLA	CHC-C1C-NC	3.67	129.78	124.20
20	A	820	CLA	CHC-C1C-NC	3.67	129.77	124.20
20	1	211	CLA	C2D-C3D-C4D	-3.67	103.14	106.30
20	B	851	CLA	C1-O2A-CGA	3.67	126.07	116.44
20	K	102	CLA	CMD-C2D-C3D	-3.67	117.82	124.68
20	B	817	CLA	C4A-NA-C1A	3.66	108.35	106.71
20	A	835	CLA	CHD-C4C-C3C	-3.66	119.45	124.84
21	F	201	LMU	O5B-C5B-C6B	3.66	115.54	106.44
20	3	312	CLA	C3C-C2C-C1C	-3.66	102.82	107.21
20	L	207	CLA	CED-O2D-CGD	3.66	124.22	115.94
20	B	803	CLA	C4-C3-C5	3.66	121.43	115.27
20	B	822	CLA	CGD-CBD-CAD	-3.66	98.88	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	838	CLA	C4A-NA-C1A	3.66	108.35	106.71
20	1	202	CLA	O2A-CGA-CBA	3.66	123.39	111.91
20	3	307	CLA	C2D-C3D-C4D	-3.66	103.15	106.30
20	R	108	CLA	C6-C5-C3	-3.66	103.86	113.45
20	B	817	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
20	A	803	CLA	O1D-CGD-CBD	-3.66	117.00	124.48
20	4	314	CLA	CHD-C4C-C3C	-3.66	119.27	124.98
20	1	211	CLA	C3D-C4D-ND	3.66	113.32	110.14
20	3	318	CLA	CHC-C1C-NC	3.65	129.75	124.20
20	B	849	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
20	1	204	CLA	CHC-C1C-NC	3.65	129.75	124.20
20	F	204	CLA	CHB-C4A-NA	3.65	129.56	124.51
20	1	215	CLA	C1-C2-C3	-3.65	119.72	126.04
20	1	215	CLA	CHC-C1C-C2C	-3.65	116.62	126.72
22	I	101	BCR	C19-C18-C17	3.65	124.54	118.94
20	A	832	CLA	CHC-C1C-NC	3.65	129.74	124.20
20	3	310	CLA	C2C-C1C-CHC	-3.65	116.94	125.67
21	C	101	LMU	C1B-C2B-C3B	3.64	117.59	110.00
20	A	810	CLA	C2A-C1A-CHA	-3.64	117.49	123.86
20	3	303	CLA	C3B-C2B-C1B	-3.64	103.17	106.29
20	1	202	CLA	CMB-C2B-C3B	3.64	131.49	124.68
20	1	214	CLA	C2A-C1A-CHA	-3.64	116.43	122.63
20	A	839	CLA	CGD-CBD-CAD	-3.64	98.95	110.73
20	B	851	CLA	O2D-CGD-CBD	3.64	117.73	111.27
21	H	107	LMU	C3'-C4'-C5'	-3.63	102.59	110.93
21	H	108	LMU	C6'-C5'-C4'	-3.63	102.75	113.33
21	R	102	LMU	C1B-C2B-C3B	3.63	117.56	110.00
20	B	808	CLA	CHC-C1C-NC	3.63	129.72	124.20
20	A	830	CLA	CHD-C4C-C3C	-3.63	119.50	124.84
20	A	815	CLA	CBC-CAC-C3C	-3.63	102.42	112.43
20	4	315	CLA	CHC-C1C-NC	3.63	129.59	124.23
20	2	315	CLA	C3B-C2B-C1B	-3.63	103.18	106.29
21	B	801	LMU	C1'-O5'-C5'	3.63	120.81	113.69
20	B	833	CLA	CHC-C1C-NC	3.62	129.70	124.20
20	4	302	CLA	CMD-C2D-C3D	-3.62	117.90	124.68
20	1	202	CLA	CHC-C1C-C2C	-3.62	116.70	126.72
20	4	316	CLA	C3D-CAD-CBD	-3.62	102.84	107.61
20	1	209	CLA	CMD-C2D-C3D	-3.62	117.90	124.68
20	A	823	CLA	CMD-C2D-C3D	-3.62	117.91	124.68
20	A	826	CLA	CHD-C4C-C3C	-3.62	119.52	124.84
20	2	312	CLA	CAA-C2A-C1A	3.62	123.83	111.97
20	B	826	CLA	C16-C15-C13	-3.62	104.23	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	201	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
21	K	106	LMU	O5B-C5B-C6B	3.61	115.42	106.44
20	A	839	CLA	C1-C2-C3	3.61	132.29	126.04
20	I	102	CLA	C3D-CAD-CBD	-3.61	102.85	107.61
20	A	850	CLA	CMC-C2C-C1C	3.60	130.53	125.04
20	1	208	CLA	C1D-CHD-C4C	-3.60	117.18	126.10
20	A	834	CLA	CAA-C2A-C3A	-3.60	102.91	112.78
20	1	201	CLA	CBA-CAA-C2A	-3.60	103.23	113.86
20	4	308	CLA	CMD-C2D-C3D	-3.60	117.94	124.68
21	R	105	LMU	O1'-C1'-C2'	3.60	113.93	108.30
21	1	219	LMU	O2B-C2B-C1B	-3.60	101.30	110.05
20	A	807	CLA	CBC-CAC-C3C	-3.60	102.51	112.43
20	H	103	CLA	O2D-CGD-CBD	3.60	117.66	111.27
20	B	811	CLA	C4A-NA-C1A	3.60	108.32	106.71
20	4	315	CLA	C4A-NA-C1A	3.60	108.32	106.71
20	A	812	CLA	C4A-NA-C1A	3.60	108.32	106.71
20	B	836	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
20	A	827	CLA	C1-O2A-CGA	3.60	125.88	116.44
20	3	301	CLA	CHC-C1C-NC	3.60	129.66	124.20
20	B	803	CLA	CED-O2D-CGD	3.59	124.07	115.94
21	R	104	LMU	O2B-C2B-C1B	3.59	118.77	110.05
20	R	108	CLA	C1-O2A-CGA	3.59	125.86	116.44
20	4	316	CLA	CHB-C4A-NA	3.59	129.48	124.51
20	A	820	CLA	CMD-C2D-C3D	-3.59	117.97	124.68
22	A	843	BCR	C33-C5-C6	-3.59	120.50	124.53
20	2	322	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
20	K	101	CLA	CMD-C2D-C3D	-3.59	117.97	124.68
20	A	822	CLA	CHC-C1C-NC	3.59	129.65	124.20
20	3	306	CLA	C3B-C2B-C1B	-3.59	103.22	106.29
20	L	201	CLA	O2A-CGA-CBA	3.58	123.15	111.91
20	B	825	CLA	CMD-C2D-C3D	-3.58	117.98	124.68
20	4	314	CLA	CAA-C2A-C3A	-3.58	107.74	116.10
22	B	845	BCR	C33-C5-C4	3.58	120.49	113.62
20	4	314	CLA	CHB-C4A-NA	3.58	129.46	124.51
20	A	816	CLA	O2A-CGA-O1A	-3.58	114.56	123.59
20	R	108	CLA	CMD-C2D-C3D	-3.58	117.98	124.68
20	4	313	CLA	CHD-C4C-NC	3.58	129.73	124.21
20	3	319	CLA	C3C-C4C-CHD	-3.58	117.39	125.22
20	2	308	CLA	CHC-C1C-C2C	-3.58	116.83	126.72
20	A	805	CLA	CHC-C1C-C2C	-3.57	116.83	126.72
20	4	303	CLA	CMD-C2D-C3D	-3.57	117.99	124.68
20	A	834	CLA	CHD-C4C-C3C	-3.57	119.58	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	107	LMU	O3'-C3'-C4'	-3.57	100.47	109.94
20	4	311	CLA	O2D-CGD-CBD	3.57	117.61	111.27
20	B	823	CLA	CMD-C2D-C3D	-3.57	118.00	124.68
20	3	311	CLA	C4A-NA-C1A	3.57	108.31	106.71
20	K	102	CLA	CHB-C4A-NA	3.57	129.44	124.51
21	A	849	LMU	O5B-C1B-C2B	3.57	117.90	110.35
20	1	202	CLA	CHD-C4C-C3C	-3.57	119.60	124.84
20	4	305	CLA	CHB-C4A-NA	3.56	129.44	124.51
22	F	203	BCR	C28-C29-C30	-3.56	101.86	114.60
21	A	849	LMU	O1'-C1'-C2'	3.56	113.87	108.30
20	A	809	CLA	C4A-NA-C1A	3.56	108.31	106.71
20	3	308	CLA	CMD-C2D-C3D	-3.56	118.01	124.68
20	K	102	CLA	O2A-CGA-O1A	-3.56	114.60	123.59
20	K	102	CLA	CHD-C4C-C3C	-3.56	119.60	124.84
20	4	318	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
22	A	845	BCR	C33-C5-C4	3.56	120.45	113.62
22	A	845	BCR	C38-C26-C27	3.56	120.45	113.62
20	4	314	CLA	CHC-C1C-NC	3.56	129.60	124.20
20	A	851	CLA	CHB-C4A-NA	3.56	129.43	124.51
20	4	318	CLA	CMB-C2B-C3B	3.55	131.33	124.68
22	F	203	BCR	C37-C22-C21	-3.55	117.95	122.92
22	B	844	BCR	C35-C13-C14	-3.55	117.95	122.92
20	A	814	CLA	CHD-C4C-C3C	-3.55	119.62	124.84
20	B	836	CLA	C4-C3-C5	3.55	121.24	115.27
21	N	101	LMU	C3B-C4B-C5B	3.55	116.57	110.24
20	4	311	CLA	C4-C3-C2	-3.55	114.58	123.68
20	4	305	CLA	CMD-C2D-C3D	-3.55	118.04	124.68
20	A	833	CLA	CHD-C4C-C3C	-3.55	119.63	124.84
20	2	303	CLA	O2A-CGA-CBA	3.54	123.03	111.91
20	A	851	CLA	O2A-C1-C2	3.54	117.95	108.64
22	I	101	BCR	C36-C18-C19	-3.54	112.50	118.08
20	A	806	CLA	CMB-C2B-C3B	3.54	131.31	124.68
21	K	106	LMU	O5B-C5B-C4B	-3.54	103.26	109.69
20	3	318	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
20	J	101	CLA	CMD-C2D-C3D	-3.53	118.07	124.68
20	B	825	CLA	C3D-CAD-CBD	-3.53	102.96	107.61
20	2	301	CLA	C3A-C4A-NA	3.53	117.32	109.92
20	4	305	CLA	CHC-C1C-C2C	-3.52	116.97	126.72
20	A	852	CLA	CHB-C4A-NA	3.52	129.38	124.51
20	F	205	CLA	CMD-C2D-C3D	-3.52	118.09	124.68
20	4	313	CLA	C4A-NA-C1A	3.52	108.29	106.71
21	2	319	LMU	O1B-C1B-C2B	3.52	117.22	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	826	CLA	CHC-C1C-NC	3.52	129.54	124.20
20	A	827	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
20	L	202	CLA	CHC-C1C-NC	3.51	129.53	124.20
22	F	203	BCR	C1-C6-C5	-3.51	117.67	122.61
20	4	311	CLA	C4-C3-C5	3.51	121.18	115.27
20	A	822	CLA	CHD-C4C-C3C	-3.51	119.68	124.84
20	B	818	CLA	CHC-C1C-NC	3.51	129.53	124.20
20	1	204	CLA	CED-O2D-CGD	3.51	123.88	115.94
20	1	202	CLA	C3A-C2A-C1A	3.51	106.59	101.34
20	A	823	CLA	CHD-C4C-C3C	-3.51	119.68	124.84
20	A	838	CLA	C3D-CAD-CBD	-3.51	102.99	107.61
20	A	805	CLA	O2D-CGD-CBD	3.50	117.49	111.27
20	1	209	CLA	CHC-C1C-NC	3.50	129.51	124.20
20	B	824	CLA	CMD-C2D-C3D	-3.50	118.13	124.68
20	A	828	CLA	C3D-CAD-CBD	-3.50	103.00	107.61
20	2	306	CLA	C3A-C4A-CHB	-3.50	119.63	123.91
22	A	844	BCR	C38-C26-C27	3.50	120.33	113.62
20	1	201	CLA	CHC-C1C-C2C	-3.50	117.05	126.72
20	A	801	CLA	C3A-C2A-C1A	3.50	106.58	101.34
20	3	309	CLA	C2D-C3D-C4D	-3.49	103.29	106.30
20	A	832	CLA	CHD-C4C-C3C	-3.49	119.71	124.84
21	H	106	LMU	C1'-O5'-C5'	-3.49	106.84	113.69
20	1	204	CLA	C4A-NA-C1A	3.49	108.27	106.71
20	A	811	CLA	CHC-C1C-C2C	-3.49	117.08	126.72
21	A	855	LMU	O2'-C2'-C3'	-3.48	102.29	110.35
20	B	806	CLA	O2A-CGA-CBA	3.48	122.84	111.91
20	3	309	CLA	C3B-C2B-C1B	-3.48	103.31	106.29
22	I	101	BCR	C33-C5-C4	3.48	120.31	113.62
21	R	102	LMU	C3B-C4B-C5B	-3.48	104.03	110.24
22	B	852	BCR	C24-C23-C22	-3.48	120.97	126.23
22	A	846	BCR	C38-C26-C27	3.48	120.30	113.62
20	J	103	CLA	C1-C2-C3	-3.48	120.03	126.04
20	B	807	CLA	O2A-CGA-CBA	3.48	122.82	111.91
22	A	847	BCR	C38-C26-C27	3.48	120.29	113.62
20	1	210	CLA	CMB-C2B-C1B	3.47	133.80	128.46
21	L	205	LMU	C1B-O1B-C4'	-3.47	109.37	117.96
20	B	832	CLA	CED-O2D-CGD	3.47	123.78	115.94
20	B	816	CLA	O2D-CGD-CBD	3.47	117.43	111.27
20	A	808	CLA	CMD-C2D-C3D	-3.47	118.19	124.68
20	L	201	CLA	C2A-C1A-CHA	-3.47	117.80	123.86
21	L	204	LMU	C4B-C3B-C2B	3.47	116.88	110.82
20	A	803	CLA	C1-C2-C3	-3.47	121.14	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	101	BCR	C38-C26-C25	-3.46	120.64	124.53
20	A	825	CLA	C1-C2-C3	-3.46	120.05	126.04
21	A	855	LMU	C3B-C4B-C5B	-3.46	104.06	110.24
20	A	851	CLA	O2D-CGD-CBD	3.46	117.41	111.27
20	2	302	CLA	CMD-C2D-C3D	-3.46	118.21	124.68
20	A	827	CLA	CHD-C4C-C3C	-3.46	119.76	124.84
21	3	322	LMU	C1B-O1B-C4'	-3.46	109.41	117.96
21	B	847	LMU	O6'-C6'-C5'	-3.46	99.43	111.29
22	J	102	BCR	C38-C26-C27	3.46	120.25	113.62
20	3	317	CLA	C3D-CAD-CBD	-3.45	103.06	107.61
22	L	210	BCR	C15-C16-C17	-3.45	116.40	123.47
22	B	844	BCR	C38-C26-C27	3.45	120.25	113.62
20	4	319	CLA	CMD-C2D-C3D	-3.45	118.22	124.68
20	1	215	CLA	C3D-CAD-CBD	-3.45	103.06	107.61
20	A	801	CLA	CHC-C1C-C2C	-3.45	117.17	126.72
22	I	103	BCR	C8-C7-C6	-3.45	117.51	127.20
21	H	106	LMU	O5B-C5B-C6B	3.45	115.01	106.44
21	N	101	LMU	O2'-C2'-C1'	3.45	118.42	110.05
22	B	852	BCR	C1-C6-C7	3.45	125.53	115.78
20	B	834	CLA	CMD-C2D-C3D	-3.45	118.23	124.68
20	B	805	CLA	CHD-C4C-C3C	-3.44	119.78	124.84
20	3	305	CLA	C2C-C1C-CHC	-3.44	117.42	125.67
20	1	208	CLA	C2B-C3B-C4B	3.44	109.23	106.29
20	1	206	CLA	CHC-C1C-NC	3.44	129.43	124.20
22	B	844	BCR	C16-C15-C14	-3.44	116.42	123.47
20	A	821	CLA	CHD-C4C-C3C	-3.44	119.78	124.84
20	R	108	CLA	CHC-C1C-C2C	-3.44	117.20	126.72
20	B	817	CLA	C1-C2-C3	-3.44	120.09	126.04
20	A	806	CLA	C1-C2-C3	-3.44	120.09	126.04
20	A	851	CLA	O2A-CGA-O1A	-3.44	114.92	123.59
21	3	322	LMU	O5B-C5B-C6B	3.44	114.98	106.44
20	H	101	CLA	CHC-C1C-C2C	-3.44	117.22	126.72
21	1	218	LMU	O4'-C4B-C5B	3.44	117.83	109.30
20	B	850	CLA	C3D-CAD-CBD	-3.43	103.08	107.61
20	B	828	CLA	CED-O2D-CGD	3.43	123.70	115.94
23	A	842	PQN	C21-C20-C18	-3.43	104.82	115.92
20	A	834	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
20	4	304	CLA	CBC-CAC-C3C	-3.43	102.97	112.43
20	B	837	CLA	O1D-CGD-CBD	-3.43	117.47	124.48
21	B	847	LMU	O2B-C2B-C1B	3.43	118.38	110.05
20	A	850	CLA	CHB-C4A-NA	3.43	129.25	124.51
20	B	830	CLA	C4-C3-C5	3.43	121.04	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	303	CLA	C3C-C4C-CHD	-3.43	117.72	125.22
22	3	314	BCR	C23-C24-C25	-3.43	117.58	127.20
20	A	802	CLA	CHB-C4A-NA	3.43	129.58	124.34
20	2	322	CLA	CHB-C4A-NA	3.42	129.25	124.51
20	1	204	CLA	CMD-C2D-C3D	-3.42	118.27	124.68
20	A	830	CLA	O2A-CGA-CBA	3.42	122.65	111.91
21	N	101	LMU	O4'-C4B-C3B	-3.42	102.44	110.35
22	I	101	BCR	C27-C26-C25	-3.42	117.76	122.73
20	H	109	CLA	CMB-C2B-C3B	3.42	131.08	124.68
20	J	103	CLA	CMD-C2D-C3D	-3.42	118.28	124.68
20	B	810	CLA	C4A-NA-C1A	3.42	108.24	106.71
20	4	313	CLA	CHC-C1C-NC	3.42	129.28	124.23
20	A	807	CLA	C3D-CAD-CBD	-3.42	103.11	107.61
22	B	844	BCR	C15-C14-C13	-3.42	122.44	127.31
22	B	852	BCR	C7-C6-C5	-3.41	113.19	121.46
20	A	816	CLA	C3D-CAD-CBD	-3.41	103.11	107.61
20	A	810	CLA	C3D-CAD-CBD	-3.41	103.11	107.61
21	1	213	LMU	O2'-C2'-C1'	-3.41	101.75	110.05
20	B	828	CLA	CGD-CBD-CAD	3.41	121.78	110.73
20	B	810	CLA	CMD-C2D-C3D	-3.41	118.30	124.68
20	B	816	CLA	O2A-CGA-CBA	3.41	122.61	111.91
20	1	205	CLA	CHB-C4A-NA	3.41	129.56	124.34
20	A	839	CLA	CMC-C2C-C3C	3.40	135.35	126.12
20	3	306	CLA	C3D-C2D-C1D	3.40	109.23	106.30
20	B	835	CLA	C1-O2A-CGA	3.40	125.36	116.44
22	I	103	BCR	C32-C1-C6	-3.40	104.79	110.30
20	1	216	CLA	C1C-NC-C4C	-3.40	105.18	106.71
21	G	101	LMU	O1B-C1B-O5B	3.39	120.16	110.67
20	B	806	CLA	CHC-C1C-C2C	-3.39	117.33	126.72
20	B	830	CLA	CMD-C2D-C3D	-3.39	118.33	124.68
20	A	810	CLA	CMA-C3A-C2A	-3.39	100.15	113.83
20	B	840	CLA	CHC-C1C-NC	3.39	129.35	124.20
22	B	844	BCR	C23-C22-C21	3.39	124.14	118.94
20	L	208	CLA	CMD-C2D-C3D	-3.39	118.34	124.68
20	2	312	CLA	CHB-C4A-NA	3.39	129.20	124.51
22	B	843	BCR	C33-C5-C4	3.39	120.12	113.62
20	B	837	CLA	C3D-CAD-CBD	-3.39	103.14	107.61
20	A	816	CLA	O1D-CGD-CBD	-3.39	117.56	124.48
20	A	827	CLA	C4A-NA-C1A	3.39	108.23	106.71
20	B	834	CLA	CHC-C1C-NC	3.38	129.34	124.20
20	A	838	CLA	CHB-C4A-NA	3.38	129.19	124.51
20	B	812	CLA	CHD-C4C-C3C	-3.38	119.87	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	313	CLA	C3D-C4D-ND	3.38	113.08	110.14
21	1	213	LMU	O5B-C5B-C4B	-3.38	103.55	109.69
20	3	303	CLA	C3D-C2D-C1D	3.38	109.21	106.30
20	2	322	CLA	O2A-CGA-CBA	3.38	122.52	111.91
20	4	311	CLA	CMD-C2D-C3D	-3.38	118.36	124.68
22	B	845	BCR	C38-C26-C27	3.38	120.11	113.62
20	1	202	CLA	C2A-C3A-C4A	-3.38	96.41	101.87
20	A	826	CLA	O2D-CGD-CBD	3.38	117.27	111.27
20	3	320	CLA	C3C-C4C-CHD	-3.37	117.83	125.22
21	F	201	LMU	O5'-C1'-C2'	-3.37	103.21	110.35
21	F	201	LMU	O3'-C3'-C2'	3.37	118.15	110.35
20	2	309	CLA	C3C-C4C-CHD	-3.37	117.84	125.22
20	A	810	CLA	CHD-C4C-C3C	-3.37	119.88	124.84
21	K	109	LMU	O1B-C4'-C5'	3.37	118.68	109.45
21	H	104	LMU	C1B-O5B-C5B	-3.37	107.07	113.69
20	3	307	CLA	C3D-C2D-C1D	3.37	109.20	106.30
21	R	104	LMU	O5B-C1B-C2B	-3.37	103.22	110.35
21	2	319	LMU	O5'-C1'-O1'	3.37	117.95	109.97
20	L	208	CLA	C4A-NA-C1A	3.37	108.22	106.71
20	3	317	CLA	CHC-C1C-NC	3.37	129.31	124.20
20	B	807	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
20	2	303	CLA	C4-C3-C2	-3.37	115.04	123.68
20	A	811	CLA	CAA-C2A-C1A	-3.36	100.95	111.97
20	B	836	CLA	C4A-NA-C1A	3.36	108.22	106.71
20	A	811	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
20	4	304	CLA	C3C-C4C-NC	-3.36	106.80	110.57
20	A	841	CLA	CHC-C1C-NC	3.36	129.30	124.20
21	H	108	LMU	O3B-C3B-C2B	-3.36	102.58	110.35
20	A	833	CLA	CHC-C1C-C2C	-3.36	117.43	126.72
20	4	306	CLA	CGD-CBD-CAD	-3.36	99.86	110.73
20	R	107	CLA	CED-O2D-CGD	3.36	123.53	115.94
21	E	101	LMU	O1B-C1B-O5B	3.36	120.05	110.67
20	B	808	CLA	C4-C3-C5	3.36	120.92	115.27
20	2	315	CLA	C3C-C4C-CHD	-3.35	117.88	125.22
20	B	827	CLA	CMA-C3A-C2A	-3.35	100.31	113.83
21	E	101	LMU	O5'-C5'-C6'	3.35	114.76	106.44
20	3	311	CLA	O2A-CGA-CBA	3.35	122.42	111.91
22	A	843	BCR	C38-C26-C27	3.35	120.05	113.62
20	4	310	CLA	CHC-C1C-NC	3.35	129.18	124.23
22	J	102	BCR	C33-C5-C4	3.35	120.05	113.62
20	4	306	CLA	CMC-C2C-C1C	3.34	130.13	125.04
20	G	102	CLA	CHB-C4A-NA	3.34	129.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	302	CLA	CHC-C1C-NC	3.34	129.27	124.20
21	R	105	LMU	C1'-C2'-C3'	3.34	116.96	110.00
20	3	302	CLA	C5-C3-C4	3.34	121.98	114.60
20	1	208	CLA	C2A-C3A-C4A	-3.34	98.94	104.18
22	B	842	BCR	C38-C26-C27	3.34	120.03	113.62
20	B	832	CLA	CHB-C4A-NA	3.34	129.12	124.51
20	2	305	CLA	CMD-C2D-C3D	-3.34	118.44	124.68
20	B	803	CLA	O2D-CGD-O1D	-3.34	117.32	123.84
22	3	314	BCR	C36-C18-C17	-3.33	118.25	122.92
20	3	309	CLA	C3D-C2D-C1D	3.33	109.17	106.30
20	B	815	CLA	CHD-C4C-C3C	-3.33	119.94	124.84
20	L	203	CLA	C4-C3-C5	3.33	120.87	115.27
20	B	813	CLA	CMB-C2B-C3B	3.33	130.91	124.68
20	A	823	CLA	O2A-CGA-CBA	3.33	122.36	111.91
22	A	847	BCR	C33-C5-C4	3.33	120.01	113.62
21	A	854	LMU	C2'-C3'-C4'	3.33	117.28	109.68
20	A	850	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
21	A	848	LMU	C1B-O5B-C5B	3.33	120.22	113.69
22	A	844	BCR	C33-C5-C4	3.33	120.01	113.62
20	3	313	CLA	O2A-C1-C2	3.33	117.37	108.64
20	A	801	CLA	CGD-CBD-CAD	3.32	121.50	110.73
20	A	815	CLA	C3A-C2A-C1A	-3.32	96.36	101.34
20	B	805	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
20	4	307	CLA	CED-O2D-CGD	3.32	123.45	115.94
21	L	204	LMU	C1'-C2'-C3'	3.32	116.91	110.00
20	A	819	CLA	CMD-C2D-C3D	-3.32	118.46	124.68
20	4	316	CLA	CHC-C1C-NC	3.32	129.24	124.20
20	1	216	CLA	C3B-C2B-C1B	-3.32	103.45	106.29
21	H	106	LMU	C1-O1'-C1'	-3.32	108.34	113.84
20	B	819	CLA	CMD-C2D-C3D	-3.32	118.47	124.68
20	3	318	CLA	CMB-C2B-C3B	3.31	130.88	124.68
20	3	307	CLA	C3D-C4D-ND	3.31	113.02	110.14
20	A	840	CLA	CAC-C3C-C4C	3.31	129.11	124.81
21	L	204	LMU	O5B-C5B-C6B	3.31	114.67	106.44
20	A	821	CLA	CMD-C2D-C3D	-3.31	118.48	124.68
21	K	106	LMU	C1B-O5B-C5B	-3.31	107.19	113.69
20	4	304	CLA	C16-C15-C13	-3.31	105.22	115.92
20	1	210	CLA	OBD-CAD-CBD	-3.31	121.17	125.89
20	4	304	CLA	C7-C6-C5	-3.31	104.37	113.36
20	4	312	CLA	C3D-C4D-ND	3.30	113.01	110.14
21	R	102	LMU	C1'-O5'-C5'	-3.30	107.20	113.69
20	B	822	CLA	C4A-NA-C1A	3.30	108.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	832	CLA	CHB-C4A-NA	3.30	129.08	124.51
20	A	819	CLA	CGD-CBD-CAD	3.30	121.42	110.73
20	A	851	CLA	O1D-CGD-CBD	-3.30	117.74	124.48
20	B	823	CLA	C4A-NA-C1A	3.30	108.19	106.71
20	2	306	CLA	C2C-C1C-CHC	-3.29	117.78	125.67
21	3	322	LMU	C3B-C4B-C5B	-3.29	104.37	110.24
20	3	306	CLA	C3D-C4D-ND	3.29	113.00	110.14
21	R	106	LMU	C1'-O5'-C5'	3.29	120.15	113.69
21	K	104	LMU	O5'-C1'-C2'	-3.29	103.38	110.35
22	I	103	BCR	C19-C18-C17	3.29	123.99	118.94
20	4	307	CLA	C6-C5-C3	-3.29	109.24	114.62
20	B	851	CLA	CMD-C2D-C3D	-3.29	118.53	124.68
20	B	850	CLA	C1-O2A-CGA	3.29	125.07	116.44
20	2	304	CLA	C2C-C1C-CHC	-3.28	117.80	125.67
20	F	206	CLA	CBA-CAA-C2A	-3.28	104.17	113.86
20	3	317	CLA	O2A-CGA-O1A	-3.28	115.31	123.59
21	R	102	LMU	O1'-C1'-C2'	3.28	113.43	108.30
20	A	814	CLA	CMD-C2D-C3D	-3.28	118.54	124.68
20	A	831	CLA	CHD-C4C-NC	3.28	129.37	124.20
20	B	824	CLA	C1-C2-C3	-3.28	120.37	126.04
20	3	316	CLA	C3D-C4D-ND	3.28	112.99	110.14
20	H	103	CLA	CED-O2D-CGD	3.28	123.35	115.94
21	2	318	LMU	C1'-C2'-C3'	3.28	116.82	110.00
20	B	825	CLA	O2A-CGA-O1A	-3.28	115.32	123.59
20	A	837	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
20	B	837	CLA	CAA-C2A-C3A	-3.28	103.81	112.78
20	A	826	CLA	CHC-C1C-NC	3.28	129.17	124.20
21	R	105	LMU	C4B-C3B-C2B	-3.27	105.11	110.82
20	1	206	CLA	CAC-C3C-C4C	3.27	129.06	124.81
20	A	837	CLA	CMB-C2B-C3B	3.27	130.80	124.68
20	L	202	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
20	4	306	CLA	CMB-C2B-C3B	3.27	130.80	124.68
20	B	822	CLA	CHB-C4A-NA	3.27	129.04	124.51
21	3	322	LMU	C1B-O5B-C5B	3.27	120.11	113.69
21	H	105	LMU	C1'-O5'-C5'	-3.27	107.27	113.69
20	A	829	CLA	O2A-CGA-CBA	3.27	122.17	111.91
20	3	302	CLA	O1D-CGD-CBD	-3.27	117.80	124.48
20	A	829	CLA	CAC-C3C-C4C	3.27	129.05	124.81
20	B	839	CLA	O2A-CGA-O1A	-3.27	115.35	123.59
20	1	206	CLA	O2A-CGA-CBA	3.27	122.16	111.91
20	B	831	CLA	O2A-CGA-CBA	3.27	122.16	111.91
20	A	838	CLA	O2A-CGA-CBA	3.26	122.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	305	CLA	C3C-C4C-CHD	-3.26	118.08	125.22
22	B	843	BCR	C38-C26-C27	3.26	119.88	113.62
22	3	314	BCR	C15-C14-C13	-3.26	122.66	127.31
22	A	846	BCR	C33-C5-C4	3.26	119.88	113.62
21	3	322	LMU	O3B-C3B-C4B	3.26	117.88	110.35
20	A	850	CLA	C4A-NA-C1A	3.26	108.17	106.71
20	A	815	CLA	CGD-CBD-CAD	3.26	121.29	110.73
20	A	830	CLA	CMD-C2D-C3D	-3.26	118.58	124.68
21	H	106	LMU	O1B-C1B-C2B	-3.26	99.66	108.10
20	2	315	CLA	C1C-NC-C4C	-3.26	105.24	106.71
20	B	851	CLA	CMA-C3A-C4A	-3.26	103.02	111.77
20	4	305	CLA	CAC-C3C-C2C	-3.26	121.96	127.53
20	B	831	CLA	CED-O2D-CGD	3.25	123.30	115.94
20	1	205	CLA	C3C-C4C-CHD	-3.25	118.09	125.22
20	B	810	CLA	C4-C3-C2	-3.25	115.33	123.68
20	B	813	CLA	C4-C3-C5	3.25	120.74	115.27
20	B	831	CLA	O2A-CGA-O1A	-3.25	115.39	123.59
20	2	311	CLA	CHD-C4C-NC	3.25	129.32	124.20
20	A	818	CLA	C1-C2-C3	-3.25	120.43	126.04
20	A	837	CLA	CAA-C2A-C1A	-3.25	101.34	111.97
20	A	841	CLA	CAC-C3C-C4C	3.24	129.02	124.81
20	A	817	CLA	CMD-C2D-C3D	-3.24	118.61	124.68
20	H	109	CLA	CMD-C2D-C3D	-3.24	118.61	124.68
20	A	836	CLA	O2A-CGA-CBA	3.24	122.08	111.91
21	1	218	LMU	O5B-C1B-C2B	-3.24	103.49	110.35
20	H	102	CLA	CED-O2D-CGD	3.24	123.27	115.94
20	2	308	CLA	C4A-NA-C1A	3.24	108.16	106.71
21	3	322	LMU	O3'-C3'-C4'	-3.24	101.36	109.94
22	B	852	BCR	C32-C1-C6	3.24	115.55	110.30
20	B	835	CLA	CHC-C1C-NC	3.24	129.11	124.20
20	A	829	CLA	CHD-C4C-NC	3.24	129.30	124.20
20	L	203	CLA	O2A-CGA-CBA	3.23	122.06	111.91
20	B	840	CLA	CGD-CBD-CAD	-3.23	101.04	114.30
20	3	319	CLA	C2C-C1C-CHC	-3.23	117.93	125.67
21	H	104	LMU	O3'-C3'-C4'	3.23	118.51	109.94
22	B	842	BCR	C33-C5-C4	3.23	119.82	113.62
20	B	849	CLA	CBC-CAC-C3C	-3.23	103.53	112.43
21	A	854	LMU	O3'-C3'-C4'	-3.23	101.39	109.94
20	2	305	CLA	C4A-NA-C1A	3.23	108.16	106.71
20	F	206	CLA	CMA-C3A-C4A	3.23	120.45	111.77
20	A	822	CLA	C1-C2-C3	-3.23	120.47	126.04
20	4	312	CLA	C2D-C3D-C4D	-3.22	103.52	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	105	LMU	O5B-C5B-C6B	3.22	114.44	106.44
20	A	835	CLA	CAA-C2A-C1A	-3.22	101.43	111.97
21	L	205	LMU	O3'-C3'-C4'	-3.22	101.42	109.94
20	F	206	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
20	B	833	CLA	O1D-CGD-CBD	-3.21	117.91	124.48
20	A	831	CLA	CAC-C3C-C2C	-3.21	122.03	127.53
20	H	102	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
21	R	103	LMU	O5B-C5B-C4B	3.21	115.53	109.69
22	A	843	BCR	C33-C5-C4	3.21	119.79	113.62
20	4	308	CLA	C1B-C2B-C3B	-3.21	103.93	106.92
20	B	813	CLA	CHC-C1C-NC	3.21	129.08	124.20
20	B	809	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
20	A	821	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
20	A	829	CLA	C3D-CAD-CBD	-3.21	103.38	107.61
20	B	809	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
20	B	825	CLA	CHB-C4A-NA	3.21	128.95	124.51
20	A	824	CLA	C1-C2-C3	-3.21	120.50	126.04
21	R	102	LMU	O5B-C1B-C2B	3.21	117.13	110.35
20	2	322	CLA	C3A-C2A-C1A	3.21	106.14	101.34
20	A	819	CLA	C4-C3-C5	3.20	120.66	115.27
20	L	207	CLA	C4A-NA-C1A	3.20	108.15	106.71
20	A	826	CLA	O2A-CGA-CBA	3.20	121.96	111.91
21	R	104	LMU	O1B-C1B-O5B	-3.20	101.73	110.67
20	B	813	CLA	O2A-CGA-CBA	3.20	121.95	111.91
22	F	203	BCR	C4-C5-C6	-3.20	118.09	122.73
20	A	835	CLA	C2A-C1A-CHA	-3.20	118.27	123.86
20	A	803	CLA	C4A-NA-C1A	3.20	108.14	106.71
20	3	304	CLA	CMD-C2D-C3D	-3.20	118.70	124.68
20	B	822	CLA	CHD-C4C-C3C	-3.19	120.14	124.84
21	H	107	LMU	O3B-C3B-C2B	3.19	117.73	110.35
20	1	203	CLA	CMC-C2C-C1C	3.19	129.90	125.04
20	B	849	CLA	C4A-NA-C1A	3.19	108.14	106.71
20	2	307	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
20	A	801	CLA	CHD-C4C-NC	3.19	129.23	124.20
20	B	819	CLA	C4A-NA-C1A	3.19	108.14	106.71
20	3	306	CLA	C2C-C1C-CHC	-3.19	118.03	125.67
20	B	829	CLA	C3D-CAD-CBD	-3.19	103.41	107.61
20	4	310	CLA	C3C-C4C-CHD	-3.19	118.24	125.22
20	A	817	CLA	CED-O2D-CGD	3.19	123.14	115.94
22	3	314	BCR	C38-C26-C27	3.18	119.73	113.62
21	H	104	LMU	C6B-C5B-C4B	3.18	120.45	113.00
20	A	840	CLA	O2D-CGD-CBD	3.18	116.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	307	CLA	C4-C3-C5	3.18	120.61	115.27
20	B	827	CLA	C2A-C1A-CHA	-3.17	118.31	123.86
21	R	101	LMU	O5'-C1'-O1'	3.17	117.49	109.97
20	B	828	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	A	809	CLA	CAC-C3C-C2C	-3.17	122.11	127.53
20	B	815	CLA	CMB-C2B-C3B	3.17	130.61	124.68
20	B	810	CLA	C5-C3-C2	3.17	127.53	121.12
20	B	822	CLA	CHC-C1C-NC	3.17	129.01	124.20
22	B	846	BCR	C33-C5-C4	3.17	119.70	113.62
20	B	823	CLA	C1-C2-C3	-3.17	120.56	126.04
20	A	822	CLA	CAC-C3C-C4C	3.17	128.92	124.81
20	B	820	CLA	C5-C3-C2	-3.17	114.71	121.12
20	3	313	CLA	O2A-CGA-CBA	3.16	121.84	111.91
20	H	101	CLA	CAC-C3C-C4C	3.16	128.92	124.81
21	2	318	LMU	O1B-C1B-C2B	3.16	116.29	108.10
20	4	304	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
20	3	302	CLA	CMB-C2B-C3B	3.16	130.59	124.68
20	1	214	CLA	C4A-NA-C1A	3.16	108.13	106.71
20	3	311	CLA	C2A-C1A-CHA	-3.16	118.33	123.86
20	4	304	CLA	CMA-C3A-C4A	3.16	120.26	111.77
22	L	210	BCR	C19-C18-C17	-3.16	114.10	118.94
21	E	101	LMU	C1'-C2'-C3'	3.16	116.57	110.00
20	B	836	CLA	O2A-CGA-CBA	3.15	121.80	111.91
21	H	105	LMU	C3'-C4'-C5'	-3.15	103.70	110.93
20	A	801	CLA	CBA-CAA-C2A	3.15	123.16	113.86
20	A	823	CLA	O2A-CGA-O1A	-3.15	115.64	123.59
20	B	817	CLA	CHC-C1C-NC	3.15	128.98	124.20
20	4	307	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
20	4	318	CLA	C1-O2A-CGA	3.15	124.71	116.44
20	F	204	CLA	CAA-C2A-C1A	-3.15	104.03	111.81
20	2	308	CLA	CGD-CBD-CAD	3.15	120.93	110.73
20	2	310	CLA	C3D-C4D-ND	3.15	112.87	110.14
20	A	820	CLA	C4-C3-C5	3.15	119.58	115.98
20	1	216	CLA	C3C-C4C-CHD	-3.15	118.33	125.22
20	4	315	CLA	C2D-C3D-C4D	-3.15	103.59	106.30
20	I	102	CLA	O2A-CGA-CBA	3.15	121.78	111.91
22	B	846	BCR	C38-C26-C27	3.14	119.66	113.62
20	A	835	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
20	F	206	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
20	3	301	CLA	CMD-C2D-C3D	-3.14	118.80	124.68
20	B	829	CLA	CHC-C1C-NC	3.14	128.97	124.20
21	R	102	LMU	C1B-O5B-C5B	3.14	119.85	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	102	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
20	A	834	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	A	854	LMU	O5'-C1'-O1'	-3.14	102.54	109.97
20	A	827	CLA	CMA-C3A-C4A	-3.14	103.34	111.77
21	E	101	LMU	O3B-C3B-C4B	-3.14	103.09	110.35
20	3	318	CLA	C1-C2-C3	-3.14	120.62	126.04
20	3	307	CLA	C2C-C1C-CHC	-3.14	118.16	125.67
21	R	103	LMU	C1'-O5'-C5'	-3.13	107.53	113.69
20	B	812	CLA	C4A-NA-C1A	3.13	108.11	106.71
20	A	829	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
20	A	818	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
21	K	109	LMU	O2B-C2B-C1B	-3.13	102.44	110.05
20	1	208	CLA	CHB-C4A-NA	3.13	129.13	124.34
23	A	842	PQN	C2M-C2-C1	3.13	121.45	116.27
20	R	107	CLA	C1-O2A-CGA	3.13	124.65	116.44
20	3	313	CLA	CAC-C3C-C2C	-3.13	122.18	127.53
21	L	205	LMU	O5B-C1B-C2B	-3.13	103.73	110.35
20	B	809	CLA	CAC-C3C-C4C	3.12	128.86	124.81
20	3	306	CLA	C3C-C4C-CHD	-3.12	118.38	125.22
20	4	314	CLA	CMC-C2C-C1C	3.12	129.79	125.04
20	A	801	CLA	C1B-C2B-C3B	-3.12	104.02	106.92
20	K	102	CLA	C3D-CAD-CBD	-3.12	103.50	107.61
21	H	108	LMU	O3'-C3'-C2'	-3.12	103.14	110.35
20	B	812	CLA	CHB-C4A-NA	3.12	128.82	124.51
21	2	318	LMU	O5B-C5B-C4B	-3.12	104.03	109.69
22	B	844	BCR	C33-C5-C6	-3.12	121.03	124.53
21	E	101	LMU	C6'-C5'-C4'	-3.11	104.27	113.33
20	2	302	CLA	C1-C2-C3	-3.11	120.66	126.04
20	A	850	CLA	C6-C7-C8	-3.11	105.86	115.92
20	A	822	CLA	CHB-C4A-NA	3.11	128.81	124.51
20	R	107	CLA	C4-C3-C5	3.11	120.50	115.27
20	3	317	CLA	O1D-CGD-CBD	-3.11	118.12	124.48
20	3	307	CLA	C3C-C4C-CHD	-3.11	118.41	125.22
20	3	308	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
22	F	202	BCR	C33-C5-C4	3.11	119.59	113.62
21	A	849	LMU	C1B-O5B-C5B	3.11	119.78	113.69
20	R	108	CLA	CAC-C3C-C4C	3.11	128.84	124.81
21	2	318	LMU	C2'-C3'-C4'	3.11	116.77	109.68
20	J	103	CLA	C4A-NA-C1A	3.11	108.10	106.71
20	L	201	CLA	C4A-NA-C1A	-3.11	105.31	106.71
20	L	202	CLA	C3D-CAD-CBD	-3.10	103.52	107.61
20	2	301	CLA	C2D-C3D-C4D	-3.10	103.63	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	850	CLA	CMB-C2B-C3B	3.10	130.48	124.68
20	3	311	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
20	B	831	CLA	CMB-C2B-C3B	3.10	130.48	124.68
20	A	809	CLA	O2A-C1-C2	3.10	116.78	108.64
20	2	322	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
20	1	211	CLA	C2A-C3A-C4A	-3.10	99.32	104.18
20	A	816	CLA	C4A-NA-C1A	3.10	108.10	106.71
20	2	304	CLA	C3C-C4C-CHD	-3.09	118.44	125.22
20	B	839	CLA	CHB-C4A-NA	3.09	128.79	124.51
20	B	819	CLA	O1D-CGD-CBD	-3.09	118.16	124.48
20	1	214	CLA	C3D-C4D-ND	3.09	112.83	110.14
20	K	103	CLA	C4A-NA-C1A	3.09	108.10	106.71
20	A	852	CLA	CHC-C1C-NC	3.09	128.89	124.20
20	2	307	CLA	C6-C5-C3	-3.09	105.35	113.45
21	A	849	LMU	C2'-C3'-C4'	3.09	116.74	109.68
20	A	816	CLA	CMD-C2D-C3D	-3.09	118.90	124.68
20	1	212	CLA	CHB-C4A-NA	3.09	129.07	124.34
21	4	321	LMU	O5B-C5B-C6B	3.09	114.12	106.44
20	B	838	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	A	820	CLA	CHB-C4A-NA	3.09	128.78	124.51
20	B	835	CLA	CMC-C2C-C1C	3.09	129.74	125.04
22	F	202	BCR	C38-C26-C27	3.08	119.54	113.62
21	L	205	LMU	O5B-C5B-C6B	3.08	114.10	106.44
20	2	306	CLA	C3C-C4C-CHD	-3.08	118.47	125.22
20	A	822	CLA	CMD-C2D-C3D	-3.08	118.91	124.68
20	B	805	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
21	L	211	LMU	O5'-C5'-C4'	-3.08	103.26	109.75
20	B	836	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
20	A	807	CLA	CMD-C2D-C3D	-3.08	118.92	124.68
20	B	821	CLA	C3A-C2A-C1A	-3.08	96.73	101.34
20	B	820	CLA	CHD-C4C-C3C	-3.08	120.31	124.84
20	A	826	CLA	CHB-C4A-NA	3.07	128.76	124.51
20	R	107	CLA	O2A-CGA-O1A	-3.07	115.83	123.59
20	B	831	CLA	CMD-C2D-C3D	-3.07	118.93	124.68
20	B	806	CLA	CMA-C3A-C2A	-3.07	101.43	113.83
20	1	204	CLA	CGD-CBD-CAD	3.07	120.69	110.73
20	1	215	CLA	C4A-NA-C1A	-3.07	105.33	106.71
20	A	811	CLA	CHB-C4A-NA	3.07	128.75	124.51
21	A	855	LMU	C6B-C5B-C4B	-3.07	105.82	113.00
20	A	801	CLA	CAC-C3C-C2C	-3.07	122.28	127.53
20	B	821	CLA	CMC-C2C-C1C	3.07	129.71	125.04
20	3	308	CLA	CHD-C4C-C3C	-3.07	120.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	E	101	LMU	C3'-C4'-C5'	-3.07	103.90	110.93
20	A	838	CLA	C1-C2-C3	-3.07	120.74	126.04
20	A	806	CLA	CMD-C2D-C3D	-3.06	118.94	124.68
20	2	312	CLA	O2A-CGA-CBA	3.06	121.52	111.91
20	3	305	CLA	CHB-C4A-NA	3.06	129.03	124.34
20	1	211	CLA	C3D-C2D-C1D	3.06	108.94	106.30
20	A	823	CLA	O2D-CGD-CBD	3.06	116.71	111.27
20	A	803	CLA	CMB-C2B-C3B	3.06	130.40	124.68
22	B	852	BCR	C29-C30-C25	3.06	115.19	110.48
20	A	830	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
20	A	811	CLA	O2D-CGD-CBD	3.05	116.70	111.27
20	3	316	CLA	CHB-C4A-NA	3.05	129.01	124.34
20	B	832	CLA	CHC-C1C-NC	3.05	128.84	124.20
21	H	105	LMU	O5'-C5'-C4'	-3.05	103.32	109.75
20	B	838	CLA	C4-C3-C5	3.05	120.40	115.27
20	2	322	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
20	A	809	CLA	C4-C3-C5	3.05	120.40	115.27
20	L	208	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
20	B	831	CLA	C4A-NA-C1A	3.05	108.08	106.71
20	A	827	CLA	O1D-CGD-CBD	-3.05	118.25	124.48
21	H	105	LMU	O3'-C3'-C2'	-3.05	103.31	110.35
20	A	813	CLA	CAA-C2A-C1A	-3.05	101.99	111.97
20	A	838	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
20	2	316	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
20	4	307	CLA	O2D-CGD-CBD	3.04	116.67	111.27
20	A	831	CLA	C2C-C1C-NC	3.04	112.82	109.97
20	A	806	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
21	H	104	LMU	O5'-C5'-C6'	3.04	113.99	106.44
20	A	831	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
20	2	322	CLA	CBC-CAC-C3C	-3.04	104.06	112.43
20	A	830	CLA	CMB-C2B-C3B	3.04	130.36	124.68
21	H	108	LMU	C3-C2-C1	-3.04	100.04	113.49
20	A	835	CLA	C4A-NA-C1A	3.03	108.07	106.71
20	4	306	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
22	F	203	BCR	C38-C26-C27	3.03	119.44	113.62
20	1	208	CLA	C3D-C2D-C1D	3.03	108.92	106.30
20	J	103	CLA	C4-C3-C5	3.03	120.37	115.27
20	4	312	CLA	C3C-C4C-CHD	-3.03	118.58	125.22
20	A	852	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
20	B	832	CLA	CMD-C2D-C3D	-3.03	119.01	124.68
20	A	809	CLA	CHD-C4C-NC	3.03	128.97	124.20
20	A	813	CLA	CHC-C1C-C2C	-3.03	118.35	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	207	CLA	CMB-C2B-C3B	3.02	130.34	124.68
20	4	318	CLA	C6-C5-C3	-3.02	109.67	114.62
20	B	806	CLA	CHD-C4C-C3C	-3.02	120.39	124.84
21	A	848	LMU	C2'-C3'-C4'	3.02	116.58	109.68
20	A	826	CLA	CMA-C3A-C4A	-3.02	103.65	111.77
20	H	109	CLA	CMC-C2C-C1C	3.02	129.63	125.04
22	F	203	BCR	C34-C9-C10	-3.02	118.70	122.92
20	R	107	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	B	827	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
20	A	818	CLA	C4-C3-C5	3.01	120.34	115.27
20	2	309	CLA	C3D-C2D-C1D	3.01	108.90	106.30
20	B	831	CLA	CAA-CBA-CGA	-3.01	104.45	113.25
20	A	839	CLA	C11-C12-C13	-3.01	106.18	115.92
20	B	831	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
20	2	316	CLA	O2A-CGA-CBA	3.01	121.36	111.91
20	A	850	CLA	C3B-C4B-NB	-3.01	105.32	109.21
22	L	210	BCR	C33-C5-C4	3.01	119.40	113.62
20	A	831	CLA	O2A-CGA-CBA	3.01	121.35	111.91
20	A	833	CLA	CAA-CBA-CGA	-3.01	107.12	113.59
20	4	309	CLA	CHB-C4A-NA	3.01	128.94	124.34
20	B	849	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
20	B	826	CLA	CMA-C3A-C2A	-3.00	101.71	113.83
20	A	805	CLA	O2A-CGA-CBA	3.00	121.34	111.91
20	A	812	CLA	CMD-C2D-C3D	-3.00	119.06	124.68
20	4	307	CLA	O1D-CGD-CBD	-3.00	118.34	124.48
20	4	311	CLA	CHC-C1C-NC	3.00	128.75	124.20
20	B	836	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
20	B	839	CLA	CAA-CBA-CGA	3.00	122.01	113.25
20	2	312	CLA	O1D-CGD-CBD	-3.00	118.35	124.48
20	A	807	CLA	O1D-CGD-CBD	-3.00	118.35	124.48
20	B	808	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
20	A	817	CLA	O1D-CGD-CBD	-2.99	118.36	124.48
20	B	820	CLA	O2D-CGD-CBD	2.99	116.59	111.27
20	B	849	CLA	CHB-C4A-NA	2.99	128.65	124.51
20	3	309	CLA	C2C-C1C-CHC	-2.99	118.51	125.67
20	A	808	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
22	I	101	BCR	C15-C16-C17	2.99	129.60	123.47
20	B	851	CLA	C4A-NA-C1A	2.99	108.05	106.71
20	B	838	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
20	1	212	CLA	C3D-C2D-C1D	2.99	108.88	106.30
20	2	303	CLA	C4-C3-C5	2.99	120.29	115.27
21	K	109	LMU	C1B-O5B-C5B	-2.98	107.83	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	822	CLA	C4-C3-C5	2.98	120.29	115.27
20	A	814	CLA	O1D-CGD-CBD	-2.98	118.38	124.48
20	H	109	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
20	A	816	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
20	1	210	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
20	B	821	CLA	CBA-CAA-C2A	2.98	122.66	113.86
20	B	822	CLA	O2A-CGA-CBA	2.98	121.26	111.91
20	1	201	CLA	CMA-C3A-C4A	2.98	119.78	111.77
20	1	214	CLA	C3C-C4C-CHD	-2.98	118.69	125.22
20	A	816	CLA	CHC-C1C-NC	2.98	128.72	124.20
20	A	804	CLA	CMB-C2B-C3B	2.98	130.25	124.68
21	H	105	LMU	C1B-O5B-C5B	2.98	119.53	113.69
21	L	204	LMU	O5'-C5'-C6'	2.98	113.84	106.44
20	A	805	CLA	CMD-C2D-C3D	-2.98	119.11	124.68
20	4	315	CLA	C1C-NC-C4C	-2.98	105.37	106.71
20	B	813	CLA	C4-C3-C2	-2.97	116.05	123.68
20	B	820	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
20	H	109	CLA	CAC-C3C-C4C	2.97	128.67	124.81
20	B	815	CLA	C3D-CAD-CBD	-2.97	103.69	107.61
20	1	210	CLA	CMA-C3A-C4A	-2.97	103.79	111.77
21	R	106	LMU	O1B-C1B-C2B	2.97	115.79	108.10
21	E	101	LMU	O5'-C5'-C4'	-2.97	103.50	109.75
21	1	218	LMU	O1B-C4'-C3'	2.97	115.17	107.28
20	B	806	CLA	C16-C15-C13	-2.97	106.33	115.92
20	L	208	CLA	CMA-C3A-C4A	-2.96	103.80	111.77
21	G	101	LMU	O3'-C3'-C4'	-2.96	102.09	109.94
20	B	807	CLA	CAA-C2A-C3A	-2.96	104.66	112.78
21	B	847	LMU	C1'-C2'-C3'	-2.96	103.82	110.00
21	2	313	LMU	O1B-C4'-C3'	2.96	115.16	107.28
20	B	806	CLA	CMD-C2D-C3D	-2.96	119.13	124.68
20	3	302	CLA	CMD-C2D-C3D	-2.96	119.13	124.68
20	B	849	CLA	C7-C6-C5	-2.96	105.31	113.36
20	2	305	CLA	CHB-C4A-NA	2.96	128.61	124.51
20	2	312	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
20	1	214	CLA	C2A-C3A-C4A	-2.96	99.54	104.18
20	L	203	CLA	CMC-C2C-C1C	2.96	129.54	125.04
20	B	839	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
20	K	103	CLA	CHC-C1C-NC	2.96	128.69	124.20
22	B	852	BCR	C19-C18-C17	-2.96	114.40	118.94
21	K	105	LMU	C1'-C2'-C3'	-2.96	103.84	110.00
20	A	801	CLA	CAA-C2A-C1A	2.96	121.66	111.97
20	A	823	CLA	CMB-C2B-C3B	2.95	130.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	313	CLA	C2B-C3B-C4B	2.95	108.82	106.29
20	B	810	CLA	CAC-C3C-C4C	2.95	128.64	124.81
20	B	804	CLA	C4A-NA-C1A	2.95	108.03	106.71
22	B	844	BCR	C36-C18-C19	2.95	122.73	118.08
20	B	849	CLA	O2D-CGD-CBD	2.95	116.52	111.27
21	R	105	LMU	O5'-C5'-C6'	2.95	113.78	106.44
20	2	312	CLA	C1-O2A-CGA	2.95	124.19	116.44
22	L	210	BCR	C15-C14-C13	2.95	131.52	127.31
20	B	807	CLA	CMA-C3A-C4A	-2.95	103.84	111.77
20	1	209	CLA	CBD-CHA-C1A	2.95	132.15	127.43
20	4	309	CLA	C2C-C1C-CHC	-2.95	118.61	125.67
20	4	305	CLA	CHD-C4C-NC	2.95	128.85	124.20
20	B	816	CLA	CHB-C4A-NA	2.95	128.59	124.51
20	A	836	CLA	C4D-C3D-CAD	2.95	110.11	108.47
20	3	318	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
20	B	851	CLA	O2A-CGA-CBA	2.95	121.15	111.91
20	B	806	CLA	C11-C12-C13	-2.94	106.40	115.92
20	A	807	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
20	K	103	CLA	C4-C3-C5	2.94	120.22	115.27
20	K	103	CLA	O2A-CGA-CBA	2.94	121.13	111.91
21	1	219	LMU	C4B-C3B-C2B	2.94	115.95	110.82
21	H	104	LMU	O1B-C1B-C2B	2.94	115.72	108.10
22	B	852	BCR	C36-C18-C17	-2.94	118.81	122.92
20	2	311	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
20	4	316	CLA	CBA-CAA-C2A	-2.94	105.19	113.86
21	L	205	LMU	O5'-C1'-O1'	-2.94	103.02	109.97
20	4	315	CLA	C3C-C4C-CHD	-2.94	118.79	125.22
20	B	840	CLA	C1B-C2B-C3B	-2.94	104.19	106.92
20	B	830	CLA	C1-C2-C3	-2.93	120.97	126.04
20	A	828	CLA	CAA-C2A-C1A	-2.93	102.36	111.97
22	I	103	BCR	C24-C25-C26	2.93	128.57	121.46
20	A	807	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
20	B	822	CLA	CAC-C3C-C2C	-2.93	122.51	127.53
20	B	804	CLA	CHB-C4A-NA	2.93	128.57	124.51
21	L	211	LMU	O5'-C5'-C6'	2.93	113.73	106.44
20	4	302	CLA	C1-C2-C3	-2.93	120.97	126.04
21	R	104	LMU	O1B-C4'-C3'	2.93	115.08	107.28
20	B	850	CLA	C6-C5-C3	2.93	121.14	113.45
20	B	821	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
21	B	801	LMU	O3B-C3B-C2B	2.93	117.13	110.35
20	B	826	CLA	C11-C12-C13	-2.93	106.44	115.92
20	1	211	CLA	CHB-C4A-NA	2.93	128.83	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	810	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
20	2	310	CLA	C4A-NA-C1A	2.93	108.02	106.71
20	A	807	CLA	C4A-NA-C1A	2.93	108.02	106.71
20	A	833	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	4	306	CLA	CHC-C1C-NC	2.93	128.64	124.20
21	R	106	LMU	C4B-C3B-C2B	-2.93	105.71	110.82
20	A	815	CLA	CAC-C3C-C4C	2.93	128.61	124.81
21	E	101	LMU	O1B-C4'-C3'	2.92	115.06	107.28
20	1	209	CLA	C1B-C2B-C3B	-2.92	104.20	106.92
20	B	807	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
20	B	829	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
20	4	307	CLA	CMA-C3A-C2A	-2.92	102.05	113.83
20	B	816	CLA	CGD-CBD-CAD	-2.92	101.27	110.73
20	A	815	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
20	B	838	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
20	B	811	CLA	CHB-C4A-NA	2.92	128.55	124.51
21	R	101	LMU	C1B-C2B-C3B	2.92	116.07	110.00
21	1	218	LMU	C3B-C4B-C5B	-2.92	105.04	110.24
20	A	812	CLA	CHB-C4A-NA	2.91	128.54	124.51
20	A	839	CLA	CBA-CAA-C2A	2.91	122.46	113.86
20	1	202	CLA	C4A-NA-C1A	2.91	108.02	106.71
20	A	827	CLA	CHB-C4A-NA	2.91	128.54	124.51
20	H	103	CLA	O2A-CGA-CBA	2.91	121.04	111.91
20	A	823	CLA	CHB-C4A-NA	2.91	128.54	124.51
21	H	106	LMU	O1B-C4'-C3'	-2.91	99.54	107.28
20	2	310	CLA	C3D-C2D-C1D	2.91	108.81	106.30
20	3	302	CLA	CAC-C3C-C4C	2.91	128.58	124.81
21	1	219	LMU	O1B-C1B-O5B	-2.91	102.55	110.67
20	B	812	CLA	CMC-C2C-C1C	2.91	129.46	125.04
20	A	831	CLA	CED-O2D-CGD	2.91	122.51	115.94
23	B	841	PQN	C16-C15-C13	-2.91	105.84	113.45
20	L	207	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
20	A	809	CLA	O2A-CGA-O1A	-2.91	116.26	123.59
20	3	313	CLA	C4-C3-C5	2.90	120.15	115.27
22	F	203	BCR	C23-C22-C21	2.90	123.39	118.94
20	B	820	CLA	CAC-C3C-C4C	2.90	128.57	124.81
20	A	814	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
20	1	210	CLA	O2A-C1-C2	2.90	116.26	108.64
20	B	822	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
21	E	101	LMU	O3'-C3'-C4'	2.90	117.62	109.94
20	A	806	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
20	3	311	CLA	C4-C3-C2	-2.89	116.25	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	105	LMU	C2'-C3'-C4'	2.89	116.29	109.68
20	I	102	CLA	CHB-C4A-NA	2.89	128.51	124.51
21	B	847	LMU	C1'-O5'-C5'	2.89	119.37	113.69
20	B	814	CLA	CMD-C2D-C3D	-2.89	119.27	124.68
20	A	841	CLA	C6-C7-C8	-2.89	106.57	115.92
20	2	308	CLA	CMD-C2D-C3D	-2.89	119.27	124.68
21	3	322	LMU	O4'-C4B-C3B	2.89	117.03	110.35
20	4	307	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
20	A	808	CLA	O2A-C1-C2	2.89	116.23	108.64
20	2	322	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	I	101	BCR	C32-C1-C31	-2.89	99.66	108.53
21	L	204	LMU	O5'-C1'-C2'	2.89	116.46	110.35
21	H	108	LMU	C1B-O5B-C5B	-2.89	108.02	113.69
20	A	834	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
20	2	322	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
20	A	823	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	3	312	CLA	C2B-C3B-C4B	2.89	108.76	106.29
20	A	804	CLA	CBA-CAA-C2A	2.89	122.38	113.86
20	A	819	CLA	CED-O2D-CGD	2.89	122.46	115.94
20	A	806	CLA	C4A-NA-C1A	2.88	108.00	106.71
20	B	827	CLA	OBD-CAD-CBD	-2.88	121.77	125.89
20	B	826	CLA	C1-C2-C3	-2.88	121.06	126.04
20	4	307	CLA	C3B-C4B-NB	2.88	112.94	109.21
20	A	852	CLA	C4A-NA-C1A	2.88	108.00	106.71
20	A	818	CLA	O2A-CGA-CBA	2.88	120.95	111.91
20	B	815	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
20	3	318	CLA	CMD-C2D-C3D	-2.88	119.29	124.68
21	L	211	LMU	O3B-C3B-C2B	-2.88	103.69	110.35
20	B	822	CLA	CMD-C2D-C3D	-2.88	119.29	124.68
20	2	310	CLA	C3C-C4C-CHD	-2.88	118.91	125.22
20	A	813	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
20	3	313	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
20	1	216	CLA	C2C-C1C-CHC	-2.88	118.78	125.67
21	4	321	LMU	C1'-C2'-C3'	2.88	115.99	110.00
20	A	833	CLA	CHB-C4A-NA	2.88	128.49	124.51
20	A	837	CLA	CMD-C2D-C3D	-2.88	119.30	124.68
20	4	313	CLA	C3C-C4C-CHD	-2.88	118.92	125.22
20	A	820	CLA	O2A-CGA-CBA	2.87	120.93	111.91
20	K	103	CLA	CAA-CBA-CGA	-2.87	104.85	113.25
20	4	310	CLA	C2C-C1C-CHC	-2.87	118.79	125.67
20	2	303	CLA	CAC-C3C-C4C	2.87	128.54	124.81
20	A	807	CLA	CED-O2D-CGD	2.87	122.44	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	306	CLA	CHB-C4A-NA	2.87	128.74	124.34
20	H	101	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
22	F	202	BCR	C28-C27-C26	-2.87	108.95	114.08
21	R	105	LMU	O5B-C5B-C6B	2.87	113.58	106.44
20	3	311	CLA	C3D-CAD-CBD	-2.87	103.82	107.61
20	A	810	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	A	836	CLA	CHB-C4A-NA	2.87	128.48	124.51
20	1	202	CLA	CAC-C3C-C2C	-2.87	122.62	127.53
20	B	851	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
20	K	102	CLA	C5-C3-C4	2.87	120.94	114.60
20	2	309	CLA	C2C-C1C-CHC	-2.87	118.80	125.67
20	1	205	CLA	C2C-C1C-CHC	-2.87	118.80	125.67
21	K	104	LMU	O2'-C2'-C1'	-2.87	103.08	110.05
20	B	815	CLA	CMD-C2D-C3D	-2.87	119.31	124.68
20	B	830	CLA	C4A-NA-C1A	2.87	108.00	106.71
20	2	315	CLA	C4A-NA-C1A	2.87	108.00	106.71
20	B	849	CLA	O2A-CGA-CBA	2.87	120.90	111.91
20	B	828	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
20	2	309	CLA	C3B-C2B-C1B	-2.86	103.84	106.29
20	B	806	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
20	A	812	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
20	K	101	CLA	CHB-C4A-NA	2.86	128.47	124.51
20	A	840	CLA	CHD-C4C-C3C	-2.86	120.63	124.84
20	1	210	CLA	CHB-C4A-NA	2.86	128.47	124.51
20	4	318	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
20	A	835	CLA	O2A-CGA-CBA	2.86	120.88	111.91
20	1	212	CLA	C3C-C4C-CHD	-2.86	118.96	125.22
20	B	809	CLA	O2A-CGA-CBA	2.86	120.87	111.91
22	I	103	BCR	C23-C22-C21	2.86	123.32	118.94
20	3	311	CLA	CBC-CAC-C3C	-2.86	104.56	112.43
20	H	101	CLA	CGD-CBD-CAD	2.86	119.98	110.73
20	B	806	CLA	CAC-C3C-C4C	2.85	128.51	124.81
21	A	849	LMU	O2B-C2B-C1B	-2.85	103.11	110.05
20	4	310	CLA	C3A-C4A-NA	2.85	115.91	109.92
20	A	825	CLA	C4-C3-C5	2.85	120.07	115.27
20	A	832	CLA	C4A-NA-C1A	2.85	107.99	106.71
20	B	803	CLA	CHB-C4A-NA	2.85	128.46	124.51
20	B	819	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
21	H	108	LMU	O5'-C1'-O1'	2.85	116.72	109.97
20	B	806	CLA	CMB-C2B-C1B	2.85	132.84	128.46
20	B	829	CLA	CED-O2D-CGD	2.85	122.38	115.94
20	2	311	CLA	CHB-C4A-NA	2.85	128.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	314	BCR	C34-C9-C10	-2.85	118.94	122.92
20	4	312	CLA	C2C-C1C-CHC	-2.85	118.86	125.67
20	3	313	CLA	CAC-C3C-C4C	2.85	128.50	124.81
20	A	819	CLA	C1-O2A-CGA	2.84	123.91	116.44
20	L	203	CLA	CMD-C2D-C3D	-2.84	119.36	124.68
20	3	311	CLA	CMC-C2C-C1C	2.84	129.37	125.04
20	H	103	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
20	A	801	CLA	CMA-C3A-C4A	2.84	119.41	111.77
20	A	806	CLA	O2A-CGA-CBA	2.84	120.82	111.91
20	B	830	CLA	CHB-C4A-NA	2.84	128.44	124.51
20	B	828	CLA	CHD-C4C-NC	2.84	128.68	124.20
20	4	311	CLA	CED-O2D-CGD	2.84	122.36	115.94
21	H	104	LMU	O3'-C3'-C2'	2.84	116.91	110.35
20	3	303	CLA	C2C-C1C-CHC	-2.84	118.87	125.67
21	A	856	LMU	O5'-C1'-C2'	2.84	116.35	110.35
21	A	855	LMU	O5B-C5B-C6B	2.84	113.49	106.44
20	3	310	CLA	C1D-CHD-C4C	-2.84	119.08	126.10
20	3	318	CLA	CAC-C3C-C4C	2.83	128.49	124.81
20	B	811	CLA	O2A-CGA-CBA	2.83	120.80	111.91
20	A	840	CLA	CHB-C4A-NA	2.83	128.43	124.51
20	2	315	CLA	C2A-C3A-C4A	-2.83	99.73	104.18
20	A	825	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
21	4	321	LMU	O5'-C5'-C4'	2.83	115.72	109.75
20	A	805	CLA	CAC-C3C-C4C	2.83	128.48	124.81
20	A	822	CLA	CMC-C2C-C1C	2.83	129.35	125.04
20	2	316	CLA	C4A-NA-C1A	2.83	107.98	106.71
20	4	315	CLA	C3B-C2B-C1B	-2.83	103.87	106.29
20	F	206	CLA	O2A-CGA-CBA	2.83	120.78	111.91
21	B	847	LMU	O1B-C4'-C5'	2.83	117.20	109.45
20	1	207	CLA	CAA-CBA-CGA	2.83	121.52	113.25
20	1	201	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
20	I	102	CLA	O1D-CGD-CBD	-2.83	118.70	124.48
20	L	202	CLA	O2A-CGA-CBA	2.83	120.78	111.91
20	3	313	CLA	O2D-CGD-CBD	2.83	116.29	111.27
20	B	814	CLA	CHB-C4A-NA	2.83	128.42	124.51
20	2	307	CLA	C11-C12-C13	-2.82	106.79	115.92
20	A	835	CLA	C1-C2-C3	-2.82	121.16	126.04
20	B	809	CLA	O1D-CGD-CBD	-2.82	118.70	124.48
20	A	840	CLA	O1D-CGD-CBD	-2.82	118.70	124.48
20	4	309	CLA	C3D-C2D-C1D	2.82	108.73	106.30
21	B	802	LMU	C1'-C2'-C3'	2.82	115.88	110.00
20	2	311	CLA	CHC-C1C-C2C	-2.82	118.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	814	CLA	C4A-NA-C1A	2.82	107.97	106.71
20	A	840	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
20	A	827	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
20	R	108	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
21	B	802	LMU	C4B-C3B-C2B	-2.82	105.90	110.82
22	B	846	BCR	C3-C4-C5	-2.82	109.04	114.08
20	4	309	CLA	C1C-NC-C4C	2.82	107.97	106.71
20	B	823	CLA	O2A-CGA-CBA	2.82	120.75	111.91
20	R	108	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
21	L	205	LMU	C1B-C2B-C3B	-2.82	104.13	110.00
20	A	806	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	L	209	CLA	CAA-C2A-C1A	2.81	121.19	111.97
20	B	817	CLA	C4-C3-C5	2.81	120.00	115.27
20	A	810	CLA	O1D-CGD-CBD	-2.81	118.74	124.48
21	A	856	LMU	O5'-C5'-C4'	-2.81	103.83	109.75
20	3	302	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
21	H	107	LMU	C1'-C2'-C3'	-2.81	104.15	110.00
20	2	322	CLA	CAC-C3C-C2C	-2.81	122.73	127.53
20	A	819	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
20	B	838	CLA	O2A-CGA-O1A	-2.80	116.51	123.59
20	3	304	CLA	CMB-C2B-C3B	2.80	130.18	124.69
20	B	816	CLA	CAC-C3C-C4C	2.80	128.45	124.81
22	3	314	BCR	C24-C23-C22	-2.80	122.00	126.23
20	A	825	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
20	B	825	CLA	CMB-C2B-C3B	2.80	129.92	124.68
20	3	311	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
20	1	212	CLA	C2A-C3A-C4A	-2.80	99.78	104.18
20	A	833	CLA	C3C-C4C-NC	-2.80	107.43	110.57
20	3	307	CLA	CHB-C4A-NA	2.80	128.63	124.34
21	A	855	LMU	C1B-C2B-C3B	2.80	115.83	110.00
21	K	106	LMU	O1B-C4'-C3'	2.80	114.72	107.28
21	H	105	LMU	O1B-C4'-C3'	2.80	114.72	107.28
20	A	818	CLA	CMB-C2B-C3B	2.80	129.91	124.68
21	L	205	LMU	O4'-C4B-C5B	-2.79	102.36	109.30
20	K	108	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
20	1	206	CLA	C1-O2A-CGA	2.79	123.77	116.44
20	2	322	CLA	C11-C12-C13	-2.79	106.89	115.92
20	B	827	CLA	O1D-CGD-CBD	-2.79	118.77	124.48
21	C	101	LMU	C4B-C3B-C2B	2.79	115.69	110.82
21	G	101	LMU	O3B-C3B-C2B	-2.79	103.90	110.35
20	B	817	CLA	CMC-C2C-C1C	2.79	129.29	125.04
21	A	856	LMU	O3'-C3'-C4'	2.79	117.33	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	207	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
20	L	201	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
21	B	847	LMU	O3B-C3B-C2B	-2.78	103.91	110.35
20	H	109	CLA	O2A-CGA-CBA	2.78	120.64	111.91
20	B	812	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
20	A	805	CLA	C1-O2A-CGA	2.78	123.74	116.44
20	A	815	CLA	CMD-C2D-C3D	-2.78	119.48	124.68
20	2	308	CLA	CHD-C4C-C3C	-2.78	120.75	124.84
20	3	313	CLA	CMD-C2D-C3D	-2.78	119.48	124.68
20	2	305	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
20	1	211	CLA	C2C-C1C-CHC	-2.78	119.02	125.67
20	3	309	CLA	C2A-C3A-C4A	-2.78	99.82	104.18
21	1	213	LMU	C6'-C5'-C4'	-2.78	105.24	113.33
20	B	850	CLA	CAA-C2A-C1A	2.78	121.08	111.97
20	B	818	CLA	O2A-CGA-CBA	2.78	120.62	111.91
20	A	839	CLA	CED-O2D-CGD	2.78	122.22	115.94
21	H	107	LMU	C1-O1'-C1'	-2.78	109.24	113.84
20	B	822	CLA	C1-O2A-CGA	2.77	123.72	116.44
20	A	802	CLA	C2A-C3A-C4A	-2.77	99.83	104.18
21	A	855	LMU	C4B-C3B-C2B	-2.77	105.98	110.82
20	B	849	CLA	CAC-C3C-C4C	2.77	128.41	124.81
20	L	202	CLA	CMD-C2D-C3D	-2.77	119.50	124.68
20	H	102	CLA	O2A-CGA-CBA	2.77	120.60	111.91
20	A	822	CLA	O2D-CGD-CBD	2.77	116.19	111.27
20	A	811	CLA	C3A-C2A-C1A	2.77	105.48	101.34
20	A	834	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
20	B	810	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
20	B	829	CLA	CMC-C2C-C1C	2.77	129.25	125.04
20	B	816	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
20	A	824	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
20	2	310	CLA	C2A-C3A-C4A	-2.76	99.85	104.18
20	B	812	CLA	O1D-CGD-CBD	-2.76	118.83	124.48
20	3	301	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	B	816	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
20	3	309	CLA	C3D-C4D-ND	2.76	112.54	110.14
21	L	204	LMU	C6'-C5'-C4'	-2.76	105.30	113.33
20	B	806	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
20	A	841	CLA	CMB-C2B-C1B	2.76	132.70	128.46
22	F	203	BCR	C35-C13-C12	2.76	122.42	118.08
20	B	811	CLA	C9-C8-C7	-2.75	101.31	111.29
20	A	815	CLA	CBA-CAA-C2A	-2.75	105.73	113.86
20	B	849	CLA	CGD-CBD-CAD	2.75	119.65	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	809	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
21	2	319	LMU	O1B-C4'-C3'	2.75	114.60	107.28
20	B	849	CLA	C16-C17-C18	-2.75	103.01	115.98
20	B	830	CLA	CAA-CBA-CGA	-2.75	105.21	113.25
20	4	316	CLA	CMB-C2B-C3B	2.75	129.82	124.68
20	B	805	CLA	O2A-CGA-CBA	2.75	120.54	111.91
21	1	218	LMU	O5'-C5'-C6'	2.75	113.27	106.44
20	J	101	CLA	CHB-C4A-NA	2.75	128.31	124.51
21	H	108	LMU	C3B-C4B-C5B	-2.75	105.34	110.24
20	A	832	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
22	I	101	BCR	C40-C30-C25	2.75	114.76	110.30
20	3	308	CLA	CHB-C4A-NA	2.75	128.31	124.51
20	B	834	CLA	C4A-NA-C1A	2.75	107.94	106.71
21	R	106	LMU	O5'-C5'-C4'	2.75	115.54	109.75
20	A	803	CLA	C5-C3-C4	2.75	120.67	114.60
20	4	318	CLA	CGD-CBD-CAD	2.75	119.63	110.73
22	B	842	BCR	C3-C4-C5	-2.74	109.18	114.08
20	K	103	CLA	C6-C7-C8	-2.74	107.06	115.92
22	F	202	BCR	C3-C4-C5	-2.74	109.18	114.08
20	A	811	CLA	CAA-CBA-CGA	2.74	121.26	113.25
20	L	209	CLA	CHC-C1C-NC	2.74	128.36	124.20
20	2	310	CLA	C2C-C1C-CHC	-2.74	119.11	125.67
20	B	823	CLA	C4-C3-C5	2.74	119.88	115.27
20	4	305	CLA	C4-C3-C5	2.74	119.88	115.27
20	B	839	CLA	CMB-C2B-C1B	2.74	132.67	128.46
20	1	215	CLA	OBD-CAD-CBD	-2.74	121.99	125.89
20	4	314	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
20	B	812	CLA	CED-O2D-CGD	2.73	122.12	115.94
20	H	101	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
20	A	840	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
20	3	312	CLA	C3A-C4A-NA	2.73	115.66	109.92
20	B	849	CLA	CMB-C2B-C3B	2.73	129.79	124.68
21	K	106	LMU	O5'-C1'-C2'	2.73	116.13	110.35
20	1	214	CLA	C2C-C1C-CHC	-2.73	119.13	125.67
22	A	843	BCR	C23-C24-C25	-2.73	119.53	127.20
20	A	825	CLA	O2A-CGA-CBA	2.73	120.48	111.91
21	A	855	LMU	C1'-O5'-C5'	-2.73	108.33	113.69
20	A	826	CLA	C6-C7-C8	-2.73	107.09	115.92
20	L	203	CLA	CHC-C1C-NC	2.73	128.34	124.20
20	4	312	CLA	CHB-C4A-NA	2.73	128.52	124.34
21	1	219	LMU	C6B-C5B-C4B	2.73	119.40	113.00
20	2	316	CLA	CMD-C2D-C3D	-2.73	119.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	102	CLA	C4-C3-C2	-2.73	116.68	123.68
20	L	208	CLA	O2A-CGA-CBA	2.73	120.47	111.91
21	2	318	LMU	O3'-C3'-C4'	-2.73	102.71	109.94
20	L	203	CLA	C4-C3-C2	-2.73	116.68	123.68
20	K	108	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
20	3	316	CLA	C3C-C4C-CHD	-2.73	119.25	125.22
21	4	301	LMU	C1B-O1B-C4'	-2.73	111.22	117.96
21	A	855	LMU	O5'-C5'-C6'	-2.72	99.66	106.44
22	F	203	BCR	C33-C5-C4	2.72	118.85	113.62
22	A	844	BCR	C8-C7-C6	-2.72	119.56	127.20
20	B	811	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
20	A	808	CLA	C1-C2-C3	-2.72	121.34	126.04
20	1	203	CLA	CAC-C3C-C4C	2.72	128.34	124.81
20	3	306	CLA	C2A-C3A-C4A	-2.72	99.92	104.18
20	2	322	CLA	CED-O2D-CGD	2.72	122.08	115.94
20	2	303	CLA	C4A-NA-C1A	2.72	107.93	106.71
21	A	856	LMU	O5'-C5'-C6'	2.71	113.18	106.44
20	F	206	CLA	C3D-CAD-CBD	-2.71	104.03	107.61
20	A	837	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
20	3	313	CLA	CMC-C2C-C1C	2.71	129.17	125.04
20	A	817	CLA	CHB-C4A-NA	2.71	128.26	124.51
20	H	102	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
20	L	209	CLA	C1-C2-C3	-2.71	122.36	126.75
20	H	101	CLA	CAC-C3C-C2C	-2.71	122.89	127.53
21	A	854	LMU	O5B-C5B-C4B	-2.71	104.77	109.69
20	R	107	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
20	A	820	CLA	C4A-NA-C1A	2.71	107.92	106.71
21	H	107	LMU	O1B-C4'-C5'	2.71	116.87	109.45
20	4	313	CLA	C1C-NC-C4C	-2.71	105.49	106.71
21	B	802	LMU	O2B-C2B-C1B	2.71	116.62	110.05
21	1	220	LMU	O1'-C1'-C2'	2.71	112.53	108.30
20	B	817	CLA	O1D-CGD-CBD	-2.71	118.95	124.48
21	A	853	LMU	C1B-O1B-C4'	-2.70	111.27	117.96
20	B	824	CLA	O2A-CGA-CBA	2.70	120.39	111.91
20	B	834	CLA	O2A-C1-C2	2.70	115.74	108.64
20	B	824	CLA	C4-C3-C5	2.70	119.82	115.27
22	J	102	BCR	C23-C24-C25	-2.70	119.61	127.20
20	A	816	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	L	203	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
20	A	808	CLA	CMB-C2B-C3B	2.70	129.73	124.68
20	B	814	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
20	3	317	CLA	CAA-CBA-CGA	2.70	121.14	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	812	CLA	CAC-C3C-C4C	2.70	128.31	124.81
20	1	203	CLA	C4A-NA-C1A	2.70	107.92	106.71
21	N	101	LMU	C1'-O5'-C5'	2.70	118.99	113.69
20	B	826	CLA	O1D-CGD-CBD	-2.70	118.96	124.48
20	1	206	CLA	C1-C2-C3	-2.70	121.38	126.04
20	B	807	CLA	CHD-C4C-C3C	-2.70	120.87	124.84
20	A	814	CLA	CMB-C2B-C1B	2.70	132.61	128.46
20	A	835	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	A	844	BCR	C23-C24-C25	-2.70	119.62	127.20
21	2	318	LMU	C4B-C3B-C2B	-2.70	106.11	110.82
20	3	317	CLA	O2A-CGA-CBA	2.70	120.37	111.91
20	1	203	CLA	CHC-C1C-NC	2.70	128.29	124.20
20	A	803	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
20	A	826	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
25	B	848	LMG	O8-C28-C29	2.70	120.37	111.91
20	3	316	CLA	C2C-C1C-CHC	-2.70	119.21	125.67
20	1	212	CLA	C2C-C1C-CHC	-2.70	119.21	125.67
21	L	211	LMU	O5B-C5B-C4B	2.70	114.59	109.69
21	H	106	LMU	C1B-O1B-C4'	-2.69	111.30	117.96
20	3	319	CLA	C2A-C3A-C4A	-2.69	99.96	104.18
21	4	322	LMU	C3B-C4B-C5B	2.69	115.04	110.24
22	B	843	BCR	C23-C24-C25	-2.69	119.64	127.20
20	4	302	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	K	106	LMU	O5'-C5'-C6'	2.69	113.13	106.44
20	4	302	CLA	C4-C3-C5	2.69	119.80	115.27
20	B	818	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
20	R	107	CLA	C4A-NA-C1A	2.69	107.92	106.71
20	A	822	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
20	F	205	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
20	H	109	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
20	J	103	CLA	CHB-C4A-NA	2.69	128.23	124.51
20	3	304	CLA	CBD-CHA-C1A	2.69	131.73	127.43
21	1	218	LMU	O3'-C3'-C4'	-2.69	102.83	109.94
20	B	830	CLA	C1-O2A-CGA	2.69	123.49	116.44
20	4	318	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
20	A	835	CLA	O1D-CGD-CBD	-2.68	118.99	124.48
20	A	805	CLA	CED-O2D-CGD	2.68	122.01	115.94
20	A	824	CLA	C4-C3-C5	2.68	119.78	115.27
21	R	106	LMU	O3B-C3B-C2B	-2.68	104.15	110.35
20	A	828	CLA	C1-C2-C3	-2.68	121.40	126.04
20	3	305	CLA	C3B-C4B-NB	2.68	112.46	110.11
22	B	846	BCR	C8-C7-C6	-2.68	119.67	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	K	103	CLA	CMC-C2C-C1C	2.68	129.12	125.04
20	A	823	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
20	A	812	CLA	O2A-CGA-CBA	2.68	120.32	111.91
20	B	838	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
20	1	202	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
20	A	803	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
20	B	814	CLA	CAC-C3C-C4C	2.68	128.28	124.81
20	B	818	CLA	C4A-NA-C1A	2.68	107.91	106.71
20	A	828	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
20	A	806	CLA	CAA-C2A-C1A	-2.67	103.21	111.97
20	K	102	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
20	A	817	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
20	A	852	CLA	CGD-CBD-CAD	2.67	119.39	110.73
21	L	205	LMU	O2'-C2'-C1'	-2.67	103.55	110.05
20	B	813	CLA	CED-O2D-CGD	2.67	121.98	115.94
22	A	843	BCR	C3-C4-C5	-2.67	109.31	114.08
22	J	102	BCR	C8-C7-C6	-2.67	119.70	127.20
20	B	840	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	L	210	BCR	C37-C22-C21	-2.67	119.18	122.92
22	I	103	BCR	C40-C30-C25	-2.67	105.97	110.30
20	A	815	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
20	B	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	A	804	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
20	H	102	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
21	K	109	LMU	O3B-C3B-C2B	2.67	116.51	110.35
20	4	315	CLA	C3D-C2D-C1D	2.67	108.60	106.30
20	2	301	CLA	C3C-C4C-NC	2.67	112.43	109.97
20	B	810	CLA	CHB-C4A-NA	2.66	128.20	124.51
20	2	308	CLA	O2A-CGA-CBA	2.66	120.27	111.91
20	A	824	CLA	O2A-CGA-CBA	2.66	120.27	111.91
21	H	104	LMU	C1B-O1B-C4'	-2.66	111.37	117.96
20	A	828	CLA	CED-O2D-CGD	2.66	121.96	115.94
21	A	848	LMU	C3'-C4'-C5'	2.66	117.03	110.93
22	B	846	BCR	C23-C24-C25	-2.66	119.72	127.20
20	2	308	CLA	CHB-C4A-NA	2.66	128.19	124.51
20	4	304	CLA	C1C-C2C-C3C	2.66	109.75	106.96
20	2	302	CLA	O2A-CGA-CBA	2.66	120.26	111.91
20	B	809	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
20	A	838	CLA	CMA-C3A-C4A	-2.66	104.62	111.77
20	3	307	CLA	C2A-C3A-C4A	-2.66	100.00	104.18
20	1	203	CLA	O2A-CGA-CBA	2.66	120.26	111.91
20	B	840	CLA	CMC-C2C-C1C	2.66	129.09	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	847	BCR	C3-C4-C5	-2.66	109.33	114.08
21	1	219	LMU	O1'-C1'-C2'	2.66	112.46	108.30
21	A	849	LMU	O3B-C3B-C2B	2.66	116.50	110.35
21	A	855	LMU	O1B-C1B-C2B	2.66	114.99	108.10
20	F	204	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
20	A	813	CLA	CAA-CBA-CGA	-2.66	105.48	113.25
20	A	838	CLA	CMB-C2B-C3B	2.66	129.65	124.68
21	H	105	LMU	O3'-C3'-C4'	-2.66	102.90	109.94
21	2	318	LMU	O5'-C5'-C6'	2.66	113.04	106.44
20	2	316	CLA	C4-C3-C5	2.66	119.74	115.27
20	B	815	CLA	O2A-CGA-CBA	2.66	120.25	111.91
21	K	105	LMU	O2'-C2'-C1'	2.66	116.50	110.05
20	3	308	CLA	CAC-C3C-C2C	-2.66	122.99	127.53
20	3	303	CLA	C3A-C2A-C1A	-2.65	100.01	104.18
20	A	813	CLA	CMD-C2D-C3D	-2.65	119.71	124.68
20	R	108	CLA	C6-C7-C8	-2.65	107.34	115.92
20	B	822	CLA	CMC-C2C-C1C	2.65	129.08	125.04
20	L	201	CLA	CMA-C3A-C4A	2.65	118.90	111.77
22	I	101	BCR	C34-C9-C8	-2.65	113.90	118.08
20	A	824	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
20	A	829	CLA	CMD-C2D-C3D	-2.65	119.72	124.68
20	B	824	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
20	A	801	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
20	4	319	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	A	830	CLA	C4A-NA-C1A	2.65	107.90	106.71
22	B	846	BCR	C28-C27-C26	-2.65	109.35	114.08
20	B	839	CLA	C4-C3-C5	2.65	119.73	115.27
20	4	308	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
21	A	855	LMU	C8-C7-C6	-2.65	100.98	114.42
21	1	219	LMU	O2'-C2'-C1'	2.65	116.48	110.05
20	1	206	CLA	C4-C3-C5	2.65	119.72	115.27
20	B	826	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
20	2	316	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
20	K	103	CLA	C1-O2A-CGA	2.65	123.39	116.44
20	A	803	CLA	O2A-CGA-CBA	2.65	120.21	111.91
21	K	104	LMU	O2B-C2B-C1B	-2.64	103.62	110.05
22	F	203	BCR	C7-C8-C9	2.64	130.23	126.23
20	2	301	CLA	C3C-C4C-CHD	-2.64	119.43	125.22
20	B	803	CLA	C3A-C2A-C1A	2.64	105.30	101.34
20	A	815	CLA	C2A-C3A-C4A	2.64	106.14	101.87
20	L	201	CLA	CMB-C2B-C3B	2.64	129.62	124.68
20	3	309	CLA	C3C-C4C-CHD	-2.64	119.44	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	219	LMU	O5'-C5'-C4'	-2.64	104.19	109.75
20	4	307	CLA	CMA-C3A-C4A	-2.64	104.68	111.77
22	3	314	BCR	C37-C22-C21	-2.64	119.23	122.92
20	1	206	CLA	C4A-NA-C1A	2.64	107.89	106.71
20	A	812	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	F	203	BCR	C39-C30-C25	2.64	114.58	110.30
20	B	818	CLA	C1-O2A-CGA	2.64	123.36	116.44
22	A	843	BCR	C8-C7-C6	-2.64	119.80	127.20
20	F	204	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
20	A	817	CLA	O2A-C1-C2	2.64	115.56	108.64
21	K	105	LMU	C1-O1'-C1'	-2.64	109.47	113.84
20	3	310	CLA	CHB-C4A-NA	2.64	128.37	124.34
20	4	302	CLA	CHC-C1C-C2C	-2.63	119.43	126.72
20	1	204	CLA	OBD-CAD-CBD	2.63	129.66	125.89
20	2	315	CLA	C2C-C1C-CHC	-2.63	119.36	125.67
21	1	220	LMU	O5B-C5B-C4B	2.63	114.48	109.69
21	G	101	LMU	O5'-C1'-C2'	-2.63	104.77	110.35
20	A	823	CLA	C4A-NA-C1A	2.63	107.89	106.71
20	B	828	CLA	C1-C2-C3	-2.63	122.50	126.75
21	R	101	LMU	C1'-O5'-C5'	-2.63	108.52	113.69
20	A	852	CLA	O2A-C1-C2	2.63	115.55	108.64
20	A	817	CLA	C1-O2A-CGA	2.63	123.34	116.44
20	L	202	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
21	4	317	LMU	O1'-C1'-C2'	2.63	112.41	108.30
20	B	809	CLA	O2A-C1-C2	2.63	115.54	108.64
20	H	101	CLA	CMA-C3A-C2A	-2.63	103.24	113.83
21	L	204	LMU	O2B-C2B-C3B	2.63	116.42	110.35
21	K	104	LMU	C1B-O5B-C5B	-2.63	108.53	113.69
21	E	101	LMU	O2B-C2B-C3B	-2.63	104.28	110.35
20	J	103	CLA	O2A-CGA-CBA	2.62	120.14	111.91
20	F	204	CLA	CBD-CHA-C1A	2.62	131.63	127.43
21	K	105	LMU	O6'-C6'-C5'	2.62	120.30	111.29
20	A	814	CLA	CED-O2D-CGD	2.62	121.87	115.94
20	B	837	CLA	CMD-C2D-C3D	-2.62	119.77	124.68
20	1	210	CLA	C2A-C3A-C4A	2.62	106.10	101.87
20	B	850	CLA	CMC-C2C-C1C	2.62	129.03	125.04
20	4	316	CLA	C3A-C2A-C1A	2.62	105.26	101.34
22	A	846	BCR	C3-C4-C5	-2.62	109.40	114.08
20	A	830	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
21	H	106	LMU	O6'-C6'-C5'	-2.62	102.31	111.29
20	A	804	CLA	C4A-NA-C1A	2.62	107.88	106.71
20	A	819	CLA	C1B-CHB-C4A	-2.62	124.93	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	838	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	A	836	CLA	CHC-C1C-C2C	-2.62	119.49	126.72
20	1	215	CLA	CMA-C3A-C4A	2.61	118.80	111.77
21	C	101	LMU	O5B-C5B-C4B	-2.61	104.95	109.69
20	4	304	CLA	C2C-C1C-NC	-2.61	107.52	109.97
21	G	101	LMU	C1'-O5'-C5'	2.61	118.82	113.69
20	B	815	CLA	CED-O2D-CGD	2.61	121.85	115.94
20	3	320	CLA	C2C-C1C-CHC	-2.61	119.41	125.67
20	B	823	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
20	H	103	CLA	CGD-CBD-CAD	-2.61	102.27	110.73
20	3	320	CLA	CHB-C4A-NA	2.61	128.33	124.34
20	A	838	CLA	C4-C3-C2	-2.61	116.99	123.68
20	H	101	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	4	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	B	851	CLA	C1-C2-C3	-2.61	121.53	126.04
20	B	817	CLA	CAA-C2A-C1A	2.61	120.52	111.97
20	G	102	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
20	2	322	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
20	2	302	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
20	B	804	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
20	A	820	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
20	A	836	CLA	OBD-CAD-CBD	-2.61	122.17	125.89
20	G	102	CLA	O2A-CGA-CBA	2.61	120.08	111.91
20	I	102	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
21	2	318	LMU	C3'-C4'-C5'	2.60	116.90	110.93
20	2	316	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
20	A	803	CLA	CMD-C2D-C3D	-2.60	119.81	124.68
20	A	850	CLA	CHC-C1C-NC	2.60	128.15	124.20
22	B	843	BCR	C28-C27-C26	-2.60	109.43	114.08
21	B	801	LMU	C4B-C3B-C2B	-2.60	106.28	110.82
22	F	203	BCR	C2-C3-C4	-2.60	105.56	111.38
20	A	850	CLA	O2A-CGA-CBA	2.60	120.07	111.91
20	3	305	CLA	C2D-C3D-C4D	-2.60	104.06	106.30
20	4	307	CLA	C4C-C3C-C2C	2.60	110.69	106.90
20	B	805	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
20	4	311	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
20	4	318	CLA	O2A-CGA-CBA	2.60	120.06	111.91
20	L	201	CLA	CHC-C1C-NC	2.59	128.14	124.20
21	E	101	LMU	O6B-C6B-C5B	-2.59	102.39	111.29
20	4	302	CLA	O2A-CGA-CBA	2.59	120.05	111.91
22	A	844	BCR	C3-C4-C5	-2.59	109.45	114.08
20	2	302	CLA	O2D-CGD-O1D	-2.59	118.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	208	CLA	CED-O2D-CGD	2.59	121.80	115.94
22	B	843	BCR	C8-C7-C6	-2.59	119.92	127.20
21	R	104	LMU	O5B-C5B-C4B	2.59	114.40	109.69
20	J	101	CLA	O2A-CGA-CBA	2.59	120.04	111.91
20	B	818	CLA	CMC-C2C-C1C	2.59	128.98	125.04
21	C	101	LMU	C6B-C5B-C4B	2.59	119.07	113.00
22	B	842	BCR	C28-C27-C26	-2.59	109.46	114.08
21	F	201	LMU	C1B-O5B-C5B	2.59	118.77	113.69
20	1	202	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	3	302	CLA	C4-C3-C2	-2.59	115.17	122.65
20	A	825	CLA	C4A-NA-C1A	2.59	107.87	106.71
20	K	101	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
20	A	838	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
22	B	845	BCR	C8-C7-C6	-2.59	119.94	127.20
21	L	211	LMU	C1B-O1B-C4'	-2.58	111.57	117.96
20	4	319	CLA	CHC-C1C-C2C	-2.58	119.57	126.72
21	R	103	LMU	O1B-C1B-C2B	2.58	114.79	108.10
20	4	314	CLA	CAC-C3C-C2C	-2.58	121.39	126.75
20	2	303	CLA	C3A-C2A-C1A	2.58	105.21	101.34
20	B	805	CLA	CAA-C2A-C1A	-2.58	103.52	111.97
21	K	104	LMU	C6'-C5'-C4'	-2.58	105.81	113.33
20	4	307	CLA	C2C-C1C-NC	-2.58	107.55	109.97
21	H	108	LMU	C1-O1'-C1'	-2.58	109.56	113.84
21	R	101	LMU	O2B-C2B-C1B	2.58	116.31	110.05
21	L	205	LMU	O5'-C5'-C6'	-2.58	100.02	106.44
20	B	823	CLA	CHB-C4A-NA	2.58	128.08	124.51
20	1	209	CLA	C4A-NA-C1A	2.58	107.87	106.71
20	A	805	CLA	C6-C7-C8	-2.58	107.58	115.92
20	A	833	CLA	CED-O2D-CGD	2.58	121.77	115.94
22	F	203	BCR	C24-C25-C26	2.58	127.71	121.46
20	B	825	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
22	A	845	BCR	C8-C7-C6	-2.58	119.96	127.20
20	A	837	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
20	2	307	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	B	806	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
21	K	106	LMU	C1'-O5'-C5'	2.58	118.75	113.69
20	A	824	CLA	C4A-NA-C1A	2.58	107.86	106.71
20	3	313	CLA	C1-O2A-CGA	2.58	123.20	116.44
20	4	308	CLA	C2A-C1A-CHA	-2.58	119.36	123.85
20	J	103	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
20	B	840	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
20	2	304	CLA	CHB-C4A-NA	2.57	128.28	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	304	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
20	B	829	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	1	208	CLA	C3C-C4C-CHD	-2.57	119.59	125.22
20	2	307	CLA	CAA-C2A-C3A	2.57	119.81	112.78
20	B	834	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	A	843	BCR	C28-C27-C26	-2.57	109.49	114.08
20	A	850	CLA	CMA-C3A-C2A	-2.57	103.47	113.83
20	2	304	CLA	C2A-C3A-C4A	-2.57	100.15	104.18
20	1	211	CLA	C3C-C4C-CHD	-2.57	119.60	125.22
21	R	101	LMU	O5B-C5B-C6B	2.57	112.82	106.44
20	A	840	CLA	C5-C3-C4	2.57	120.27	114.60
20	2	307	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
20	2	316	CLA	CMB-C2B-C3B	2.57	129.48	124.68
20	A	803	CLA	CHB-C4A-NA	2.57	128.06	124.51
20	B	803	CLA	CAA-C2A-C1A	-2.56	103.57	111.97
20	B	834	CLA	CHB-C4A-NA	2.56	128.06	124.51
20	A	850	CLA	O2A-C1-C2	2.56	115.37	108.64
21	B	801	LMU	O3'-C3'-C2'	2.56	116.27	110.35
20	G	102	CLA	CAC-C3C-C4C	-2.56	121.48	124.81
20	B	835	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
20	2	309	CLA	CHB-C4A-NA	2.56	128.26	124.34
20	A	808	CLA	CAA-CBA-CGA	2.56	120.73	113.25
22	B	842	BCR	C8-C7-C6	-2.56	120.02	127.20
20	2	322	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
22	B	845	BCR	C23-C24-C25	-2.55	120.03	127.20
20	B	839	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
20	1	206	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
20	1	216	CLA	C2A-C3A-C4A	-2.55	100.17	104.18
20	I	102	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
20	F	206	CLA	C2C-C1C-NC	2.55	112.36	109.97
22	J	102	BCR	C3-C4-C5	-2.55	109.52	114.08
22	B	845	BCR	C28-C27-C26	-2.55	109.52	114.08
20	1	206	CLA	CMB-C2B-C3B	2.55	129.45	124.68
22	A	846	BCR	C23-C24-C25	-2.55	120.04	127.20
20	A	826	CLA	C4A-NA-C1A	2.55	107.85	106.71
21	A	855	LMU	C1-O1'-C1'	-2.55	109.61	113.84
22	L	210	BCR	C28-C27-C26	-2.55	109.53	114.08
20	2	303	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
21	K	109	LMU	O2'-C2'-C3'	-2.55	104.46	110.35
20	H	109	CLA	C1-C2-C3	2.55	130.45	126.04
20	A	838	CLA	C6-C7-C8	-2.55	107.69	115.92
20	1	207	CLA	O2A-CGA-CBA	2.55	119.90	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	301	CLA	CHD-C4C-NC	2.55	128.14	124.21
22	A	844	BCR	C28-C27-C26	-2.55	109.53	114.08
20	B	807	CLA	CMD-C2D-C3D	-2.55	119.92	124.68
22	L	210	BCR	C8-C7-C6	-2.55	120.05	127.20
20	1	216	CLA	C2D-C3D-C4D	-2.54	104.11	106.30
20	A	818	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
20	B	837	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	4	302	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
20	1	201	CLA	CMA-C3A-C2A	2.54	124.08	113.83
22	A	846	BCR	C8-C7-C6	-2.54	120.06	127.20
20	B	851	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
20	A	826	CLA	C11-C10-C8	-2.54	107.71	115.92
21	4	322	LMU	O2B-C2B-C3B	-2.54	104.48	110.35
21	H	106	LMU	C3'-C4'-C5'	2.54	116.74	110.93
20	4	313	CLA	C2D-C1D-ND	-2.54	107.93	110.14
20	A	834	CLA	C1-O2A-CGA	2.53	123.09	116.44
20	A	830	CLA	CHB-C4A-NA	2.53	128.02	124.51
20	B	805	CLA	C1-C2-C3	2.53	130.42	126.04
20	3	301	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	2	306	CLA	CHB-C4A-NA	2.53	128.21	124.34
25	B	848	LMG	C8-O7-C10	-2.53	111.56	117.79
20	4	312	CLA	C2A-C3A-C4A	-2.53	100.21	104.18
20	A	833	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
21	H	108	LMU	O1'-C1-C2	-2.53	100.71	109.56
20	1	204	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
20	3	317	CLA	CMB-C2B-C3B	2.53	129.41	124.68
20	4	311	CLA	O2A-CGA-CBA	2.53	119.84	111.91
22	B	843	BCR	C3-C4-C5	-2.53	109.57	114.08
20	H	102	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
20	B	833	CLA	CMD-C2D-C3D	-2.52	119.95	124.68
20	J	101	CLA	CHC-C1C-C2C	-2.52	119.74	126.72
20	B	829	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
22	F	202	BCR	C8-C7-C6	-2.52	120.11	127.20
20	K	108	CLA	O2A-CGA-CBA	2.52	119.83	111.91
22	B	844	BCR	C32-C1-C6	2.52	114.39	110.30
20	2	301	CLA	C3D-C2D-C1D	2.52	108.48	106.30
20	B	803	CLA	C1-C2-C3	-2.52	121.68	126.04
20	A	841	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	J	102	BCR	C28-C27-C26	-2.52	109.58	114.08
20	B	827	CLA	C7-C6-C5	-2.52	106.51	113.36
20	B	851	CLA	CED-O2D-CGD	2.52	121.64	115.94
21	2	317	LMU	C1B-O1B-C4'	-2.52	111.73	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	847	BCR	C23-C24-C25	-2.52	120.13	127.20
20	B	829	CLA	O2A-CGA-CBA	2.52	119.81	111.91
20	B	817	CLA	O2A-CGA-CBA	2.52	119.81	111.91
20	4	305	CLA	C1-O2A-CGA	2.52	123.05	116.44
20	B	849	CLA	C11-C10-C8	-2.52	107.78	115.92
21	N	101	LMU	O1B-C4'-C3'	2.52	113.97	107.28
20	3	316	CLA	C2A-C3A-C4A	-2.51	100.23	104.18
20	L	208	CLA	CAC-C3C-C4C	2.51	128.07	124.81
20	H	101	CLA	O2D-CGD-CBD	2.51	115.73	111.27
20	2	303	CLA	CAA-C2A-C1A	-2.51	103.74	111.97
20	B	830	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
20	B	819	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
20	A	818	CLA	CED-O2D-CGD	2.51	121.62	115.94
20	2	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	A	817	CLA	C4A-NA-C1A	2.51	107.83	106.71
20	B	812	CLA	CAC-C3C-C2C	-2.51	123.23	127.53
20	1	208	CLA	C3A-C4A-NA	2.51	115.19	109.92
20	B	826	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
21	D	201	LMU	C1B-O1B-C4'	-2.51	111.76	117.96
20	4	319	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
20	1	210	CLA	C3A-C2A-C1A	-2.51	97.58	101.34
20	B	851	CLA	C6-C7-C8	-2.51	107.82	115.92
20	B	813	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
20	B	811	CLA	C1-C2-C3	2.51	130.38	126.04
20	B	835	CLA	CAC-C3C-C4C	2.51	128.06	124.81
20	3	311	CLA	CMD-C2D-C3D	-2.51	119.99	124.68
20	A	811	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
20	B	807	CLA	CAC-C3C-C4C	2.50	128.06	124.81
20	L	209	CLA	CAA-CBA-CGA	-2.50	105.94	113.25
20	B	803	CLA	CMD-C2D-C3D	-2.50	119.99	124.68
20	B	831	CLA	C3A-C2A-C1A	2.50	105.09	101.34
20	1	203	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	A	851	CLA	CMB-C2B-C3B	2.50	129.36	124.68
20	L	202	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
20	H	103	CLA	C1-O2A-CGA	2.50	123.00	116.44
20	4	305	CLA	O2A-CGA-CBA	2.50	119.75	111.91
21	1	217	LMU	C1B-O1B-C4'	-2.50	111.78	117.96
20	3	304	CLA	C4A-NA-C1A	2.50	107.83	106.71
20	A	838	CLA	CHC-C1C-NC	2.50	127.99	124.20
20	A	825	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
20	1	202	CLA	C4-C3-C2	-2.50	117.28	123.68
20	4	303	CLA	C1B-CHB-C4A	-2.50	125.17	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	104	LMU	O5'-C5'-C4'	2.49	115.01	109.75
20	J	101	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
20	F	205	CLA	C2A-C1A-CHA	-2.49	119.50	123.85
22	F	203	BCR	C12-C13-C14	2.49	122.77	118.94
20	A	851	CLA	CHC-C1C-C2C	-2.49	119.82	126.72
20	B	823	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
20	A	828	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
20	H	102	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
20	A	801	CLA	CHB-C4A-NA	2.49	127.96	124.51
20	A	832	CLA	O2A-CGA-CBA	2.49	119.72	111.91
20	1	216	CLA	CHB-C4A-NA	2.49	128.15	124.34
20	3	305	CLA	C3D-C4D-ND	2.49	112.30	110.14
20	A	828	CLA	CMD-C2D-C3D	-2.49	120.03	124.68
22	L	210	BCR	C30-C25-C24	2.49	122.81	115.78
20	A	839	CLA	C1-O2A-CGA	2.49	122.96	116.44
20	H	101	CLA	C3C-C4C-NC	-2.48	107.79	110.57
20	B	808	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
20	A	818	CLA	CMD-C2D-C3D	-2.48	120.03	124.68
20	2	311	CLA	C5-C3-C4	2.48	120.09	114.60
20	4	304	CLA	CHA-C1A-NA	-2.48	120.71	126.40
20	R	108	CLA	C3B-C4B-NB	2.48	112.42	109.21
20	B	830	CLA	CAA-C2A-C1A	-2.48	103.85	111.97
20	3	318	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
21	1	219	LMU	O5'-C5'-C6'	2.48	112.60	106.44
21	1	213	LMU	C1'-O5'-C5'	-2.48	108.82	113.69
22	3	314	BCR	C28-C27-C26	-2.48	109.65	114.08
20	B	819	CLA	CMB-C2B-C3B	2.48	129.31	124.68
20	2	302	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
21	R	104	LMU	O4'-C4B-C5B	2.47	115.44	109.30
21	4	320	LMU	C1B-O1B-C4'	-2.47	111.84	117.96
21	B	801	LMU	O1B-C1B-C2B	2.47	114.51	108.10
20	A	815	CLA	C1-O2A-CGA	2.47	122.93	116.44
22	A	844	BCR	C11-C12-C13	-2.47	119.47	126.42
20	3	308	CLA	CED-O2D-CGD	2.47	121.53	115.94
20	A	829	CLA	CHD-C4C-C3C	-2.47	121.21	124.84
20	B	822	CLA	C2C-C1C-NC	2.47	112.29	109.97
23	A	842	PQN	O1-C1-C2	2.47	123.46	120.25
20	H	101	CLA	C4-C3-C2	-2.47	117.34	123.68
20	K	101	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
22	A	847	BCR	C35-C13-C14	-2.47	119.47	122.92
20	4	311	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
20	B	812	CLA	O2A-CGA-CBA	2.47	119.65	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	828	CLA	CMC-C2C-C1C	2.47	128.80	125.04
20	A	816	CLA	O2A-CGA-CBA	2.47	119.65	111.91
22	A	847	BCR	C20-C19-C18	-2.47	119.49	126.42
20	A	813	CLA	CMB-C2B-C3B	2.47	129.29	124.68
20	2	311	CLA	CAC-C3C-C2C	-2.46	123.31	127.53
20	4	303	CLA	CHB-C4A-NA	2.46	127.92	124.51
20	4	308	CLA	CBD-CHA-C1A	2.46	131.37	127.43
22	I	101	BCR	C29-C30-C25	-2.46	106.69	110.48
20	B	833	CLA	CMB-C2B-C3B	2.46	129.28	124.68
20	1	207	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
20	3	318	CLA	C4-C3-C5	2.46	119.41	115.27
20	R	107	CLA	C4-C3-C2	-2.46	117.37	123.68
20	A	816	CLA	CMB-C2B-C3B	2.46	129.28	124.68
20	4	312	CLA	C3D-C2D-C1D	2.46	108.42	106.30
20	J	103	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
20	1	204	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
21	K	106	LMU	O4'-C4B-C3B	2.46	116.03	110.35
20	A	819	CLA	CMB-C2B-C3B	2.46	129.28	124.68
21	K	105	LMU	C3B-C4B-C5B	-2.45	105.86	110.24
20	A	833	CLA	CAC-C3C-C2C	-2.45	123.33	127.53
22	A	847	BCR	C8-C7-C6	-2.45	120.31	127.20
20	3	305	CLA	C3D-C2D-C1D	2.45	108.42	106.30
20	K	108	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	B	808	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	F	203	BCR	C32-C1-C6	-2.45	106.32	110.30
20	A	804	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
22	B	852	BCR	C32-C1-C31	-2.45	101.01	108.53
20	G	102	CLA	CED-O2D-CGD	2.45	121.48	115.94
20	B	805	CLA	C6-C7-C8	-2.45	108.00	115.92
20	F	205	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
20	1	215	CLA	C11-C12-C13	-2.45	108.00	115.92
21	L	211	LMU	O3'-C3'-C4'	-2.45	103.45	109.94
20	B	835	CLA	O2A-CGA-CBA	2.45	119.59	111.91
20	2	301	CLA	CHB-C4A-NA	2.45	128.09	124.34
20	A	808	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
20	2	307	CLA	CMD-C2D-C3D	-2.45	120.10	124.68
20	2	316	CLA	CAC-C3C-C4C	2.45	127.98	124.81
20	3	317	CLA	CHC-C1C-C2C	-2.45	119.96	126.72
20	A	826	CLA	CMB-C2B-C3B	2.45	129.25	124.68
20	A	827	CLA	O2A-CGA-CBA	2.44	119.58	111.91
20	A	827	CLA	CGD-CBD-CAD	2.44	118.65	110.73
22	B	844	BCR	C35-C13-C12	2.44	121.93	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	806	CLA	C3C-C4C-NC	-2.44	107.83	110.57
20	A	831	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
20	A	852	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
22	A	846	BCR	C35-C13-C14	-2.44	119.50	122.92
20	A	841	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
20	B	838	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
20	B	849	CLA	C12-C11-C10	-2.44	102.02	113.24
20	I	102	CLA	CMD-C2D-C3D	-2.44	120.11	124.68
22	3	314	BCR	C8-C7-C6	-2.44	120.35	127.20
22	I	101	BCR	C8-C9-C10	2.44	122.69	118.94
20	F	204	CLA	CMA-C3A-C4A	-2.44	105.22	111.77
20	A	839	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
20	A	810	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
20	2	305	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
20	A	818	CLA	C1-O2A-CGA	2.44	122.83	116.44
21	L	205	LMU	C3B-C4B-C5B	-2.44	105.89	110.24
21	1	218	LMU	O1B-C4'-C5'	2.43	116.12	109.45
21	3	321	LMU	C1B-O1B-C4'	-2.43	111.94	117.96
20	R	108	CLA	O1A-CGA-CBA	-2.43	114.24	123.73
21	H	107	LMU	O5B-C5B-C4B	-2.43	105.28	109.69
21	R	104	LMU	C1B-O1B-C4'	2.43	123.98	117.96
20	A	824	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	B	847	LMU	O1'-C1'-C2'	-2.43	104.51	108.30
22	B	846	BCR	C11-C12-C13	-2.43	119.59	126.42
22	A	844	BCR	C20-C19-C18	-2.43	119.59	126.42
20	B	833	CLA	CED-O2D-CGD	2.43	121.43	115.94
22	B	844	BCR	C39-C30-C25	-2.43	106.36	110.30
20	3	302	CLA	O2A-CGA-CBA	2.43	119.53	111.91
20	K	103	CLA	CMD-C2D-C3D	-2.43	120.14	124.68
20	B	837	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
21	H	105	LMU	O2'-C2'-C1'	-2.43	104.15	110.05
20	B	807	CLA	O2A-C1-C2	2.43	115.01	108.64
20	B	808	CLA	O2A-CGA-CBA	2.43	119.52	111.91
20	A	818	CLA	C4A-NA-C1A	2.43	107.80	106.71
21	F	201	LMU	O3'-C3'-C4'	-2.43	103.51	109.94
21	K	104	LMU	O5'-C5'-C4'	2.43	114.87	109.75
20	A	852	CLA	O2A-CGA-CBA	2.42	119.51	111.91
20	B	807	CLA	C11-C12-C13	-2.42	108.09	115.92
20	2	316	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
20	A	821	CLA	CAA-C2A-C3A	2.42	120.31	114.26
20	B	807	CLA	C3A-C2A-C1A	2.42	104.97	101.34
20	A	819	CLA	O2D-CGD-O1D	-2.42	119.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	845	BCR	C3-C4-C5	-2.42	109.75	114.08
20	3	304	CLA	CHB-C4A-NA	2.42	127.86	124.51
20	A	823	CLA	C14-C13-C12	2.42	120.05	111.29
20	1	215	CLA	C4-C3-C5	2.42	119.34	115.27
20	A	815	CLA	C5-C3-C4	2.42	119.94	114.60
21	H	104	LMU	C4B-C3B-C2B	-2.42	106.60	110.82
20	B	824	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
22	F	202	BCR	C23-C24-C25	-2.42	120.42	127.20
22	A	845	BCR	C23-C24-C25	-2.42	120.42	127.20
22	B	845	BCR	C37-C22-C21	-2.42	119.54	122.92
20	B	804	CLA	CMB-C2B-C3B	2.41	129.19	124.68
20	A	805	CLA	O1A-CGA-CBA	-2.41	114.32	123.73
20	A	836	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
20	A	807	CLA	CBA-CAA-C2A	-2.41	106.74	113.86
20	B	818	CLA	CMB-C2B-C3B	2.41	129.19	124.68
20	B	805	CLA	C3C-C4C-NC	-2.41	107.87	110.57
21	F	201	LMU	C6'-C5'-C4'	-2.41	106.31	113.33
20	A	826	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
20	A	841	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	K	103	CLA	C4-C3-C2	-2.41	117.50	123.68
20	A	802	CLA	C2C-C1C-CHC	-2.41	119.90	125.67
20	L	208	CLA	CMB-C2B-C3B	2.41	129.18	124.68
20	L	203	CLA	CMA-C3A-C4A	2.41	118.24	111.77
20	2	310	CLA	C2B-C3B-C4B	2.41	108.35	106.29
21	A	848	LMU	O6'-C6'-C5'	-2.41	103.04	111.29
20	K	103	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	806	CLA	CED-O2D-CGD	2.41	121.38	115.94
20	B	834	CLA	O2A-CGA-CBA	2.40	119.45	111.91
20	A	808	CLA	C1-O2A-CGA	2.40	122.75	116.44
20	4	319	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
20	B	834	CLA	CED-O2D-CGD	2.40	121.37	115.94
20	B	824	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
20	A	828	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
20	B	828	CLA	CMD-C2D-C3D	-2.40	120.19	124.68
20	A	804	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	A	807	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
20	2	308	CLA	C1-O2A-CGA	2.40	122.73	116.44
20	A	819	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
20	4	315	CLA	C2C-C1C-CHC	-2.40	119.93	125.67
20	A	801	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
20	B	817	CLA	CHC-C1C-C2C	-2.40	120.10	126.72
20	L	209	CLA	CMC-C2C-C1C	2.39	128.69	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	842	BCR	C23-C24-C25	-2.39	120.48	127.20
20	3	317	CLA	CMD-C2D-C3D	-2.39	120.20	124.68
22	A	843	BCR	C11-C12-C13	-2.39	119.69	126.42
22	J	102	BCR	C11-C12-C13	-2.39	119.70	126.42
20	B	805	CLA	C4-C3-C5	2.39	119.30	115.27
20	4	307	CLA	C4-C3-C2	-2.39	117.54	123.68
21	4	317	LMU	C4B-C3B-C2B	-2.39	106.65	110.82
21	A	855	LMU	O1'-C1'-C2'	2.39	112.03	108.30
20	1	210	CLA	C6-C5-C3	-2.39	101.92	113.58
20	A	835	CLA	O2A-C1-C2	2.39	114.91	108.64
20	1	204	CLA	CHB-C4A-NA	2.39	127.81	124.51
20	A	808	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
20	1	215	CLA	C11-C10-C8	-2.39	108.21	115.92
20	B	803	CLA	C2A-C1A-CHA	-2.39	119.69	123.86
20	B	818	CLA	O1D-CGD-CBD	-2.38	119.60	124.48
20	A	826	CLA	C4-C3-C2	-2.38	117.56	123.68
20	4	306	CLA	CED-O2D-CGD	2.38	121.33	115.94
20	A	815	CLA	CED-O2D-CGD	2.38	121.33	115.94
21	L	205	LMU	O4'-C4B-C3B	2.38	115.86	110.35
22	I	101	BCR	C20-C19-C18	2.38	133.11	126.42
20	A	836	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
20	A	831	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	3	314	BCR	C35-C13-C12	2.38	121.83	118.08
20	B	851	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
20	B	811	CLA	C2C-C1C-NC	-2.38	107.74	109.97
21	4	322	LMU	C1B-C2B-C3B	2.38	114.95	110.00
20	3	317	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	B	851	CLA	CMA-C3A-C2A	-2.38	104.23	113.83
20	L	202	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
22	A	847	BCR	C28-C27-C26	-2.38	109.83	114.08
20	2	322	CLA	CMA-C3A-C4A	-2.38	105.38	111.77
20	B	832	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	B	818	CLA	CMA-C3A-C2A	-2.38	104.24	113.83
22	B	843	BCR	C11-C12-C13	-2.38	119.74	126.42
20	4	306	CLA	CAC-C3C-C2C	-2.38	123.46	127.53
20	L	209	CLA	CMA-C3A-C4A	2.38	118.16	111.77
20	B	825	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
20	A	837	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	B	846	BCR	C20-C19-C18	-2.38	119.74	126.42
21	1	213	LMU	O5'-C1'-C2'	-2.37	105.32	110.35
20	A	821	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	H	109	CLA	C4-C3-C5	2.37	119.26	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	109	CLA	CAC-C3C-C2C	-2.37	123.47	127.53
20	A	814	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	H	108	LMU	C2'-C3'-C4'	-2.37	104.27	109.68
20	3	303	CLA	CHB-C4A-NA	2.37	127.97	124.34
20	B	832	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
22	3	314	BCR	C33-C5-C4	2.37	118.17	113.62
21	A	856	LMU	O1B-C4'-C5'	2.37	115.94	109.45
20	4	304	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
20	B	825	CLA	CAA-C2A-C1A	-2.37	104.22	111.97
20	L	209	CLA	O2A-CGA-CBA	2.37	119.33	111.91
20	B	808	CLA	C4A-NA-C1A	2.36	107.77	106.71
20	B	825	CLA	O2A-C1-C2	2.36	114.84	108.64
20	A	828	CLA	C5-C3-C2	-2.36	116.34	121.12
20	A	827	CLA	C4-C3-C5	2.36	119.25	115.27
21	1	213	LMU	O5B-C1B-C2B	-2.36	105.35	110.35
21	K	105	LMU	O5B-C5B-C6B	2.36	112.30	106.44
20	4	303	CLA	CAC-C3C-C4C	2.36	128.63	125.04
20	B	837	CLA	CED-O2D-CGD	2.36	121.27	115.94
20	4	318	CLA	CMA-C3A-C2A	-2.36	104.32	113.83
20	A	809	CLA	C5-C3-C2	-2.36	116.35	121.12
20	4	307	CLA	C5-C3-C2	2.36	125.89	121.12
22	A	847	BCR	C34-C9-C10	-2.36	119.62	122.92
20	3	318	CLA	C4A-NA-C1A	2.36	107.77	106.71
21	L	205	LMU	O3'-C3'-C2'	2.36	115.79	110.35
21	K	104	LMU	O4'-C4B-C3B	2.36	115.79	110.35
20	B	839	CLA	CMD-C2D-C3D	-2.35	120.27	124.68
20	G	102	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
21	B	847	LMU	O3'-C3'-C4'	-2.35	103.70	109.94
20	F	204	CLA	CGD-CBD-CAD	-2.35	104.65	114.30
20	H	101	CLA	CED-O2D-CGD	2.35	121.26	115.94
22	B	845	BCR	C35-C13-C14	-2.35	119.63	122.92
20	A	808	CLA	O2A-CGA-CBA	2.35	119.29	111.91
20	2	305	CLA	CMB-C2B-C3B	2.35	129.08	124.68
21	L	204	LMU	O1B-C1B-C2B	2.35	114.19	108.10
20	A	850	CLA	CMD-C2D-C3D	-2.35	120.28	124.68
20	4	315	CLA	C3D-C4D-ND	2.35	112.18	110.14
20	B	850	CLA	CBA-CAA-C2A	-2.35	106.93	113.86
22	J	102	BCR	C20-C19-C18	-2.35	119.82	126.42
20	A	852	CLA	C16-C15-C13	-2.35	108.33	115.92
22	A	846	BCR	C37-C22-C21	-2.35	119.64	122.92
20	A	828	CLA	CAA-CBA-CGA	2.35	120.11	113.25
20	B	815	CLA	CAC-C3C-C4C	2.35	127.85	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	836	CLA	OBD-CAD-C3D	-2.35	124.09	127.98
22	B	845	BCR	C36-C18-C17	-2.35	119.64	122.92
21	1	220	LMU	C1B-O5B-C5B	2.34	118.29	113.69
22	F	203	BCR	C20-C19-C18	-2.34	119.83	126.42
20	A	829	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
20	J	103	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
21	R	106	LMU	O4'-C4B-C3B	2.34	115.76	110.35
20	A	823	CLA	C4-C3-C2	-2.34	117.67	123.68
20	3	311	CLA	C1-O2A-CGA	2.34	122.58	116.44
22	B	844	BCR	C1-C6-C7	2.34	122.40	115.78
20	H	101	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
20	1	207	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
21	H	107	LMU	O5B-C5B-C6B	2.34	112.25	106.44
20	A	819	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	L	204	LMU	O5'-C5'-C4'	2.34	114.68	109.75
21	3	322	LMU	C2'-C3'-C4'	-2.34	104.35	109.68
20	B	830	CLA	C3A-C2A-C1A	2.34	104.84	101.34
21	H	105	LMU	O5B-C5B-C4B	-2.34	105.45	109.69
21	A	855	LMU	O5B-C5B-C4B	-2.34	105.45	109.69
20	A	815	CLA	CMC-C2C-C1C	2.34	128.60	125.04
22	A	846	BCR	C28-C27-C26	-2.33	109.91	114.08
20	B	833	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
22	I	101	BCR	C16-C15-C14	-2.33	118.69	123.47
22	A	845	BCR	C28-C27-C26	-2.33	109.91	114.08
20	A	821	CLA	CED-O2D-CGD	2.33	121.21	115.94
20	1	216	CLA	C3D-C4D-ND	2.33	112.17	110.14
20	B	825	CLA	C1-C2-C3	-2.33	122.01	126.04
21	R	103	LMU	O1'-C1'-C2'	2.33	111.94	108.30
20	2	301	CLA	C3D-C4D-ND	2.33	112.16	110.14
20	B	829	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
20	K	103	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
20	4	319	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	A	810	CLA	CED-O2D-CGD	2.33	121.20	115.94
20	A	837	CLA	CGD-CBD-CAD	2.33	118.27	110.73
21	4	321	LMU	C3'-C4'-C5'	2.33	116.26	110.93
20	B	832	CLA	CHC-C1C-C2C	-2.33	120.29	126.72
20	B	815	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
20	3	313	CLA	C3C-C4C-NC	-2.32	107.97	110.57
20	A	805	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	2	316	CLA	CED-O2D-CGD	2.32	121.19	115.94
20	B	805	CLA	CMB-C2B-C1B	2.32	132.03	128.46
21	K	104	LMU	O1'-C1-C2	-2.32	101.43	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	820	CLA	C1-C2-C3	-2.32	122.03	126.04
20	A	851	CLA	CED-O2D-CGD	2.32	121.19	115.94
20	1	201	CLA	CAA-C2A-C1A	2.32	119.58	111.97
20	B	815	CLA	C1-O2A-CGA	2.32	122.53	116.44
20	B	830	CLA	C9-C8-C10	2.32	119.68	111.29
21	H	108	LMU	C1'-C2'-C3'	-2.32	105.17	110.00
22	B	842	BCR	C11-C12-C13	-2.32	119.91	126.42
20	L	207	CLA	CHC-C1C-C2C	-2.31	120.32	126.72
20	A	818	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
20	B	812	CLA	O2A-C1-C2	2.31	114.72	108.64
22	B	843	BCR	C20-C19-C18	-2.31	119.91	126.42
20	4	306	CLA	CAA-C2A-C3A	2.31	119.11	112.78
21	L	205	LMU	C1-O1'-C1'	-2.31	110.00	113.84
20	B	821	CLA	CHC-C1C-NC	2.31	127.71	124.20
20	B	828	CLA	CHD-C4C-C3C	-2.31	121.44	124.84
21	A	856	LMU	C2'-C3'-C4'	-2.31	104.41	109.68
20	3	301	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
20	B	811	CLA	CAC-C3C-C4C	-2.31	121.81	124.81
21	K	105	LMU	O4'-C4B-C5B	2.31	115.03	109.30
20	A	831	CLA	C5-C3-C2	-2.31	116.45	121.12
20	A	825	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	A	855	LMU	O4'-C4B-C5B	-2.31	103.57	109.30
20	3	308	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	B	831	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
20	3	311	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
21	K	104	LMU	O5B-C1B-C2B	-2.30	105.47	110.35
22	B	845	BCR	C11-C12-C13	-2.30	119.94	126.42
20	4	302	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
20	4	313	CLA	C2A-C3A-C4A	-2.30	100.57	104.18
21	K	106	LMU	C2'-C3'-C4'	-2.30	104.43	109.68
20	A	850	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
21	B	802	LMU	O5'-C5'-C4'	-2.30	104.91	109.75
20	B	829	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
22	A	843	BCR	C20-C19-C18	-2.30	119.96	126.42
20	R	107	CLA	CGD-CBD-CAD	-2.30	103.30	110.73
20	3	313	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
20	1	204	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	R	109	LMU	C1B-O1B-C4'	-2.30	112.28	117.96
20	A	852	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
20	A	829	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
20	4	316	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
20	A	830	CLA	O2A-CGA-O1A	-2.29	117.80	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	822	CLA	CAC-C3C-C2C	-2.29	123.61	127.53
22	A	846	BCR	C34-C9-C10	-2.29	119.71	122.92
20	2	308	CLA	C11-C10-C8	-2.29	108.51	115.92
22	F	202	BCR	C11-C12-C13	-2.29	119.98	126.42
20	3	302	CLA	CED-O2D-CGD	2.29	121.12	115.94
20	B	806	CLA	C1-C2-C3	-2.29	122.08	126.04
22	B	842	BCR	C20-C19-C18	-2.29	119.98	126.42
20	4	310	CLA	C2B-C3B-C4B	2.29	108.25	106.29
20	B	850	CLA	CMD-C2D-C3D	-2.29	120.39	124.68
21	R	103	LMU	C3B-C4B-C5B	-2.29	106.16	110.24
20	A	813	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
22	B	852	BCR	C2-C1-C6	2.29	114.00	110.48
20	2	307	CLA	C3C-C4C-NC	-2.29	108.00	110.57
22	A	846	BCR	C36-C18-C17	-2.29	119.72	122.92
20	A	839	CLA	CHB-C4A-NA	2.29	127.67	124.51
21	L	211	LMU	C1'-C2'-C3'	-2.29	105.24	110.00
20	R	108	CLA	CMB-C2B-C1B	2.28	131.97	128.46
21	4	321	LMU	O2'-C2'-C3'	-2.28	105.07	110.35
20	A	807	CLA	C3C-C4C-NC	-2.28	108.01	110.57
20	B	822	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
20	1	214	CLA	C1C-NC-C4C	-2.28	105.68	106.71
21	H	106	LMU	O3'-C3'-C4'	-2.28	103.90	109.94
20	L	202	CLA	CBA-CAA-C2A	2.28	120.60	113.86
20	A	820	CLA	CMB-C2B-C3B	2.28	128.95	124.68
20	B	832	CLA	CMB-C2B-C3B	2.28	128.95	124.68
20	1	208	CLA	C2C-C1C-CHC	-2.28	120.21	125.67
20	A	826	CLA	C1-O2A-CGA	2.28	122.43	116.44
20	K	101	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
20	G	102	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
20	F	205	CLA	CHB-C4A-NA	2.28	127.66	124.51
20	L	207	CLA	C1-O2A-CGA	2.28	122.42	116.44
21	2	318	LMU	C1'-O5'-C5'	2.28	118.16	113.69
21	2	313	LMU	O5'-C5'-C6'	2.28	112.10	106.44
20	B	809	CLA	CAC-C3C-C2C	-2.28	123.63	127.53
20	A	815	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
20	2	308	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
20	I	102	CLA	C4-C3-C5	2.28	119.10	115.27
20	A	818	CLA	CAA-C2A-C1A	-2.28	104.52	111.97
20	2	308	CLA	C6-C7-C8	-2.28	108.56	115.92
20	2	308	CLA	CMB-C2B-C3B	2.27	128.93	124.68
20	1	206	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
21	R	103	LMU	O5'-C5'-C6'	-2.27	100.78	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	829	CLA	CGD-CBD-CAD	2.27	118.10	110.73
21	N	101	LMU	C6B-C5B-C4B	-2.27	107.68	113.00
20	1	214	CLA	C2B-C3B-C4B	2.27	108.23	106.29
20	B	826	CLA	C12-C11-C10	-2.27	102.80	113.24
20	1	214	CLA	C3A-C4A-NA	2.27	114.69	109.92
22	A	847	BCR	C37-C22-C21	-2.27	119.74	122.92
20	A	829	CLA	CBA-CAA-C2A	2.27	120.56	113.86
20	B	828	CLA	CHB-C4A-NA	2.27	127.65	124.51
20	4	313	CLA	CHB-C4A-NA	2.27	127.81	124.34
21	H	105	LMU	O2B-C2B-C3B	-2.27	105.11	110.35
20	K	108	CLA	C5-C3-C4	2.27	119.61	114.60
20	B	814	CLA	CED-O2D-CGD	2.27	121.06	115.94
20	B	831	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	B	845	BCR	C20-C19-C18	-2.27	120.05	126.42
20	1	201	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
20	L	203	CLA	CED-O2D-CGD	2.27	121.06	115.94
22	A	845	BCR	C20-C19-C18	-2.26	120.06	126.42
20	A	826	CLA	C4-C3-C5	2.26	119.08	115.27
20	B	821	CLA	O2A-C1-C2	2.26	114.58	108.64
20	2	304	CLA	C3B-C4B-NB	2.26	112.09	110.11
20	4	306	CLA	C3D-CAD-CBD	-2.26	104.62	107.61
20	4	309	CLA	C2A-C3A-C4A	-2.26	100.63	104.18
21	R	102	LMU	O5B-C5B-C4B	2.26	113.80	109.69
20	A	835	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
20	G	102	CLA	CAA-C2A-C1A	2.26	119.39	111.97
20	B	808	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	B	810	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
20	A	808	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
22	F	203	BCR	C15-C16-C17	-2.26	118.84	123.47
20	A	835	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
20	B	838	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
20	K	102	CLA	CED-O2D-CGD	2.26	121.05	115.94
20	B	849	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
20	B	833	CLA	C4A-NA-C1A	2.26	107.72	106.71
20	H	102	CLA	CMD-C2D-C3D	-2.26	120.45	124.68
20	B	813	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
20	A	809	CLA	C1-C2-C3	2.26	129.95	126.04
20	A	816	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
21	R	103	LMU	C1-O1'-C1'	-2.26	110.10	113.84
20	F	206	CLA	CMC-C2C-C1C	2.26	128.47	125.04
20	K	108	CLA	CHB-C4A-NA	2.25	127.63	124.51
20	2	304	CLA	C3A-C4A-NA	2.25	114.65	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	845	BCR	C3-C4-C5	-2.25	110.06	114.08
21	G	101	LMU	O5B-C5B-C4B	-2.25	105.60	109.69
22	I	101	BCR	C10-C11-C12	-2.25	116.19	123.22
20	1	203	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
21	H	105	LMU	O1'-C1'-C2'	2.25	111.82	108.30
20	A	822	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
20	B	817	CLA	C4-C3-C2	-2.25	117.91	123.68
20	H	109	CLA	O2A-C1-C2	2.25	114.54	108.64
20	B	821	CLA	C7-C6-C5	-2.25	107.26	113.36
20	B	822	CLA	CAA-C2A-C1A	2.25	119.33	111.97
20	A	824	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
20	L	201	CLA	CMC-C2C-C1C	-2.25	121.62	125.04
20	B	830	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	B	820	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
20	L	207	CLA	CMB-C2B-C3B	2.24	128.87	124.68
20	1	210	CLA	CMB-C2B-C3B	-2.24	120.48	124.68
20	A	840	CLA	O2A-CGA-CBA	2.24	118.94	111.91
21	R	105	LMU	C1B-O5B-C5B	2.24	118.09	113.69
20	A	832	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
22	B	844	BCR	C33-C5-C4	2.24	117.92	113.62
21	R	104	LMU	O5'-C5'-C4'	2.24	114.47	109.75
21	K	105	LMU	C5-C4-C3	-2.24	103.05	114.42
20	B	850	CLA	O2A-CGA-CBA	2.24	118.94	111.91
20	B	803	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
20	H	102	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
20	1	211	CLA	C3A-C4A-NA	2.24	114.61	109.92
20	B	808	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	A	845	BCR	C11-C12-C13	-2.24	120.13	126.42
20	A	829	CLA	C1-O2A-CGA	2.24	122.31	116.44
20	B	839	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
20	A	839	CLA	CAC-C3C-C2C	2.23	131.35	127.53
20	4	303	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
22	F	202	BCR	C20-C19-C18	-2.23	120.14	126.42
20	A	835	CLA	C3C-C4C-NC	-2.23	108.07	110.57
20	L	202	CLA	C1-O2A-CGA	2.23	122.30	116.44
21	B	801	LMU	O5'-C1'-C2'	2.23	115.08	110.35
20	R	108	CLA	O2A-C1-C2	2.23	114.50	108.64
20	A	829	CLA	CHB-C4A-NA	2.23	127.60	124.51
21	E	101	LMU	C6-C5-C4	-2.23	103.10	114.42
20	2	310	CLA	C3A-C4A-NA	2.23	114.60	109.92
20	B	820	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	3	322	LMU	C1'-C2'-C3'	-2.23	105.36	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	817	CLA	C4-C3-C5	2.23	119.02	115.27
20	A	806	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
20	2	302	CLA	CHB-C4A-NA	2.23	127.59	124.51
20	A	809	CLA	C2C-C1C-NC	2.22	112.06	109.97
21	2	318	LMU	O5'-C1'-C2'	2.22	115.06	110.35
20	A	813	CLA	CAC-C3C-C4C	2.22	127.69	124.81
20	B	810	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
20	L	202	CLA	C4-C3-C2	-2.22	117.98	123.68
20	2	307	CLA	C16-C17-C18	-2.22	105.51	115.98
20	A	820	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
21	L	205	LMU	O1B-C4'-C5'	2.22	115.53	109.45
20	A	830	CLA	C4-C3-C5	2.22	119.00	115.27
20	A	835	CLA	CMB-C2B-C3B	2.22	128.83	124.68
20	A	812	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
20	R	107	CLA	CAC-C3C-C4C	2.22	127.69	124.81
20	2	305	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
20	2	307	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
20	L	207	CLA	CMD-C2D-C3D	-2.22	120.53	124.68
21	2	318	LMU	C3B-C4B-C5B	2.22	114.19	110.24
20	3	309	CLA	C3A-C4A-NA	2.22	114.57	109.92
22	I	101	BCR	C15-C14-C13	2.22	130.47	127.31
20	L	209	CLA	CMB-C2B-C3B	2.21	128.82	124.68
21	4	321	LMU	C4B-C3B-C2B	2.21	114.69	110.82
20	A	841	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
21	B	847	LMU	O5'-C5'-C6'	-2.21	100.93	106.44
20	A	805	CLA	C4-C3-C5	2.21	118.99	115.27
22	B	845	BCR	C34-C9-C10	-2.21	119.82	122.92
21	A	855	LMU	C1'-C2'-C3'	2.21	114.60	110.00
22	I	103	BCR	C3-C2-C1	-2.21	106.70	114.60
20	F	206	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
22	B	846	BCR	C35-C13-C14	-2.21	119.83	122.92
22	B	844	BCR	C2-C1-C6	2.21	113.88	110.48
20	4	308	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	L	210	BCR	C23-C24-C25	-2.21	121.00	127.20
20	B	834	CLA	C1-C2-C3	-2.21	122.23	126.04
21	R	102	LMU	C8-C7-C6	-2.21	103.23	114.42
21	R	101	LMU	O5B-C1B-C2B	-2.20	105.68	110.35
20	B	828	CLA	CMB-C2B-C3B	2.20	128.80	124.68
20	A	826	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
22	B	852	BCR	C23-C22-C21	2.20	122.32	118.94
21	A	848	LMU	C3B-C4B-C5B	2.20	114.17	110.24
21	H	107	LMU	O2B-C2B-C3B	2.20	115.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	817	CLA	CMB-C2B-C3B	2.20	128.79	124.68
20	3	308	CLA	C3B-C4B-NB	2.20	112.05	109.21
20	1	205	CLA	C2D-C1D-ND	-2.20	108.23	110.14
21	1	213	LMU	O1B-C4'-C3'	2.20	113.12	107.28
20	2	305	CLA	CED-O2D-CGD	2.20	120.91	115.94
20	3	318	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
21	H	104	LMU	O1B-C1B-O5B	2.20	116.81	110.67
22	A	846	BCR	C30-C25-C26	-2.20	119.52	122.61
20	A	840	CLA	C4A-NA-C1A	2.20	107.69	106.71
20	B	840	CLA	CMD-C2D-C3D	-2.20	120.57	124.68
20	B	806	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
21	K	106	LMU	O2'-C2'-C1'	2.19	115.38	110.05
20	A	804	CLA	O2D-CGD-CBD	2.19	115.17	111.27
22	B	846	BCR	C37-C22-C21	-2.19	119.85	122.92
20	A	830	CLA	C1-O2A-CGA	2.19	122.20	116.44
20	B	827	CLA	O2A-CGA-CBA	2.19	118.79	111.91
20	A	813	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
20	B	837	CLA	O2A-CGA-CBA	2.19	118.78	111.91
20	A	818	CLA	CHB-C4A-NA	2.19	127.54	124.51
20	H	103	CLA	CHB-C4A-NA	2.19	127.54	124.51
20	A	818	CLA	C4-C3-C2	-2.19	118.06	123.68
20	A	820	CLA	CED-O2D-CGD	2.19	120.89	115.94
20	B	825	CLA	C4-C3-C5	2.19	118.95	115.27
22	B	843	BCR	C37-C22-C21	-2.19	119.86	122.92
20	B	819	CLA	O2A-CGA-CBA	2.19	120.88	112.23
20	B	812	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
22	A	847	BCR	C1-C6-C5	-2.19	119.53	122.61
20	A	811	CLA	CAC-C3C-C4C	2.19	127.65	124.81
20	1	204	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
21	K	104	LMU	C1'-O5'-C5'	2.19	117.98	113.69
20	1	206	CLA	CBC-CAC-C3C	2.19	118.46	112.43
22	B	852	BCR	C11-C10-C9	2.19	130.43	127.31
21	A	854	LMU	C6B-C5B-C4B	-2.19	107.88	113.00
22	A	843	BCR	C27-C26-C25	-2.19	119.56	122.73
20	3	312	CLA	C3C-C4C-CHD	-2.19	120.43	125.22
20	2	303	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
21	1	213	LMU	O4'-C4B-C3B	-2.18	105.30	110.35
21	H	108	LMU	O5B-C5B-C6B	-2.18	101.01	106.44
20	G	102	CLA	CAA-CBA-CGA	-2.18	106.88	113.25
20	B	816	CLA	CED-O2D-CGD	2.18	120.87	115.94
20	A	850	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
20	A	834	CLA	O2A-CGA-CBA	2.18	118.75	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	I	102	CLA	C1-O2A-CGA	2.18	122.16	116.44
20	4	311	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	I	103	BCR	C31-C1-C6	-2.18	106.77	110.30
22	B	842	BCR	C36-C18-C17	-2.18	119.87	122.92
22	A	845	BCR	C35-C13-C14	-2.18	119.87	122.92
20	1	212	CLA	C2B-C3B-C4B	2.18	108.15	106.29
20	A	834	CLA	CHB-C4A-NA	2.18	127.52	124.51
20	1	209	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
20	2	322	CLA	C2A-C3A-C4A	-2.18	98.35	101.87
21	R	104	LMU	O2B-C2B-C3B	-2.18	105.32	110.35
22	A	846	BCR	C11-C12-C13	-2.17	120.31	126.42
20	B	826	CLA	O2A-C1-C2	2.17	114.34	108.64
22	B	843	BCR	C35-C13-C14	-2.17	119.88	122.92
20	1	211	CLA	C2B-C3B-C4B	2.17	108.14	106.29
20	B	850	CLA	CAC-C3C-C2C	-2.17	123.82	127.53
20	A	803	CLA	O2A-C1-C2	2.17	114.34	108.64
20	4	307	CLA	CAC-C3C-C4C	-2.17	122.00	124.81
20	2	303	CLA	CED-O2D-CGD	2.17	120.84	115.94
20	A	851	CLA	C4-C3-C5	2.17	118.91	115.27
20	B	833	CLA	CHB-C4A-NA	2.17	127.51	124.51
20	A	832	CLA	C1-O2A-CGA	2.16	122.12	116.44
22	L	210	BCR	C24-C23-C22	-2.16	122.96	126.23
20	B	809	CLA	C1-O2A-CGA	2.16	122.12	116.44
20	3	305	CLA	C1C-NC-C4C	2.16	107.68	106.71
20	A	829	CLA	CAC-C3C-C2C	-2.16	123.83	127.53
20	B	804	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
20	3	313	CLA	CGD-CBD-CAD	2.16	117.74	110.73
20	H	102	CLA	C4A-NA-C1A	2.16	107.68	106.71
22	A	845	BCR	C1-C6-C5	-2.16	119.57	122.61
20	B	803	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
20	A	838	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
21	H	104	LMU	O5B-C1B-C2B	2.16	114.92	110.35
20	B	840	CLA	CAC-C3C-C4C	2.16	128.32	125.04
20	B	813	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
20	J	101	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
22	B	845	BCR	C1-C6-C5	-2.16	119.58	122.61
20	A	838	CLA	O2A-C1-C2	2.16	114.30	108.64
22	A	847	BCR	C30-C25-C26	-2.16	119.58	122.61
20	A	826	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
20	B	805	CLA	CMA-C3A-C4A	-2.15	105.98	111.77
20	A	813	CLA	C4-C3-C5	2.15	118.90	115.27
20	2	322	CLA	C6-C5-C3	-2.15	107.81	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	301	CLA	CAC-C3C-C4C	2.15	128.32	125.04
20	A	810	CLA	C3B-C4B-NB	-2.15	106.43	109.21
21	L	211	LMU	O1B-C1B-O5B	2.15	116.69	110.67
20	1	203	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
20	H	109	CLA	C1-O2A-CGA	2.15	122.09	116.44
21	R	101	LMU	O5B-C5B-C4B	2.15	113.60	109.69
20	1	201	CLA	C2C-C1C-NC	2.15	111.99	109.97
22	A	846	BCR	C20-C19-C18	-2.15	120.38	126.42
21	2	320	LMU	O5B-C5B-C6B	2.15	111.78	106.44
20	A	822	CLA	CGD-CBD-CAD	2.15	117.70	110.73
20	A	816	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
20	B	828	CLA	CAC-C3C-C2C	-2.15	123.86	127.53
23	A	842	PQN	C8-C7-C6	2.15	123.46	120.19
20	2	307	CLA	CHB-C4A-NA	2.15	127.48	124.51
21	F	201	LMU	O5'-C1'-O1'	-2.15	104.89	109.97
20	4	309	CLA	C3B-C4B-NB	2.14	111.98	110.11
21	R	106	LMU	O2B-C2B-C1B	2.14	115.25	110.05
20	B	828	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
22	B	852	BCR	C23-C24-C25	-2.14	121.19	127.20
20	B	806	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
20	B	816	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
20	A	816	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
20	2	316	CLA	C4-C3-C2	-2.14	118.19	123.68
21	B	801	LMU	C1'-C2'-C3'	-2.14	105.54	110.00
20	A	807	CLA	O2A-CGA-CBA	2.14	120.69	112.23
21	1	213	LMU	O6B-C6B-C5B	-2.14	103.95	111.29
20	L	208	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	2	322	CLA	CMD-C2D-C3D	-2.14	120.68	124.68
22	A	845	BCR	C36-C18-C17	-2.14	119.93	122.92
21	R	104	LMU	C6'-C5'-C4'	-2.14	107.10	113.33
22	I	103	BCR	C28-C27-C26	-2.14	110.26	114.08
20	H	109	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	A	847	BCR	C11-C12-C13	-2.14	120.42	126.42
21	H	106	LMU	O1'-C1-C2	2.14	117.05	109.56
21	2	319	LMU	C1-O1'-C1'	2.14	117.38	113.84
21	A	854	LMU	C4-C3-C2	-2.14	103.58	114.42
22	B	842	BCR	C34-C9-C10	-2.14	119.93	122.92
20	3	317	CLA	CAA-C2A-C1A	2.13	118.97	111.97
20	3	308	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
20	H	103	CLA	CAC-C3C-C4C	2.13	127.58	124.81
20	B	838	CLA	C1-C2-C3	-2.13	122.35	126.04
21	R	102	LMU	O2B-C2B-C3B	-2.13	105.42	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	811	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	B	802	LMU	O4'-C4B-C3B	2.13	115.28	110.35
20	3	308	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
20	B	811	CLA	C5-C3-C2	-2.13	116.81	121.12
22	B	843	BCR	C36-C18-C17	-2.13	119.94	122.92
21	A	854	LMU	C4B-C3B-C2B	2.13	114.54	110.82
20	4	303	CLA	CAA-C2A-C1A	-2.13	106.55	111.81
20	A	839	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
20	4	313	CLA	C2C-C1C-CHC	-2.13	120.57	125.67
21	C	101	LMU	O4'-C4B-C5B	2.13	114.58	109.30
20	L	207	CLA	CHB-C4A-NA	2.13	127.45	124.51
20	2	305	CLA	O2A-CGA-CBA	2.13	118.58	111.91
20	A	807	CLA	CHD-C4C-C3C	-2.13	121.71	124.84
21	2	319	LMU	O5'-C5'-C6'	2.13	111.72	106.44
20	B	803	CLA	C5-C3-C2	-2.12	116.82	121.12
22	B	844	BCR	C8-C7-C6	-2.12	121.24	127.20
20	B	813	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
20	A	822	CLA	CMB-C2B-C3B	2.12	128.65	124.68
20	4	315	CLA	C2A-C3A-C4A	-2.12	100.85	104.18
20	1	206	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
20	4	319	CLA	C4A-NA-C1A	2.12	107.66	106.71
22	F	202	BCR	C34-C9-C10	-2.12	119.96	122.92
22	I	101	BCR	C2-C1-C6	-2.12	107.22	110.48
20	2	301	CLA	C3B-C4B-NB	-2.12	108.25	110.11
20	3	301	CLA	CMB-C2B-C1B	2.12	131.72	128.46
20	A	829	CLA	CMB-C2B-C3B	2.12	128.64	124.68
20	B	827	CLA	CMB-C2B-C1B	2.11	131.71	128.46
20	B	816	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
20	4	316	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
20	L	208	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
20	A	833	CLA	C3B-C4B-NB	2.11	111.94	109.21
20	2	305	CLA	CGD-CBD-CAD	-2.11	103.89	110.73
20	A	841	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
20	2	311	CLA	O2A-CGA-CBA	2.11	118.53	111.91
20	B	809	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	B	823	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
20	B	824	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	3	310	CLA	C3C-C4C-NC	-2.11	108.03	109.97
20	2	309	CLA	C3B-C4B-NB	2.11	111.95	110.11
20	L	201	CLA	CHB-C4A-NA	2.11	127.42	124.51
21	B	847	LMU	O2'-C2'-C3'	-2.10	105.48	110.35
20	A	807	CLA	CMB-C2B-C3B	2.10	128.62	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	820	CLA	CHC-C1C-C2C	-2.10	120.90	126.72
20	A	804	CLA	C1-C2-C3	2.10	129.68	126.04
21	R	104	LMU	C1'-C2'-C3'	2.10	114.37	110.00
22	B	846	BCR	C34-C9-C10	-2.10	119.98	122.92
22	J	102	BCR	C27-C26-C25	-2.10	119.68	122.73
21	C	101	LMU	O1B-C1B-C2B	2.10	113.54	108.10
20	B	820	CLA	O2A-C1-C2	2.10	114.16	108.64
23	A	842	PQN	O1-C1-C10	-2.10	118.16	121.56
20	F	206	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
20	3	312	CLA	C2C-C3C-C4C	2.10	109.73	107.21
20	L	208	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
20	3	319	CLA	C2B-C3B-C4B	2.10	108.08	106.29
20	B	834	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
22	J	102	BCR	C4-C5-C6	-2.09	119.69	122.73
20	K	102	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
21	1	220	LMU	O3B-C3B-C4B	-2.09	105.51	110.35
22	B	843	BCR	C34-C9-C10	-2.09	119.99	122.92
20	3	318	CLA	C5-C3-C2	-2.09	116.89	121.12
20	3	307	CLA	C2B-C3B-C4B	2.09	108.08	106.29
21	E	101	LMU	O5B-C1B-C2B	-2.09	105.93	110.35
20	A	811	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
21	A	849	LMU	C1'-C2'-C3'	2.09	114.34	110.00
20	R	108	CLA	CHB-C4A-NA	2.09	127.40	124.51
20	L	202	CLA	CED-O2D-CGD	2.09	120.66	115.94
21	E	101	LMU	O2'-C2'-C3'	-2.08	105.53	110.35
20	A	803	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
20	B	825	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
20	B	825	CLA	CAC-C3C-C2C	2.08	131.09	127.53
22	B	844	BCR	C11-C12-C13	-2.08	120.56	126.42
20	A	836	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
20	A	819	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
20	3	313	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
22	F	203	BCR	C8-C9-C10	-2.08	115.75	118.94
20	A	805	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
20	A	829	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
21	A	849	LMU	C1B-C2B-C3B	2.08	114.33	110.00
20	F	204	CLA	CAA-C2A-C3A	-2.08	111.24	116.10
20	B	831	CLA	C1-O2A-CGA	2.08	121.90	116.44
22	A	844	BCR	C34-C9-C10	-2.08	120.01	122.92
21	K	106	LMU	C6-C5-C4	-2.08	103.87	114.42
20	4	303	CLA	CMC-C2C-C1C	2.08	128.20	125.04
20	A	823	CLA	C1-C2-C3	-2.08	122.45	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	303	CLA	C1-C2-C3	2.08	129.64	126.04
22	A	843	BCR	C4-C5-C6	-2.08	119.71	122.73
20	B	839	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
20	3	301	CLA	CAA-C2A-C3A	-2.08	111.25	116.10
20	B	817	CLA	O2A-C1-C2	2.08	114.09	108.64
20	B	839	CLA	CED-O2D-CGD	2.08	120.64	115.94
20	L	207	CLA	C5-C3-C4	2.08	119.19	114.60
20	2	315	CLA	C3A-C4A-NA	2.08	114.28	109.92
20	B	825	CLA	C7-C6-C5	-2.08	107.72	113.36
20	4	305	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
22	F	202	BCR	C35-C13-C14	-2.07	120.02	122.92
20	H	102	CLA	CMB-C2B-C3B	2.07	128.56	124.68
21	R	102	LMU	O6B-C6B-C5B	-2.07	104.17	111.29
20	2	303	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
20	A	826	CLA	C3A-C2A-C1A	2.07	104.44	101.34
20	L	209	CLA	CHB-C4A-NA	2.07	127.38	124.51
22	A	845	BCR	C37-C22-C21	-2.07	120.02	122.92
20	3	313	CLA	C5-C3-C2	-2.07	116.92	121.12
20	B	838	CLA	CBA-CAA-C2A	2.07	119.98	113.86
20	L	209	CLA	CHA-C1A-NA	-2.07	121.65	126.40
20	B	828	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
20	B	809	CLA	C5-C3-C2	-2.07	116.93	121.12
20	F	204	CLA	C3C-C4C-NC	-2.07	108.31	110.57
22	B	846	BCR	C36-C18-C17	-2.07	120.03	122.92
20	A	840	CLA	CMB-C2B-C3B	2.07	128.55	124.68
20	4	305	CLA	C3A-C2A-C1A	2.07	104.43	101.34
20	1	210	CLA	C3B-C4B-NB	2.06	111.88	109.21
20	L	203	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
20	A	822	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
22	B	845	BCR	C30-C25-C26	-2.06	119.71	122.61
20	3	309	CLA	CHB-C4A-NA	2.06	127.49	124.34
20	A	828	CLA	C6-C7-C8	-2.06	109.26	115.92
21	1	218	LMU	O5'-C1'-C2'	-2.06	105.99	110.35
20	A	851	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
20	B	803	CLA	O2A-CGA-CBA	2.06	118.37	111.91
20	A	822	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
20	A	809	CLA	CMB-C2B-C1B	2.06	131.63	128.46
23	B	841	PQN	C11-C3-C4	2.06	120.70	118.50
20	R	108	CLA	CAA-CBA-CGA	2.06	119.26	113.25
20	I	102	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
20	B	806	CLA	C4-C3-C5	2.06	118.73	115.27
20	1	205	CLA	C2B-C3B-C4B	2.06	108.05	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	205	CLA	C4A-NA-C1A	2.06	107.63	106.71
20	4	316	CLA	C1-O2A-CGA	2.05	122.88	116.11
20	B	817	CLA	CHB-C4A-NA	2.05	127.35	124.51
20	A	818	CLA	C6-C7-C8	-2.05	109.28	115.92
20	A	836	CLA	CAA-C2A-C1A	2.05	118.70	111.97
21	A	849	LMU	C4B-C3B-C2B	-2.05	107.24	110.82
21	N	101	LMU	C1B-O1B-C4'	-2.05	112.89	117.96
20	A	810	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
22	A	844	BCR	C27-C26-C25	-2.05	119.75	122.73
20	3	311	CLA	C1-C2-C3	-2.05	122.50	126.04
22	A	845	BCR	C30-C25-C26	-2.05	119.72	122.61
20	2	308	CLA	C2C-C1C-NC	2.05	111.89	109.97
20	B	837	CLA	CHB-C4A-NA	2.05	127.35	124.51
20	2	311	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
20	4	311	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
21	R	104	LMU	C1-O1'-C1'	2.05	117.23	113.84
22	A	845	BCR	C34-C9-C10	-2.05	120.06	122.92
20	A	832	CLA	CED-O2D-CGD	2.05	120.57	115.94
21	2	318	LMU	O6B-C6B-C5B	2.05	118.31	111.29
20	A	827	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
21	H	105	LMU	C1B-O1B-C4'	-2.04	112.90	117.96
20	B	817	CLA	C11-C10-C8	-2.04	109.32	115.92
20	2	315	CLA	CHB-C4A-NA	2.04	127.47	124.34
21	H	107	LMU	C1B-C2B-C3B	-2.04	105.75	110.00
20	B	810	CLA	CAA-CBA-CGA	2.04	119.21	113.25
20	A	836	CLA	CAC-C3C-C4C	2.04	127.46	124.81
20	1	207	CLA	CAC-C3C-C4C	2.04	127.45	124.81
21	1	213	LMU	C1B-C2B-C3B	-2.04	105.75	110.00
22	I	103	BCR	C4-C5-C6	-2.04	119.78	122.73
20	A	837	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
20	B	805	CLA	O2A-C1-C2	-2.03	103.29	108.64
20	B	824	CLA	CMB-C2B-C3B	2.03	128.49	124.68
20	B	808	CLA	C1-C2-C3	-2.03	122.52	126.04
20	1	216	CLA	C3A-C4A-NA	2.03	114.19	109.92
21	K	105	LMU	C6B-C5B-C4B	-2.03	108.24	113.00
20	L	207	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
20	4	304	CLA	CAC-C3C-C4C	2.03	127.45	124.81
21	R	106	LMU	C3'-C4'-C5'	2.03	115.59	110.93
21	K	105	LMU	O1B-C1B-C2B	-2.03	102.83	108.10
20	4	311	CLA	C1-C2-C3	2.03	129.56	126.04
20	K	108	CLA	C4A-NA-C1A	2.03	107.62	106.71
20	3	302	CLA	C3B-C4B-NB	2.03	111.83	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	818	CLA	C3A-C2A-C1A	2.03	104.38	101.34
21	1	220	LMU	O3B-C3B-C2B	2.03	115.04	110.35
20	A	841	CLA	O2A-CGA-CBA	2.03	118.27	111.91
20	B	850	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
20	H	101	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
21	K	106	LMU	O3'-C3'-C4'	2.03	115.31	109.94
22	F	202	BCR	C36-C18-C17	-2.03	120.08	122.92
20	F	205	CLA	CMA-C3A-C2A	-2.03	111.37	116.10
20	L	208	CLA	CMC-C2C-C1C	2.03	128.12	125.04
20	A	833	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
20	A	801	CLA	CMA-C3A-C2A	2.03	122.00	113.83
20	B	819	CLA	CGD-CBD-CAD	2.02	117.29	110.73
23	B	841	PQN	C14-C13-C12	-2.02	118.49	123.68
20	1	207	CLA	CMC-C2C-C1C	2.02	128.12	125.04
20	A	809	CLA	CHB-C4A-NA	2.02	127.31	124.51
20	A	809	CLA	CMA-C3A-C4A	2.02	117.21	111.77
20	3	306	CLA	C2B-C3B-C4B	2.02	108.02	106.29
20	2	312	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
20	L	201	CLA	C3A-C2A-C1A	-2.02	98.31	101.34
20	4	310	CLA	C3D-C2D-C1D	2.02	108.04	106.30
21	R	103	LMU	O5B-C5B-C6B	2.02	111.46	106.44
21	R	105	LMU	C1'-O5'-C5'	-2.02	109.72	113.69
20	R	107	CLA	CMB-C2B-C3B	2.02	128.46	124.68
20	3	319	CLA	C3A-C4A-NA	2.02	114.16	109.92
20	2	312	CLA	O2A-C1-C2	2.02	113.94	108.64
20	F	205	CLA	CAA-C2A-C3A	-2.02	111.38	116.10
20	4	314	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
20	B	805	CLA	CMA-C3A-C2A	-2.02	105.68	113.83
20	B	838	CLA	CMA-C3A-C2A	-2.02	105.68	113.83
20	H	103	CLA	CBA-CAA-C2A	-2.02	107.91	113.86
21	R	105	LMU	C3'-C4'-C5'	2.02	115.55	110.93
20	2	310	CLA	CHB-C4A-NA	2.02	127.43	124.34
21	F	201	LMU	O5'-C5'-C4'	-2.02	105.50	109.75
20	3	301	CLA	C2A-C1A-CHA	-2.02	120.33	123.85
20	L	203	CLA	C1-O2A-CGA	2.02	121.74	116.44
20	3	307	CLA	C3A-C4A-NA	2.02	114.15	109.92
21	B	847	LMU	O2'-C2'-C1'	-2.02	105.15	110.05
21	F	201	LMU	O1B-C4'-C3'	-2.02	101.92	107.28
20	3	318	CLA	CED-O2D-CGD	2.02	120.50	115.94
20	B	814	CLA	CBA-CAA-C2A	-2.01	107.92	113.86
21	E	101	LMU	C4-C3-C2	-2.01	104.20	114.42
20	B	828	CLA	CMA-C3A-C2A	-2.01	105.70	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	834	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
20	A	832	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
20	2	306	CLA	C3A-C2A-C1A	-2.01	101.02	104.18
22	A	844	BCR	C35-C13-C14	-2.01	120.11	122.92
20	1	207	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
22	B	842	BCR	C35-C13-C14	-2.01	120.11	122.92
22	3	314	BCR	C39-C30-C25	-2.01	107.04	110.30
20	B	810	CLA	O2A-CGA-CBA	2.01	118.21	111.91
20	A	851	CLA	C4A-NA-C1A	2.01	107.61	106.71
20	B	816	CLA	CMB-C2B-C3B	2.01	128.44	124.68
20	3	318	CLA	O2A-C1-C2	2.01	113.91	108.64
20	B	811	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
21	K	106	LMU	C1B-C2B-C3B	-2.01	105.82	110.00
21	4	321	LMU	C1'-O5'-C5'	2.01	117.63	113.69
20	B	803	CLA	C3B-C4B-NB	-2.01	106.62	109.21
20	B	811	CLA	C3C-C4C-NC	-2.01	108.32	110.57
20	A	811	CLA	O2A-CGA-CBA	2.01	118.20	111.91
20	B	849	CLA	CMA-C3A-C2A	-2.00	105.74	113.83
20	B	837	CLA	C4A-NA-C1A	2.00	107.61	106.71
20	2	305	CLA	C1-O2A-CGA	2.00	121.70	116.44
20	A	828	CLA	CHB-C4A-NA	2.00	127.28	124.51
20	B	836	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
20	A	824	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
20	B	811	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
20	F	205	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (610) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	J	103	CLA	C8
20	J	103	CLA	NC
20	J	103	CLA	ND
20	J	103	CLA	NA
20	4	316	CLA	NC
20	4	316	CLA	ND
20	4	316	CLA	NA
20	A	809	CLA	NC
20	A	809	CLA	ND
20	A	809	CLA	NA
20	3	303	CLA	NC
20	3	303	CLA	ND
20	3	303	CLA	NA

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Mol	Chain	Res	Type	Atom
20	B	825	CLA	C8
20	B	825	CLA	NC
20	B	825	CLA	ND
20	B	825	CLA	NA
20	B	806	CLA	C8
20	B	806	CLA	NC
20	B	806	CLA	ND
20	B	806	CLA	NA
20	B	851	CLA	C8
20	B	851	CLA	NC
20	B	851	CLA	ND
20	B	851	CLA	NA
20	A	851	CLA	C8
20	A	851	CLA	NC
20	A	851	CLA	ND
20	A	851	CLA	NA
20	2	303	CLA	C8
20	2	303	CLA	NC
20	2	303	CLA	ND
20	2	303	CLA	NA
20	B	836	CLA	C8
20	B	836	CLA	NC
20	B	836	CLA	ND
20	B	836	CLA	NA
20	3	308	CLA	NC
20	3	308	CLA	ND
20	3	308	CLA	NA
20	4	302	CLA	C8
20	4	302	CLA	NC
20	4	302	CLA	ND
20	4	302	CLA	NA
20	A	827	CLA	C8
20	A	827	CLA	NC
20	A	827	CLA	ND
20	A	827	CLA	NA
20	A	816	CLA	NC
20	A	816	CLA	ND
20	A	816	CLA	NA
20	1	203	CLA	NC
20	1	203	CLA	ND
20	1	203	CLA	NA
20	2	305	CLA	NC

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Mol	Chain	Res	Type	Atom
20	2	305	CLA	ND
20	2	305	CLA	NA
20	1	209	CLA	NC
20	1	209	CLA	ND
20	1	209	CLA	NA
20	2	322	CLA	C8
20	2	322	CLA	NC
20	2	322	CLA	ND
20	2	322	CLA	NA
20	A	818	CLA	C8
20	A	818	CLA	NC
20	A	818	CLA	ND
20	A	818	CLA	NA
20	A	841	CLA	C8
20	A	841	CLA	NC
20	A	841	CLA	ND
20	A	841	CLA	NA
20	F	206	CLA	C2A
20	F	206	CLA	NA
20	F	206	CLA	CBD
20	F	206	CLA	NC
20	F	206	CLA	ND
20	F	206	CLA	C3A
20	4	305	CLA	C8
20	4	305	CLA	NC
20	4	305	CLA	ND
20	4	305	CLA	NA
20	B	811	CLA	C8
20	B	811	CLA	NC
20	B	811	CLA	ND
20	B	811	CLA	NA
20	3	310	CLA	NC
20	3	310	CLA	ND
20	3	310	CLA	NA
20	L	202	CLA	C8
20	L	202	CLA	NC
20	L	202	CLA	ND
20	L	202	CLA	NA
20	B	814	CLA	NC
20	B	814	CLA	ND
20	B	814	CLA	NA
20	2	310	CLA	NC

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Mol	Chain	Res	Type	Atom
20	2	310	CLA	ND
20	2	310	CLA	NA
20	4	306	CLA	NC
20	4	306	CLA	ND
20	4	306	CLA	NA
20	A	812	CLA	NC
20	A	812	CLA	ND
20	A	812	CLA	NA
20	2	308	CLA	C8
20	2	308	CLA	NC
20	2	308	CLA	ND
20	2	308	CLA	NA
20	A	805	CLA	C8
20	A	805	CLA	NC
20	A	805	CLA	ND
20	A	805	CLA	NA
20	4	304	CLA	C8
20	4	304	CLA	CBD
20	4	304	CLA	NC
20	4	304	CLA	ND
20	4	304	CLA	NA
20	K	102	CLA	NC
20	K	102	CLA	ND
20	K	102	CLA	NA
20	B	829	CLA	NC
20	B	829	CLA	ND
20	B	829	CLA	NA
20	2	316	CLA	C8
20	2	316	CLA	NC
20	2	316	CLA	ND
20	2	316	CLA	NA
20	B	834	CLA	NC
20	B	834	CLA	ND
20	B	834	CLA	NA
20	1	211	CLA	NC
20	1	211	CLA	ND
20	1	211	CLA	NA
20	A	833	CLA	NC
20	A	833	CLA	ND
20	A	833	CLA	NA
20	A	814	CLA	NC
20	A	814	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	814	CLA	NA
20	F	205	CLA	NC
20	F	205	CLA	ND
20	F	205	CLA	NA
20	G	102	CLA	NC
20	G	102	CLA	ND
20	G	102	CLA	NA
20	4	313	CLA	NC
20	4	313	CLA	ND
20	4	313	CLA	NA
20	B	826	CLA	C8
20	B	826	CLA	NC
20	B	826	CLA	ND
20	B	826	CLA	NA
20	3	305	CLA	NC
20	3	305	CLA	ND
20	3	305	CLA	NA
20	A	824	CLA	C8
20	A	824	CLA	NC
20	A	824	CLA	ND
20	A	824	CLA	NA
20	B	804	CLA	NC
20	B	804	CLA	ND
20	B	804	CLA	NA
20	R	107	CLA	C8
20	R	107	CLA	NC
20	R	107	CLA	ND
20	R	107	CLA	NA
20	B	812	CLA	C8
20	B	812	CLA	NC
20	B	812	CLA	ND
20	B	812	CLA	NA
20	3	306	CLA	NC
20	3	306	CLA	ND
20	3	306	CLA	NA
20	B	818	CLA	NC
20	B	818	CLA	ND
20	B	818	CLA	NA
20	2	306	CLA	NC
20	2	306	CLA	ND
20	2	306	CLA	NA
21	R	101	LMU	C2B

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Mol	Chain	Res	Type	Atom
20	B	820	CLA	C8
20	B	820	CLA	NC
20	B	820	CLA	ND
20	B	820	CLA	NA
20	4	308	CLA	NC
20	4	308	CLA	ND
20	4	308	CLA	NA
20	A	825	CLA	C8
20	A	825	CLA	NC
20	A	825	CLA	ND
20	A	825	CLA	NA
20	B	807	CLA	C8
20	B	807	CLA	NC
20	B	807	CLA	ND
20	B	807	CLA	NA
20	A	838	CLA	C8
20	A	838	CLA	NC
20	A	838	CLA	ND
20	A	838	CLA	NA
20	4	314	CLA	NC
20	4	314	CLA	ND
20	4	314	CLA	NA
20	A	837	CLA	NC
20	A	837	CLA	ND
20	A	837	CLA	NA
20	1	201	CLA	NC
20	1	201	CLA	ND
20	1	201	CLA	NA
20	B	850	CLA	C8
20	B	850	CLA	NC
20	B	850	CLA	ND
20	B	850	CLA	NA
20	1	208	CLA	NC
20	1	208	CLA	ND
20	1	208	CLA	NA
20	2	307	CLA	C8
20	2	307	CLA	NC
20	2	307	CLA	ND
20	2	307	CLA	NA
20	A	801	CLA	NC
20	A	801	CLA	C2A
20	A	801	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	801	CLA	NA
20	A	801	CLA	CBD
20	3	309	CLA	NC
20	3	309	CLA	ND
20	3	309	CLA	NA
20	B	816	CLA	C8
20	B	816	CLA	NC
20	B	816	CLA	ND
20	B	816	CLA	NA
20	B	830	CLA	C8
20	B	830	CLA	NC
20	B	830	CLA	ND
20	B	830	CLA	NA
20	1	207	CLA	C2A
20	1	207	CLA	NC
20	1	207	CLA	ND
20	1	207	CLA	NA
20	3	313	CLA	C8
20	3	313	CLA	NC
20	3	313	CLA	ND
20	3	313	CLA	NA
20	3	316	CLA	NC
20	3	316	CLA	ND
20	3	316	CLA	NA
20	A	811	CLA	C8
20	A	811	CLA	NC
20	A	811	CLA	ND
20	A	811	CLA	NA
20	2	315	CLA	NC
20	2	315	CLA	ND
20	2	315	CLA	NA
20	H	102	CLA	C8
20	H	102	CLA	NC
20	H	102	CLA	ND
20	H	102	CLA	NA
20	4	319	CLA	NC
20	4	319	CLA	ND
20	4	319	CLA	NA
20	B	815	CLA	C8
20	B	815	CLA	NC
20	B	815	CLA	ND
20	B	815	CLA	NA

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Mol	Chain	Res	Type	Atom
20	A	810	CLA	NC
20	A	810	CLA	ND
20	A	810	CLA	NA
20	B	849	CLA	C8
20	B	849	CLA	NC
20	B	849	CLA	ND
20	B	849	CLA	NA
20	3	302	CLA	NC
20	3	302	CLA	ND
20	3	302	CLA	NA
20	4	311	CLA	C8
20	4	311	CLA	NC
20	4	311	CLA	ND
20	4	311	CLA	NA
20	B	805	CLA	C8
20	B	805	CLA	NC
20	B	805	CLA	ND
20	B	805	CLA	NA
20	A	822	CLA	C8
20	A	822	CLA	NC
20	A	822	CLA	ND
20	A	822	CLA	NA
20	1	214	CLA	NC
20	1	214	CLA	ND
20	1	214	CLA	NA
20	A	850	CLA	C8
20	A	850	CLA	NC
20	A	850	CLA	ND
20	A	850	CLA	NA
20	K	103	CLA	C8
20	K	103	CLA	NC
20	K	103	CLA	ND
20	K	103	CLA	NA
20	J	101	CLA	NC
20	J	101	CLA	ND
20	J	101	CLA	NA
20	B	838	CLA	C8
20	B	838	CLA	NC
20	B	838	CLA	ND
20	B	838	CLA	NA
23	B	841	PQN	C23
20	A	802	CLA	NC

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Mol	Chain	Res	Type	Atom
20	A	802	CLA	ND
20	A	802	CLA	NA
20	B	822	CLA	NC
20	B	822	CLA	ND
20	B	822	CLA	NA
20	A	852	CLA	C8
20	A	852	CLA	NC
20	A	852	CLA	ND
20	A	852	CLA	NA
20	A	819	CLA	C8
20	A	819	CLA	NC
20	A	819	CLA	ND
20	A	819	CLA	NA
20	A	813	CLA	NC
20	A	813	CLA	ND
20	A	813	CLA	NA
20	1	204	CLA	NC
20	1	204	CLA	ND
20	1	204	CLA	NA
20	B	824	CLA	C8
20	B	824	CLA	NC
20	B	824	CLA	ND
20	B	824	CLA	NA
20	L	207	CLA	NC
20	L	207	CLA	ND
20	L	207	CLA	NA
20	A	808	CLA	C8
20	A	808	CLA	NC
20	A	808	CLA	ND
20	A	808	CLA	NA
20	A	803	CLA	NC
20	A	803	CLA	ND
20	A	803	CLA	NA
20	B	821	CLA	NC
20	B	821	CLA	ND
20	B	821	CLA	NA
20	B	833	CLA	NC
20	B	833	CLA	ND
20	B	833	CLA	NA
20	3	318	CLA	C8
20	3	318	CLA	NC
20	3	318	CLA	ND

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Mol	Chain	Res	Type	Atom
20	3	318	CLA	NA
20	1	205	CLA	NC
20	1	205	CLA	ND
20	1	205	CLA	NA
20	4	315	CLA	NC
20	4	315	CLA	ND
20	4	315	CLA	NA
20	3	311	CLA	C8
20	3	311	CLA	NC
20	3	311	CLA	ND
20	3	311	CLA	NA
20	2	311	CLA	NC
20	2	311	CLA	ND
20	2	311	CLA	NA
20	A	832	CLA	NC
20	A	832	CLA	ND
20	A	832	CLA	NA
20	A	817	CLA	NC
20	A	817	CLA	ND
20	A	817	CLA	NA
20	R	108	CLA	C8
20	R	108	CLA	NC
20	R	108	CLA	ND
20	R	108	CLA	NA
20	2	304	CLA	NC
20	2	304	CLA	ND
20	2	304	CLA	NA
20	H	101	CLA	C8
20	H	101	CLA	NC
20	H	101	CLA	ND
20	H	101	CLA	NA
20	A	821	CLA	NC
20	A	821	CLA	ND
20	A	821	CLA	NA
20	A	839	CLA	C2A
20	A	839	CLA	NC
20	A	839	CLA	ND
20	A	839	CLA	NA
20	3	317	CLA	NC
20	3	317	CLA	ND
20	3	317	CLA	NA
20	3	320	CLA	NC

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Mol	Chain	Res	Type	Atom
20	3	320	CLA	ND
20	3	320	CLA	NA
20	B	817	CLA	C8
20	B	817	CLA	NC
20	B	817	CLA	ND
20	B	817	CLA	NA
20	L	209	CLA	CBD
20	L	209	CLA	NC
20	L	209	CLA	ND
20	L	209	CLA	NA
20	B	827	CLA	C8
20	B	827	CLA	NC
20	B	827	CLA	ND
20	B	827	CLA	NA
20	I	102	CLA	C8
20	I	102	CLA	NC
20	I	102	CLA	ND
20	I	102	CLA	NA
20	B	810	CLA	C8
20	B	810	CLA	NC
20	B	810	CLA	ND
20	B	810	CLA	NA
20	3	307	CLA	NC
20	3	307	CLA	ND
20	3	307	CLA	NA
20	1	216	CLA	NC
20	1	216	CLA	ND
20	1	216	CLA	NA
20	4	307	CLA	NC
20	4	307	CLA	C2A
20	4	307	CLA	ND
20	4	307	CLA	NA
20	4	310	CLA	NC
20	4	310	CLA	ND
20	4	310	CLA	NA
20	B	840	CLA	NC
20	B	840	CLA	ND
20	B	840	CLA	NA
20	B	828	CLA	NC
20	B	828	CLA	ND
20	B	828	CLA	NA
20	B	823	CLA	C8

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Mol	Chain	Res	Type	Atom
20	B	823	CLA	NC
20	B	823	CLA	ND
20	B	823	CLA	NA
20	A	804	CLA	C8
20	A	804	CLA	NC
20	A	804	CLA	ND
20	A	804	CLA	NA
20	A	836	CLA	NC
20	A	836	CLA	ND
20	A	836	CLA	NA
20	1	215	CLA	C8
20	1	215	CLA	NC
20	1	215	CLA	ND
20	1	215	CLA	NA
20	1	210	CLA	CBD
20	1	210	CLA	NC
20	1	210	CLA	ND
20	1	210	CLA	NA
20	K	108	CLA	NC
20	K	108	CLA	ND
20	K	108	CLA	NA
20	B	809	CLA	C8
20	B	809	CLA	NC
20	B	809	CLA	ND
20	B	809	CLA	NA
20	A	829	CLA	NC
20	A	829	CLA	ND
20	A	829	CLA	NA
20	A	834	CLA	NC
20	A	834	CLA	ND
20	A	834	CLA	NA
20	A	820	CLA	NC
20	A	820	CLA	ND
20	A	820	CLA	NA
20	B	831	CLA	NC
20	B	831	CLA	ND
20	B	831	CLA	NA
20	B	803	CLA	C8
20	B	803	CLA	NC
20	B	803	CLA	ND
20	B	803	CLA	NA
20	B	808	CLA	C8

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Mol	Chain	Res	Type	Atom
20	B	808	CLA	NC
20	B	808	CLA	ND
20	B	808	CLA	NA
20	3	301	CLA	NC
20	3	301	CLA	ND
20	3	301	CLA	NA
20	B	837	CLA	NC
20	B	837	CLA	ND
20	B	837	CLA	NA
20	4	303	CLA	NC
20	4	303	CLA	ND
20	4	303	CLA	NA
20	H	103	CLA	C8
20	H	103	CLA	NC
20	H	103	CLA	ND
20	H	103	CLA	NA
20	K	101	CLA	NC
20	K	101	CLA	ND
20	K	101	CLA	NA
20	B	835	CLA	C8
20	B	835	CLA	NC
20	B	835	CLA	ND
20	B	835	CLA	NA
20	3	319	CLA	NC
20	3	319	CLA	ND
20	3	319	CLA	NA
20	B	839	CLA	C8
20	B	839	CLA	NC
20	B	839	CLA	ND
20	B	839	CLA	NA
20	2	301	CLA	NC
20	2	301	CLA	ND
20	2	301	CLA	NA
20	1	202	CLA	C8
20	1	202	CLA	NC
20	1	202	CLA	ND
20	1	202	CLA	NA
20	1	206	CLA	C8
20	1	206	CLA	NC
20	1	206	CLA	ND
20	1	206	CLA	NA
20	A	807	CLA	NC

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Mol	Chain	Res	Type	Atom
20	A	807	CLA	ND
20	A	807	CLA	NA
20	B	832	CLA	NC
20	B	832	CLA	ND
20	B	832	CLA	NA
20	B	813	CLA	C8
20	B	813	CLA	NC
20	B	813	CLA	ND
20	B	813	CLA	NA
20	A	830	CLA	C8
20	A	830	CLA	NC
20	A	830	CLA	ND
20	A	830	CLA	NA
20	3	304	CLA	NC
20	3	304	CLA	ND
20	3	304	CLA	NA
23	A	842	PQN	C23
20	A	831	CLA	C8
20	A	831	CLA	NC
20	A	831	CLA	ND
20	A	831	CLA	NA
20	A	815	CLA	NC
20	A	815	CLA	ND
20	A	815	CLA	NA
20	A	840	CLA	NC
20	A	840	CLA	ND
20	A	840	CLA	NA
20	2	309	CLA	NC
20	2	309	CLA	ND
20	2	309	CLA	NA
20	4	309	CLA	NC
20	4	309	CLA	ND
20	4	309	CLA	NA
20	A	826	CLA	C8
20	A	826	CLA	NC
20	A	826	CLA	ND
20	A	826	CLA	NA
20	4	312	CLA	NC
20	4	312	CLA	ND
20	4	312	CLA	NA
20	F	204	CLA	NC
20	F	204	CLA	ND

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Mol	Chain	Res	Type	Atom
20	F	204	CLA	NA
20	3	312	CLA	NC
20	3	312	CLA	ND
20	3	312	CLA	NA
20	H	109	CLA	C8
20	H	109	CLA	NC
20	H	109	CLA	ND
20	H	109	CLA	NA
20	1	212	CLA	NC
20	1	212	CLA	ND
20	1	212	CLA	NA
20	L	203	CLA	C8
20	L	203	CLA	NC
20	L	203	CLA	ND
20	L	203	CLA	NA
20	L	201	CLA	C2A
20	L	201	CLA	NC
20	L	201	CLA	ND
20	L	201	CLA	NA
20	L	201	CLA	C3A
20	B	819	CLA	NC
20	B	819	CLA	ND
20	B	819	CLA	NA
20	2	302	CLA	NC
20	2	302	CLA	ND
20	2	302	CLA	NA
20	A	823	CLA	C8
20	A	823	CLA	NC
20	A	823	CLA	ND
20	A	823	CLA	NA
20	A	828	CLA	C8
20	A	828	CLA	NC
20	A	828	CLA	ND
20	A	828	CLA	NA
20	2	312	CLA	NC
20	2	312	CLA	ND
20	2	312	CLA	NA
20	L	208	CLA	NC
20	L	208	CLA	ND
20	L	208	CLA	NA
20	4	318	CLA	NC
20	4	318	CLA	ND

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Mol	Chain	Res	Type	Atom
20	4	318	CLA	NA
20	A	806	CLA	C8
20	A	806	CLA	NC
20	A	806	CLA	ND
20	A	806	CLA	NA
20	A	835	CLA	C8
20	A	835	CLA	NC
20	A	835	CLA	ND
20	A	835	CLA	NA

All (2773) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	J	103	CLA	C3A-C2A-CAA-CBA
20	J	103	CLA	C2A-CAA-CBA-CGA
20	J	103	CLA	CHA-CBD-CGD-O1D
20	J	103	CLA	CHA-CBD-CGD-O2D
20	J	103	CLA	CBD-CGD-O2D-CED
22	B	852	BCR	C11-C12-C13-C14
22	B	852	BCR	C11-C12-C13-C35
22	B	852	BCR	C20-C21-C22-C23
22	B	852	BCR	C20-C21-C22-C37
22	B	852	BCR	C21-C22-C23-C24
22	B	852	BCR	C37-C22-C23-C24
20	4	316	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	O2A-C1-C2-C3
20	B	825	CLA	C3A-C2A-CAA-CBA
20	B	825	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	O1D-CGD-O2D-CED
20	A	851	CLA	C6-C7-C8-C9
20	2	303	CLA	C1A-C2A-CAA-CBA
20	2	303	CLA	C3A-C2A-CAA-CBA
20	2	303	CLA	CAD-CBD-CGD-O1D
20	2	303	CLA	CAD-CBD-CGD-O2D
20	2	303	CLA	C4-C3-C5-C6
20	3	308	CLA	C1A-C2A-CAA-CBA
20	4	302	CLA	C2C-C3C-CAC-CBC
20	4	302	CLA	C4C-C3C-CAC-CBC
20	4	302	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	4	302	CLA	C4-C3-C5-C6
20	A	816	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	CBD-CGD-O2D-CED
20	2	305	CLA	C2-C1-O2A-CGA
22	B	843	BCR	C1-C6-C7-C8
22	B	843	BCR	C5-C6-C7-C8
22	B	843	BCR	C18-C19-C20-C21
22	B	843	BCR	C20-C21-C22-C23
22	B	843	BCR	C20-C21-C22-C37
22	B	843	BCR	C23-C24-C25-C30
21	4	317	LMU	C2'-C1'-O1'-C1
21	4	317	LMU	O5'-C1'-O1'-C1
20	2	322	CLA	C1A-C2A-CAA-CBA
20	2	322	CLA	C3A-C2A-CAA-CBA
20	2	322	CLA	CHA-CBD-CGD-O1D
20	2	322	CLA	CHA-CBD-CGD-O2D
20	2	322	CLA	CAD-CBD-CGD-O1D
20	2	322	CLA	CBD-CGD-O2D-CED
20	A	818	CLA	C1A-C2A-CAA-CBA
20	A	818	CLA	C3A-C2A-CAA-CBA
20	A	818	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	CAD-CBD-CGD-O1D
20	A	818	CLA	CAD-CBD-CGD-O2D
20	A	818	CLA	CBD-CGD-O2D-CED
22	B	844	BCR	C20-C21-C22-C23
22	B	844	BCR	C20-C21-C22-C37
22	B	844	BCR	C37-C22-C23-C24
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
21	4	320	LMU	O5'-C1'-O1'-C1
22	A	845	BCR	C5-C6-C7-C8
22	A	845	BCR	C7-C8-C9-C10
22	A	845	BCR	C11-C12-C13-C14
22	A	845	BCR	C11-C12-C13-C35
22	A	845	BCR	C17-C18-C19-C20
22	A	845	BCR	C36-C18-C19-C20
22	A	845	BCR	C21-C22-C23-C24
22	A	845	BCR	C37-C22-C23-C24
21	L	211	LMU	C2'-C1'-O1'-C1
21	L	211	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	L	211	LMU	C2-C1-O1'-C1'
20	F	206	CLA	C1A-C2A-CAA-CBA
20	F	206	CLA	C3A-C2A-CAA-CBA
20	F	206	CLA	CBD-CGD-O2D-CED
20	F	206	CLA	O1D-CGD-O2D-CED
21	1	217	LMU	C2'-C1'-O1'-C1
21	1	217	LMU	O5'-C1'-O1'-C1
21	2	313	LMU	C2-C1-O1'-C1'
20	B	811	CLA	CHA-CBD-CGD-O1D
20	B	811	CLA	CAD-CBD-CGD-O1D
21	A	848	LMU	C2-C1-O1'-C1'
20	L	202	CLA	C1A-C2A-CAA-CBA
20	L	202	CLA	CHA-CBD-CGD-O1D
20	L	202	CLA	CHA-CBD-CGD-O2D
20	L	202	CLA	CBD-CGD-O2D-CED
20	L	202	CLA	C4-C3-C5-C6
20	B	814	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C2C-C3C-CAC-CBC
20	B	814	CLA	C4C-C3C-CAC-CBC
20	B	814	CLA	CBD-CGD-O2D-CED
22	A	847	BCR	C17-C18-C19-C20
22	A	847	BCR	C36-C18-C19-C20
22	A	847	BCR	C18-C19-C20-C21
22	A	847	BCR	C23-C24-C25-C26
22	A	847	BCR	C23-C24-C25-C30
21	N	101	LMU	C2'-C1'-O1'-C1
21	N	101	LMU	C2-C1-O1'-C1'
20	4	306	CLA	CBD-CGD-O2D-CED
21	4	322	LMU	C2'-C1'-O1'-C1
21	4	322	LMU	O5'-C1'-O1'-C1
21	K	105	LMU	C2'-C1'-O1'-C1
21	K	105	LMU	O5'-C1'-O1'-C1
21	L	205	LMU	C2-C1-O1'-C1'
21	H	107	LMU	C2'-C1'-O1'-C1
21	H	107	LMU	O5'-C1'-O1'-C1
20	2	308	CLA	CBA-CGA-O2A-C1
20	2	308	CLA	O1A-CGA-O2A-C1
20	A	805	CLA	C1A-C2A-CAA-CBA
20	A	805	CLA	C3A-C2A-CAA-CBA
20	A	805	CLA	C2-C3-C5-C6
20	A	805	CLA	C4-C3-C5-C6
20	4	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	4	304	CLA	C3A-C2A-CAA-CBA
20	4	304	CLA	CHA-CBD-CGD-O1D
20	4	304	CLA	CHA-CBD-CGD-O2D
21	L	204	LMU	C2-C1-O1'-C1'
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C2C-C3C-CAC-CBC
20	B	829	CLA	C4C-C3C-CAC-CBC
20	B	829	CLA	CHA-CBD-CGD-O1D
20	B	829	CLA	CHA-CBD-CGD-O2D
20	2	316	CLA	C2-C1-O2A-CGA
20	2	316	CLA	CBD-CGD-O2D-CED
20	2	316	CLA	C14-C13-C15-C16
20	B	834	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C2-C3-C5-C6
20	B	834	CLA	C4-C3-C5-C6
20	A	833	CLA	C1A-C2A-CAA-CBA
20	A	833	CLA	C3A-C2A-CAA-CBA
20	A	814	CLA	C1A-C2A-CAA-CBA
20	A	814	CLA	C2A-CAA-CBA-CGA
20	F	205	CLA	CBD-CGD-O2D-CED
20	G	102	CLA	CAD-CBD-CGD-O1D
20	G	102	CLA	CBD-CGD-O2D-CED
20	G	102	CLA	C2-C3-C5-C6
20	G	102	CLA	C4-C3-C5-C6
20	B	826	CLA	C3A-C2A-CAA-CBA
20	A	824	CLA	C2-C1-O2A-CGA
20	A	824	CLA	C2C-C3C-CAC-CBC
20	A	824	CLA	C4C-C3C-CAC-CBC
20	A	824	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	R	107	CLA	C1A-C2A-CAA-CBA
20	R	107	CLA	CHA-CBD-CGD-O1D
20	R	107	CLA	CHA-CBD-CGD-O2D
20	R	107	CLA	CBD-CGD-O2D-CED
20	R	107	CLA	C2-C3-C5-C6
20	R	107	CLA	C4-C3-C5-C6
20	B	812	CLA	C1A-C2A-CAA-CBA
20	B	812	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	CBD-CGD-O2D-CED
20	B	818	CLA	O1D-CGD-O2D-CED
21	R	101	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	R	101	LMU	O5'-C1'-O1'-C1
20	B	820	CLA	C1A-C2A-CAA-CBA
20	B	820	CLA	C3A-C2A-CAA-CBA
20	A	825	CLA	C1A-C2A-CAA-CBA
20	A	825	CLA	O2A-C1-C2-C3
20	B	807	CLA	C11-C10-C8-C9
20	B	807	CLA	C12-C13-C15-C16
20	A	838	CLA	C1A-C2A-CAA-CBA
20	A	838	CLA	C3A-C2A-CAA-CBA
21	A	853	LMU	C2'-C1'-O1'-C1
21	A	853	LMU	O5'-C1'-O1'-C1
21	A	853	LMU	C2-C1-O1'-C1'
20	A	837	CLA	CBD-CGD-O2D-CED
20	1	201	CLA	C1A-C2A-CAA-CBA
20	1	201	CLA	C3A-C2A-CAA-CBA
20	1	201	CLA	CBA-CGA-O2A-C1
20	1	201	CLA	CHA-CBD-CGD-O1D
20	1	201	CLA	CHA-CBD-CGD-O2D
20	B	850	CLA	C2-C3-C5-C6
20	B	850	CLA	C4-C3-C5-C6
20	2	307	CLA	C1A-C2A-CAA-CBA
20	2	307	CLA	CBD-CGD-O2D-CED
22	B	845	BCR	C9-C10-C11-C12
22	B	845	BCR	C17-C18-C19-C20
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C21-C22-C23-C24
22	B	845	BCR	C37-C22-C23-C24
20	A	801	CLA	CAD-CBD-CGD-O1D
20	A	801	CLA	CAD-CBD-CGD-O2D
20	A	801	CLA	CBD-CGD-O2D-CED
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C3A-C2A-CAA-CBA
20	B	830	CLA	C1A-C2A-CAA-CBA
20	1	207	CLA	C2-C3-C5-C6
20	1	207	CLA	C4-C3-C5-C6
20	3	313	CLA	CBD-CGD-O2D-CED
20	3	313	CLA	C2-C3-C5-C6
20	3	313	CLA	C4-C3-C5-C6
22	A	844	BCR	C1-C6-C7-C8
22	A	844	BCR	C5-C6-C7-C8
22	A	844	BCR	C7-C8-C9-C10
22	A	844	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	A	844	BCR	C11-C12-C13-C14
22	A	844	BCR	C11-C12-C13-C35
22	A	844	BCR	C18-C19-C20-C21
22	A	844	BCR	C20-C21-C22-C37
22	A	844	BCR	C21-C22-C23-C24
22	A	844	BCR	C37-C22-C23-C24
20	A	811	CLA	CBD-CGD-O2D-CED
21	H	108	LMU	C2'-C1'-O1'-C1
21	H	108	LMU	O5'-C1'-O1'-C1
22	I	103	BCR	C11-C12-C13-C14
22	I	103	BCR	C11-C12-C13-C35
22	I	103	BCR	C17-C18-C19-C20
22	I	103	BCR	C36-C18-C19-C20
22	I	103	BCR	C18-C19-C20-C21
22	I	103	BCR	C19-C20-C21-C22
22	I	103	BCR	C20-C21-C22-C23
22	I	103	BCR	C20-C21-C22-C37
21	E	101	LMU	C2'-C1'-O1'-C1
21	E	101	LMU	O5'-C1'-O1'-C1
20	H	102	CLA	CAD-CBD-CGD-O1D
20	H	102	CLA	CAD-CBD-CGD-O2D
20	H	102	CLA	CBD-CGD-O2D-CED
21	R	105	LMU	C2'-C1'-O1'-C1
21	R	105	LMU	O5'-C1'-O1'-C1
20	4	319	CLA	CHA-CBD-CGD-O1D
20	4	319	CLA	CHA-CBD-CGD-O2D
20	4	319	CLA	CBD-CGD-O2D-CED
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	815	CLA	C3A-C2A-CAA-CBA
20	B	815	CLA	C2A-CAA-CBA-CGA
20	B	815	CLA	CBD-CGD-O2D-CED
22	F	202	BCR	C5-C6-C7-C8
22	F	202	BCR	C18-C19-C20-C21
20	A	810	CLA	CBD-CGD-O2D-CED
22	L	210	BCR	C1-C6-C7-C8
22	L	210	BCR	C7-C8-C9-C10
22	L	210	BCR	C7-C8-C9-C34
22	L	210	BCR	C20-C21-C22-C23
22	L	210	BCR	C20-C21-C22-C37
22	L	210	BCR	C21-C22-C23-C24
22	L	210	BCR	C37-C22-C23-C24
21	R	102	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
21	K	104	LMU	C2B-C1B-O1B-C4'
21	K	104	LMU	C2'-C1'-O1'-C1
21	K	104	LMU	O5'-C1'-O1'-C1
20	4	311	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C2-C1-O2A-CGA
20	B	805	CLA	CAD-CBD-CGD-O1D
20	B	805	CLA	CAD-CBD-CGD-O2D
20	A	822	CLA	C1A-C2A-CAA-CBA
22	J	102	BCR	C5-C6-C7-C8
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
22	J	102	BCR	C18-C19-C20-C21
22	J	102	BCR	C20-C21-C22-C23
22	J	102	BCR	C20-C21-C22-C37
20	A	850	CLA	C3A-C2A-CAA-CBA
20	A	850	CLA	CBA-CGA-O2A-C1
20	K	103	CLA	C1A-C2A-CAA-CBA
20	K	103	CLA	C3A-C2A-CAA-CBA
20	K	103	CLA	C2-C1-O2A-CGA
20	K	103	CLA	CHA-CBD-CGD-O1D
20	K	103	CLA	CHA-CBD-CGD-O2D
21	H	106	LMU	O5'-C1'-O1'-C1
20	B	838	CLA	C2A-CAA-CBA-CGA
23	B	841	PQN	C12-C13-C15-C16
23	B	841	PQN	C14-C13-C15-C16
20	A	852	CLA	CHA-CBD-CGD-O1D
20	A	852	CLA	CHA-CBD-CGD-O2D
20	A	852	CLA	O2A-C1-C2-C3
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA
20	A	813	CLA	CBD-CGD-O2D-CED
20	1	204	CLA	C1A-C2A-CAA-CBA
20	1	204	CLA	CBD-CGD-O2D-CED
20	1	204	CLA	O1D-CGD-O2D-CED
20	B	824	CLA	C1A-C2A-CAA-CBA
20	B	824	CLA	C3A-C2A-CAA-CBA
20	L	207	CLA	C1A-C2A-CAA-CBA
20	L	207	CLA	C3A-C2A-CAA-CBA
20	L	207	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	K	106	LMU	C2'-C1'-O1'-C1
21	K	106	LMU	C2-C1-O1'-C1'
20	B	821	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	CBD-CGD-O2D-CED
20	B	821	CLA	C6-C7-C8-C9
20	B	833	CLA	CBD-CGD-O2D-CED
20	3	318	CLA	C2-C3-C5-C6
20	3	318	CLA	C4-C3-C5-C6
21	H	104	LMU	C2'-C1'-O1'-C1
21	H	104	LMU	O5'-C1'-O1'-C1
21	H	104	LMU	C2-C1-O1'-C1'
20	3	311	CLA	C1A-C2A-CAA-CBA
20	3	311	CLA	C3A-C2A-CAA-CBA
20	3	311	CLA	CAD-CBD-CGD-O1D
20	3	311	CLA	CAD-CBD-CGD-O2D
21	R	106	LMU	C2'-C1'-O1'-C1
21	R	106	LMU	O5'-C1'-O1'-C1
21	R	106	LMU	C2-C1-O1'-C1'
20	2	311	CLA	CHA-CBD-CGD-O1D
20	2	311	CLA	CHA-CBD-CGD-O2D
22	F	203	BCR	C7-C8-C9-C10
22	F	203	BCR	C7-C8-C9-C34
22	F	203	BCR	C15-C16-C17-C18
22	F	203	BCR	C18-C19-C20-C21
22	F	203	BCR	C19-C20-C21-C22
22	F	203	BCR	C20-C21-C22-C23
22	F	203	BCR	C20-C21-C22-C37
20	A	832	CLA	C1A-C2A-CAA-CBA
20	A	832	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	CAD-CBD-CGD-O1D
20	A	817	CLA	C1A-C2A-CAA-CBA
20	A	817	CLA	C3A-C2A-CAA-CBA
20	A	817	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	CHA-CBD-CGD-O1D
20	A	817	CLA	CHA-CBD-CGD-O2D
20	A	817	CLA	CBD-CGD-O2D-CED
20	R	108	CLA	O1A-CGA-O2A-C1
20	R	108	CLA	CHA-CBD-CGD-O1D
20	R	108	CLA	CAD-CBD-CGD-O1D
20	R	108	CLA	CAD-CBD-CGD-O2D
20	H	101	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	H	101	CLA	C3A-C2A-CAA-CBA
20	H	101	CLA	C2-C1-O2A-CGA
20	H	101	CLA	CAD-CBD-CGD-O1D
20	H	101	CLA	CAD-CBD-CGD-O2D
20	H	101	CLA	CBD-CGD-O2D-CED
20	A	821	CLA	C1A-C2A-CAA-CBA
20	A	821	CLA	C3A-C2A-CAA-CBA
20	A	839	CLA	C1A-C2A-CAA-CBA
20	A	839	CLA	C2C-C3C-CAC-CBC
20	A	839	CLA	C4C-C3C-CAC-CBC
20	A	839	CLA	C2-C3-C5-C6
20	A	839	CLA	C4-C3-C5-C6
20	3	317	CLA	C1A-C2A-CAA-CBA
21	R	104	LMU	O5'-C1'-O1'-C1
21	R	104	LMU	C2-C1-O1'-C1'
21	A	849	LMU	C2-C1-O1'-C1'
20	B	817	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	817	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	C4-C3-C5-C6
20	L	209	CLA	C1A-C2A-CAA-CBA
20	L	209	CLA	C3A-C2A-CAA-CBA
20	L	209	CLA	C2C-C3C-CAC-CBC
20	L	209	CLA	C4C-C3C-CAC-CBC
20	B	827	CLA	CHA-CBD-CGD-O1D
20	B	827	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	CAD-CBD-CGD-O1D
21	4	321	LMU	C2'-C1'-O1'-C1
21	4	321	LMU	O5'-C1'-O1'-C1
20	I	102	CLA	CHA-CBD-CGD-O1D
20	I	102	CLA	CHA-CBD-CGD-O2D
21	3	321	LMU	C2'-C1'-O1'-C1
21	3	321	LMU	O5'-C1'-O1'-C1
21	2	320	LMU	O5'-C1'-O1'-C1
21	2	320	LMU	C2-C1-O1'-C1'
21	H	105	LMU	O5'-C1'-O1'-C1
21	H	105	LMU	C2-C1-O1'-C1'
21	2	318	LMU	C2'-C1'-O1'-C1
21	2	318	LMU	O5'-C1'-O1'-C1
21	1	218	LMU	C2-C1-O1'-C1'
21	D	201	LMU	O5'-C1'-O1'-C1
21	1	213	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	1	213	LMU	C2-C1-O1'-C1'
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	CHA-CBD-CGD-O1D
20	B	828	CLA	CHA-CBD-CGD-O2D
20	B	828	CLA	CBD-CGD-O2D-CED
20	B	828	CLA	O1D-CGD-O2D-CED
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	C2C-C3C-CAC-CBC
20	B	823	CLA	C4C-C3C-CAC-CBC
20	B	823	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	C2-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
20	B	823	CLA	C11-C10-C8-C9
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	O1A-CGA-O2A-C1
22	I	101	BCR	C1-C6-C7-C8
22	I	101	BCR	C5-C6-C7-C8
22	I	101	BCR	C17-C18-C19-C20
22	I	101	BCR	C19-C20-C21-C22
20	1	215	CLA	CBA-CGA-O2A-C1
20	1	215	CLA	O1A-CGA-O2A-C1
20	1	215	CLA	C2C-C3C-CAC-CBC
20	1	215	CLA	C4C-C3C-CAC-CBC
20	1	215	CLA	CHA-CBD-CGD-O1D
20	1	215	CLA	CHA-CBD-CGD-O2D
20	1	215	CLA	CBD-CGD-O2D-CED
20	1	215	CLA	O1D-CGD-O2D-CED
20	1	215	CLA	O2A-C1-C2-C3
20	1	215	CLA	C4-C3-C5-C6
20	1	215	CLA	C11-C12-C13-C14
20	1	210	CLA	CBD-CGD-O2D-CED
20	1	210	CLA	C2-C3-C5-C6
20	1	210	CLA	C4-C3-C5-C6
20	K	108	CLA	O2A-C1-C2-C3
21	B	802	LMU	O5'-C1'-O1'-C1
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	846	BCR	C18-C19-C20-C21
22	B	846	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	B	846	BCR	C37-C22-C23-C24
20	B	809	CLA	C1A-C2A-CAA-CBA
20	B	809	CLA	C3A-C2A-CAA-CBA
20	B	809	CLA	CBA-CGA-O2A-C1
20	B	809	CLA	O1A-CGA-O2A-C1
20	A	834	CLA	C1A-C2A-CAA-CBA
20	A	834	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	C1A-C2A-CAA-CBA
20	A	820	CLA	CAD-CBD-CGD-O1D
20	A	820	CLA	CAD-CBD-CGD-O2D
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	831	CLA	C3A-C2A-CAA-CBA
20	B	831	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	O2A-C1-C2-C3
20	B	803	CLA	C2A-CAA-CBA-CGA
20	B	808	CLA	C1A-C2A-CAA-CBA
20	B	808	CLA	O2A-C1-C2-C3
21	2	317	LMU	O5'-C1'-O1'-C1
21	A	855	LMU	C2'-C1'-O1'-C1
21	A	855	LMU	O5'-C1'-O1'-C1
22	B	842	BCR	C7-C8-C9-C10
22	B	842	BCR	C7-C8-C9-C34
22	B	842	BCR	C17-C18-C19-C20
22	B	842	BCR	C36-C18-C19-C20
22	B	842	BCR	C18-C19-C20-C21
22	B	842	BCR	C20-C21-C22-C23
22	B	842	BCR	C20-C21-C22-C37
20	H	103	CLA	C2A-CAA-CBA-CGA
20	H	103	CLA	C2-C3-C5-C6
20	H	103	CLA	C4-C3-C5-C6
20	K	101	CLA	C2A-CAA-CBA-CGA
20	B	839	CLA	C3A-C2A-CAA-CBA
21	4	301	LMU	O5'-C1'-O1'-C1
20	1	202	CLA	CBD-CGD-O2D-CED
20	1	202	CLA	C2-C3-C5-C6
20	1	202	CLA	C4-C3-C5-C6
25	B	848	LMG	O6-C1-O1-C7
25	B	848	LMG	C11-C10-O7-C8
20	1	206	CLA	C1A-C2A-CAA-CBA
20	1	206	CLA	C2C-C3C-CAC-CBC
20	1	206	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	1	206	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	CBD-CGD-O2D-CED
20	B	832	CLA	C1A-C2A-CAA-CBA
20	B	832	CLA	C3A-C2A-CAA-CBA
20	B	832	CLA	CHA-CBD-CGD-O1D
20	B	832	CLA	CHA-CBD-CGD-O2D
20	B	832	CLA	CAD-CBD-CGD-O1D
20	B	832	CLA	CAD-CBD-CGD-O2D
20	B	832	CLA	CBD-CGD-O2D-CED
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	CHA-CBD-CGD-O1D
20	B	813	CLA	CHA-CBD-CGD-O2D
20	B	813	CLA	CAD-CBD-CGD-O1D
20	B	813	CLA	CAD-CBD-CGD-O2D
21	C	101	LMU	C2'-C1'-O1'-C1
21	C	101	LMU	O5'-C1'-O1'-C1
20	A	830	CLA	CBD-CGD-O2D-CED
23	A	842	PQN	C12-C13-C15-C16
23	A	842	PQN	C14-C13-C15-C16
20	A	815	CLA	C1A-C2A-CAA-CBA
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	815	CLA	CBA-CGA-O2A-C1
20	A	815	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	CBD-CGD-O2D-CED
20	A	840	CLA	C3A-C2A-CAA-CBA
20	A	840	CLA	CHA-CBD-CGD-O1D
20	A	840	CLA	CHA-CBD-CGD-O2D
20	A	840	CLA	CBD-CGD-O2D-CED
20	A	840	CLA	O1D-CGD-O2D-CED
22	A	846	BCR	C1-C6-C7-C8
22	A	846	BCR	C5-C6-C7-C8
22	A	846	BCR	C7-C8-C9-C10
22	A	846	BCR	C7-C8-C9-C34
22	A	846	BCR	C11-C12-C13-C35
22	A	846	BCR	C18-C19-C20-C21
22	A	846	BCR	C20-C21-C22-C23
22	A	846	BCR	C20-C21-C22-C37
22	A	846	BCR	C37-C22-C23-C24
22	A	846	BCR	C23-C24-C25-C30
22	3	314	BCR	C18-C19-C20-C21
22	3	314	BCR	C20-C21-C22-C23
22	3	314	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	3	314	BCR	C21-C22-C23-C24
22	3	314	BCR	C37-C22-C23-C24
21	1	220	LMU	C2'-C1'-O1'-C1
21	1	220	LMU	O5'-C1'-O1'-C1
21	1	220	LMU	C2-C1-O1'-C1'
20	H	109	CLA	O2A-C1-C2-C3
20	L	203	CLA	CBD-CGD-O2D-CED
20	L	203	CLA	C2-C3-C5-C6
20	L	203	CLA	C4-C3-C5-C6
21	R	109	LMU	O5B-C1B-O1B-C4'
21	R	109	LMU	O5'-C1'-O1'-C1
21	R	109	LMU	C2-C1-O1'-C1'
20	L	201	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	C3A-C2A-CAA-CBA
20	L	201	CLA	C2-C1-O2A-CGA
20	L	201	CLA	C2C-C3C-CAC-CBC
20	L	201	CLA	C4C-C3C-CAC-CBC
20	B	819	CLA	CBA-CGA-O2A-C1
20	B	819	CLA	CBD-CGD-O2D-CED
20	2	302	CLA	C1A-C2A-CAA-CBA
20	2	302	CLA	C3A-C2A-CAA-CBA
20	2	302	CLA	O2A-C1-C2-C3
20	A	828	CLA	C1A-C2A-CAA-CBA
20	A	828	CLA	C3A-C2A-CAA-CBA
20	A	828	CLA	CHA-CBD-CGD-O1D
20	A	828	CLA	CHA-CBD-CGD-O2D
20	A	828	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	CBA-CGA-O2A-C1
20	2	312	CLA	O1A-CGA-O2A-C1
20	L	208	CLA	CBD-CGD-O2D-CED
20	4	318	CLA	C1A-C2A-CAA-CBA
22	A	843	BCR	C18-C19-C20-C21
22	A	843	BCR	C20-C21-C22-C23
22	A	843	BCR	C20-C21-C22-C37
22	A	843	BCR	C21-C22-C23-C24
22	A	843	BCR	C37-C22-C23-C24
21	F	201	LMU	C2'-C1'-O1'-C1
21	F	201	LMU	O5'-C1'-O1'-C1
21	2	319	LMU	C2B-C1B-O1B-C4'
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	O1A-CGA-O2A-C1
20	A	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	835	CLA	CHA-CBD-CGD-O1D
20	A	835	CLA	CHA-CBD-CGD-O2D
20	A	816	CLA	C4C-C3C-CAC-CBC
20	B	811	CLA	C4C-C3C-CAC-CBC
20	4	306	CLA	C4C-C3C-CAC-CBC
21	K	105	LMU	C3'-C4'-O1B-C1B
21	4	301	LMU	C5'-C4'-O1B-C1B
20	3	308	CLA	O1D-CGD-O2D-CED
20	A	816	CLA	O1D-CGD-O2D-CED
20	L	202	CLA	O1D-CGD-O2D-CED
20	B	814	CLA	O1D-CGD-O2D-CED
20	F	205	CLA	O1D-CGD-O2D-CED
20	A	801	CLA	O1D-CGD-O2D-CED
20	4	319	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	O1D-CGD-O2D-CED
20	J	101	CLA	O1D-CGD-O2D-CED
20	L	207	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	O1D-CGD-O2D-CED
20	H	103	CLA	O1D-CGD-O2D-CED
20	A	807	CLA	O1D-CGD-O2D-CED
20	A	815	CLA	O1D-CGD-O2D-CED
20	A	823	CLA	O1D-CGD-O2D-CED
21	K	105	LMU	O5B-C1B-O1B-C4'
21	B	801	LMU	O5B-C1B-O1B-C4'
21	E	101	LMU	O5B-C1B-O1B-C4'
20	2	307	CLA	C15-C16-C17-C18
20	B	825	CLA	C2C-C3C-CAC-CBC
20	B	825	CLA	C4C-C3C-CAC-CBC
20	2	303	CLA	C2C-C3C-CAC-CBC
20	4	305	CLA	C2C-C3C-CAC-CBC
20	B	811	CLA	C2C-C3C-CAC-CBC
20	4	306	CLA	C2C-C3C-CAC-CBC
21	H	107	LMU	C3'-C4'-O1B-C1B
20	K	102	CLA	C2C-C3C-CAC-CBC
20	G	102	CLA	C2C-C3C-CAC-CBC
21	R	101	LMU	C3'-C4'-O1B-C1B
20	1	201	CLA	C2C-C3C-CAC-CBC
20	3	313	CLA	C2C-C3C-CAC-CBC
20	3	313	CLA	C4C-C3C-CAC-CBC
20	4	319	CLA	C2C-C3C-CAC-CBC
21	R	103	LMU	C3'-C4'-O1B-C1B
21	2	317	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
20	B	839	CLA	C2C-C3C-CAC-CBC
20	B	839	CLA	C4C-C3C-CAC-CBC
20	B	819	CLA	C2C-C3C-CAC-CBC
20	4	316	CLA	O1D-CGD-O2D-CED
20	1	203	CLA	O1D-CGD-O2D-CED
20	2	322	CLA	O1D-CGD-O2D-CED
20	A	818	CLA	O1D-CGD-O2D-CED
20	4	306	CLA	O1D-CGD-O2D-CED
20	R	107	CLA	O1D-CGD-O2D-CED
20	A	837	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	O1D-CGD-O2D-CED
20	3	313	CLA	O1D-CGD-O2D-CED
20	A	811	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	O1D-CGD-O2D-CED
20	H	101	CLA	O1D-CGD-O2D-CED
20	B	823	CLA	O1D-CGD-O2D-CED
20	B	831	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	O1D-CGD-O2D-CED
20	A	830	CLA	O1D-CGD-O2D-CED
20	L	203	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	O1D-CGD-O2D-CED
20	L	208	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	O1D-CGD-O2D-CED
20	4	316	CLA	CBD-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	B	851	CLA	CBD-CGD-O2D-CED
20	3	308	CLA	CBD-CGD-O2D-CED
20	1	203	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBD-CGD-O2D-CED
20	A	825	CLA	CBD-CGD-O2D-CED
20	1	201	CLA	CBD-CGD-O2D-CED
20	B	850	CLA	CBD-CGD-O2D-CED
20	B	830	CLA	CBD-CGD-O2D-CED
20	1	207	CLA	CBD-CGD-O2D-CED
20	B	849	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	CBD-CGD-O2D-CED
20	A	822	CLA	CBD-CGD-O2D-CED
20	K	103	CLA	CBD-CGD-O2D-CED
20	J	101	CLA	CBD-CGD-O2D-CED
20	A	839	CLA	CBD-CGD-O2D-CED
20	L	209	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	I	102	CLA	CBD-CGD-O2D-CED
20	A	804	CLA	CBD-CGD-O2D-CED
20	B	809	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	CBD-CGD-O2D-CED
20	H	103	CLA	CBD-CGD-O2D-CED
20	B	835	CLA	CBD-CGD-O2D-CED
20	1	206	CLA	CBD-CGD-O2D-CED
20	B	813	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	CBD-CGD-O2D-CED
20	H	109	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	CBD-CGD-O2D-CED
20	R	107	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	A	850	CLA	O1A-CGA-O2A-C1
20	3	318	CLA	O1A-CGA-O2A-C1
20	A	832	CLA	O1A-CGA-O2A-C1
20	B	808	CLA	O1A-CGA-O2A-C1
20	B	837	CLA	O1A-CGA-O2A-C1
20	H	103	CLA	O1A-CGA-O2A-C1
20	4	316	CLA	O1A-CGA-O2A-C1
21	K	106	LMU	O5B-C1B-O1B-C4'
21	K	105	LMU	C2B-C1B-O1B-C4'
21	B	801	LMU	C2B-C1B-O1B-C4'
21	E	101	LMU	C2B-C1B-O1B-C4'
20	A	816	CLA	C2C-C3C-CAC-CBC
20	4	305	CLA	C4C-C3C-CAC-CBC
21	4	322	LMU	C5'-C4'-O1B-C1B
20	K	102	CLA	C4C-C3C-CAC-CBC
20	1	201	CLA	C4C-C3C-CAC-CBC
20	A	801	CLA	C2C-C3C-CAC-CBC
20	A	801	CLA	C4C-C3C-CAC-CBC
20	4	319	CLA	C4C-C3C-CAC-CBC
21	K	109	LMU	C5'-C4'-O1B-C1B
20	A	819	CLA	C4C-C3C-CAC-CBC
20	1	204	CLA	C2C-C3C-CAC-CBC
20	B	821	CLA	C2C-C3C-CAC-CBC
20	B	821	CLA	C4C-C3C-CAC-CBC
21	2	320	LMU	C5'-C4'-O1B-C1B
21	1	218	LMU	C3'-C4'-O1B-C1B
21	B	847	LMU	C5'-C4'-O1B-C1B
20	A	815	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	A	848	LMU	C4B-C5B-C6B-O6B
20	J	103	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	O1D-CGD-O2D-CED
20	B	825	CLA	O1D-CGD-O2D-CED
20	B	806	CLA	O1D-CGD-O2D-CED
20	A	814	CLA	O1D-CGD-O2D-CED
20	1	207	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	O1D-CGD-O2D-CED
20	K	103	CLA	O1D-CGD-O2D-CED
20	1	210	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	O1D-CGD-O2D-CED
20	B	813	CLA	O1D-CGD-O2D-CED
20	A	826	CLA	O1D-CGD-O2D-CED
20	4	316	CLA	CBA-CGA-O2A-C1
20	2	303	CLA	C4C-C3C-CAC-CBC
20	1	203	CLA	C2-C1-O2A-CGA
20	G	102	CLA	C4C-C3C-CAC-CBC
20	A	811	CLA	C4C-C3C-CAC-CBC
20	J	101	CLA	C2C-C3C-CAC-CBC
20	J	101	CLA	C4C-C3C-CAC-CBC
20	1	204	CLA	C4C-C3C-CAC-CBC
21	A	849	LMU	C5'-C4'-O1B-C1B
20	B	819	CLA	C4C-C3C-CAC-CBC
25	B	848	LMG	C8-C9-O8-C28
21	L	211	LMU	O5B-C1B-O1B-C4'
21	1	217	LMU	O5B-C1B-O1B-C4'
21	2	313	LMU	O5B-C1B-O1B-C4'
21	H	108	LMU	O5B-C1B-O1B-C4'
21	R	105	LMU	O5B-C1B-O1B-C4'
21	R	102	LMU	O5B-C1B-O1B-C4'
21	A	849	LMU	O5B-C1B-O1B-C4'
21	G	101	LMU	O5B-C1B-O1B-C4'
20	G	102	CLA	O1D-CGD-O2D-CED
20	A	824	CLA	O1D-CGD-O2D-CED
20	H	102	CLA	O1D-CGD-O2D-CED
20	4	311	CLA	O1D-CGD-O2D-CED
20	B	833	CLA	O1D-CGD-O2D-CED
20	1	202	CLA	O1D-CGD-O2D-CED
20	B	832	CLA	O1D-CGD-O2D-CED
20	B	834	CLA	CBA-CGA-O2A-C1
20	R	107	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	3	318	CLA	CBA-CGA-O2A-C1
20	A	832	CLA	CBA-CGA-O2A-C1
20	B	837	CLA	CBA-CGA-O2A-C1
20	H	103	CLA	CBA-CGA-O2A-C1
20	4	305	CLA	CBD-CGD-O2D-CED
20	A	812	CLA	CBD-CGD-O2D-CED
20	A	833	CLA	CBD-CGD-O2D-CED
20	B	816	CLA	CBD-CGD-O2D-CED
20	3	318	CLA	CBD-CGD-O2D-CED
20	R	108	CLA	CBD-CGD-O2D-CED
20	3	317	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CBD-CGD-O2D-CED
20	B	851	CLA	C2C-C3C-CAC-CBC
20	B	851	CLA	C4C-C3C-CAC-CBC
20	A	811	CLA	C2C-C3C-CAC-CBC
20	A	819	CLA	C2C-C3C-CAC-CBC
20	A	832	CLA	C2C-C3C-CAC-CBC
20	A	832	CLA	C4C-C3C-CAC-CBC
20	A	815	CLA	C4C-C3C-CAC-CBC
21	1	220	LMU	C3'-C4'-O1B-C1B
20	2	302	CLA	C2C-C3C-CAC-CBC
20	2	302	CLA	C4C-C3C-CAC-CBC
20	2	312	CLA	C2C-C3C-CAC-CBC
20	J	103	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	O1A-CGA-O2A-C1
20	2	316	CLA	O1A-CGA-O2A-C1
20	B	834	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	2	307	CLA	O1A-CGA-O2A-C1
20	1	207	CLA	O1A-CGA-O2A-C1
20	3	313	CLA	O1A-CGA-O2A-C1
20	B	849	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	A	852	CLA	O1A-CGA-O2A-C1
20	K	108	CLA	O1A-CGA-O2A-C1
20	1	202	CLA	O1A-CGA-O2A-C1
20	1	206	CLA	O1A-CGA-O2A-C1
20	A	840	CLA	O1A-CGA-O2A-C1
20	A	826	CLA	O1A-CGA-O2A-C1
20	1	201	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	O1D-CGD-O2D-CED
20	A	813	CLA	O1D-CGD-O2D-CED
20	B	821	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	C4C-C3C-CAC-CBC
20	H	101	CLA	C2C-C3C-CAC-CBC
20	H	101	CLA	C4C-C3C-CAC-CBC
20	B	835	CLA	C4C-C3C-CAC-CBC
20	2	312	CLA	C4C-C3C-CAC-CBC
21	4	317	LMU	O5'-C5'-C6'-O6'
20	2	316	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	O1D-CGD-O2D-CED
20	A	834	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	C2C-C3C-CAC-CBC
20	A	825	CLA	C4C-C3C-CAC-CBC
20	B	827	CLA	C2C-C3C-CAC-CBC
20	B	827	CLA	C4C-C3C-CAC-CBC
21	B	802	LMU	C3'-C4'-O1B-C1B
20	A	832	CLA	CBD-CGD-O2D-CED
20	4	307	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	O1D-CGD-O2D-CED
25	B	848	LMG	O9-C10-O7-C8
20	B	814	CLA	CBA-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1
21	1	219	LMU	C3'-C4'-O1B-C1B
20	B	835	CLA	C2C-C3C-CAC-CBC
20	B	814	CLA	O1A-CGA-O2A-C1
20	4	302	CLA	C3-C5-C6-C7
20	A	816	CLA	C3-C5-C6-C7
20	4	305	CLA	C3-C5-C6-C7
20	B	811	CLA	C3-C5-C6-C7
20	A	805	CLA	C3-C5-C6-C7
20	A	838	CLA	C3-C5-C6-C7
20	B	850	CLA	C3-C5-C6-C7
20	B	805	CLA	C3-C5-C6-C7
20	B	838	CLA	C3-C5-C6-C7
20	A	819	CLA	C3-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7
20	B	835	CLA	C3-C5-C6-C7
20	A	830	CLA	C3-C5-C6-C7
20	A	826	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	828	CLA	C3-C5-C6-C7
20	A	841	CLA	CBA-CGA-O2A-C1
20	F	206	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	A	801	CLA	CBA-CGA-O2A-C1
20	3	313	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	849	CLA	CBA-CGA-O2A-C1
20	A	852	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	CBA-CGA-O2A-C1
20	R	108	CLA	CBA-CGA-O2A-C1
20	K	108	CLA	CBA-CGA-O2A-C1
20	B	808	CLA	CBA-CGA-O2A-C1
20	1	202	CLA	CBA-CGA-O2A-C1
20	1	206	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	C2C-C3C-CAC-CBC
21	A	856	LMU	C3'-C4'-O1B-C1B
21	R	104	LMU	O5B-C5B-C6B-O6B
20	B	829	CLA	CBD-CGD-O2D-CED
21	A	853	LMU	C3'-C4'-O1B-C1B
20	1	207	CLA	C2C-C3C-CAC-CBC
20	4	318	CLA	C2C-C3C-CAC-CBC
21	R	101	LMU	C4'-C5'-C6'-O6'
21	D	201	LMU	C4'-C5'-C6'-O6'
21	1	220	LMU	C4B-C5B-C6B-O6B
20	A	837	CLA	C2-C1-O2A-CGA
21	3	322	LMU	C2B-C1B-O1B-C4'
20	A	836	CLA	C2C-C3C-CAC-CBC
20	1	206	CLA	C4-C3-C5-C6
21	K	105	LMU	C4B-C5B-C6B-O6B
20	L	202	CLA	C2-C3-C5-C6
20	B	812	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	CBD-CGD-O2D-CED
20	L	202	CLA	C2A-CAA-CBA-CGA
20	A	805	CLA	C2A-CAA-CBA-CGA
20	K	102	CLA	C2A-CAA-CBA-CGA
20	B	820	CLA	C2A-CAA-CBA-CGA
20	A	850	CLA	C2A-CAA-CBA-CGA
20	A	832	CLA	C2A-CAA-CBA-CGA
20	A	817	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	H	109	CLA	C2A-CAA-CBA-CGA
20	A	809	CLA	O1A-CGA-O2A-C1
20	2	312	CLA	O1D-CGD-O2D-CED
20	A	827	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	R	108	CLA	C3-C5-C6-C7
20	B	839	CLA	C3-C5-C6-C7
20	J	103	CLA	CBA-CGA-O2A-C1
20	2	316	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
20	2	307	CLA	CBA-CGA-O2A-C1
20	1	207	CLA	CBA-CGA-O2A-C1
20	H	102	CLA	CBA-CGA-O2A-C1
20	B	817	CLA	CBA-CGA-O2A-C1
20	L	209	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	803	CLA	CBA-CGA-O2A-C1
20	A	840	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
21	2	313	LMU	O5'-C5'-C6'-O6'
21	H	107	LMU	O5B-C5B-C6B-O6B
21	H	108	LMU	O5B-C5B-C6B-O6B
21	R	106	LMU	O5B-C5B-C6B-O6B
21	1	213	LMU	O5B-C5B-C6B-O6B
21	4	320	LMU	C4'-C5'-C6'-O6'
21	R	103	LMU	C4B-C5B-C6B-O6B
21	H	104	LMU	C2B-C1B-O1B-C4'
21	H	107	LMU	C6-C7-C8-C9
21	H	105	LMU	C3-C4-C5-C6
20	B	830	CLA	O1D-CGD-O2D-CED
20	B	827	CLA	O1D-CGD-O2D-CED
20	J	103	CLA	C2C-C3C-CAC-CBC
21	A	854	LMU	C2-C3-C4-C5
20	4	318	CLA	C4C-C3C-CAC-CBC
21	3	322	LMU	O5B-C1B-O1B-C4'
21	H	107	LMU	O5B-C1B-O1B-C4'
21	4	321	LMU	O5B-C1B-O1B-C4'
20	A	825	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	O1D-CGD-O2D-CED
21	G	101	LMU	O5'-C5'-C6'-O6'
21	1	220	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	B	801	LMU	C4B-C5B-C6B-O6B
21	K	104	LMU	C4'-C5'-C6'-O6'
20	F	206	CLA	O1A-CGA-O2A-C1
20	A	801	CLA	O1A-CGA-O2A-C1
20	H	102	CLA	O1A-CGA-O2A-C1
20	4	319	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	A	836	CLA	O1A-CGA-O2A-C1
21	E	101	LMU	C1-C2-C3-C4
21	G	101	LMU	C11-C10-C9-C8
20	B	832	CLA	C2A-CAA-CBA-CGA
20	B	819	CLA	O1A-CGA-O2A-C1
22	B	852	BCR	C19-C20-C21-C22
22	B	844	BCR	C19-C20-C21-C22
22	A	847	BCR	C19-C20-C21-C22
22	F	203	BCR	C13-C14-C15-C16
22	A	846	BCR	C19-C20-C21-C22
22	3	314	BCR	C19-C20-C21-C22
22	A	843	BCR	C9-C10-C11-C12
21	4	321	LMU	C2B-C1B-O1B-C4'
21	R	105	LMU	O5B-C5B-C6B-O6B
21	R	104	LMU	O5'-C5'-C6'-O6'
21	D	201	LMU	O5B-C5B-C6B-O6B
21	F	201	LMU	O5B-C5B-C6B-O6B
20	1	207	CLA	C4C-C3C-CAC-CBC
21	R	104	LMU	C3'-C4'-O1B-C1B
20	A	827	CLA	CBD-CGD-O2D-CED
20	2	316	CLA	C3-C5-C6-C7
20	A	822	CLA	C3-C5-C6-C7
20	A	809	CLA	CBA-CGA-O2A-C1
20	2	305	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	CBA-CGA-O2A-C1
20	4	311	CLA	CBA-CGA-O2A-C1
20	A	839	CLA	CBA-CGA-O2A-C1
20	A	836	CLA	CBA-CGA-O2A-C1
20	H	109	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	CBA-CGA-O2A-C1
21	B	847	LMU	C6-C7-C8-C9
20	L	209	CLA	O1A-CGA-O2A-C1
21	H	107	LMU	C2B-C1B-O1B-C4'
21	R	105	LMU	O5'-C5'-C6'-O6'
21	R	103	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
21	4	321	LMU	O5B-C5B-C6B-O6B
21	2	318	LMU	O5B-C5B-C6B-O6B
21	1	219	LMU	O5'-C5'-C6'-O6'
21	4	317	LMU	C4'-C5'-C6'-O6'
21	1	217	LMU	C4'-C5'-C6'-O6'
21	R	106	LMU	C4B-C5B-C6B-O6B
20	B	850	CLA	O1D-CGD-O2D-CED
20	I	102	CLA	O1D-CGD-O2D-CED
20	B	835	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	C5-C6-C7-C8
21	N	101	LMU	C11-C10-C9-C8
20	K	108	CLA	C2C-C3C-CAC-CBC
21	F	201	LMU	C7-C8-C9-C10
21	A	853	LMU	O5B-C1B-O1B-C4'
20	A	852	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBD-CGD-O2D-CED
21	L	204	LMU	O5'-C5'-C6'-O6'
21	F	201	LMU	O5'-C5'-C6'-O6'
21	A	848	LMU	C2-C3-C4-C5
20	4	319	CLA	C2-C1-O2A-CGA
21	K	109	LMU	C5-C6-C7-C8
21	R	102	LMU	C6-C7-C8-C9
21	R	102	LMU	C11-C10-C9-C8
21	H	106	LMU	C5-C6-C7-C8
21	K	106	LMU	C2-C3-C4-C5
21	R	104	LMU	C11-C10-C9-C8
21	D	201	LMU	C7-C8-C9-C10
21	B	847	LMU	C11-C10-C9-C8
21	1	219	LMU	C7-C8-C9-C10
21	B	847	LMU	O5B-C1B-O1B-C4'
20	2	305	CLA	O1A-CGA-O2A-C1
21	A	853	LMU	C2-C3-C4-C5
21	A	854	LMU	C4-C5-C6-C7
21	R	106	LMU	C2-C3-C4-C5
21	4	321	LMU	C7-C8-C9-C10
21	H	105	LMU	C6-C7-C8-C9
21	4	321	LMU	O5'-C5'-C6'-O6'
21	D	201	LMU	O5'-C5'-C6'-O6'
21	A	856	LMU	O5'-C5'-C6'-O6'
21	4	322	LMU	C4B-C5B-C6B-O6B
21	R	103	LMU	C4'-C5'-C6'-O6'
21	R	104	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	1	213	LMU	C4B-C5B-C6B-O6B
21	1	219	LMU	C4'-C5'-C6'-O6'
21	G	101	LMU	C4'-C5'-C6'-O6'
21	A	848	LMU	C3'-C4'-O1B-C1B
21	1	218	LMU	C1-C2-C3-C4
20	K	103	CLA	C3-C5-C6-C7
20	H	103	CLA	C3-C5-C6-C7
23	A	842	PQN	C13-C15-C16-C17
20	L	203	CLA	C3-C5-C6-C7
20	4	319	CLA	CBA-CGA-O2A-C1
20	3	317	CLA	O1D-CGD-O2D-CED
21	4	320	LMU	O5'-C5'-C6'-O6'
21	1	217	LMU	O5'-C5'-C6'-O6'
21	R	101	LMU	O5'-C5'-C6'-O6'
21	A	853	LMU	O5'-C5'-C6'-O6'
21	R	105	LMU	C4B-C5B-C6B-O6B
21	2	317	LMU	C4'-C5'-C6'-O6'
21	L	211	LMU	C5-C6-C7-C8
21	E	101	LMU	C3-C4-C5-C6
21	K	106	LMU	C4-C5-C6-C7
20	A	837	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	O1A-CGA-O2A-C1
20	A	828	CLA	O1A-CGA-O2A-C1
21	H	106	LMU	O1'-C1-C2-C3
20	A	852	CLA	C2C-C3C-CAC-CBC
21	A	848	LMU	O5B-C5B-C6B-O6B
21	L	205	LMU	O5B-C5B-C6B-O6B
21	B	801	LMU	O5B-C5B-C6B-O6B
21	3	321	LMU	O5'-C5'-C6'-O6'
21	H	105	LMU	O5'-C5'-C6'-O6'
20	A	851	CLA	C4-C3-C5-C6
20	B	824	CLA	C4-C3-C5-C6
20	A	831	CLA	C4-C3-C5-C6
20	4	318	CLA	C4-C3-C5-C6
21	L	205	LMU	C4B-C5B-C6B-O6B
21	H	107	LMU	C4B-C5B-C6B-O6B
21	L	204	LMU	C4'-C5'-C6'-O6'
21	F	201	LMU	C4B-C5B-C6B-O6B
20	A	851	CLA	C2-C3-C5-C6
20	2	303	CLA	C2-C3-C5-C6
20	B	824	CLA	C2-C3-C5-C6
20	B	817	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	1	215	CLA	C2-C3-C5-C6
20	A	831	CLA	C2-C3-C5-C6
20	4	318	CLA	C2-C3-C5-C6
20	B	811	CLA	C2A-CAA-CBA-CGA
20	B	812	CLA	C2A-CAA-CBA-CGA
20	A	838	CLA	C2A-CAA-CBA-CGA
20	B	819	CLA	C2A-CAA-CBA-CGA
20	H	109	CLA	O1D-CGD-O2D-CED
21	K	105	LMU	O5B-C5B-C6B-O6B
21	L	204	LMU	O5B-C5B-C6B-O6B
21	K	104	LMU	O5'-C5'-C6'-O6'
21	R	103	LMU	O5B-C5B-C6B-O6B
21	A	855	LMU	O5B-C5B-C6B-O6B
20	4	311	CLA	O1A-CGA-O2A-C1
20	A	839	CLA	O1A-CGA-O2A-C1
20	B	803	CLA	O1A-CGA-O2A-C1
21	F	201	LMU	C4'-C5'-C6'-O6'
21	N	101	LMU	O5'-C1'-O1'-C1
21	L	205	LMU	O5'-C1'-O1'-C1
21	A	854	LMU	O5'-C1'-O1'-C1
21	K	106	LMU	O5'-C1'-O1'-C1
21	B	847	LMU	O5'-C1'-O1'-C1
21	H	108	LMU	C4-C5-C6-C7
21	H	108	LMU	C6-C7-C8-C9
21	R	106	LMU	C6-C7-C8-C9
21	K	104	LMU	O5B-C1B-O1B-C4'
20	A	838	CLA	CBA-CGA-O2A-C1
20	2	305	CLA	C2C-C3C-CAC-CBC
20	B	838	CLA	C2C-C3C-CAC-CBC
21	R	109	LMU	C7-C8-C9-C10
20	L	208	CLA	C2C-C3C-CAC-CBC
21	K	109	LMU	O5'-C5'-C6'-O6'
21	H	108	LMU	C4B-C5B-C6B-O6B
21	2	317	LMU	O5B-C1B-O1B-C4'
21	K	105	LMU	C3-C4-C5-C6
20	A	836	CLA	C4C-C3C-CAC-CBC
20	B	816	CLA	O1D-CGD-O2D-CED
20	B	849	CLA	O1D-CGD-O2D-CED
20	H	109	CLA	O1A-CGA-O2A-C1
21	A	848	LMU	C4'-C5'-C6'-O6'
21	R	101	LMU	C4B-C5B-C6B-O6B
21	D	201	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	A	855	LMU	C4B-C5B-C6B-O6B
21	2	313	LMU	C5'-C4'-O1B-C1B
21	2	318	LMU	C3-C4-C5-C6
20	1	201	CLA	O1D-CGD-O2D-CED
20	L	209	CLA	O1D-CGD-O2D-CED
20	4	307	CLA	O1D-CGD-O2D-CED
20	A	831	CLA	O1D-CGD-O2D-CED
20	2	302	CLA	CBD-CGD-O2D-CED
21	N	101	LMU	O5B-C1B-O1B-C4'
20	B	851	CLA	O1D-CGD-O2D-CED
20	A	838	CLA	O1A-CGA-O2A-C1
21	3	322	LMU	C3-C4-C5-C6
20	A	812	CLA	C3-C5-C6-C7
20	4	305	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBA-CGA-O2A-C1
20	K	102	CLA	CBA-CGA-O2A-C1
20	L	207	CLA	CBA-CGA-O2A-C1
20	2	311	CLA	CBA-CGA-O2A-C1
20	3	317	CLA	CBA-CGA-O2A-C1
20	1	210	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	CBA-CGA-O2A-C1
25	B	848	LMG	C29-C28-O8-C9
20	2	302	CLA	CBA-CGA-O2A-C1
21	H	104	LMU	C1-C2-C3-C4
20	4	302	CLA	CBD-CGD-O2D-CED
20	B	838	CLA	CBD-CGD-O2D-CED
20	A	819	CLA	CBD-CGD-O2D-CED
20	B	810	CLA	CBD-CGD-O2D-CED
21	2	319	LMU	C2-C3-C4-C5
22	I	103	BCR	C9-C10-C11-C12
22	L	210	BCR	C19-C20-C21-C22
22	B	846	BCR	C19-C20-C21-C22
21	K	104	LMU	C11-C10-C9-C8
21	A	855	LMU	C5-C6-C7-C8
21	R	105	LMU	C4'-C5'-C6'-O6'
21	R	104	LMU	C4'-C5'-C6'-O6'
21	3	321	LMU	C4'-C5'-C6'-O6'
21	H	105	LMU	C4'-C5'-C6'-O6'
21	A	856	LMU	C4'-C5'-C6'-O6'
21	B	801	LMU	C6-C7-C8-C9
21	4	320	LMU	C7-C8-C9-C10
21	A	848	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
21	1	219	LMU	C3-C4-C5-C6
20	A	831	CLA	C2C-C3C-CAC-CBC
21	2	313	LMU	C4'-C5'-C6'-O6'
21	L	204	LMU	C4B-C5B-C6B-O6B
21	H	105	LMU	C4B-C5B-C6B-O6B
20	B	825	CLA	C8-C10-C11-C12
20	A	841	CLA	C15-C16-C17-C18
20	B	830	CLA	C13-C15-C16-C17
20	3	313	CLA	C5-C6-C7-C8
20	A	819	CLA	C10-C11-C12-C13
20	A	808	CLA	C5-C6-C7-C8
20	B	803	CLA	C15-C16-C17-C18
20	A	817	CLA	C3-C5-C6-C7
21	4	320	LMU	C2'-C1'-O1'-C1
21	B	802	LMU	C2'-C1'-O1'-C1
21	2	317	LMU	C2'-C1'-O1'-C1
21	R	109	LMU	C2'-C1'-O1'-C1
21	2	319	LMU	C2'-C1'-O1'-C1
21	R	103	LMU	C7-C8-C9-C10
25	B	848	LMG	O10-C28-O8-C9
21	A	853	LMU	C2B-C1B-O1B-C4'
21	4	322	LMU	O5B-C5B-C6B-O6B
21	B	802	LMU	O5B-C5B-C6B-O6B
21	2	317	LMU	O5'-C5'-C6'-O6'
20	J	103	CLA	C11-C12-C13-C14
20	B	825	CLA	C6-C7-C8-C9
20	B	851	CLA	C14-C13-C15-C16
20	B	836	CLA	C11-C12-C13-C14
20	A	818	CLA	C6-C7-C8-C9
20	4	304	CLA	C6-C7-C8-C9
20	B	812	CLA	C14-C13-C15-C16
20	A	825	CLA	C11-C10-C8-C9
20	A	825	CLA	C14-C13-C15-C16
20	B	830	CLA	C11-C10-C8-C9
20	B	849	CLA	C11-C12-C13-C14
20	A	852	CLA	C11-C10-C8-C9
20	B	824	CLA	C11-C12-C13-C14
20	B	821	CLA	C14-C13-C15-C16
20	3	311	CLA	C11-C12-C13-C14
20	3	311	CLA	C14-C13-C15-C16
20	A	839	CLA	C6-C7-C8-C9
20	B	827	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	C11-C10-C8-C9
20	B	803	CLA	C14-C13-C15-C16
20	B	808	CLA	C11-C10-C8-C9
20	1	202	CLA	C11-C10-C8-C9
23	A	842	PQN	C21-C22-C23-C24
20	A	823	CLA	C11-C10-C8-C9
20	A	823	CLA	C14-C13-C15-C16
20	A	826	CLA	C15-C16-C17-C18
20	4	302	CLA	C2A-CAA-CBA-CGA
20	R	107	CLA	C2A-CAA-CBA-CGA
20	A	837	CLA	C2A-CAA-CBA-CGA
22	B	844	BCR	C11-C12-C13-C35
22	A	845	BCR	C7-C8-C9-C34
22	I	103	BCR	C37-C22-C23-C24
22	F	202	BCR	C37-C22-C23-C24
22	J	102	BCR	C36-C18-C19-C20
22	I	101	BCR	C36-C18-C19-C20
22	B	846	BCR	C7-C8-C9-C34
22	A	846	BCR	C36-C18-C19-C20
22	3	314	BCR	C36-C18-C19-C20
22	A	843	BCR	C7-C8-C9-C34
22	B	844	BCR	C21-C22-C23-C24
22	I	103	BCR	C21-C22-C23-C24
22	F	202	BCR	C21-C22-C23-C24
22	B	846	BCR	C7-C8-C9-C10
22	A	846	BCR	C21-C22-C23-C24
22	3	314	BCR	C17-C18-C19-C20
21	A	853	LMU	C4B-C5B-C6B-O6B
20	2	311	CLA	O1A-CGA-O2A-C1
20	A	834	CLA	O1A-CGA-O2A-C1
20	B	851	CLA	C10-C11-C12-C13
20	A	850	CLA	C10-C11-C12-C13
20	B	839	CLA	C15-C16-C17-C18
20	3	318	CLA	O1D-CGD-O2D-CED
21	B	801	LMU	C7-C8-C9-C10
20	4	318	CLA	CBD-CGD-O2D-CED
21	L	211	LMU	O5B-C5B-C6B-O6B
21	1	218	LMU	O5'-C5'-C6'-O6'
21	A	853	LMU	C4'-C5'-C6'-O6'
21	K	109	LMU	C4'-C5'-C6'-O6'
21	R	109	LMU	C5'-C4'-O1B-C1B
20	A	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	811	CLA	C3-C5-C6-C7
20	3	311	CLA	C3-C5-C6-C7
20	B	851	CLA	C13-C15-C16-C17
20	2	303	CLA	C8-C10-C11-C12
20	A	827	CLA	C5-C6-C7-C8
20	L	202	CLA	C5-C6-C7-C8
20	L	202	CLA	C13-C15-C16-C17
20	B	830	CLA	C10-C11-C12-C13
20	A	811	CLA	C5-C6-C7-C8
20	A	850	CLA	C5-C6-C7-C8
20	B	827	CLA	C15-C16-C17-C18
20	A	831	CLA	C5-C6-C7-C8
20	4	316	CLA	C2C-C3C-CAC-CBC
21	N	101	LMU	C2B-C1B-O1B-C4'
20	J	103	CLA	C4C-C3C-CAC-CBC
21	H	104	LMU	C4-C5-C6-C7
20	3	317	CLA	C2C-C3C-CAC-CBC
21	C	101	LMU	O5'-C5'-C6'-O6'
21	R	101	LMU	C1-C2-C3-C4
21	H	108	LMU	C1-C2-C3-C4
20	A	818	CLA	C10-C11-C12-C13
20	A	841	CLA	C8-C10-C11-C12
20	B	807	CLA	C15-C16-C17-C18
20	4	311	CLA	C5-C6-C7-C8
23	B	841	PQN	C15-C16-C17-C18
20	3	311	CLA	C5-C6-C7-C8
20	R	108	CLA	C8-C10-C11-C12
20	B	817	CLA	C10-C11-C12-C13
20	B	803	CLA	C13-C15-C16-C17
20	B	808	CLA	C10-C11-C12-C13
20	1	206	CLA	C8-C10-C11-C12
21	R	109	LMU	C3'-C4'-O1B-C1B
21	R	101	LMU	O5B-C5B-C6B-O6B
21	A	853	LMU	O1'-C1-C2-C3
21	H	108	LMU	C5-C6-C7-C8
21	1	213	LMU	C3'-C4'-O1B-C1B
21	L	205	LMU	C4'-C5'-C6'-O6'
20	B	812	CLA	C13-C15-C16-C17
20	B	820	CLA	C5-C6-C7-C8
20	B	807	CLA	C8-C10-C11-C12
20	A	811	CLA	C10-C11-C12-C13
20	B	808	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	H	103	CLA	C5-C6-C7-C8
20	A	809	CLA	C2C-C3C-CAC-CBC
21	K	106	LMU	O1'-C1-C2-C3
20	A	812	CLA	O1D-CGD-O2D-CED
20	B	837	CLA	O1D-CGD-O2D-CED
21	4	317	LMU	O5B-C5B-C6B-O6B
20	A	805	CLA	C2-C1-O2A-CGA
20	4	307	CLA	C2-C1-O2A-CGA
20	1	206	CLA	C2-C1-O2A-CGA
20	A	823	CLA	C2-C1-O2A-CGA
21	L	205	LMU	O1'-C1-C2-C3
21	F	201	LMU	O1'-C1-C2-C3
20	J	103	CLA	C8-C10-C11-C12
20	B	836	CLA	C8-C10-C11-C12
20	3	313	CLA	C13-C15-C16-C17
20	B	838	CLA	C10-C11-C12-C13
20	B	824	CLA	C15-C16-C17-C18
20	I	102	CLA	C5-C6-C7-C8
23	A	842	PQN	C25-C26-C27-C28
20	R	107	CLA	C8-C10-C11-C12
20	B	804	CLA	C2A-CAA-CBA-CGA
20	B	812	CLA	C5-C6-C7-C8
20	B	816	CLA	C10-C11-C12-C13
20	A	852	CLA	C8-C10-C11-C12
20	B	810	CLA	C5-C6-C7-C8
20	J	103	CLA	C6-C7-C8-C10
20	B	825	CLA	C6-C7-C8-C10
20	B	806	CLA	C11-C10-C8-C7
20	2	322	CLA	C11-C12-C13-C15
20	A	841	CLA	C11-C10-C8-C7
20	B	811	CLA	C6-C7-C8-C10
20	L	202	CLA	C12-C13-C15-C16
20	2	308	CLA	C12-C13-C15-C16
20	4	304	CLA	C12-C13-C15-C16
20	3	313	CLA	C11-C10-C8-C7
20	A	850	CLA	C12-C13-C15-C16
20	A	808	CLA	C6-C7-C8-C10
20	A	808	CLA	C12-C13-C15-C16
20	B	821	CLA	C11-C12-C13-C15
20	3	318	CLA	C11-C10-C8-C7
20	3	311	CLA	C6-C7-C8-C10
20	3	311	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	839	CLA	C12-C13-C15-C16
20	1	215	CLA	C11-C10-C8-C7
21	2	318	LMU	C1-C2-C3-C4
20	B	821	CLA	C3-C5-C6-C7
20	L	207	CLA	O1A-CGA-O2A-C1
20	2	302	CLA	O1A-CGA-O2A-C1
20	A	852	CLA	C4C-C3C-CAC-CBC
22	F	203	BCR	C9-C10-C11-C12
20	A	812	CLA	C2A-CAA-CBA-CGA
20	A	824	CLA	C2A-CAA-CBA-CGA
20	A	808	CLA	C2A-CAA-CBA-CGA
20	3	317	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
20	A	836	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C2A-CAA-CBA-CGA
20	4	305	CLA	O1D-CGD-O2D-CED
20	B	829	CLA	O1D-CGD-O2D-CED
20	A	832	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	O1D-CGD-O2D-CED
20	B	806	CLA	C13-C15-C16-C17
23	B	841	PQN	C18-C20-C21-C22
20	3	311	CLA	C15-C16-C17-C18
20	1	215	CLA	C5-C6-C7-C8
23	A	842	PQN	C20-C21-C22-C23
20	H	109	CLA	C8-C10-C11-C12
21	B	801	LMU	O1'-C1-C2-C3
21	A	855	LMU	O1'-C1-C2-C3
20	A	812	CLA	O1A-CGA-O2A-C1
20	3	317	CLA	O1A-CGA-O2A-C1
21	4	301	LMU	C4'-C5'-C6'-O6'
21	2	313	LMU	O5'-C1'-O1'-C1
20	2	303	CLA	C13-C15-C16-C17
20	B	836	CLA	C13-C15-C16-C17
20	B	812	CLA	C10-C11-C12-C13
20	A	838	CLA	C13-C15-C16-C17
21	2	313	LMU	O1'-C1-C2-C3
21	H	106	LMU	C3'-C4'-O1B-C1B
21	1	218	LMU	O1'-C1-C2-C3
21	1	220	LMU	O1'-C1-C2-C3
21	L	205	LMU	O5'-C5'-C6'-O6'
21	A	855	LMU	O5'-C5'-C6'-O6'
21	R	109	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	4	321	LMU	C4B-C5B-C6B-O6B
20	A	813	CLA	C3-C5-C6-C7
20	B	827	CLA	C3-C5-C6-C7
21	1	219	LMU	C1-C2-C3-C4
20	2	316	CLA	C8-C10-C11-C12
20	2	307	CLA	C8-C10-C11-C12
20	B	815	CLA	C8-C10-C11-C12
23	B	841	PQN	C20-C21-C22-C23
20	A	819	CLA	C5-C6-C7-C8
20	3	318	CLA	C8-C10-C11-C12
20	B	827	CLA	C5-C6-C7-C8
20	A	823	CLA	C15-C16-C17-C18
20	1	203	CLA	CBA-CGA-O2A-C1
20	4	305	CLA	O1A-CGA-O2A-C1
20	K	102	CLA	O1A-CGA-O2A-C1
21	H	107	LMU	C9-C10-C11-C12
21	H	104	LMU	C2-C3-C4-C5
21	2	317	LMU	O1'-C1-C2-C3
20	B	811	CLA	C8-C10-C11-C12
20	4	304	CLA	C8-C10-C11-C12
20	B	850	CLA	C13-C15-C16-C17
20	B	849	CLA	C10-C11-C12-C13
20	A	850	CLA	C8-C10-C11-C12
20	A	852	CLA	C15-C16-C17-C18
20	R	108	CLA	C5-C6-C7-C8
20	A	806	CLA	C5-C6-C7-C8
21	H	105	LMU	O5B-C5B-C6B-O6B
20	B	815	CLA	C10-C11-C12-C13
20	B	838	CLA	C4C-C3C-CAC-CBC
20	A	818	CLA	C5-C6-C7-C8
20	A	818	CLA	C15-C16-C17-C18
20	A	805	CLA	C13-C15-C16-C17
20	A	825	CLA	C8-C10-C11-C12
20	K	103	CLA	C13-C15-C16-C17
20	B	824	CLA	C8-C10-C11-C12
20	B	821	CLA	C13-C15-C16-C17
20	3	311	CLA	C8-C10-C11-C12
20	B	835	CLA	C5-C6-C7-C8
20	B	812	CLA	C3-C5-C6-C7
21	R	109	LMU	C4B-C5B-C6B-O6B
20	B	838	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	826	CLA	C10-C11-C12-C13
21	2	318	LMU	C4B-C5B-C6B-O6B
20	A	833	CLA	O1D-CGD-O2D-CED
21	K	105	LMU	C5-C6-C7-C8
21	R	106	LMU	O1'-C1-C2-C3
20	K	108	CLA	C4C-C3C-CAC-CBC
20	B	808	CLA	C15-C16-C17-C18
20	B	804	CLA	C2C-C3C-CAC-CBC
21	R	109	LMU	C9-C10-C11-C12
20	B	824	CLA	C2A-CAA-CBA-CGA
20	A	830	CLA	C2A-CAA-CBA-CGA
20	A	811	CLA	C16-C17-C18-C19
20	B	838	CLA	C16-C17-C18-C19
21	E	101	LMU	O5'-C5'-C6'-O6'
20	B	816	CLA	C3-C5-C6-C7
20	A	831	CLA	C3-C5-C6-C7
20	B	816	CLA	CBA-CGA-O2A-C1
20	L	201	CLA	CBA-CGA-O2A-C1
20	B	851	CLA	C15-C16-C17-C18
21	3	321	LMU	O1'-C1-C2-C3
21	3	322	LMU	C5-C6-C7-C8
22	J	102	BCR	C19-C20-C21-C22
22	I	101	BCR	C9-C10-C11-C12
21	4	317	LMU	C2-C3-C4-C5
21	2	313	LMU	C6-C7-C8-C9
21	3	322	LMU	C6-C7-C8-C9
20	B	839	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	C10-C11-C12-C13
22	A	847	BCR	C20-C21-C22-C37
22	B	845	BCR	C20-C21-C22-C37
22	F	202	BCR	C20-C21-C22-C37
21	L	211	LMU	C6-C7-C8-C9
21	N	101	LMU	C4-C5-C6-C7
21	L	205	LMU	C6-C7-C8-C9
21	A	853	LMU	C7-C8-C9-C10
21	H	108	LMU	C3-C4-C5-C6
21	R	106	LMU	C3-C4-C5-C6
21	3	321	LMU	C4-C5-C6-C7
21	B	802	LMU	C4-C5-C6-C7
21	A	856	LMU	C6-C7-C8-C9
21	4	301	LMU	C3-C4-C5-C6
25	B	848	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
21	C	101	LMU	C11-C10-C9-C8
21	1	220	LMU	C4-C5-C6-C7
21	2	319	LMU	C3-C4-C5-C6
20	B	816	CLA	O1A-CGA-O2A-C1
20	1	210	CLA	O1A-CGA-O2A-C1
20	3	313	CLA	C16-C17-C18-C19
20	3	311	CLA	C16-C17-C18-C19
20	A	828	CLA	C16-C17-C18-C19
20	B	824	CLA	CBA-CGA-O2A-C1
21	L	211	LMU	C11-C10-C9-C8
21	4	322	LMU	C4-C5-C6-C7
21	H	104	LMU	C3-C4-C5-C6
21	A	849	LMU	C5-C6-C7-C8
21	R	109	LMU	C11-C10-C9-C8
20	A	830	CLA	C15-C16-C17-C18
21	2	319	LMU	C4B-C5B-C6B-O6B
21	K	105	LMU	C11-C10-C9-C8
21	H	107	LMU	C2-C3-C4-C5
21	B	801	LMU	C11-C10-C9-C8
21	A	854	LMU	C11-C10-C9-C8
25	B	848	LMG	C32-C33-C34-C35
21	A	854	LMU	O5'-C5'-C6'-O6'
21	A	848	LMU	C11-C10-C9-C8
20	2	307	CLA	C2C-C3C-CAC-CBC
21	A	855	LMU	C3-C4-C5-C6
21	C	101	LMU	C7-C8-C9-C10
21	1	220	LMU	C2-C3-C4-C5
21	R	105	LMU	O1'-C1-C2-C3
21	R	105	LMU	C2-C3-C4-C5
20	B	822	CLA	C5-C6-C7-C8
20	A	813	CLA	C5-C6-C7-C8
21	R	104	LMU	O1'-C1-C2-C3
21	G	101	LMU	C2-C3-C4-C5
21	C	101	LMU	C6-C7-C8-C9
20	2	307	CLA	C3-C5-C6-C7
20	R	108	CLA	O1D-CGD-O2D-CED
20	A	820	CLA	O1D-CGD-O2D-CED
21	3	322	LMU	C2'-C1'-O1'-C1
21	L	205	LMU	C2'-C1'-O1'-C1
22	B	845	BCR	C20-C21-C22-C23
22	A	844	BCR	C20-C21-C22-C23
22	F	202	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	H	106	LMU	C2'-C1'-O1'-C1
21	H	105	LMU	C2'-C1'-O1'-C1
21	B	847	LMU	C2'-C1'-O1'-C1
21	A	856	LMU	C2'-C1'-O1'-C1
21	4	301	LMU	C2'-C1'-O1'-C1
25	B	848	LMG	C2-C1-O1-C7
21	4	320	LMU	C3'-C4'-O1B-C1B
21	4	320	LMU	C5'-C4'-O1B-C1B
21	L	204	LMU	C6-C7-C8-C9
20	F	205	CLA	C2C-C3C-CAC-CBC
21	E	101	LMU	C11-C10-C9-C8
21	1	218	LMU	C5-C6-C7-C8
20	B	838	CLA	O1A-CGA-O2A-C1
20	A	851	CLA	C16-C17-C18-C20
20	B	836	CLA	C16-C17-C18-C19
20	A	827	CLA	C6-C7-C8-C9
20	A	841	CLA	C16-C17-C18-C20
20	4	311	CLA	C6-C7-C8-C9
20	3	318	CLA	C16-C17-C18-C19
20	B	835	CLA	C11-C12-C13-C14
20	A	835	CLA	C16-C17-C18-C19
21	A	853	LMU	O5B-C5B-C6B-O6B
20	B	808	CLA	C4-C3-C5-C6
21	4	320	LMU	C4-C5-C6-C7
21	K	105	LMU	C6-C7-C8-C9
21	A	849	LMU	C6-C7-C8-C9
21	1	213	LMU	C5-C6-C7-C8
21	A	856	LMU	C7-C8-C9-C10
21	L	211	LMU	C4B-C5B-C6B-O6B
20	F	206	CLA	C2-C3-C5-C6
20	J	103	CLA	C11-C10-C8-C9
20	B	806	CLA	C11-C10-C8-C9
20	B	806	CLA	C11-C12-C13-C14
20	A	851	CLA	C11-C12-C13-C14
20	L	202	CLA	C11-C10-C8-C9
20	A	824	CLA	C11-C12-C13-C14
20	2	307	CLA	C11-C10-C8-C9
20	B	849	CLA	C11-C10-C8-C9
20	3	311	CLA	C6-C7-C8-C9
20	A	839	CLA	C14-C13-C15-C16
21	K	105	LMU	C4-C5-C6-C7
21	H	107	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	K	106	LMU	C3-C4-C5-C6
21	R	104	LMU	C5-C6-C7-C8
21	2	317	LMU	C7-C8-C9-C10
20	B	808	CLA	C8-C10-C11-C12
20	B	826	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	C2A-CAA-CBA-CGA
20	A	829	CLA	C2A-CAA-CBA-CGA
22	J	102	BCR	C37-C22-C23-C24
22	B	842	BCR	C37-C22-C23-C24
20	2	305	CLA	C4C-C3C-CAC-CBC
21	4	317	LMU	C7-C8-C9-C10
21	K	104	LMU	C4-C5-C6-C7
21	3	321	LMU	C11-C10-C9-C8
21	1	218	LMU	C3-C4-C5-C6
21	1	213	LMU	O1'-C1-C2-C3
22	J	102	BCR	C21-C22-C23-C24
22	B	842	BCR	C21-C22-C23-C24
22	A	846	BCR	C11-C12-C13-C14
22	A	843	BCR	C7-C8-C9-C10
20	A	850	CLA	C3-C5-C6-C7
20	4	304	CLA	C5-C6-C7-C8
21	K	106	LMU	C7-C8-C9-C10
21	4	321	LMU	C6-C7-C8-C9
25	B	848	LMG	C15-C16-C17-C18
21	4	317	LMU	C11-C10-C9-C8
21	4	322	LMU	C2-C3-C4-C5
20	A	812	CLA	C5-C6-C7-C8
21	L	205	LMU	C2-C3-C4-C5
21	L	205	LMU	C5-C6-C7-C8
21	D	201	LMU	C2-C3-C4-C5
21	4	301	LMU	C4-C5-C6-C7
25	B	848	LMG	C37-C38-C39-C40
25	B	848	LMG	C40-C41-C42-C43
21	3	322	LMU	O5'-C5'-C6'-O6'
21	B	847	LMU	O5B-C5B-C6B-O6B
20	A	851	CLA	C16-C17-C18-C19
20	A	841	CLA	C16-C17-C18-C19
20	2	308	CLA	C16-C17-C18-C20
20	B	812	CLA	C16-C17-C18-C19
20	2	307	CLA	C16-C17-C18-C19
20	2	307	CLA	C16-C17-C18-C20
23	A	842	PQN	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
20	A	828	CLA	C16-C17-C18-C20
20	2	316	CLA	C10-C11-C12-C13
20	A	838	CLA	C5-C6-C7-C8
20	1	215	CLA	C8-C10-C11-C12
21	A	853	LMU	C5-C6-C7-C8
21	R	105	LMU	C7-C8-C9-C10
21	K	106	LMU	C9-C10-C11-C12
21	4	321	LMU	C3-C4-C5-C6
21	3	321	LMU	C2-C3-C4-C5
21	2	320	LMU	C7-C8-C9-C10
21	1	213	LMU	C1-C2-C3-C4
20	4	318	CLA	O1D-CGD-O2D-CED
21	2	313	LMU	C11-C10-C9-C8
21	4	322	LMU	C3-C4-C5-C6
21	L	204	LMU	C4-C5-C6-C7
21	R	101	LMU	C11-C10-C9-C8
21	H	106	LMU	C7-C8-C9-C10
21	H	105	LMU	C4-C5-C6-C7
21	A	856	LMU	C4-C5-C6-C7
20	A	851	CLA	C13-C15-C16-C17
20	1	203	CLA	O1A-CGA-O2A-C1
21	K	105	LMU	C2-C3-C4-C5
21	2	320	LMU	C2-C3-C4-C5
21	2	318	LMU	C2-C3-C4-C5
21	B	802	LMU	C5-C6-C7-C8
21	1	219	LMU	C6-C7-C8-C9
20	1	202	CLA	C2C-C3C-CAC-CBC
25	B	848	LMG	C35-C36-C37-C38
20	2	308	CLA	C3-C5-C6-C7
21	H	105	LMU	C1-C2-C3-C4
21	1	213	LMU	C6-C7-C8-C9
21	2	317	LMU	C4-C5-C6-C7
20	A	809	CLA	C3A-C2A-CAA-CBA
20	1	203	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	L	202	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C3A-C2A-CAA-CBA
20	2	316	CLA	C3A-C2A-CAA-CBA
20	A	814	CLA	C3A-C2A-CAA-CBA
20	R	107	CLA	C3A-C2A-CAA-CBA
20	A	825	CLA	C3A-C2A-CAA-CBA
20	4	311	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	803	CLA	C3A-C2A-CAA-CBA
20	1	215	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	C3A-C2A-CAA-CBA
20	1	206	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C3A-C2A-CAA-CBA
20	L	208	CLA	C3A-C2A-CAA-CBA
20	A	806	CLA	C3A-C2A-CAA-CBA
20	B	839	CLA	C10-C11-C12-C13
21	3	322	LMU	C1-C2-C3-C4
21	R	103	LMU	C1-C2-C3-C4
21	R	109	LMU	C1-C2-C3-C4
21	E	101	LMU	C2-C1-O1'-C1'
21	A	854	LMU	C2-C1-O1'-C1'
21	A	853	LMU	C11-C10-C9-C8
21	2	318	LMU	C4-C5-C6-C7
25	B	848	LMG	C13-C14-C15-C16
21	2	319	LMU	C5-C6-C7-C8
20	A	824	CLA	C16-C17-C18-C19
20	3	313	CLA	C16-C17-C18-C20
20	A	808	CLA	C16-C17-C18-C19
21	A	848	LMU	C5-C6-C7-C8
21	N	101	LMU	C3-C4-C5-C6
21	L	204	LMU	C7-C8-C9-C10
21	H	106	LMU	C4-C5-C6-C7
21	A	854	LMU	C1-C2-C3-C4
21	A	848	LMU	C3-C4-C5-C6
20	A	841	CLA	O2A-C1-C2-C3
20	4	311	CLA	C3-C5-C6-C7
20	B	817	CLA	C5-C6-C7-C8
20	F	206	CLA	C4-C3-C5-C6
20	B	812	CLA	C4-C3-C5-C6
20	A	825	CLA	C4-C3-C5-C6
20	B	807	CLA	C4-C3-C5-C6
20	A	835	CLA	C4-C3-C5-C6
20	J	101	CLA	CBA-CGA-O2A-C1
20	A	823	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	C2-C3-C5-C6
20	A	825	CLA	C2-C3-C5-C6
20	B	807	CLA	C2-C3-C5-C6
20	1	206	CLA	C2-C3-C5-C6
20	A	835	CLA	C2-C3-C5-C6
21	K	104	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	R	103	LMU	O1'-C1-C2-C3
21	G	101	LMU	O1'-C1-C2-C3
21	K	109	LMU	C7-C8-C9-C10
21	A	854	LMU	O1'-C1-C2-C3
21	D	201	LMU	C3-C4-C5-C6
20	A	827	CLA	O1D-CGD-O2D-CED
21	H	106	LMU	O5'-C5'-C6'-O6'
20	4	305	CLA	C6-C7-C8-C10
20	B	850	CLA	C16-C17-C18-C19
20	B	830	CLA	C16-C17-C18-C20
20	4	311	CLA	C6-C7-C8-C10
20	B	838	CLA	C16-C17-C18-C20
20	A	835	CLA	C16-C17-C18-C20
21	4	317	LMU	C4-C5-C6-C7
21	L	211	LMU	C3-C4-C5-C6
20	L	202	CLA	C10-C11-C12-C13
20	B	822	CLA	C3-C5-C6-C7
20	1	206	CLA	C3-C5-C6-C7
21	A	853	LMU	C1-C2-C3-C4
20	L	208	CLA	C4C-C3C-CAC-CBC
20	B	824	CLA	O1A-CGA-O2A-C1
21	2	313	LMU	C4-C5-C6-C7
21	A	849	LMU	C11-C10-C9-C8
21	L	211	LMU	C1-C2-C3-C4
21	4	301	LMU	C1-C2-C3-C4
20	B	830	CLA	C2-C1-O2A-CGA
21	A	849	LMU	C2-C3-C4-C5
21	1	220	LMU	C7-C8-C9-C10
21	3	322	LMU	O5B-C5B-C6B-O6B
20	A	851	CLA	C15-C16-C17-C18
20	B	836	CLA	C15-C16-C17-C18
20	A	824	CLA	C10-C11-C12-C13
20	A	850	CLA	C13-C15-C16-C17
20	A	828	CLA	C8-C10-C11-C12
21	N	101	LMU	C7-C8-C9-C10
21	4	301	LMU	C2-C3-C4-C5
21	C	101	LMU	C5-C6-C7-C8
20	A	811	CLA	C16-C17-C18-C20
22	B	843	BCR	C23-C24-C25-C26
22	A	845	BCR	C1-C6-C7-C8
22	A	845	BCR	C23-C24-C25-C26
22	A	845	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	F	202	BCR	C1-C6-C7-C8
22	F	202	BCR	C23-C24-C25-C26
22	F	202	BCR	C23-C24-C25-C30
22	L	210	BCR	C5-C6-C7-C8
22	J	102	BCR	C1-C6-C7-C8
22	B	846	BCR	C23-C24-C25-C26
22	B	842	BCR	C23-C24-C25-C26
22	B	842	BCR	C23-C24-C25-C30
22	A	846	BCR	C23-C24-C25-C26
21	R	103	LMU	C4-C5-C6-C7
21	1	218	LMU	C6-C7-C8-C9
20	B	827	CLA	CBA-CGA-O2A-C1
20	4	305	CLA	C5-C6-C7-C8
20	B	805	CLA	C10-C11-C12-C13
20	I	102	CLA	C8-C10-C11-C12
21	R	105	LMU	C1-C2-C3-C4
21	2	313	LMU	C2-C3-C4-C5
21	R	101	LMU	C2-C3-C4-C5
21	E	101	LMU	C4-C5-C6-C7
21	R	106	LMU	C9-C10-C11-C12
21	2	318	LMU	C7-C8-C9-C10
21	1	213	LMU	C5'-C4'-O1B-C1B
21	1	219	LMU	C5'-C4'-O1B-C1B
21	R	102	LMU	O5'-C5'-C6'-O6'
21	H	105	LMU	C2B-C1B-O1B-C4'
21	K	109	LMU	C9-C10-C11-C12
21	H	106	LMU	C9-C10-C11-C12
20	2	316	CLA	C5-C6-C7-C8
21	B	802	LMU	O5'-C5'-C6'-O6'
21	2	313	LMU	C7-C8-C9-C10
21	B	801	LMU	C5-C6-C7-C8
21	K	109	LMU	C11-C10-C9-C8
20	A	830	CLA	C4-C3-C5-C6
20	J	103	CLA	C11-C10-C8-C7
20	B	806	CLA	C11-C12-C13-C15
20	B	851	CLA	C6-C7-C8-C10
20	A	851	CLA	C11-C12-C13-C15
20	2	303	CLA	C12-C13-C15-C16
20	A	824	CLA	C11-C12-C13-C15
20	B	812	CLA	C11-C10-C8-C7
20	B	812	CLA	C12-C13-C15-C16
20	A	825	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	2	307	CLA	C11-C10-C8-C7
20	B	830	CLA	C11-C12-C13-C15
20	A	811	CLA	C6-C7-C8-C10
20	A	811	CLA	C12-C13-C15-C16
20	B	849	CLA	C6-C7-C8-C10
20	B	849	CLA	C11-C10-C8-C7
23	B	841	PQN	C21-C22-C23-C25
20	A	852	CLA	C6-C7-C8-C10
20	A	808	CLA	C11-C12-C13-C15
20	3	311	CLA	C11-C12-C13-C15
20	A	839	CLA	C6-C7-C8-C10
20	B	827	CLA	C6-C7-C8-C10
20	B	827	CLA	C11-C10-C8-C7
20	B	810	CLA	C2-C3-C5-C6
20	1	215	CLA	C11-C12-C13-C15
20	A	830	CLA	C2-C3-C5-C6
20	A	826	CLA	C11-C12-C13-C15
20	L	201	CLA	C2-C3-C5-C6
20	A	823	CLA	C12-C13-C15-C16
21	R	106	LMU	C1-C2-C3-C4
20	J	101	CLA	O1A-CGA-O2A-C1
20	A	823	CLA	O1A-CGA-O2A-C1
21	H	106	LMU	C5'-C4'-O1B-C1B
20	B	817	CLA	C8-C10-C11-C12
20	A	823	CLA	C10-C11-C12-C13
20	A	836	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	C6-C7-C8-C10
20	I	102	CLA	C11-C12-C13-C14
20	A	852	CLA	O1D-CGD-O2D-CED
21	K	105	LMU	O5'-C5'-C6'-O6'
21	1	219	LMU	C11-C10-C9-C8
20	B	829	CLA	C2A-CAA-CBA-CGA
20	A	840	CLA	C2A-CAA-CBA-CGA
21	A	848	LMU	C6-C7-C8-C9
21	R	103	LMU	C9-C10-C11-C12
21	R	109	LMU	C2-C3-C4-C5
21	R	109	LMU	C5-C6-C7-C8
20	A	823	CLA	C2C-C3C-CAC-CBC
21	3	322	LMU	C7-C8-C9-C10
21	1	213	LMU	C3-C4-C5-C6
20	J	103	CLA	C12-C13-C15-C16
21	F	201	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	A	855	LMU	C4'-C5'-C6'-O6'
20	B	806	CLA	C10-C11-C12-C13
20	B	826	CLA	C5-C6-C7-C8
21	L	204	LMU	C1-C2-C3-C4
21	K	109	LMU	C1-C2-C3-C4
21	R	106	LMU	C4-C5-C6-C7
21	A	849	LMU	O1'-C1-C2-C3
22	B	845	BCR	C18-C19-C20-C21
21	R	102	LMU	C2-C3-C4-C5
21	4	301	LMU	C5-C6-C7-C8
20	A	831	CLA	C4C-C3C-CAC-CBC
20	B	838	CLA	C8-C10-C11-C12
20	A	852	CLA	C13-C15-C16-C17
20	B	827	CLA	C10-C11-C12-C13
20	K	101	CLA	CBD-CGD-O2D-CED
20	L	201	CLA	O1A-CGA-O2A-C1
21	2	318	LMU	C5-C6-C7-C8
20	B	830	CLA	C3-C5-C6-C7
20	B	808	CLA	C3-C5-C6-C7
21	D	201	LMU	C2'-C1'-O1'-C1
20	2	311	CLA	O1D-CGD-O2D-CED
20	B	836	CLA	C16-C17-C18-C20
20	I	102	CLA	C11-C12-C13-C15
21	A	856	LMU	C5-C6-C7-C8
21	N	101	LMU	O5B-C5B-C6B-O6B
20	2	322	CLA	C8-C10-C11-C12
20	A	805	CLA	C15-C16-C17-C18
20	B	849	CLA	C5-C6-C7-C8
20	3	311	CLA	C13-C15-C16-C17
20	A	823	CLA	C5-C6-C7-C8
20	L	201	CLA	C4-C3-C5-C6
20	A	812	CLA	C2-C3-C5-C6
20	B	808	CLA	C2-C3-C5-C6
20	3	317	CLA	C4C-C3C-CAC-CBC
20	J	103	CLA	C6-C7-C8-C9
20	B	851	CLA	C6-C7-C8-C9
20	2	303	CLA	C14-C13-C15-C16
20	A	841	CLA	C11-C12-C13-C14
20	B	811	CLA	C11-C10-C8-C9
20	L	202	CLA	C14-C13-C15-C16
20	2	308	CLA	C14-C13-C15-C16
20	A	805	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	825	CLA	C6-C7-C8-C9
20	B	830	CLA	C11-C12-C13-C14
20	3	313	CLA	C11-C10-C8-C9
20	A	811	CLA	C11-C12-C13-C14
23	B	841	PQN	C21-C22-C23-C24
20	B	821	CLA	C11-C12-C13-C14
20	3	318	CLA	C11-C10-C8-C9
20	B	808	CLA	C14-C13-C15-C16
20	A	826	CLA	C11-C12-C13-C14
20	A	828	CLA	C11-C10-C8-C9
21	K	109	LMU	C2-C3-C4-C5
21	2	313	LMU	C1-C2-C3-C4
21	R	102	LMU	C1-C2-C3-C4
20	4	316	CLA	C4C-C3C-CAC-CBC
21	K	104	LMU	O1'-C1-C2-C3
20	B	851	CLA	CBA-CGA-O2A-C1
22	B	846	BCR	C36-C18-C19-C20
22	3	314	BCR	C11-C12-C13-C35
22	3	314	BCR	C11-C12-C13-C14
20	B	827	CLA	O1A-CGA-O2A-C1
20	J	103	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	A	816	CLA	C1A-C2A-CAA-CBA
20	1	203	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	A	801	CLA	C1A-C2A-CAA-CBA
20	4	311	CLA	C1A-C2A-CAA-CBA
20	A	850	CLA	C1A-C2A-CAA-CBA
20	J	101	CLA	C1A-C2A-CAA-CBA
20	A	803	CLA	C1A-C2A-CAA-CBA
20	R	108	CLA	C1A-C2A-CAA-CBA
20	A	804	CLA	C1A-C2A-CAA-CBA
20	1	215	CLA	C1A-C2A-CAA-CBA
20	B	837	CLA	C1A-C2A-CAA-CBA
20	B	839	CLA	C1A-C2A-CAA-CBA
21	4	301	LMU	O5'-C5'-C6'-O6'
20	1	202	CLA	C1A-C2A-CAA-CBA
20	A	840	CLA	C1A-C2A-CAA-CBA
20	L	208	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	818	CLA	C16-C17-C18-C20
20	B	826	CLA	C16-C17-C18-C20
20	B	812	CLA	C16-C17-C18-C20
20	3	318	CLA	C16-C17-C18-C20
22	I	101	BCR	C15-C16-C17-C18
22	B	842	BCR	C19-C20-C21-C22
20	2	302	CLA	O1D-CGD-O2D-CED
20	B	825	CLA	C5-C6-C7-C8
20	A	824	CLA	C5-C6-C7-C8
20	A	830	CLA	C13-C15-C16-C17
25	B	848	LMG	C11-C12-C13-C14
20	2	303	CLA	C10-C11-C12-C13
20	A	805	CLA	C5-C6-C7-C8
20	B	850	CLA	C15-C16-C17-C18
20	B	839	CLA	O1D-CGD-O2D-CED
21	L	211	LMU	C2-C3-C4-C5
21	1	217	LMU	C5'-C4'-O1B-C1B
21	L	205	LMU	C1-C2-C3-C4
21	G	101	LMU	C1-C2-C3-C4
20	A	818	CLA	C16-C17-C18-C19
20	A	824	CLA	C16-C17-C18-C20
20	B	835	CLA	C11-C12-C13-C15
20	L	201	CLA	C6-C7-C8-C10
21	B	802	LMU	C11-C10-C9-C8
21	2	317	LMU	C5-C6-C7-C8
21	A	856	LMU	C11-C10-C9-C8
20	B	806	CLA	C15-C16-C17-C18
20	A	852	CLA	C10-C11-C12-C13
20	A	825	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	C4-C3-C5-C6
20	B	810	CLA	C4-C3-C5-C6
20	3	308	CLA	C3A-C2A-CAA-CBA
21	1	217	LMU	C3'-C4'-O1B-C1B
21	L	204	LMU	C11-C10-C9-C8
20	B	804	CLA	C4C-C3C-CAC-CBC
21	K	105	LMU	C4'-C5'-C6'-O6'
21	L	205	LMU	C11-C10-C9-C8
21	K	104	LMU	C3-C4-C5-C6
21	H	106	LMU	C2-C3-C4-C5
20	A	811	CLA	C8-C10-C11-C12
20	A	828	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	L	209	CLA	C2A-CAA-CBA-CGA
20	2	308	CLA	C16-C17-C18-C19
21	2	320	LMU	O5B-C5B-C6B-O6B
21	2	320	LMU	C9-C10-C11-C12
21	D	201	LMU	C9-C10-C11-C12
20	A	831	CLA	CBA-CGA-O2A-C1
21	H	108	LMU	O5'-C5'-C6'-O6'
21	K	109	LMU	O5B-C5B-C6B-O6B
21	R	101	LMU	C9-C10-C11-C12
21	1	219	LMU	C9-C10-C11-C12
21	H	106	LMU	C4'-C5'-C6'-O6'
20	4	302	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	O1D-CGD-O2D-CED
20	A	816	CLA	C6-C7-C8-C9
25	B	848	LMG	C17-C18-C19-C20
21	G	101	LMU	C5-C6-C7-C8
21	F	201	LMU	C11-C10-C9-C8
21	2	319	LMU	C9-C10-C11-C12
21	4	320	LMU	O5B-C5B-C6B-O6B
20	2	322	CLA	C14-C13-C15-C16
21	2	317	LMU	C9-C10-C11-C12
21	1	217	LMU	C2-C3-C4-C5
20	A	813	CLA	C6-C7-C8-C9
21	A	854	LMU	C4'-C5'-C6'-O6'
21	B	801	LMU	O5'-C5'-C6'-O6'
21	G	101	LMU	C4-C5-C6-C7
20	B	851	CLA	O1A-CGA-O2A-C1
20	2	308	CLA	C2C-C3C-CAC-CBC
21	A	849	LMU	C9-C10-C11-C12
21	D	201	LMU	C6-C7-C8-C9
21	B	802	LMU	C3-C4-C5-C6
21	E	101	LMU	O5B-C5B-C6B-O6B
21	K	106	LMU	O5B-C5B-C6B-O6B
21	K	106	LMU	O5'-C5'-C6'-O6'
21	H	104	LMU	O5'-C5'-C6'-O6'
21	R	106	LMU	O5'-C5'-C6'-O6'
21	2	317	LMU	O5B-C5B-C6B-O6B
21	2	319	LMU	O5'-C5'-C6'-O6'
20	B	816	CLA	C4-C3-C5-C6
20	B	849	CLA	C4-C3-C5-C6
21	A	848	LMU	C9-C10-C11-C12
21	H	104	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	H	104	LMU	C9-C10-C11-C12
20	B	816	CLA	C2-C3-C5-C6
25	B	848	LMG	C10-C11-C12-C13
20	2	322	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	CBA-CGA-O2A-C1
21	N	101	LMU	C5-C6-C7-C8
21	A	849	LMU	C3-C4-C5-C6
20	B	838	CLA	C5-C6-C7-C8
20	A	819	CLA	C8-C10-C11-C12
20	H	101	CLA	C5-C6-C7-C8
21	A	853	LMU	C4-C5-C6-C7
21	R	105	LMU	C5'-C4'-O1B-C1B
25	B	848	LMG	C9-C8-O7-C10
20	A	827	CLA	C2A-CAA-CBA-CGA
20	B	850	CLA	C2A-CAA-CBA-CGA
20	R	108	CLA	C2A-CAA-CBA-CGA
20	1	210	CLA	C2A-CAA-CBA-CGA
20	A	816	CLA	C2-C1-O2A-CGA
21	R	104	LMU	C9-C10-C11-C12
21	L	211	LMU	C7-C8-C9-C10
21	B	847	LMU	C2-C3-C4-C5
21	2	318	LMU	O5B-C1B-O1B-C4'
21	R	104	LMU	O5B-C1B-O1B-C4'
21	4	322	LMU	C5-C6-C7-C8
21	G	101	LMU	C6-C7-C8-C9
22	A	847	BCR	C20-C21-C22-C23
21	R	104	LMU	C2'-C1'-O1'-C1
20	J	101	CLA	CAA-CBA-CGA-O2A
21	3	322	LMU	C2-C3-C4-C5
21	R	105	LMU	C5-C6-C7-C8
21	1	220	LMU	C3-C4-C5-C6
20	A	808	CLA	C15-C16-C17-C18
20	2	322	CLA	O1A-CGA-O2A-C1
20	A	825	CLA	O1A-CGA-O2A-C1
21	4	317	LMU	C1-C2-C3-C4
21	K	106	LMU	C1-C2-C3-C4
25	B	848	LMG	C39-C40-C41-C42
20	B	827	CLA	C4-C3-C5-C6
20	J	103	CLA	C11-C12-C13-C15
20	B	825	CLA	C11-C10-C8-C7
20	B	806	CLA	C12-C13-C15-C16
20	B	851	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	851	CLA	C6-C7-C8-C10
20	B	836	CLA	C11-C10-C8-C7
20	2	322	CLA	C11-C10-C8-C7
20	A	841	CLA	C11-C12-C13-C15
20	2	308	CLA	C11-C10-C8-C7
20	A	805	CLA	C11-C10-C8-C7
20	B	826	CLA	C11-C12-C13-C15
20	B	812	CLA	C6-C7-C8-C10
20	A	838	CLA	C6-C7-C8-C10
20	2	307	CLA	C12-C13-C15-C16
20	B	805	CLA	C6-C7-C8-C10
20	A	850	CLA	C11-C10-C8-C7
20	K	103	CLA	C11-C10-C8-C7
20	K	103	CLA	C12-C13-C15-C16
20	B	838	CLA	C11-C10-C8-C7
20	A	852	CLA	C11-C10-C8-C7
20	A	852	CLA	C12-C13-C15-C16
20	3	311	CLA	C12-C13-C15-C16
20	R	108	CLA	C6-C7-C8-C10
20	B	817	CLA	C11-C12-C13-C15
20	B	823	CLA	C6-C7-C8-C10
20	B	823	CLA	C11-C10-C8-C7
20	B	803	CLA	C12-C13-C15-C16
20	B	808	CLA	C11-C10-C8-C7
20	B	808	CLA	C12-C13-C15-C16
20	B	835	CLA	C6-C7-C8-C10
20	1	202	CLA	C11-C10-C8-C7
20	A	823	CLA	C11-C10-C8-C7
20	A	823	CLA	C11-C12-C13-C15
20	A	803	CLA	CAA-CBA-CGA-O2A
21	L	204	LMU	C5-C6-C7-C8
21	A	854	LMU	C5-C6-C7-C8
20	B	825	CLA	C11-C10-C8-C9
20	B	806	CLA	C6-C7-C8-C9
20	B	806	CLA	C14-C13-C15-C16
20	2	322	CLA	C11-C10-C8-C9
20	2	322	CLA	C11-C12-C13-C14
20	A	841	CLA	C11-C10-C8-C9
20	4	304	CLA	C11-C12-C13-C14
20	4	304	CLA	C14-C13-C15-C16
20	B	826	CLA	C11-C12-C13-C14
20	A	838	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	811	CLA	C6-C7-C8-C9
20	B	815	CLA	C11-C10-C8-C9
20	K	103	CLA	C11-C10-C8-C9
20	K	103	CLA	C11-C12-C13-C14
20	K	103	CLA	C14-C13-C15-C16
20	A	852	CLA	C6-C7-C8-C9
20	A	852	CLA	C14-C13-C15-C16
20	3	311	CLA	C11-C10-C8-C9
20	B	817	CLA	C11-C10-C8-C9
20	B	827	CLA	C6-C7-C8-C9
20	1	215	CLA	C11-C10-C8-C9
20	B	835	CLA	C6-C7-C8-C9
20	A	826	CLA	C6-C7-C8-C9
20	A	823	CLA	C11-C12-C13-C14
20	A	804	CLA	C2C-C3C-CAC-CBC
20	A	822	CLA	CBA-CGA-O2A-C1
22	I	103	BCR	C7-C8-C9-C34
20	A	838	CLA	C16-C17-C18-C20
20	B	810	CLA	C6-C7-C8-C9
21	H	104	LMU	C5'-C4'-O1B-C1B
22	I	103	BCR	C7-C8-C9-C10
22	A	846	BCR	C17-C18-C19-C20
21	H	104	LMU	O5B-C1B-O1B-C4'
21	4	320	LMU	C5-C6-C7-C8
20	B	822	CLA	C6-C7-C8-C9
21	1	219	LMU	C5-C6-C7-C8
20	A	811	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	CBA-CGA-O2A-C1
20	A	829	CLA	CBA-CGA-O2A-C1
21	A	856	LMU	C1-C2-C3-C4
20	A	809	CLA	C4C-C3C-CAC-CBC
21	K	106	LMU	C6-C7-C8-C9
21	F	201	LMU	C3'-C4'-O1B-C1B
20	4	318	CLA	C3-C5-C6-C7
21	1	218	LMU	C4'-C5'-C6'-O6'
21	L	204	LMU	C2-C3-C4-C5
21	A	856	LMU	C2-C3-C4-C5
21	4	301	LMU	O1'-C1-C2-C3
21	1	220	LMU	C6-C7-C8-C9
20	K	103	CLA	CBA-CGA-O2A-C1
20	B	849	CLA	CAA-CBA-CGA-O2A
21	3	322	LMU	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	3	321	LMU	C5-C6-C7-C8
20	J	103	CLA	C4-C3-C5-C6
20	B	849	CLA	C2-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
21	H	108	LMU	C3'-C4'-O1B-C1B
20	B	835	CLA	C10-C11-C12-C13
20	A	831	CLA	O1A-CGA-O2A-C1
21	L	205	LMU	C7-C8-C9-C10
20	2	305	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	C6-C7-C8-C10
21	R	105	LMU	C3'-C4'-O1B-C1B
20	A	830	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	C3A-C2A-CAA-CBA
20	A	820	CLA	C3A-C2A-CAA-CBA
20	B	803	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	B	849	CLA	C8-C10-C11-C12
21	K	105	LMU	C2-C1-O1'-C1'
21	H	108	LMU	C2-C1-O1'-C1'
21	R	103	LMU	C2-C1-O1'-C1'
21	4	321	LMU	C2-C1-O1'-C1'
21	3	321	LMU	C2-C1-O1'-C1'
21	2	317	LMU	C2-C1-O1'-C1'
21	G	101	LMU	C2-C1-O1'-C1'
21	1	217	LMU	C11-C10-C9-C8
20	A	819	CLA	C13-C15-C16-C17
20	B	823	CLA	C5-C6-C7-C8
21	B	801	LMU	C9-C10-C11-C12
20	B	850	CLA	C16-C17-C18-C20
20	3	311	CLA	C16-C17-C18-C20
20	A	820	CLA	CBA-CGA-O2A-C1
20	B	839	CLA	CBA-CGA-O2A-C1
20	L	203	CLA	CBA-CGA-O2A-C1
21	2	313	LMU	C3'-C4'-O1B-C1B
21	L	204	LMU	C9-C10-C11-C12
21	R	102	LMU	C3-C4-C5-C6
20	B	820	CLA	O1A-CGA-O2A-C1
20	B	809	CLA	C6-C7-C8-C10
20	J	103	CLA	C2-C3-C5-C6
21	3	321	LMU	C7-C8-C9-C10
20	2	307	CLA	C4C-C3C-CAC-CBC
20	B	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	853	LMU	C5'-C4'-O1B-C1B
21	A	854	LMU	C6-C7-C8-C9
20	A	819	CLA	O1D-CGD-O2D-CED
21	4	320	LMU	O5B-C1B-O1B-C4'
20	B	825	CLA	C10-C11-C12-C13
21	K	109	LMU	O1'-C1-C2-C3
21	K	106	LMU	C5-C6-C7-C8
21	F	201	LMU	C2-C3-C4-C5
20	4	306	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	CBA-CGA-O2A-C1
21	R	102	LMU	C5-C6-C7-C8
21	1	219	LMU	O1'-C1-C2-C3
20	4	305	CLA	C6-C7-C8-C9
20	A	805	CLA	C16-C17-C18-C20
20	4	304	CLA	C16-C17-C18-C20
20	B	821	CLA	C16-C17-C18-C20
21	N	101	LMU	O1'-C1-C2-C3
21	K	104	LMU	C9-C10-C11-C12
20	A	825	CLA	C5-C6-C7-C8
20	B	827	CLA	C13-C15-C16-C17
20	K	103	CLA	O1A-CGA-O2A-C1
20	A	829	CLA	O1A-CGA-O2A-C1
21	K	105	LMU	C9-C10-C11-C12
21	2	320	LMU	C6-C7-C8-C9
21	B	847	LMU	C3-C4-C5-C6
21	H	105	LMU	O5B-C1B-O1B-C4'
20	3	318	CLA	C5-C6-C7-C8
21	R	102	LMU	C3'-C4'-O1B-C1B
25	B	848	LMG	C41-C42-C43-C44
21	A	855	LMU	O5B-C1B-O1B-C4'
20	4	302	CLA	C6-C7-C8-C10
20	B	826	CLA	C16-C17-C18-C19
20	A	808	CLA	C16-C17-C18-C20
20	A	830	CLA	C16-C17-C18-C19
23	A	842	PQN	C26-C27-C28-C29
20	B	806	CLA	C8-C10-C11-C12
20	2	316	CLA	C13-C15-C16-C17
20	B	850	CLA	C5-C6-C7-C8
20	4	306	CLA	C2-C1-O2A-CGA
20	A	838	CLA	C2-C1-O2A-CGA
20	A	832	CLA	C2-C1-O2A-CGA
20	A	804	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	C2-C1-O2A-CGA
20	H	109	CLA	C2-C1-O2A-CGA
21	A	848	LMU	O5'-C5'-C6'-O6'
20	B	811	CLA	C6-C7-C8-C9
20	B	826	CLA	C6-C7-C8-C9
20	B	812	CLA	C6-C7-C8-C9
20	B	830	CLA	C14-C13-C15-C16
20	A	811	CLA	C14-C13-C15-C16
20	B	849	CLA	C6-C7-C8-C9
20	B	805	CLA	C6-C7-C8-C9
20	B	805	CLA	C11-C10-C8-C9
20	B	838	CLA	C11-C10-C8-C9
20	A	808	CLA	C11-C10-C8-C9
20	A	808	CLA	C11-C12-C13-C14
20	A	830	CLA	C6-C7-C8-C9
21	1	218	LMU	C7-C8-C9-C10
20	2	308	CLA	C13-C15-C16-C17
23	B	841	PQN	C23-C25-C26-C27
20	2	302	CLA	C4-C3-C5-C6
21	4	322	LMU	C1-C2-C3-C4
20	L	208	CLA	C2A-CAA-CBA-CGA
23	B	841	PQN	C26-C27-C28-C30
20	L	201	CLA	C6-C7-C8-C9
22	B	845	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	A	843	BCR	C23-C24-C25-C26
21	B	801	LMU	C3-C4-C5-C6
21	A	848	LMU	O1'-C1-C2-C3
20	A	822	CLA	O1A-CGA-O2A-C1
22	B	844	BCR	C11-C12-C13-C14
20	F	205	CLA	C4C-C3C-CAC-CBC
21	C	101	LMU	C3'-C4'-O1B-C1B
20	4	304	CLA	C2C-C3C-CAC-CBC
20	A	823	CLA	C4C-C3C-CAC-CBC
20	B	805	CLA	C11-C12-C13-C15
20	A	839	CLA	C16-C17-C18-C20
20	J	103	CLA	C14-C13-C15-C16
20	1	206	CLA	C14-C13-C15-C16
20	B	850	CLA	C10-C11-C12-C13
20	B	806	CLA	C6-C7-C8-C10
20	A	818	CLA	C12-C13-C15-C16
20	B	811	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	826	CLA	C6-C7-C8-C10
20	B	807	CLA	C11-C10-C8-C7
20	B	830	CLA	C12-C13-C15-C16
20	K	103	CLA	C11-C12-C13-C15
20	A	852	CLA	C11-C12-C13-C15
20	A	808	CLA	C11-C10-C8-C7
20	B	821	CLA	C6-C7-C8-C10
20	B	817	CLA	C11-C10-C8-C7
20	B	827	CLA	C11-C12-C13-C15
20	1	215	CLA	C6-C7-C8-C10
20	B	839	CLA	C11-C12-C13-C15
20	A	830	CLA	C11-C10-C8-C7
20	A	826	CLA	C6-C7-C8-C10
20	A	835	CLA	C12-C13-C15-C16
20	H	101	CLA	C3-C5-C6-C7
21	2	319	LMU	C11-C10-C9-C8
20	B	824	CLA	C5-C6-C7-C8
22	B	852	BCR	C13-C14-C15-C16
22	B	852	BCR	C15-C16-C17-C18
22	A	846	BCR	C13-C14-C15-C16
20	B	824	CLA	CBD-CGD-O2D-CED
21	B	802	LMU	C5'-C4'-O1B-C1B
21	1	213	LMU	C2-C3-C4-C5
21	N	101	LMU	C6-C7-C8-C9
21	B	801	LMU	C4-C5-C6-C7
20	4	304	CLA	CBA-CGA-O2A-C1
20	1	206	CLA	C12-C13-C15-C16
21	H	104	LMU	C4B-C5B-C6B-O6B
21	2	313	LMU	C5-C6-C7-C8
20	A	808	CLA	C13-C15-C16-C17
20	3	308	CLA	CAD-CBD-CGD-O2D
20	1	203	CLA	CAD-CBD-CGD-O2D
20	2	322	CLA	CAD-CBD-CGD-O2D
20	A	812	CLA	CAD-CBD-CGD-O2D
20	K	102	CLA	CAD-CBD-CGD-O2D
20	B	834	CLA	CAD-CBD-CGD-O2D
20	G	102	CLA	CAD-CBD-CGD-O2D
20	B	838	CLA	CAD-CBD-CGD-O2D
20	L	209	CLA	CAD-CBD-CGD-O2D
20	B	810	CLA	CAD-CBD-CGD-O2D
20	A	804	CLA	CAD-CBD-CGD-O2D
20	A	834	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	801	CLA	CAA-CBA-CGA-O2A
20	H	109	CLA	C4-C3-C5-C6
20	B	830	CLA	C16-C17-C18-C19
20	B	803	CLA	C16-C17-C18-C19
21	3	322	LMU	O5'-C1'-O1'-C1
20	A	811	CLA	C13-C15-C16-C17
20	H	109	CLA	C2-C3-C5-C6
20	A	839	CLA	C13-C15-C16-C17
21	3	322	LMU	C4'-C5'-C6'-O6'
20	A	851	CLA	C2A-CAA-CBA-CGA
20	A	804	CLA	C6-C7-C8-C10
20	B	809	CLA	C6-C7-C8-C9
21	4	321	LMU	C2-C3-C4-C5
25	B	848	LMG	C38-C39-C40-C41
20	A	851	CLA	CHA-CBD-CGD-O1D
20	A	851	CLA	CHA-CBD-CGD-O2D
20	B	836	CLA	CHA-CBD-CGD-O1D
20	A	841	CLA	CHA-CBD-CGD-O1D
20	A	841	CLA	CHA-CBD-CGD-O2D
20	4	305	CLA	CHA-CBD-CGD-O1D
20	4	305	CLA	CHA-CBD-CGD-O2D
20	B	811	CLA	CHA-CBD-CGD-O2D
20	A	805	CLA	CHA-CBD-CGD-O1D
20	3	313	CLA	CHA-CBD-CGD-O1D
20	3	313	CLA	CHA-CBD-CGD-O2D
20	B	849	CLA	CHA-CBD-CGD-O1D
20	B	849	CLA	CHA-CBD-CGD-O2D
20	A	850	CLA	CHA-CBD-CGD-O1D
20	A	850	CLA	CHA-CBD-CGD-O2D
20	A	808	CLA	CHA-CBD-CGD-O1D
20	A	808	CLA	CHA-CBD-CGD-O2D
20	B	821	CLA	CHA-CBD-CGD-O1D
20	B	821	CLA	CHA-CBD-CGD-O2D
20	B	833	CLA	CHA-CBD-CGD-O1D
20	B	833	CLA	CHA-CBD-CGD-O2D
20	B	803	CLA	CHA-CBD-CGD-O1D
20	A	831	CLA	CHA-CBD-CGD-O1D
20	A	831	CLA	CHA-CBD-CGD-O2D
20	B	819	CLA	CHA-CBD-CGD-O1D
20	B	819	CLA	CHA-CBD-CGD-O2D
20	4	318	CLA	CHA-CBD-CGD-O1D
20	4	318	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	825	CLA	C3-C5-C6-C7
20	B	826	CLA	C3-C5-C6-C7
20	A	824	CLA	C3-C5-C6-C7
20	3	302	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	O1A-CGA-O2A-C1
20	A	820	CLA	O1A-CGA-O2A-C1
20	L	203	CLA	O1A-CGA-O2A-C1
20	3	302	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	C8-C10-C11-C12
21	1	217	LMU	C4-C5-C6-C7
20	A	805	CLA	C16-C17-C18-C19
20	K	101	CLA	O1D-CGD-O2D-CED
20	A	808	CLA	C3-C5-C6-C7
20	H	101	CLA	C4-C3-C5-C6
20	B	807	CLA	C14-C13-C15-C16
20	A	850	CLA	C14-C13-C15-C16
20	A	808	CLA	C6-C7-C8-C9
20	A	808	CLA	C14-C13-C15-C16
20	B	817	CLA	C11-C12-C13-C14
20	1	215	CLA	C6-C7-C8-C9
21	4	320	LMU	C2-C3-C4-C5
21	C	101	LMU	C5'-C4'-O1B-C1B
21	3	322	LMU	C11-C10-C9-C8
21	4	320	LMU	C11-C10-C9-C8
20	B	823	CLA	C2A-CAA-CBA-CGA
20	R	108	CLA	C10-C11-C12-C13
20	A	813	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	C2C-C3C-CAC-CBC
22	J	102	BCR	C17-C18-C19-C20
20	2	316	CLA	C1A-C2A-CAA-CBA
20	A	837	CLA	C1A-C2A-CAA-CBA
20	B	850	CLA	C1A-C2A-CAA-CBA
20	B	835	CLA	C1A-C2A-CAA-CBA
20	B	851	CLA	C16-C17-C18-C20
20	B	820	CLA	C6-C7-C8-C9
20	B	813	CLA	C11-C12-C13-C14
20	J	103	CLA	C2-C1-O2A-CGA
20	A	834	CLA	C2-C1-O2A-CGA
22	B	852	BCR	C9-C10-C11-C12
22	3	314	BCR	C15-C16-C17-C18
20	B	810	CLA	C3-C5-C6-C7
20	4	306	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	811	CLA	O1A-CGA-O2A-C1
20	A	839	CLA	C16-C17-C18-C19
21	B	847	LMU	C1-C2-C3-C4
21	K	109	LMU	C3'-C4'-O1B-C1B
21	H	105	LMU	C7-C8-C9-C10
20	B	803	CLA	C16-C17-C18-C20
20	B	806	CLA	CAD-CBD-CGD-O1D
20	B	836	CLA	CAD-CBD-CGD-O1D
20	4	302	CLA	CAD-CBD-CGD-O1D
20	2	308	CLA	CAD-CBD-CGD-O1D
20	B	850	CLA	CAD-CBD-CGD-O1D
20	J	101	CLA	CAD-CBD-CGD-O1D
20	B	833	CLA	CAD-CBD-CGD-O1D
20	H	103	CLA	CAD-CBD-CGD-O1D
20	B	835	CLA	CAD-CBD-CGD-O1D
20	A	826	CLA	CAD-CBD-CGD-O1D
20	2	302	CLA	C2-C3-C5-C6
20	A	835	CLA	CAD-CBD-CGD-O1D
21	G	101	LMU	C9-C10-C11-C12
21	A	855	LMU	C2-C3-C4-C5
20	A	839	CLA	C5-C6-C7-C8
21	4	317	LMU	C3-C4-C5-C6
20	4	302	CLA	C6-C7-C8-C9
20	B	816	CLA	C11-C12-C13-C15
20	A	805	CLA	C11-C12-C13-C15
20	4	304	CLA	C11-C12-C13-C15
20	2	316	CLA	C12-C13-C15-C16
20	B	812	CLA	C11-C12-C13-C15
20	A	825	CLA	C11-C10-C8-C7
20	B	830	CLA	C11-C10-C8-C7
20	B	815	CLA	C11-C10-C8-C7
20	B	849	CLA	C11-C12-C13-C15
20	A	850	CLA	C6-C7-C8-C10
20	K	103	CLA	C6-C7-C8-C10
20	B	824	CLA	C11-C12-C13-C15
20	3	318	CLA	C11-C12-C13-C15
20	H	101	CLA	C2-C3-C5-C6
20	A	839	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C12-C13-C15-C16
20	I	102	CLA	C11-C10-C8-C7
20	B	803	CLA	C11-C10-C8-C7
20	B	839	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	A	842	PQN	C22-C23-C25-C26
20	A	828	CLA	C6-C7-C8-C10
20	B	807	CLA	C3-C5-C6-C7
22	F	202	BCR	C9-C10-C11-C12
21	C	101	LMU	C2-C1-O1'-C1'
20	B	839	CLA	O1A-CGA-O2A-C1
21	L	204	LMU	C3'-C4'-O1B-C1B
20	2	307	CLA	C2A-CAA-CBA-CGA
20	3	311	CLA	C2A-CAA-CBA-CGA
20	4	304	CLA	C16-C17-C18-C19
20	A	830	CLA	C16-C17-C18-C20
20	2	308	CLA	C4C-C3C-CAC-CBC
20	4	318	CLA	CAA-CBA-CGA-O2A
21	B	801	LMU	C3'-C4'-O1B-C1B
21	R	104	LMU	C5'-C4'-O1B-C1B
21	B	801	LMU	C2-C3-C4-C5
21	C	101	LMU	O1'-C1-C2-C3
20	1	202	CLA	C8-C10-C11-C12
21	4	317	LMU	O1'-C1-C2-C3
20	B	813	CLA	C10-C11-C12-C13
20	B	836	CLA	C11-C10-C8-C9
20	A	818	CLA	C14-C13-C15-C16
20	A	805	CLA	C11-C12-C13-C14
20	A	852	CLA	C11-C12-C13-C14
20	A	835	CLA	C14-C13-C15-C16
20	4	304	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	O1D-CGD-O2D-CED
21	2	319	LMU	O5B-C5B-C6B-O6B
21	A	849	LMU	C7-C8-C9-C10
20	3	318	CLA	C10-C11-C12-C13
21	R	109	LMU	C3-C4-C5-C6
20	H	103	CLA	C6-C7-C8-C9
22	B	846	BCR	C17-C18-C19-C20
21	1	219	LMU	C4-C5-C6-C7
21	A	855	LMU	C2B-C1B-O1B-C4'
20	B	823	CLA	C3-C5-C6-C7
21	4	322	LMU	C11-C10-C9-C8
20	A	824	CLA	C13-C15-C16-C17
20	A	838	CLA	C16-C17-C18-C19
20	3	318	CLA	C13-C15-C16-C17
20	A	826	CLA	C13-C15-C16-C17
20	A	834	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	4	322	LMU	O1'-C1-C2-C3
21	4	322	LMU	C6-C7-C8-C9
20	R	108	CLA	CAA-CBA-CGA-O2A
21	E	101	LMU	C9-C10-C11-C12
20	L	207	CLA	C2A-CAA-CBA-CGA
20	H	101	CLA	C2A-CAA-CBA-CGA
20	B	837	CLA	C2A-CAA-CBA-CGA
20	A	809	CLA	C2-C1-O2A-CGA
20	B	836	CLA	C2-C1-O2A-CGA
20	2	322	CLA	C2-C1-O2A-CGA
20	A	841	CLA	C2-C1-O2A-CGA
20	B	829	CLA	C2-C1-O2A-CGA
20	B	850	CLA	C2-C1-O2A-CGA
20	B	824	CLA	C2-C1-O2A-CGA
20	A	808	CLA	C2-C1-O2A-CGA
20	A	840	CLA	C2-C1-O2A-CGA
21	F	201	LMU	C6-C7-C8-C9
21	4	301	LMU	C6-C7-C8-C9
20	A	807	CLA	CAA-CBA-CGA-O2A
21	A	849	LMU	C1-C2-C3-C4
20	B	808	CLA	O1D-CGD-O2D-CED
21	A	856	LMU	C5'-C4'-O1B-C1B
20	B	806	CLA	C5-C6-C7-C8
21	1	217	LMU	C7-C8-C9-C10
21	4	321	LMU	C4-C5-C6-C7
21	B	801	LMU	C1-C2-C3-C4
20	B	814	CLA	CAA-CBA-CGA-O2A
20	A	812	CLA	C6-C7-C8-C9
20	B	821	CLA	C16-C17-C18-C19
21	A	856	LMU	O5'-C1'-O1'-C1
20	B	831	CLA	C2A-CAA-CBA-CGA
21	1	217	LMU	C5-C6-C7-C8
21	R	105	LMU	C9-C10-C11-C12
21	2	318	LMU	O1'-C1-C2-C3
21	A	849	LMU	C4-C5-C6-C7
20	A	841	CLA	C4-C3-C5-C6
20	A	818	CLA	C6-C7-C8-C10
20	A	811	CLA	C11-C12-C13-C15
20	A	850	CLA	C11-C12-C13-C15
20	B	821	CLA	C12-C13-C15-C16
20	A	828	CLA	C11-C10-C8-C7
21	4	320	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	2	308	CLA	C11-C10-C8-C9
20	B	812	CLA	C11-C10-C8-C9
20	B	849	CLA	C14-C13-C15-C16
20	K	103	CLA	C6-C7-C8-C9
20	B	827	CLA	C11-C12-C13-C14
20	B	823	CLA	C6-C7-C8-C9
20	B	839	CLA	C11-C12-C13-C14
20	A	830	CLA	C11-C10-C8-C9
22	L	210	BCR	C15-C16-C17-C18
20	H	103	CLA	C6-C7-C8-C10
21	C	101	LMU	C9-C10-C11-C12
20	1	206	CLA	C2A-CAA-CBA-CGA
20	3	313	CLA	C10-C11-C12-C13
22	F	203	BCR	C11-C12-C13-C35
21	A	848	LMU	C4-C5-C6-C7
20	H	101	CLA	O1A-CGA-O2A-C1
20	H	102	CLA	C5-C6-C7-C8
20	B	824	CLA	C13-C15-C16-C17
20	L	201	CLA	C5-C6-C7-C8
20	2	322	CLA	C12-C13-C15-C16
20	2	322	CLA	C4-C3-C5-C6
20	A	814	CLA	C4C-C3C-CAC-CBC
23	B	841	PQN	C26-C27-C28-C29
20	A	819	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	C11-C12-C13-C14
20	B	825	CLA	CAA-CBA-CGA-O2A
21	R	104	LMU	C3-C4-C5-C6
20	1	202	CLA	C5-C6-C7-C8
20	A	827	CLA	O1A-CGA-O2A-C1
20	A	827	CLA	CBA-CGA-O2A-C1
20	3	302	CLA	CBA-CGA-O2A-C1
22	A	845	BCR	C13-C14-C15-C16
20	A	819	CLA	O1A-CGA-O2A-C1
21	F	201	LMU	C4-C5-C6-C7
20	B	811	CLA	CAA-CBA-CGA-O2A
20	B	812	CLA	C8-C10-C11-C12
20	A	835	CLA	C13-C15-C16-C17
21	2	313	LMU	C9-C10-C11-C12
21	2	319	LMU	O5B-C1B-O1B-C4'
20	A	850	CLA	C4-C3-C5-C6
20	B	830	CLA	O1A-CGA-O2A-C1
21	4	321	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	F	206	CLA	C2-C1-O2A-CGA
20	K	102	CLA	C2-C1-O2A-CGA
20	R	107	CLA	C2-C1-O2A-CGA
20	B	827	CLA	C2-C1-O2A-CGA
21	R	102	LMU	C5'-C4'-O1B-C1B
21	1	220	LMU	C5'-C4'-O1B-C1B
20	B	825	CLA	C2A-CAA-CBA-CGA
20	3	313	CLA	C2A-CAA-CBA-CGA
20	4	316	CLA	C3A-C2A-CAA-CBA
20	4	302	CLA	C3A-C2A-CAA-CBA
20	A	812	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C3A-C2A-CAA-CBA
20	2	307	CLA	C3A-C2A-CAA-CBA
20	4	307	CLA	C3A-C2A-CAA-CBA
20	A	834	CLA	C3A-C2A-CAA-CBA
20	B	835	CLA	C3A-C2A-CAA-CBA
20	A	822	CLA	C6-C7-C8-C10
22	B	845	BCR	C13-C14-C15-C16
20	B	830	CLA	CBA-CGA-O2A-C1
20	A	835	CLA	CBA-CGA-O2A-C1
21	A	853	LMU	C6-C7-C8-C9
20	A	805	CLA	C14-C13-C15-C16
20	A	850	CLA	C6-C7-C8-C9
20	A	839	CLA	C11-C12-C13-C14
20	A	830	CLA	C11-C12-C13-C14
20	B	824	CLA	C16-C17-C18-C20
20	A	835	CLA	C15-C16-C17-C18
21	R	104	LMU	C2-C3-C4-C5
22	B	852	BCR	C11-C10-C9-C34
22	B	844	BCR	C11-C10-C9-C34
22	A	847	BCR	C35-C13-C14-C15
22	F	203	BCR	C16-C17-C18-C36
21	A	848	LMU	C1-C2-C3-C4
20	A	811	CLA	C4-C3-C5-C6
20	B	833	CLA	C1A-C2A-CAA-CBA
20	4	307	CLA	C1A-C2A-CAA-CBA
20	B	803	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	C6-C7-C8-C10
20	B	835	CLA	C11-C10-C8-C7
20	A	835	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	K	101	CLA	C2C-C3C-CAC-CBC
20	4	306	CLA	C2A-CAA-CBA-CGA
20	I	102	CLA	C2A-CAA-CBA-CGA
20	A	838	CLA	C15-C16-C17-C18
20	B	812	CLA	C15-C16-C17-C18
20	2	322	CLA	C3-C5-C6-C7
20	B	827	CLA	C8-C10-C11-C12
20	2	307	CLA	C4-C3-C5-C6
20	A	841	CLA	C2-C3-C5-C6
21	2	317	LMU	C3-C4-C5-C6
21	4	320	LMU	C2B-C1B-O1B-C4'
21	N	101	LMU	C5'-C4'-O1B-C1B
20	A	852	CLA	C16-C17-C18-C20
22	B	852	BCR	C11-C10-C9-C8
22	B	844	BCR	C11-C10-C9-C8
22	A	847	BCR	C12-C13-C14-C15
22	F	203	BCR	C16-C17-C18-C19
21	K	105	LMU	O1'-C1-C2-C3
21	B	802	LMU	C1-C2-C3-C4
22	A	845	BCR	C19-C20-C21-C22
22	F	202	BCR	C13-C14-C15-C16
22	A	843	BCR	C13-C14-C15-C16
25	B	848	LMG	C31-C32-C33-C34
20	B	808	CLA	C13-C15-C16-C17
20	A	830	CLA	C8-C10-C11-C12
20	1	202	CLA	C4C-C3C-CAC-CBC
20	A	851	CLA	C2-C1-O2A-CGA
20	4	302	CLA	C2-C1-O2A-CGA
20	4	311	CLA	C2-C1-O2A-CGA
20	A	850	CLA	C2-C3-C5-C6
20	L	208	CLA	C2-C1-O2A-CGA
20	A	830	CLA	C10-C11-C12-C13
20	B	839	CLA	CAA-CBA-CGA-O2A
20	B	813	CLA	C6-C7-C8-C9
20	A	823	CLA	C3-C5-C6-C7
20	J	101	CLA	CAA-CBA-CGA-O1A
20	B	805	CLA	CAA-CBA-CGA-O2A
20	3	311	CLA	CAA-CBA-CGA-O2A
21	2	319	LMU	C1-C2-C3-C4
21	C	101	LMU	C4'-C5'-C6'-O6'
20	B	803	CLA	C5-C6-C7-C8
20	4	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	D	201	LMU	C2B-C1B-O1B-C4'
20	H	109	CLA	C3-C5-C6-C7
22	A	843	BCR	C23-C24-C25-C30
20	A	836	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	CAA-CBA-CGA-O2A
20	A	824	CLA	C8-C10-C11-C12
22	A	844	BCR	C13-C14-C15-C16
20	R	108	CLA	C4-C3-C5-C6
20	A	851	CLA	C8-C10-C11-C12
21	N	101	LMU	C9-C10-C11-C12
20	A	826	CLA	C16-C17-C18-C19
21	D	201	LMU	O5B-C1B-O1B-C4'
20	B	849	CLA	CAA-CBA-CGA-O1A
20	B	808	CLA	C2A-CAA-CBA-CGA
20	B	816	CLA	C5-C6-C7-C8
20	A	826	CLA	C4-C3-C5-C6
20	A	803	CLA	CAA-CBA-CGA-O1A
20	2	316	CLA	C11-C10-C8-C7
20	B	849	CLA	C12-C13-C15-C16
20	H	101	CLA	CBA-CGA-O2A-C1
21	2	319	LMU	C7-C8-C9-C10
20	B	803	CLA	CAA-CBA-CGA-O2A
20	B	838	CLA	C13-C15-C16-C17
20	B	818	CLA	CAA-CBA-CGA-O2A
20	H	103	CLA	CAA-CBA-CGA-O2A
20	B	826	CLA	C4-C3-C5-C6
20	B	830	CLA	C4-C3-C5-C6
20	A	804	CLA	C4-C3-C5-C6
20	A	835	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	C2-C3-C5-C6
20	A	838	CLA	CAA-CBA-CGA-O2A
20	A	850	CLA	CAA-CBA-CGA-O2A
20	B	824	CLA	CAA-CBA-CGA-O2A
20	B	819	CLA	CAA-CBA-CGA-O2A
21	D	201	LMU	C5-C6-C7-C8
21	H	106	LMU	C2B-C1B-O1B-C4'
20	B	816	CLA	C6-C7-C8-C9
20	3	318	CLA	C11-C12-C13-C14
20	I	102	CLA	C11-C10-C8-C9
20	B	839	CLA	C14-C13-C15-C16
23	A	842	PQN	C24-C23-C25-C26
20	2	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	K	102	CLA	C3A-C2A-CAA-CBA
20	A	811	CLA	C3A-C2A-CAA-CBA
20	A	822	CLA	C3A-C2A-CAA-CBA
20	1	204	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C3A-C2A-CAA-CBA
21	C	101	LMU	C3-C4-C5-C6
20	I	102	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	CAD-CBD-CGD-O2D
20	B	811	CLA	CAD-CBD-CGD-O2D
20	B	826	CLA	CAD-CBD-CGD-O2D
20	A	838	CLA	CAD-CBD-CGD-O2D
20	A	837	CLA	CAD-CBD-CGD-O2D
20	4	311	CLA	CAD-CBD-CGD-O2D
20	B	822	CLA	CAD-CBD-CGD-O2D
20	A	819	CLA	CAD-CBD-CGD-O2D
20	A	813	CLA	CAD-CBD-CGD-O2D
20	A	803	CLA	CAD-CBD-CGD-O2D
20	A	832	CLA	CAD-CBD-CGD-O2D
20	3	317	CLA	CAD-CBD-CGD-O2D
20	B	827	CLA	CAD-CBD-CGD-O2D
20	4	307	CLA	CAD-CBD-CGD-O2D
20	B	823	CLA	CAD-CBD-CGD-O2D
20	H	109	CLA	CAD-CBD-CGD-O2D
20	A	823	CLA	CAD-CBD-CGD-O2D
20	2	312	CLA	CAD-CBD-CGD-O2D
20	B	805	CLA	C11-C12-C13-C14
20	A	852	CLA	C16-C17-C18-C19
20	B	806	CLA	C2C-C3C-CAC-CBC
20	B	830	CLA	C5-C6-C7-C8
20	A	826	CLA	C10-C11-C12-C13
20	B	828	CLA	C2-C1-O2A-CGA
20	A	805	CLA	CAA-CBA-CGA-O2A
20	A	837	CLA	CAA-CBA-CGA-O2A
20	2	312	CLA	CAA-CBA-CGA-O2A
21	G	101	LMU	C5'-C4'-O1B-C1B
20	A	824	CLA	C4-C3-C5-C6
21	G	101	LMU	O5'-C1'-O1'-C1
20	A	824	CLA	C2-C3-C5-C6
20	2	307	CLA	C2-C3-C5-C6
20	B	830	CLA	C2-C3-C5-C6
20	A	811	CLA	C2-C3-C5-C6
20	4	304	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	2	318	LMU	C2B-C1B-O1B-C4'
20	2	305	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	CAA-CBA-CGA-O2A
21	A	856	LMU	C9-C10-C11-C12
20	B	851	CLA	O2A-C1-C2-C3
20	A	838	CLA	O2A-C1-C2-C3
20	1	207	CLA	O2A-C1-C2-C3
20	A	817	CLA	O2A-C1-C2-C3
20	B	823	CLA	O2A-C1-C2-C3
21	4	317	LMU	C4B-C5B-C6B-O6B
20	A	819	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C8-C10-C11-C12
20	B	836	CLA	CHA-CBD-CGD-O2D
20	A	827	CLA	CHA-CBD-CGD-O1D
20	2	316	CLA	CHA-CBD-CGD-O1D
20	2	316	CLA	CHA-CBD-CGD-O2D
20	B	826	CLA	CHA-CBD-CGD-O1D
20	B	826	CLA	CHA-CBD-CGD-O2D
22	F	202	BCR	C15-C16-C17-C18
20	4	311	CLA	CHA-CBD-CGD-O2D
20	B	805	CLA	CHA-CBD-CGD-O1D
20	B	805	CLA	CHA-CBD-CGD-O2D
20	3	318	CLA	CHA-CBD-CGD-O1D
20	3	318	CLA	CHA-CBD-CGD-O2D
20	R	108	CLA	CHA-CBD-CGD-O2D
20	A	839	CLA	CHA-CBD-CGD-O1D
20	A	839	CLA	CHA-CBD-CGD-O2D
20	B	817	CLA	CHA-CBD-CGD-O1D
20	B	817	CLA	CHA-CBD-CGD-O2D
20	B	803	CLA	CHA-CBD-CGD-O2D
20	B	839	CLA	CHA-CBD-CGD-O1D
20	B	839	CLA	CHA-CBD-CGD-O2D
20	1	202	CLA	CHA-CBD-CGD-O1D
20	1	202	CLA	CHA-CBD-CGD-O2D
20	2	312	CLA	CHA-CBD-CGD-O1D
20	2	312	CLA	CHA-CBD-CGD-O2D
20	L	208	CLA	CHA-CBD-CGD-O1D
20	L	207	CLA	C2C-C3C-CAC-CBC
20	A	826	CLA	C2-C3-C5-C6
20	J	103	CLA	C3-C5-C6-C7
20	A	830	CLA	C5-C6-C7-C8
20	1	206	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	A	825	CLA	C10-C11-C12-C13
21	H	108	LMU	C5'-C4'-O1B-C1B
20	A	816	CLA	C2A-CAA-CBA-CGA
20	B	811	CLA	CBA-CGA-O2A-C1
20	A	825	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	CAA-CBA-CGA-O2A
20	1	210	CLA	CAA-CBA-CGA-O2A
20	B	826	CLA	C2-C3-C5-C6
20	B	813	CLA	C6-C7-C8-C10
20	B	813	CLA	C11-C10-C8-C7
20	A	819	CLA	C16-C17-C18-C20
21	R	104	LMU	C2B-C1B-O1B-C4'
21	4	322	LMU	C4'-C5'-C6'-O6'
20	B	836	CLA	C14-C13-C15-C16
20	B	812	CLA	C11-C12-C13-C14
20	2	307	CLA	C14-C13-C15-C16
20	A	850	CLA	C11-C12-C13-C14
20	A	828	CLA	C6-C7-C8-C9
21	R	109	LMU	O1'-C1-C2-C3
20	A	805	CLA	C2C-C3C-CAC-CBC
21	4	321	LMU	C9-C10-C11-C12
20	A	850	CLA	C16-C17-C18-C19
20	B	809	CLA	C2C-C3C-CAC-CBC
21	G	101	LMU	C3-C4-C5-C6
20	A	852	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
20	4	304	CLA	C4C-C3C-CAC-CBC
20	K	103	CLA	CAA-CBA-CGA-O2A
20	I	102	CLA	CAA-CBA-CGA-O1A
21	1	217	LMU	C9-C10-C11-C12
20	4	302	CLA	C1A-C2A-CAA-CBA
20	2	305	CLA	C1A-C2A-CAA-CBA
20	A	812	CLA	C1A-C2A-CAA-CBA
20	K	102	CLA	C1A-C2A-CAA-CBA
20	B	819	CLA	C1A-C2A-CAA-CBA
20	A	806	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	CAA-CBA-CGA-O1A
20	B	824	CLA	CAA-CBA-CGA-O1A
20	2	303	CLA	C2-C1-O2A-CGA
20	B	821	CLA	C2-C1-O2A-CGA
20	B	834	CLA	CAA-CBA-CGA-O1A
20	B	819	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	E	101	LMU	O1'-C1-C2-C3
20	B	822	CLA	CBD-CGD-O2D-CED
20	B	818	CLA	CAA-CBA-CGA-O1A
20	B	803	CLA	CAA-CBA-CGA-O1A
20	H	103	CLA	CAA-CBA-CGA-O1A
20	B	851	CLA	C4-C3-C5-C6
20	H	102	CLA	CAA-CBA-CGA-O2A
20	A	805	CLA	CAA-CBA-CGA-O1A
20	A	850	CLA	CAA-CBA-CGA-O1A
20	K	103	CLA	CAA-CBA-CGA-O1A
20	A	810	CLA	C2A-CAA-CBA-CGA
21	H	107	LMU	C5'-C4'-O1B-C1B
20	A	838	CLA	CAA-CBA-CGA-O1A
20	A	811	CLA	CAA-CBA-CGA-O1A
20	2	303	CLA	CBA-CGA-O2A-C1
22	B	845	BCR	C1-C6-C7-C8
22	B	845	BCR	C5-C6-C7-C8
22	B	845	BCR	C23-C24-C25-C30
22	3	314	BCR	C1-C6-C7-C8
22	3	314	BCR	C5-C6-C7-C8
20	A	840	CLA	C2C-C3C-CAC-CBC
20	A	825	CLA	CAA-CBA-CGA-O1A
20	A	837	CLA	CAA-CBA-CGA-O1A
20	2	312	CLA	CAA-CBA-CGA-O1A
20	B	851	CLA	CAA-CBA-CGA-O2A
20	B	822	CLA	C4-C3-C5-C6
20	2	322	CLA	C2-C3-C5-C6
20	A	851	CLA	CAD-CBD-CGD-O1D
20	4	306	CLA	CAD-CBD-CGD-O1D
20	A	805	CLA	CAD-CBD-CGD-O1D
20	F	205	CLA	CAD-CBD-CGD-O1D
20	B	804	CLA	CAD-CBD-CGD-O1D
20	A	825	CLA	CAD-CBD-CGD-O1D
20	B	824	CLA	CAD-CBD-CGD-O1D
20	A	804	CLA	CAD-CBD-CGD-O1D
20	1	210	CLA	CAD-CBD-CGD-O1D
20	A	820	CLA	C2-C3-C5-C6
20	K	101	CLA	CAD-CBD-CGD-O1D
20	4	318	CLA	CAD-CBD-CGD-O1D
21	A	855	LMU	C9-C10-C11-C12
20	2	308	CLA	C11-C12-C13-C14
20	B	838	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	838	CLA	C14-C13-C15-C16
20	A	819	CLA	C14-C13-C15-C16
20	B	813	CLA	C11-C10-C8-C9
21	E	101	LMU	C6-C7-C8-C9
21	4	301	LMU	C7-C8-C9-C10
25	B	848	LMG	C28-C29-C30-C31
20	H	102	CLA	CAA-CBA-CGA-O1A
20	1	206	CLA	CAA-CBA-CGA-O1A
21	H	105	LMU	O1'-C1-C2-C3
20	B	836	CLA	CAA-CBA-CGA-O2A
20	A	817	CLA	CAA-CBA-CGA-O2A
20	A	830	CLA	CAA-CBA-CGA-O2A
20	A	835	CLA	C8-C10-C11-C12
20	A	801	CLA	C2-C1-O2A-CGA
21	1	213	LMU	C4-C5-C6-C7
20	4	316	CLA	CAA-CBA-CGA-O2A
20	2	308	CLA	CAA-CBA-CGA-O2A
20	B	812	CLA	CAA-CBA-CGA-O2A
20	3	318	CLA	CAA-CBA-CGA-O2A
20	1	202	CLA	CAA-CBA-CGA-O2A
21	H	105	LMU	C5-C6-C7-C8
20	2	303	CLA	O1A-CGA-O2A-C1
20	B	836	CLA	C6-C7-C8-C10
20	B	836	CLA	C11-C12-C13-C15
20	A	811	CLA	C11-C10-C8-C7
20	B	838	CLA	C6-C7-C8-C10
20	A	819	CLA	C12-C13-C15-C16
20	A	804	CLA	C2-C3-C5-C6
23	A	842	PQN	C21-C22-C23-C25
20	H	109	CLA	C11-C10-C8-C7
20	4	316	CLA	CAA-CBA-CGA-O1A
20	A	801	CLA	CAA-CBA-CGA-O1A
21	A	855	LMU	C1-C2-C3-C4
20	A	808	CLA	C2C-C3C-CAC-CBC
21	R	103	LMU	C2-C3-C4-C5
20	A	813	CLA	CAA-CBA-CGA-O2A
20	3	311	CLA	O1A-CGA-O2A-C1
22	B	845	BCR	C7-C8-C9-C10
20	B	836	CLA	CAA-CBA-CGA-O1A
22	B	842	BCR	C15-C16-C17-C18
20	A	805	CLA	C10-C11-C12-C13
20	A	850	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	A	830	CLA	CAA-CBA-CGA-O1A
21	1	217	LMU	C4B-C5B-C6B-O6B
21	H	105	LMU	C3'-C4'-O1B-C1B
21	L	211	LMU	C4'-C5'-C6'-O6'
20	A	836	CLA	CAA-CBA-CGA-O2A
20	A	833	CLA	C2A-CAA-CBA-CGA
20	B	824	CLA	C10-C11-C12-C13
20	A	828	CLA	C10-C11-C12-C13
20	B	851	CLA	CAA-CBA-CGA-O1A
21	R	103	LMU	C5-C6-C7-C8
20	2	303	CLA	C5-C6-C7-C8
20	B	830	CLA	C8-C10-C11-C12
20	B	805	CLA	C4-C3-C5-C6
20	B	820	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

227 monomers are involved in 3721 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	CLA	28	0
22	B	852	BCR	13	0
20	4	316	CLA	6	0
20	A	809	CLA	26	0
20	B	825	CLA	25	0
20	B	806	CLA	20	0
20	B	851	CLA	51	0
20	A	851	CLA	36	0
20	2	303	CLA	13	0
20	B	836	CLA	44	0
20	3	308	CLA	2	0
20	4	304	CLA	24	0
20	4	302	CLA	26	0
20	A	827	CLA	21	0
20	A	816	CLA	36	0
20	1	203	CLA	13	0
20	2	305	CLA	13	0
20	1	209	CLA	11	0
22	B	843	BCR	17	0
21	4	317	LMU	4	0
20	2	322	CLA	35	0
20	A	818	CLA	29	0
22	B	844	BCR	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	101	BCR	19	0
20	A	841	CLA	30	0
20	F	206	CLA	15	0
21	1	217	LMU	10	0
21	2	313	LMU	3	1
20	4	305	CLA	20	0
21	4	320	LMU	9	5
20	B	811	CLA	29	0
20	3	310	CLA	7	0
20	B	814	CLA	24	0
22	A	847	BCR	63	0
21	N	101	LMU	36	0
20	4	306	CLA	9	0
21	4	322	LMU	1	0
22	F	203	BCR	45	0
22	A	845	BCR	45	0
20	A	812	CLA	4	0
21	L	205	LMU	4	0
21	H	107	LMU	11	0
20	2	308	CLA	9	0
20	A	805	CLA	28	0
20	B	829	CLA	13	0
20	K	102	CLA	11	0
20	2	316	CLA	6	0
20	B	834	CLA	4	0
20	1	211	CLA	5	0
20	A	833	CLA	18	1
20	A	814	CLA	35	0
20	F	205	CLA	15	0
20	G	102	CLA	20	0
20	4	313	CLA	5	0
20	B	826	CLA	33	0
20	3	305	CLA	1	0
20	A	824	CLA	86	0
20	B	804	CLA	9	0
20	R	107	CLA	10	0
20	B	812	CLA	20	0
20	3	306	CLA	3	0
20	B	818	CLA	9	0
21	L	204	LMU	3	0
21	R	101	LMU	6	0
20	B	820	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	825	CLA	79	0
20	B	807	CLA	23	0
20	A	838	CLA	42	0
20	4	314	CLA	7	0
20	A	837	CLA	18	0
20	1	201	CLA	13	0
20	B	850	CLA	41	0
24	C	103	SF4	4	0
20	2	307	CLA	18	0
22	B	845	BCR	32	0
20	A	801	CLA	9	0
21	B	801	LMU	13	0
20	3	309	CLA	5	0
20	B	816	CLA	15	0
20	B	830	CLA	29	0
20	1	207	CLA	6	1
20	3	313	CLA	25	0
22	A	844	BCR	24	0
20	3	311	CLA	20	0
20	A	811	CLA	22	0
21	H	108	LMU	38	0
21	E	101	LMU	30	0
20	H	102	CLA	15	0
21	A	848	LMU	3	0
20	L	202	CLA	26	0
22	F	202	BCR	31	0
20	A	810	CLA	4	0
20	B	849	CLA	22	0
21	K	109	LMU	6	0
22	L	210	BCR	51	0
21	R	102	LMU	20	0
21	K	104	LMU	8	0
20	3	302	CLA	28	0
20	4	311	CLA	17	0
20	B	805	CLA	19	0
21	1	219	LMU	20	0
21	B	802	LMU	4	0
22	J	102	BCR	41	0
20	A	850	CLA	20	0
20	K	103	CLA	3	0
21	H	106	LMU	29	0
20	J	101	CLA	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	322	LMU	8	0
23	B	841	PQN	32	0
20	B	822	CLA	25	0
20	A	852	CLA	27	0
20	A	819	CLA	45	0
20	A	813	CLA	20	0
20	1	204	CLA	5	0
21	A	854	LMU	42	0
20	B	824	CLA	50	0
20	A	808	CLA	26	0
21	K	106	LMU	47	0
20	A	803	CLA	14	0
20	B	821	CLA	39	0
20	B	833	CLA	23	0
20	3	318	CLA	17	0
21	H	104	LMU	21	0
21	R	103	LMU	25	0
20	4	315	CLA	3	0
20	B	815	CLA	24	0
20	2	311	CLA	18	0
22	I	103	BCR	46	0
20	A	832	CLA	16	0
20	A	817	CLA	12	0
20	R	108	CLA	12	0
20	1	215	CLA	52	0
20	2	304	CLA	5	0
20	H	101	CLA	31	0
20	A	821	CLA	10	0
20	A	839	CLA	42	0
20	3	317	CLA	3	0
21	R	104	LMU	11	0
21	A	849	LMU	4	0
20	B	817	CLA	19	0
20	4	319	CLA	11	0
20	L	209	CLA	13	0
20	B	823	CLA	62	0
24	A	857	SF4	19	0
20	B	827	CLA	32	0
24	C	102	SF4	4	0
21	4	321	LMU	2	0
20	I	102	CLA	12	0
21	3	321	LMU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	320	LMU	0	2
20	B	810	CLA	17	0
20	L	207	CLA	9	0
20	3	307	CLA	16	0
21	H	105	LMU	12	0
21	2	318	LMU	6	0
20	4	307	CLA	15	0
21	1	218	LMU	8	0
20	4	310	CLA	3	0
21	D	201	LMU	12	0
21	1	213	LMU	8	0
20	B	840	CLA	2	0
20	B	828	CLA	11	0
21	K	105	LMU	35	0
20	A	804	CLA	28	0
20	A	836	CLA	19	0
20	A	822	CLA	34	0
20	1	210	CLA	9	0
20	K	108	CLA	25	0
21	L	211	LMU	3	0
21	B	847	LMU	28	30
22	B	846	BCR	52	0
20	B	809	CLA	6	0
20	A	829	CLA	11	0
20	A	834	CLA	10	0
20	A	820	CLA	17	0
20	B	831	CLA	16	0
20	B	803	CLA	28	0
20	B	808	CLA	21	0
21	2	317	LMU	12	0
21	A	855	LMU	27	0
20	3	301	CLA	1	0
20	B	837	CLA	25	0
22	B	842	BCR	10	0
20	4	303	CLA	6	0
20	H	103	CLA	3	0
21	A	853	LMU	8	0
20	K	101	CLA	19	1
20	B	835	CLA	16	0
20	B	839	CLA	26	0
20	B	838	CLA	28	0
21	4	301	LMU	7	0

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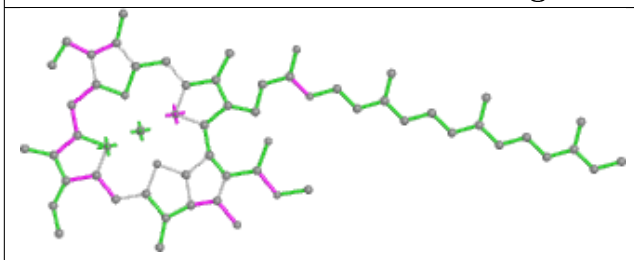
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	202	CLA	40	0
25	B	848	LMG	30	0
21	G	101	LMU	19	0
20	1	206	CLA	16	0
20	A	807	CLA	29	0
20	B	832	CLA	22	0
20	B	813	CLA	13	0
20	A	830	CLA	38	0
20	3	304	CLA	14	0
23	A	842	PQN	15	0
20	A	831	CLA	16	0
20	A	815	CLA	44	0
20	A	840	CLA	8	0
20	4	309	CLA	1	0
20	A	826	CLA	63	0
22	A	846	BCR	37	0
21	R	106	LMU	2	0
20	4	312	CLA	4	0
22	3	314	BCR	19	28
20	F	204	CLA	1	0
20	H	109	CLA	17	0
20	L	203	CLA	17	0
21	R	109	LMU	20	5
20	L	201	CLA	35	0
20	B	819	CLA	21	0
20	2	302	CLA	17	0
20	A	823	CLA	18	0
20	A	828	CLA	17	0
20	2	312	CLA	10	0
20	L	208	CLA	22	0
20	4	318	CLA	19	0
22	A	843	BCR	45	0
21	F	201	LMU	19	0
21	2	319	LMU	4	0
20	A	806	CLA	21	0
20	A	835	CLA	19	0

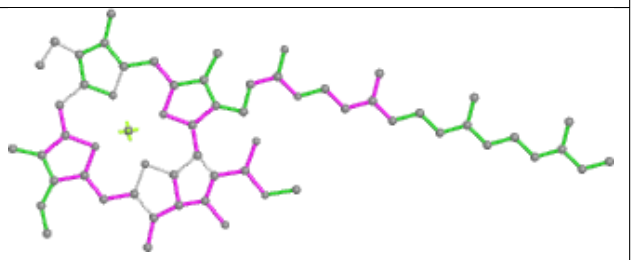
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

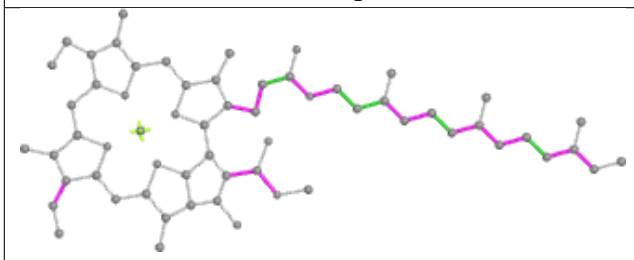
Ligand CLA J 103



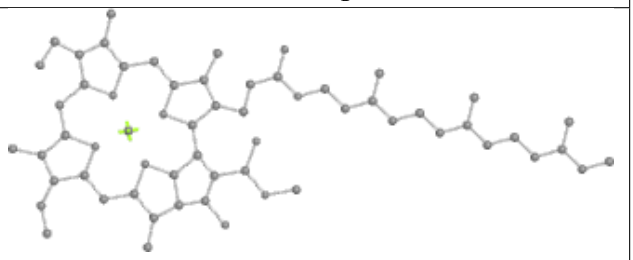
Bond lengths



Bond angles

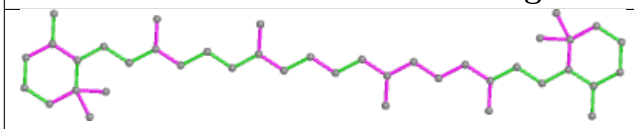


Torsions

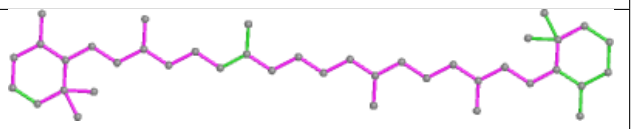


Rings

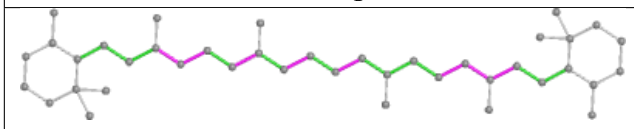
Ligand BCR B 852



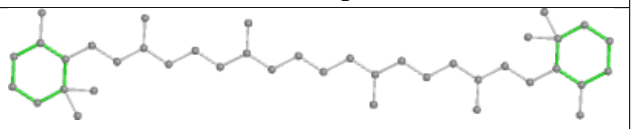
Bond lengths



Bond angles

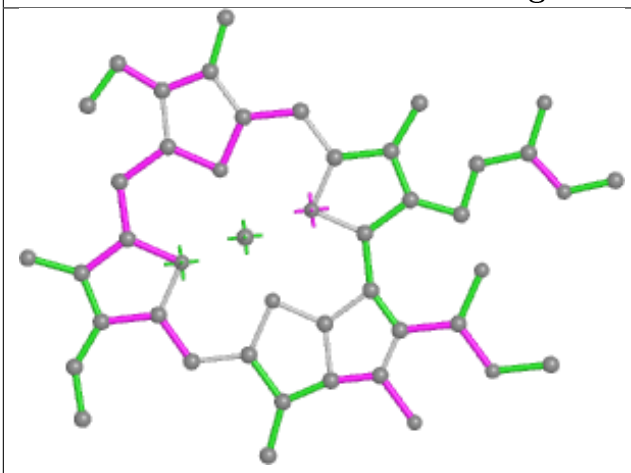


Torsions



Rings

Ligand CLA 4 316



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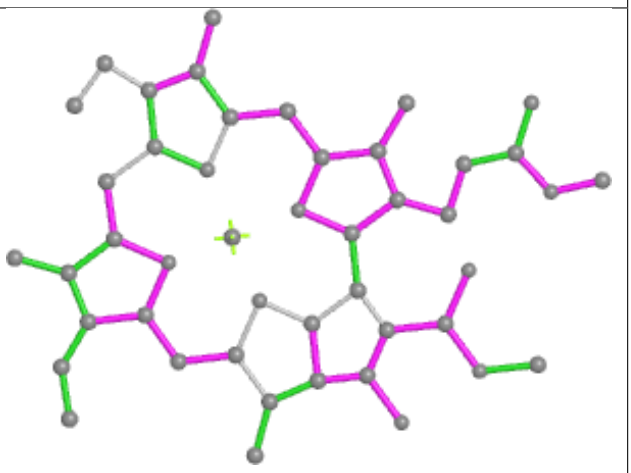
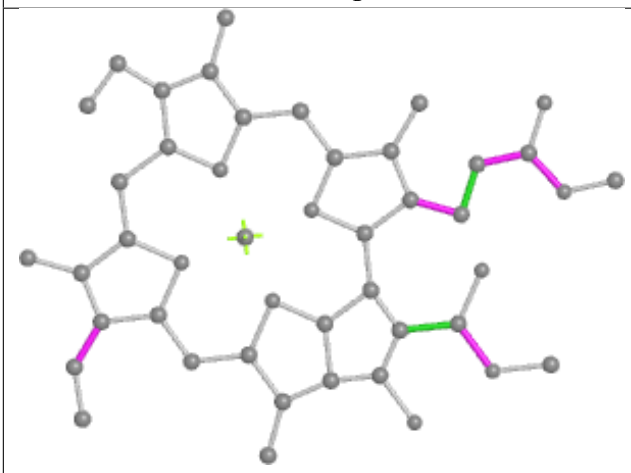
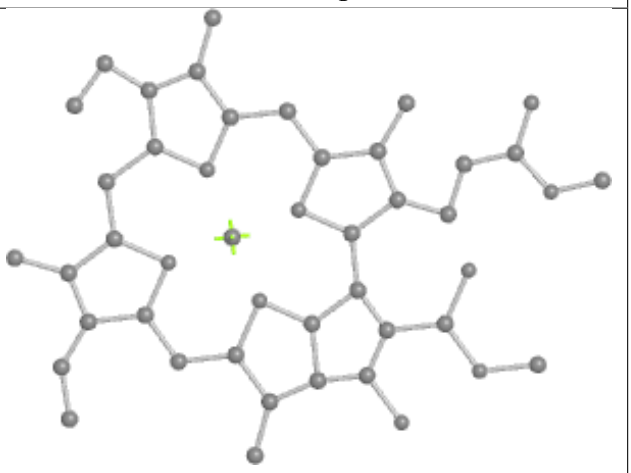


Bond angles

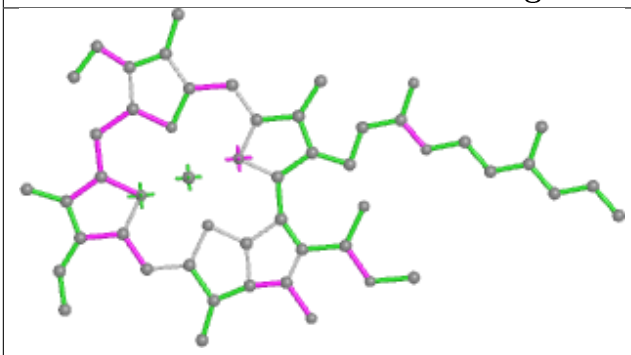


Torsions

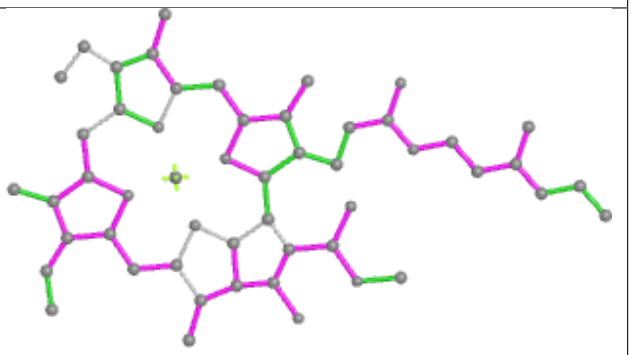


Rings

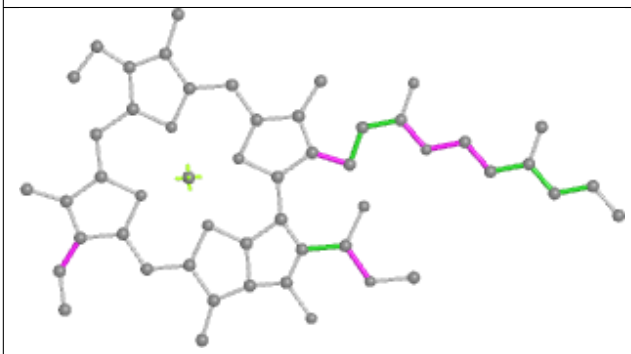
Ligand CLA A 809



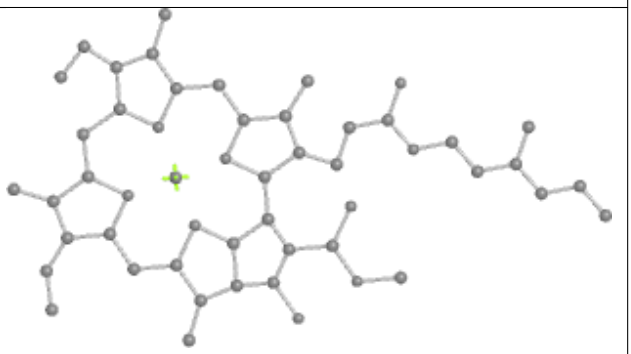
Bond lengths



Bond angles

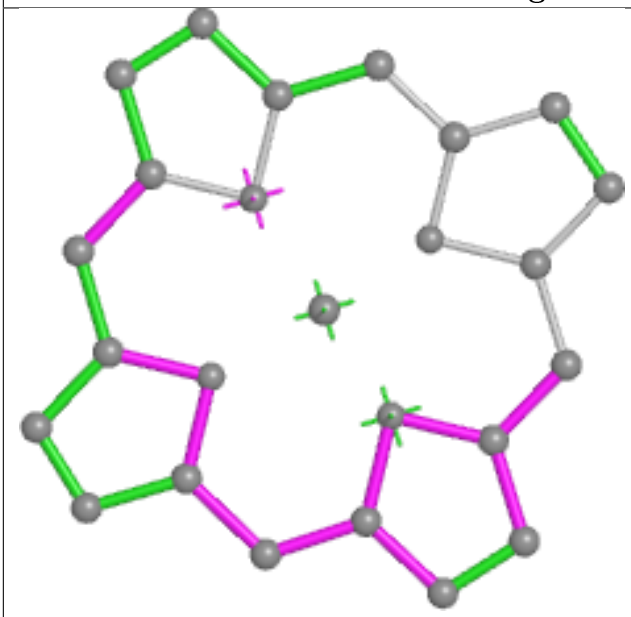


Torsions

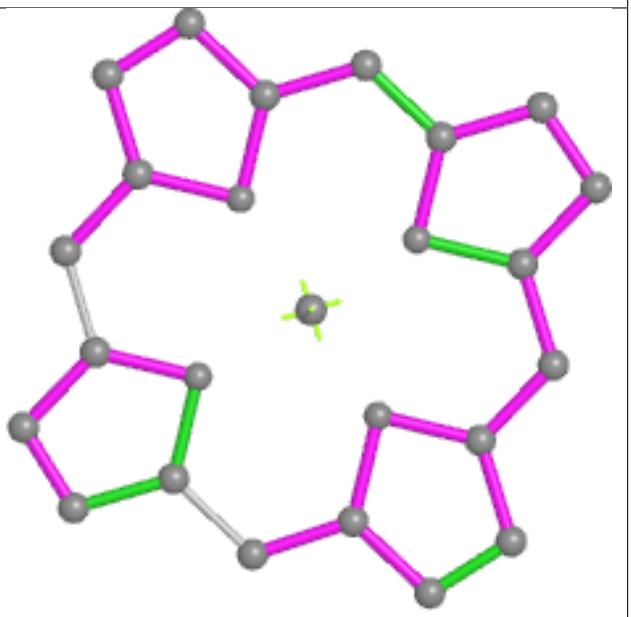


Rings

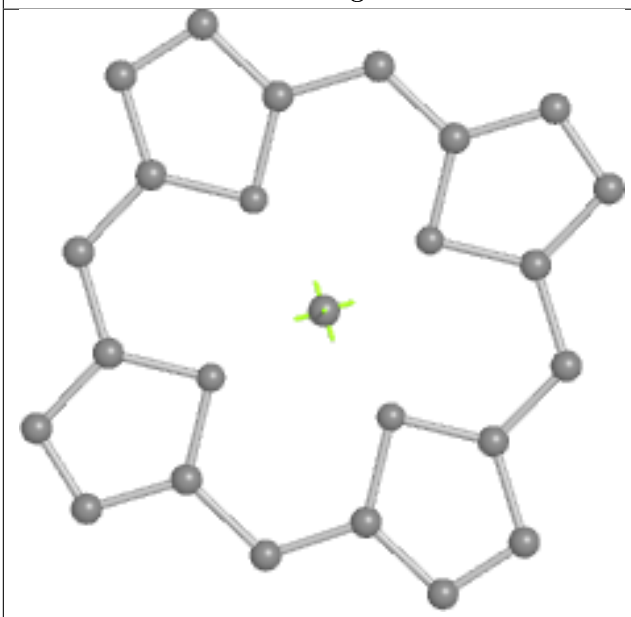
Ligand CLA 3 303



Bond lengths



Bond angles



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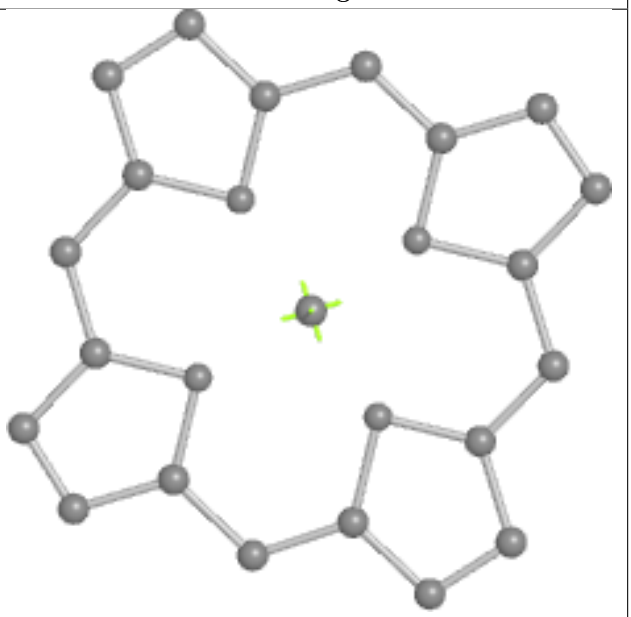
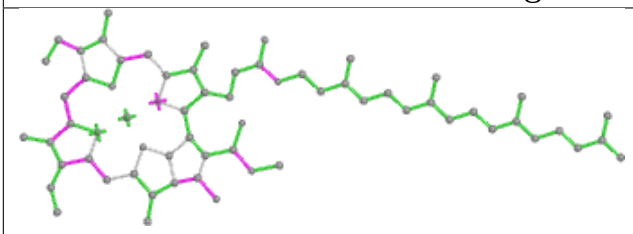


Rings

Ligand CLA B 825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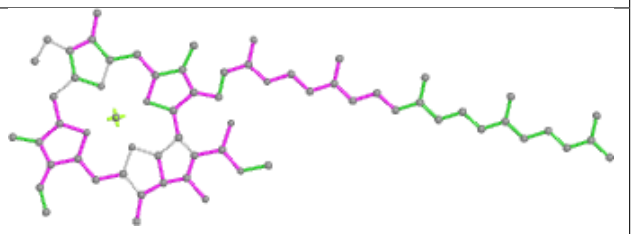
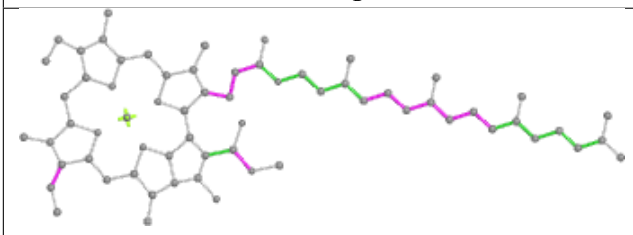
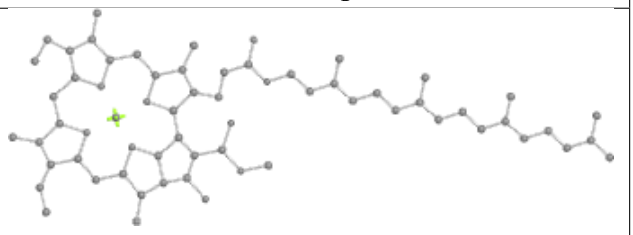
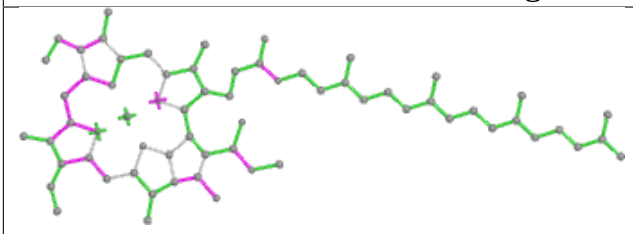
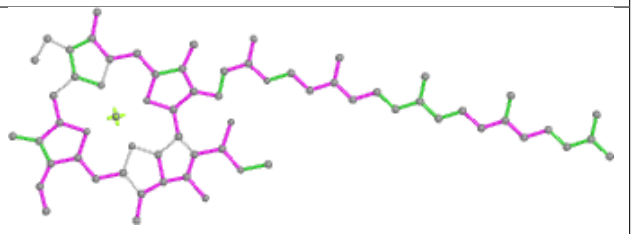

Bond angles

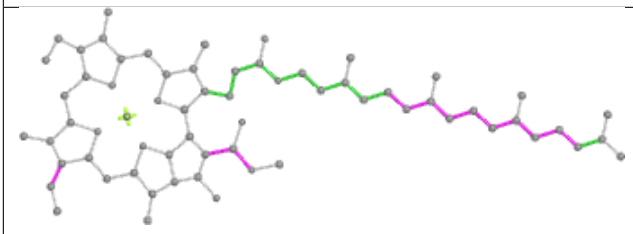

Torsions

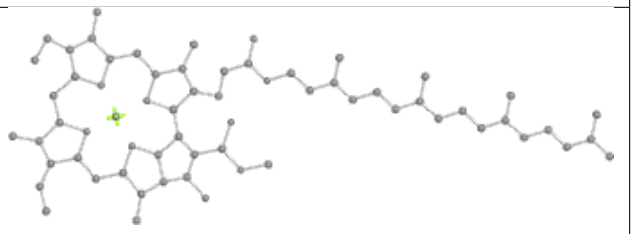

Rings

Ligand CLA B 806

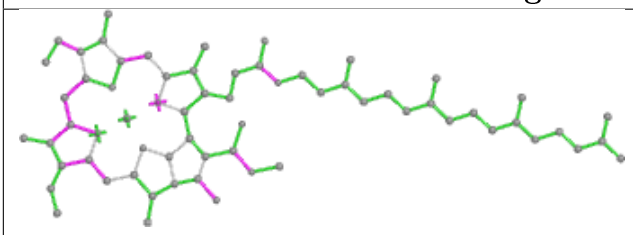

Bond lengths

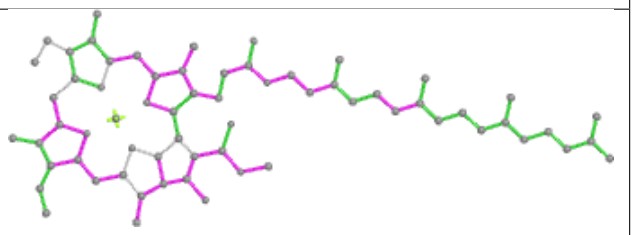

Bond angles

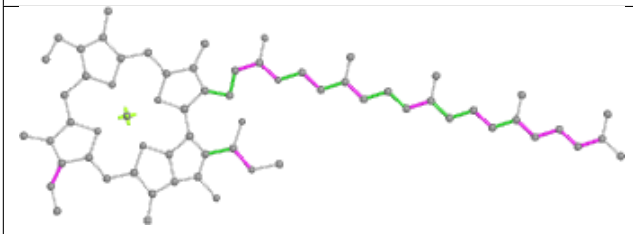

Torsions

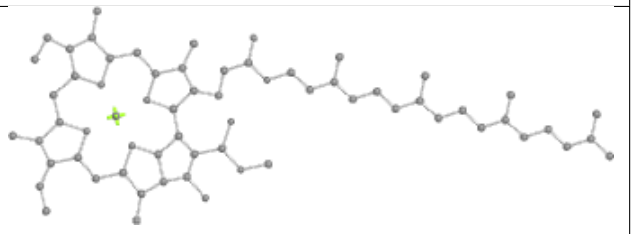

Rings

Ligand CLA B 851

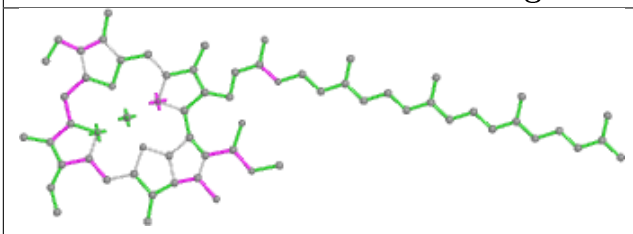

Bond lengths


Bond angles

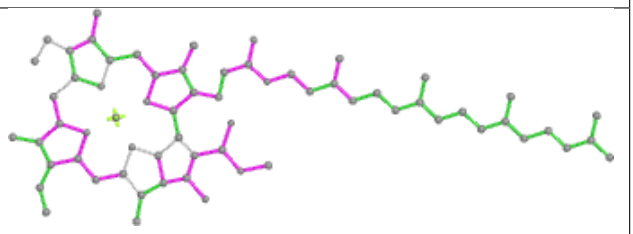

Torsions


Rings

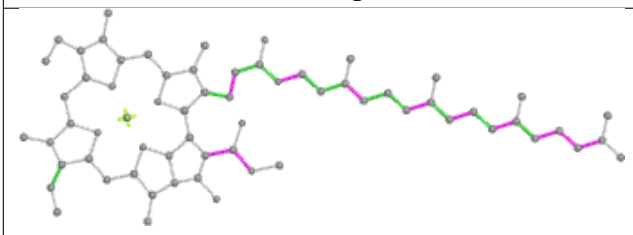
Ligand CLA A 851



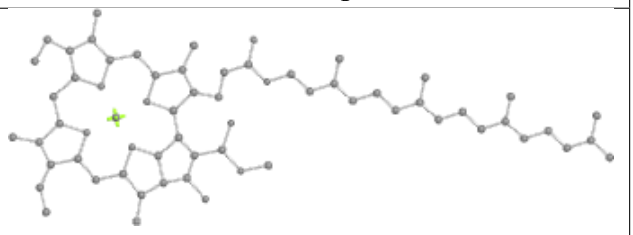
Bond lengths



Bond angles

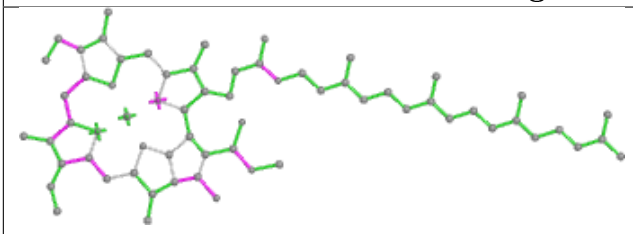


Torsions

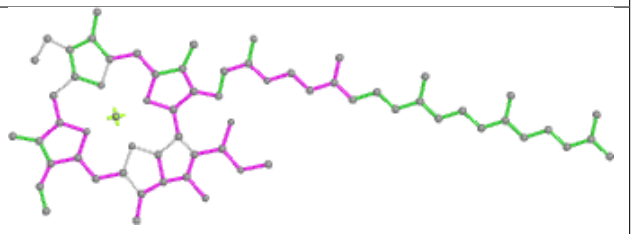


Rings

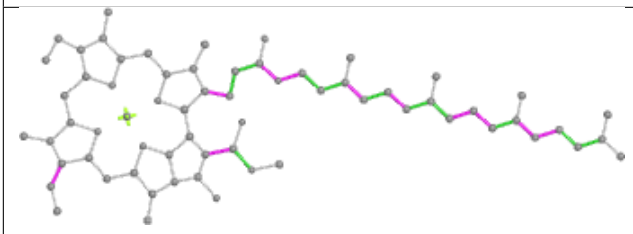
Ligand CLA 2 303



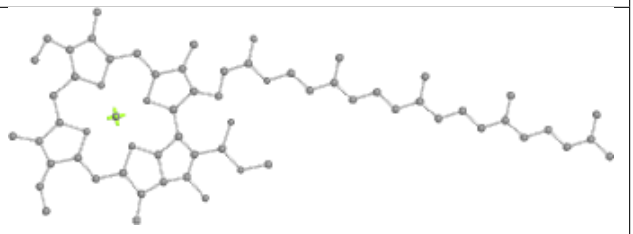
Bond lengths



Bond angles

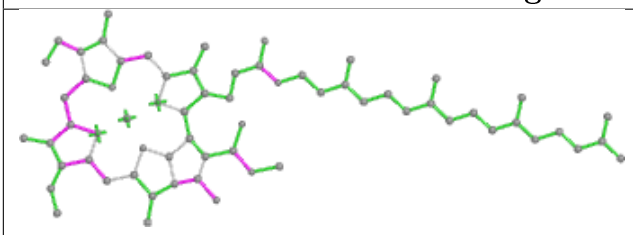


Torsions

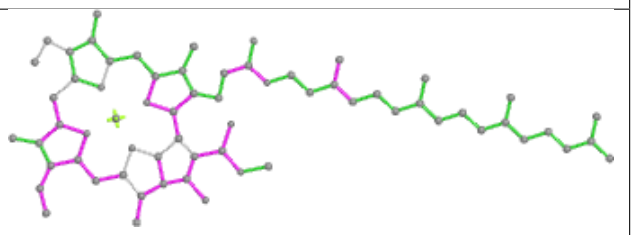


Rings

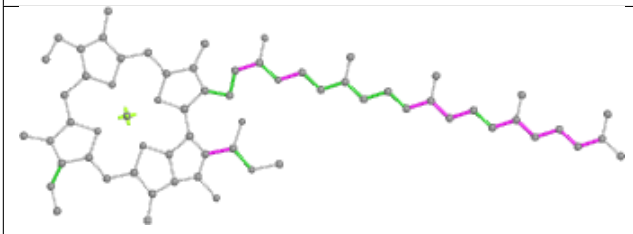
Ligand CLA B 836



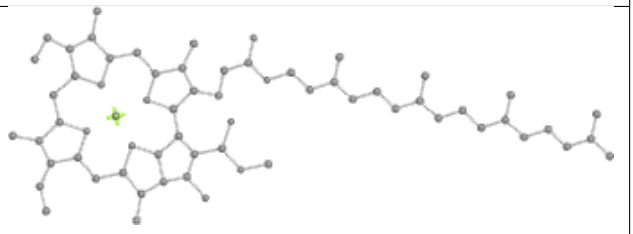
Bond lengths



Bond angles

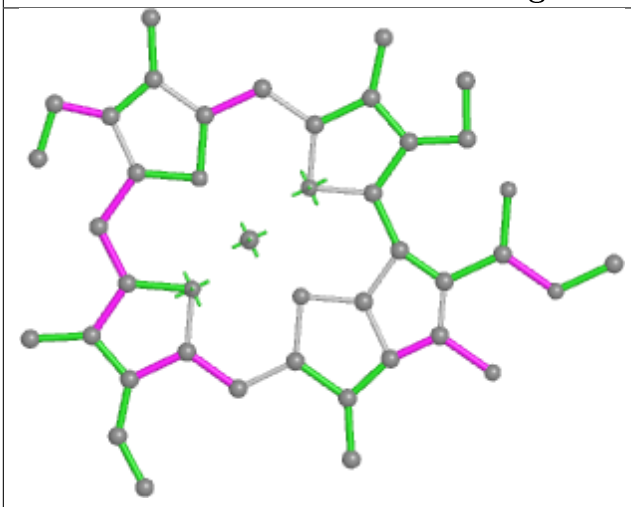


Torsions

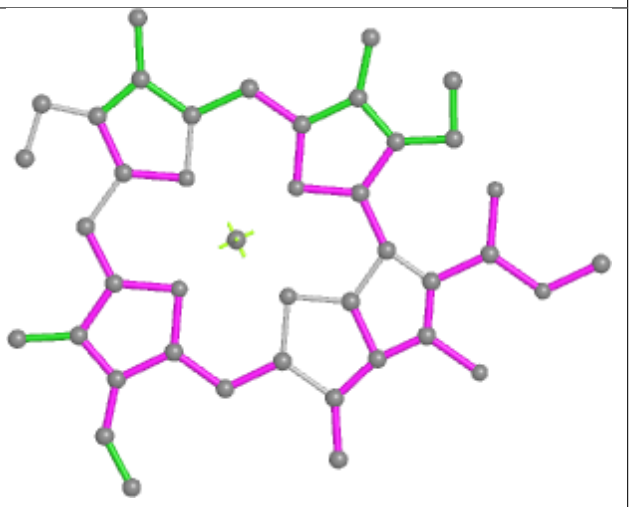


Rings

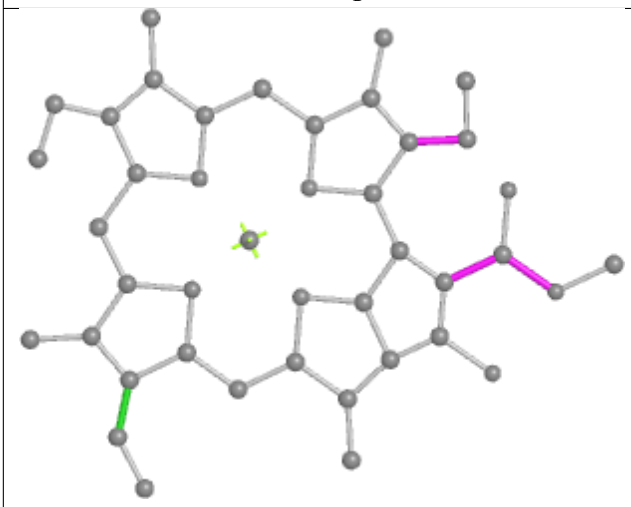
Ligand CLA 3 308



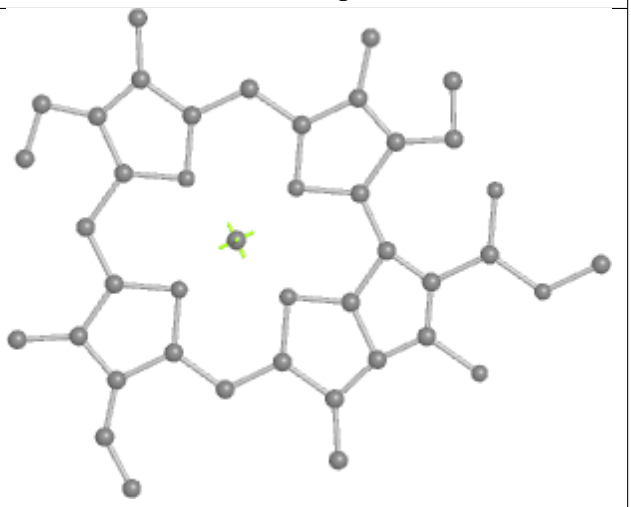
Bond lengths



Bond angles

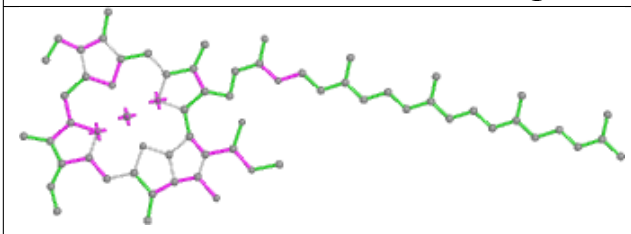


Torsions

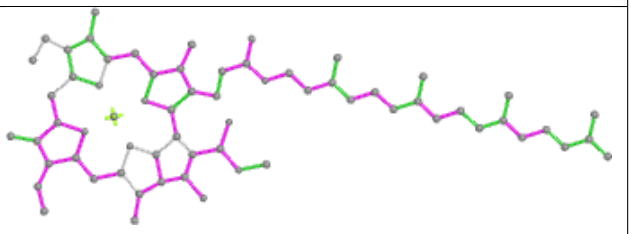


Rings

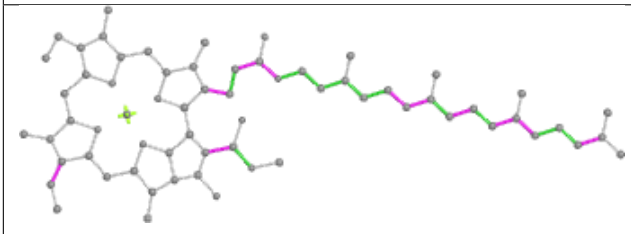
Ligand CLA 4 304



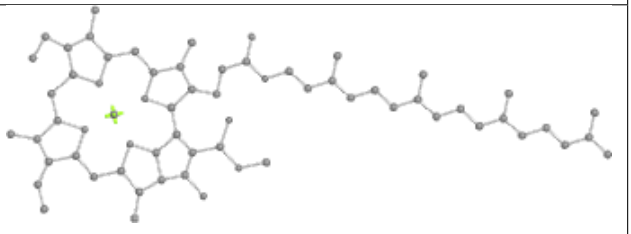
Bond lengths



Bond angles

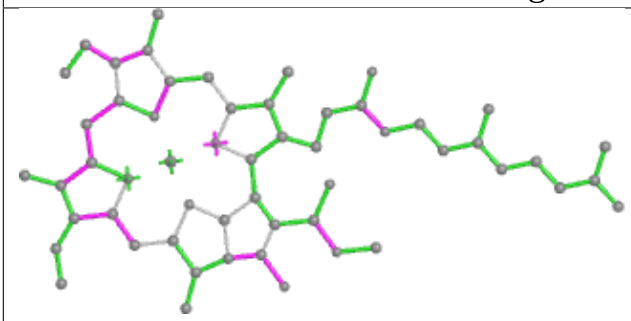


Torsions

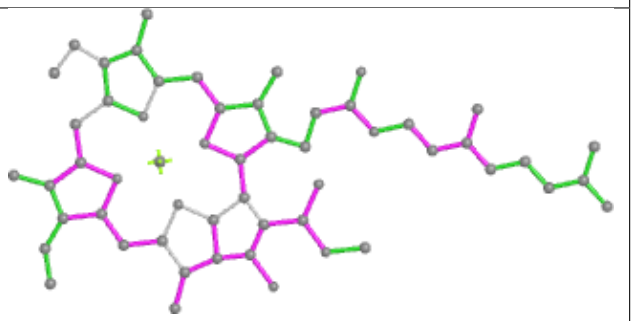


Rings

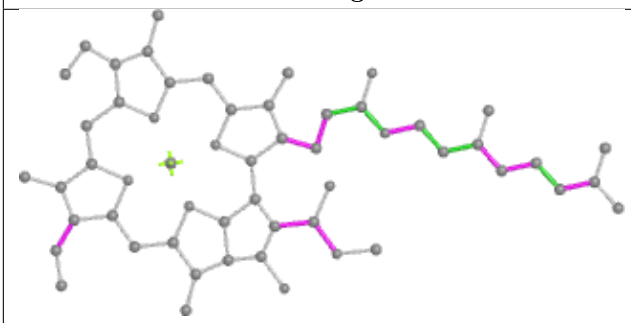
Ligand CLA 4 302



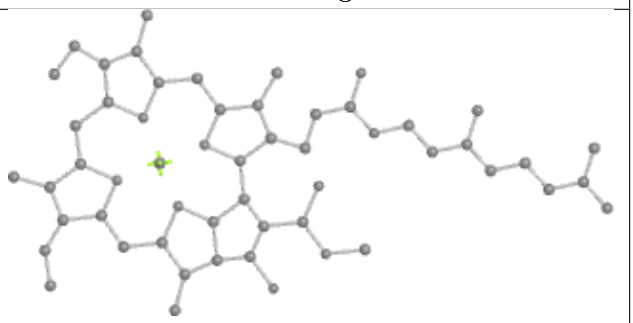
Bond lengths



Bond angles

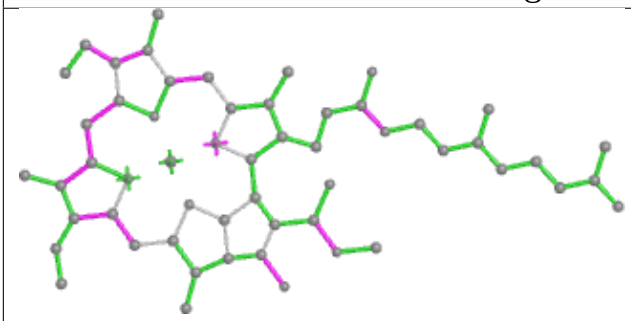


Torsions

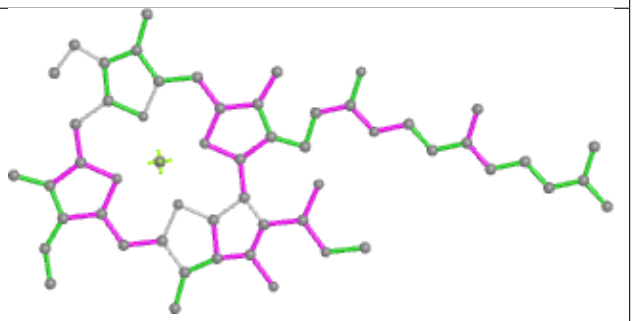


Rings

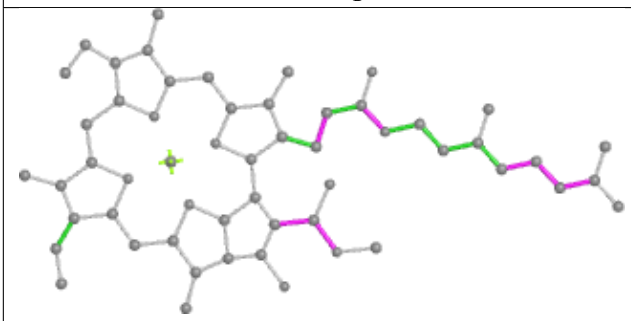
Ligand CLA A 827



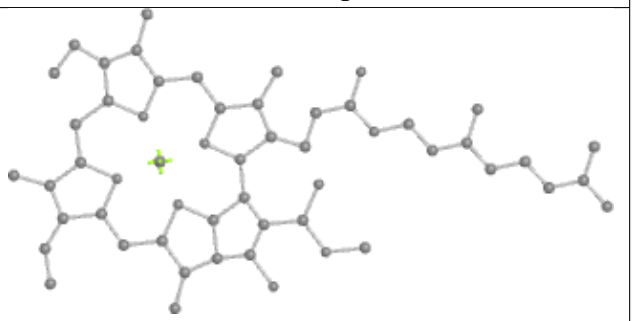
Bond lengths



Bond angles

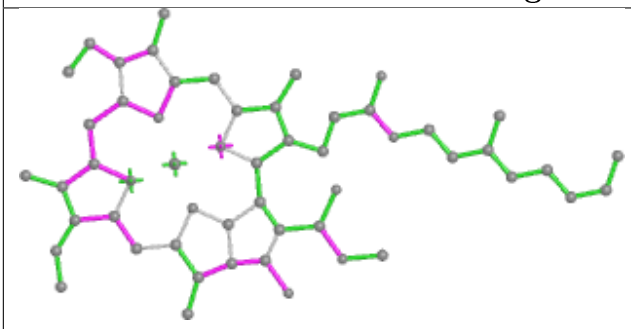


Torsions

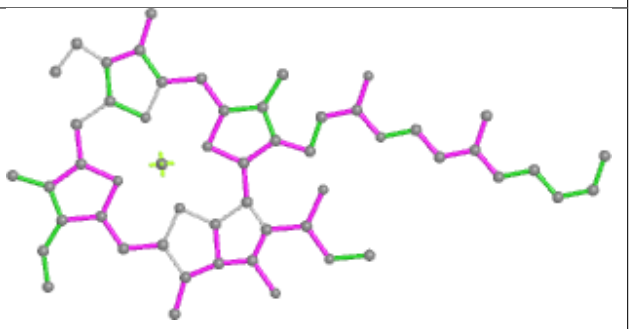


Rings

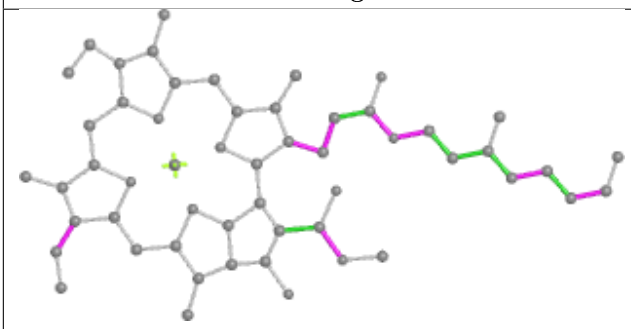
Ligand CLA A 816



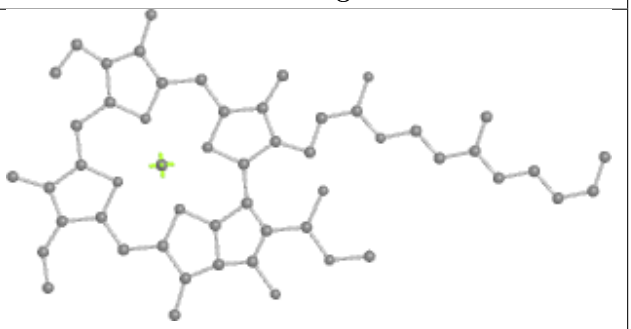
Bond lengths



Bond angles

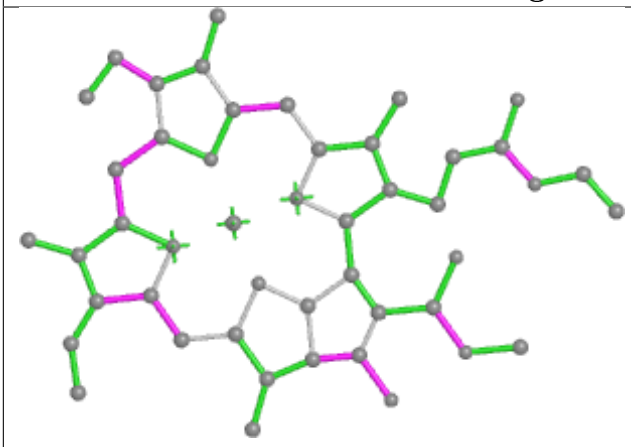


Torsions

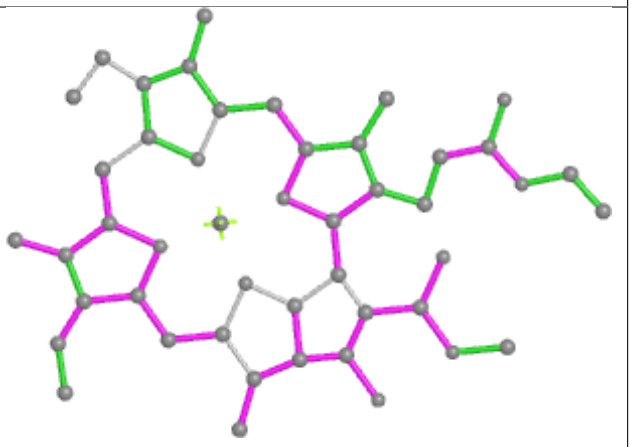


Rings

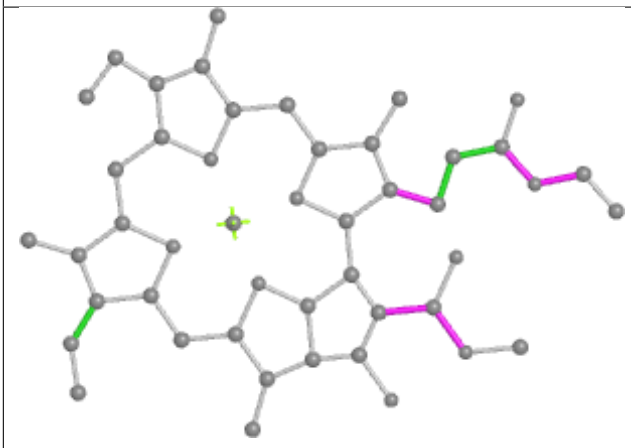
Ligand CLA 1 203



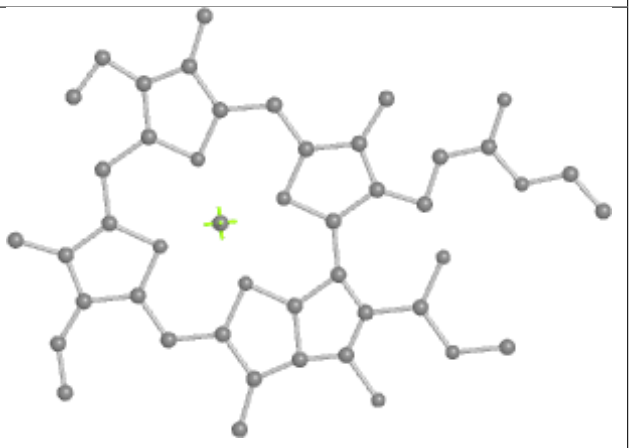
Bond lengths



Bond angles

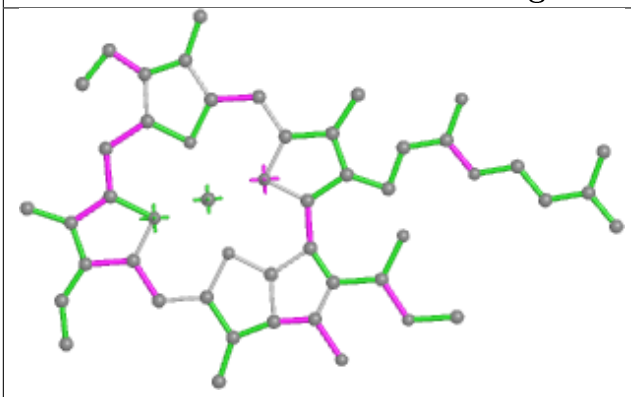


Torsions

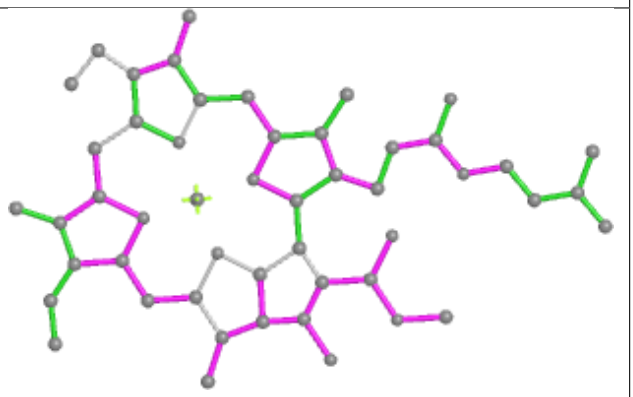


Rings

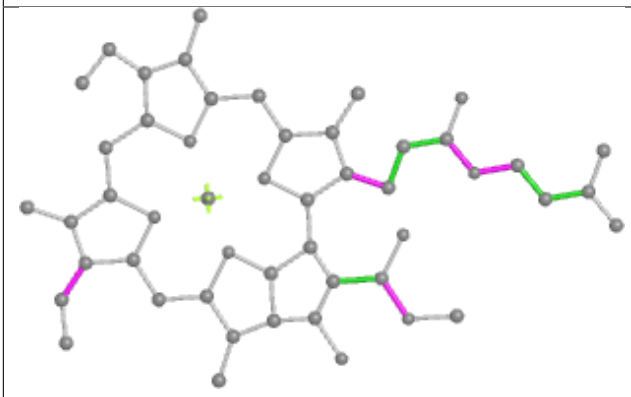
Ligand CLA 2 305



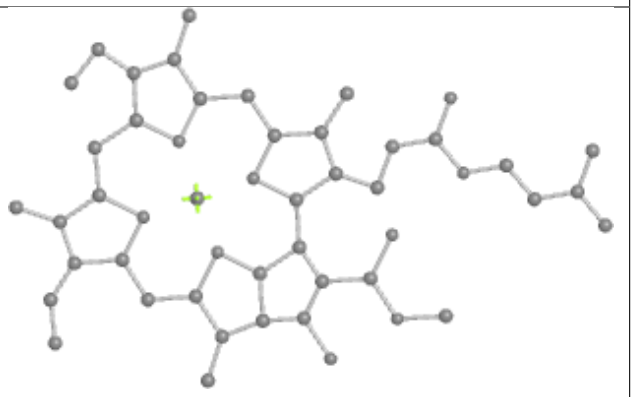
Bond lengths



Bond angles

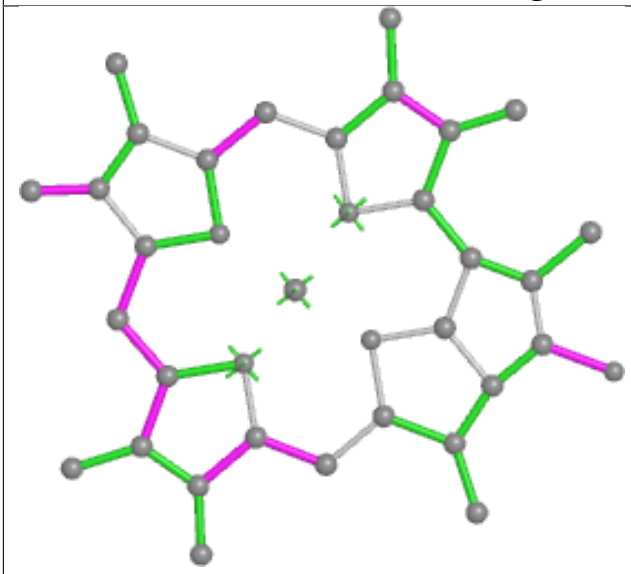


Torsions

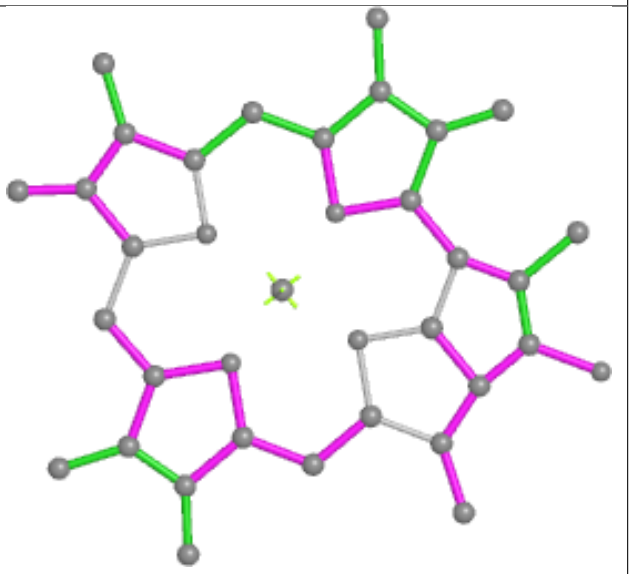


Rings

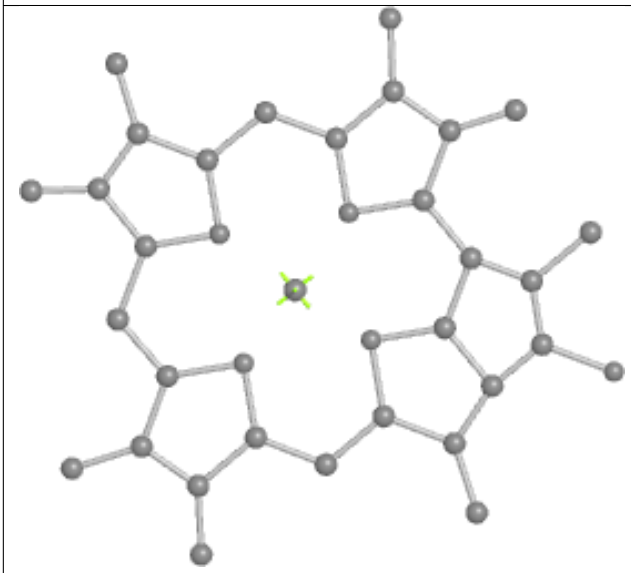
Ligand CLA 1 209



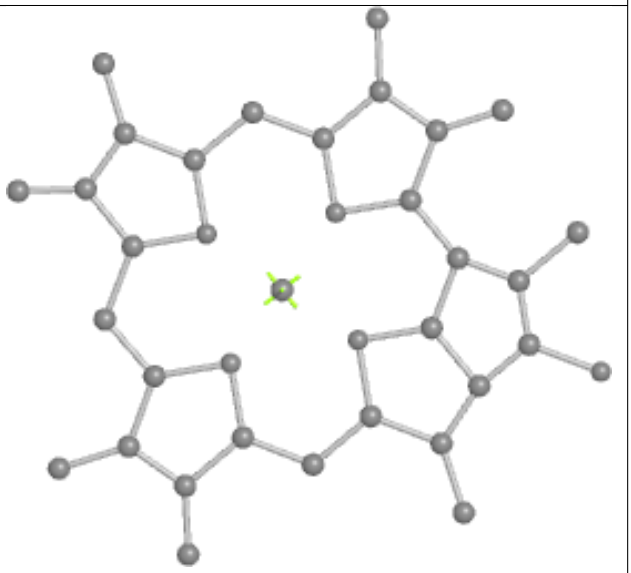
Bond lengths



Bond angles

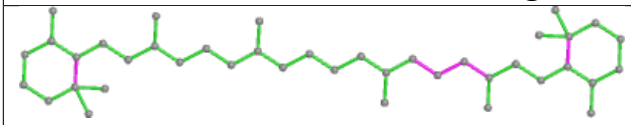


Torsions

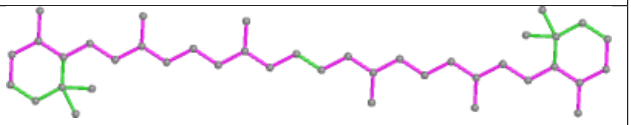


Rings

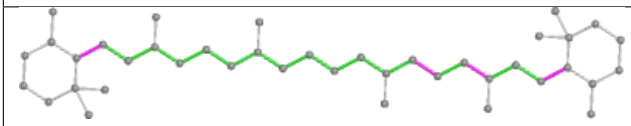
Ligand BCR B 843



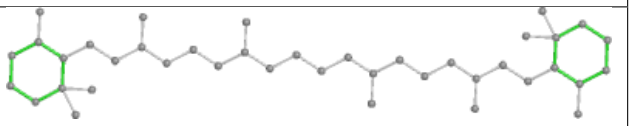
Bond lengths



Bond angles

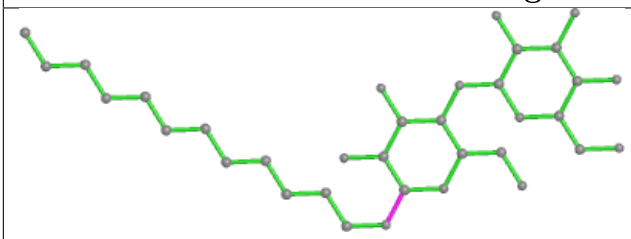


Torsions

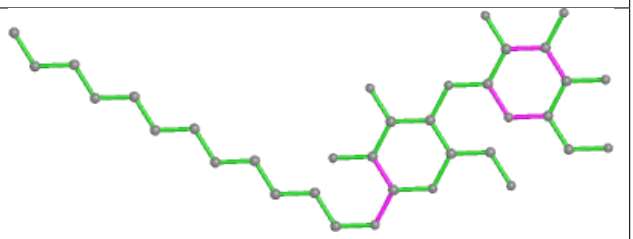


Rings

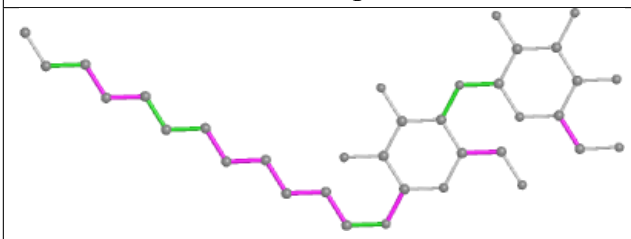
Ligand LMU 4 317



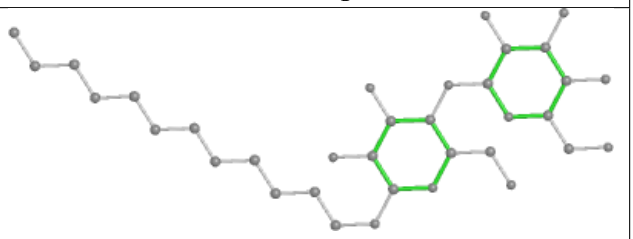
Bond lengths



Bond angles

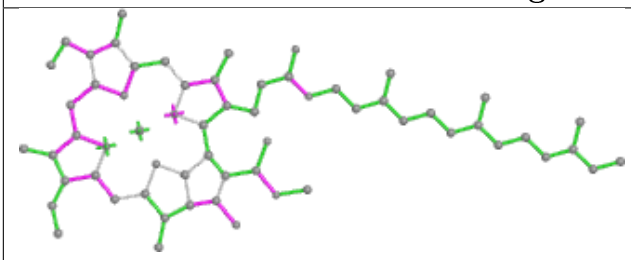


Torsions

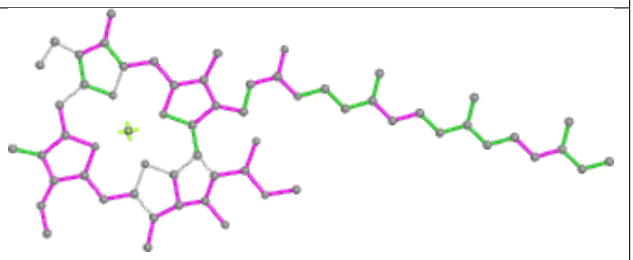


Rings

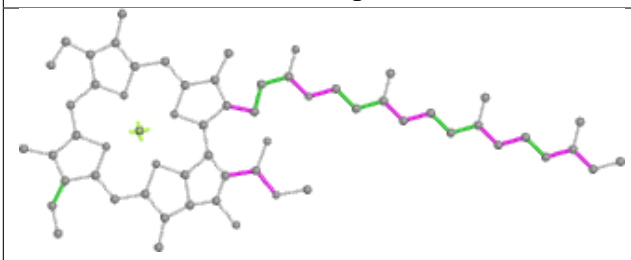
Ligand CLA 2 322



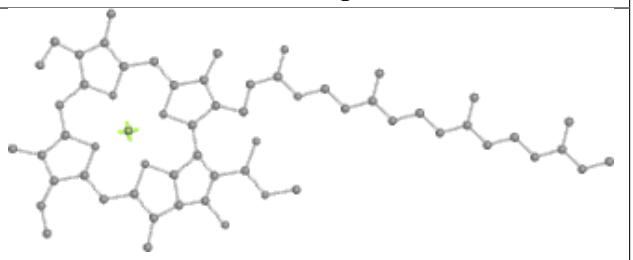
Bond lengths



Bond angles

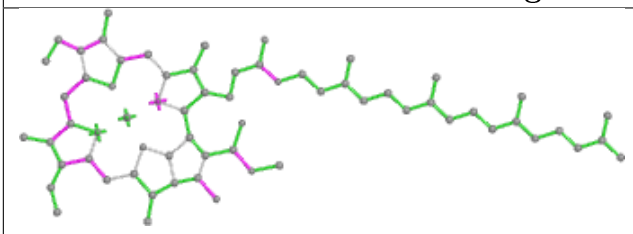


Torsions

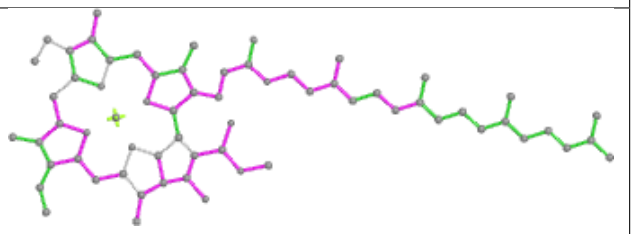


Rings

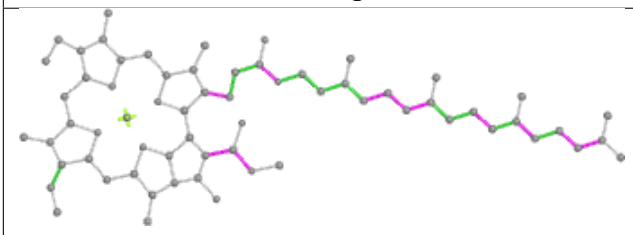
Ligand CLA A 818



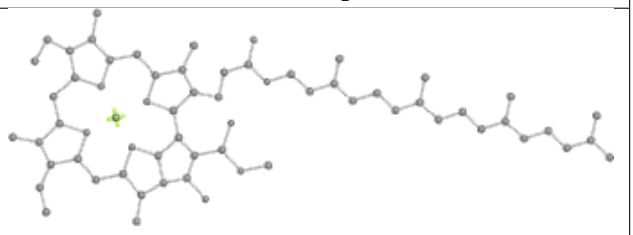
Bond lengths



Bond angles

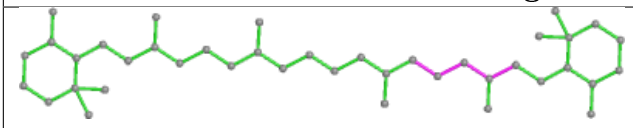


Torsions

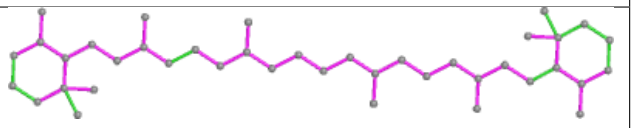


Rings

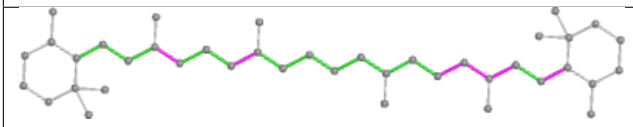
Ligand BCR B 844



Bond lengths



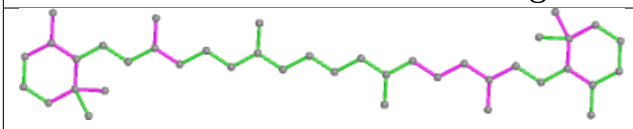
Bond angles



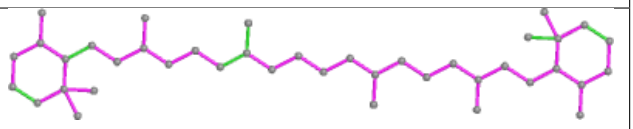
Torsions

Rings

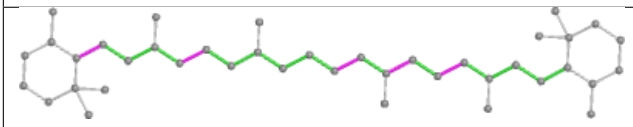
Ligand BCR I 101



Bond lengths



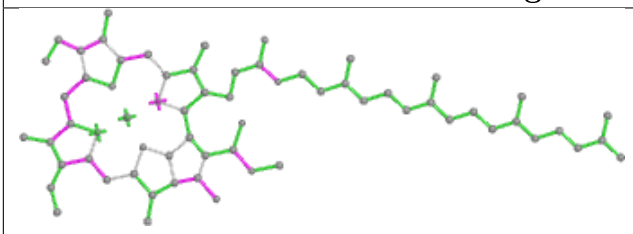
Bond angles



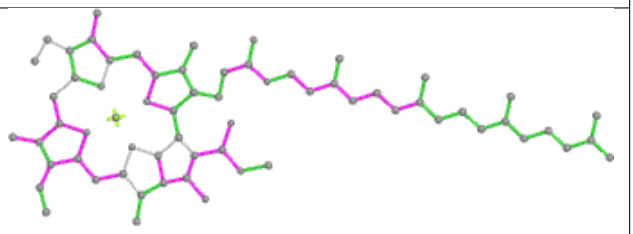
Torsions

Rings

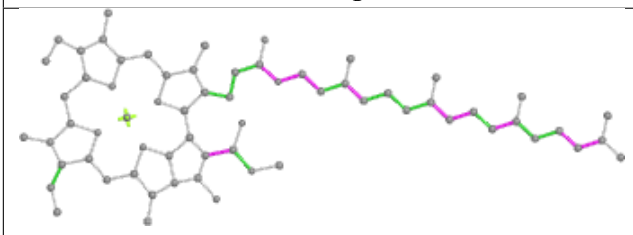
Ligand CLA A 841



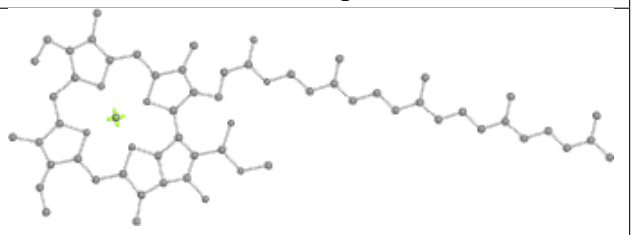
Bond lengths



Bond angles

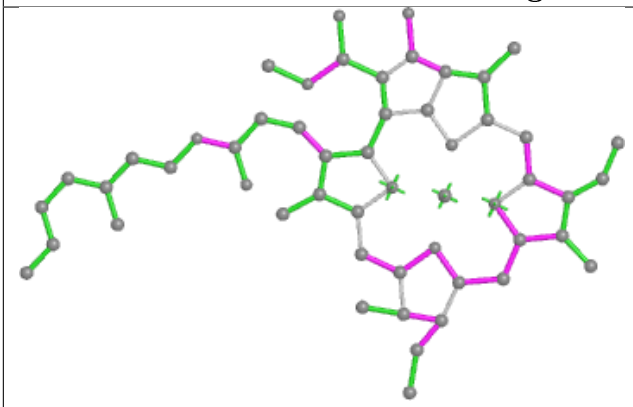


Torsions

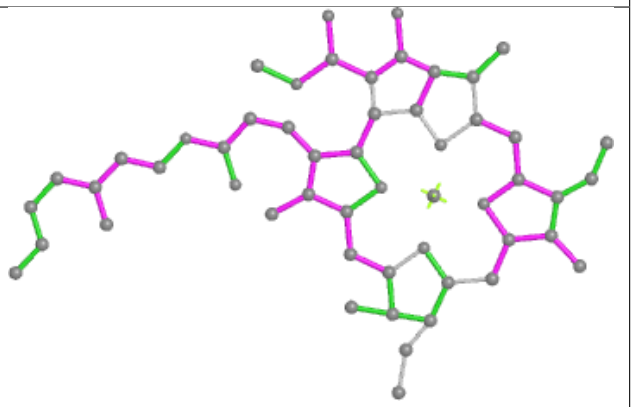


Rings

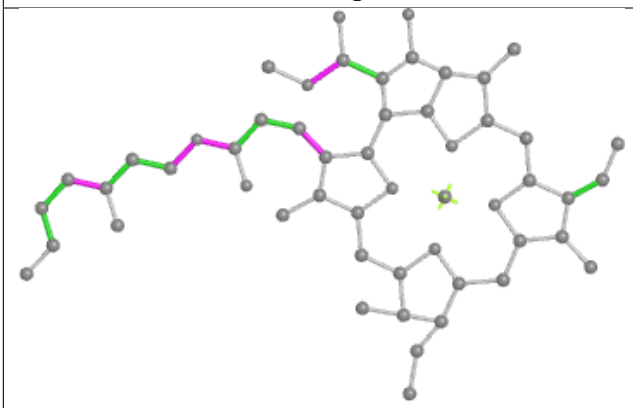
Ligand CLA F 206



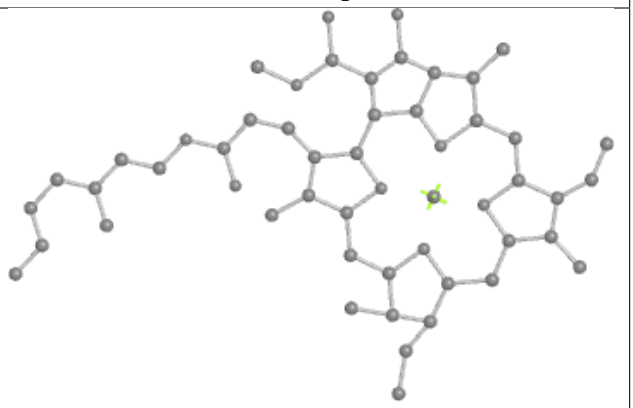
Bond lengths



Bond angles

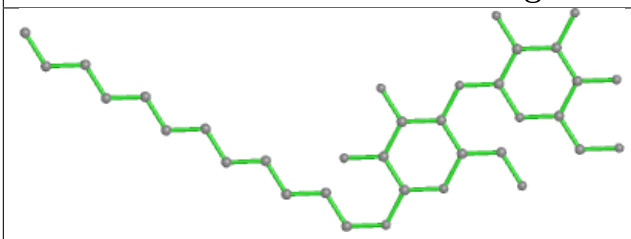


Torsions



Rings

Ligand LMU 1 217



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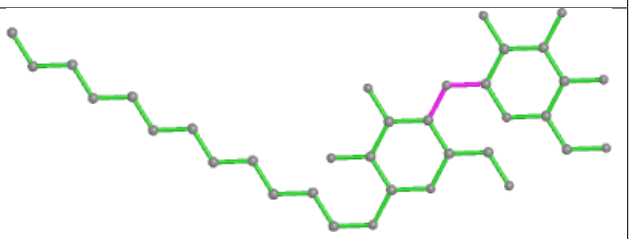
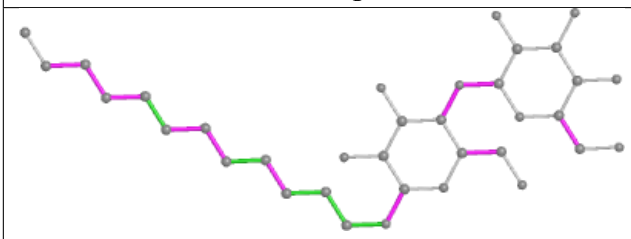
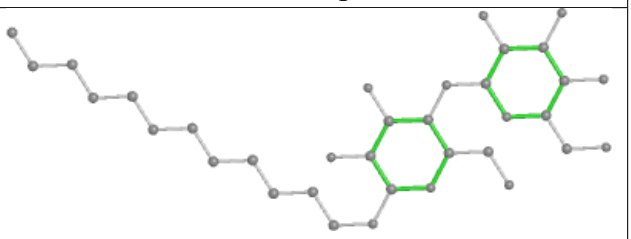


Bond angles

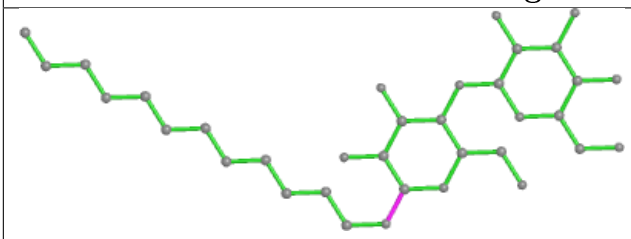


Torsions

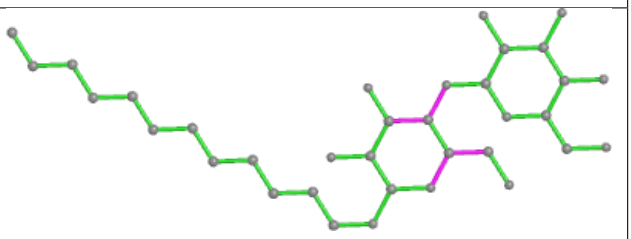


Rings

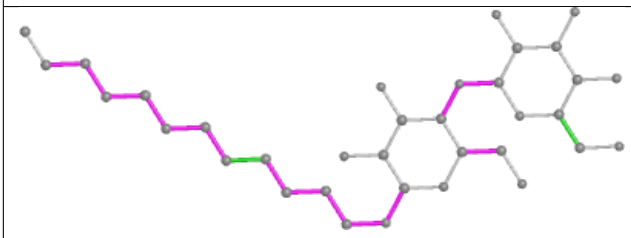
Ligand LMU 2 313



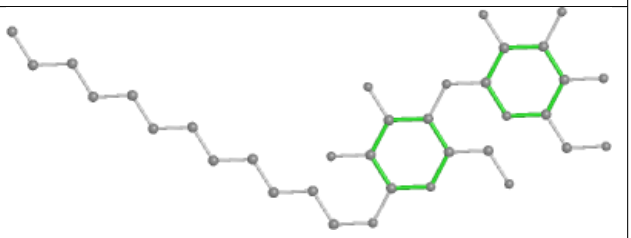
Bond lengths



Bond angles

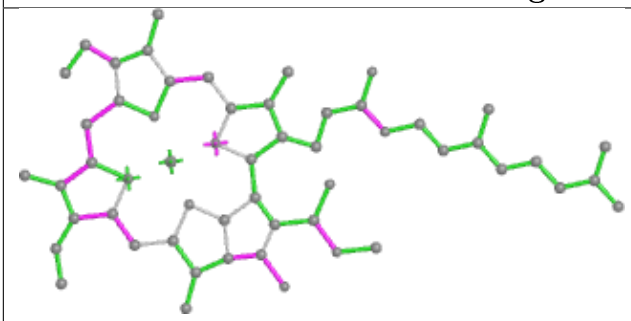


Torsions

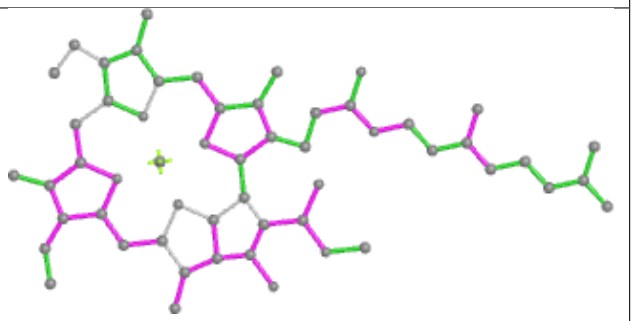


Rings

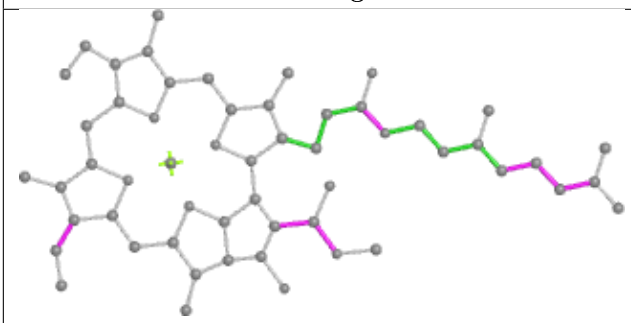
Ligand CLA 4 305



Bond lengths



Bond angles



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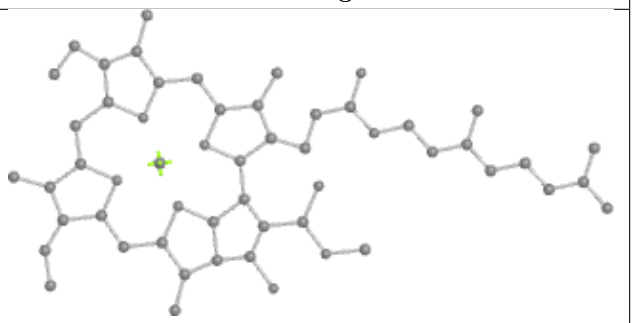
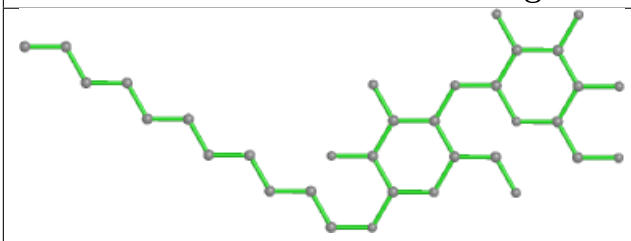


Rings

Ligand LMU 4 320



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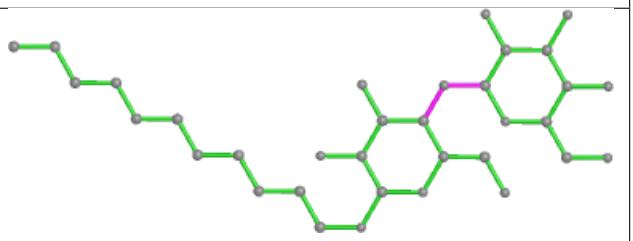
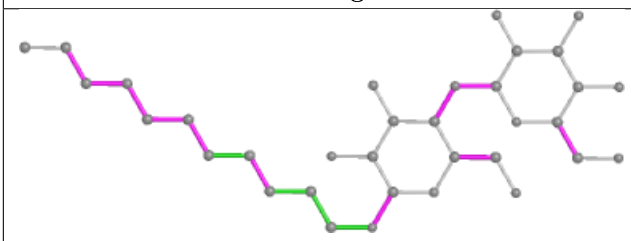
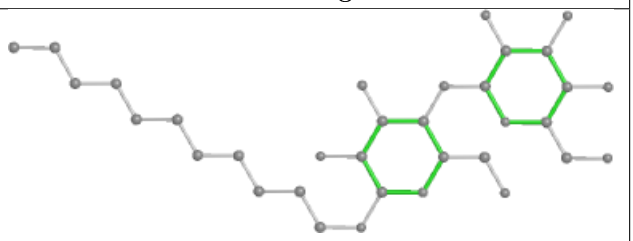


Bond angles

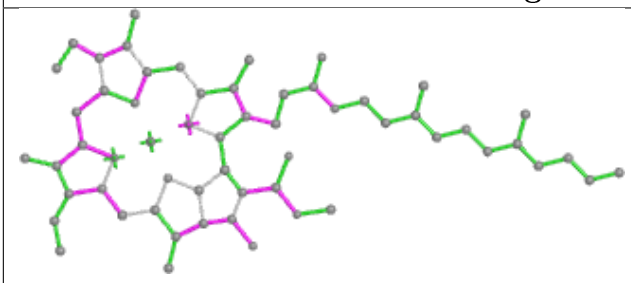


Torsions



Rings

Ligand CLA B 811



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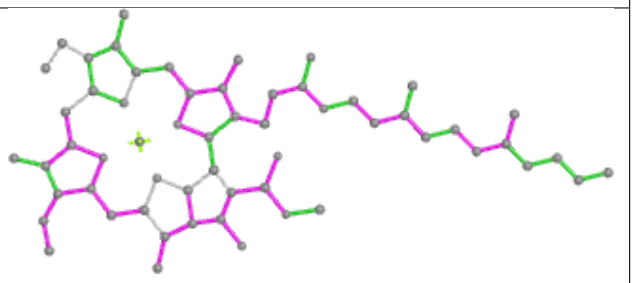
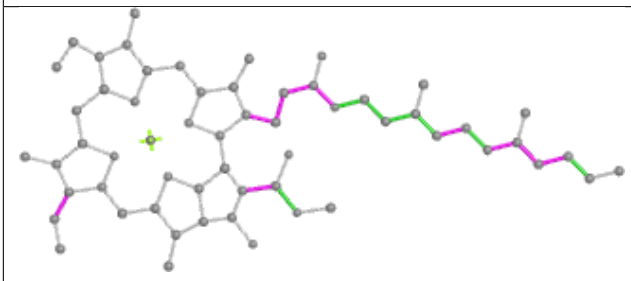
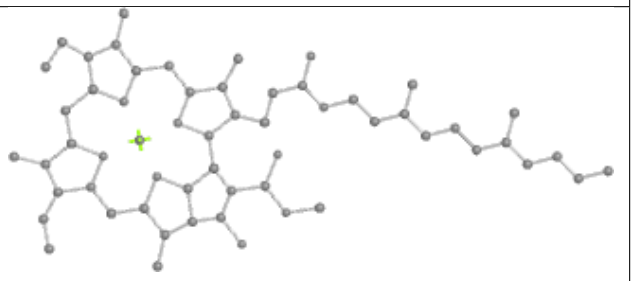


Bond angles

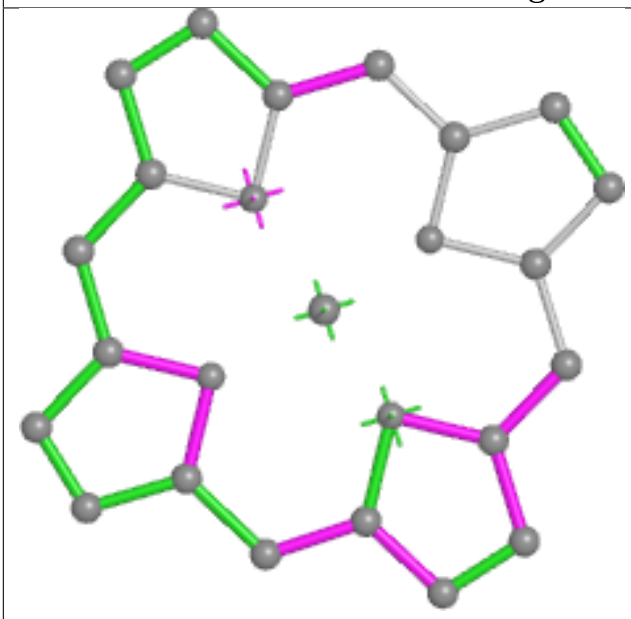


Torsions

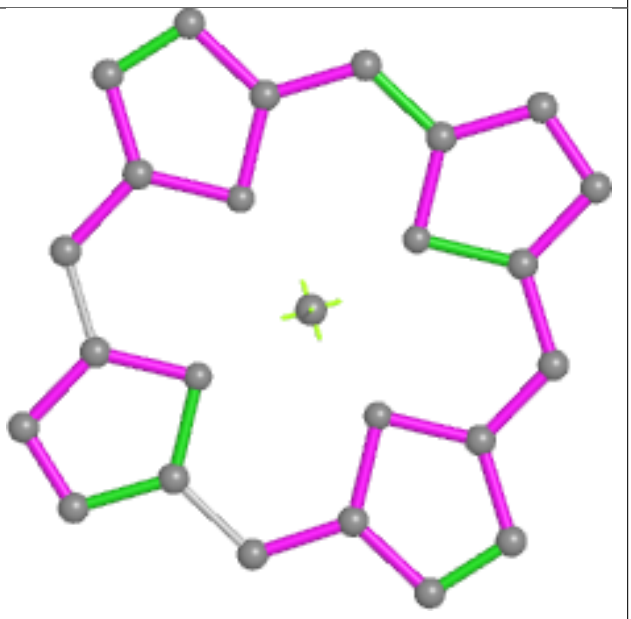


Rings

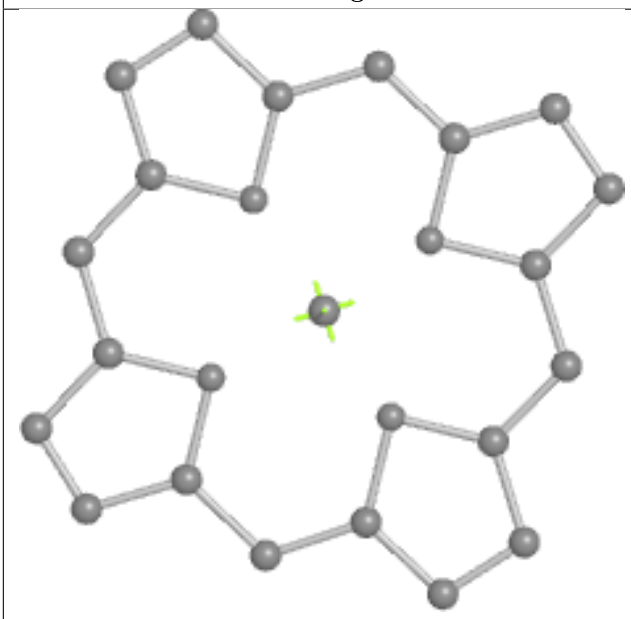
Ligand CLA 3 310



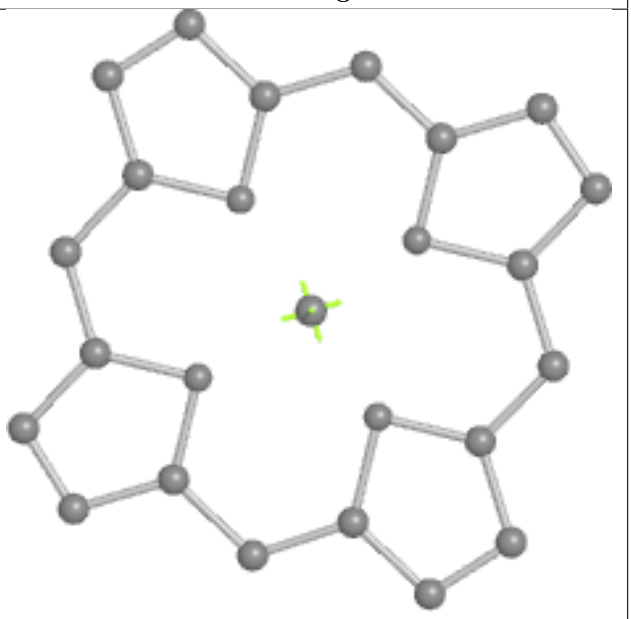
Bond lengths



Bond angles

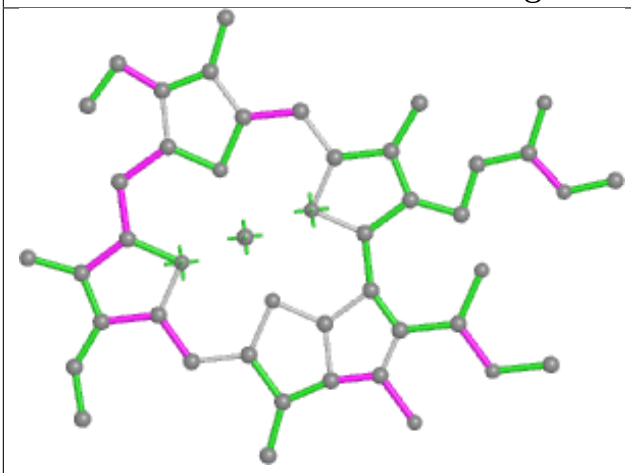


Torsions

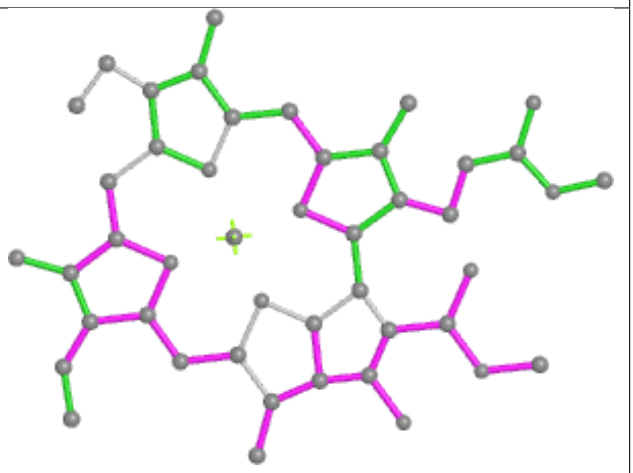


Rings

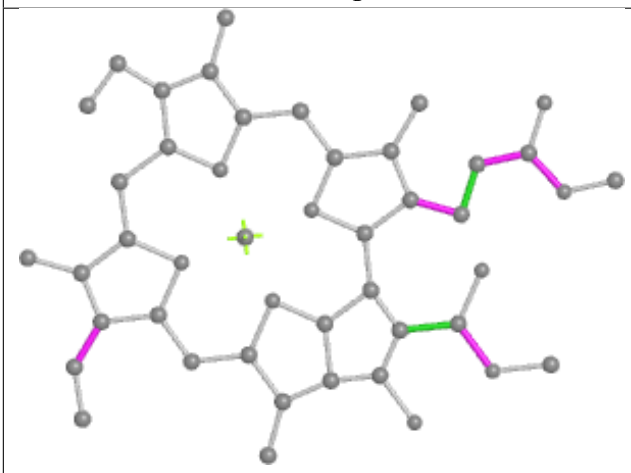
Ligand CLA B 814



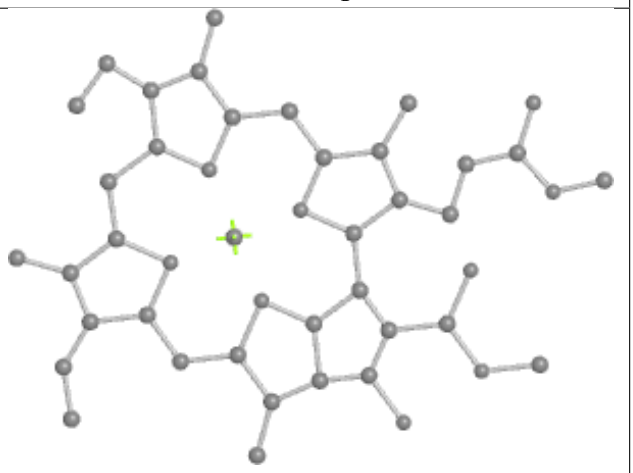
Bond lengths



Bond angles

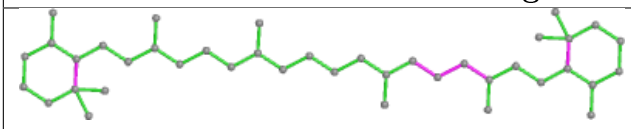


Torsions

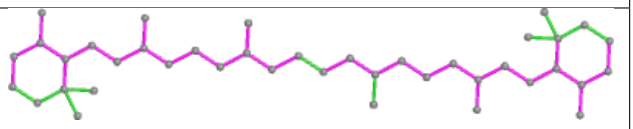


Rings

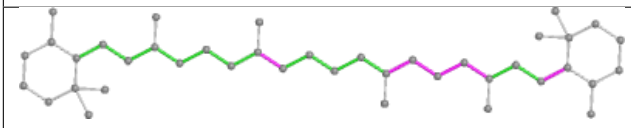
Ligand BCR A 847



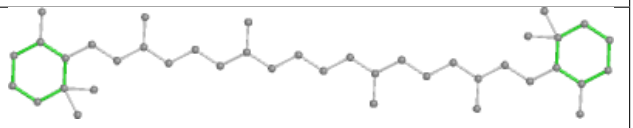
Bond lengths



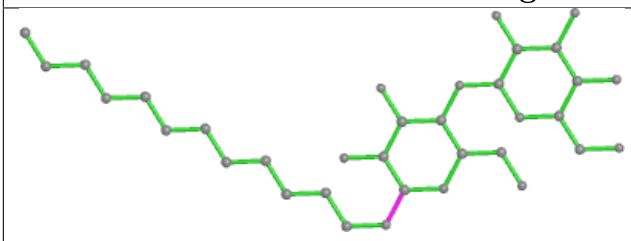
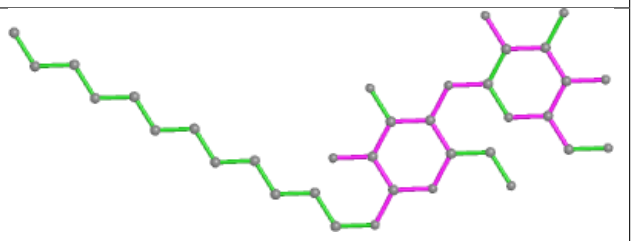
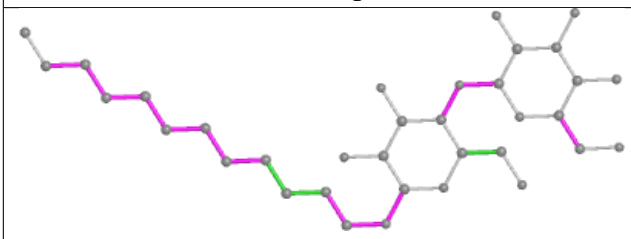
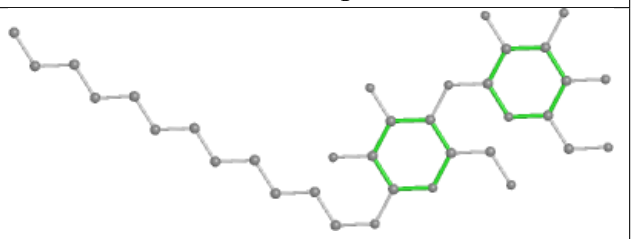
Bond angles



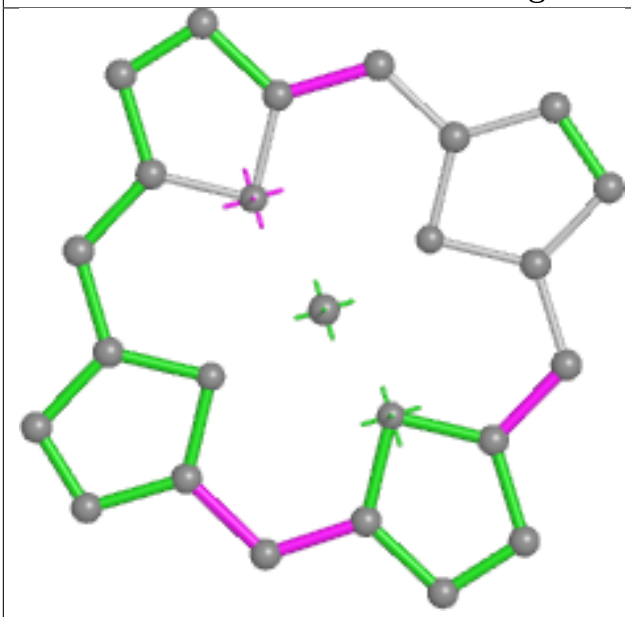
Torsions



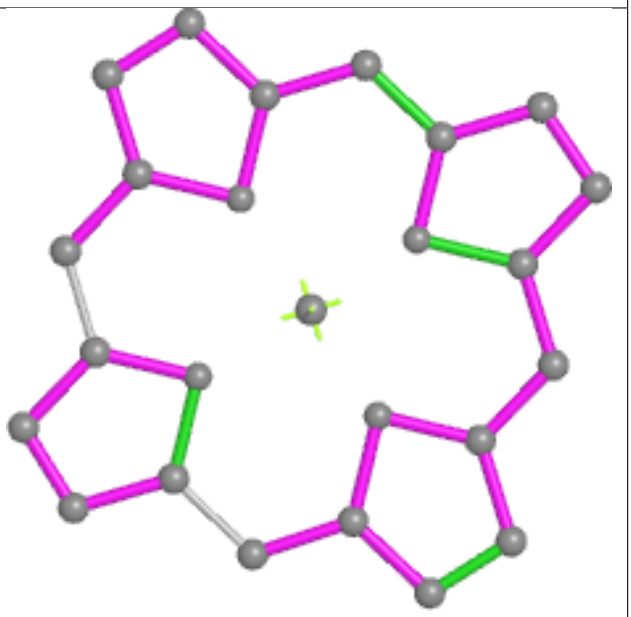
Rings

Ligand LMU N 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

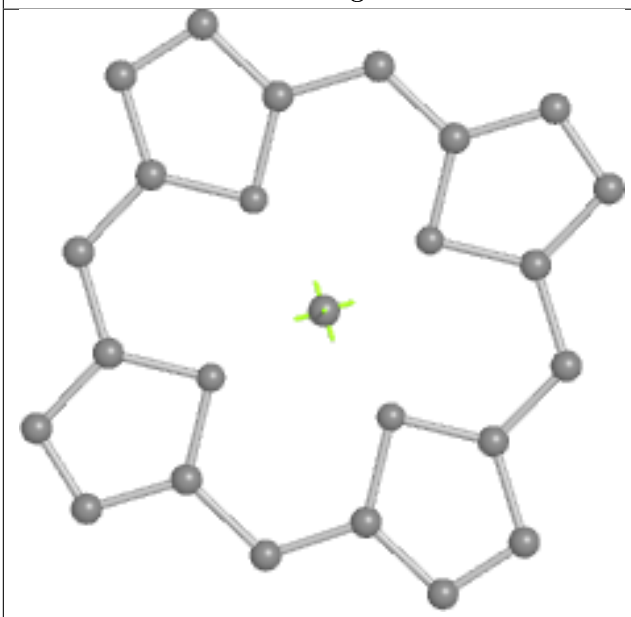
Ligand CLA 2 310



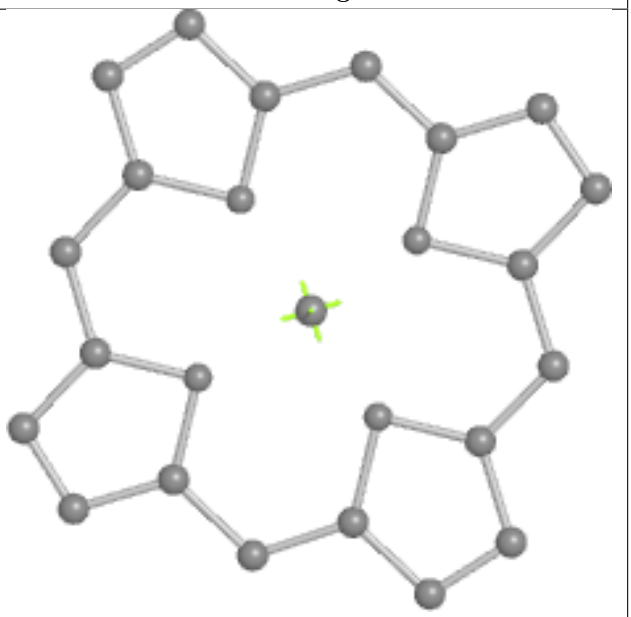
Bond lengths



Bond angles

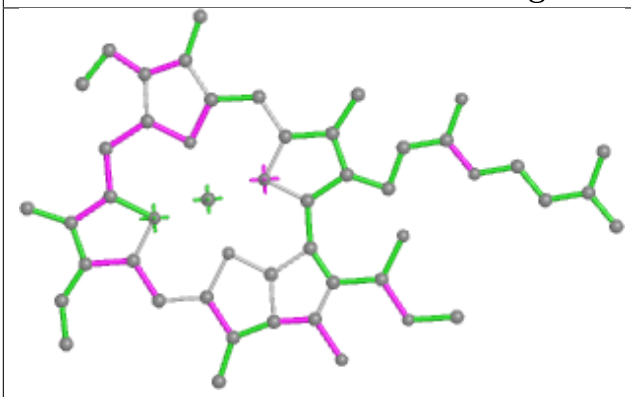


Torsions

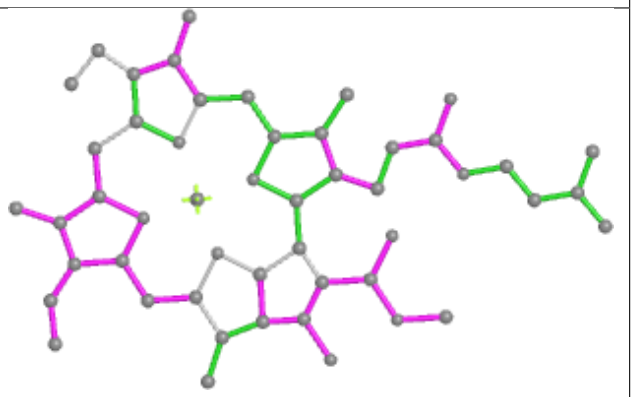


Rings

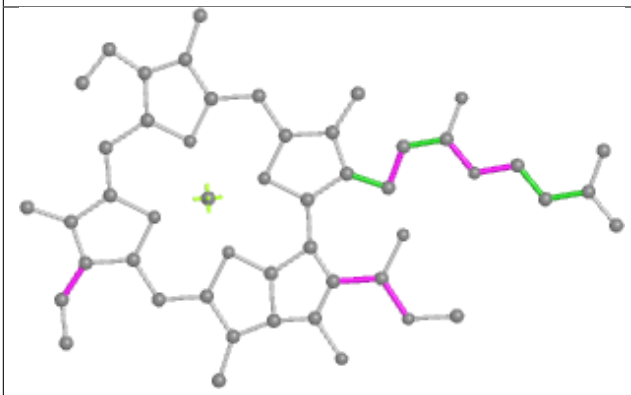
Ligand CLA 4 306



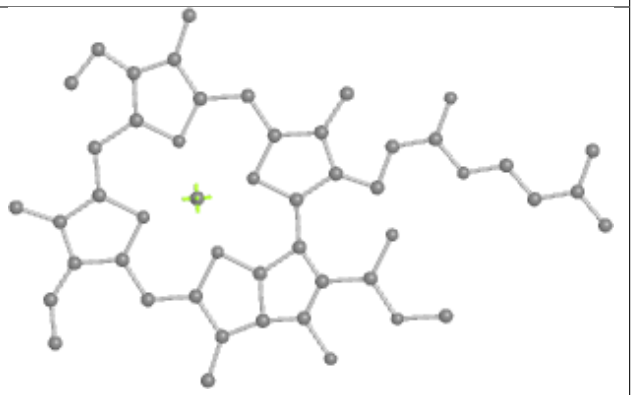
Bond lengths



Bond angles

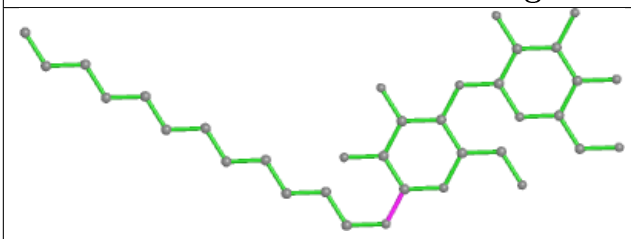


Torsions

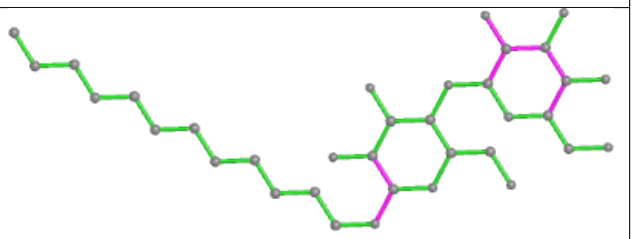


Rings

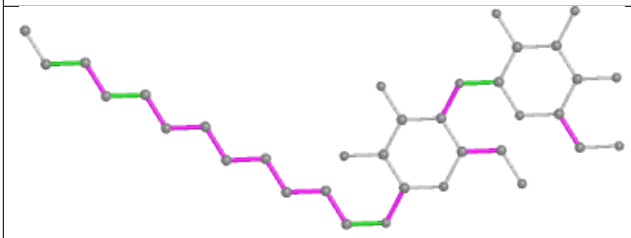
Ligand LMU 4 322



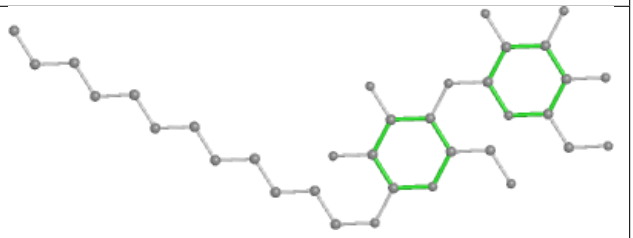
Bond lengths



Bond angles

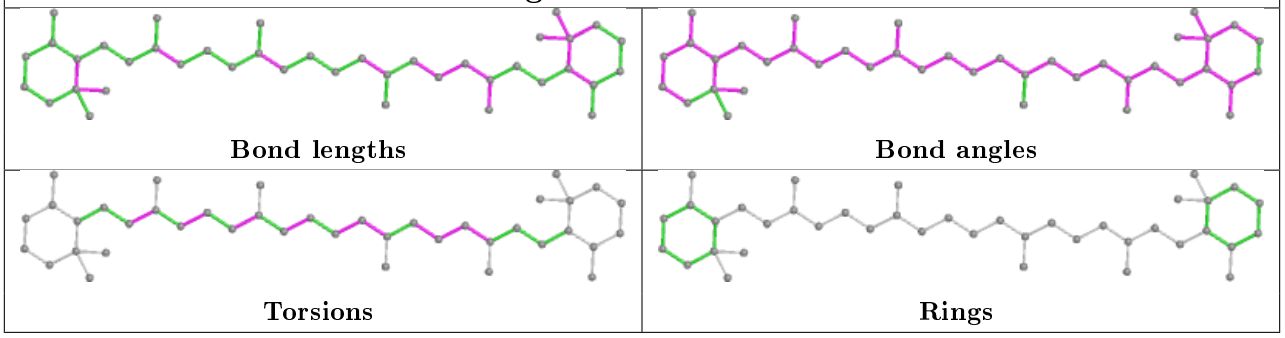


Torsions

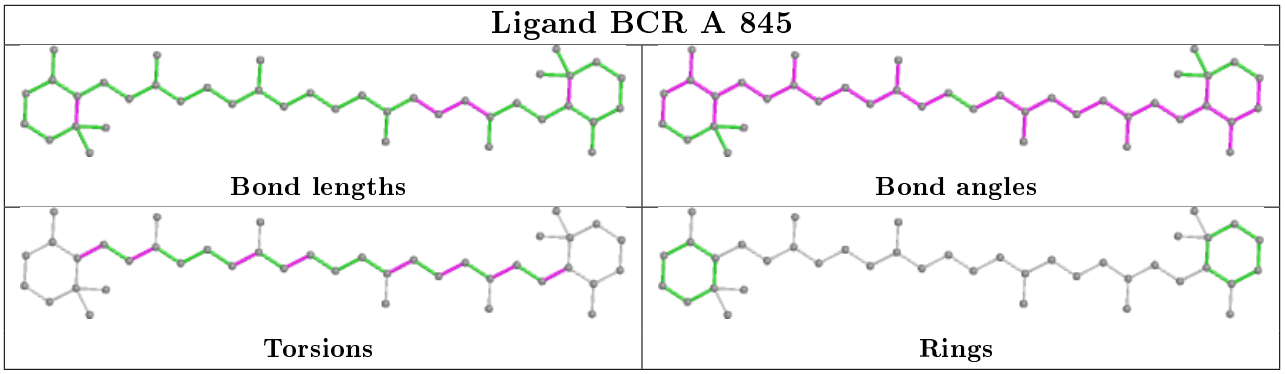


Rings

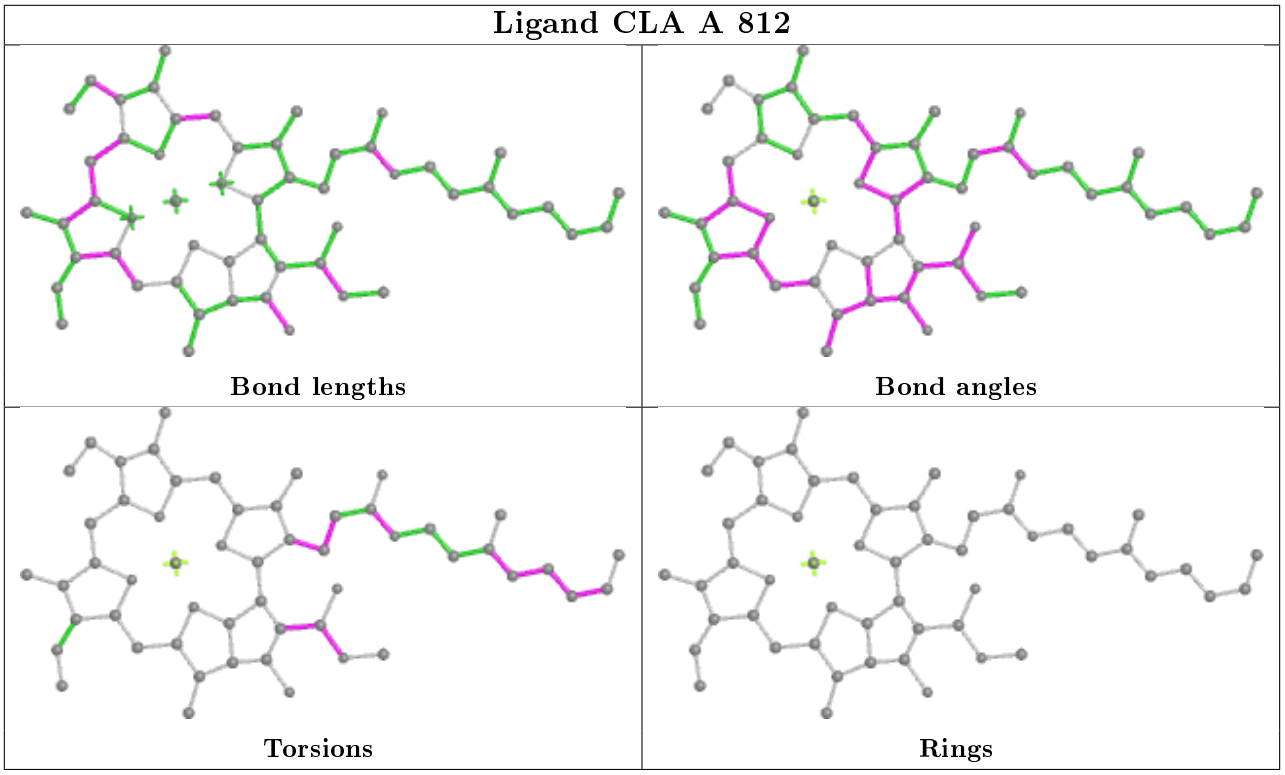
Ligand BCR F 203



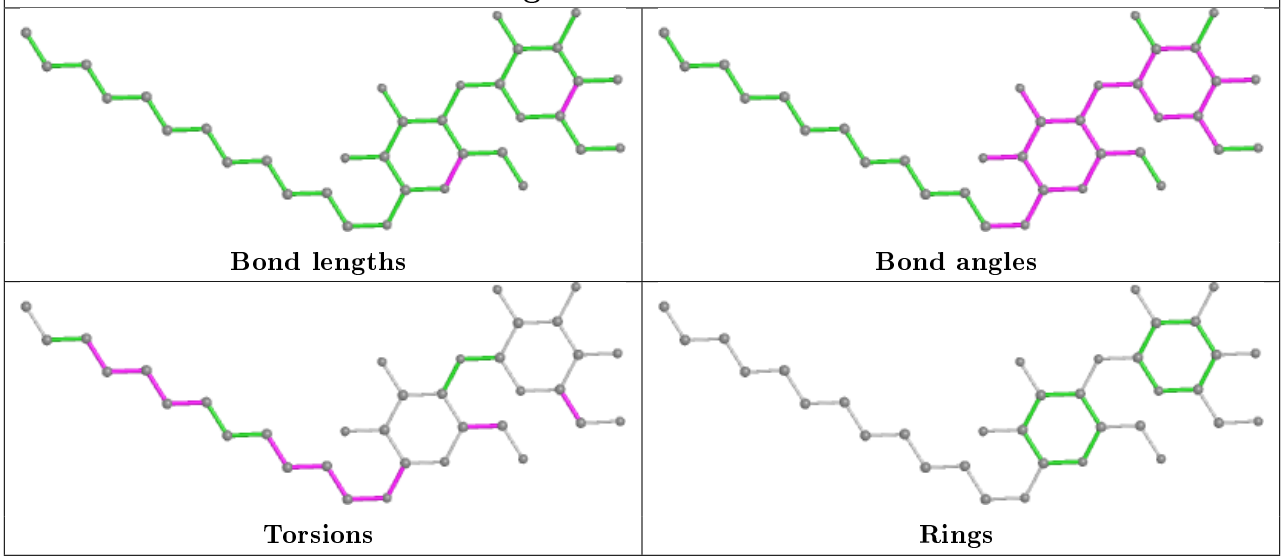
Ligand BCR A 845



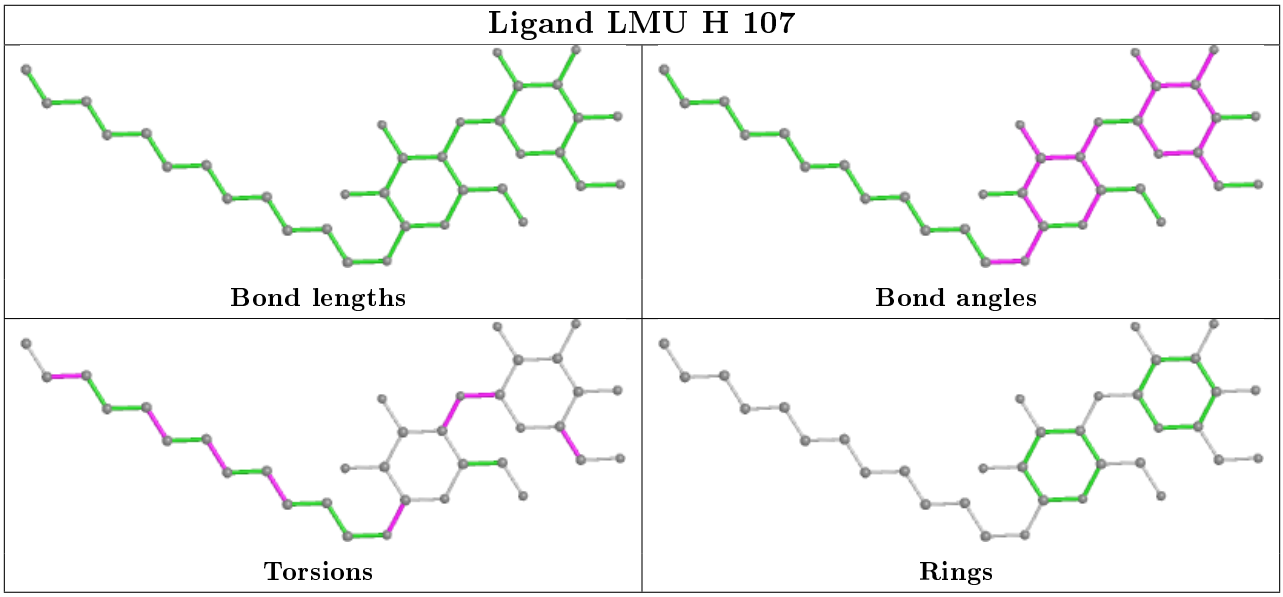
Ligand CLA A 812



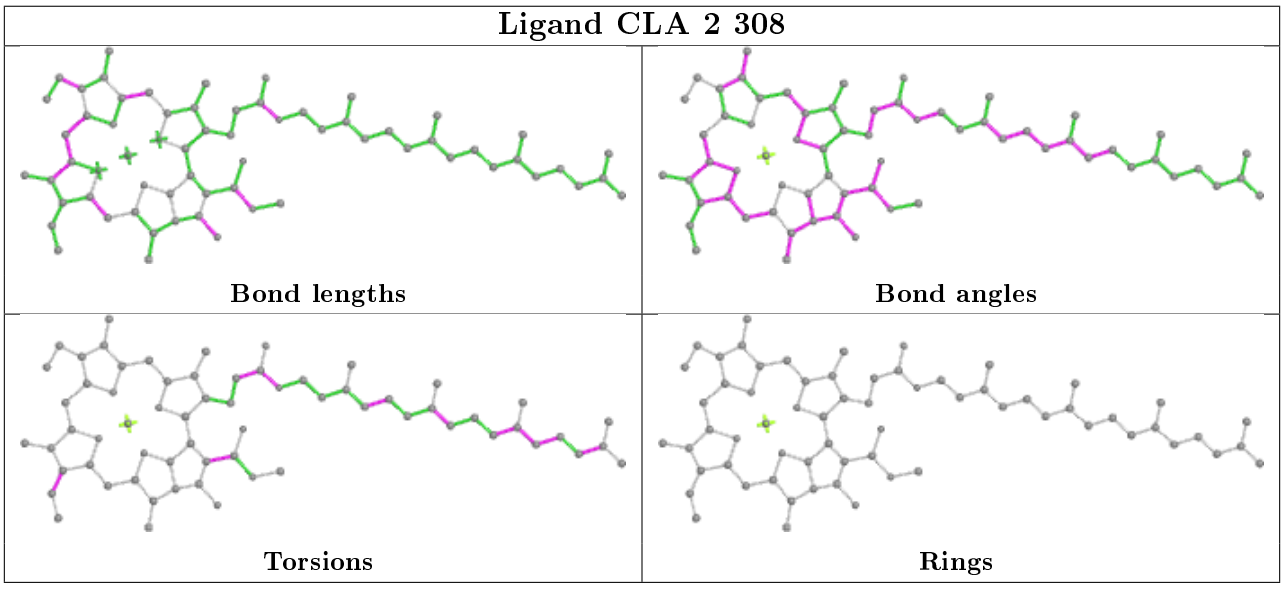
Ligand LMU L 205



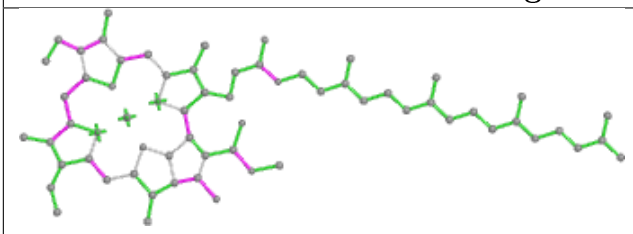
Ligand LMU H 107



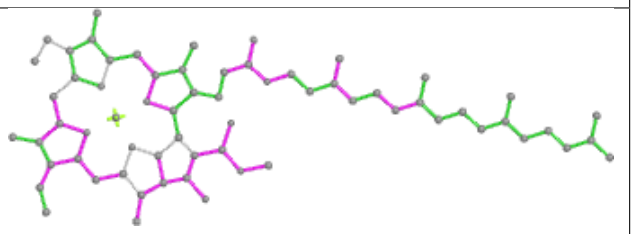
Ligand CLA 2 308



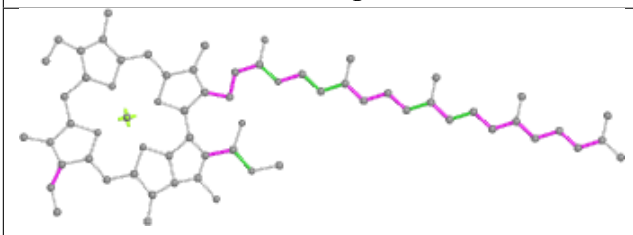
Ligand CLA A 805



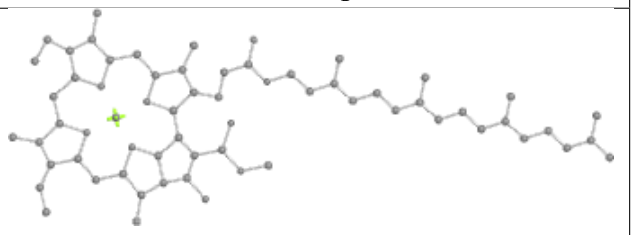
Bond lengths



Bond angles

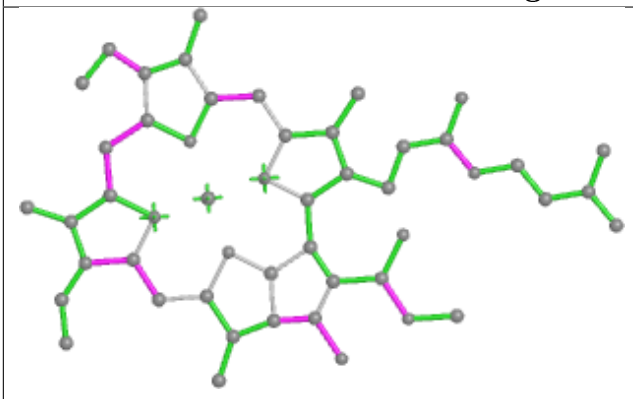


Torsions

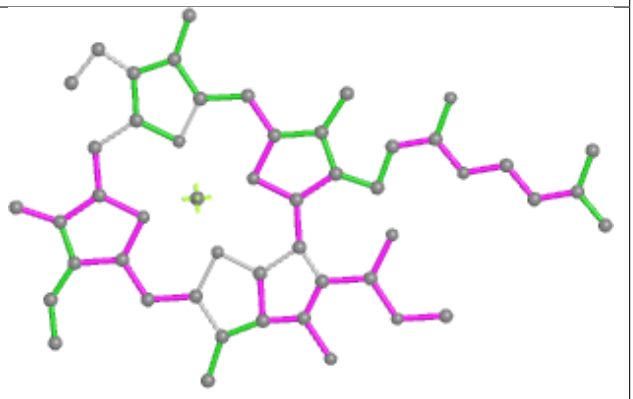


Rings

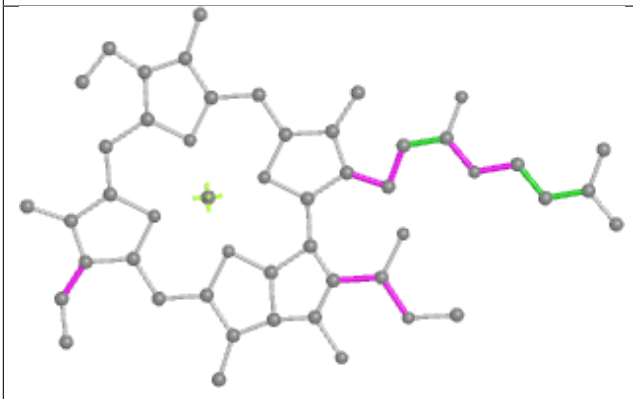
Ligand CLA B 829



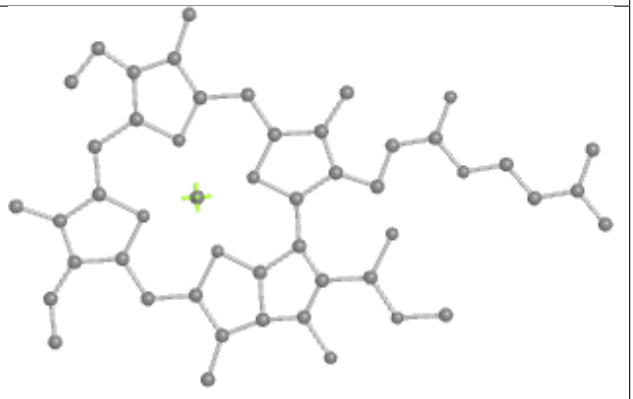
Bond lengths



Bond angles

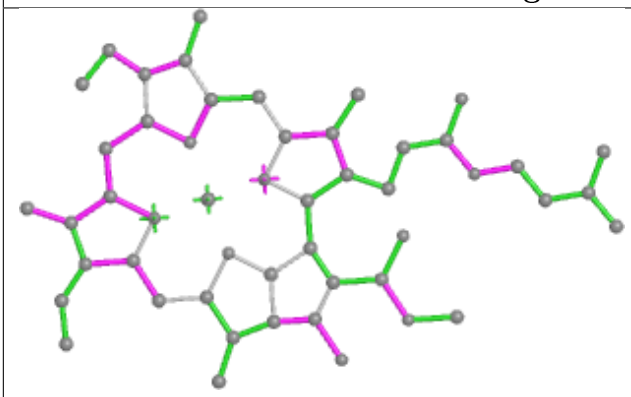


Torsions

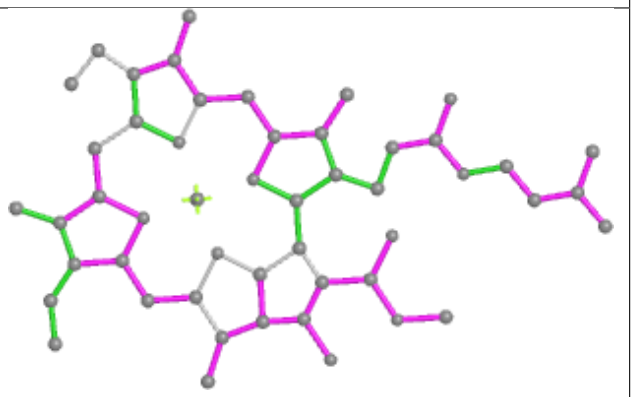


Rings

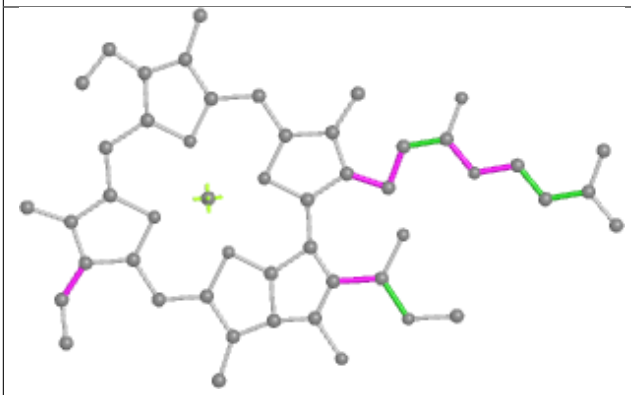
Ligand CLA K 102



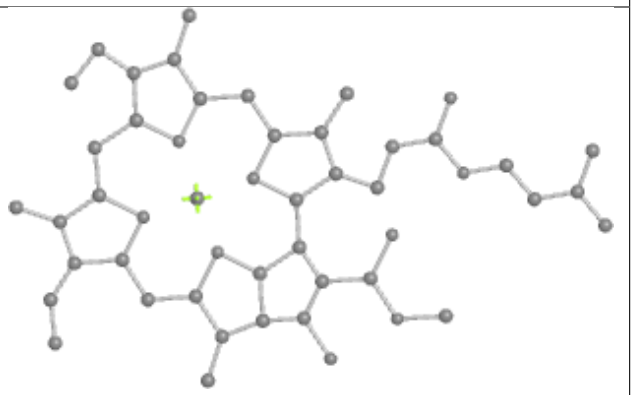
Bond lengths



Bond angles

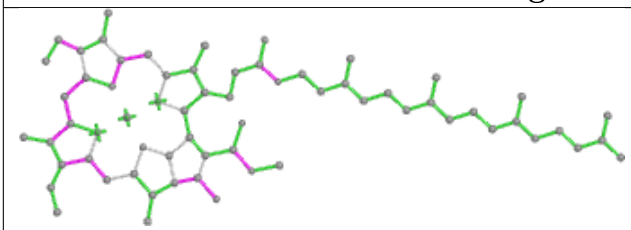


Torsions

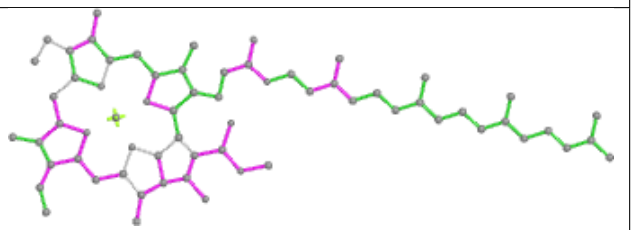


Rings

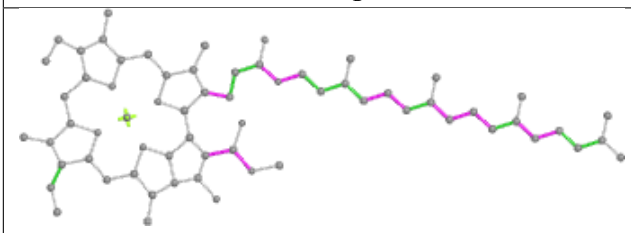
Ligand CLA 2 316



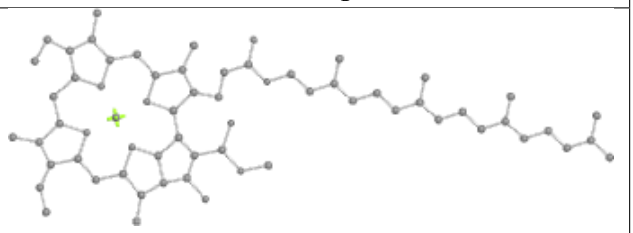
Bond lengths



Bond angles

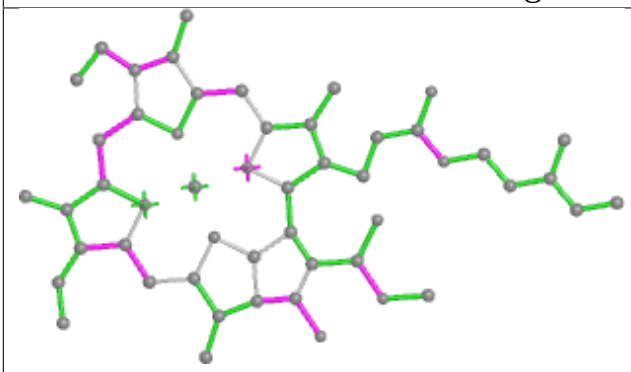


Torsions

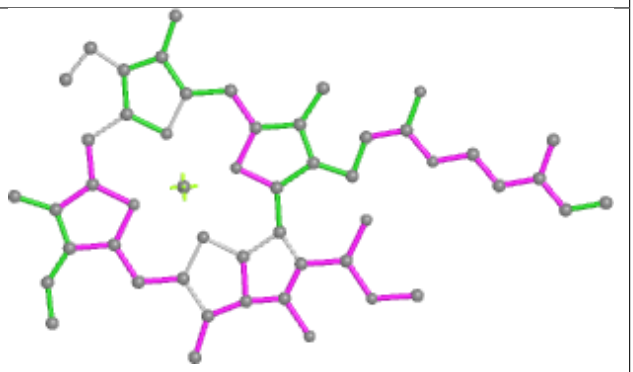


Rings

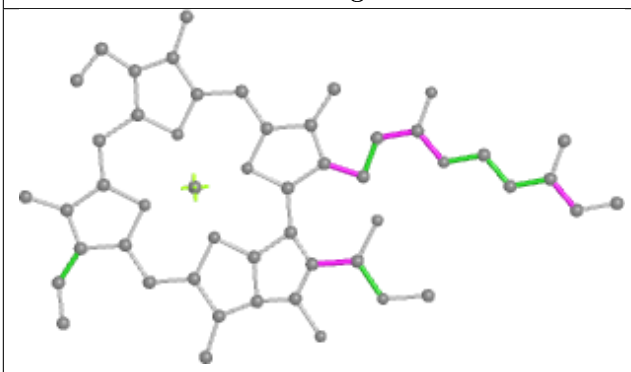
Ligand CLA B 834



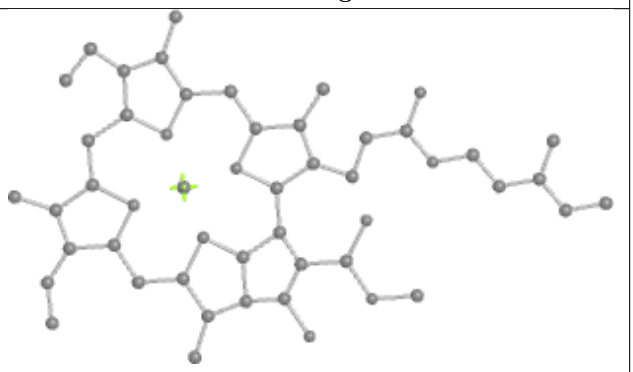
Bond lengths



Bond angles

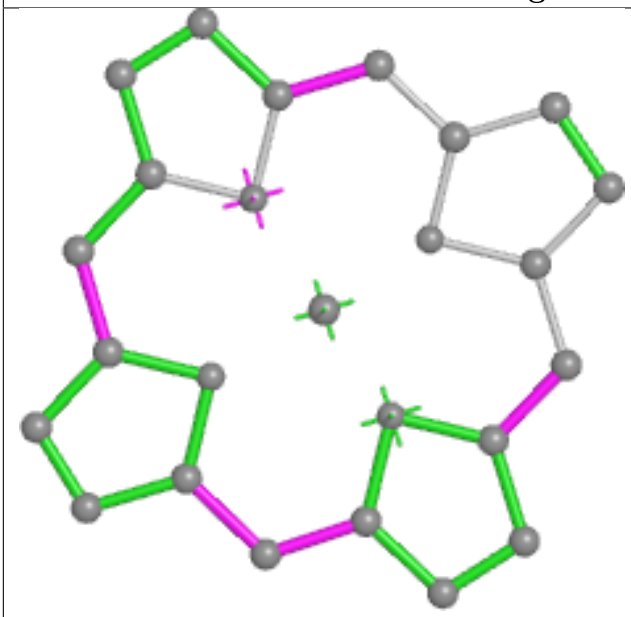


Torsions

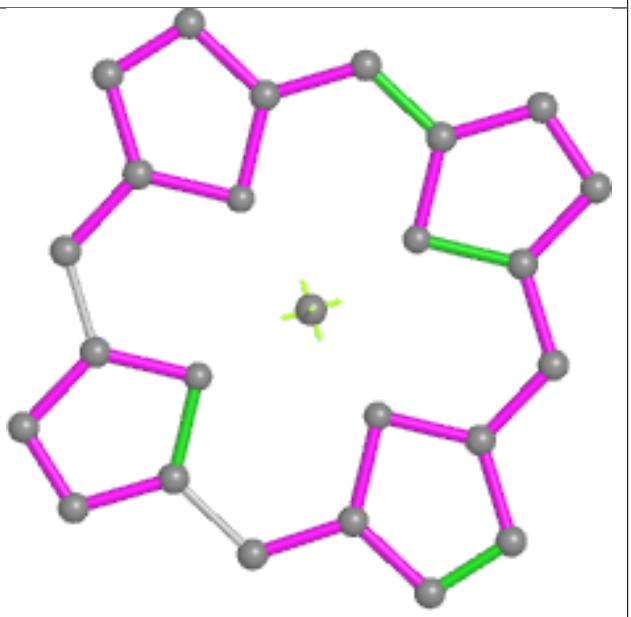


Rings

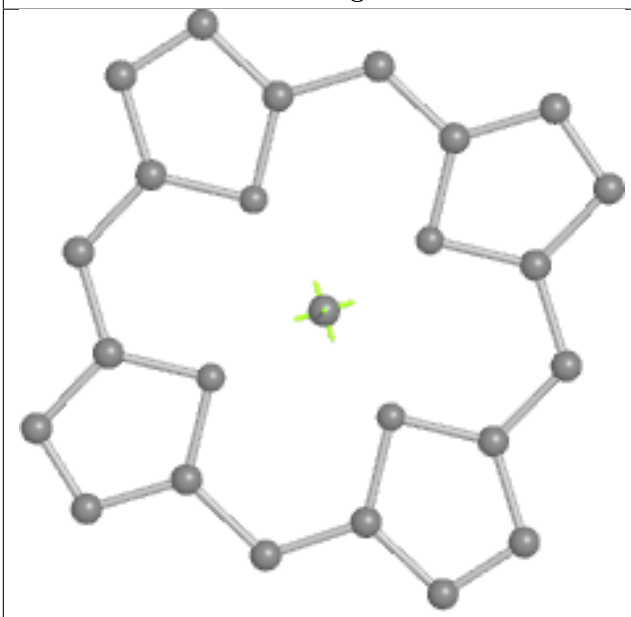
Ligand CLA 1 211



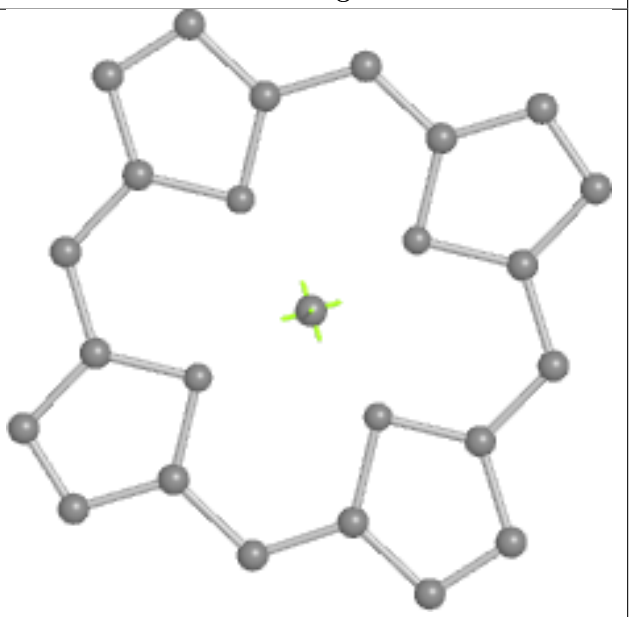
Bond lengths



Bond angles

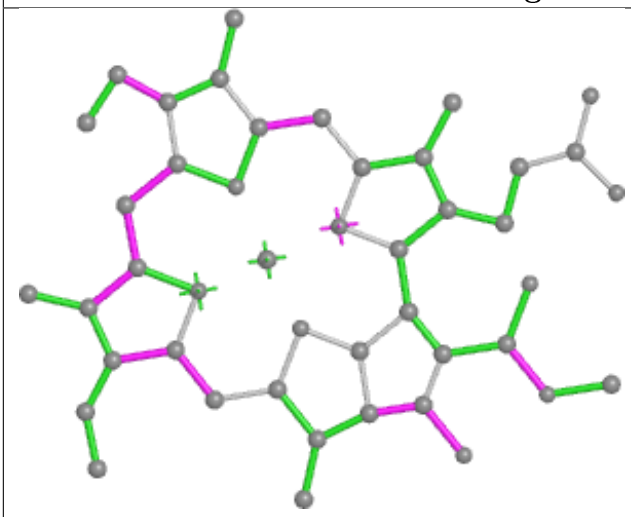


Torsions

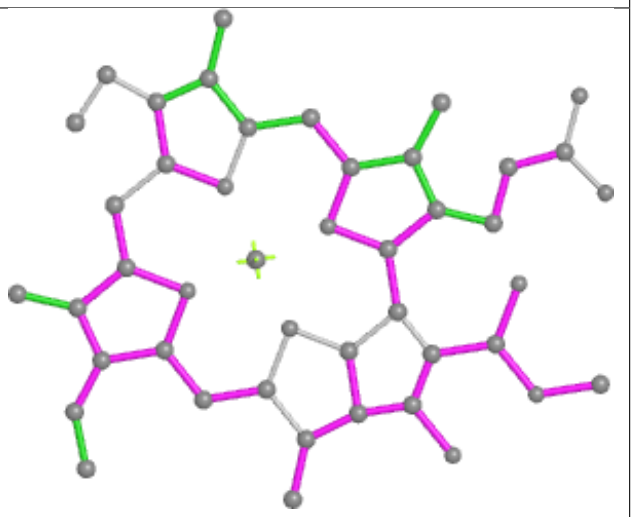


Rings

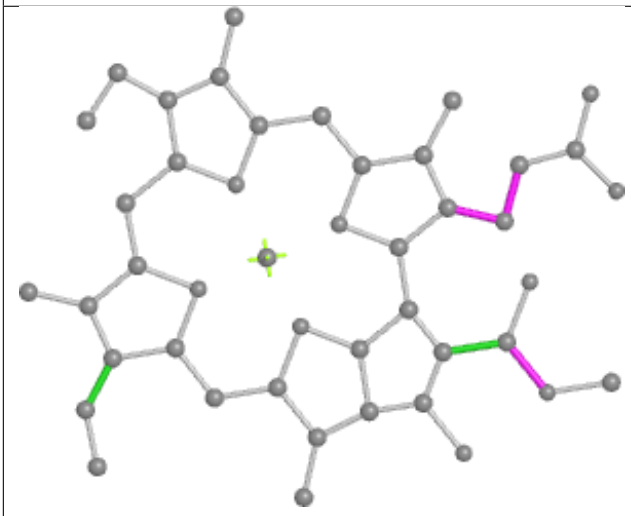
Ligand CLA A 833



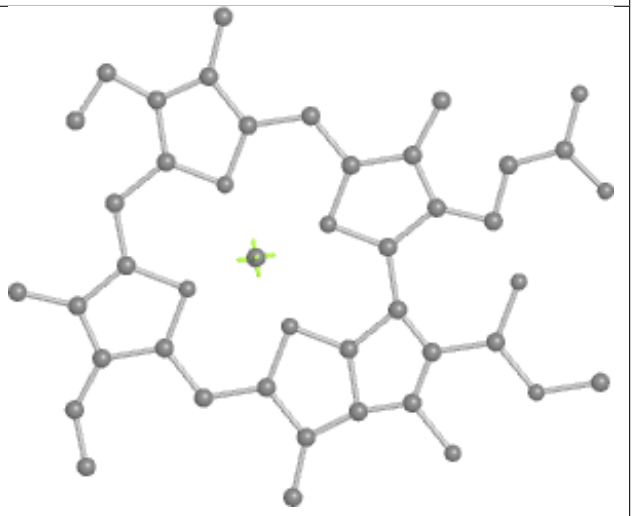
Bond lengths



Bond angles

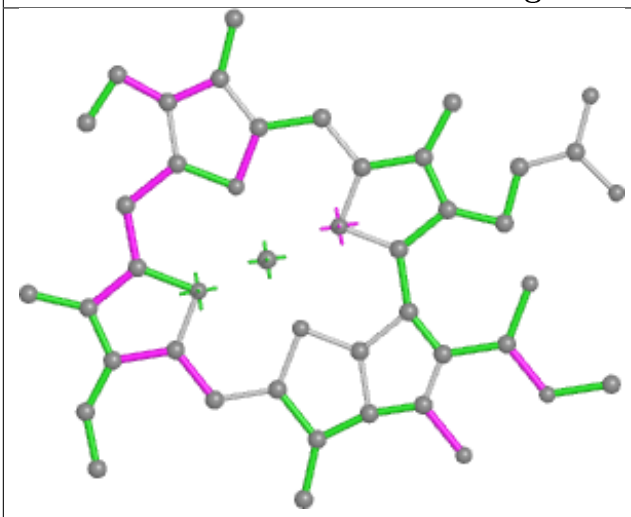


Torsions

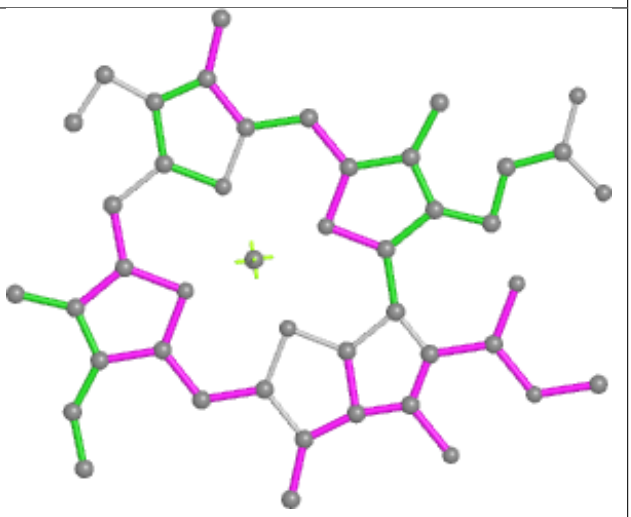


Rings

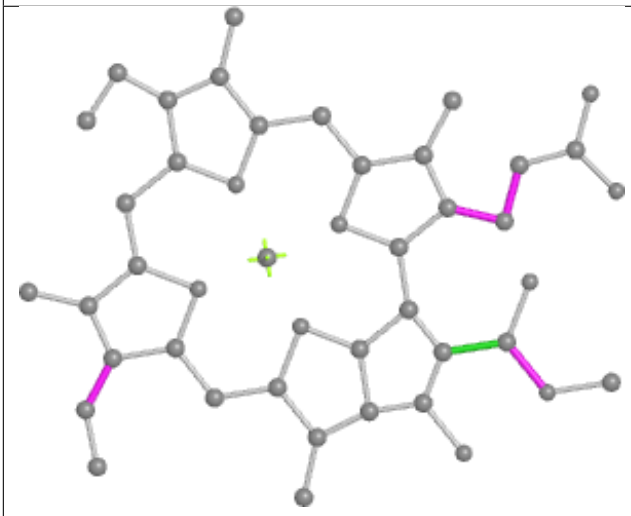
Ligand CLA A 814



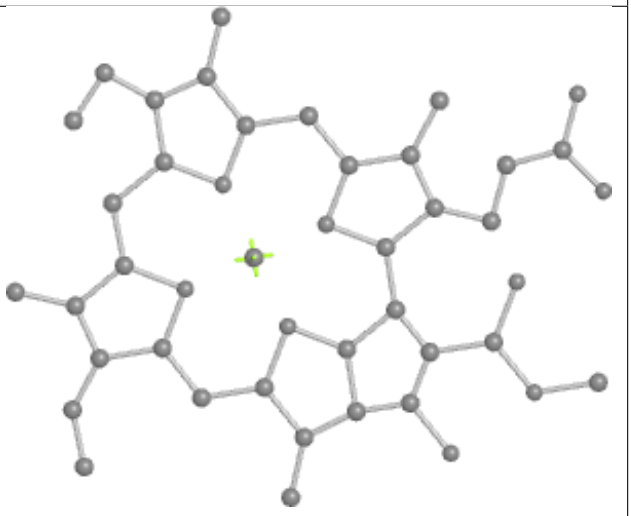
Bond lengths



Bond angles

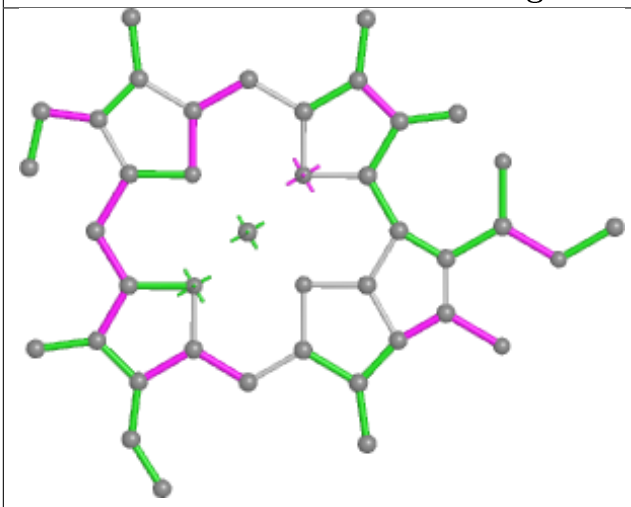


Torsions

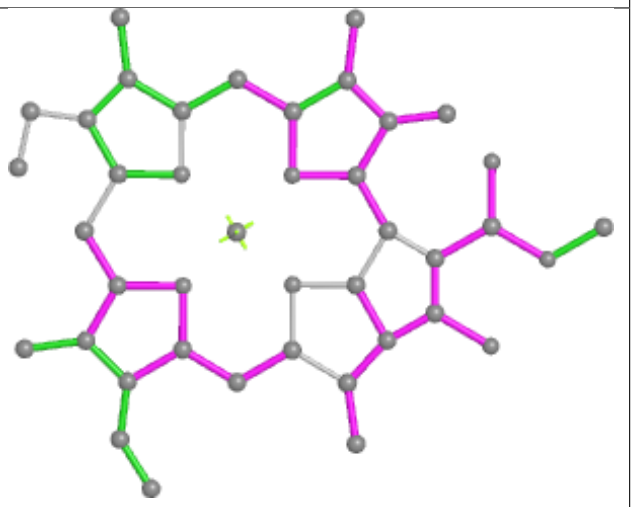


Rings

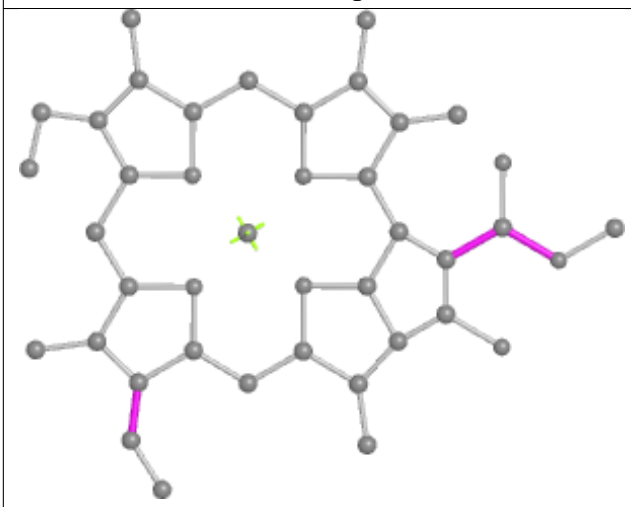
Ligand CLA F 205



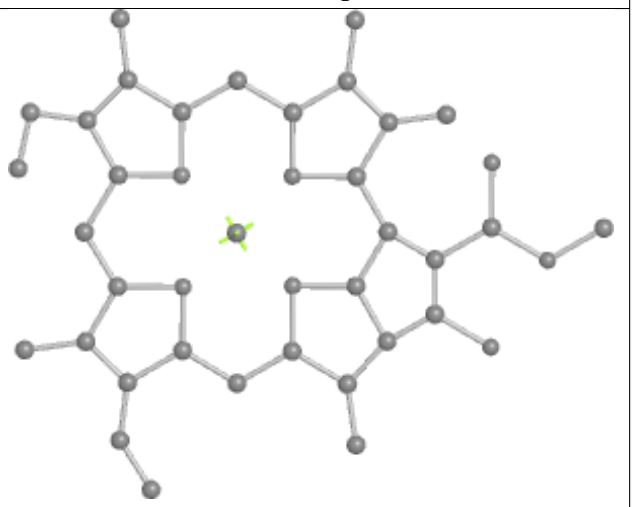
Bond lengths



Bond angles

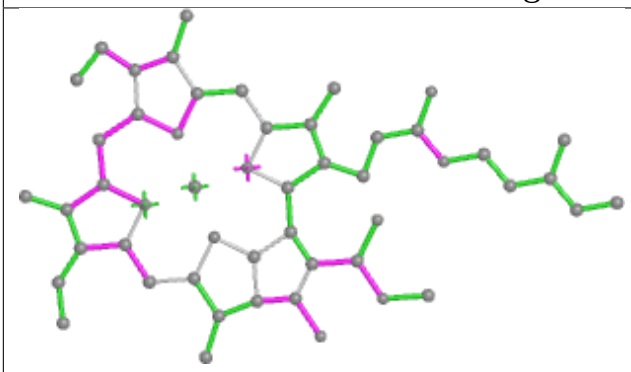


Torsions

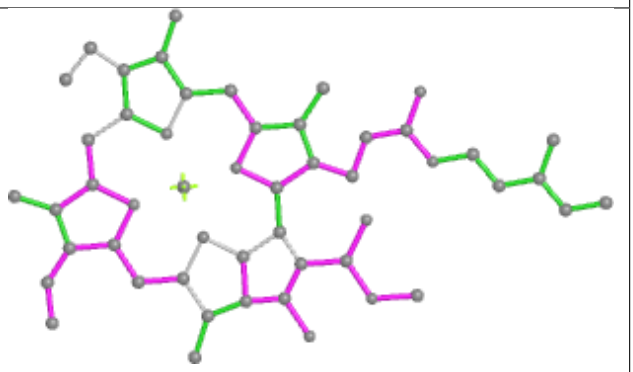


Rings

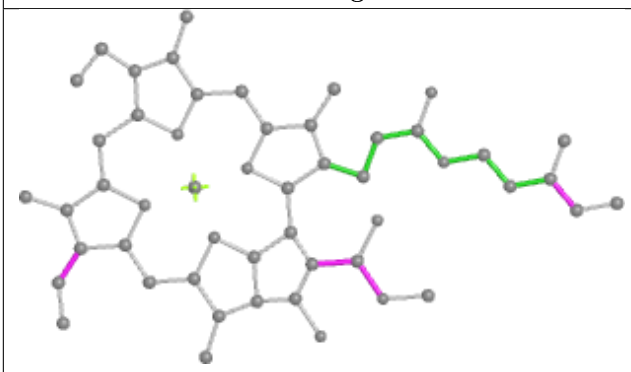
Ligand CLA G 102



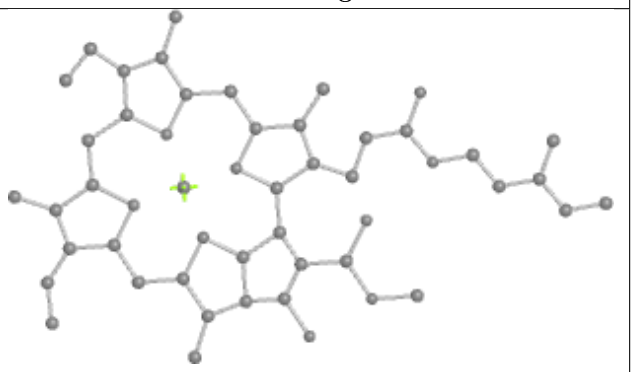
Bond lengths



Bond angles

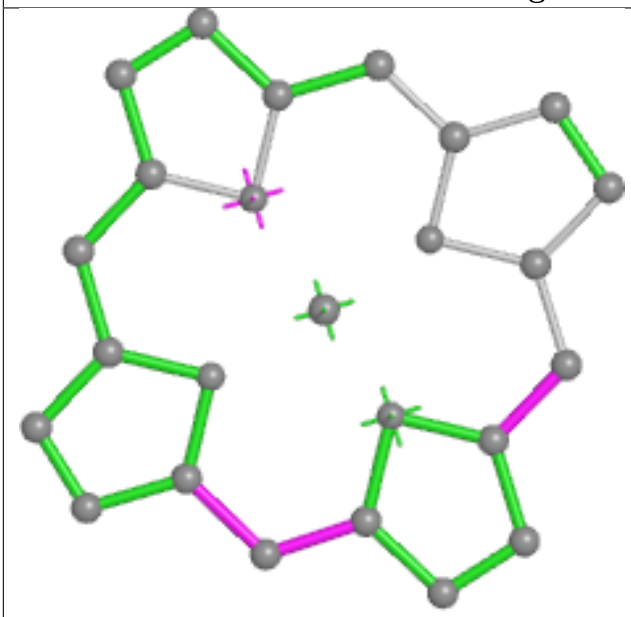


Torsions

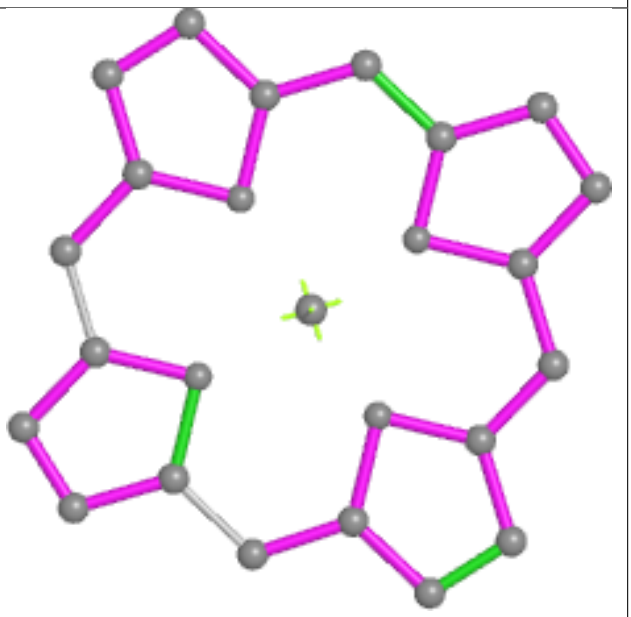


Rings

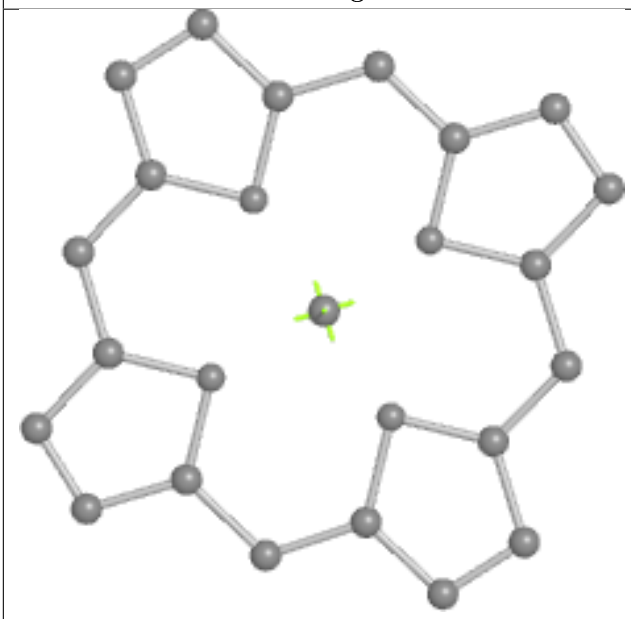
Ligand CLA 4 313



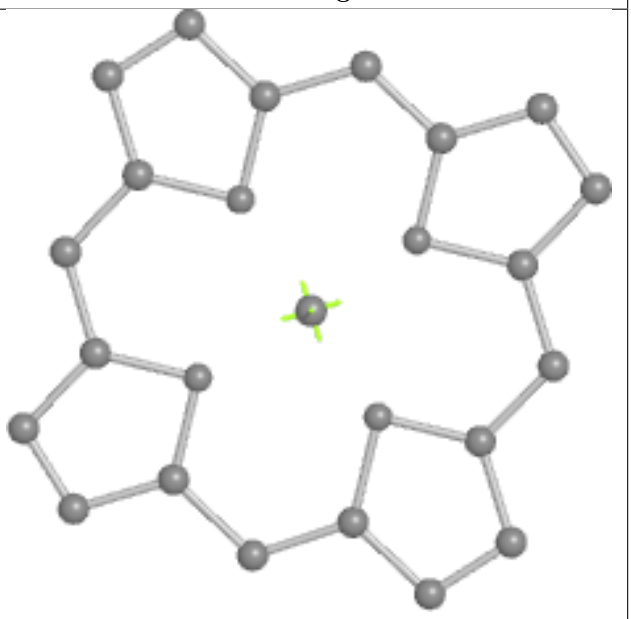
Bond lengths



Bond angles

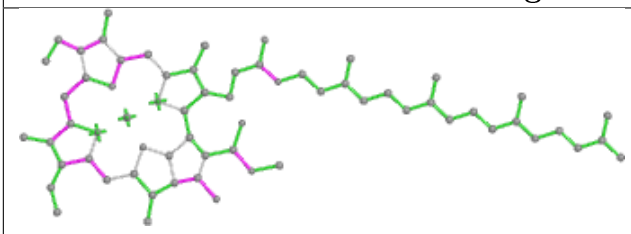


Torsions

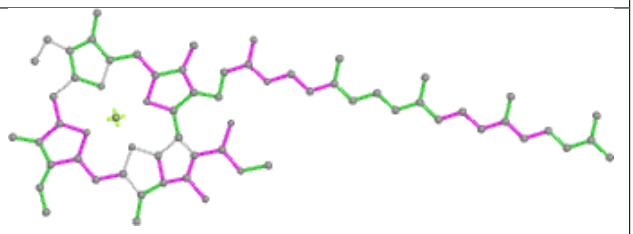


Rings

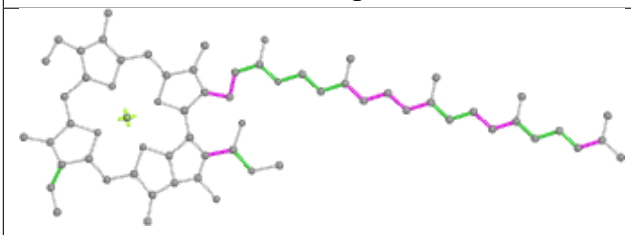
Ligand CLA B 826



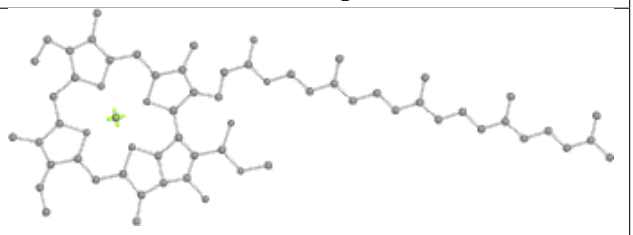
Bond lengths



Bond angles

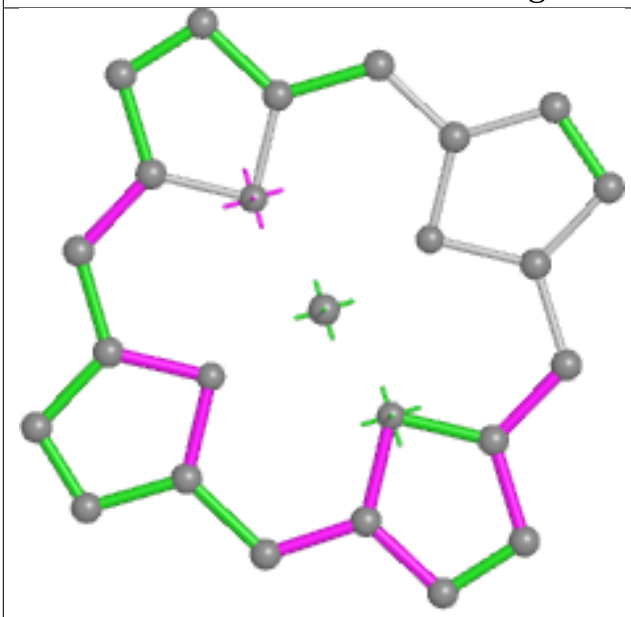


Torsions

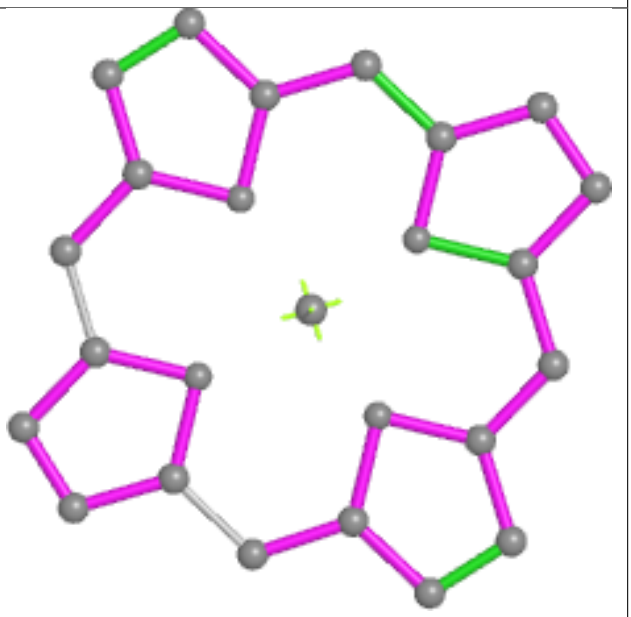


Rings

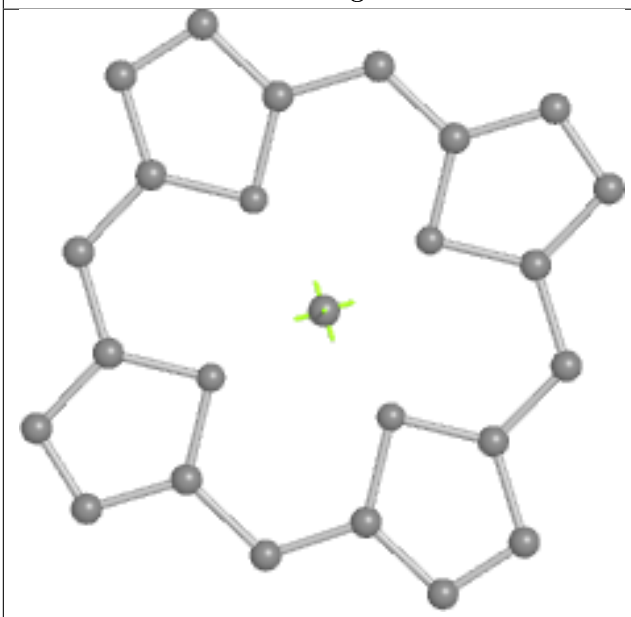
Ligand CLA 3 305



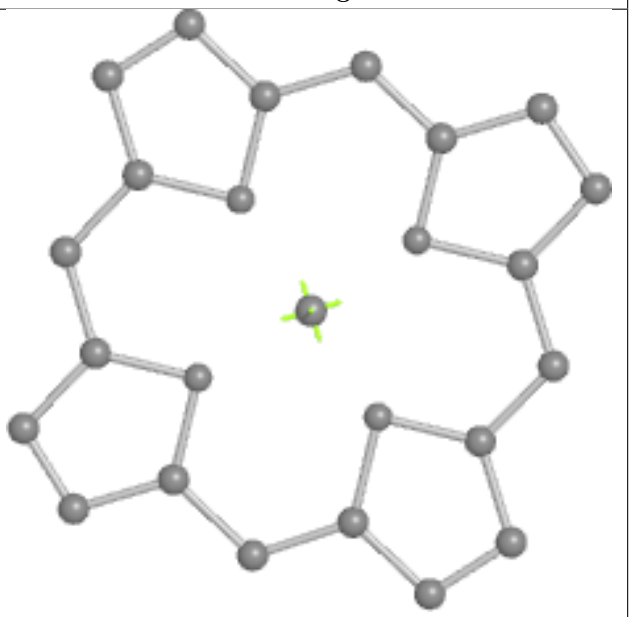
Bond lengths



Bond angles

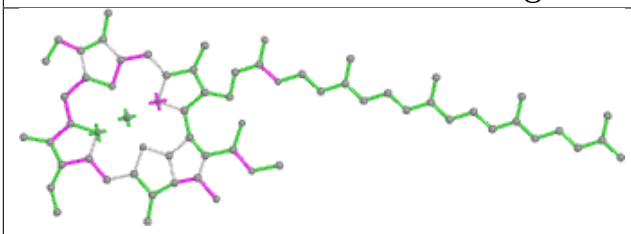


Torsions

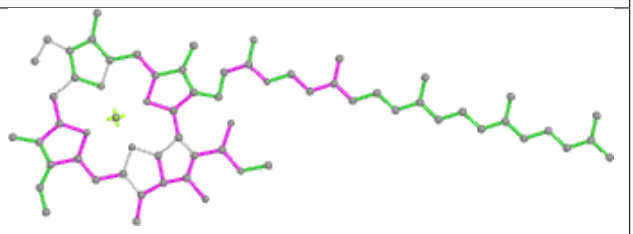


Rings

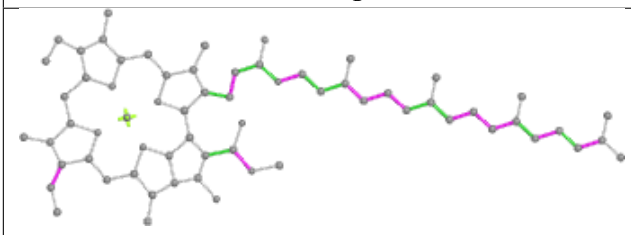
Ligand CLA A 824



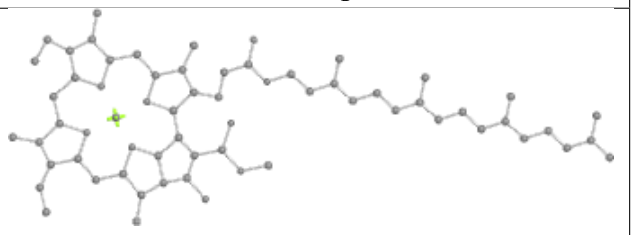
Bond lengths



Bond angles

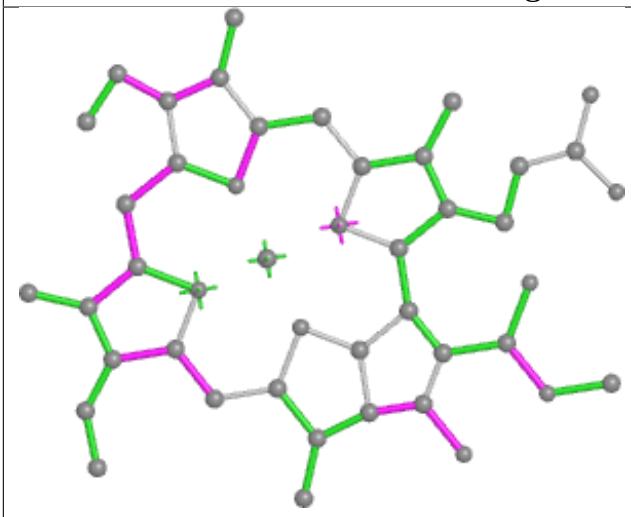


Torsions

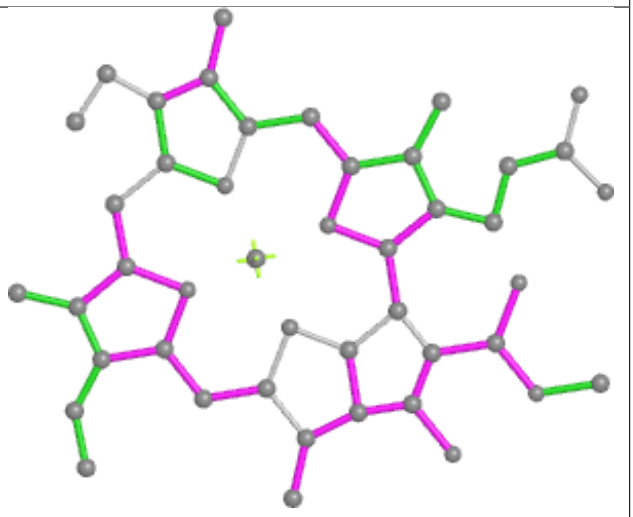


Rings

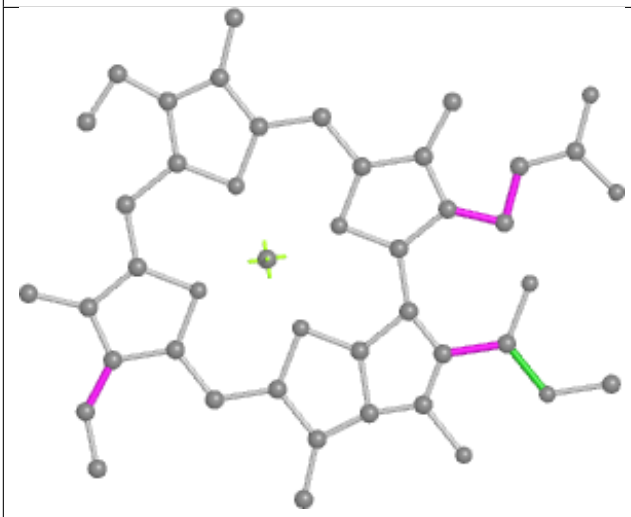
Ligand CLA B 804



Bond lengths



Bond angles



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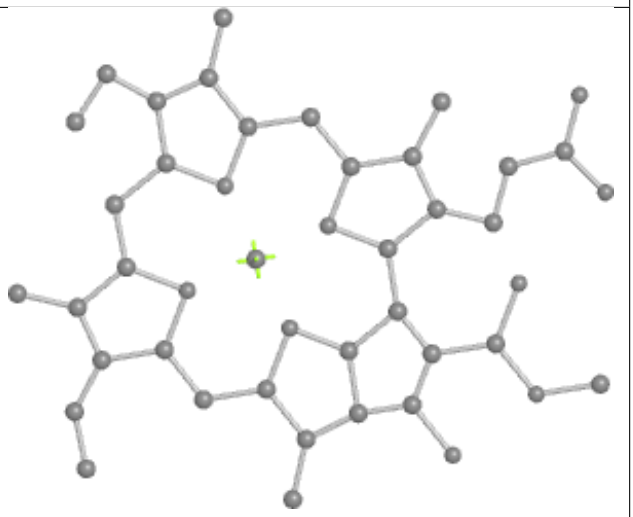
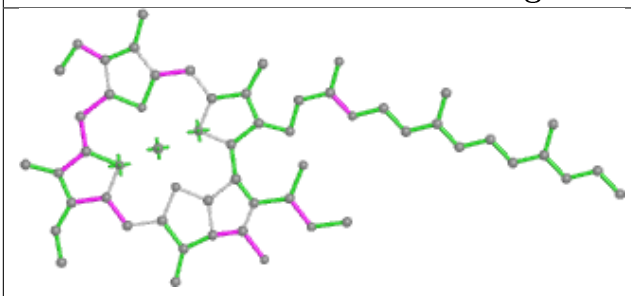


Rings

Ligand CLA R 107



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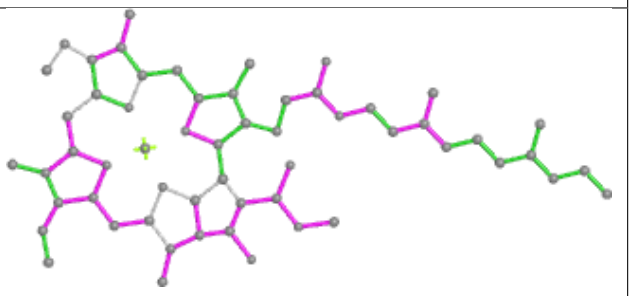
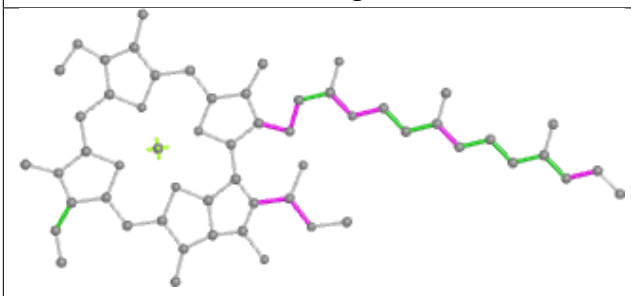
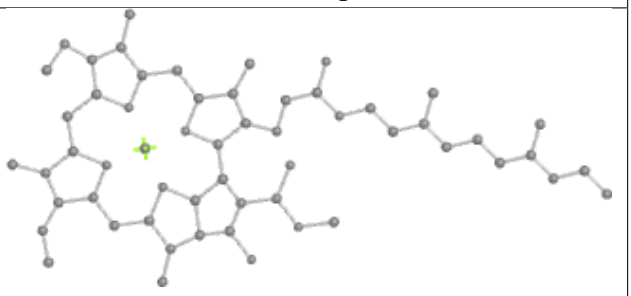


Bond angles

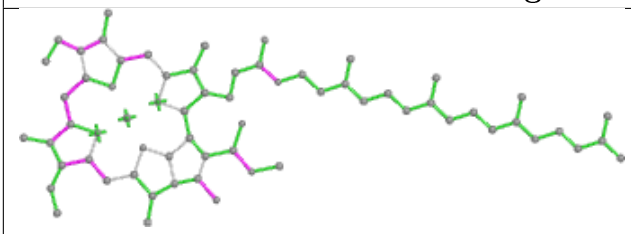


Torsions

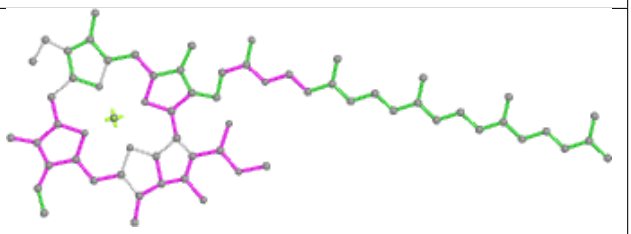


Rings

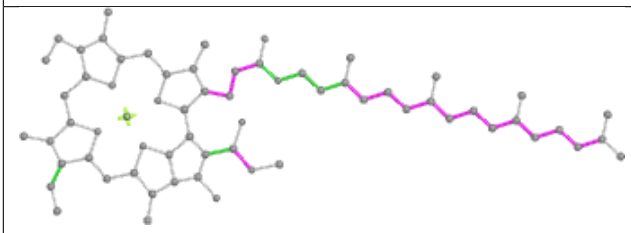
Ligand CLA B 812



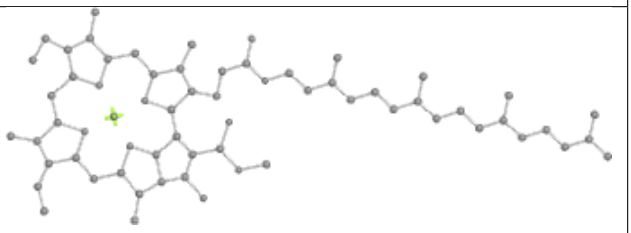
Bond lengths



Bond angles

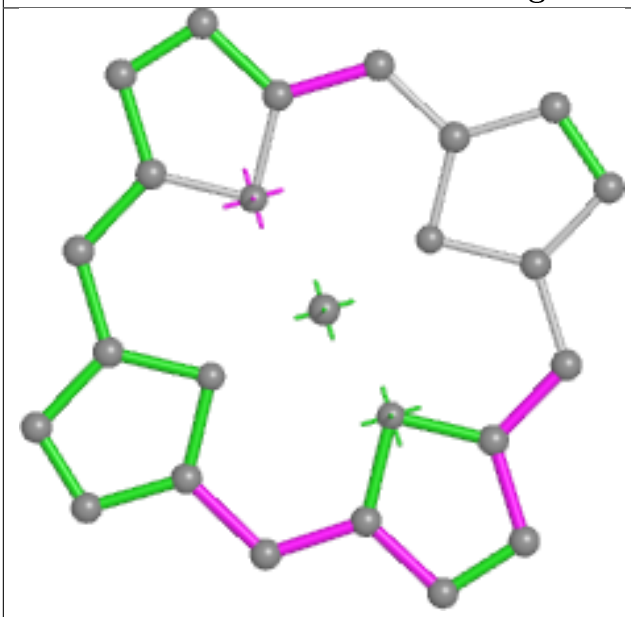


Torsions

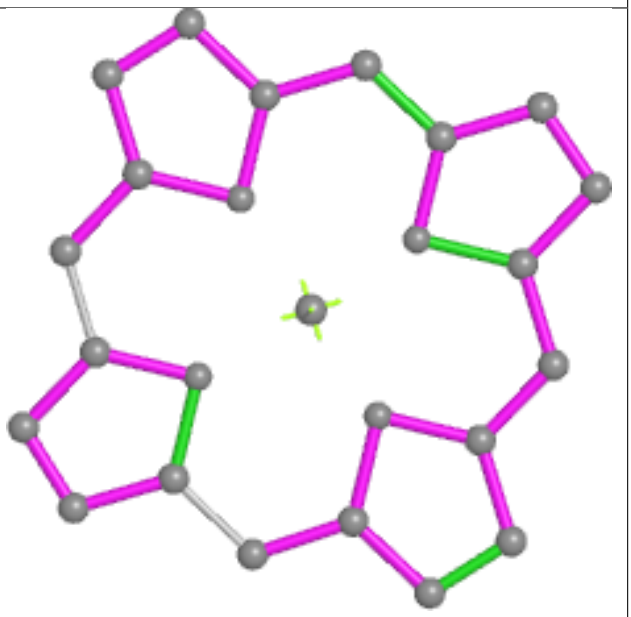


Rings

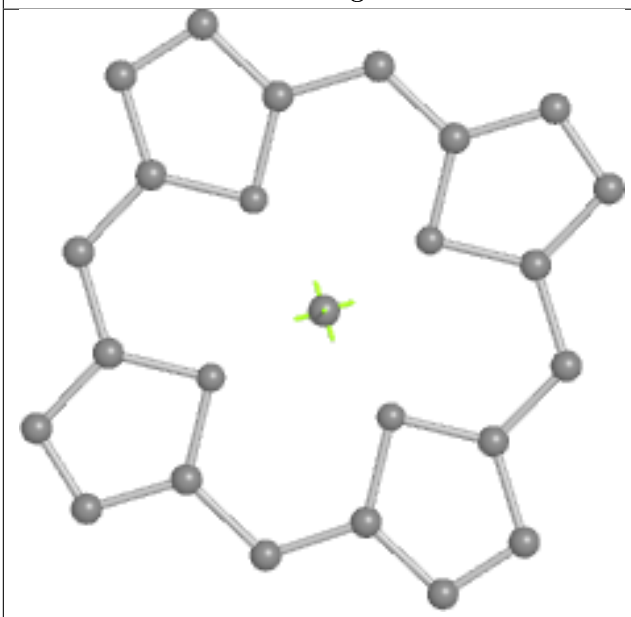
Ligand CLA 3 306



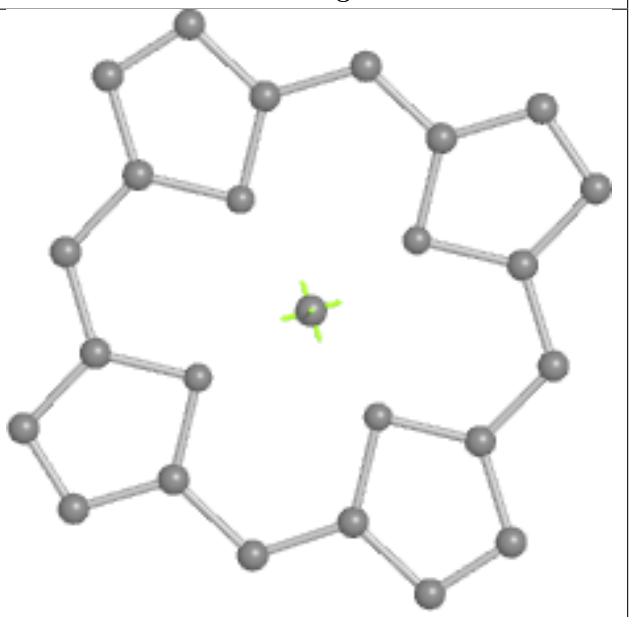
Bond lengths



Bond angles

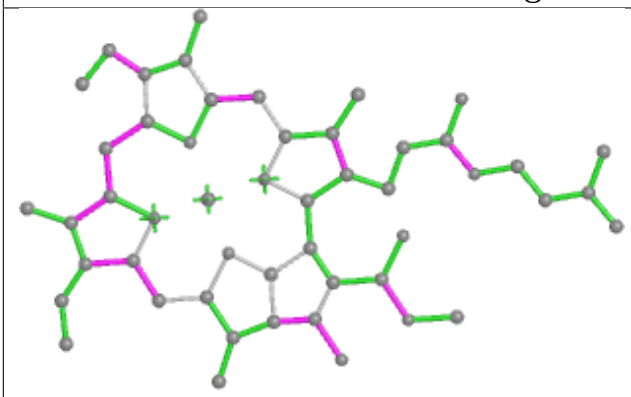


Torsions

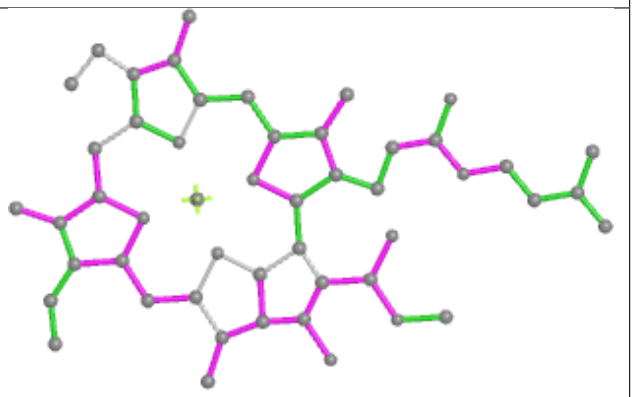


Rings

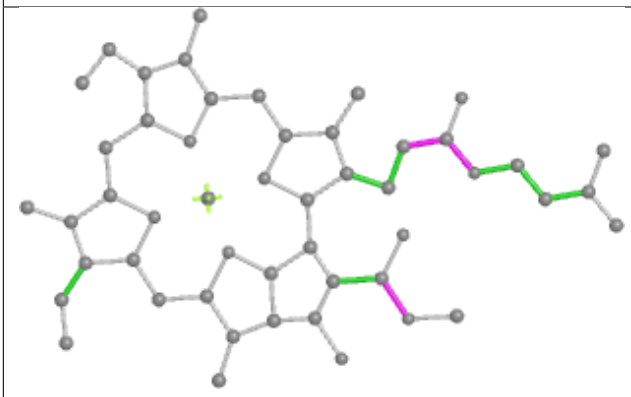
Ligand CLA B 818



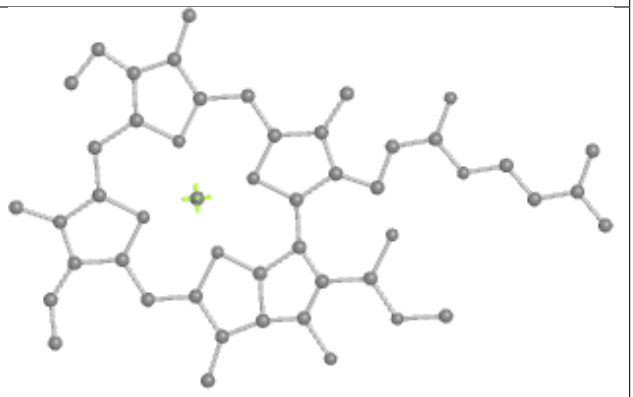
Bond lengths



Bond angles

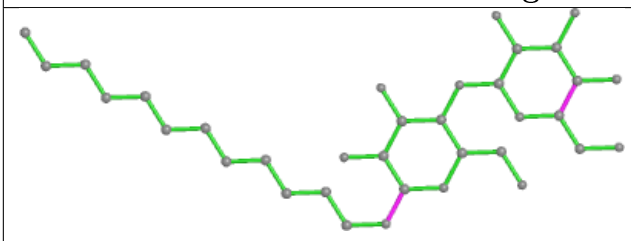


Torsions

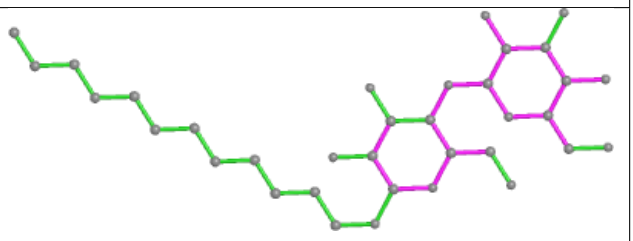


Rings

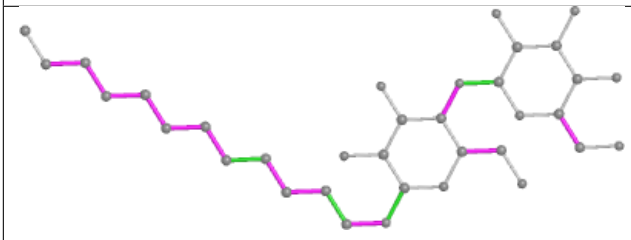
Ligand LMU L 204



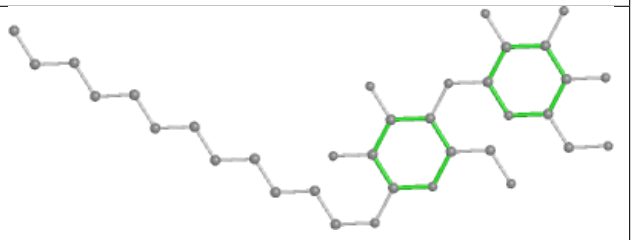
Bond lengths



Bond angles

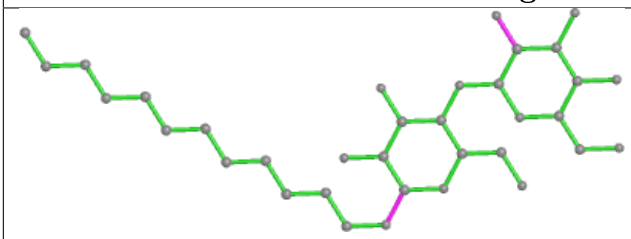


Torsions

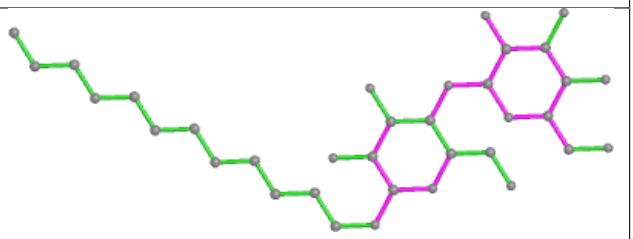


Rings

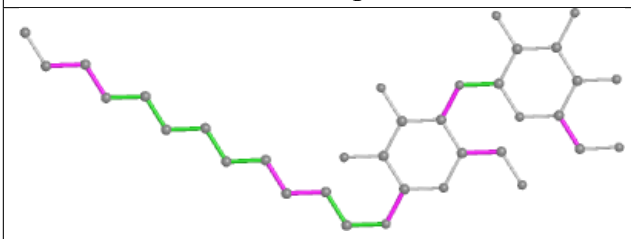
Ligand LMU R 101



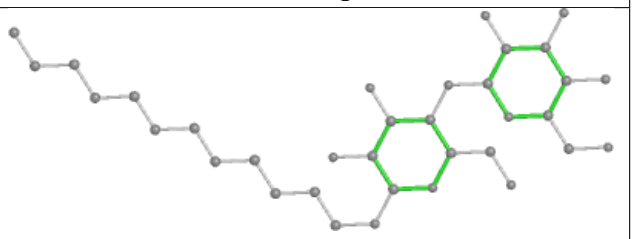
Bond lengths



Bond angles

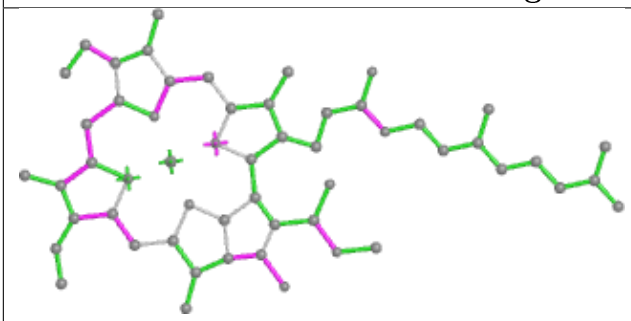


Torsions

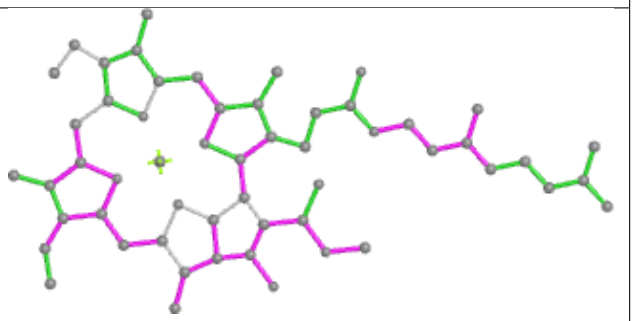


Rings

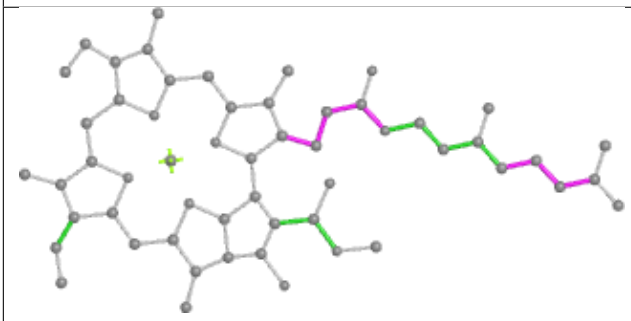
Ligand CLA B 820



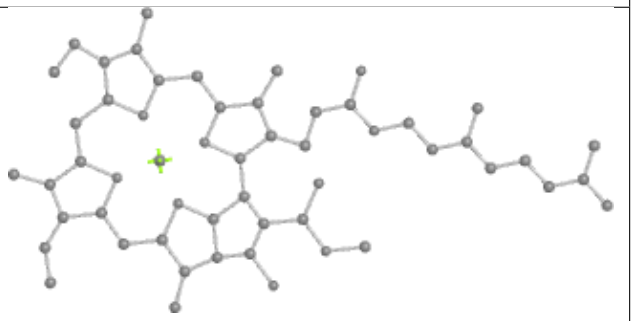
Bond lengths



Bond angles

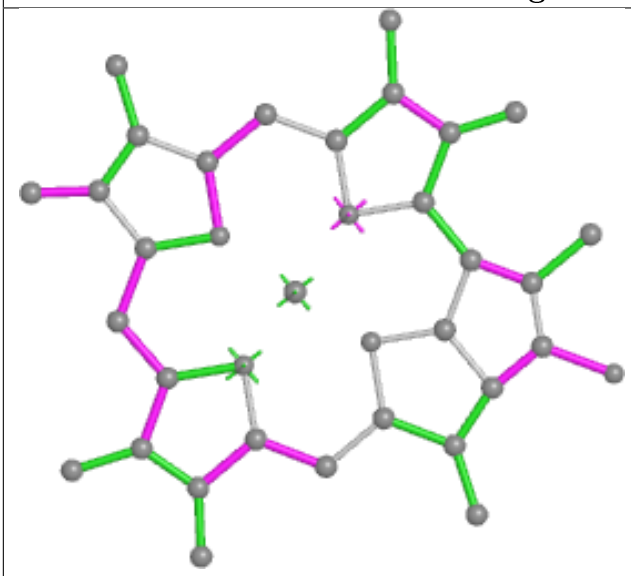


Torsions

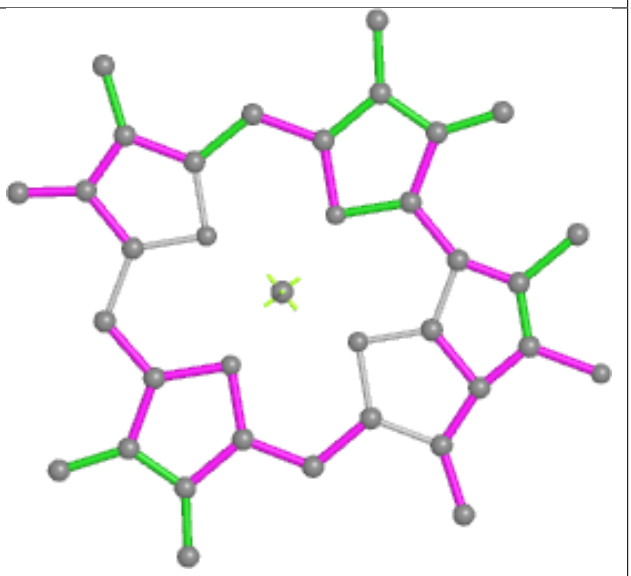


Rings

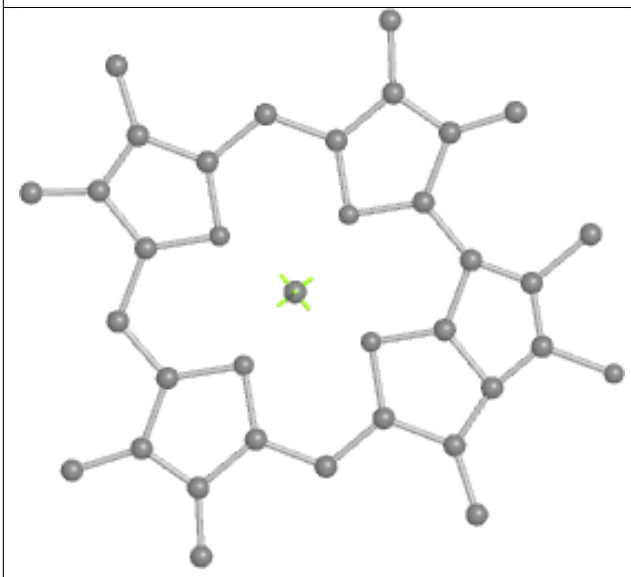
Ligand CLA 4 308



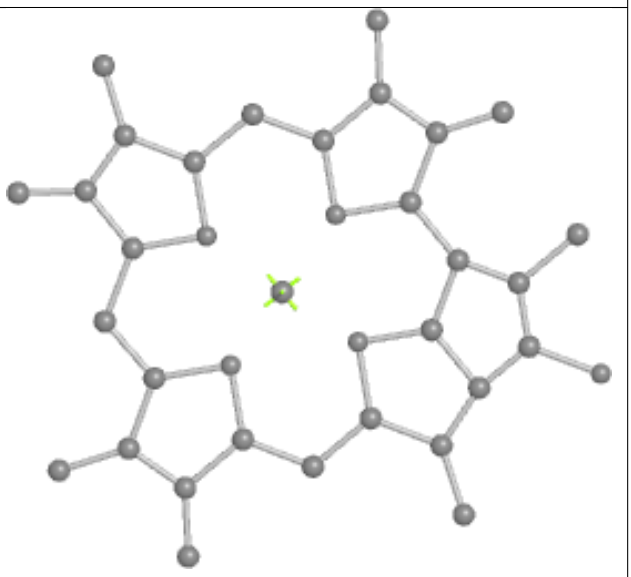
Bond lengths



Bond angles

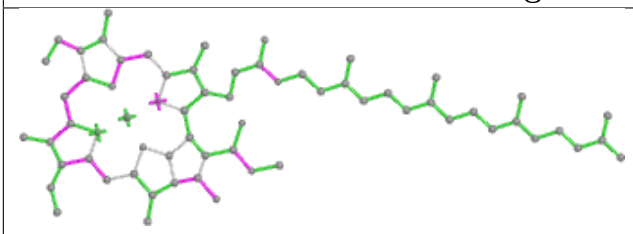


Torsions

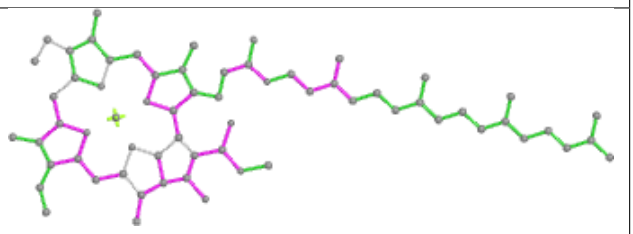


Rings

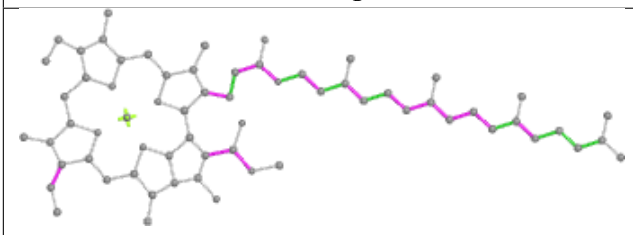
Ligand CLA A 825



Bond lengths



Bond angles



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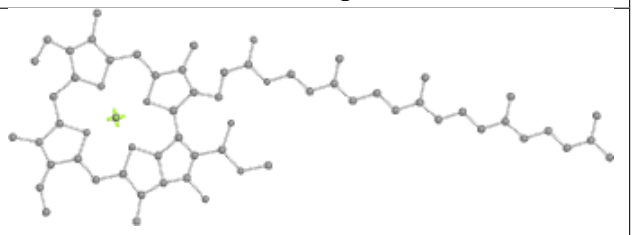
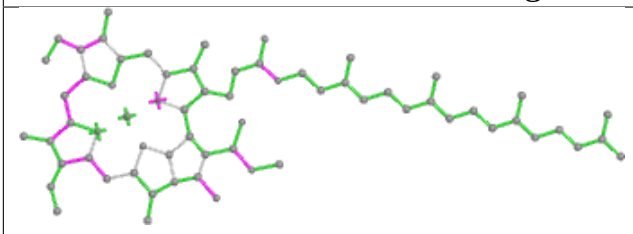


Rings

Ligand CLA B 807



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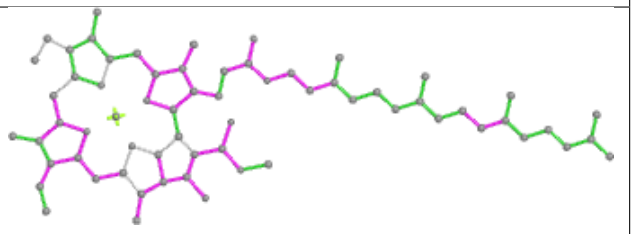
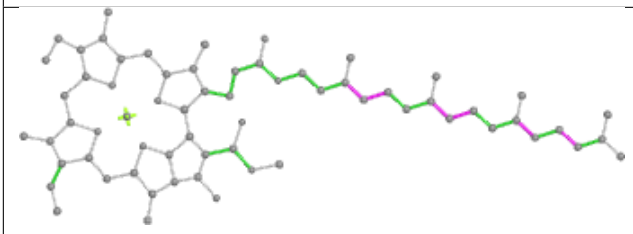


Bond angles



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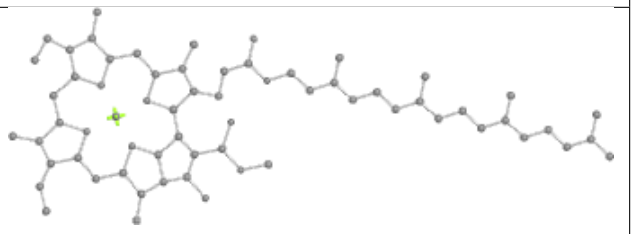
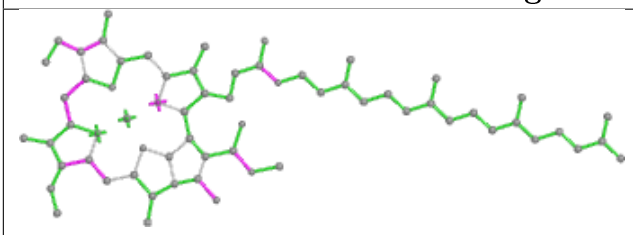
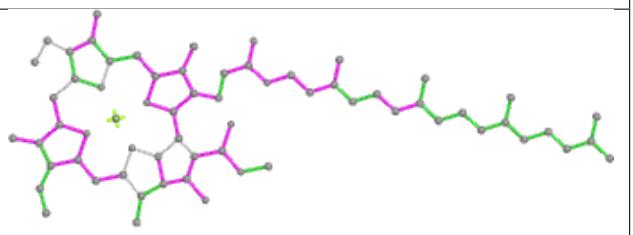


Rings

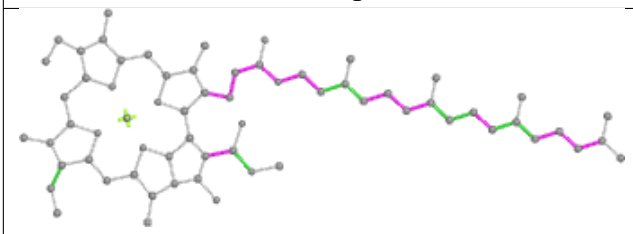
Ligand CLA A 838



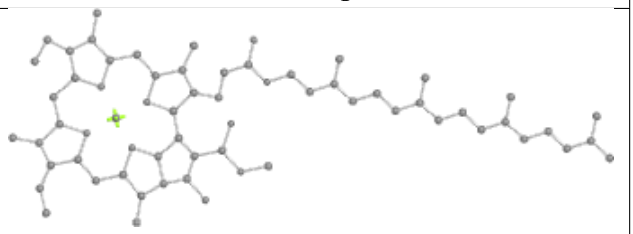
Bond lengths



Bond angles

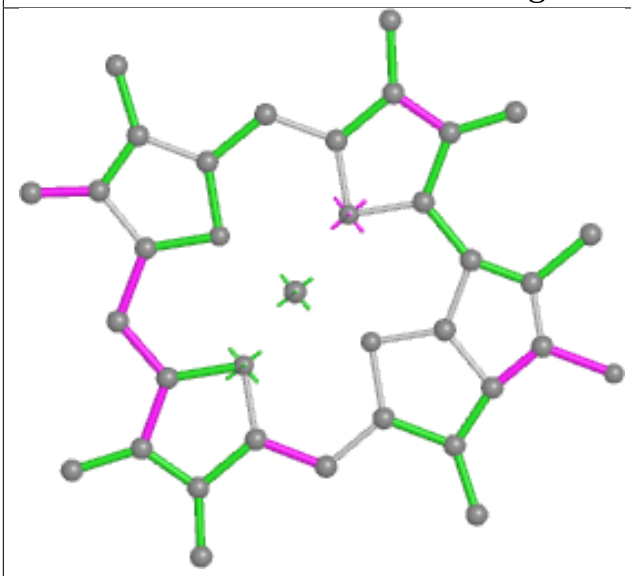


Torsions



Rings

Ligand CLA 4 314



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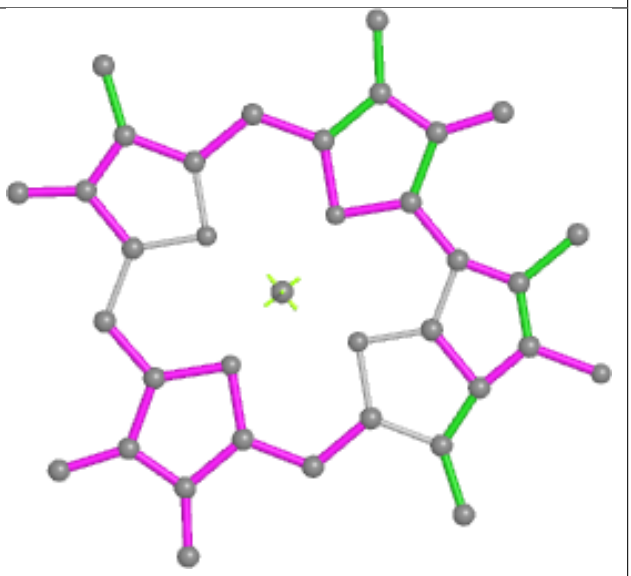
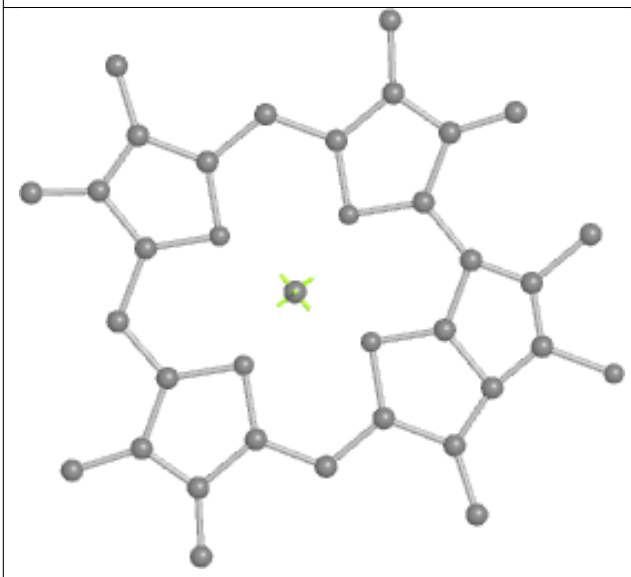


Bond angles



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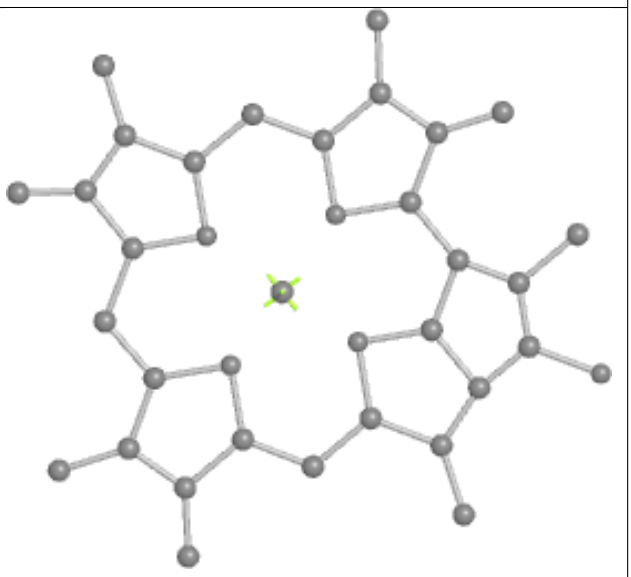
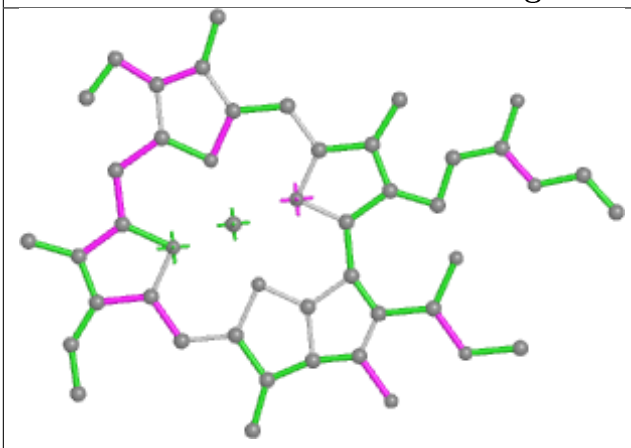
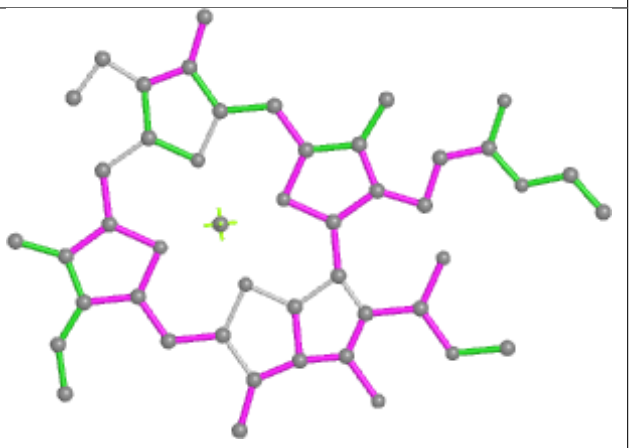


Rings

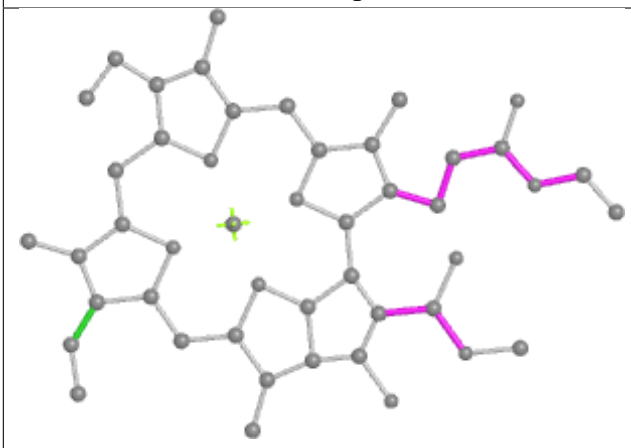
Ligand CLA A 837



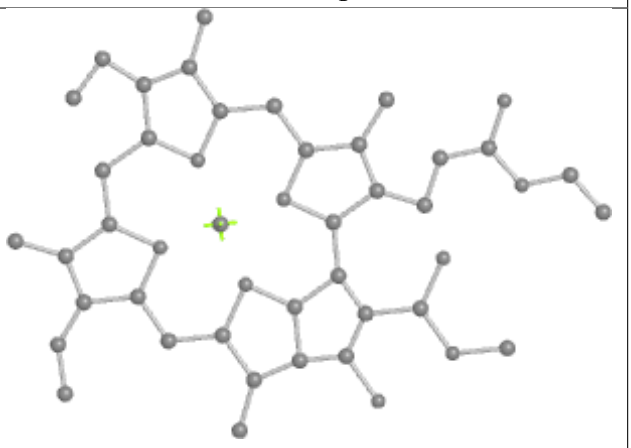
Bond lengths



Bond angles

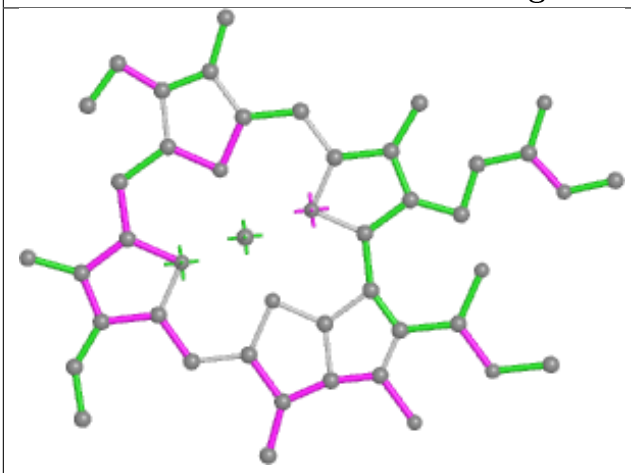


Torsions

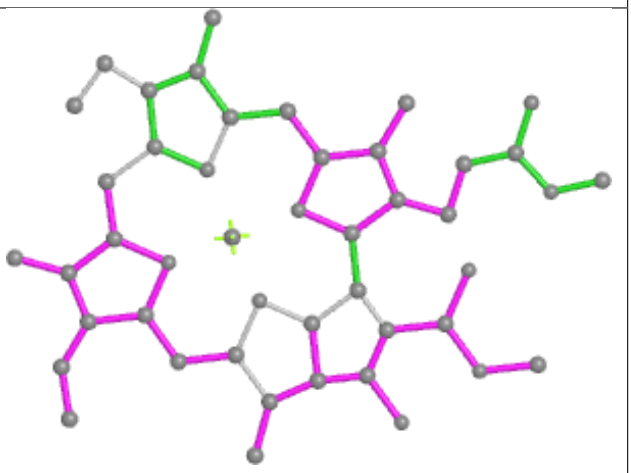


Rings

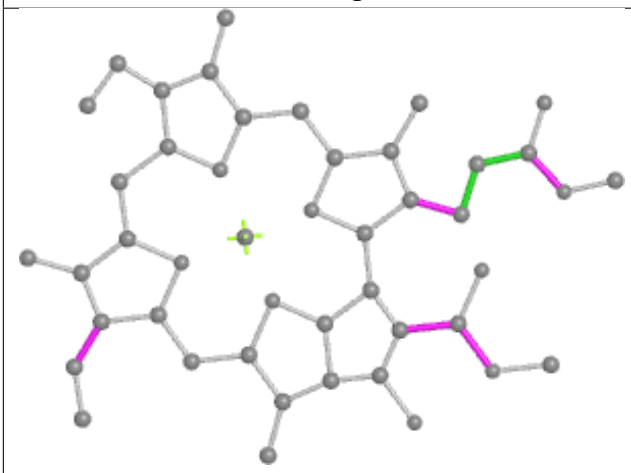
Ligand CLA 1 201



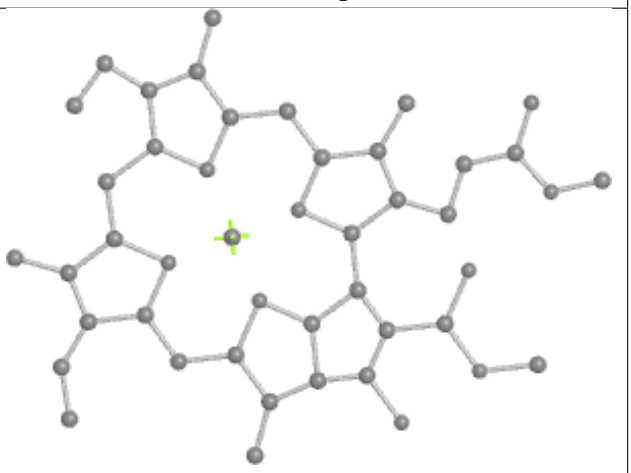
Bond lengths



Bond angles

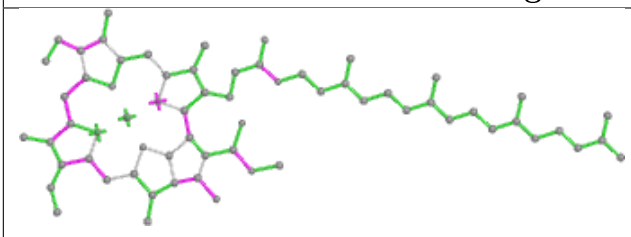


Torsions

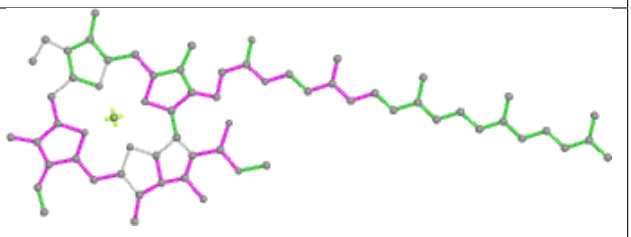


Rings

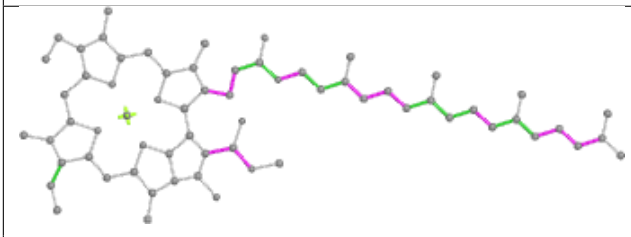
Ligand CLA B 850



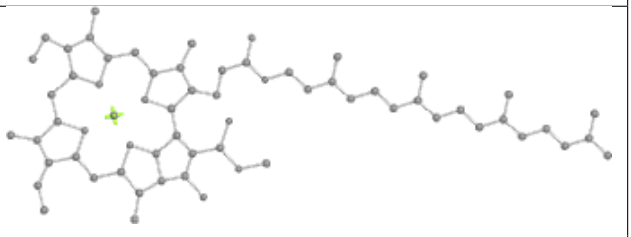
Bond lengths



Bond angles

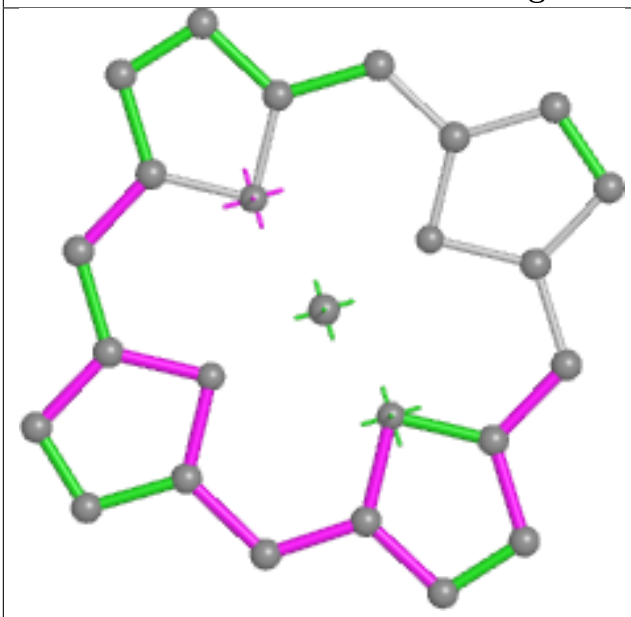


Torsions

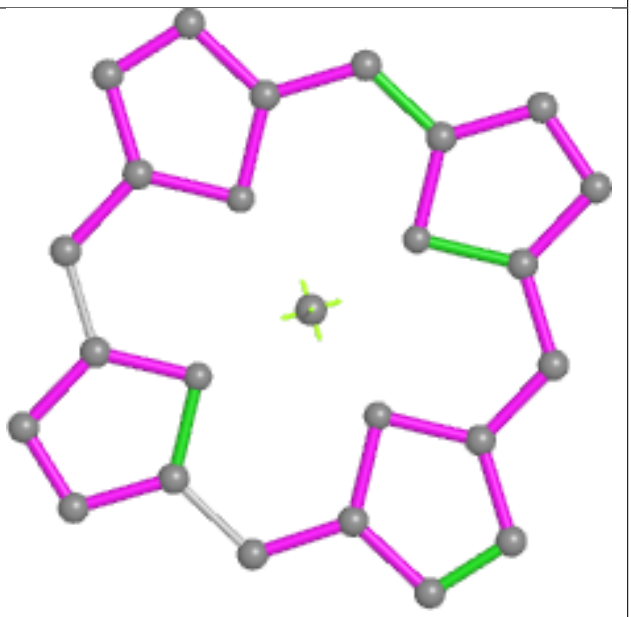


Rings

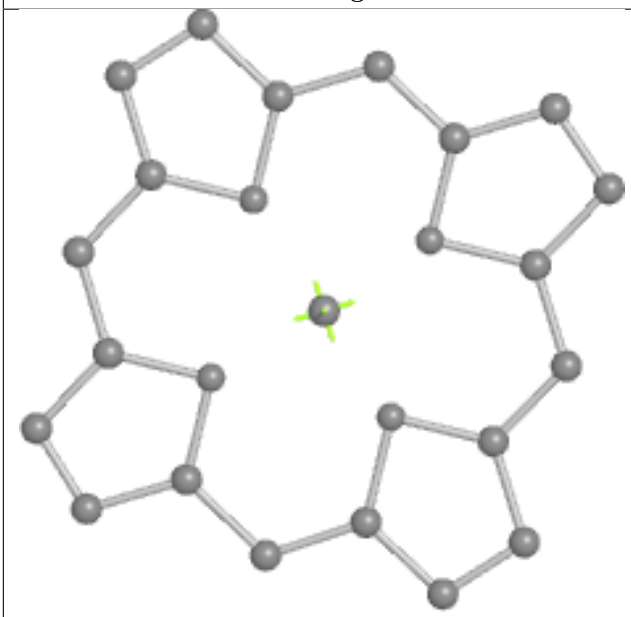
Ligand CLA 1 208



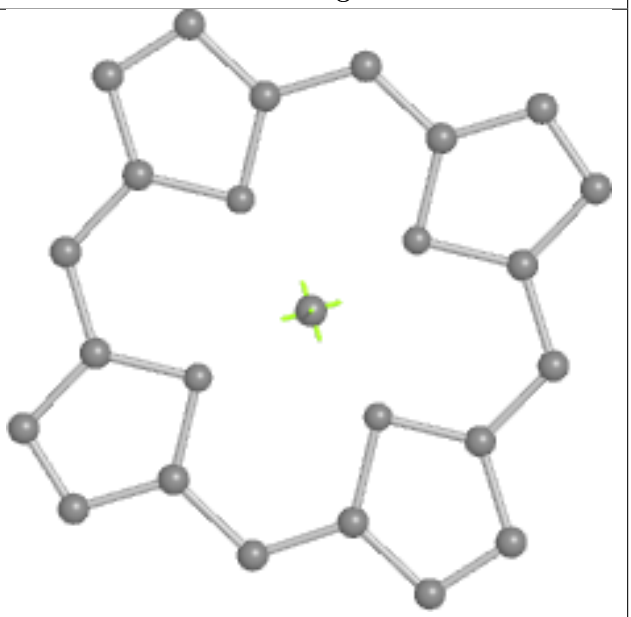
Bond lengths



Bond angles

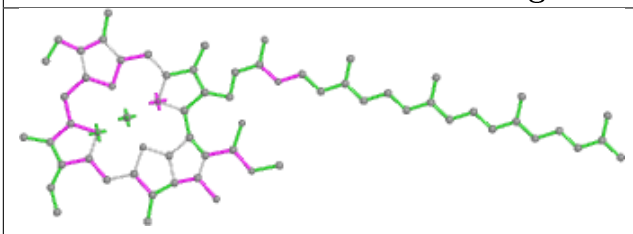


Torsions

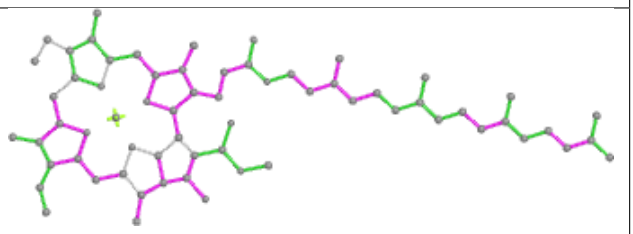


Rings

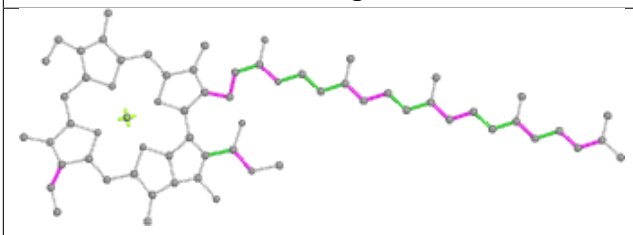
Ligand CLA 2 307



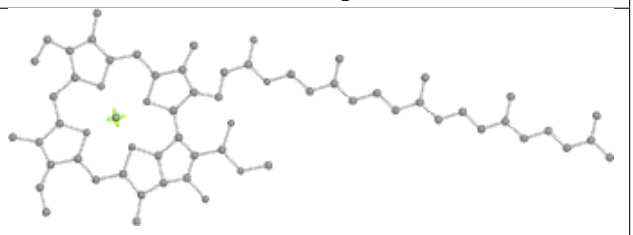
Bond lengths



Bond angles

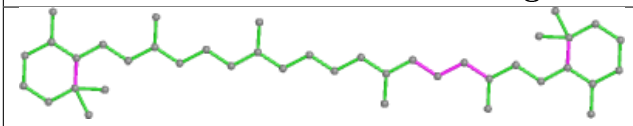


Torsions

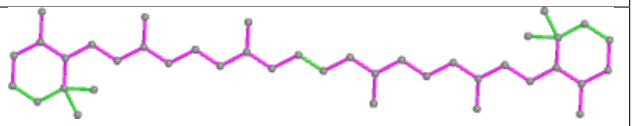


Rings

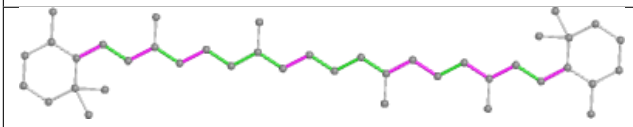
Ligand BCR B 845



Bond lengths



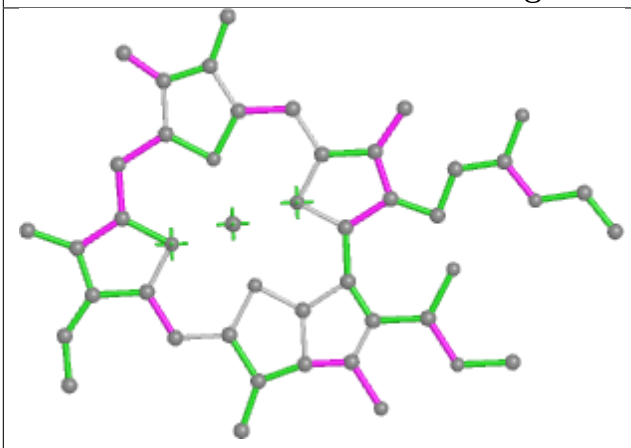
Bond angles



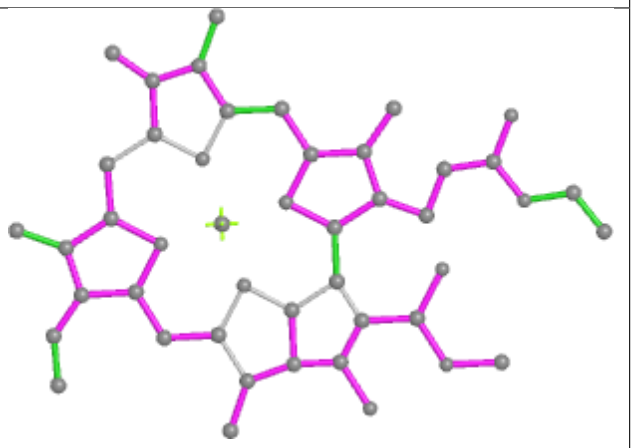
Torsions

Rings

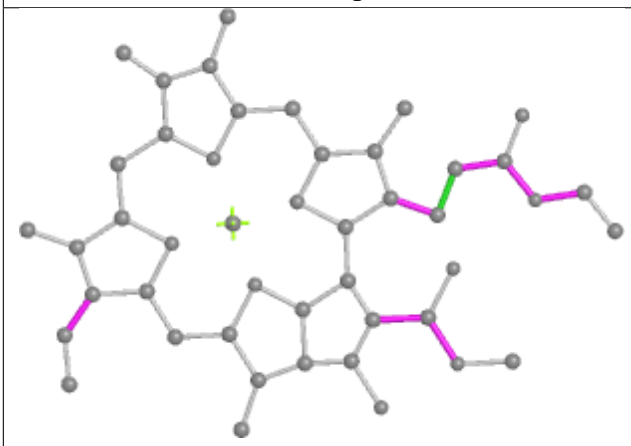
Ligand CLA A 801



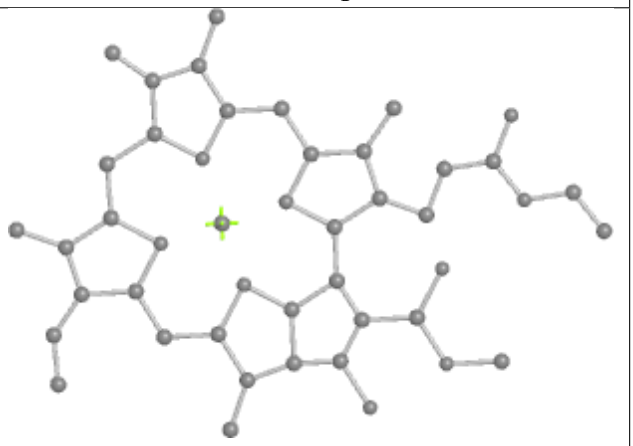
Bond lengths



Bond angles

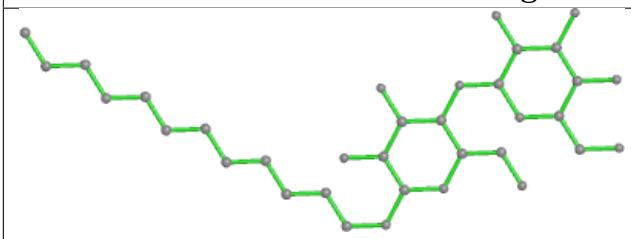


Torsions

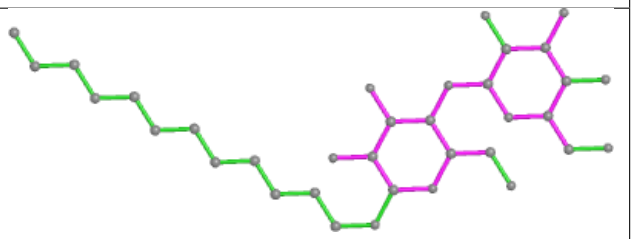


Rings

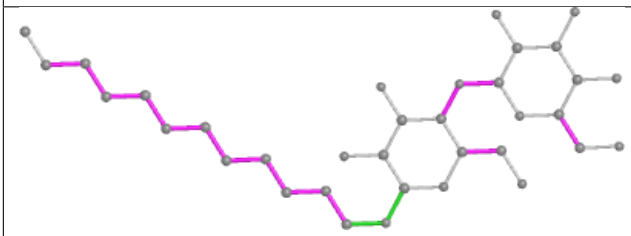
Ligand LMU B 801



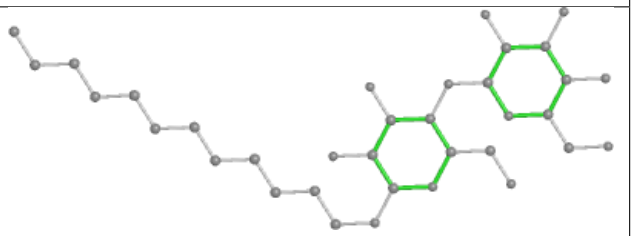
Bond lengths



Bond angles

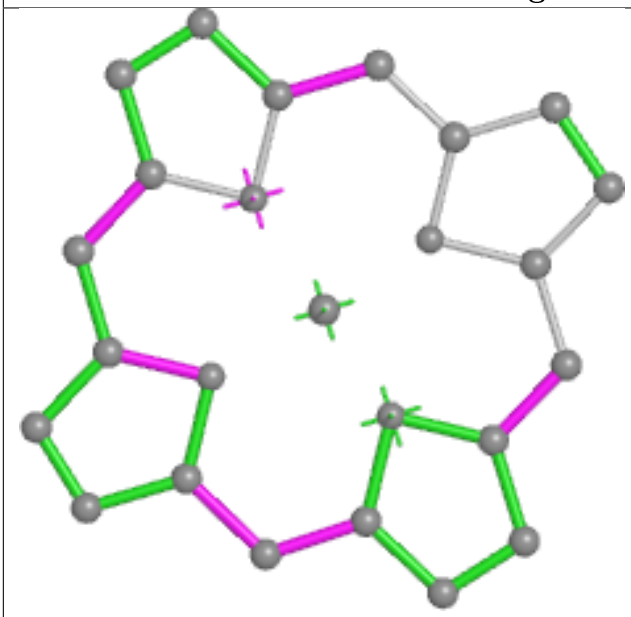


Torsions

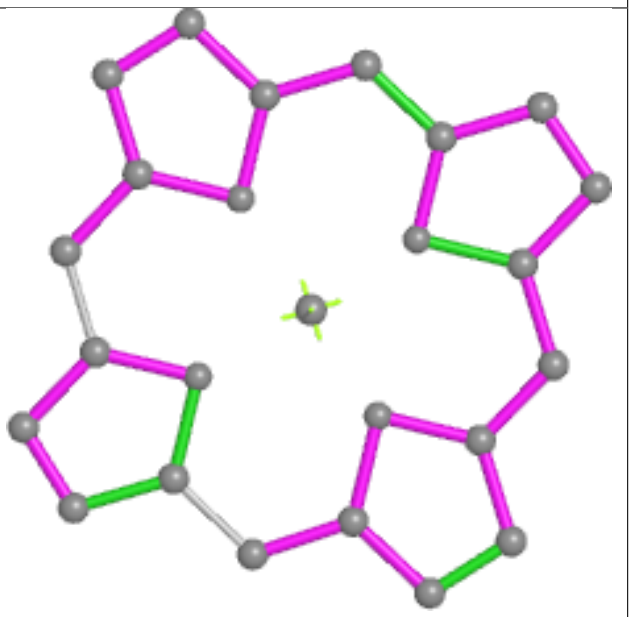


Rings

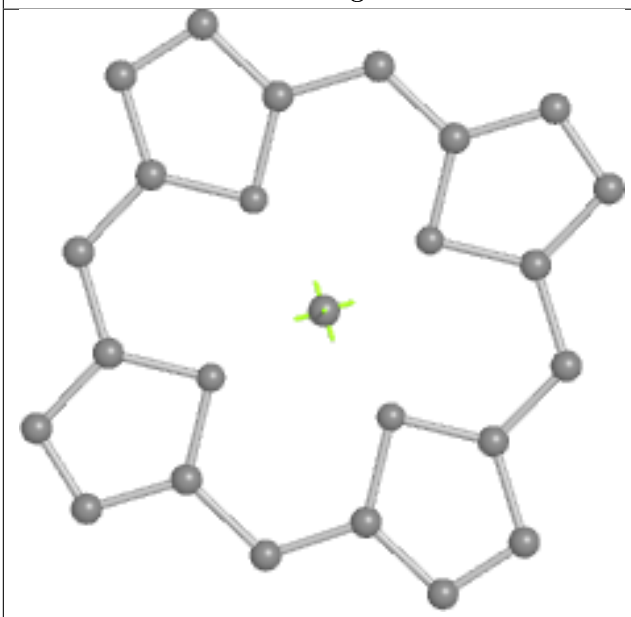
Ligand CLA 3 309



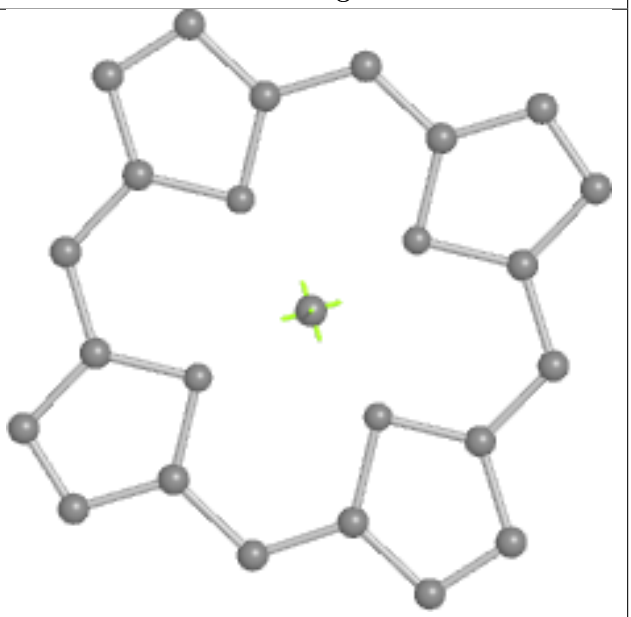
Bond lengths



Bond angles

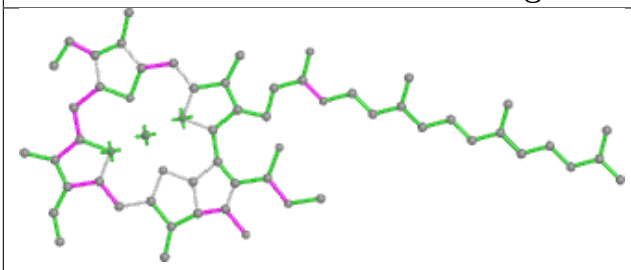


Torsions

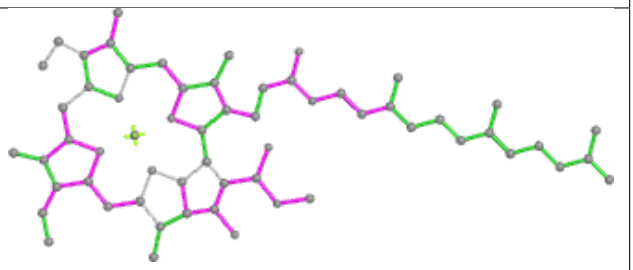


Rings

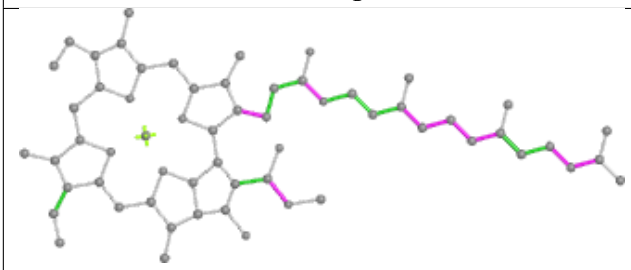
Ligand CLA B 816



Bond lengths



Bond angles



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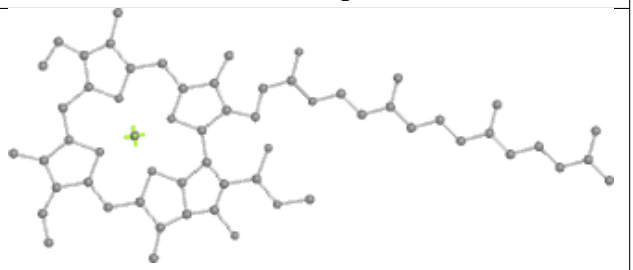
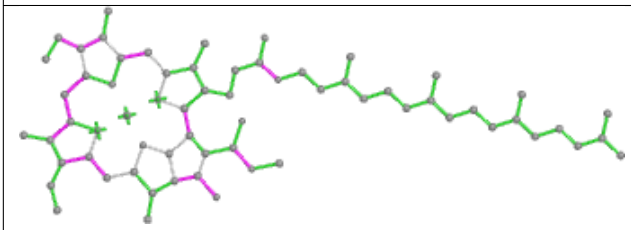
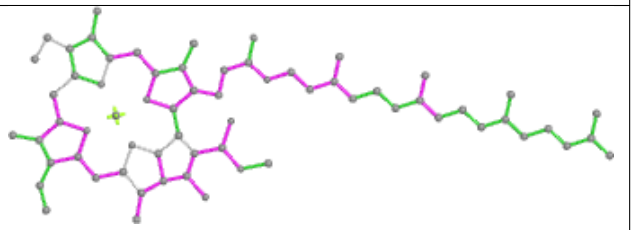


Rings

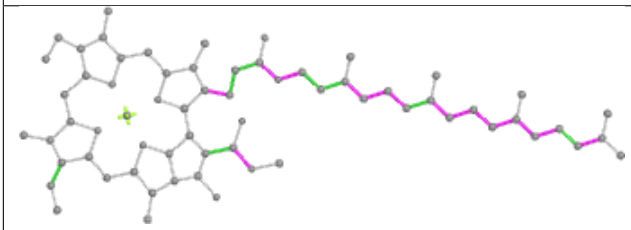
Ligand CLA B 830



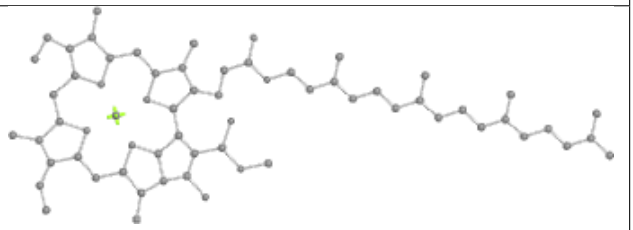
Bond lengths



Bond angles

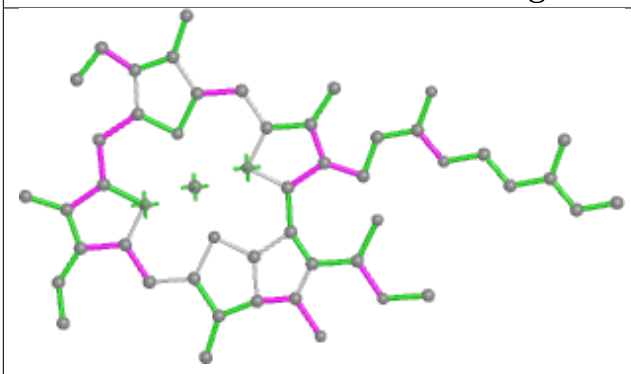


Torsions

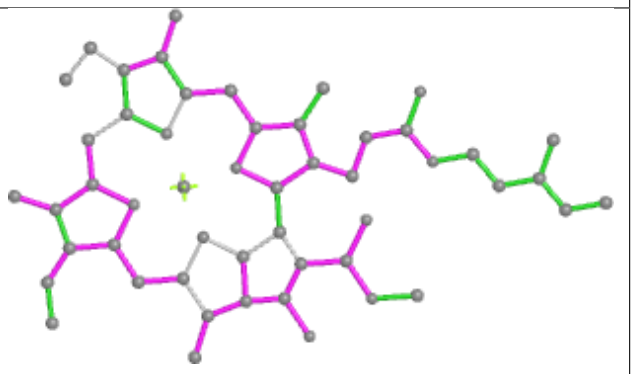


Rings

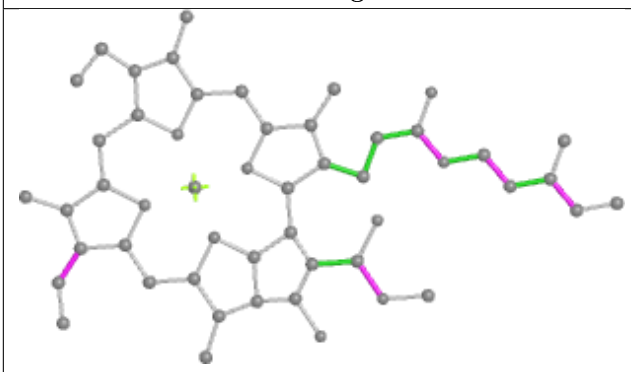
Ligand CLA 1 207



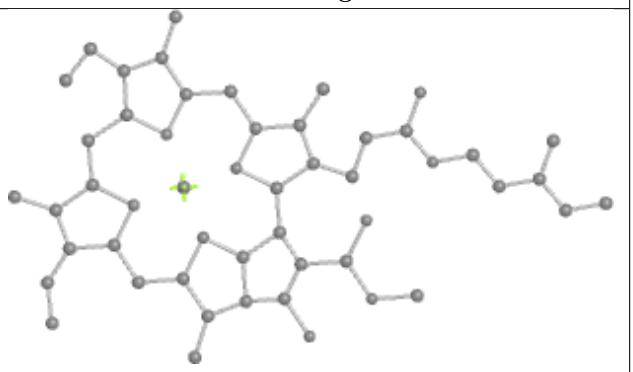
Bond lengths



Bond angles

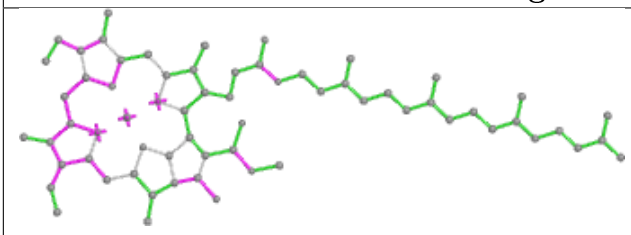


Torsions



Rings

Ligand CLA 3 313



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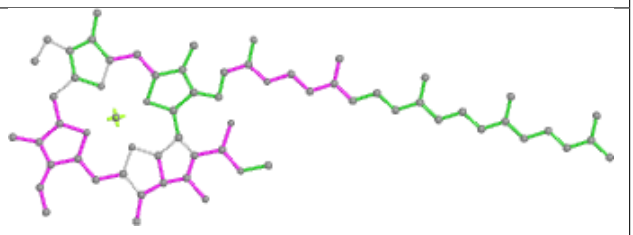
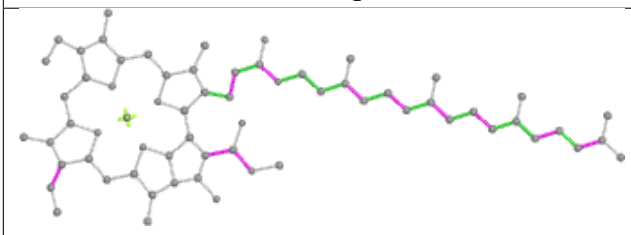
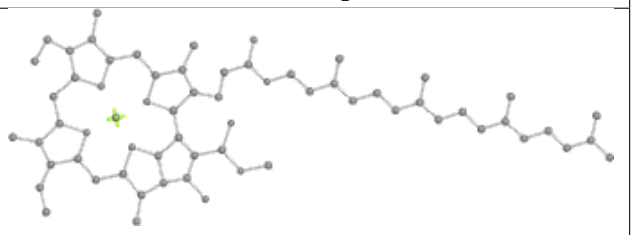


Bond angles

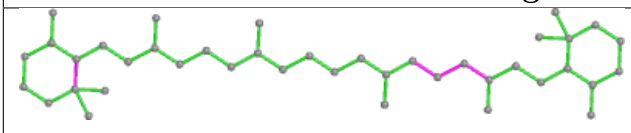


Torsions



Rings

Ligand BCR A 844



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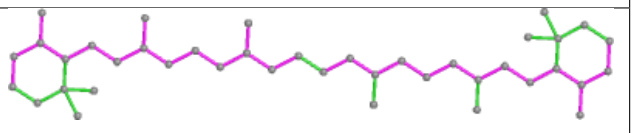
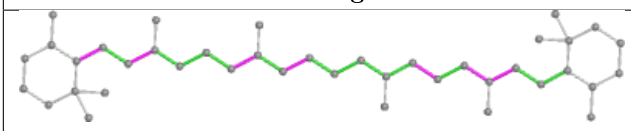


Bond angles



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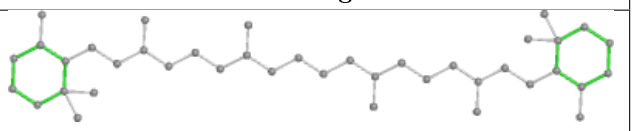
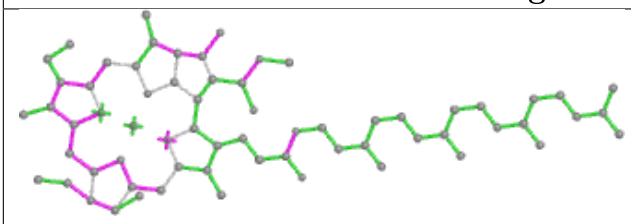


Rings

Ligand CLA 3 311



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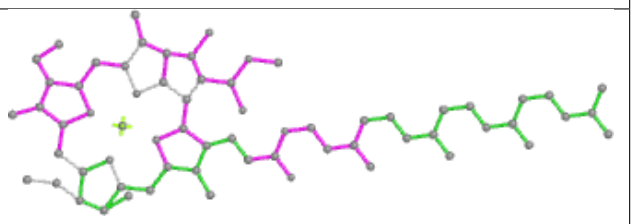
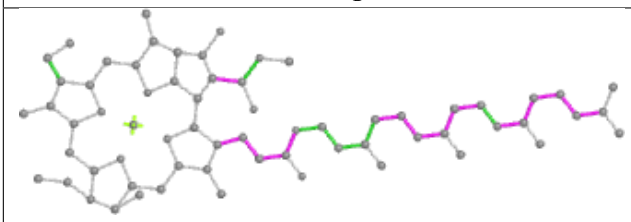
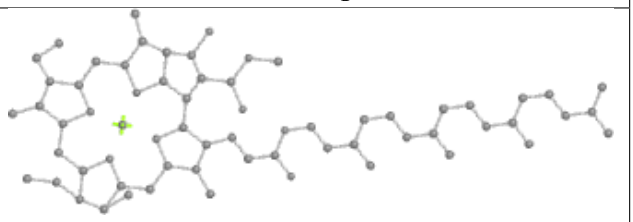


Bond angles

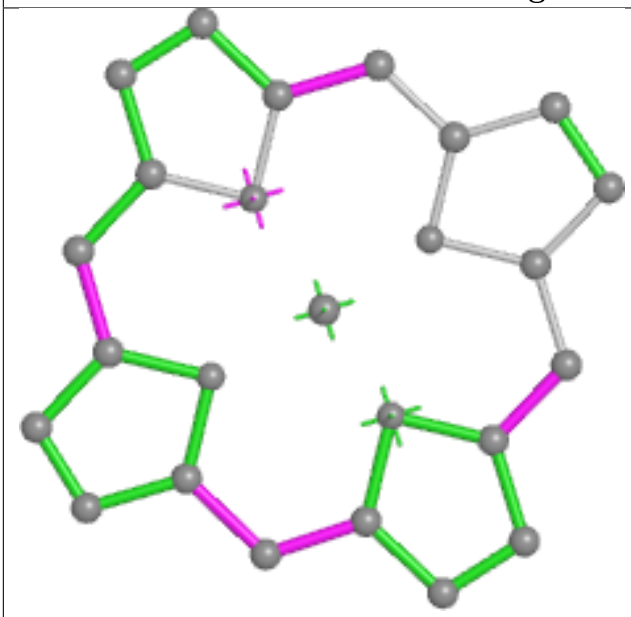


Torsions

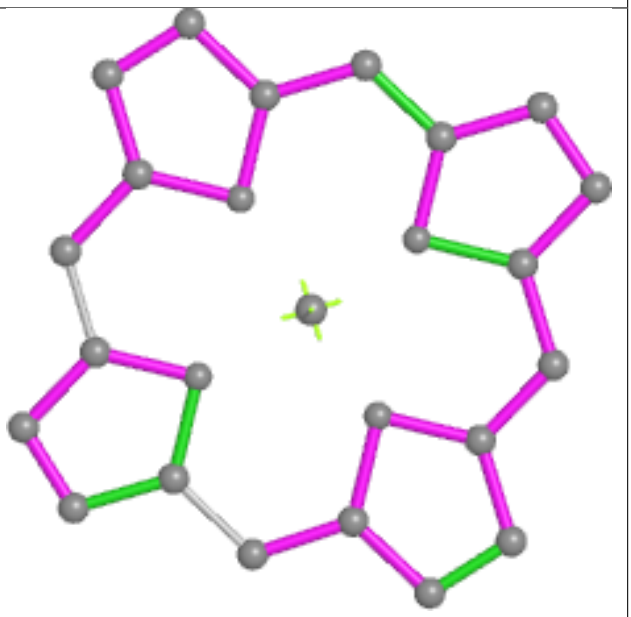


Rings

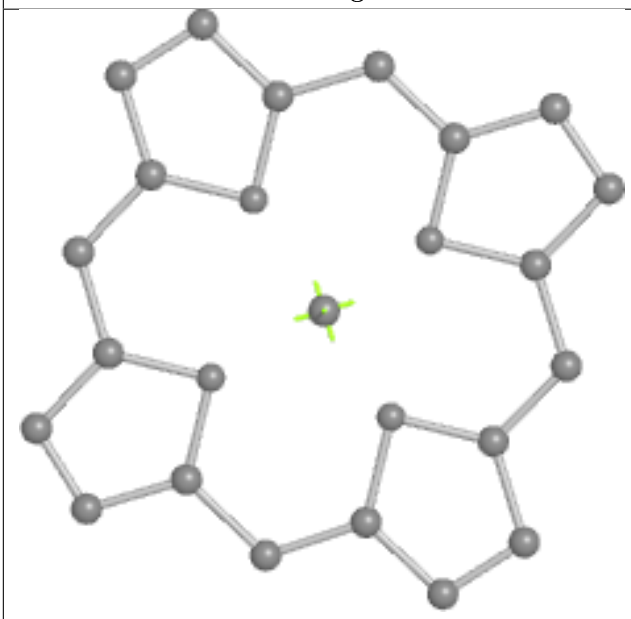
Ligand CLA 3 316



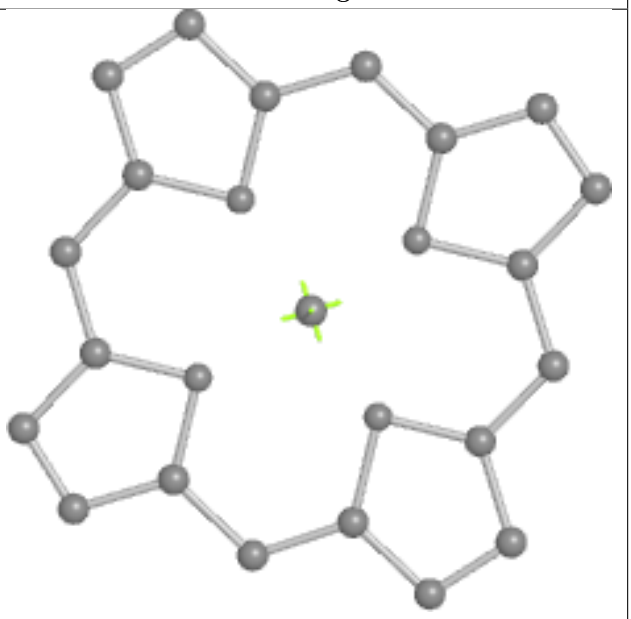
Bond lengths



Bond angles

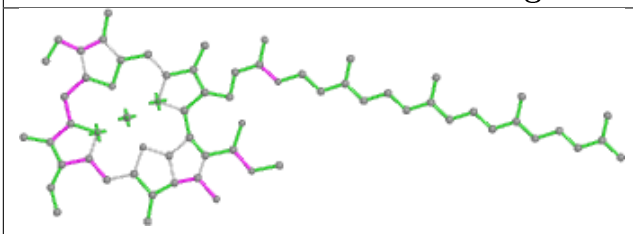


Torsions

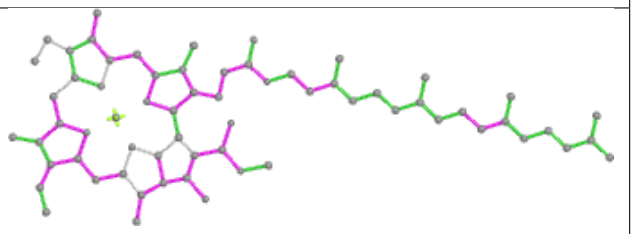


Rings

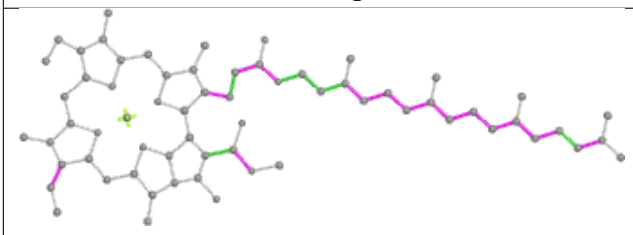
Ligand CLA A 811



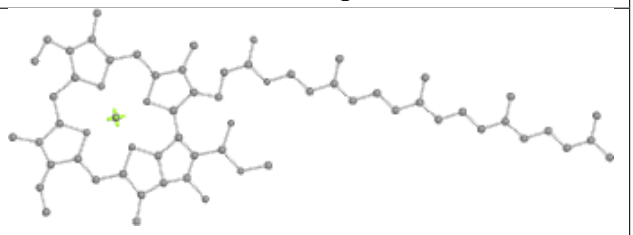
Bond lengths



Bond angles

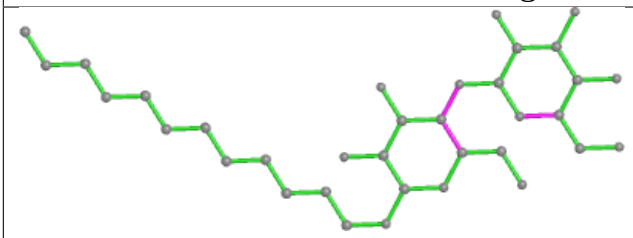


Torsions

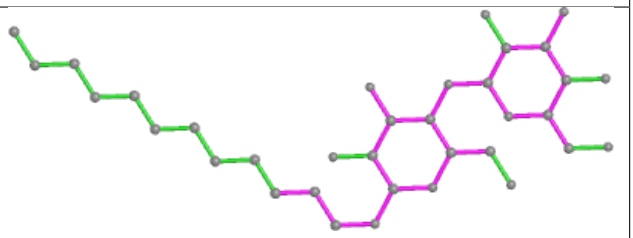


Rings

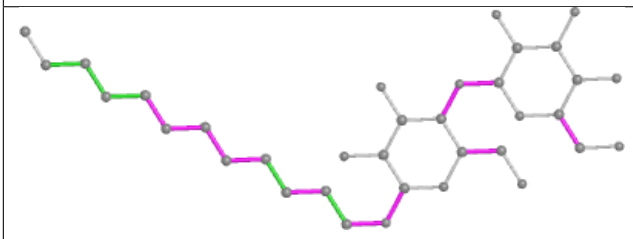
Ligand LMU H 108



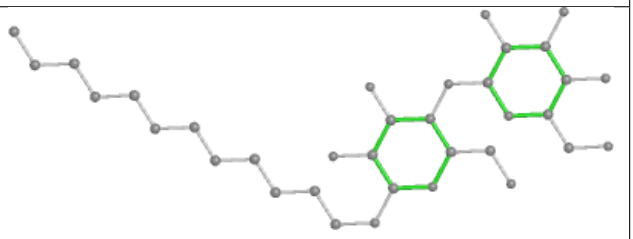
Bond lengths



Bond angles

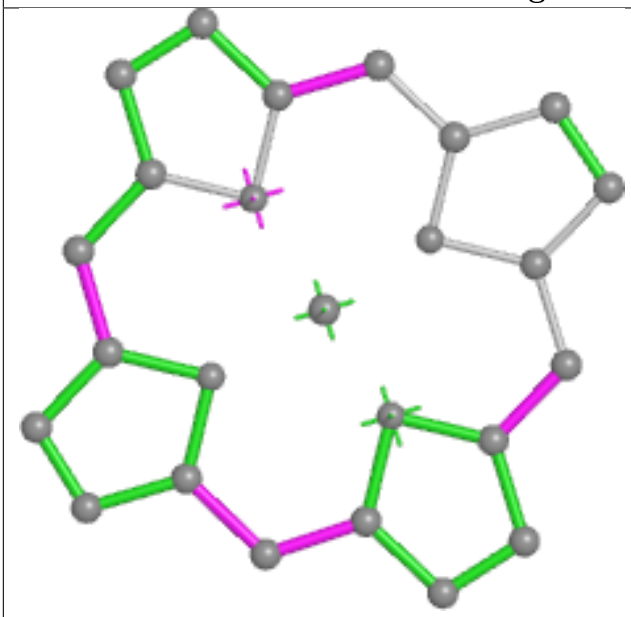


Torsions

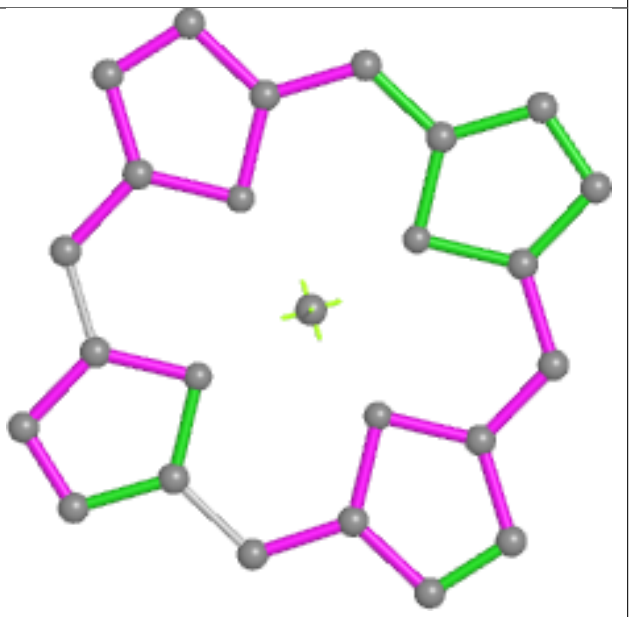


Rings

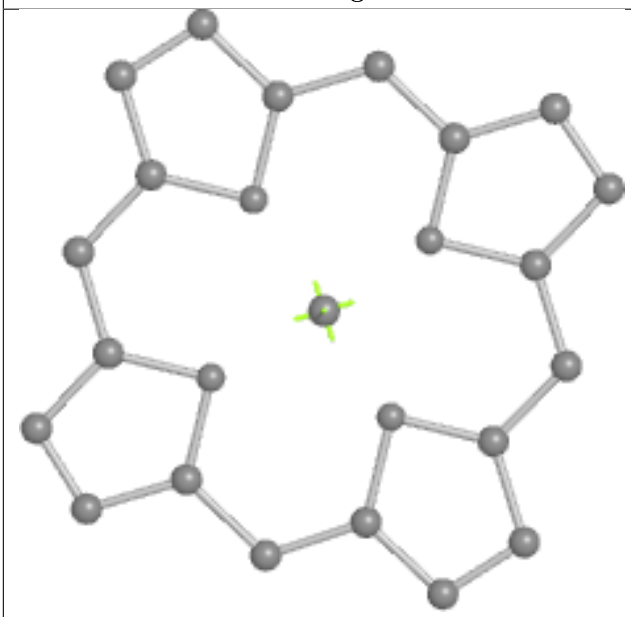
Ligand CLA 2 315



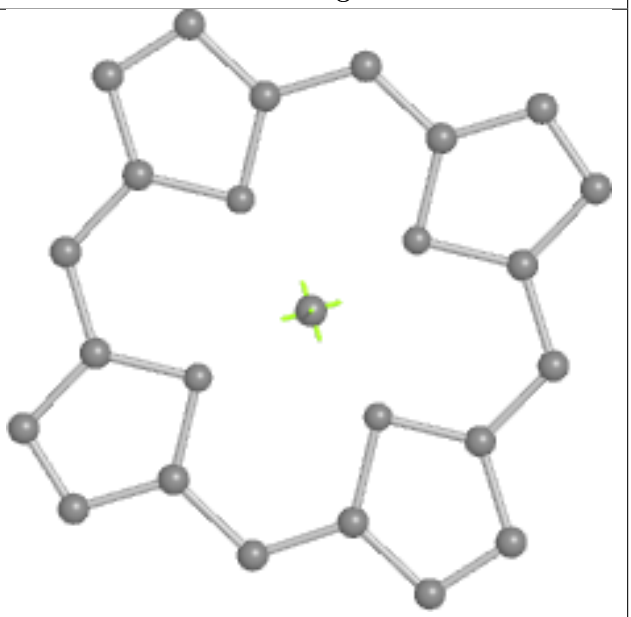
Bond lengths



Bond angles

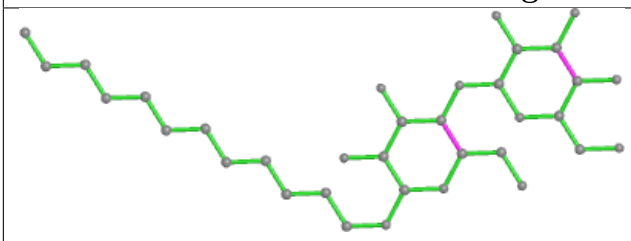


Torsions

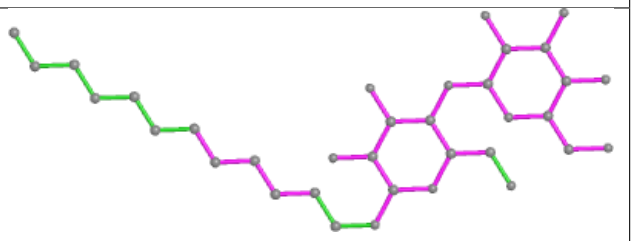


Rings

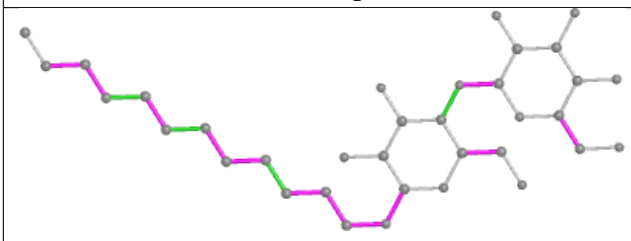
Ligand LMU E 101



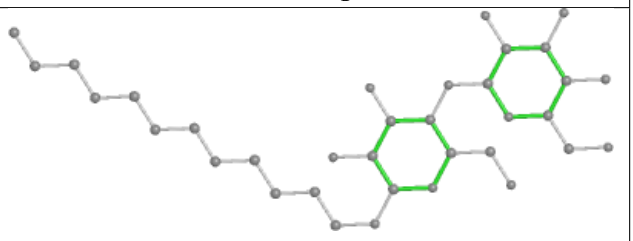
Bond lengths



Bond angles

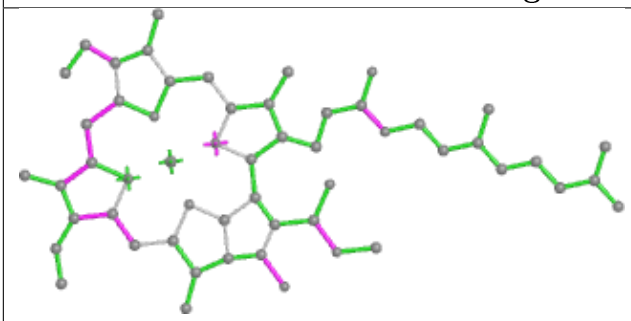


Torsions

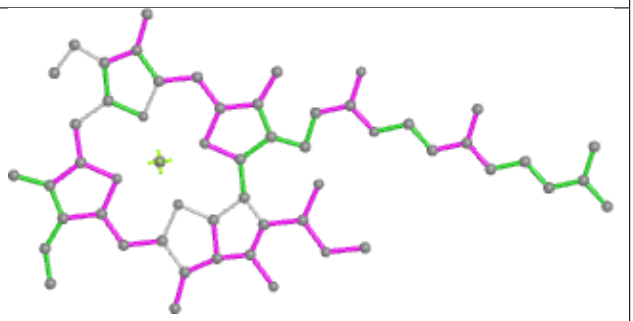


Rings

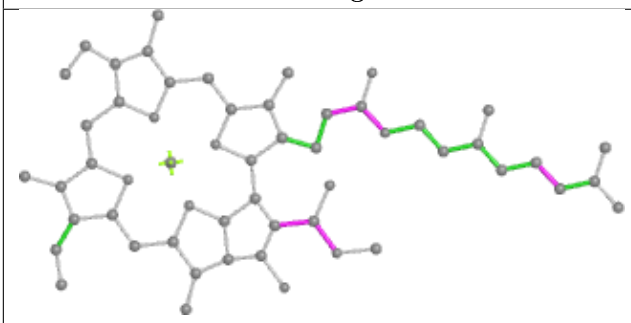
Ligand CLA H 102



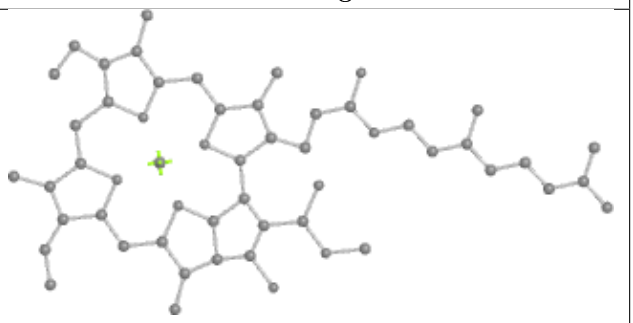
Bond lengths



Bond angles

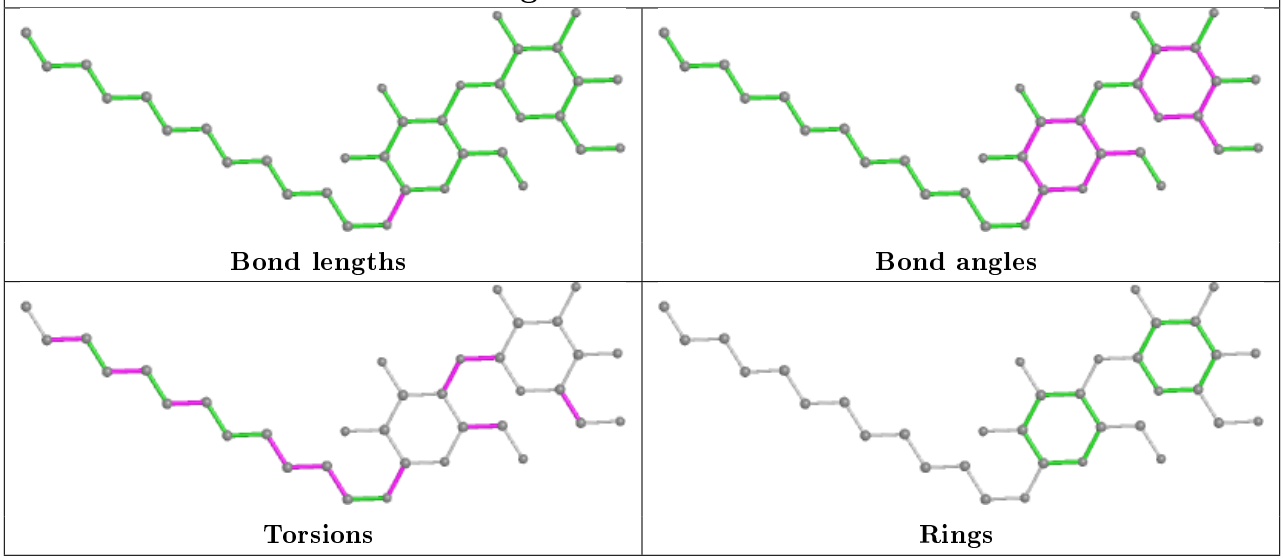


Torsions

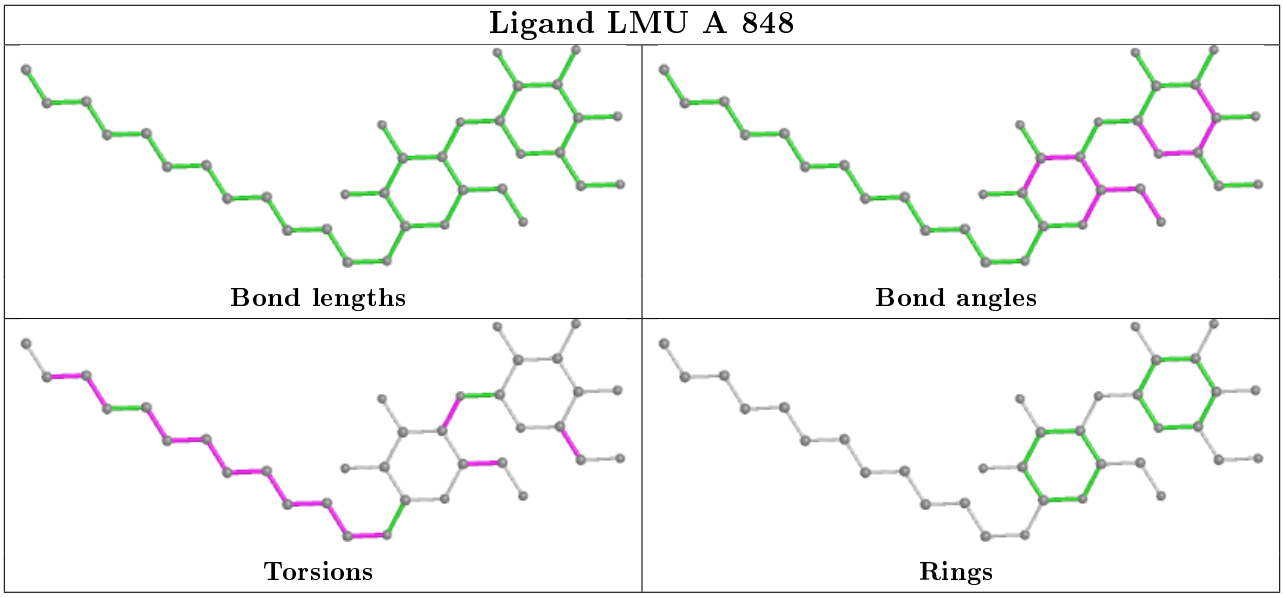


Rings

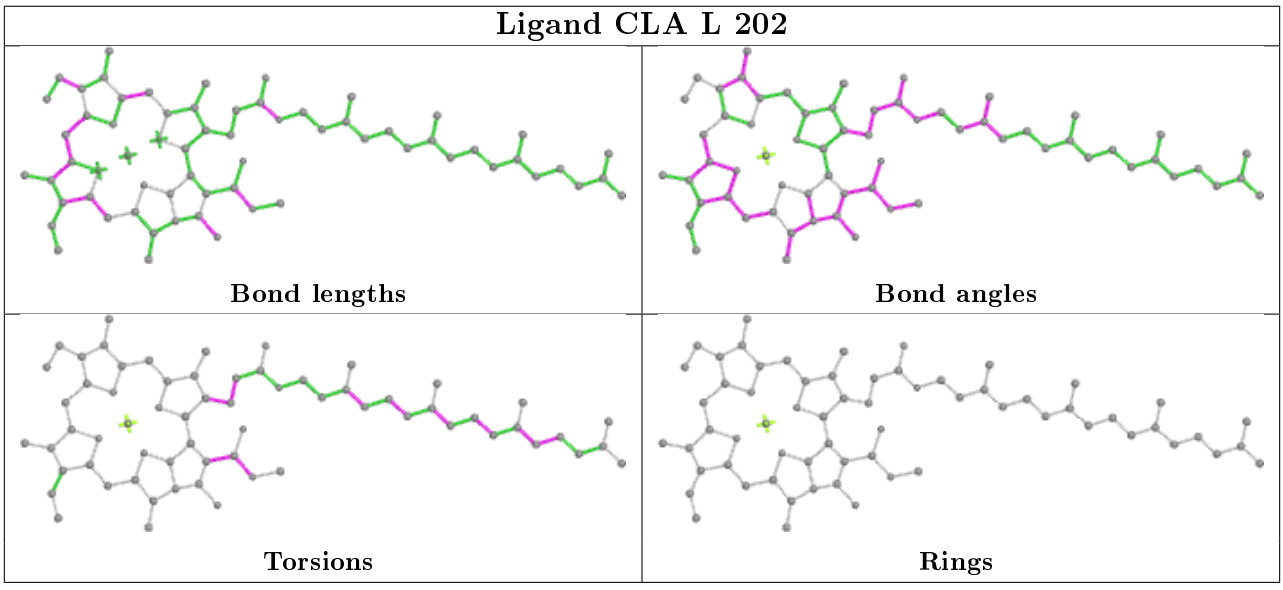
Ligand LMU R 105



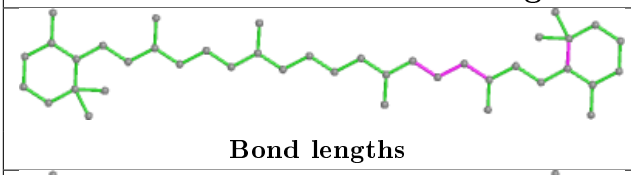
Ligand LMU A 848



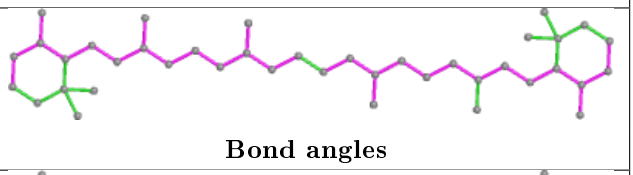
Ligand CLA L 202



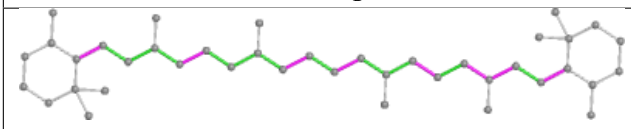
Ligand BCR F 202



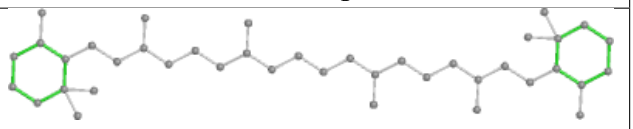
Bond lengths



Bond angles

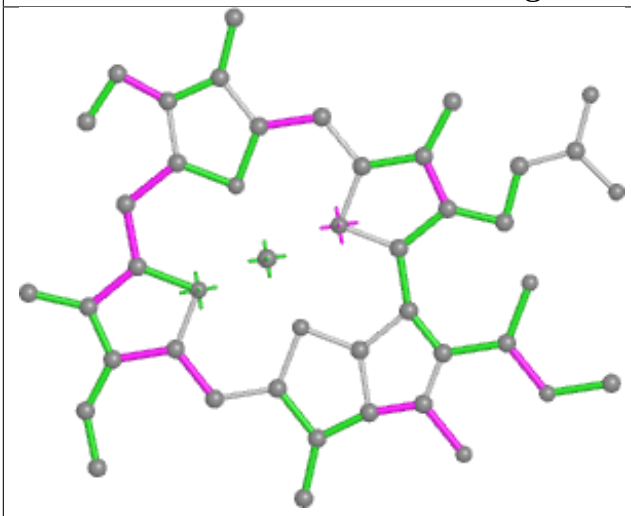


Torsions

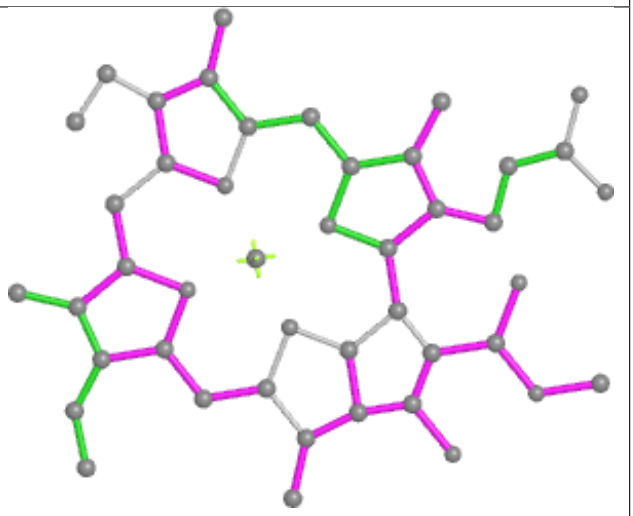


Rings

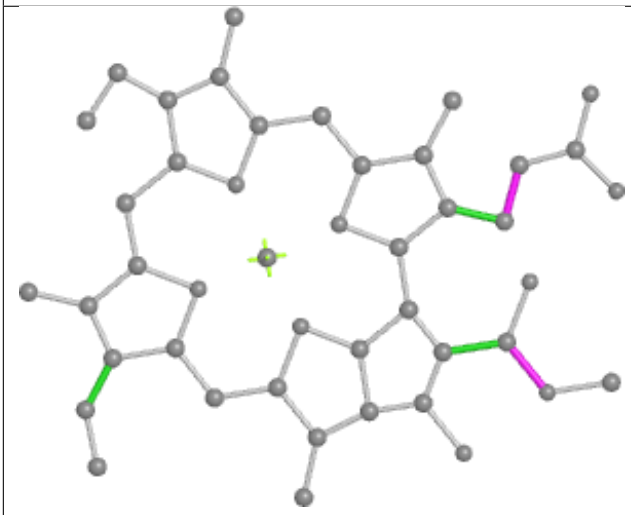
Ligand CLA A 810



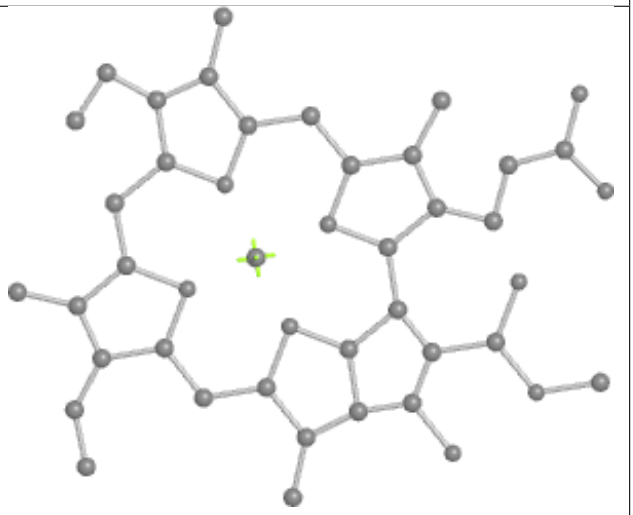
Bond lengths



Bond angles

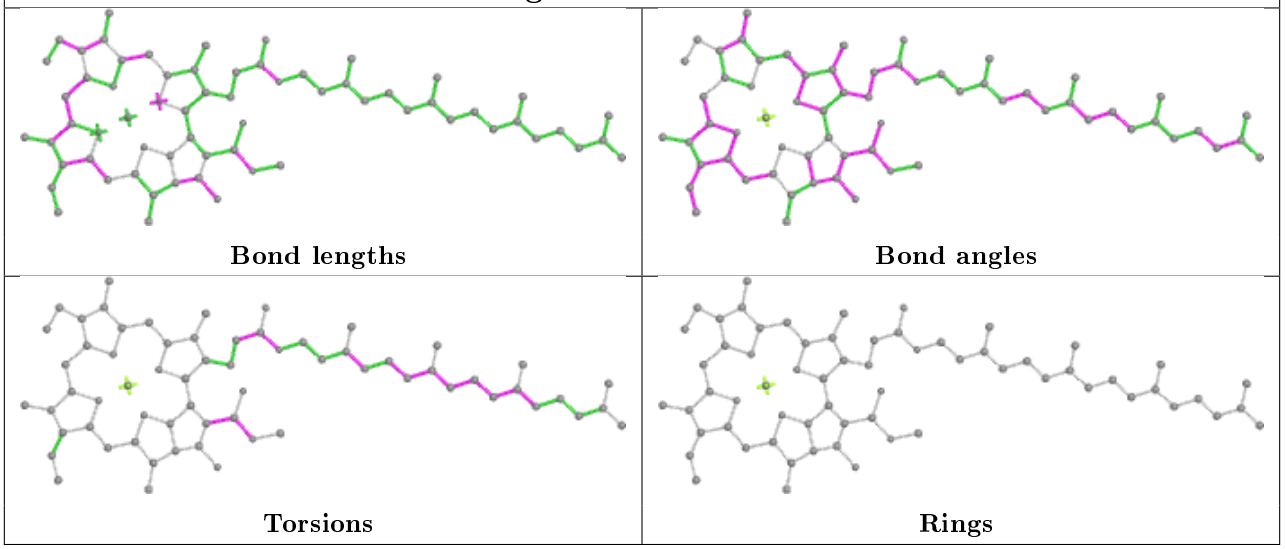


Torsions

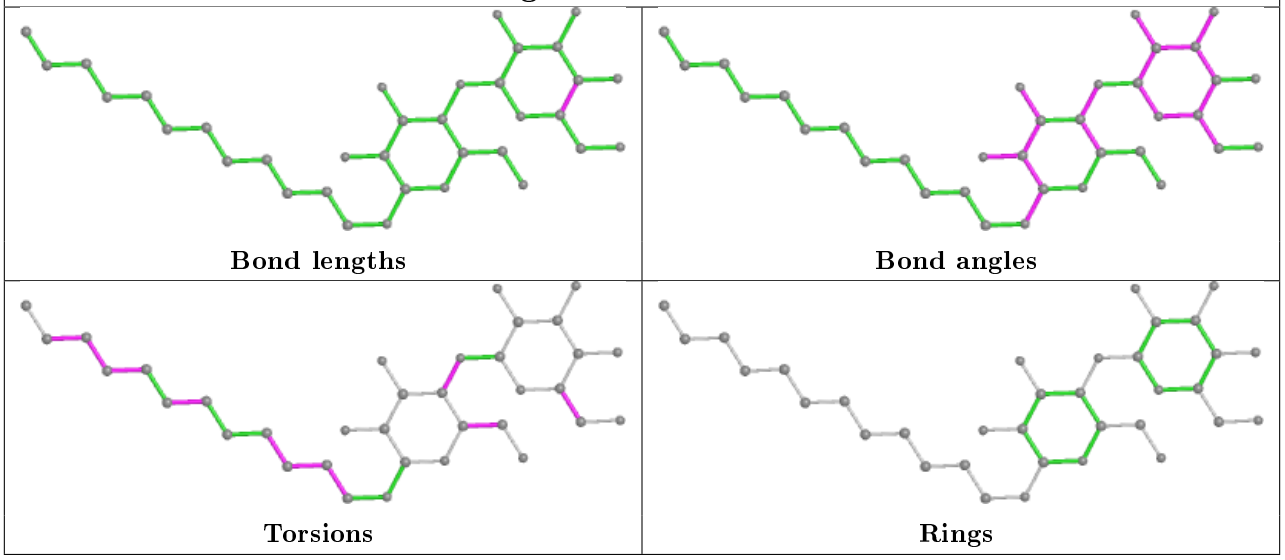


Rings

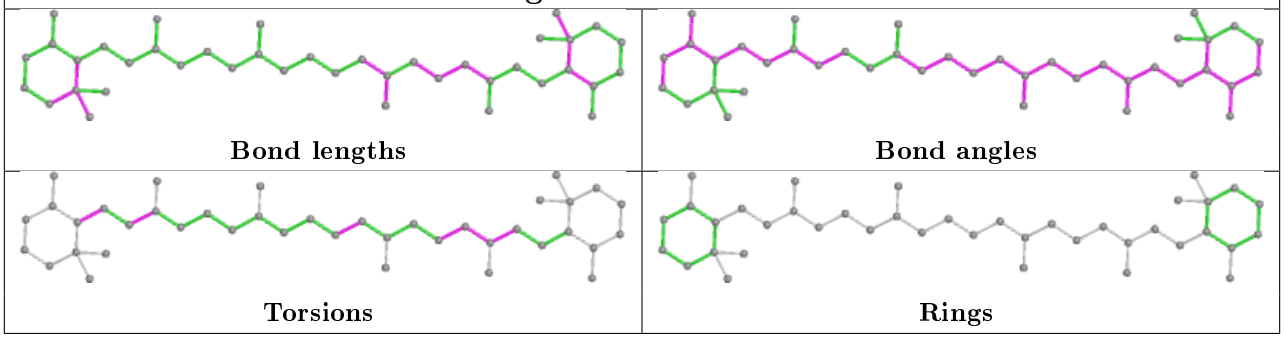
Ligand CLA B 849



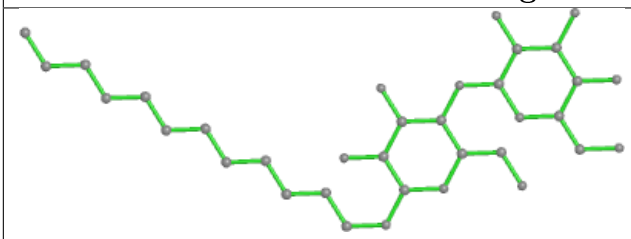
Ligand LMU K 109



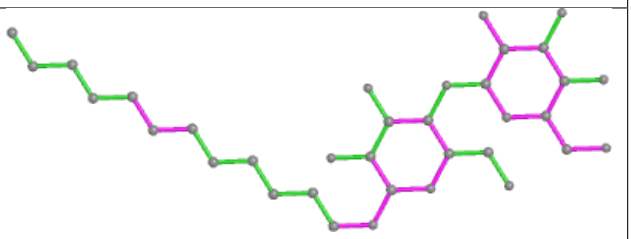
Ligand BCR L 210



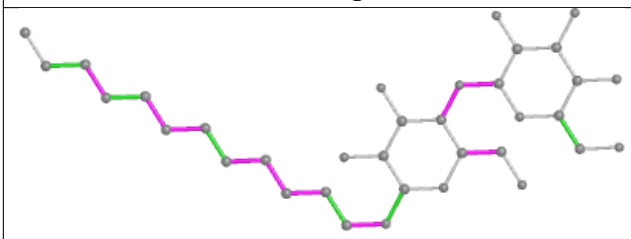
Ligand LMU R 102



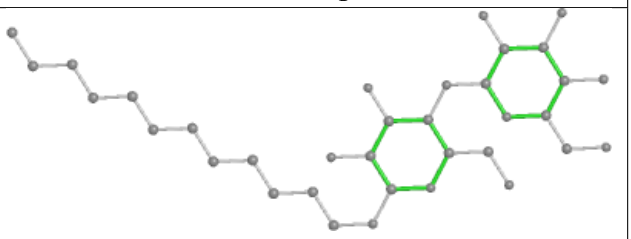
Bond lengths



Bond angles

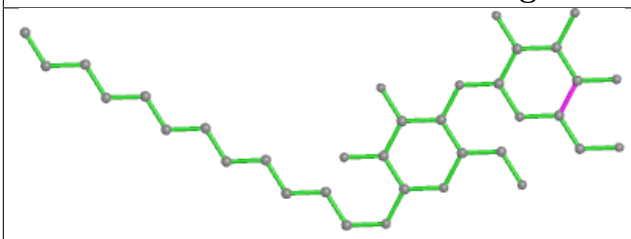


Torsions

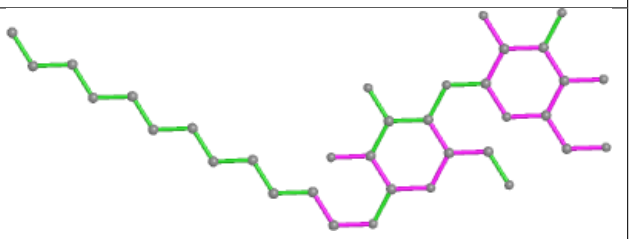


Rings

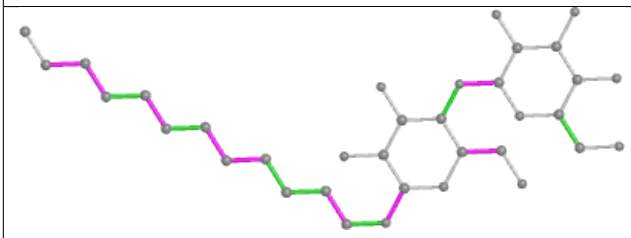
Ligand LMU K 104



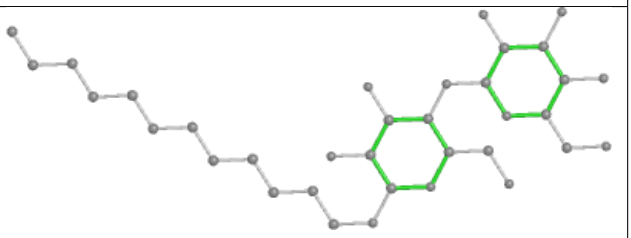
Bond lengths



Bond angles

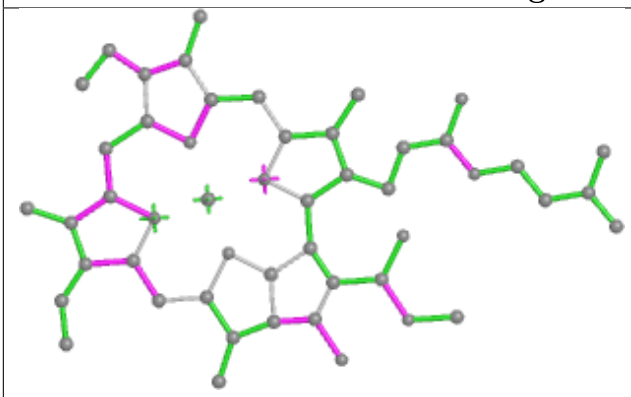


Torsions

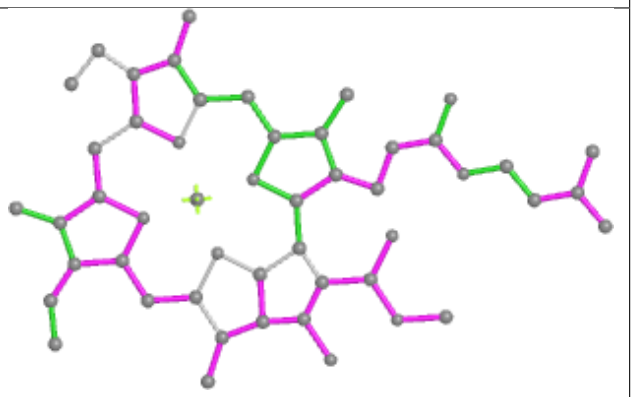


Rings

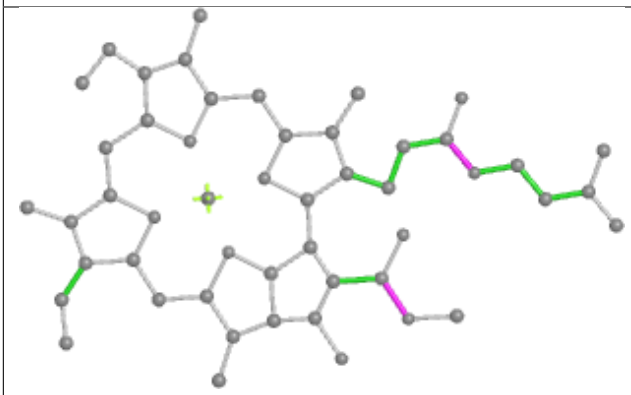
Ligand CLA 3 302



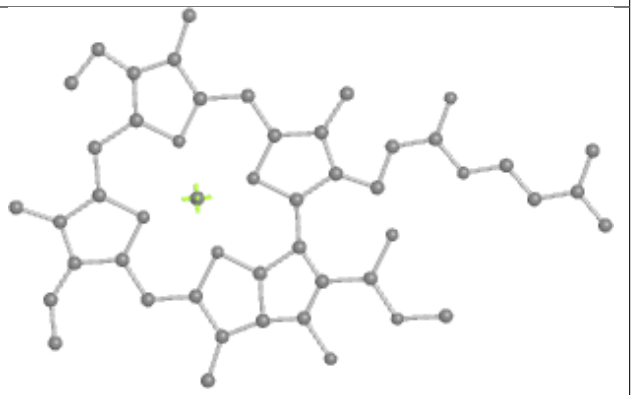
Bond lengths



Bond angles

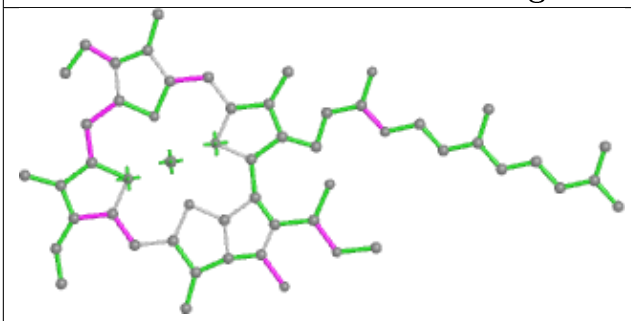


Torsions

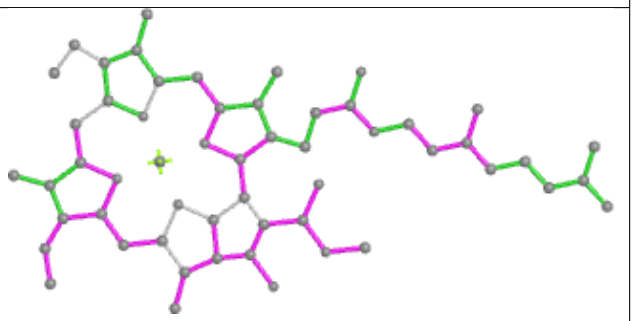


Rings

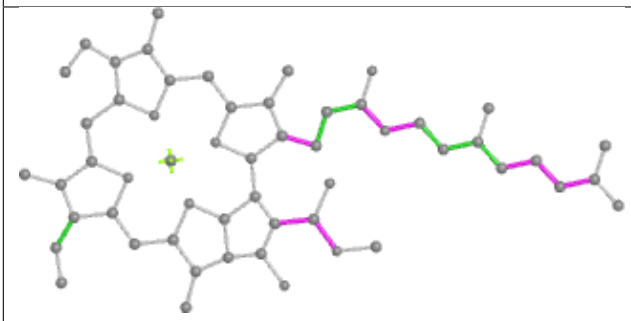
Ligand CLA 4 311



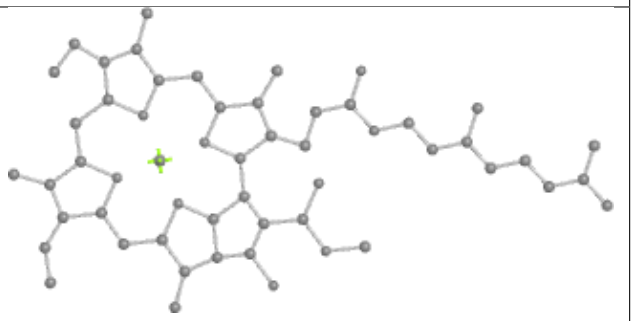
Bond lengths



Bond angles

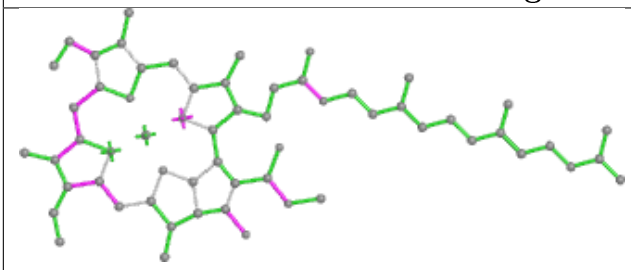


Torsions

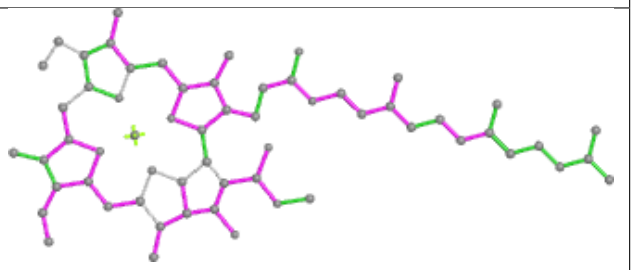


Rings

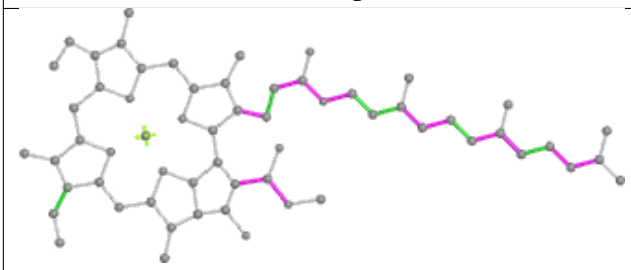
Ligand CLA B 805



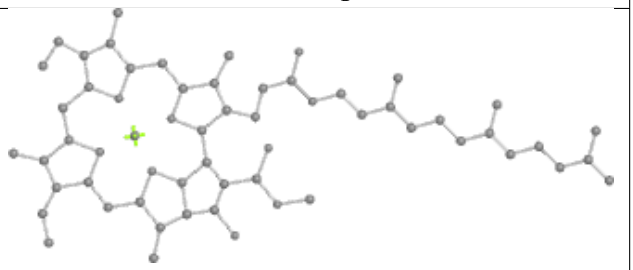
Bond lengths



Bond angles

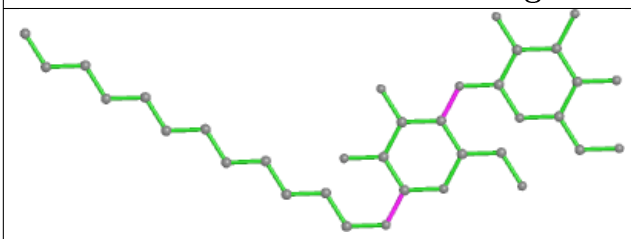


Torsions

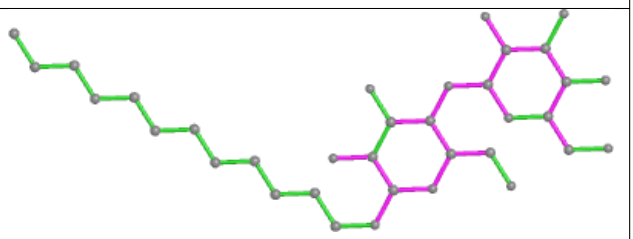


Rings

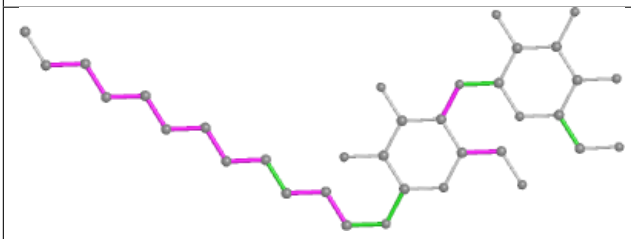
Ligand LMU 1 219



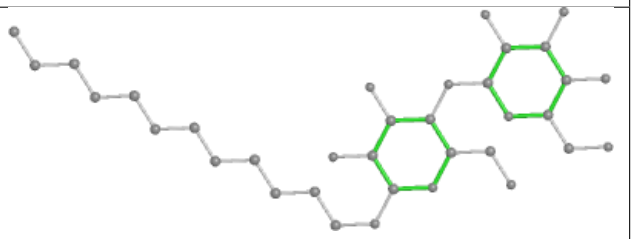
Bond lengths



Bond angles

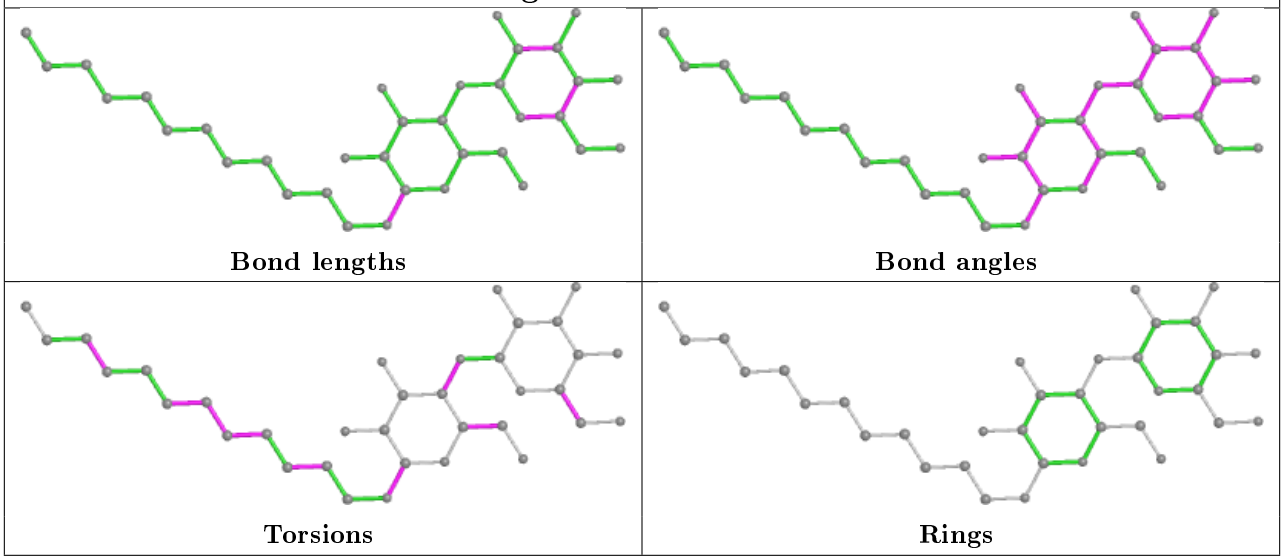


Torsions

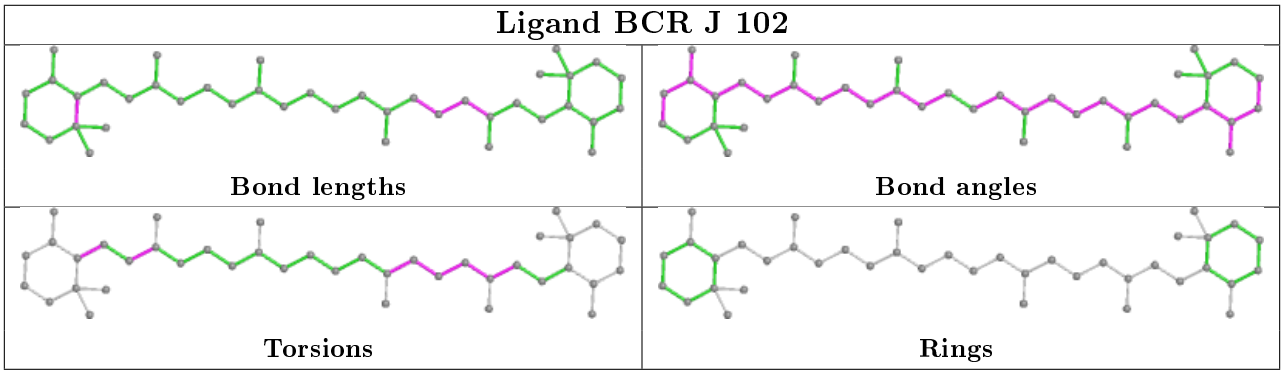


Rings

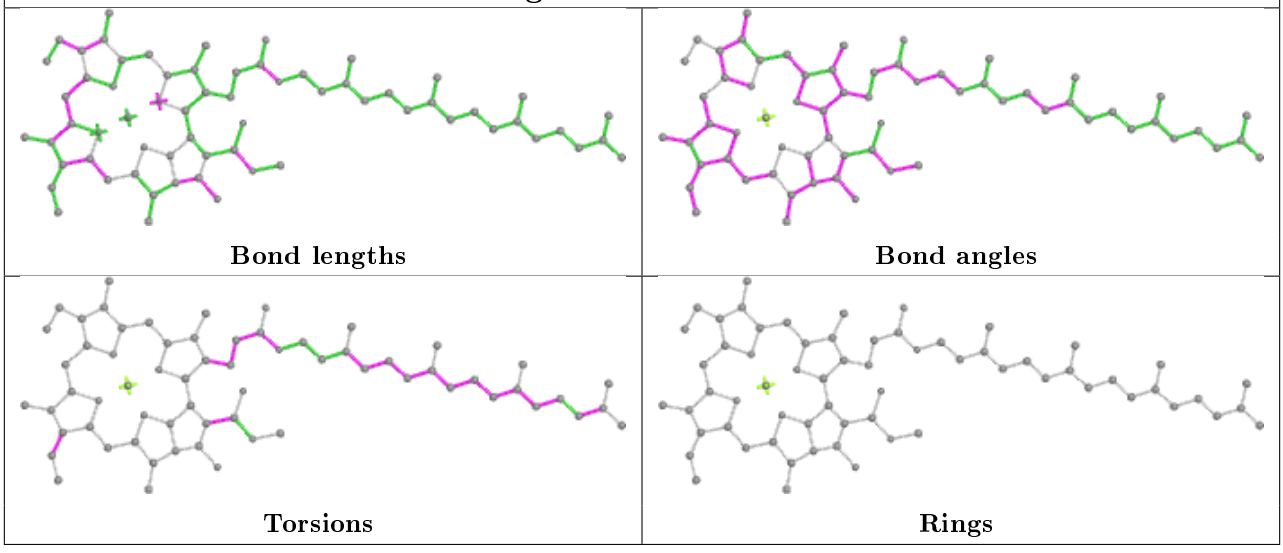
Ligand LMU B 802



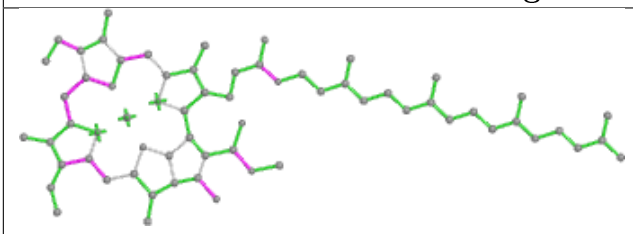
Ligand BCR J 102



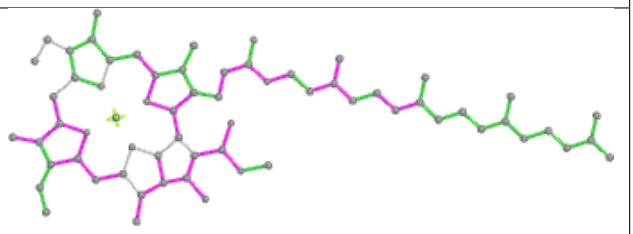
Ligand CLA A 850



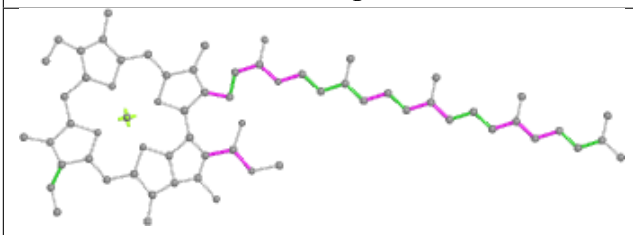
Ligand CLA K 103



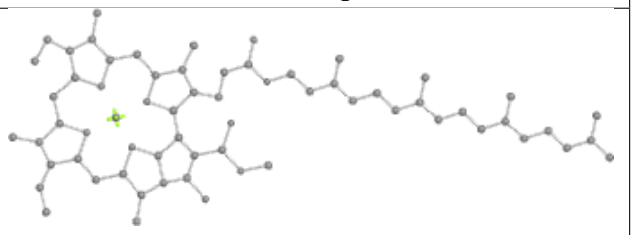
Bond lengths



Bond angles

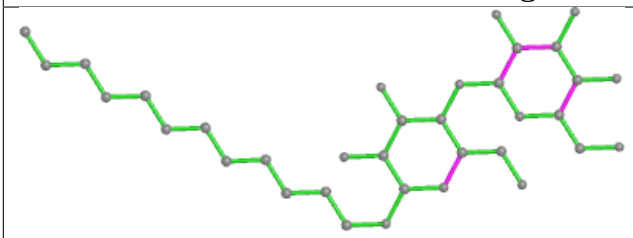


Torsions

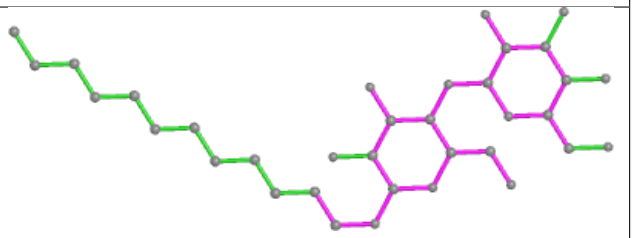


Rings

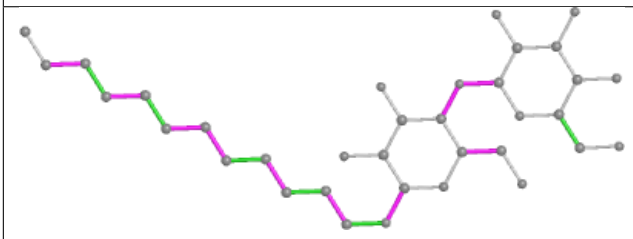
Ligand LMU H 106



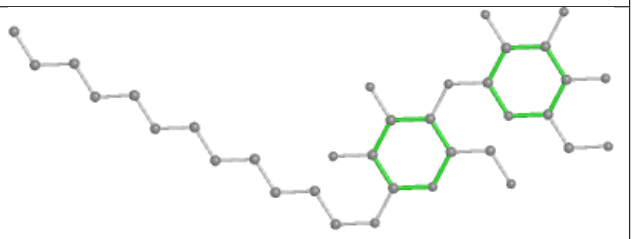
Bond lengths



Bond angles

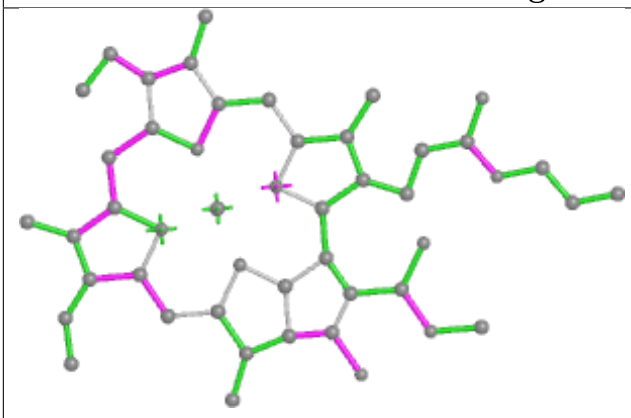


Torsions

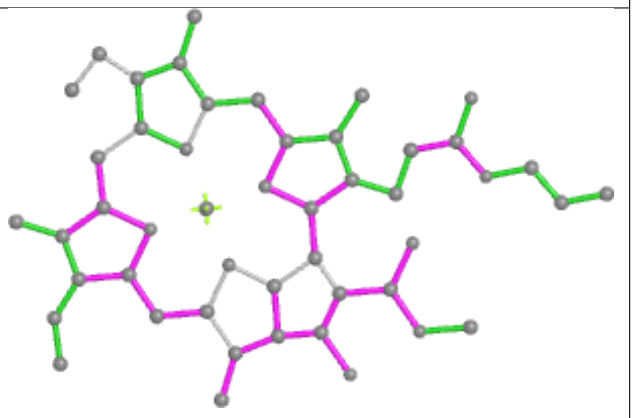


Rings

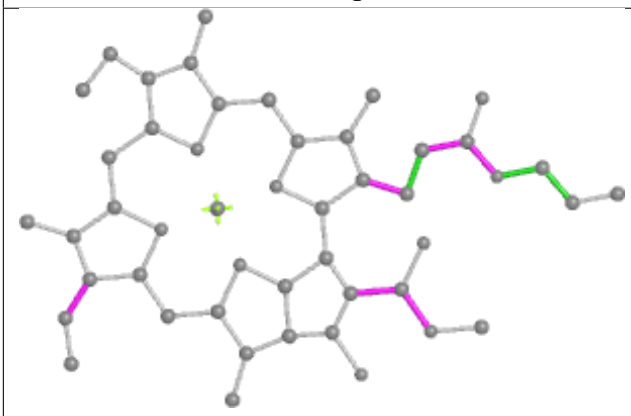
Ligand CLA J 101



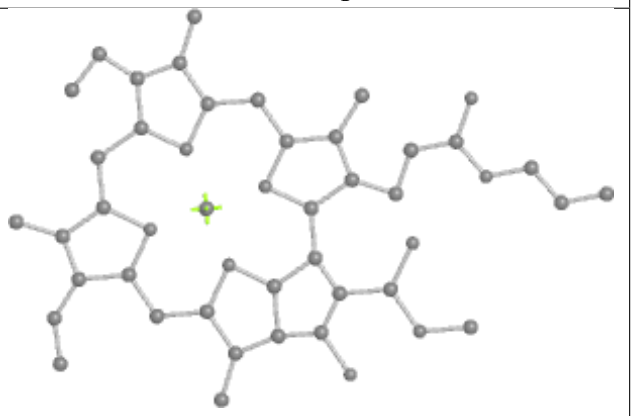
Bond lengths



Bond angles

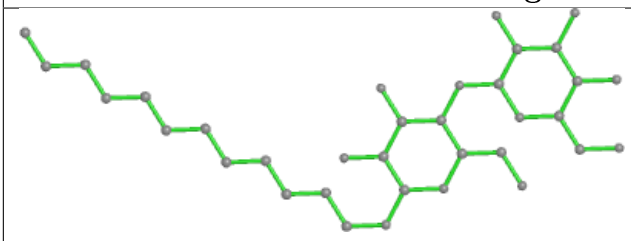


Torsions

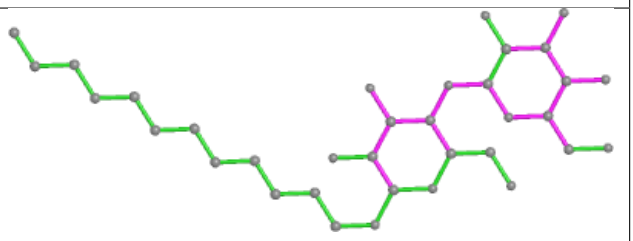


Rings

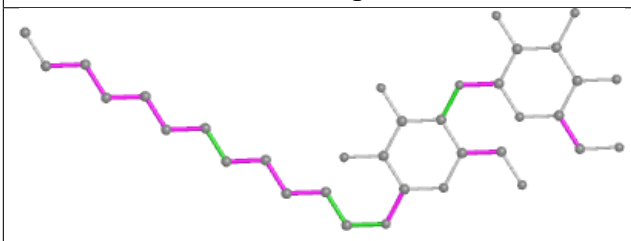
Ligand LMU 3 322



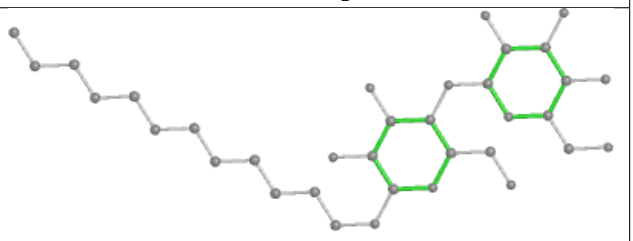
Bond lengths



Bond angles

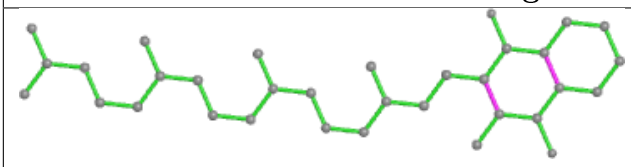


Torsions

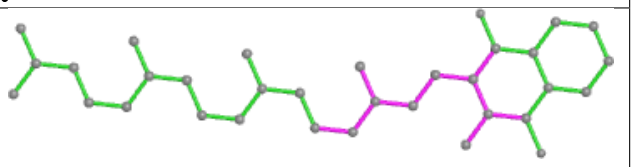


Rings

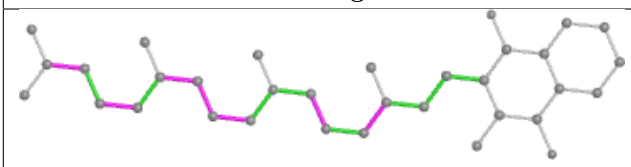
Ligand PQN B 841



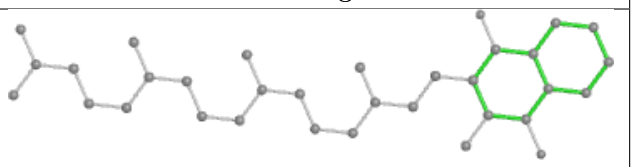
Bond lengths



Bond angles

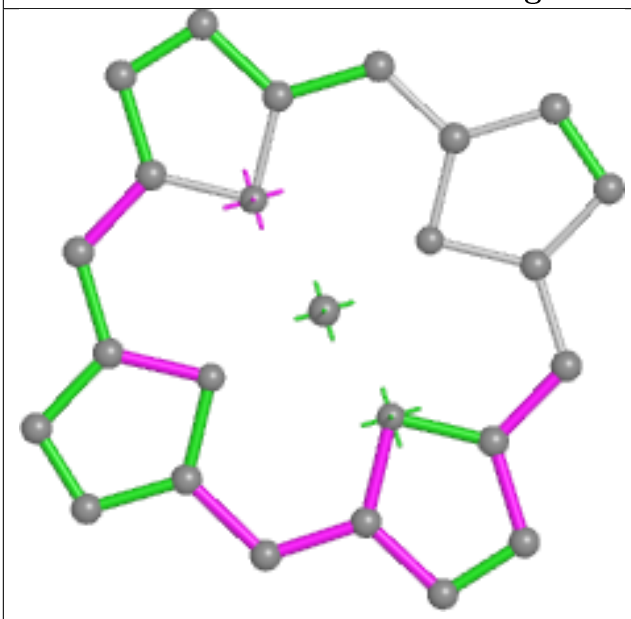


Torsions

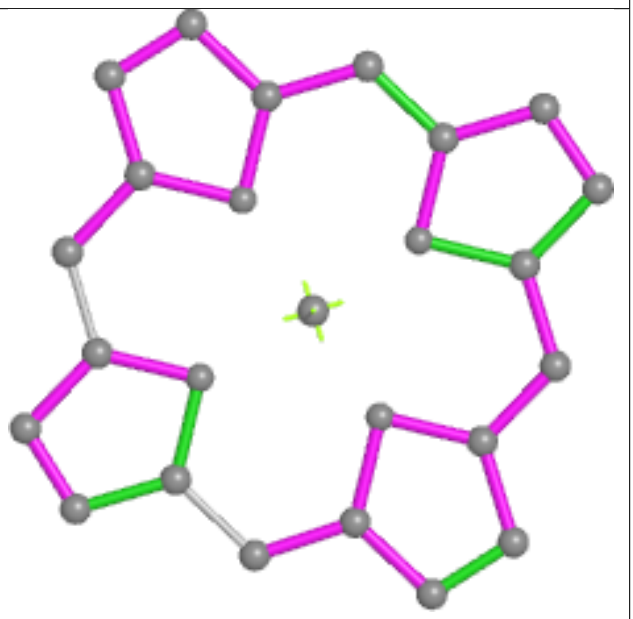


Rings

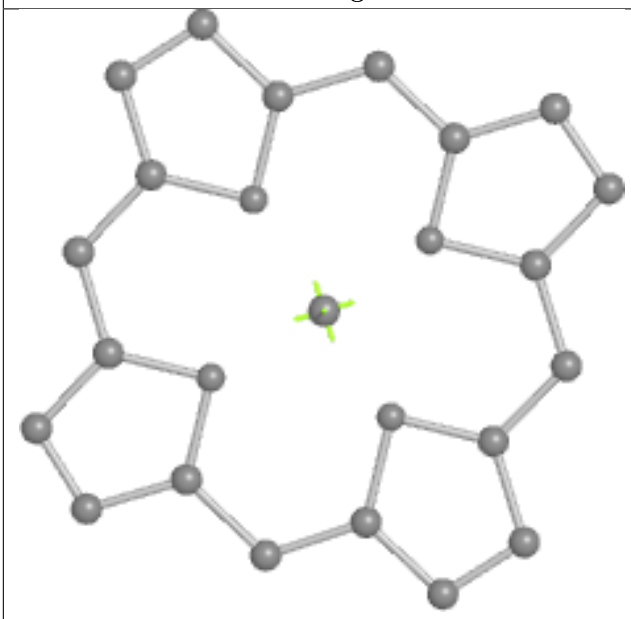
Ligand CLA A 802



Bond lengths



Bond angles



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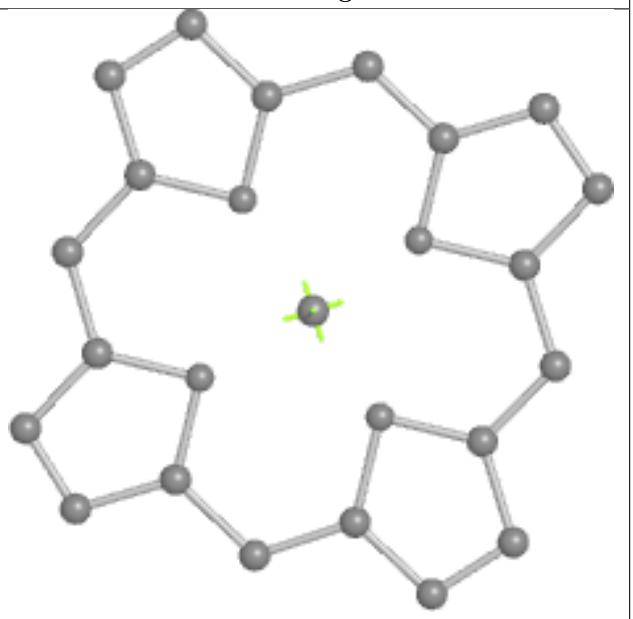
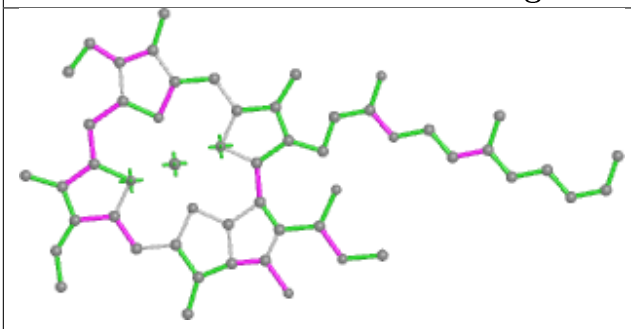


Rings

Ligand CLA B 822



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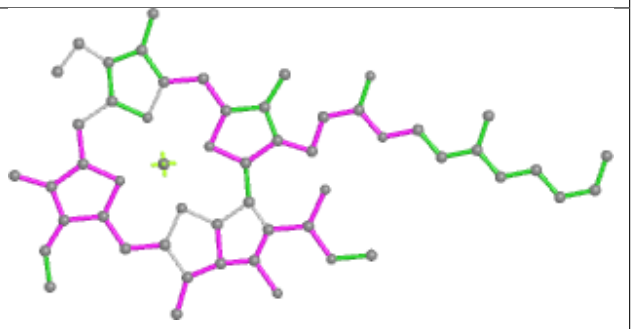
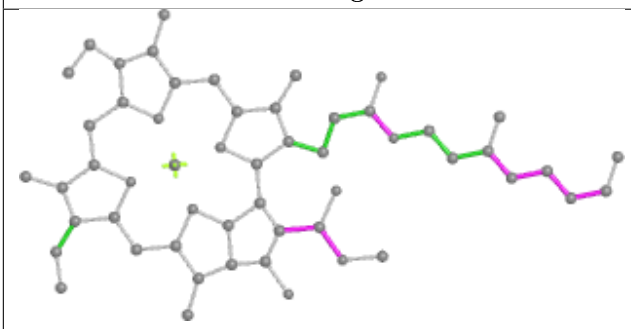
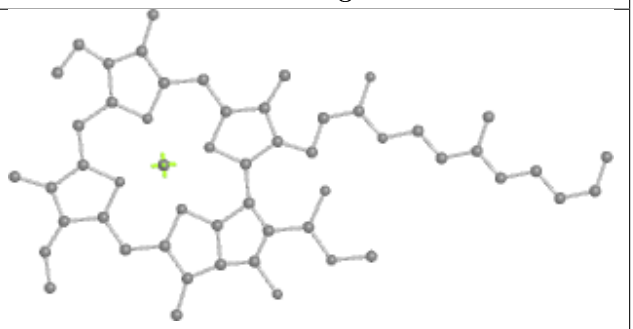


Bond angles

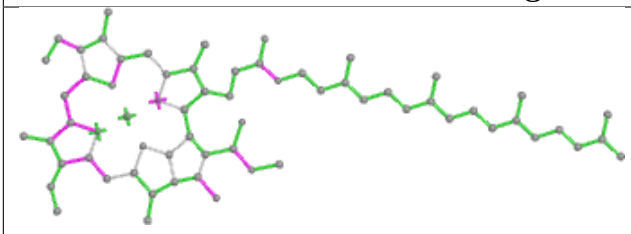


Torsions

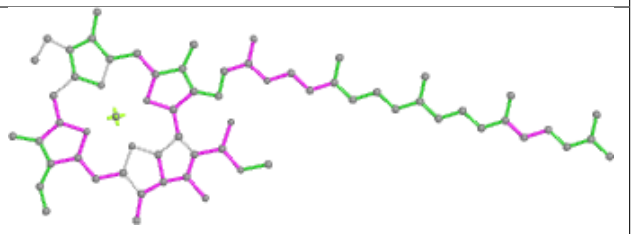


Rings

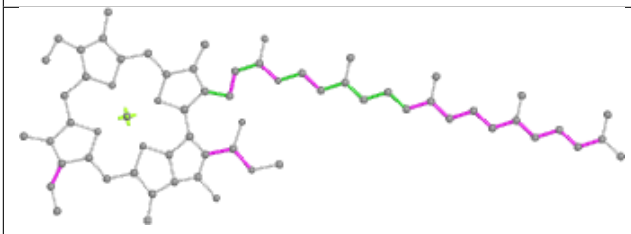
Ligand CLA A 852



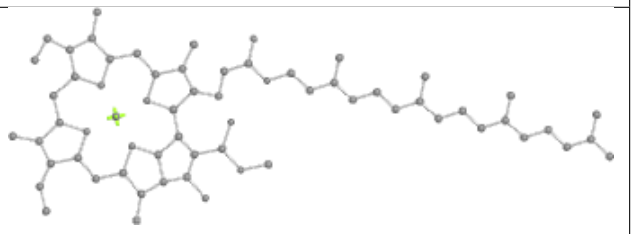
Bond lengths



Bond angles

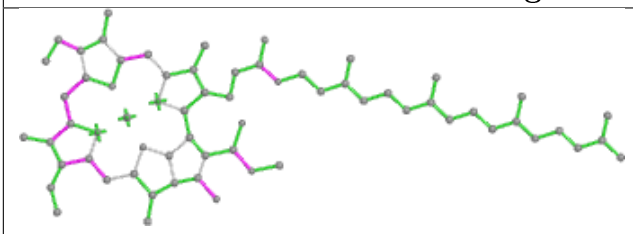


Torsions

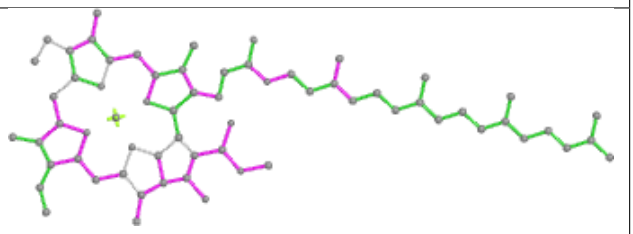


Rings

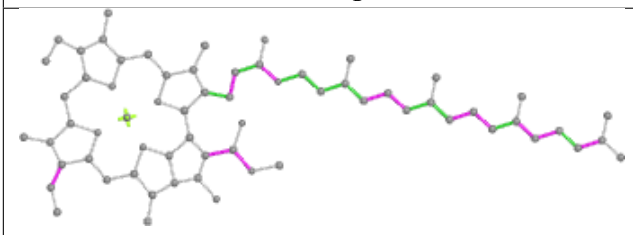
Ligand CLA A 819



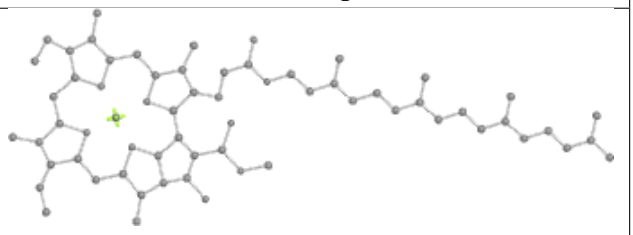
Bond lengths



Bond angles

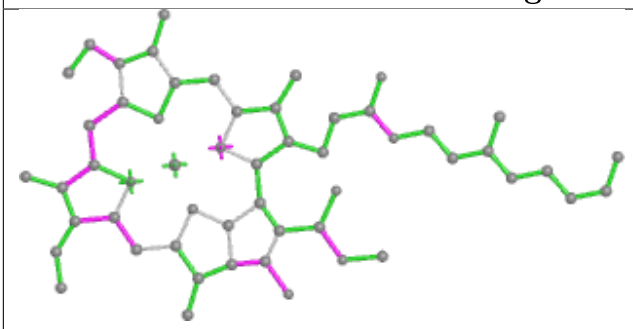


Torsions

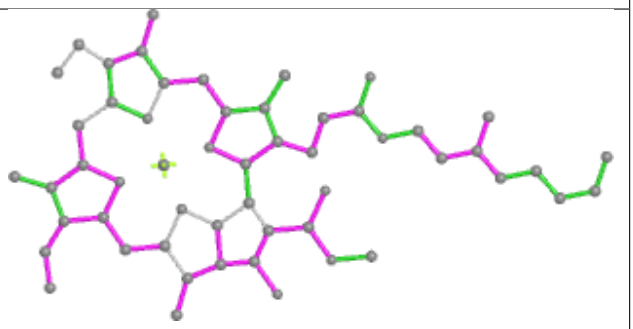


Rings

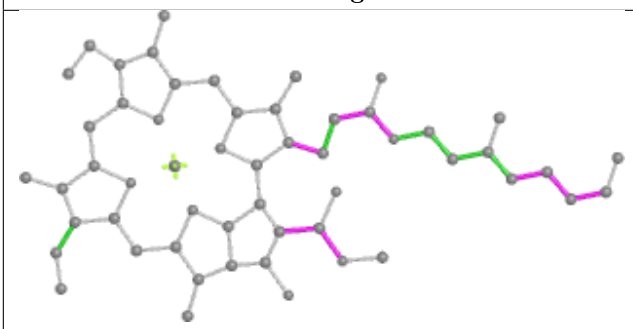
Ligand CLA A 813



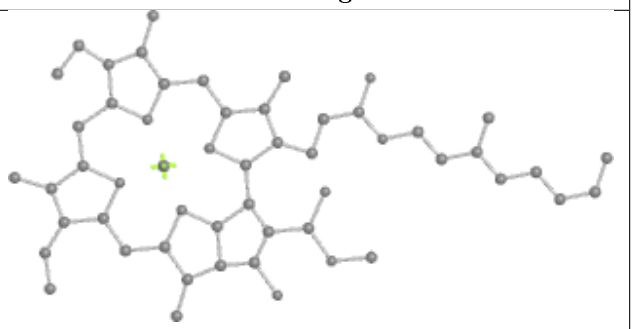
Bond lengths



Bond angles

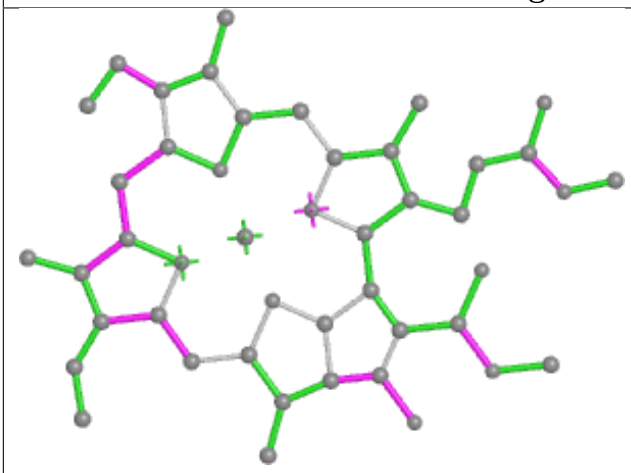


Torsions

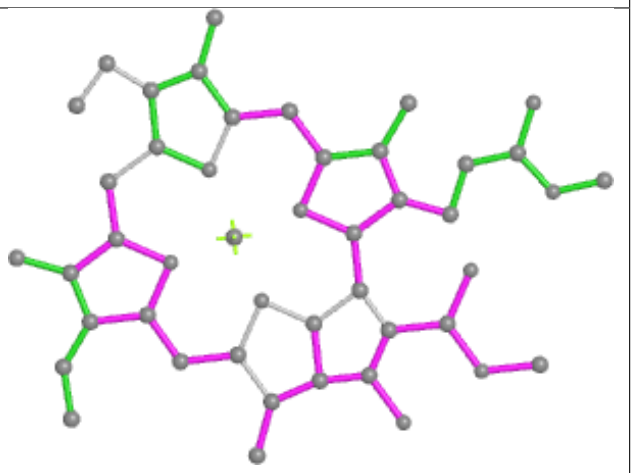


Rings

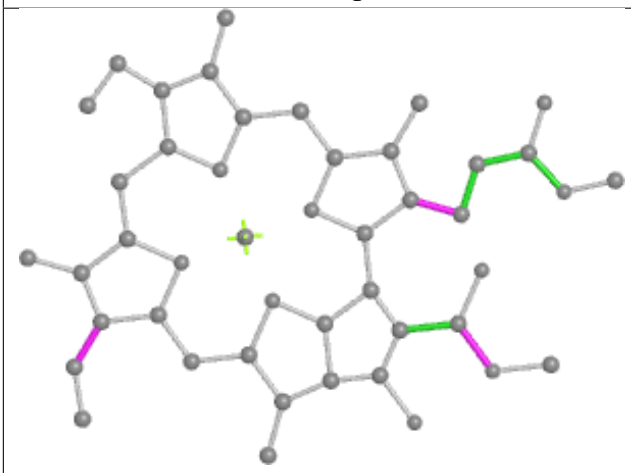
Ligand CLA 1 204



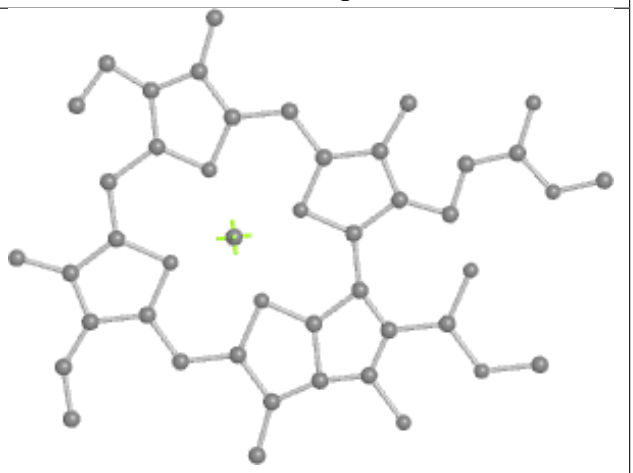
Bond lengths



Bond angles

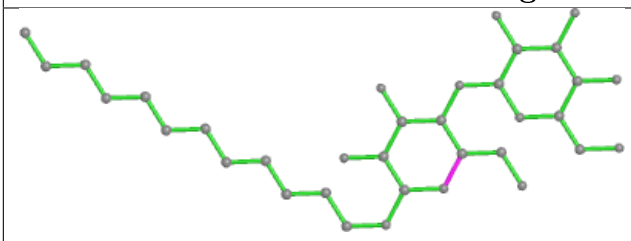


Torsions

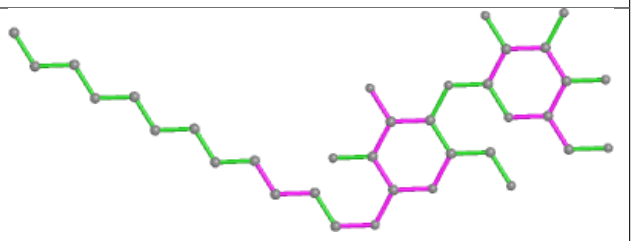


Rings

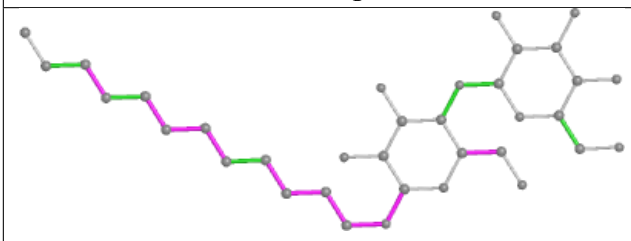
Ligand LMU A 854



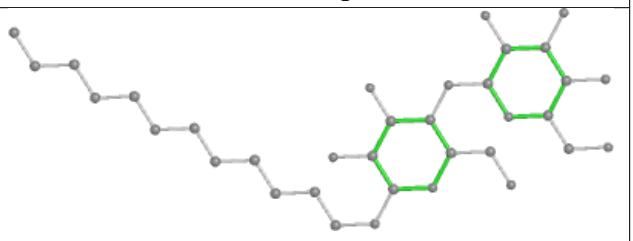
Bond lengths



Bond angles

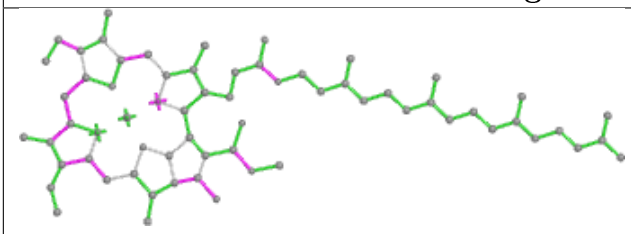


Torsions

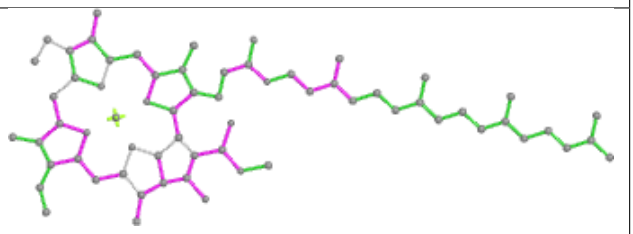


Rings

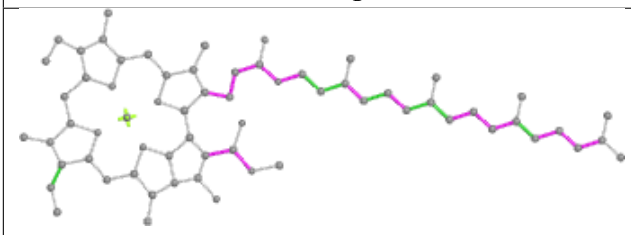
Ligand CLA B 824



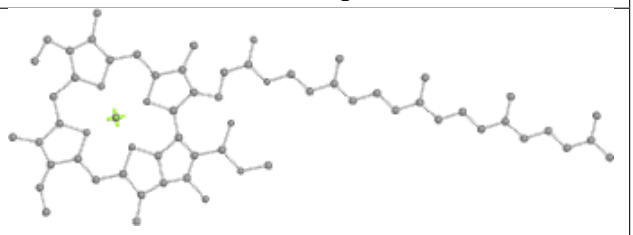
Bond lengths



Bond angles

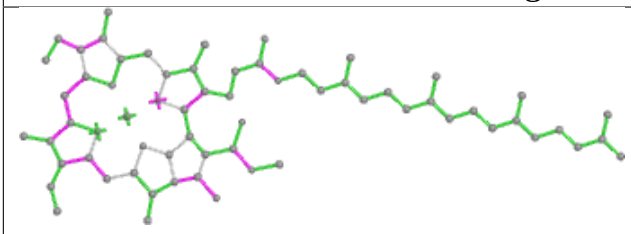


Torsions

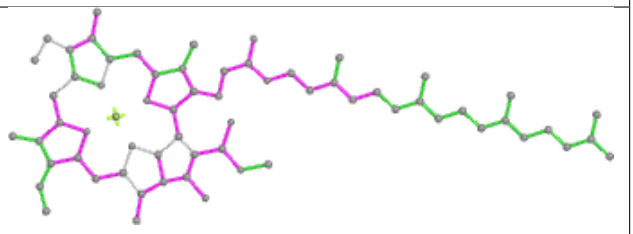


Rings

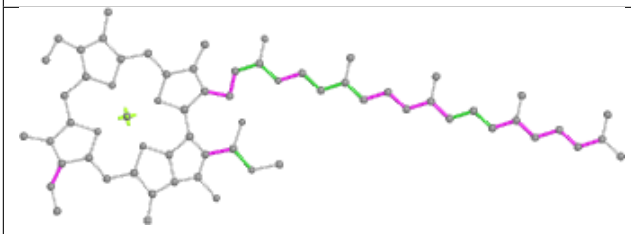
Ligand CLA A 808



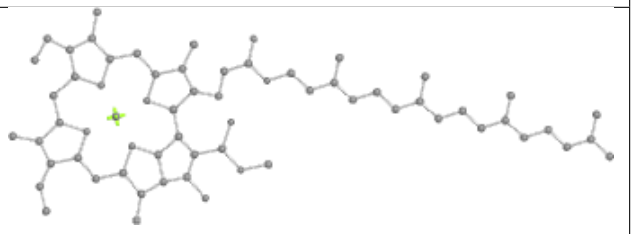
Bond lengths



Bond angles

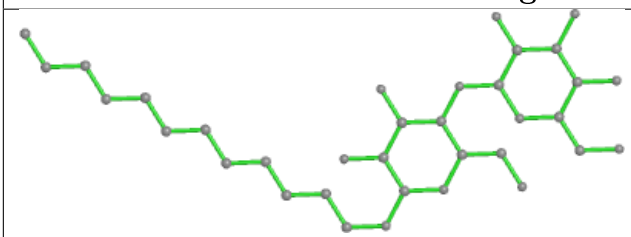


Torsions

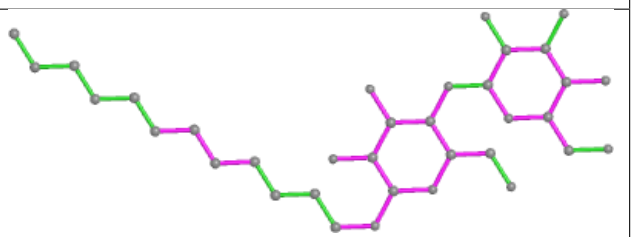


Rings

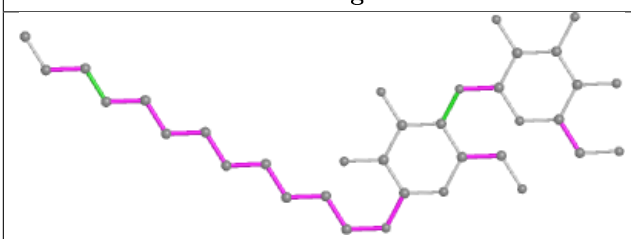
Ligand LMU K 106



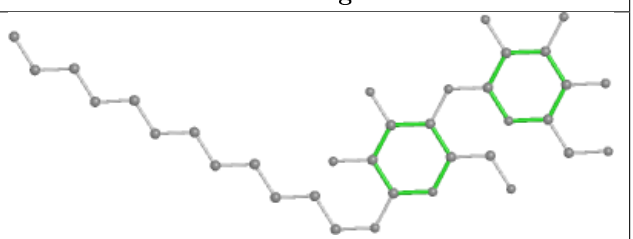
Bond lengths



Bond angles

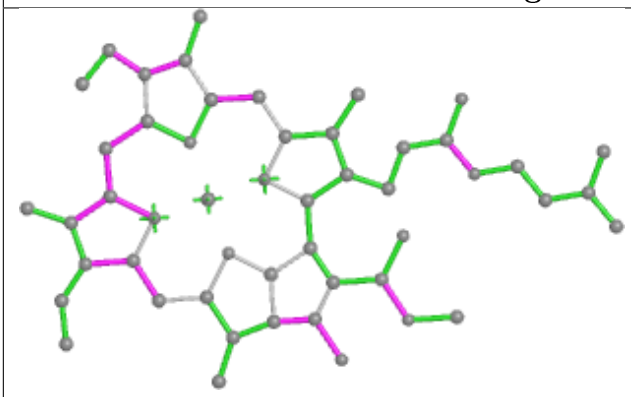


Torsions

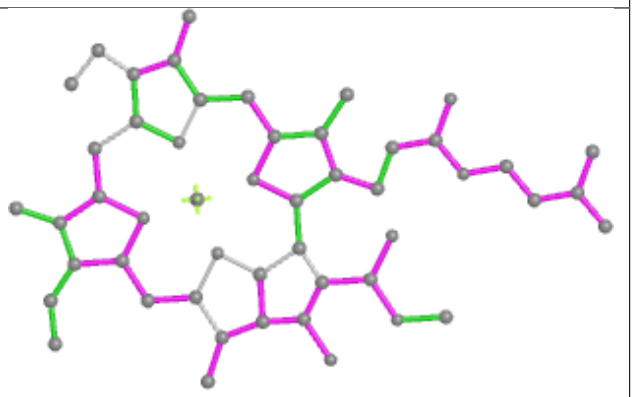


Rings

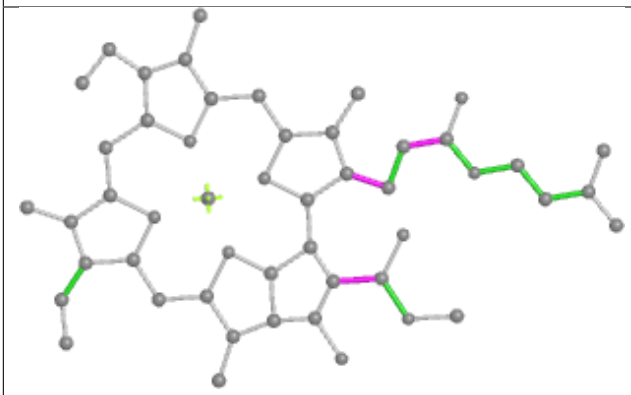
Ligand CLA A 803



Bond lengths



Bond angles



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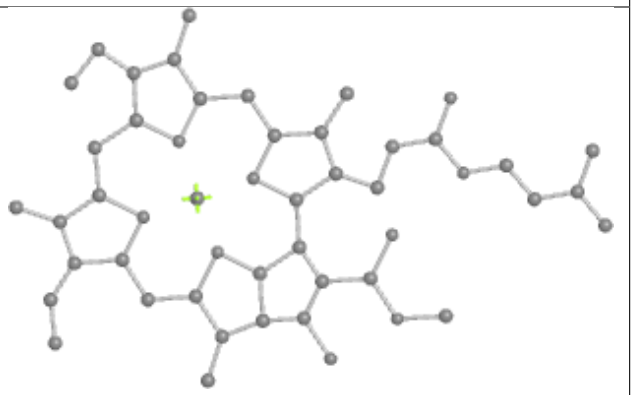
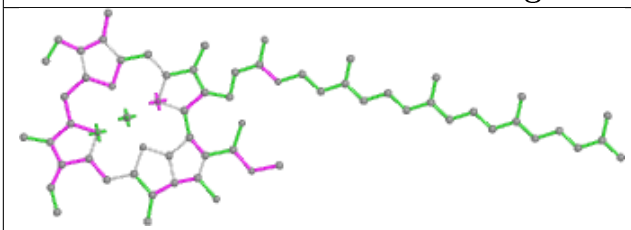
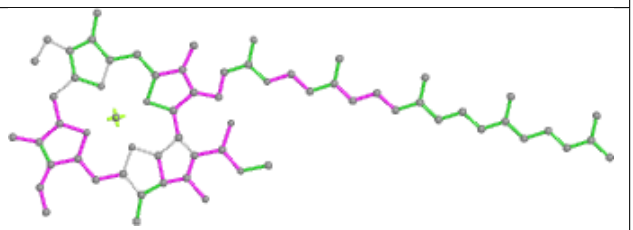


Rings

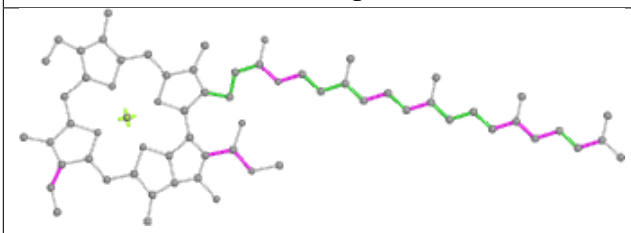
Ligand CLA B 821



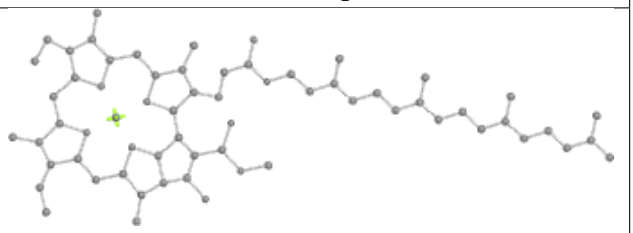
Bond lengths



Bond angles

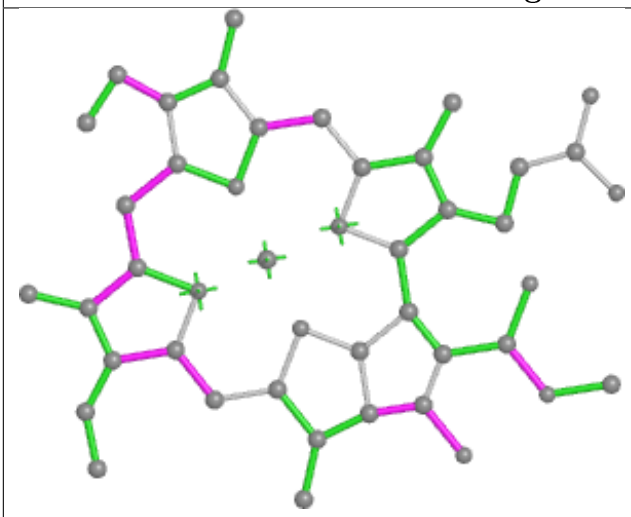


Torsions

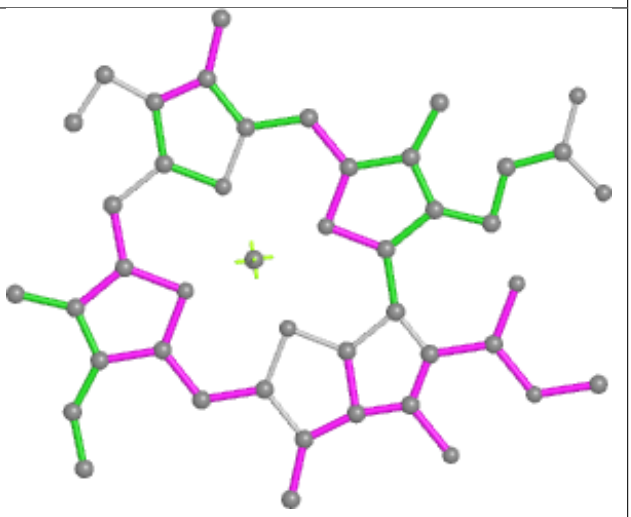


Rings

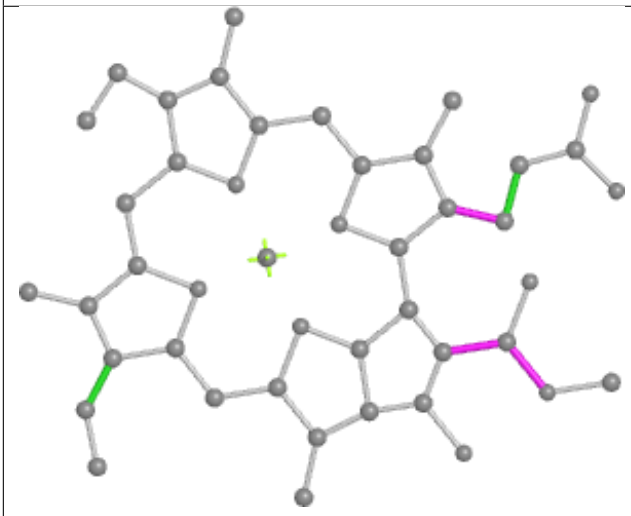
Ligand CLA B 833



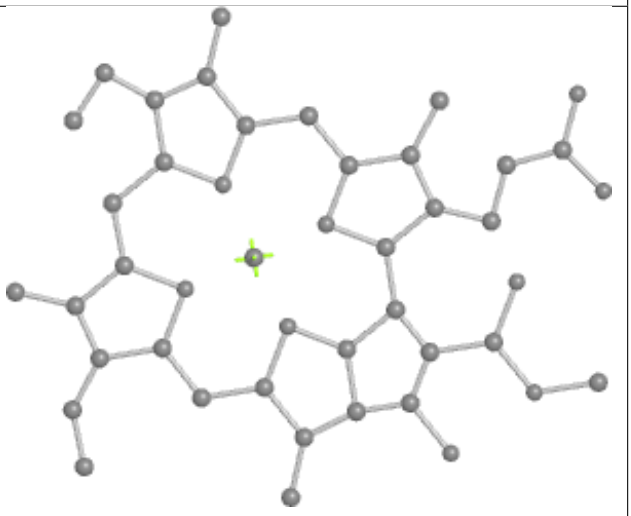
Bond lengths



Bond angles

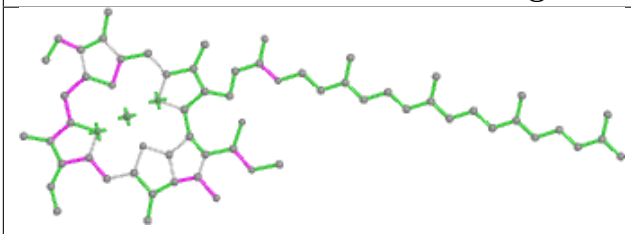


Torsions

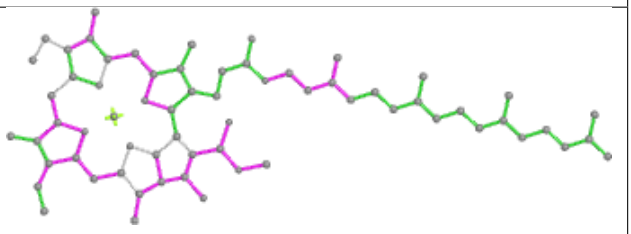


Rings

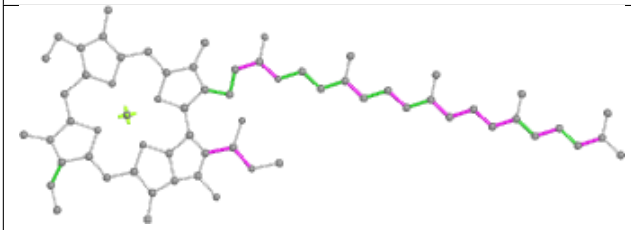
Ligand CLA 3 318



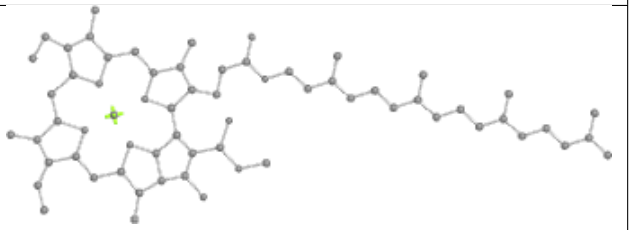
Bond lengths



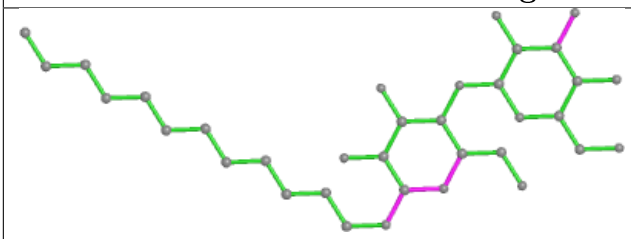
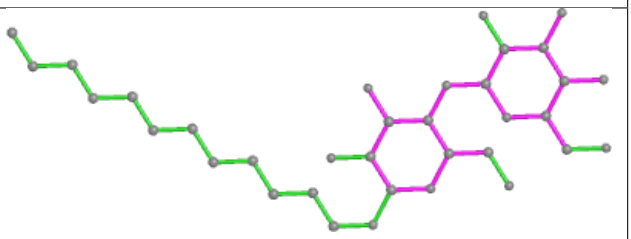
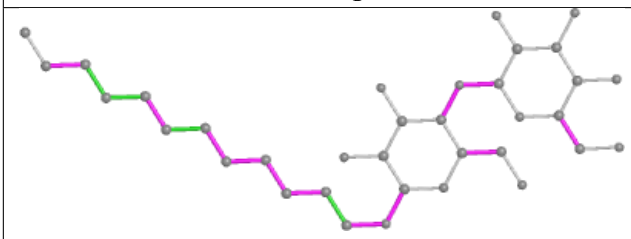
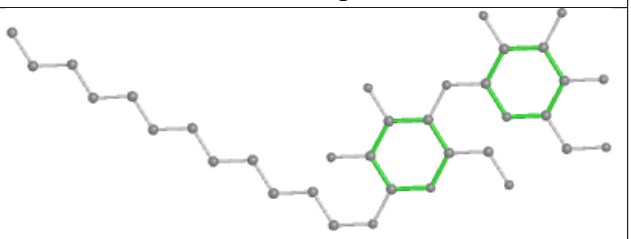
Bond angles

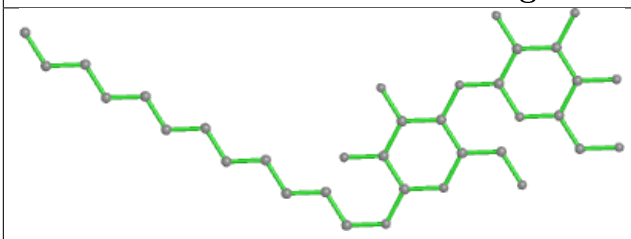
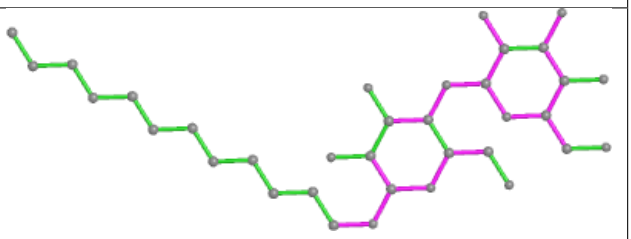
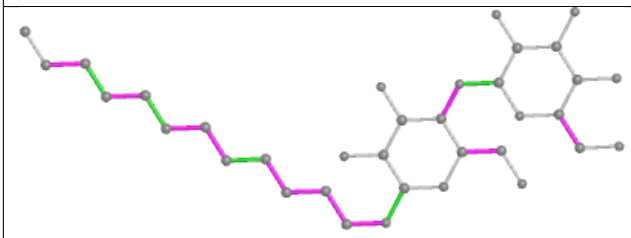
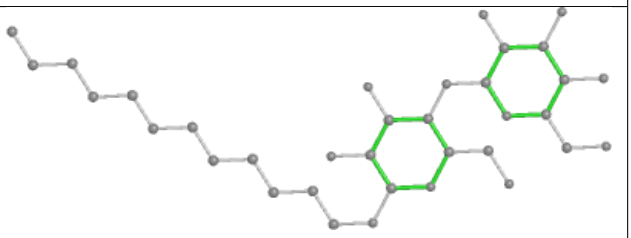


Torsions

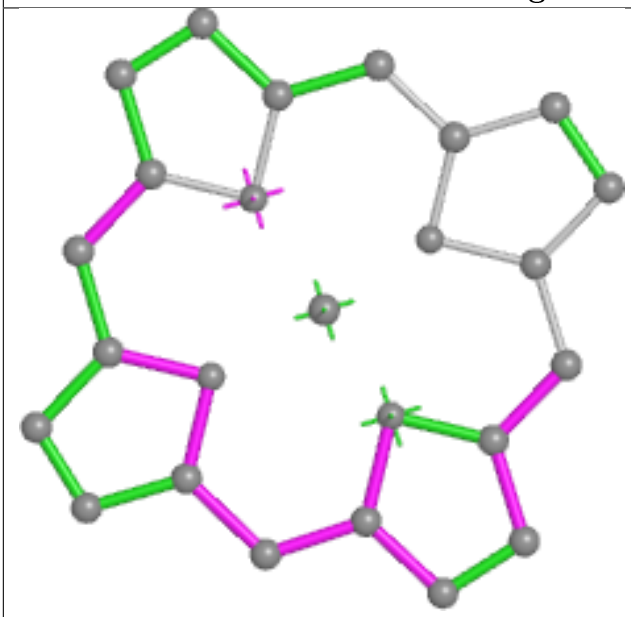


Rings

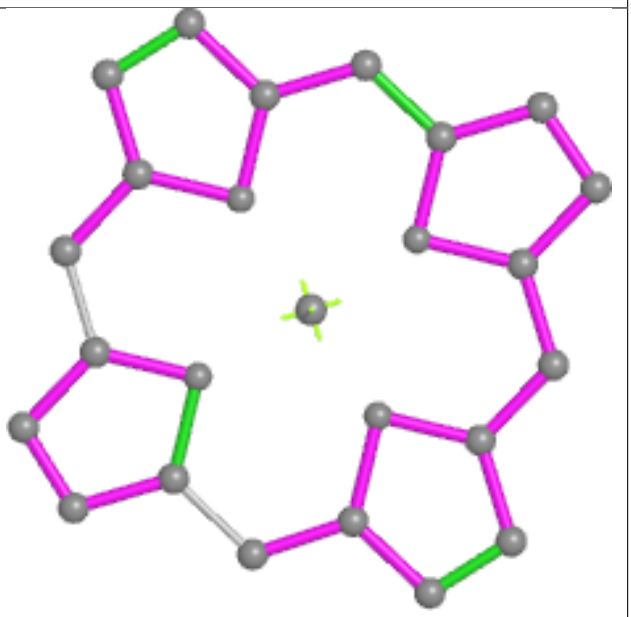
Ligand LMU H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU R 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

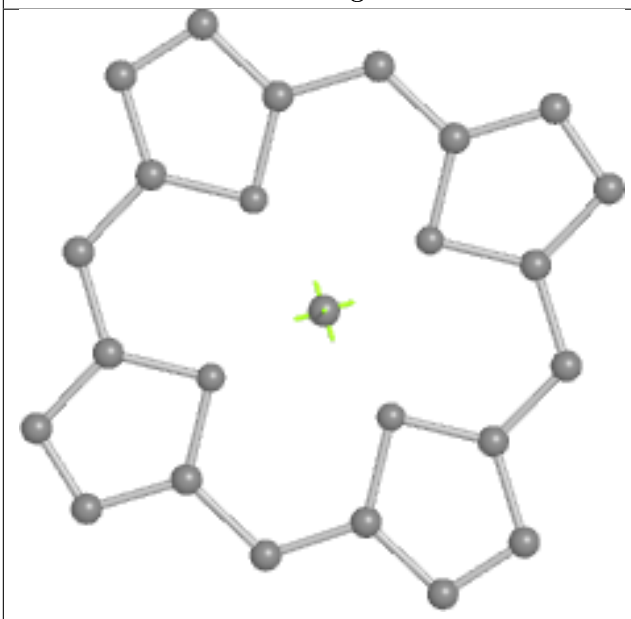
Ligand CLA 1 205



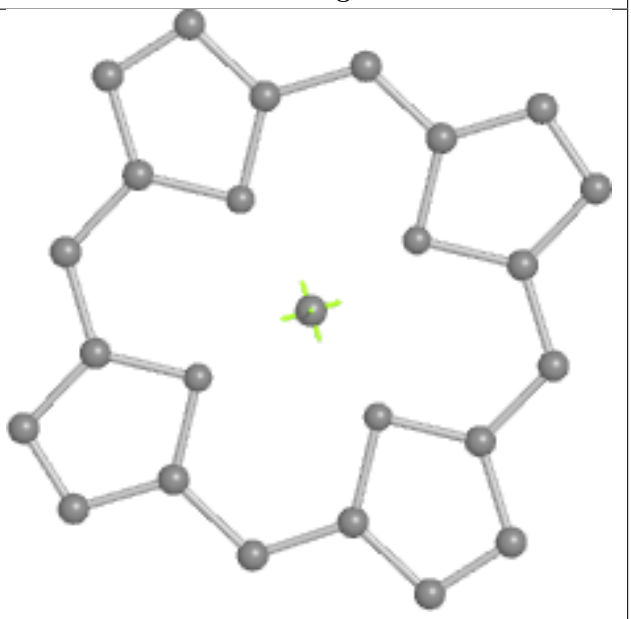
Bond lengths



Bond angles

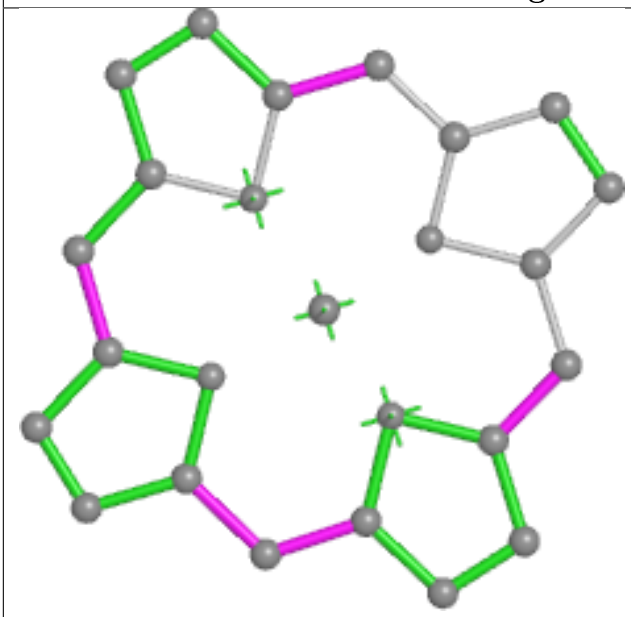


Torsions

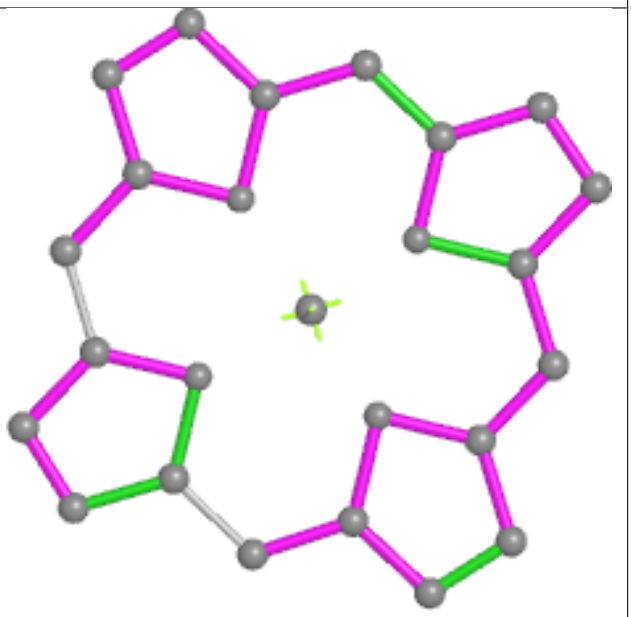


Rings

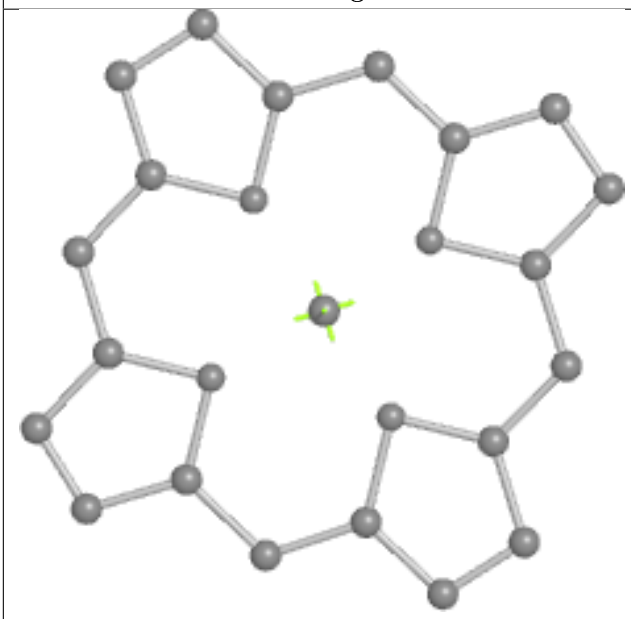
Ligand CLA 4 315



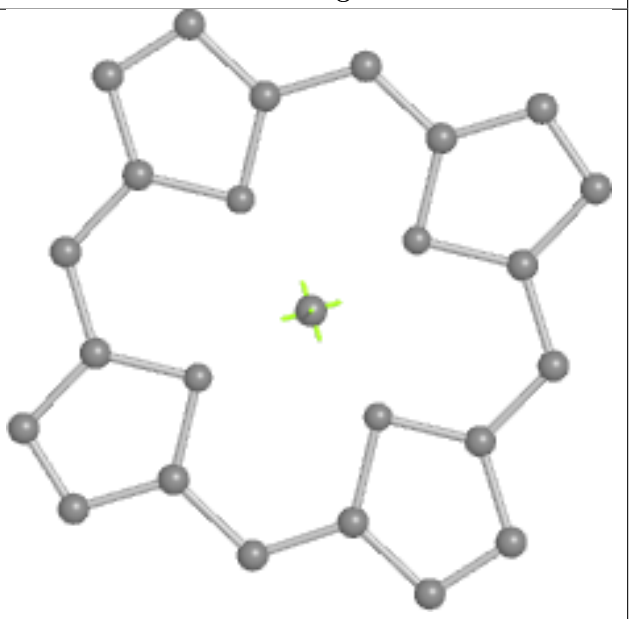
Bond lengths



Bond angles

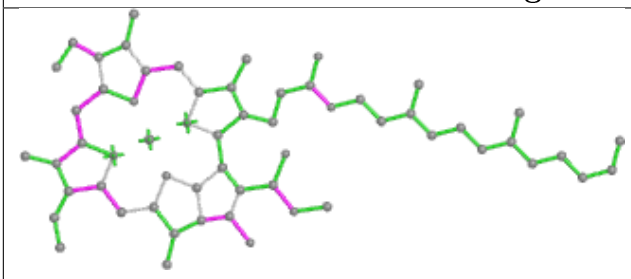


Torsions

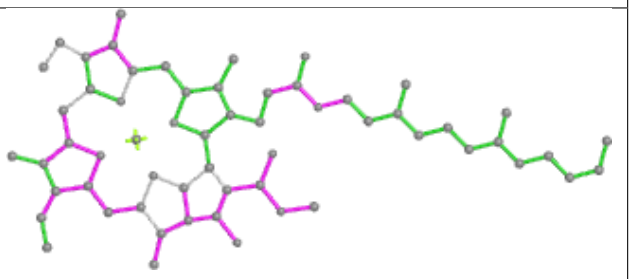


Rings

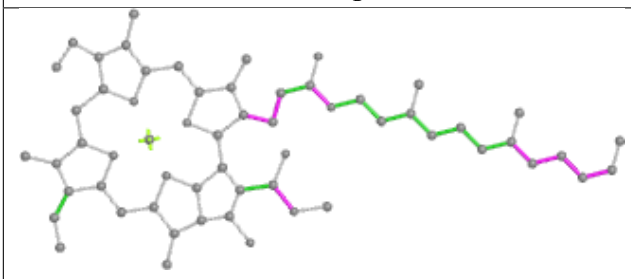
Ligand CLA B 815



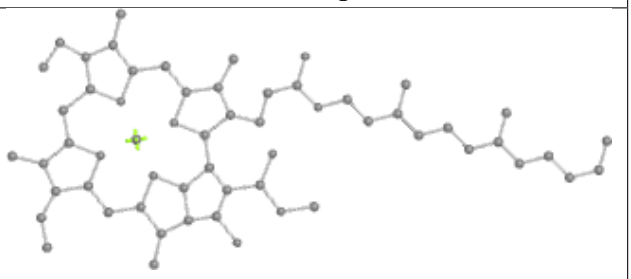
Bond lengths



Bond angles

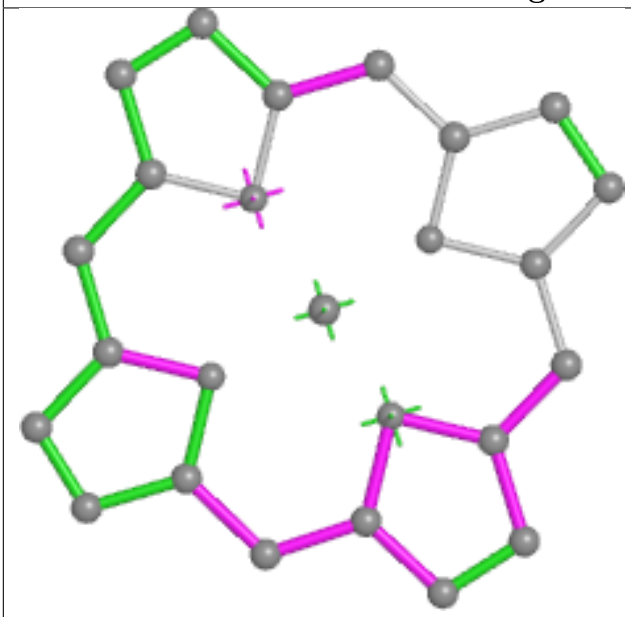


Torsions

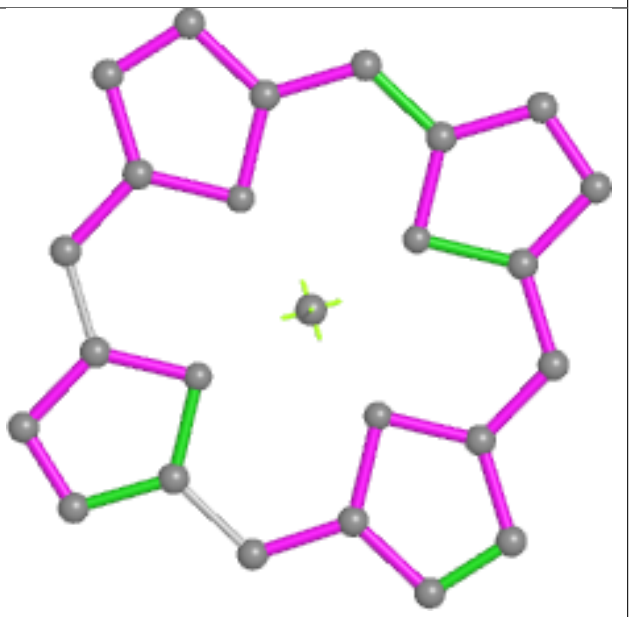


Rings

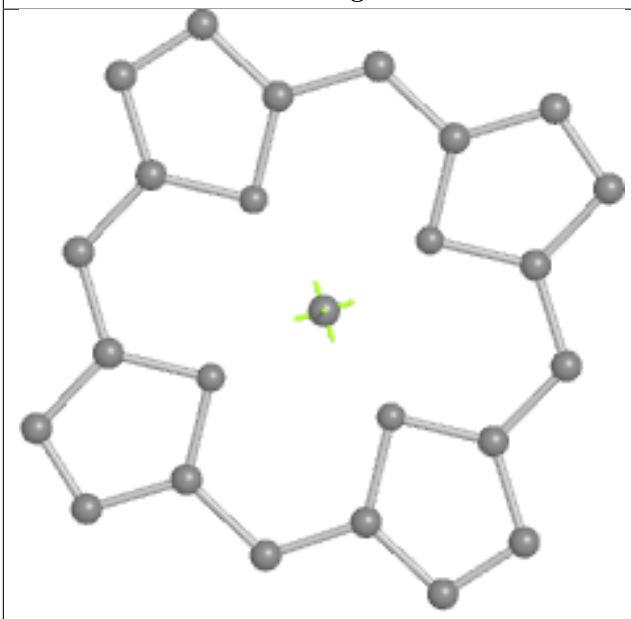
Ligand CLA 2 306



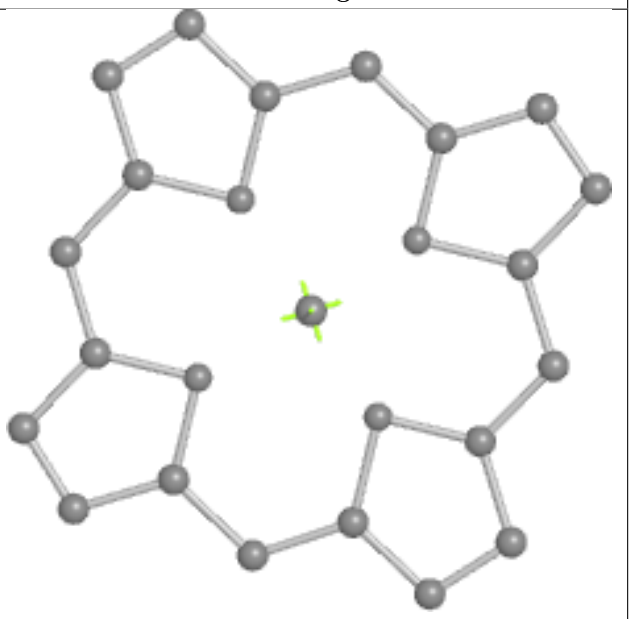
Bond lengths



Bond angles

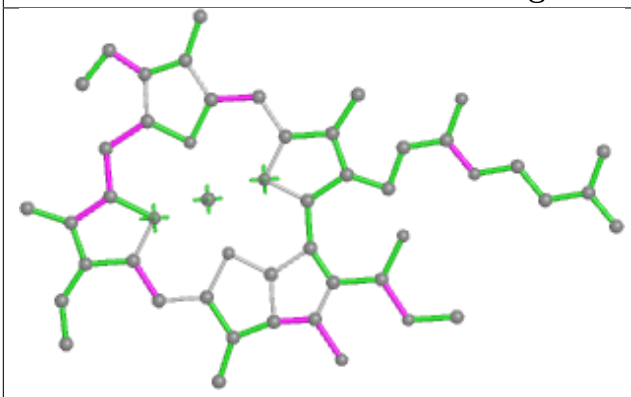


Torsions

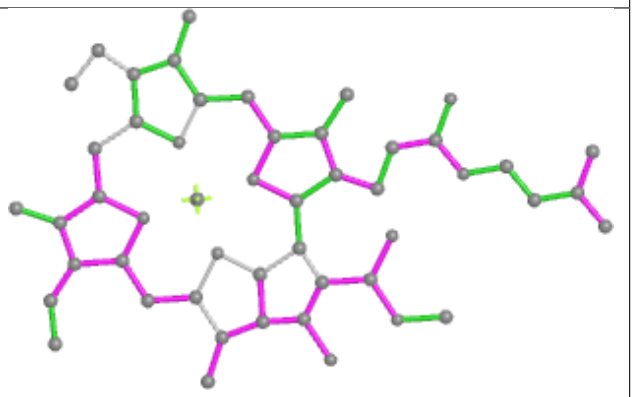


Rings

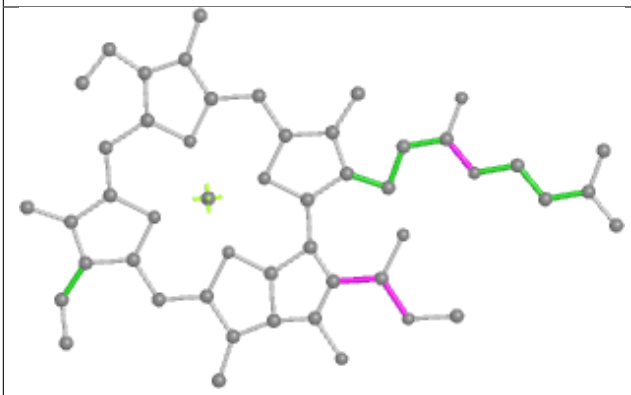
Ligand CLA 2 311



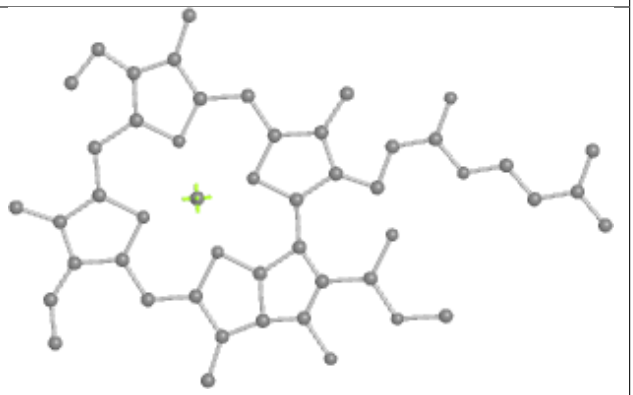
Bond lengths



Bond angles

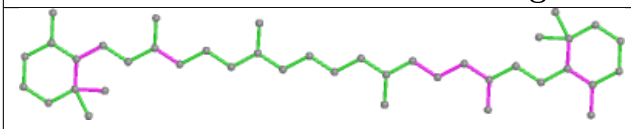


Torsions

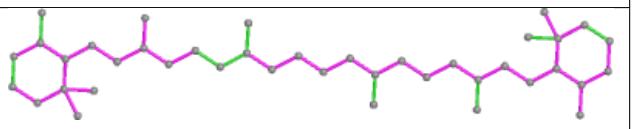


Rings

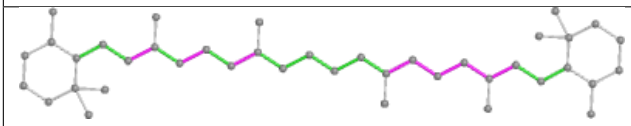
Ligand BCR I 103



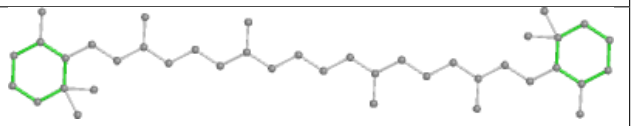
Bond lengths



Bond angles

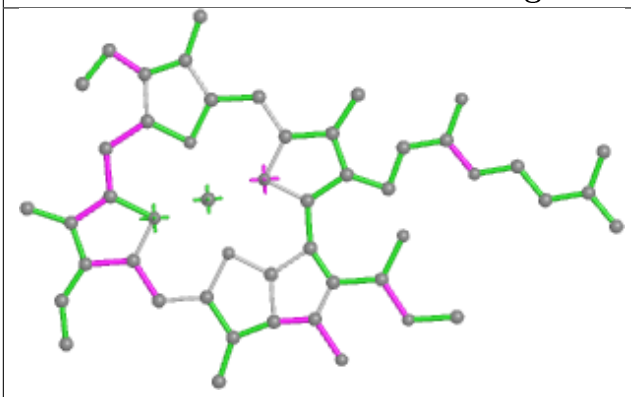


Torsions

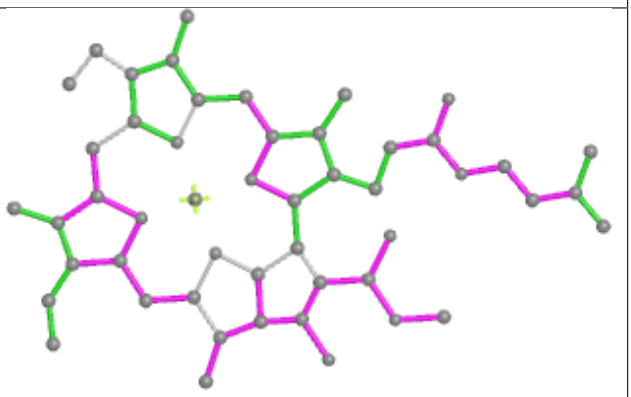


Rings

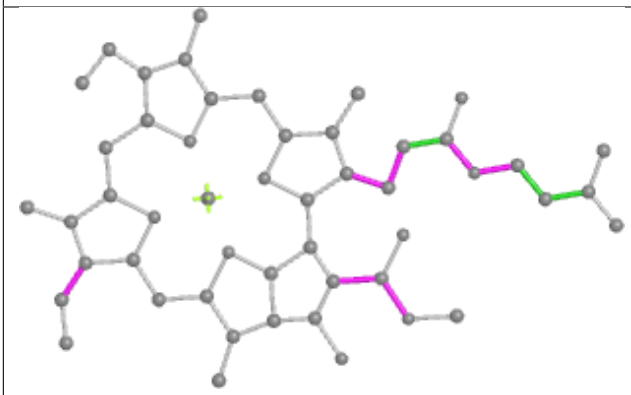
Ligand CLA A 832



Bond lengths



Bond angles



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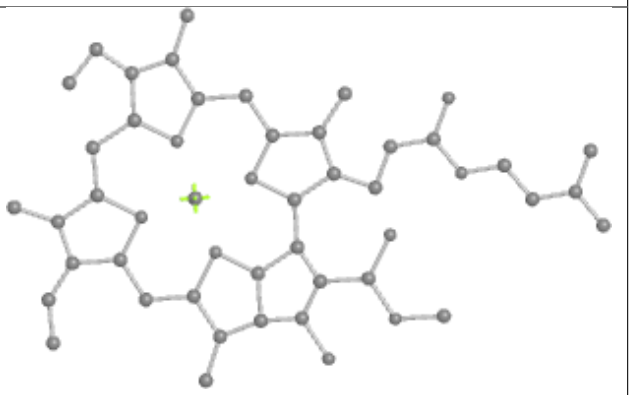
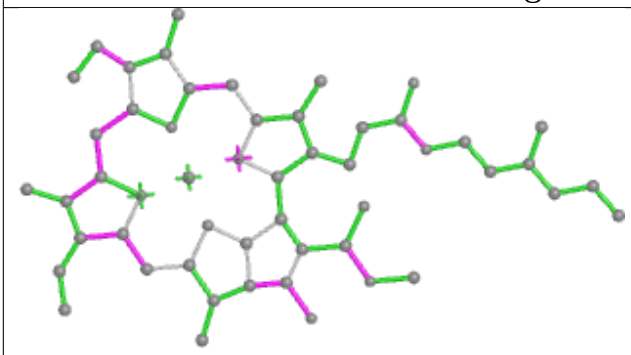
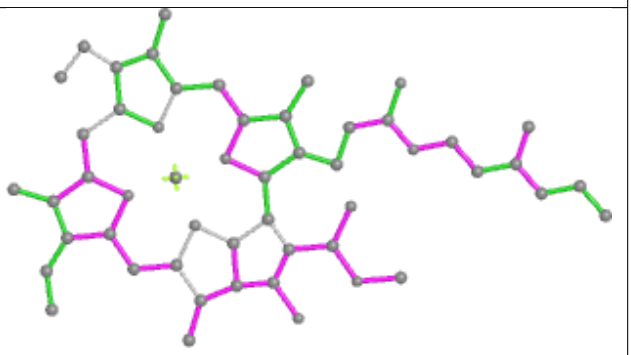


Rings

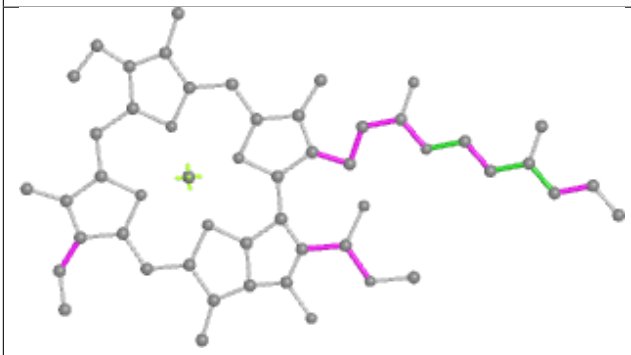
Ligand CLA A 817



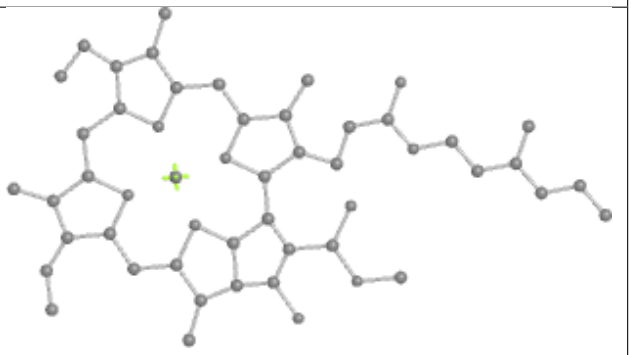
Bond lengths



Bond angles

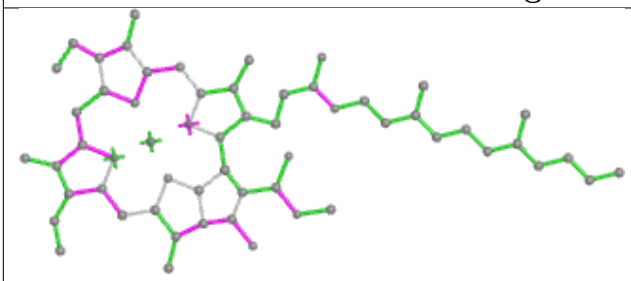


Torsions

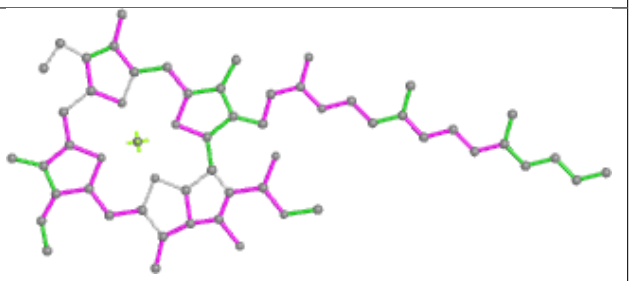


Rings

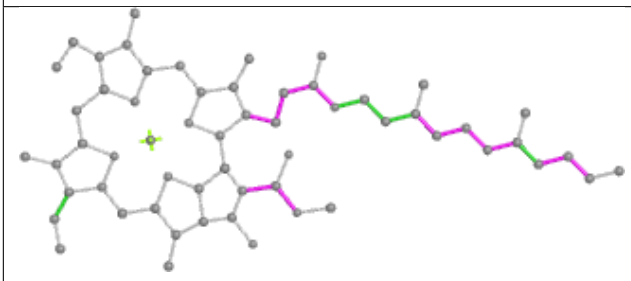
Ligand CLA R 108



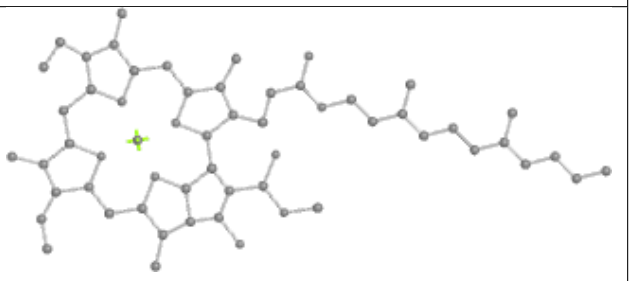
Bond lengths



Bond angles

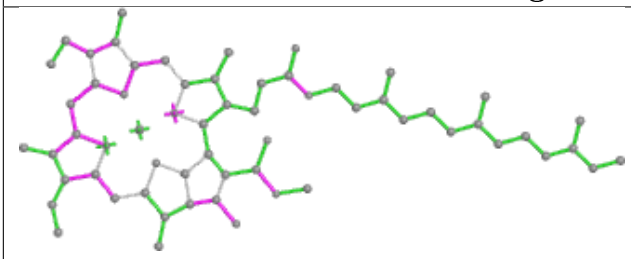


Torsions

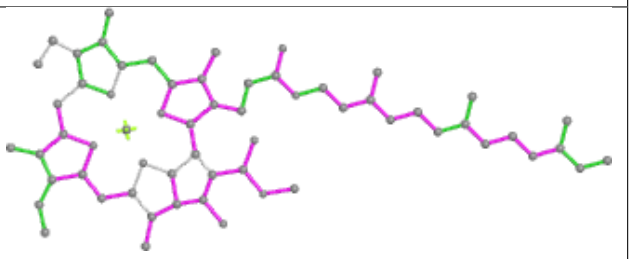


Rings

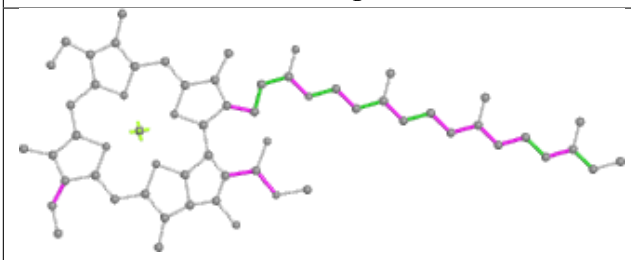
Ligand CLA 1 215



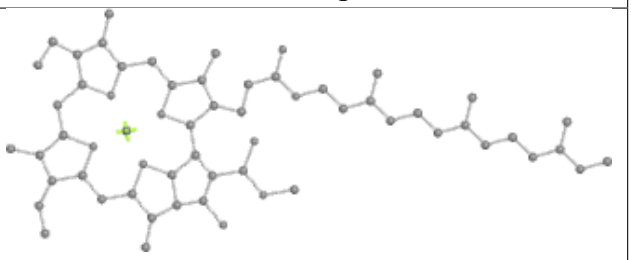
Bond lengths



Bond angles

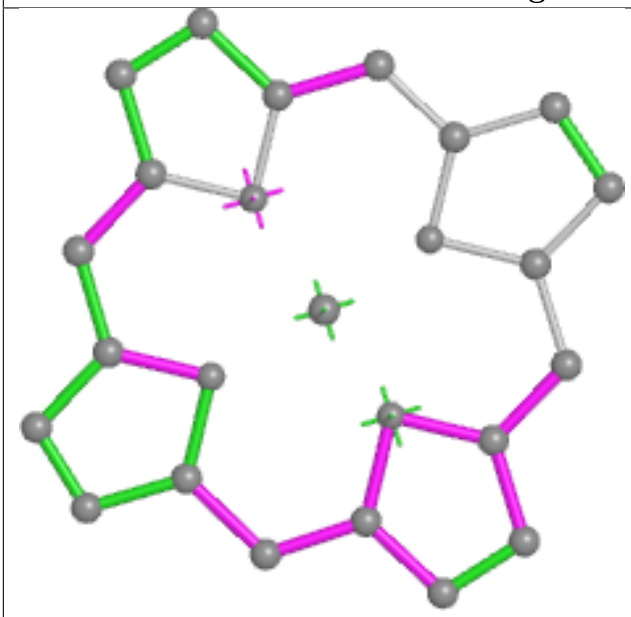


Torsions

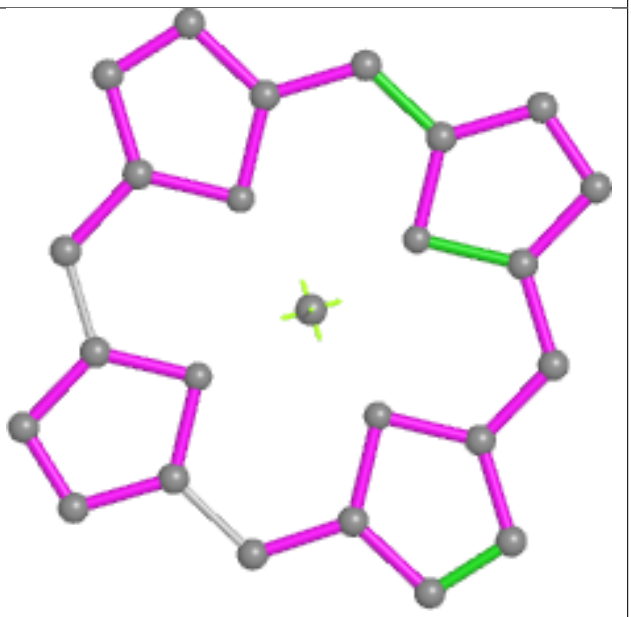


Rings

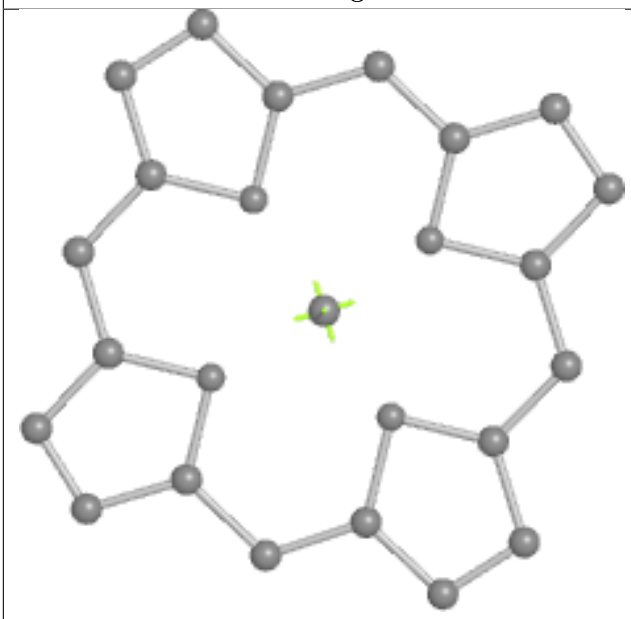
Ligand CLA 2 304



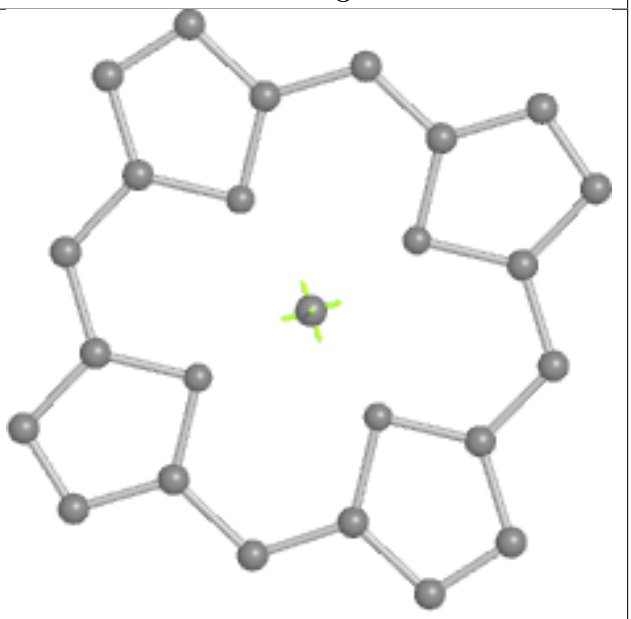
Bond lengths



Bond angles

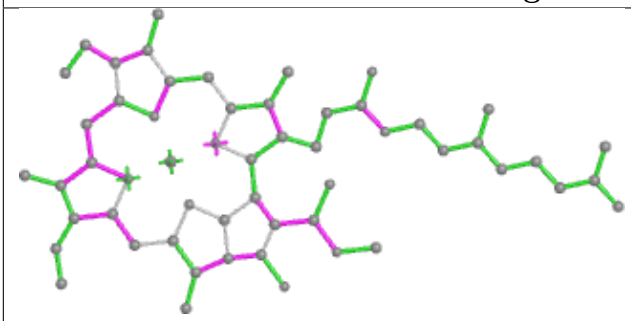


Torsions

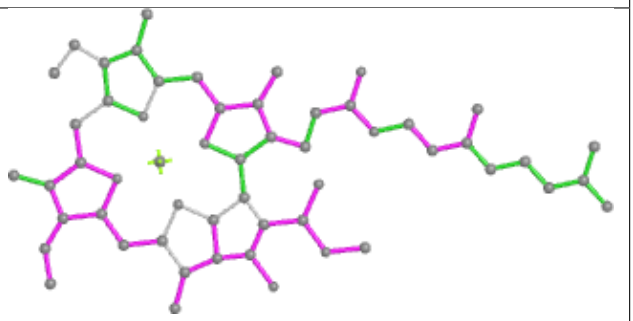


Rings

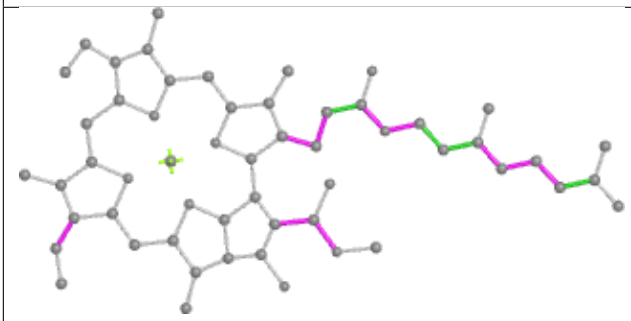
Ligand CLA H 101



Bond lengths



Bond angles



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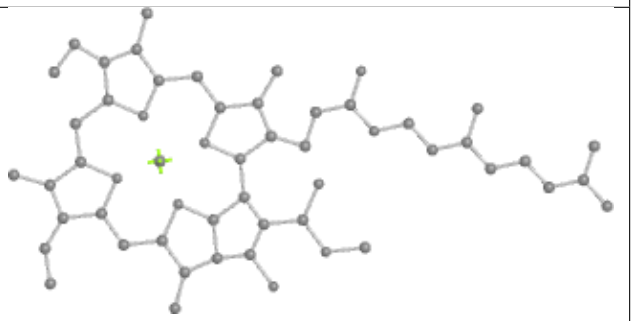
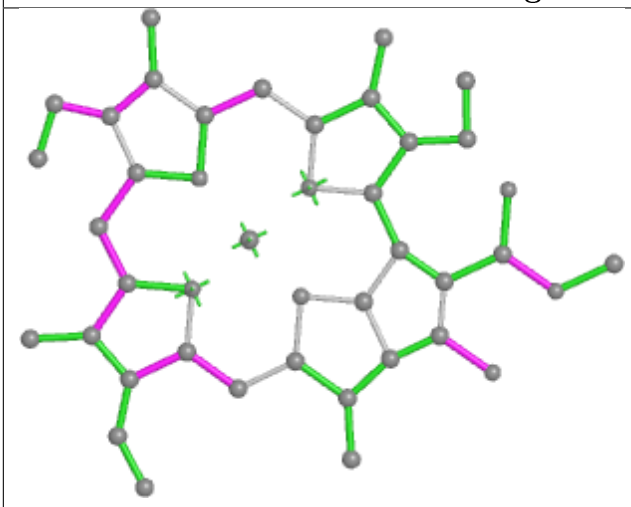
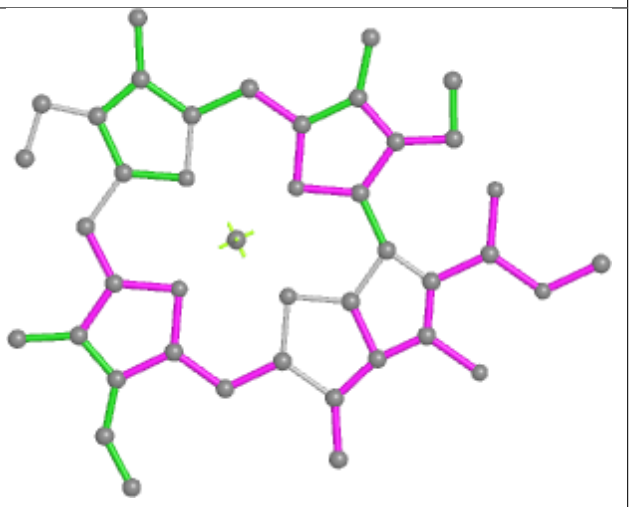


Rings

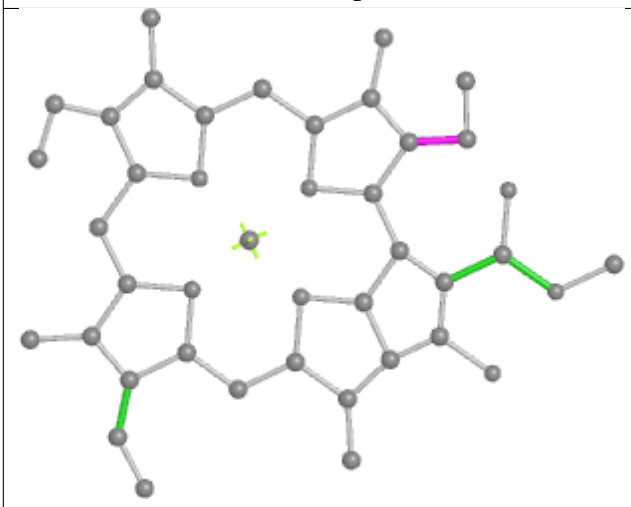
Ligand CLA A 821



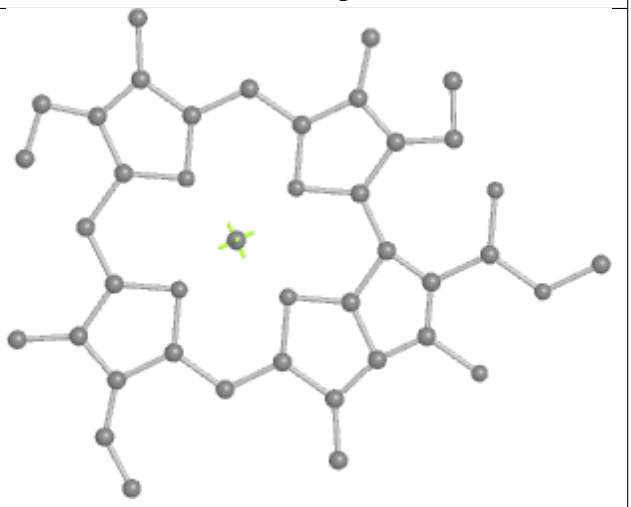
Bond lengths



Bond angles

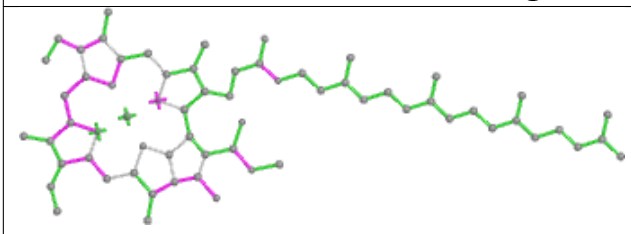


Torsions

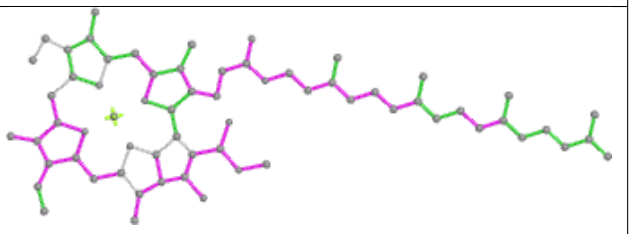


Rings

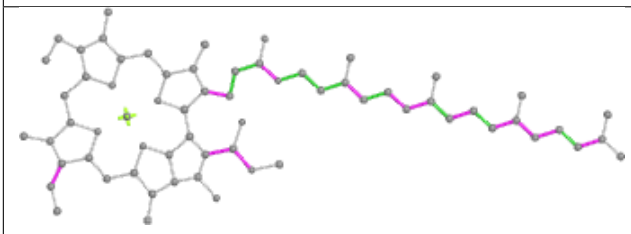
Ligand CLA A 839



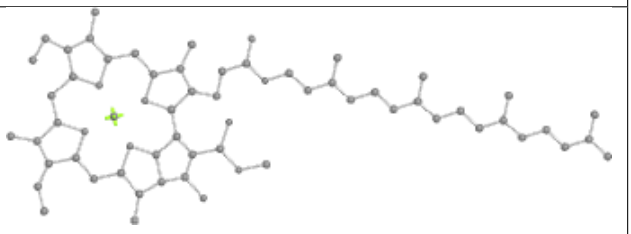
Bond lengths



Bond angles

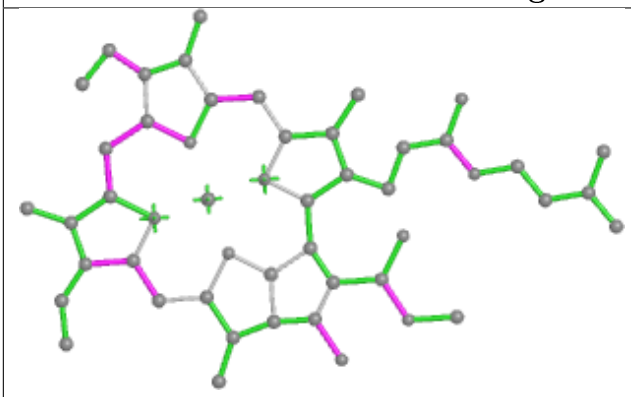


Torsions

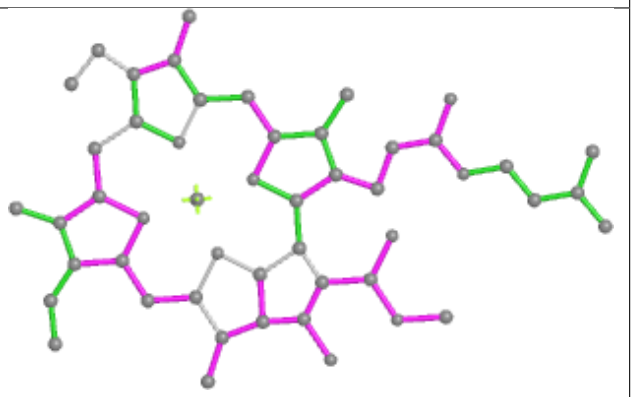


Rings

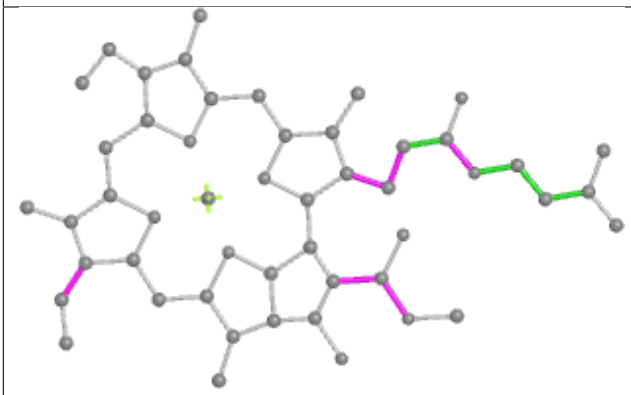
Ligand CLA 3 317



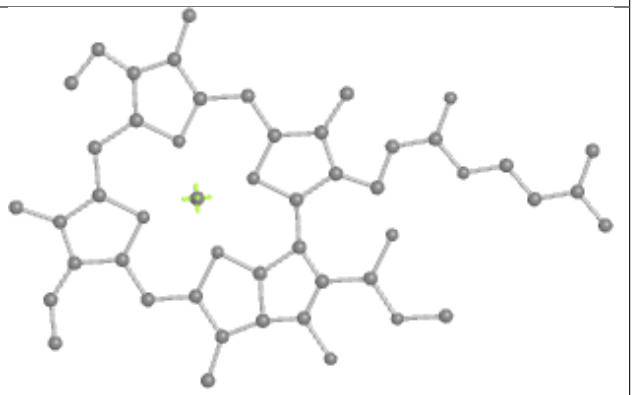
Bond lengths



Bond angles

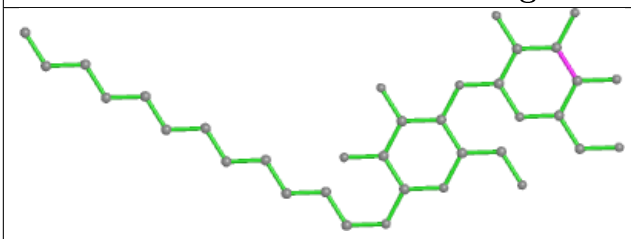


Torsions

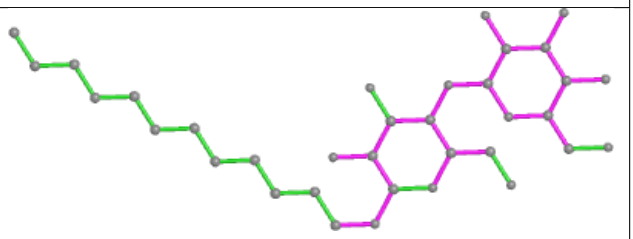


Rings

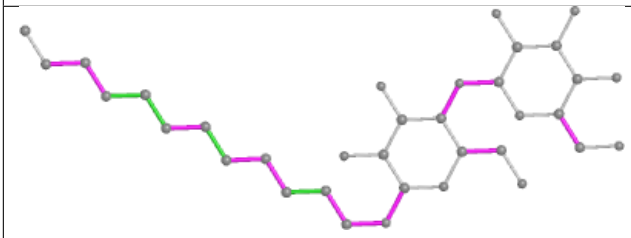
Ligand LMU R 104



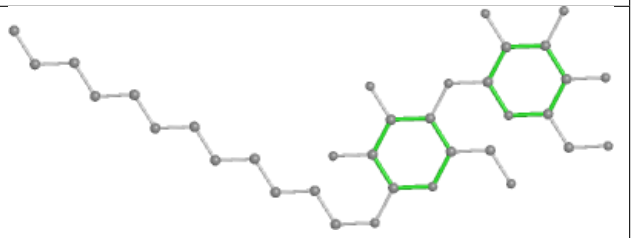
Bond lengths



Bond angles

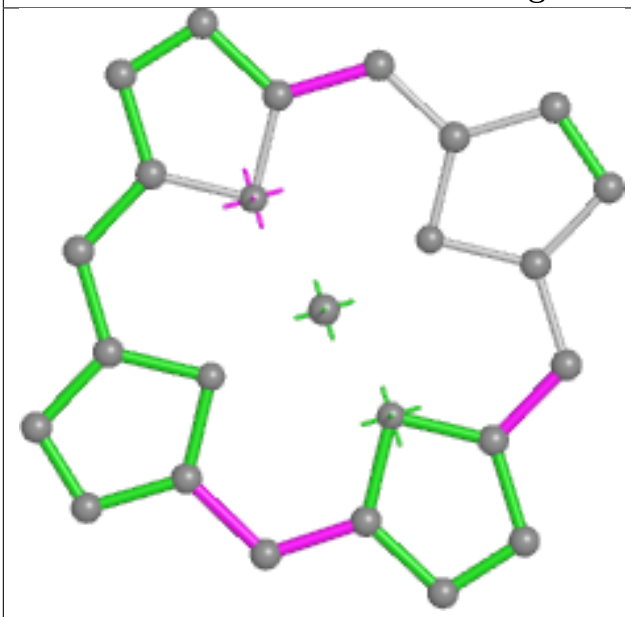


Torsions

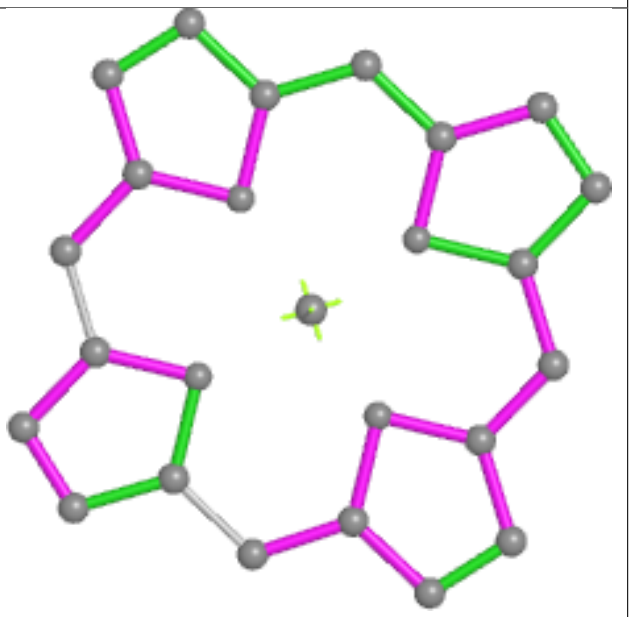


Rings

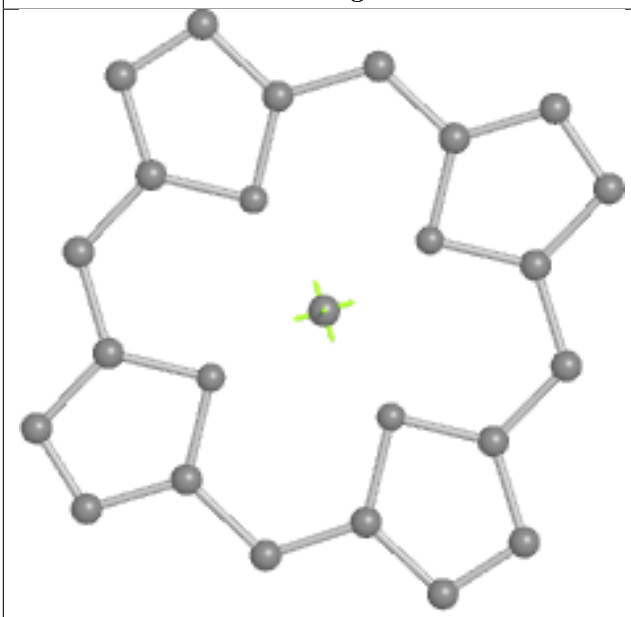
Ligand CLA 3 320



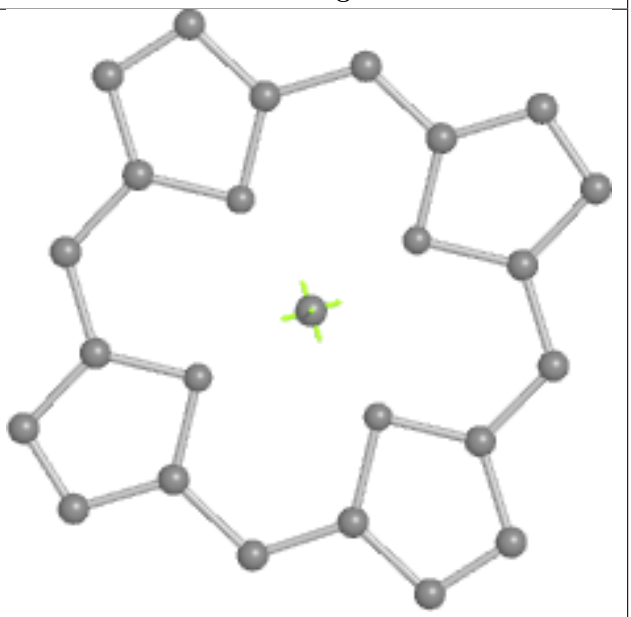
Bond lengths



Bond angles

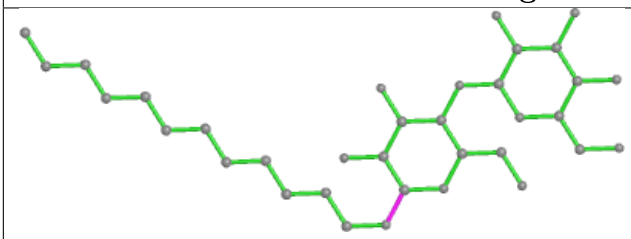


Torsions

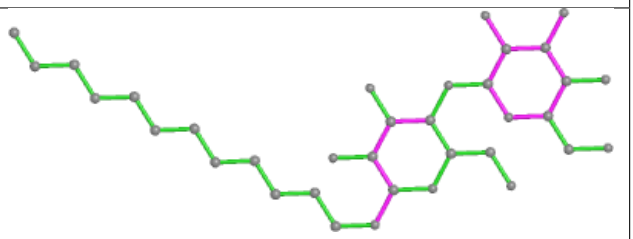


Rings

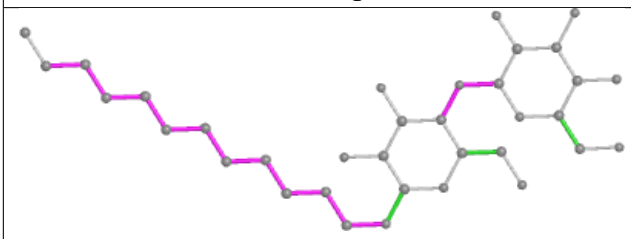
Ligand LMU A 849



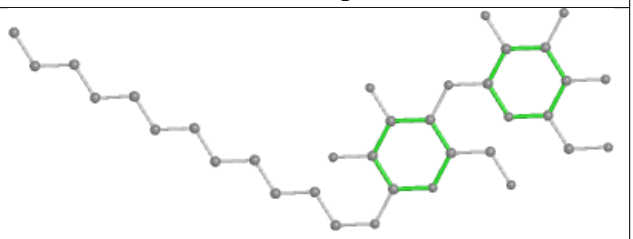
Bond lengths



Bond angles

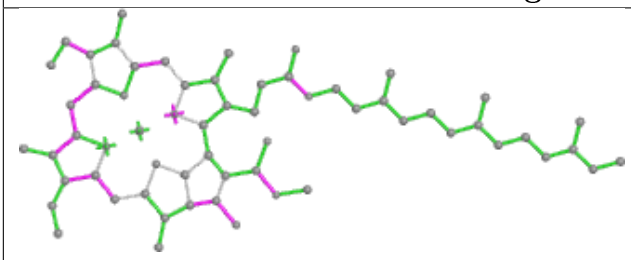


Torsions

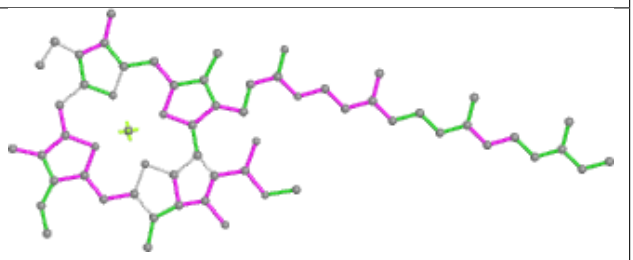


Rings

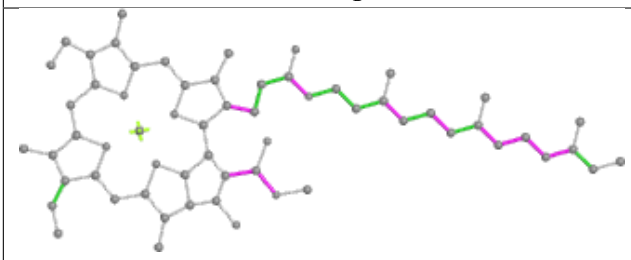
Ligand CLA B 817



Bond lengths



Bond angles



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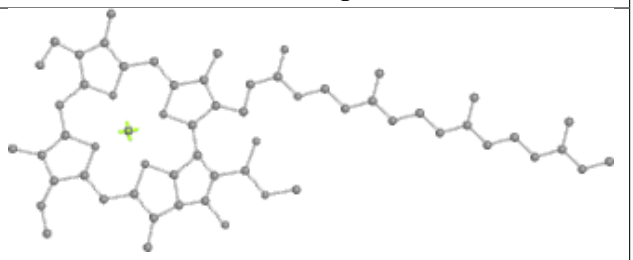
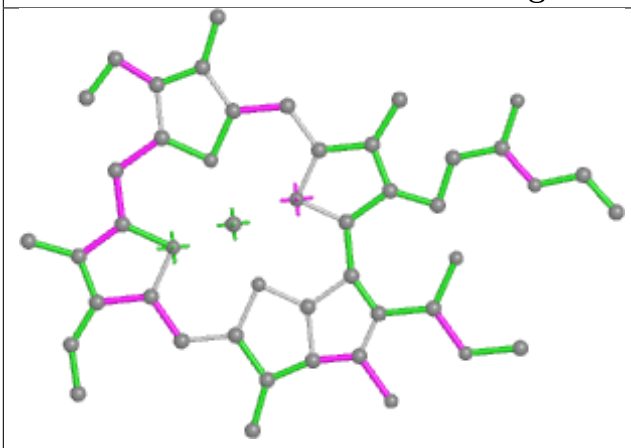


Rings

Ligand CLA 4 319



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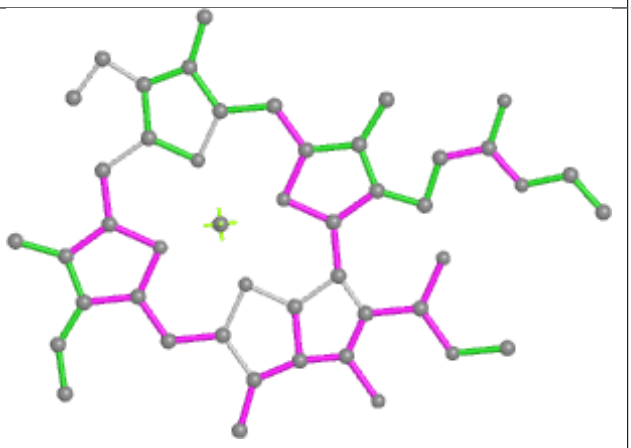
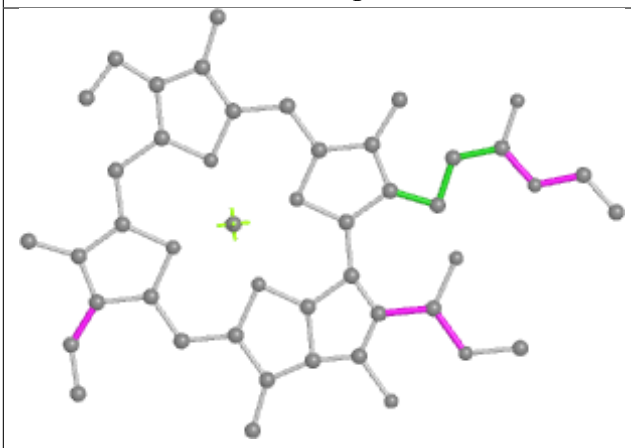
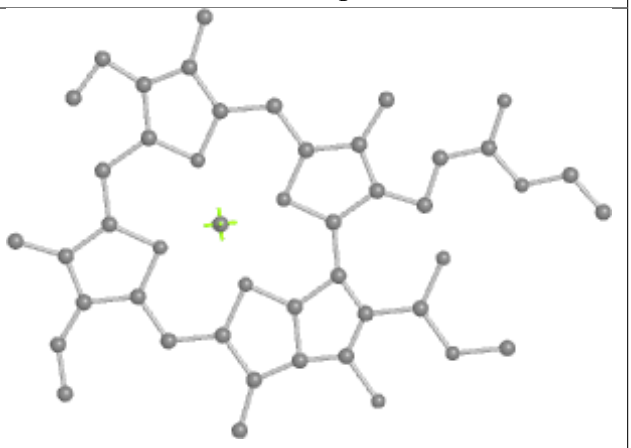


Bond angles

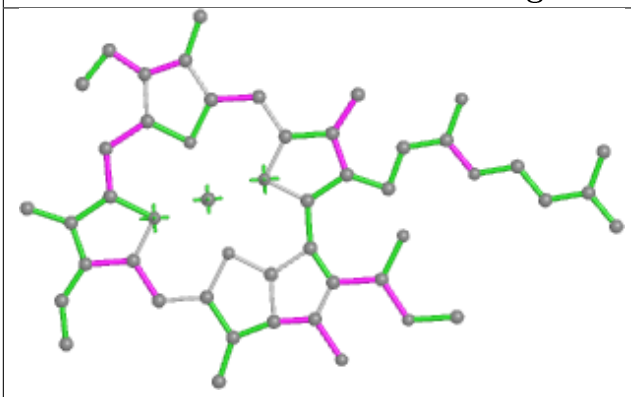


Torsions

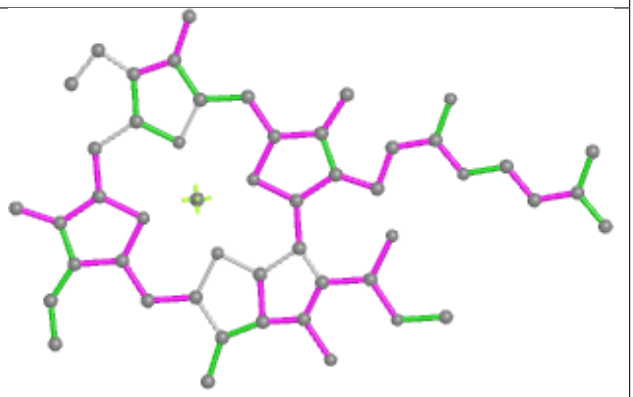


Rings

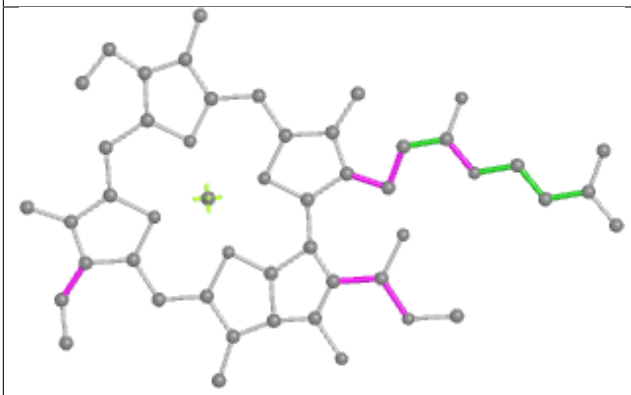
Ligand CLA L 209



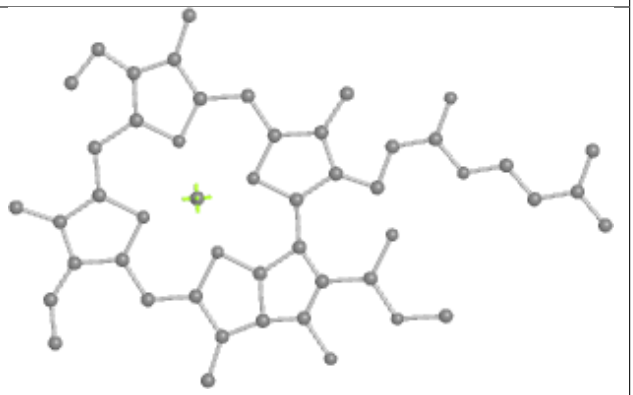
Bond lengths



Bond angles

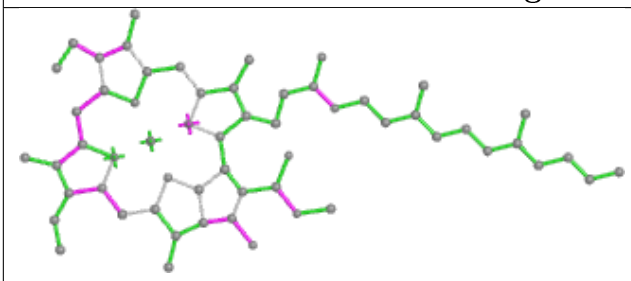


Torsions

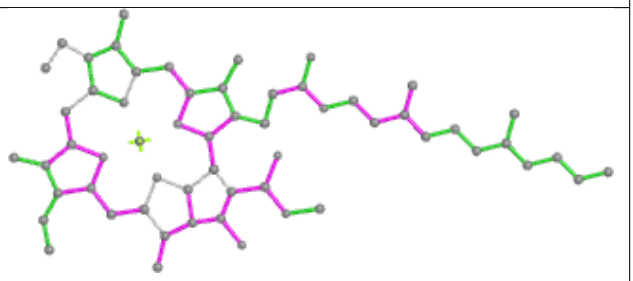


Rings

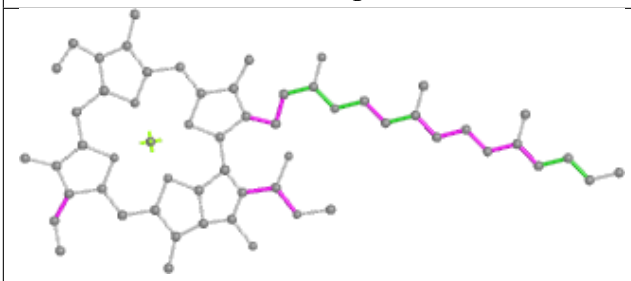
Ligand CLA B 823



Bond lengths



Bond angles



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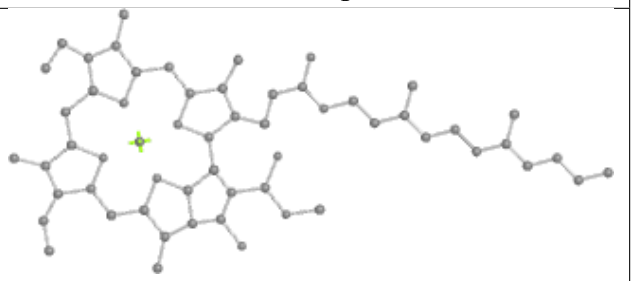
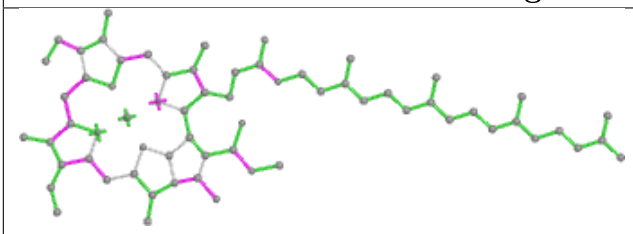
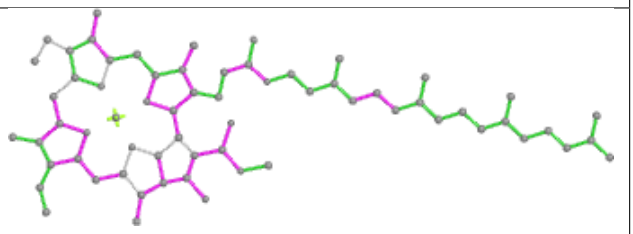


Rings

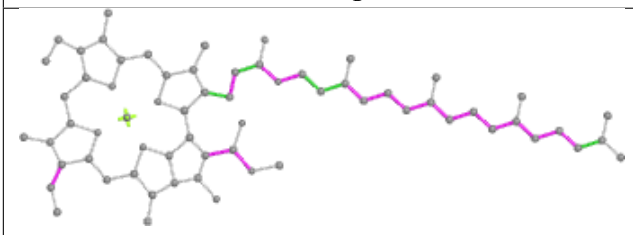
Ligand CLA B 827



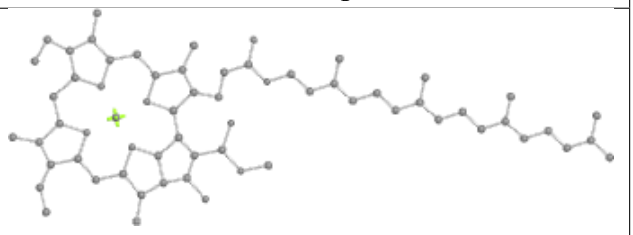
Bond lengths



Bond angles

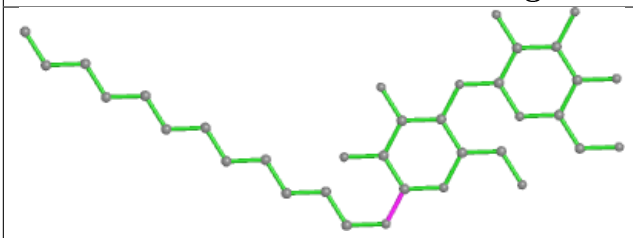


Torsions

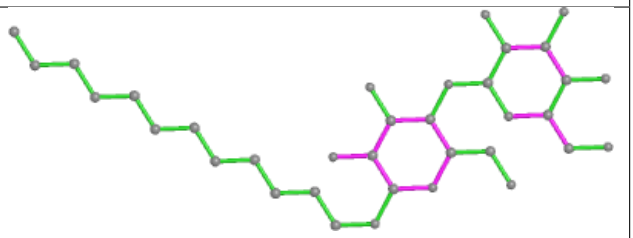


Rings

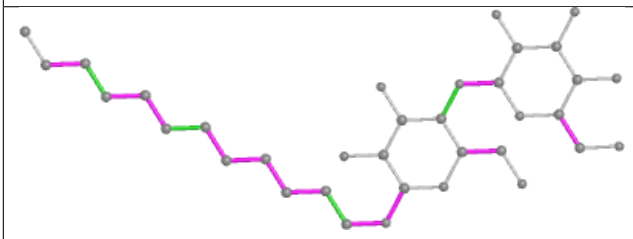
Ligand LMU 4 321



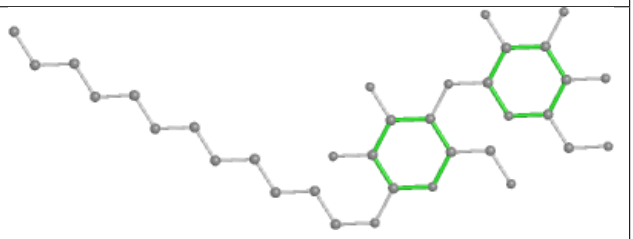
Bond lengths



Bond angles

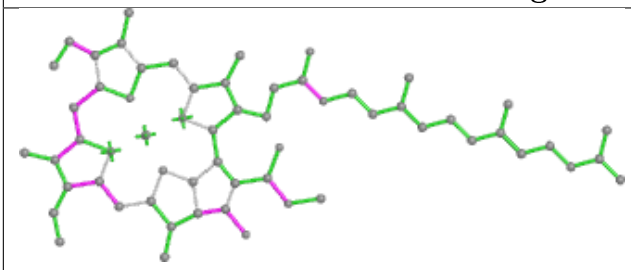


Torsions



Rings

Ligand CLA I 102



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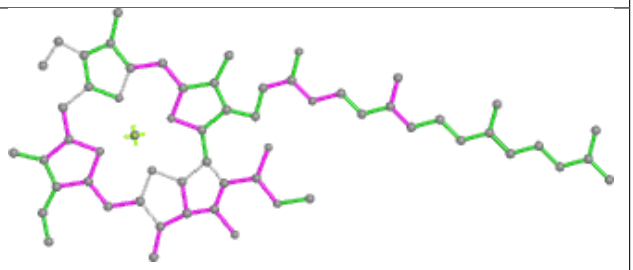
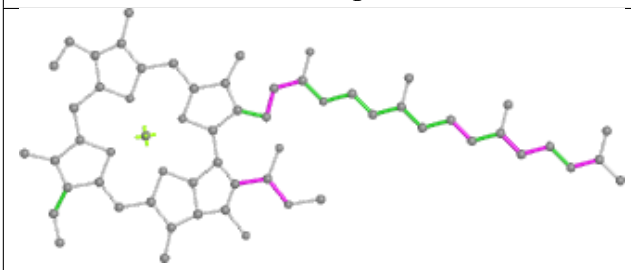
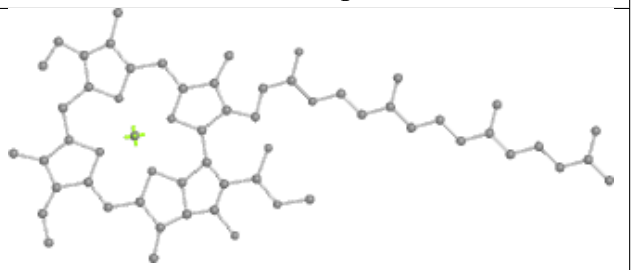


Bond angles

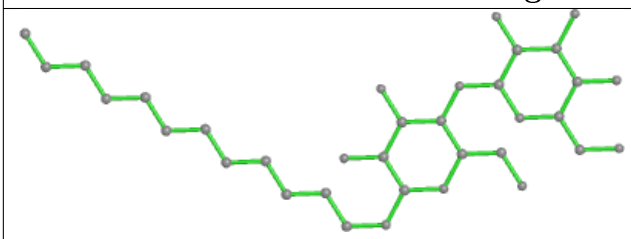


Torsions

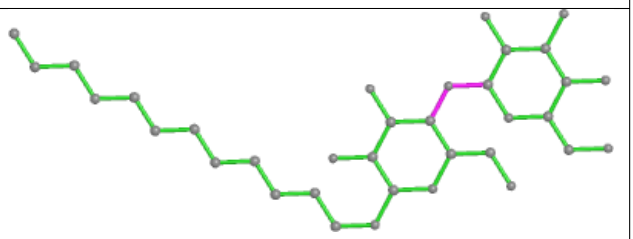


Rings

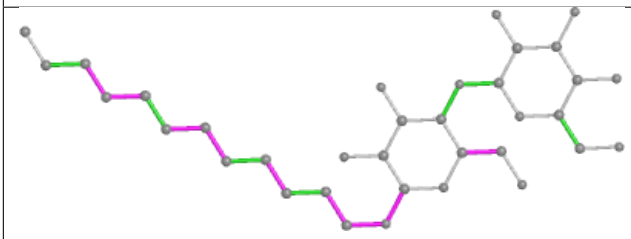
Ligand LMU 3 321



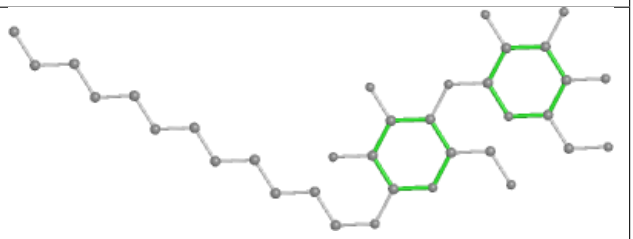
Bond lengths



Bond angles

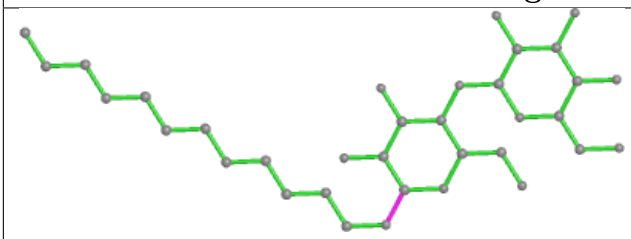


Torsions

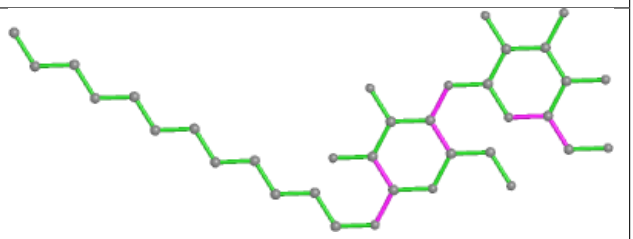


Rings

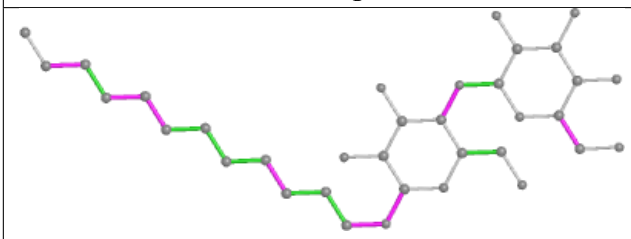
Ligand LMU 2 320



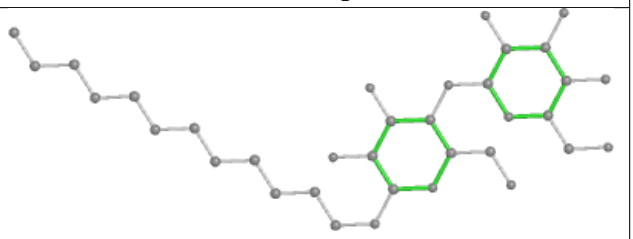
Bond lengths



Bond angles

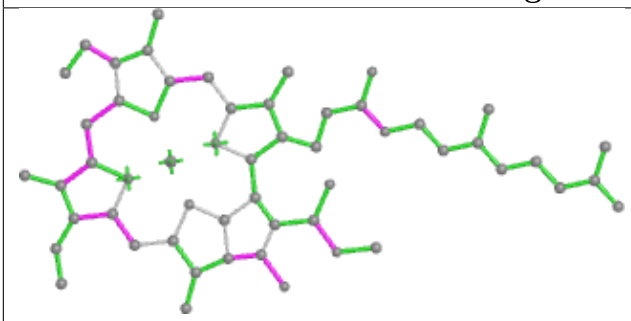


Torsions

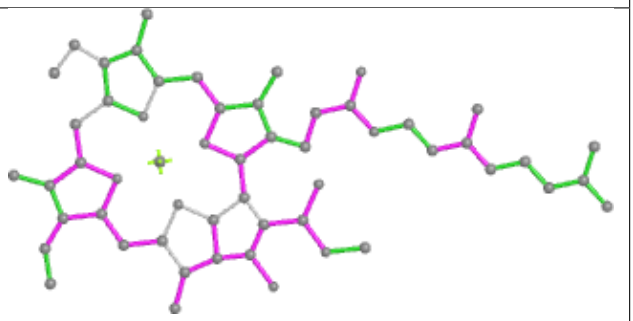


Rings

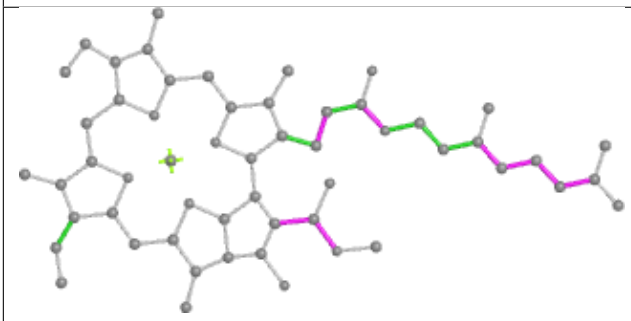
Ligand CLA B 810



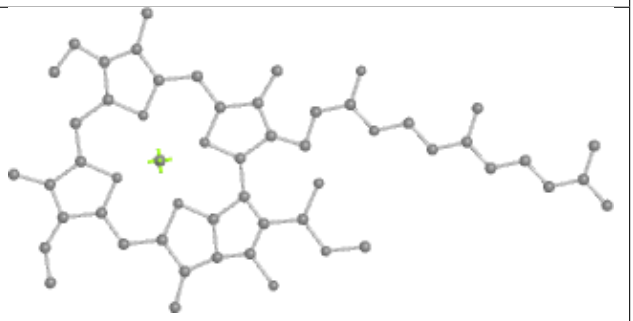
Bond lengths



Bond angles

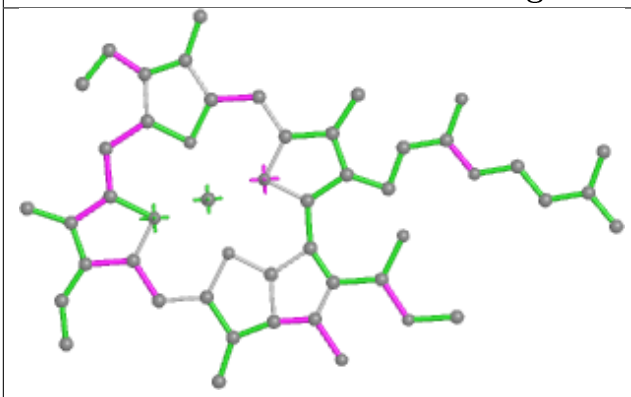


Torsions

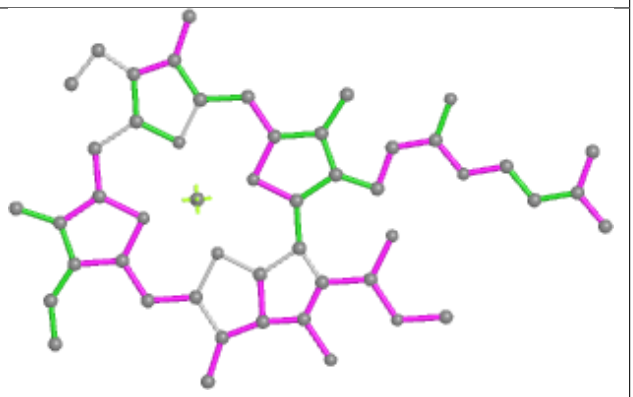


Rings

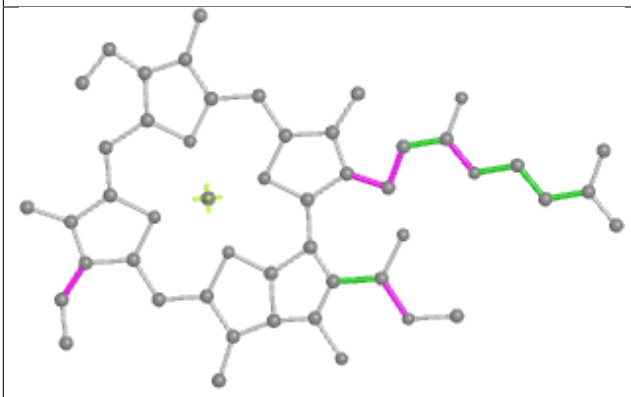
Ligand CLA L 207



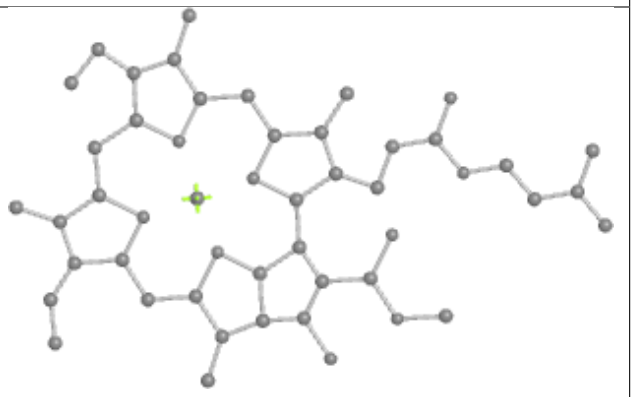
Bond lengths



Bond angles

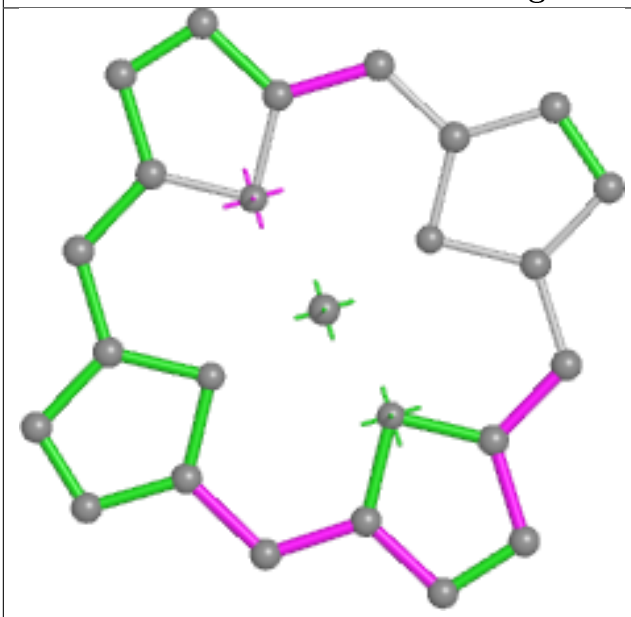


Torsions

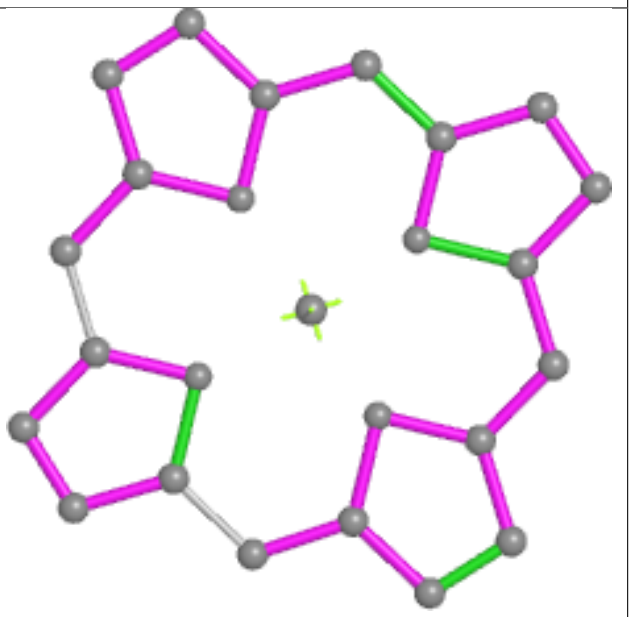


Rings

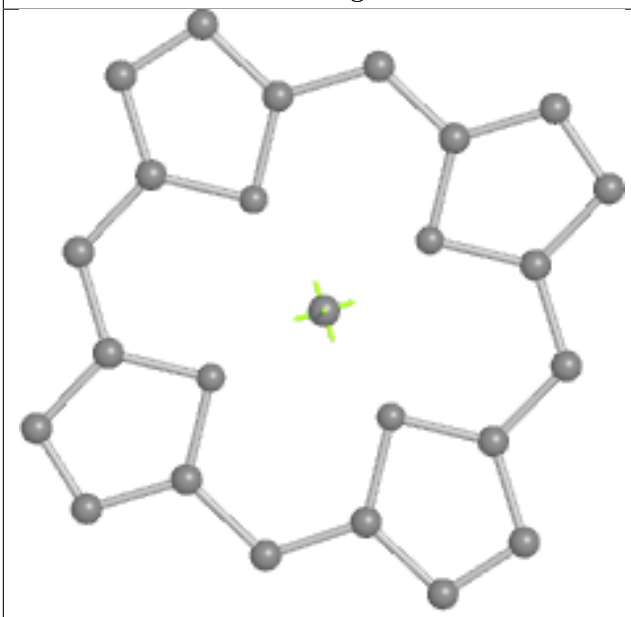
Ligand CLA 3 307



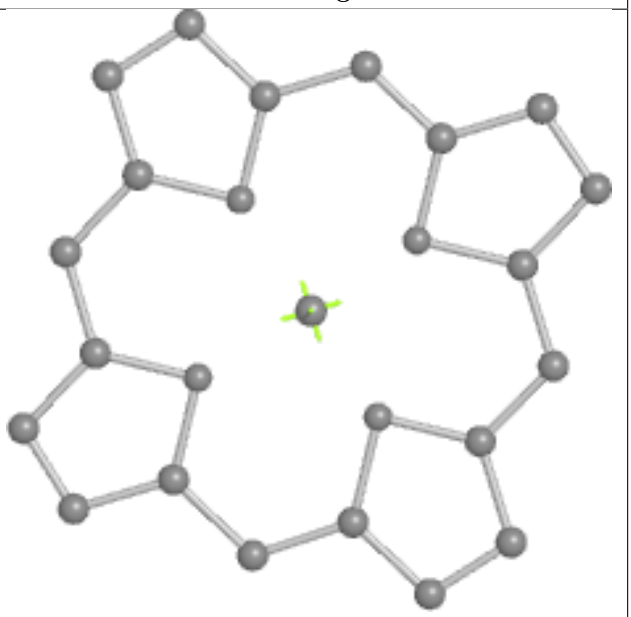
Bond lengths



Bond angles

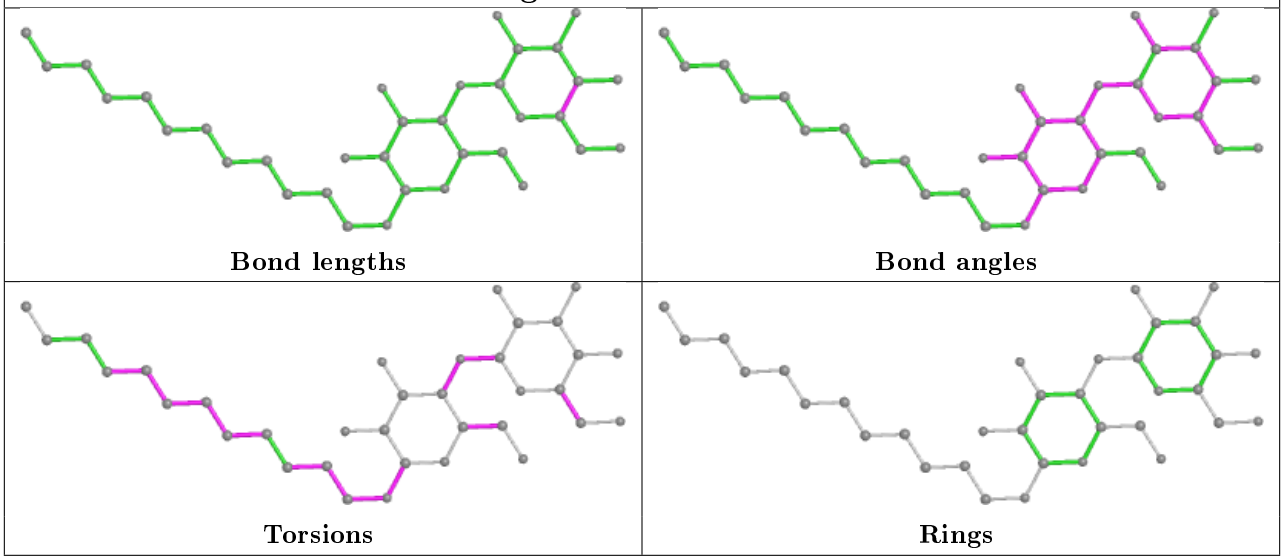


Torsions

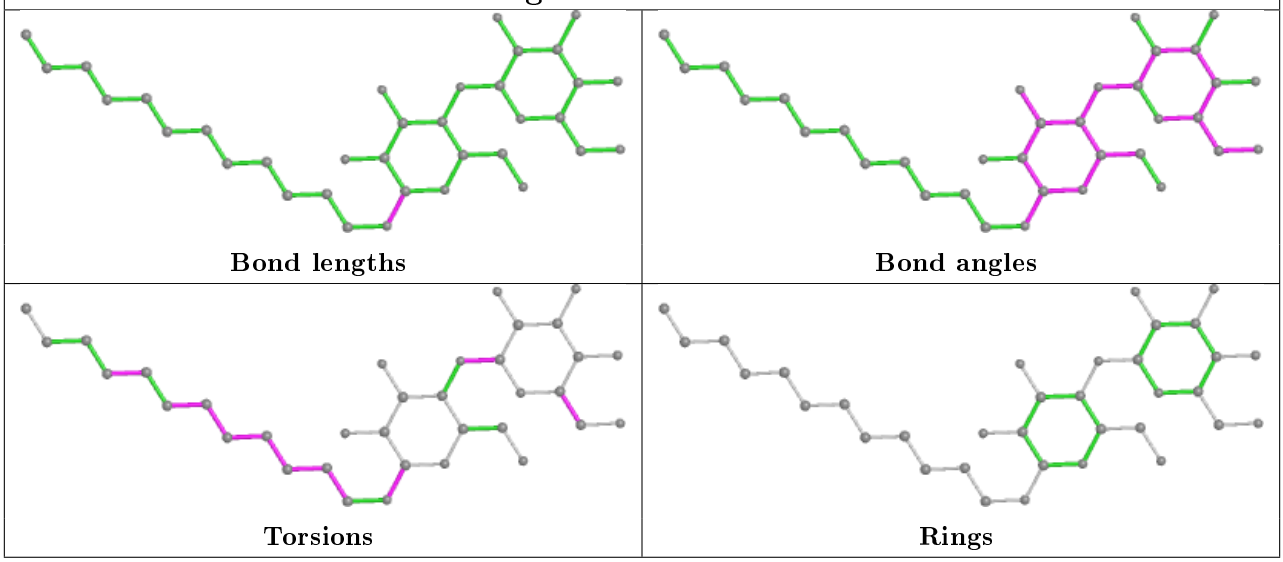


Rings

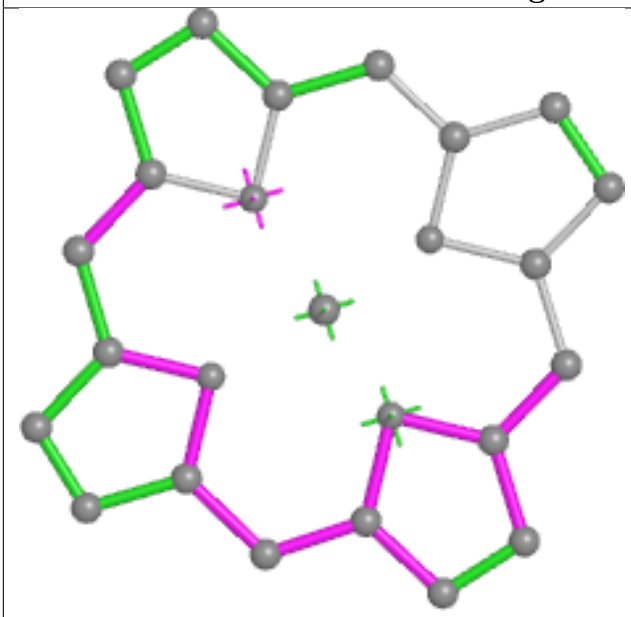
Ligand LMU H 105



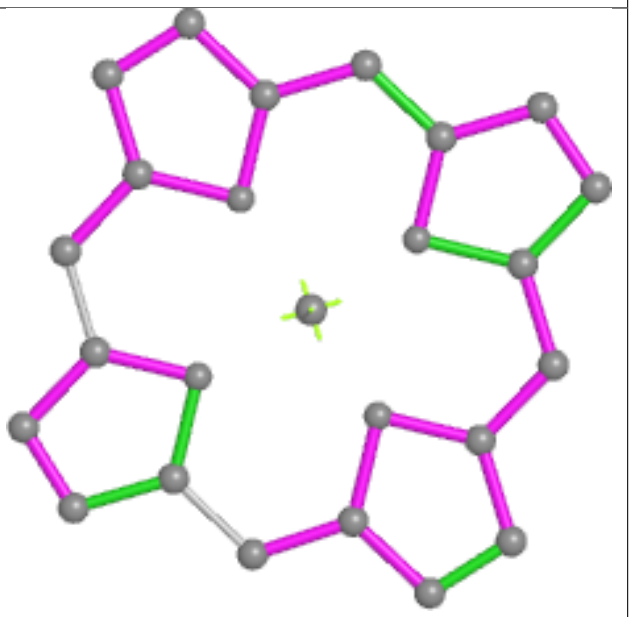
Ligand LMU 2 318



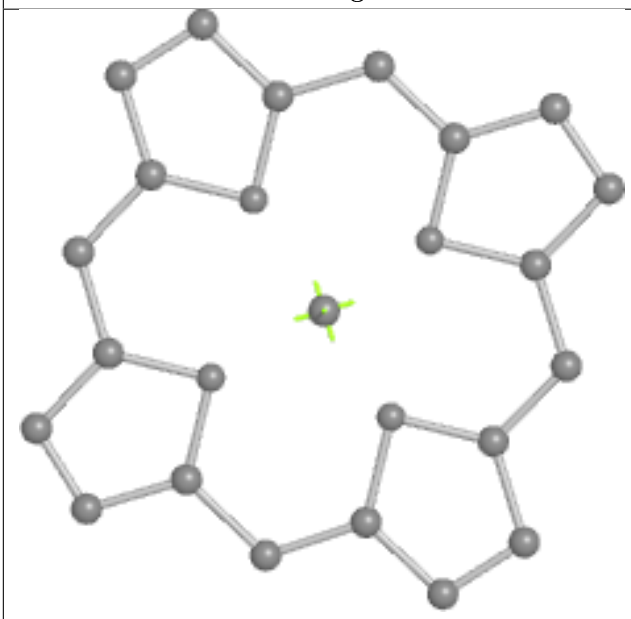
Ligand CLA 1 216



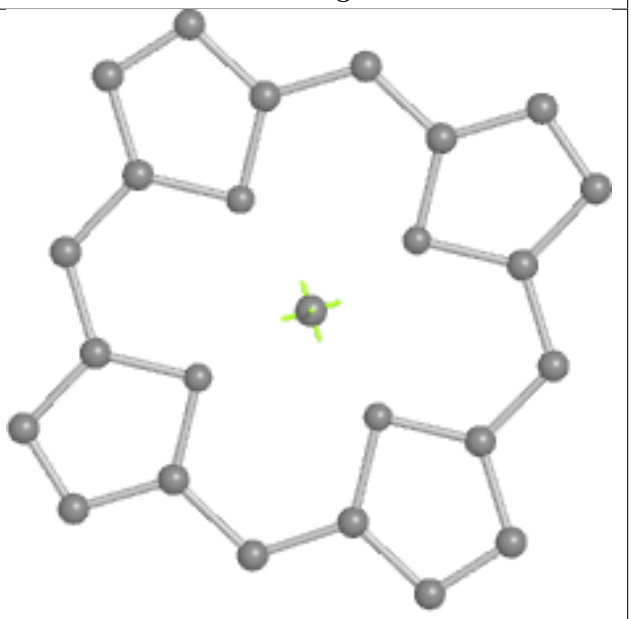
Bond lengths



Bond angles

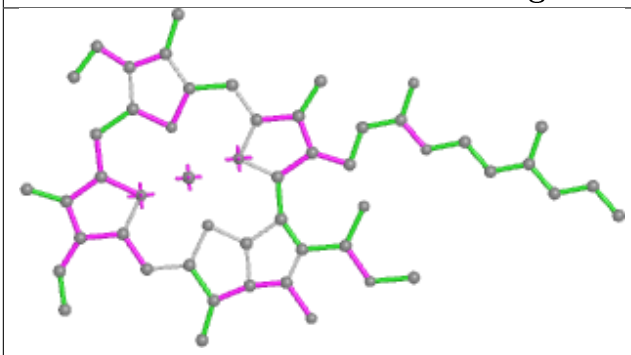


Torsions

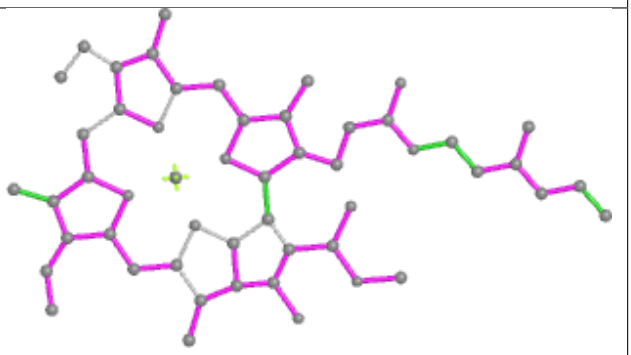


Rings

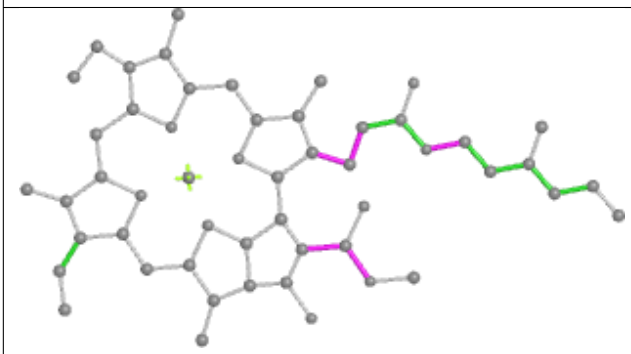
Ligand CLA 4 307



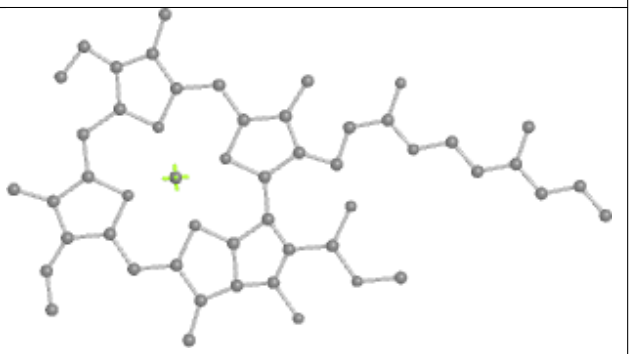
Bond lengths



Bond angles

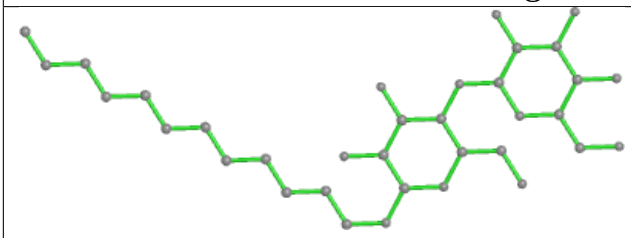


Torsions



Rings

Ligand LMU 1 218



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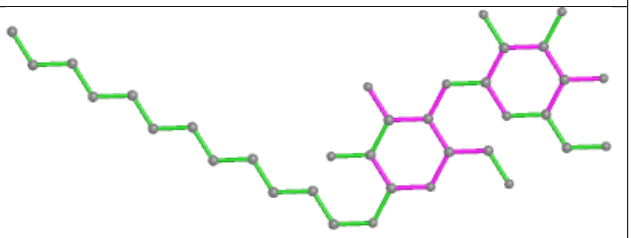
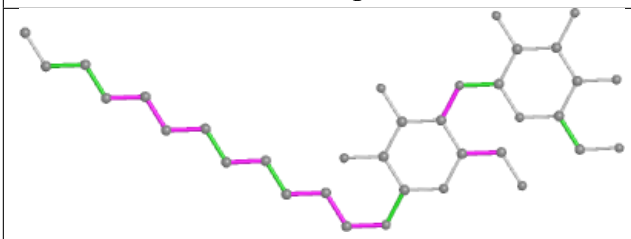
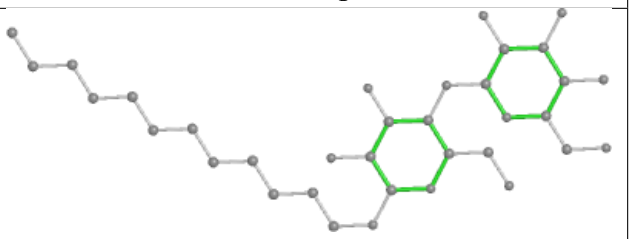


Bond angles

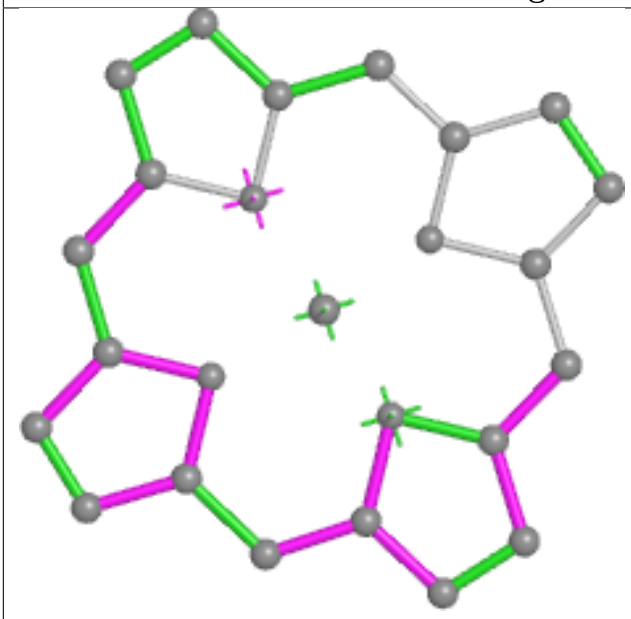


Torsions



Rings

Ligand CLA 4 310



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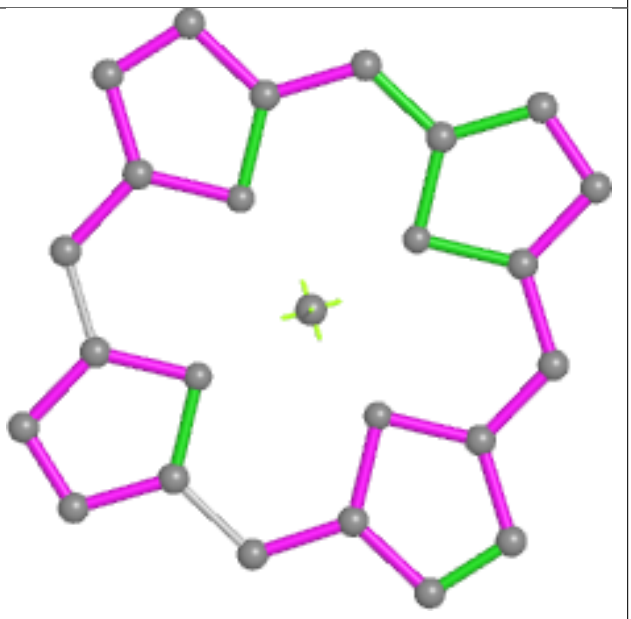
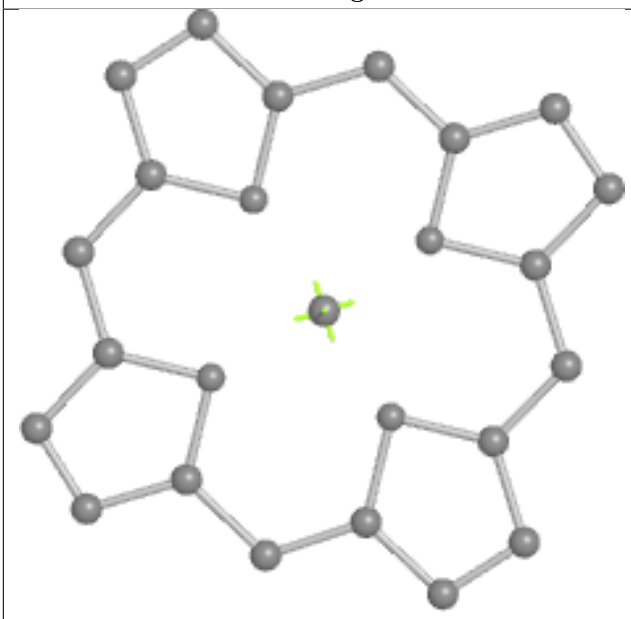
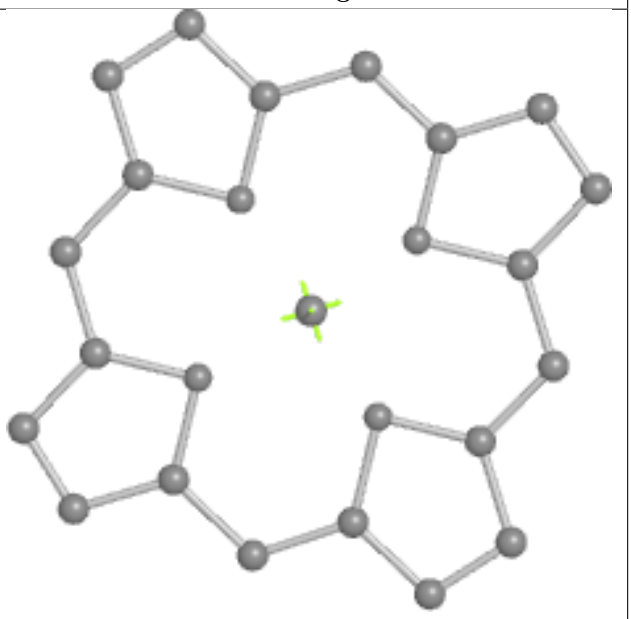


Bond angles

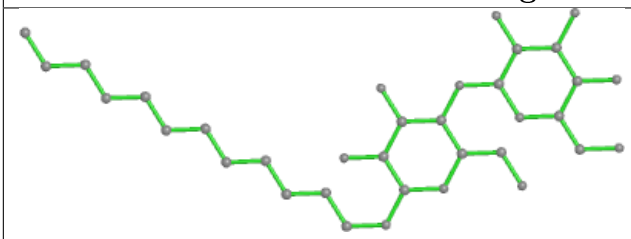


Torsions

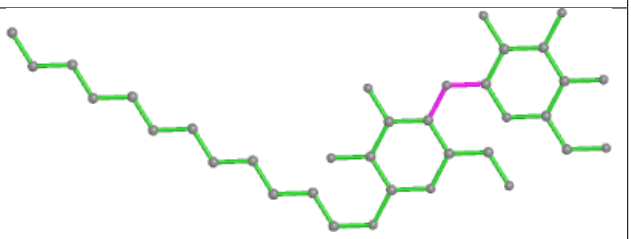


Rings

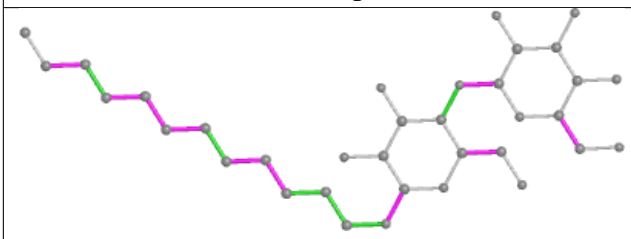
Ligand LMU D 201



Bond lengths



Bond angles



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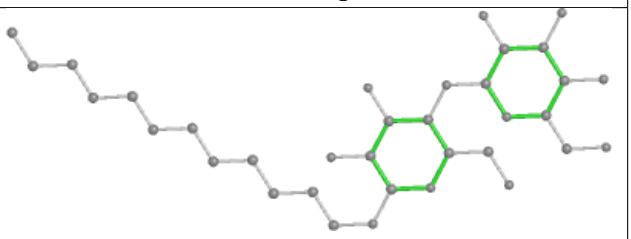
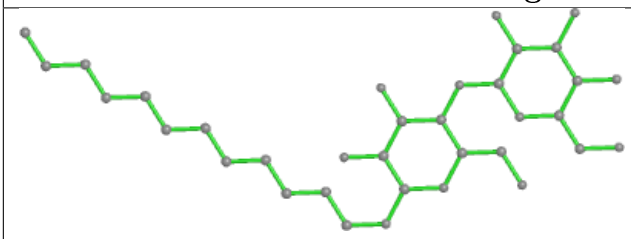
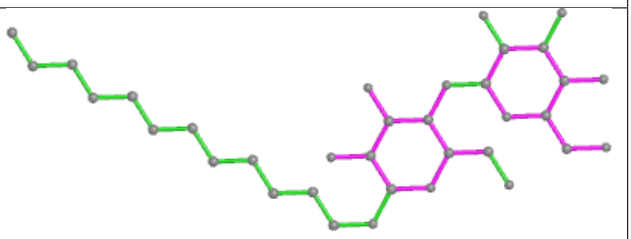


Rings

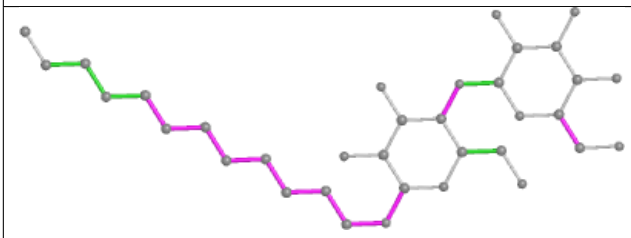
Ligand LMU 1 213



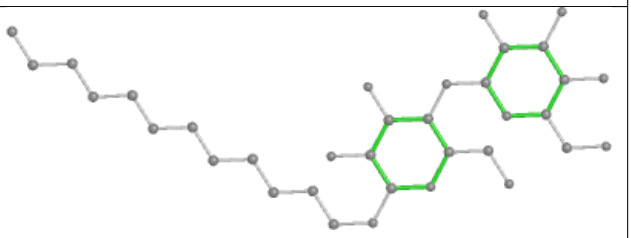
Bond lengths



Bond angles

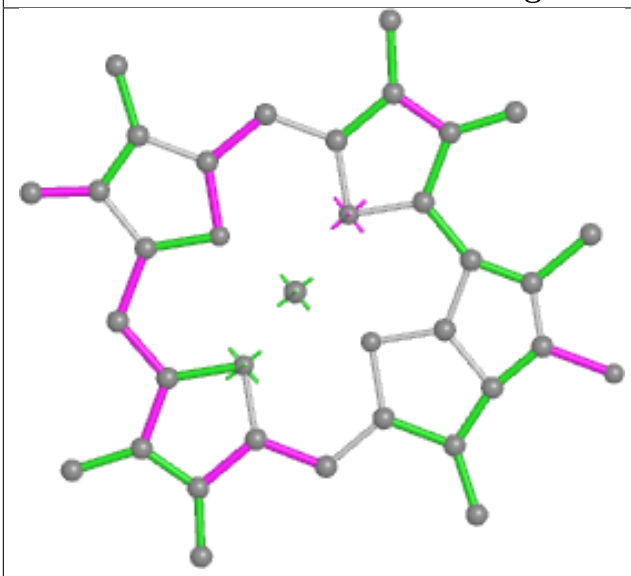


Torsions

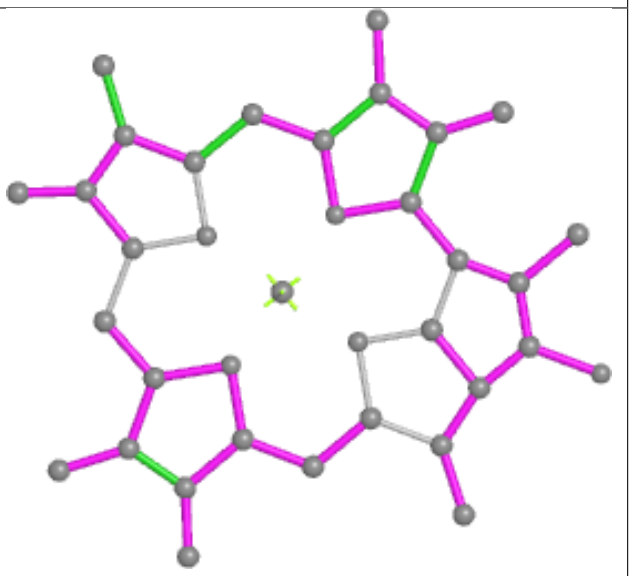


Rings

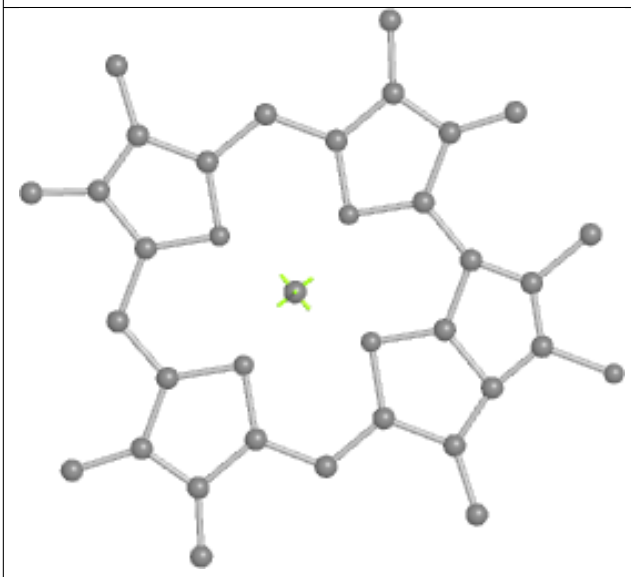
Ligand CLA B 840



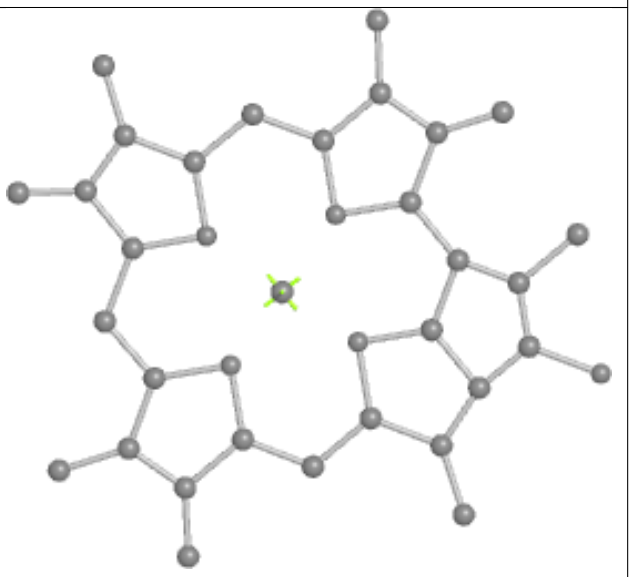
Bond lengths



Bond angles

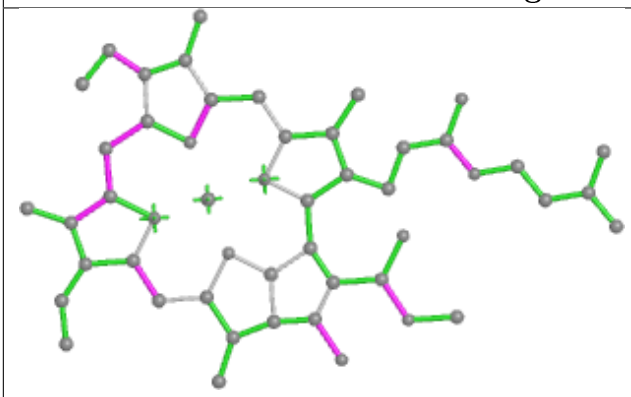


Torsions

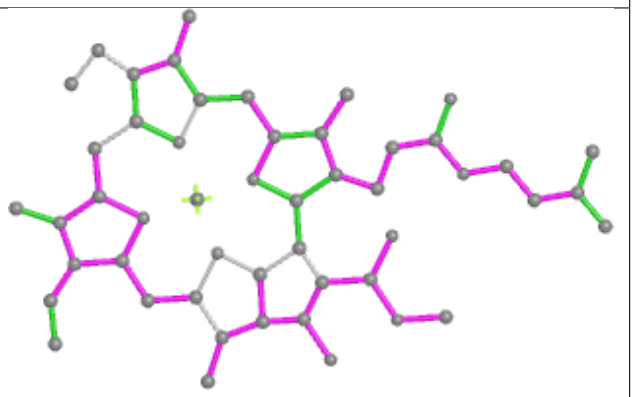


Rings

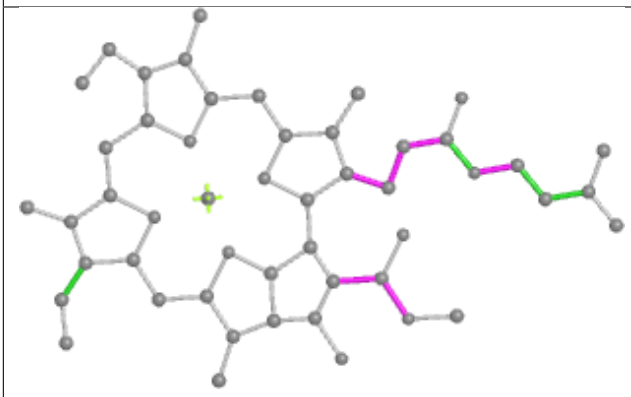
Ligand CLA B 828



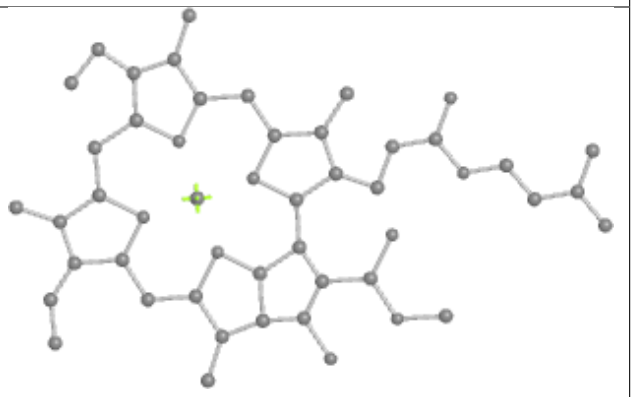
Bond lengths



Bond angles

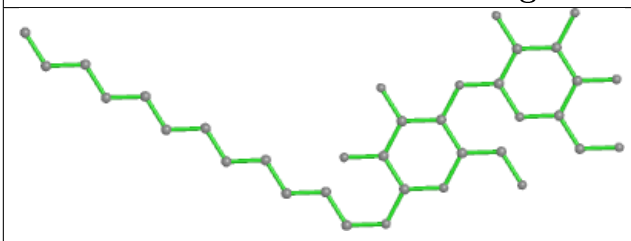


Torsions

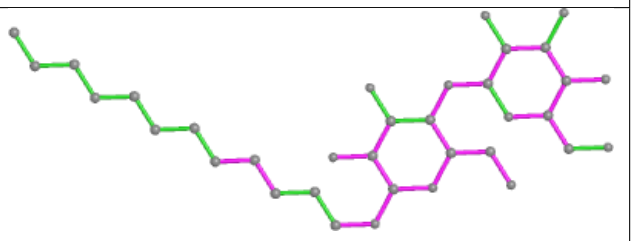


Rings

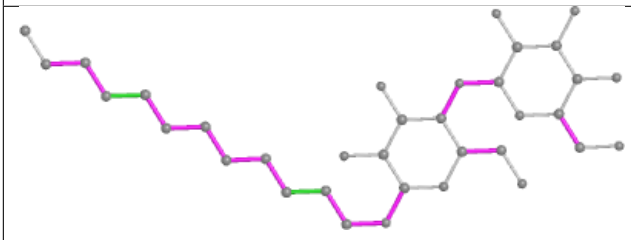
Ligand LMU K 105



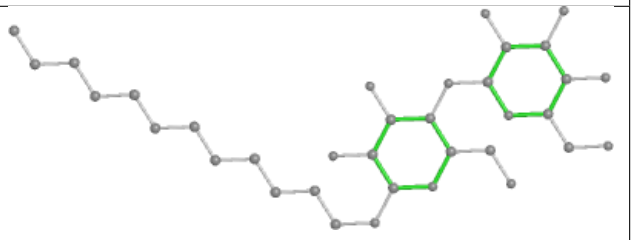
Bond lengths



Bond angles

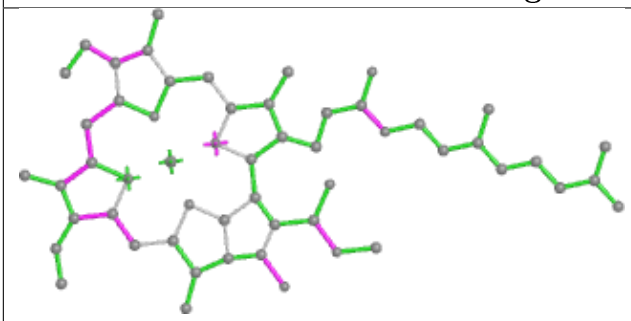


Torsions

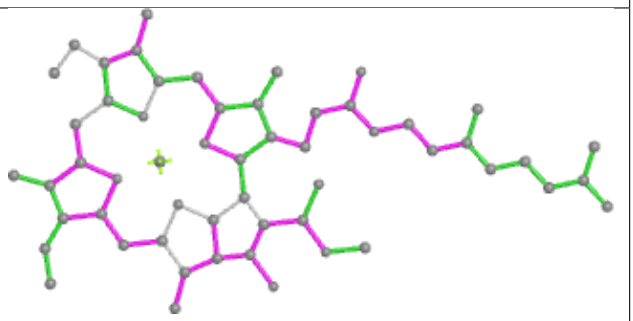


Rings

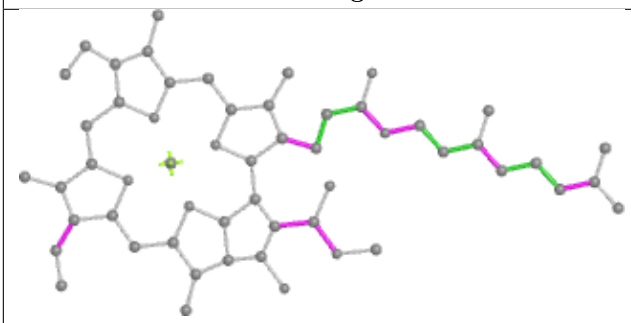
Ligand CLA A 804



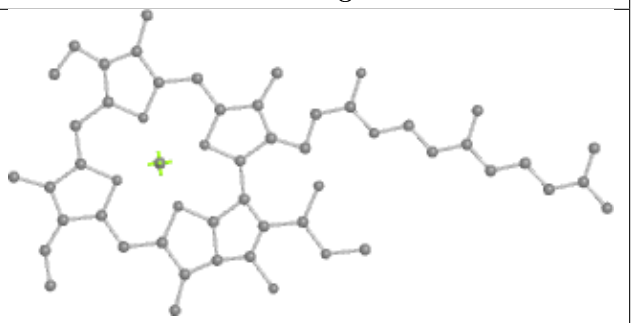
Bond lengths



Bond angles

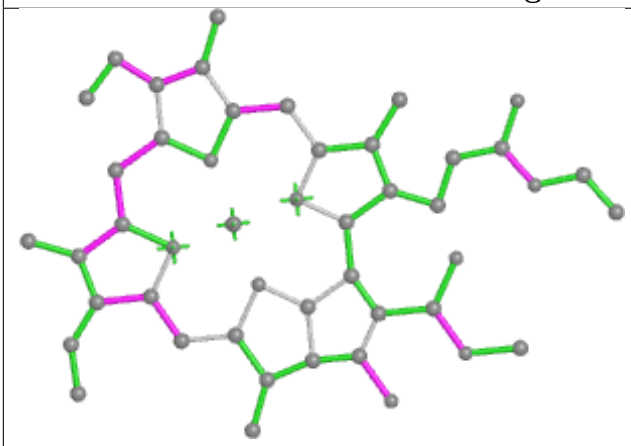


Torsions

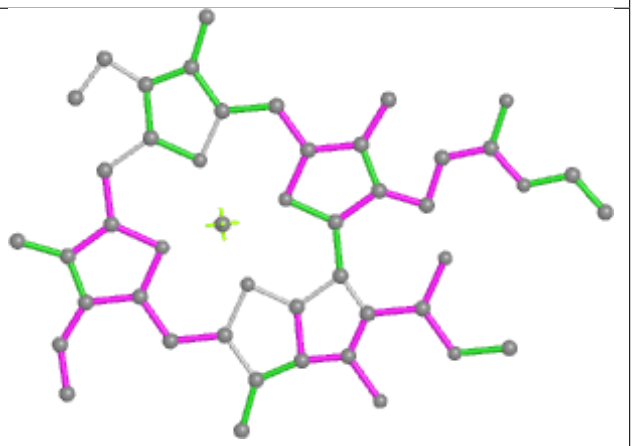


Rings

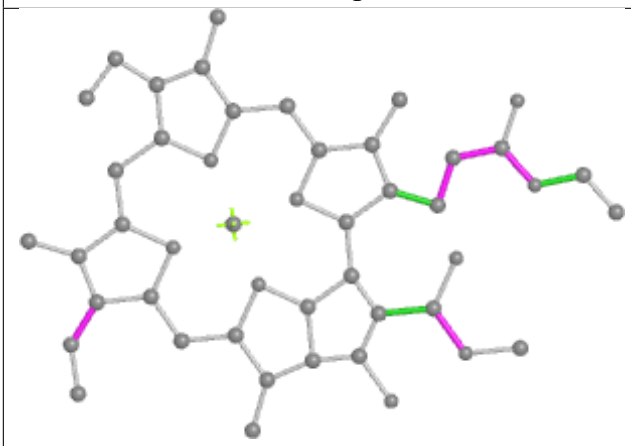
Ligand CLA A 836



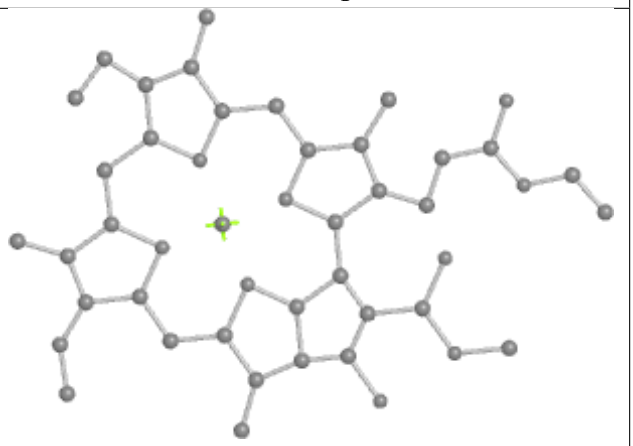
Bond lengths



Bond angles

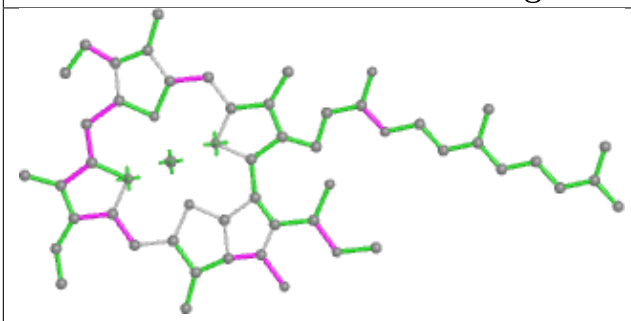


Torsions

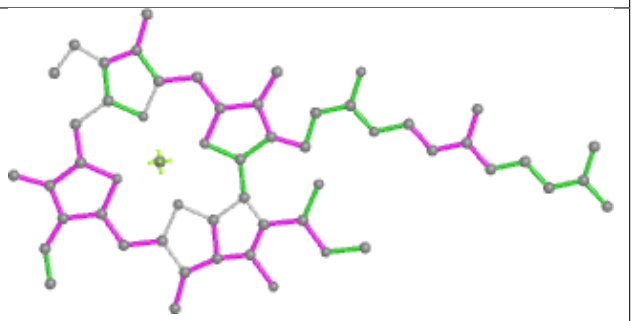


Rings

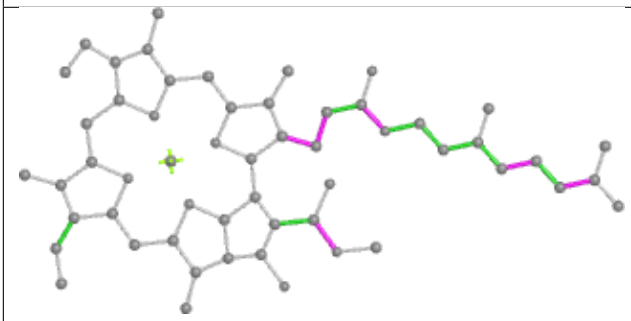
Ligand CLA A 822



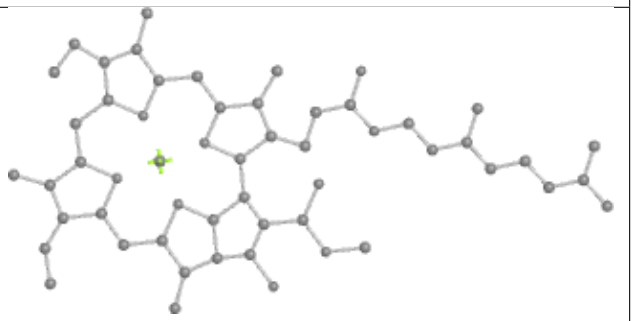
Bond lengths



Bond angles

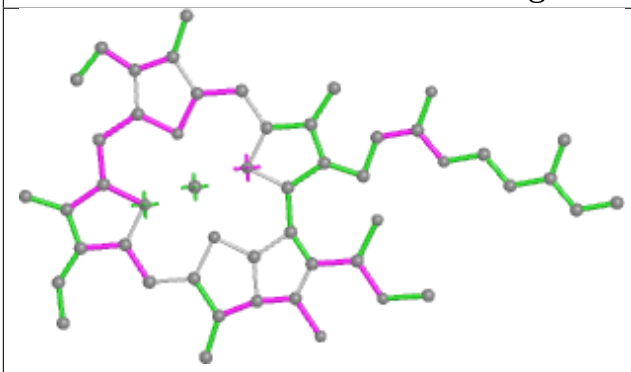


Torsions

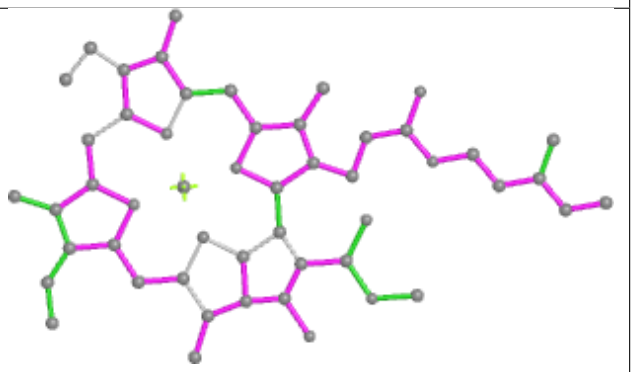


Rings

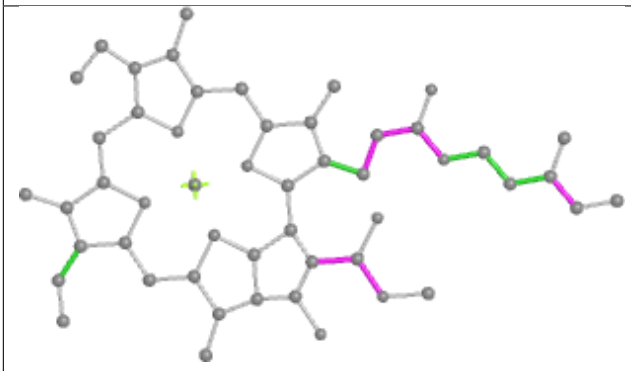
Ligand CLA 1 210



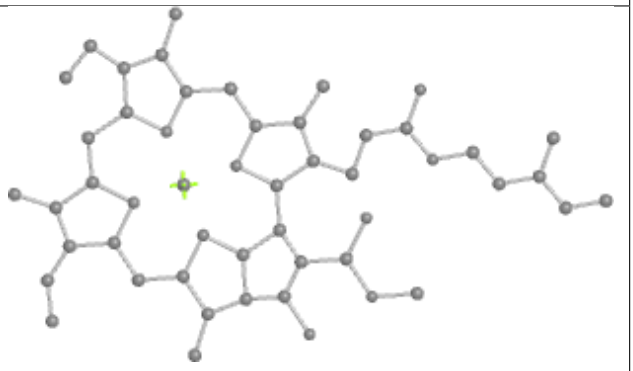
Bond lengths



Bond angles

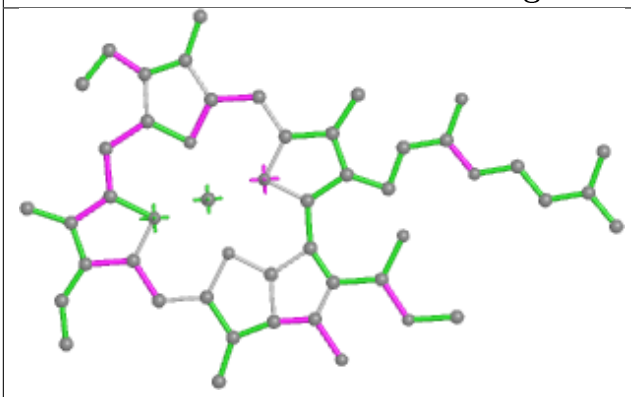


Torsions

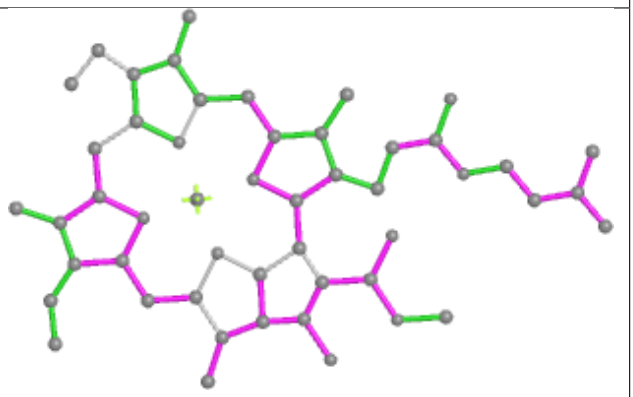


Rings

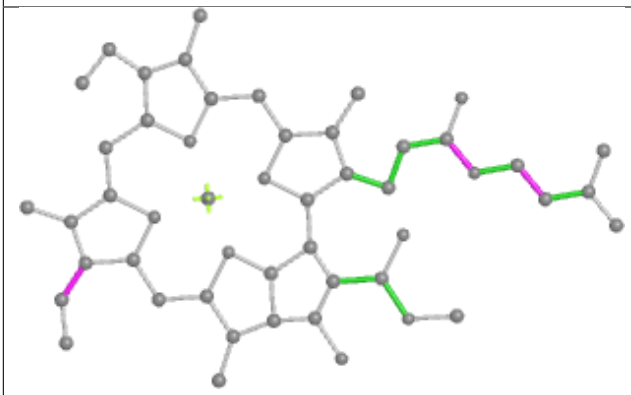
Ligand CLA K 108



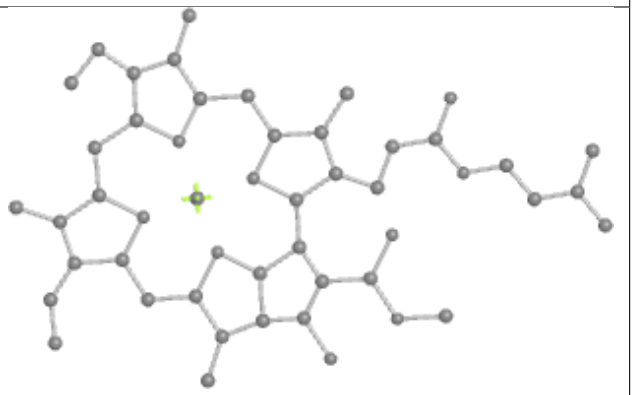
Bond lengths



Bond angles

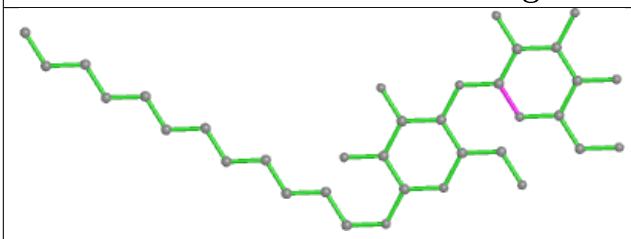


Torsions

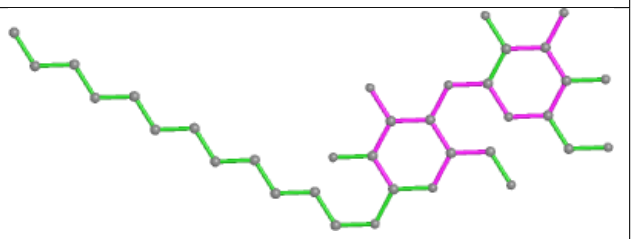


Rings

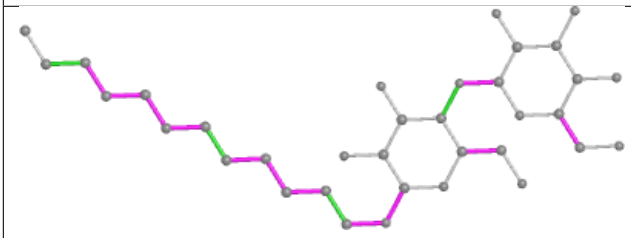
Ligand LMU L 211



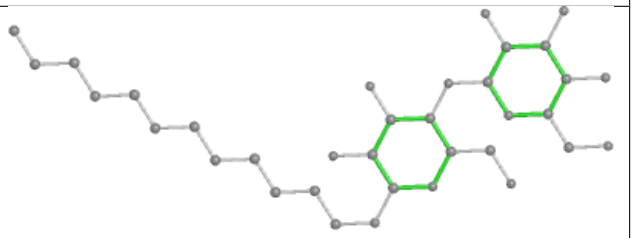
Bond lengths



Bond angles

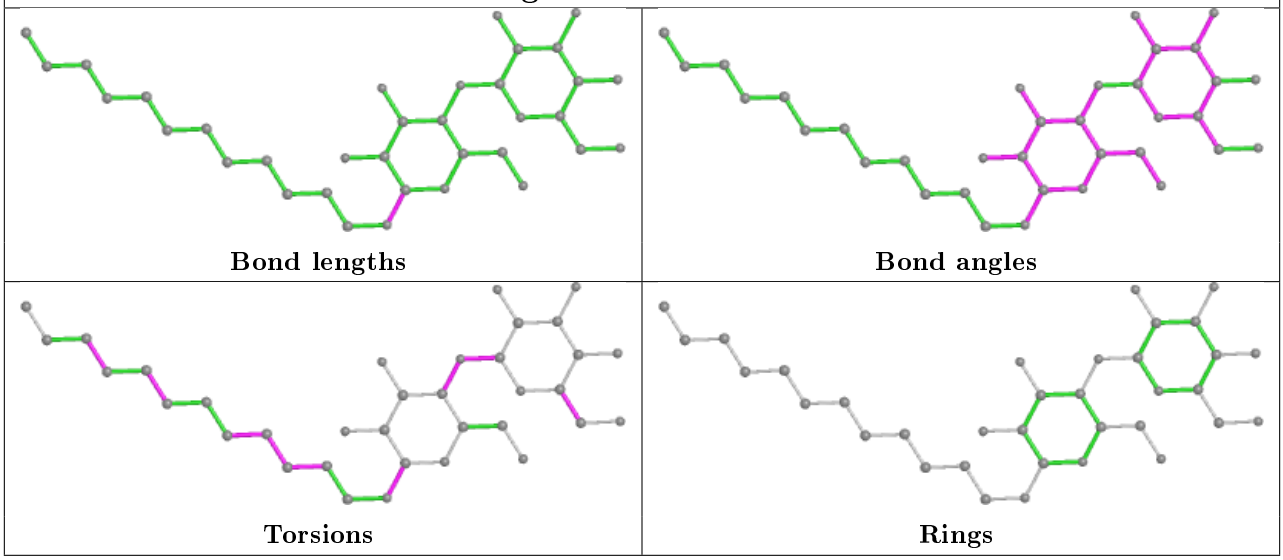


Torsions

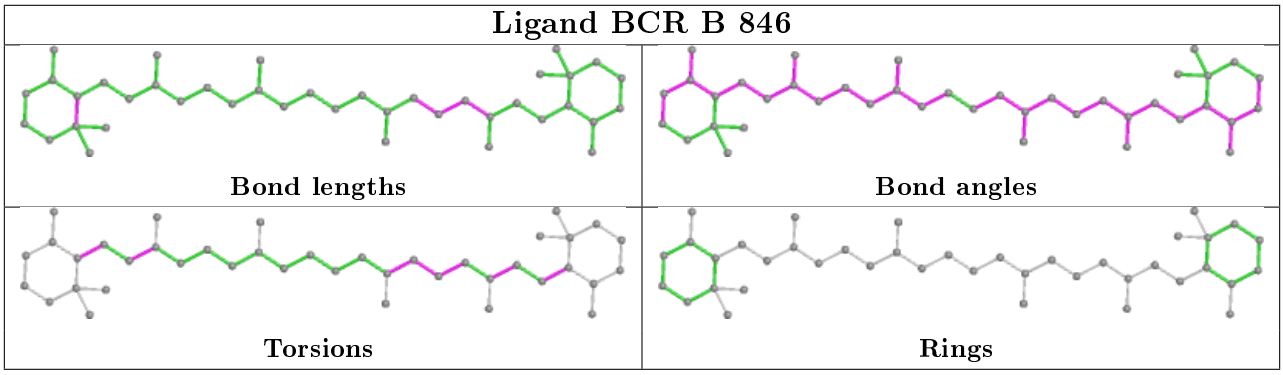


Rings

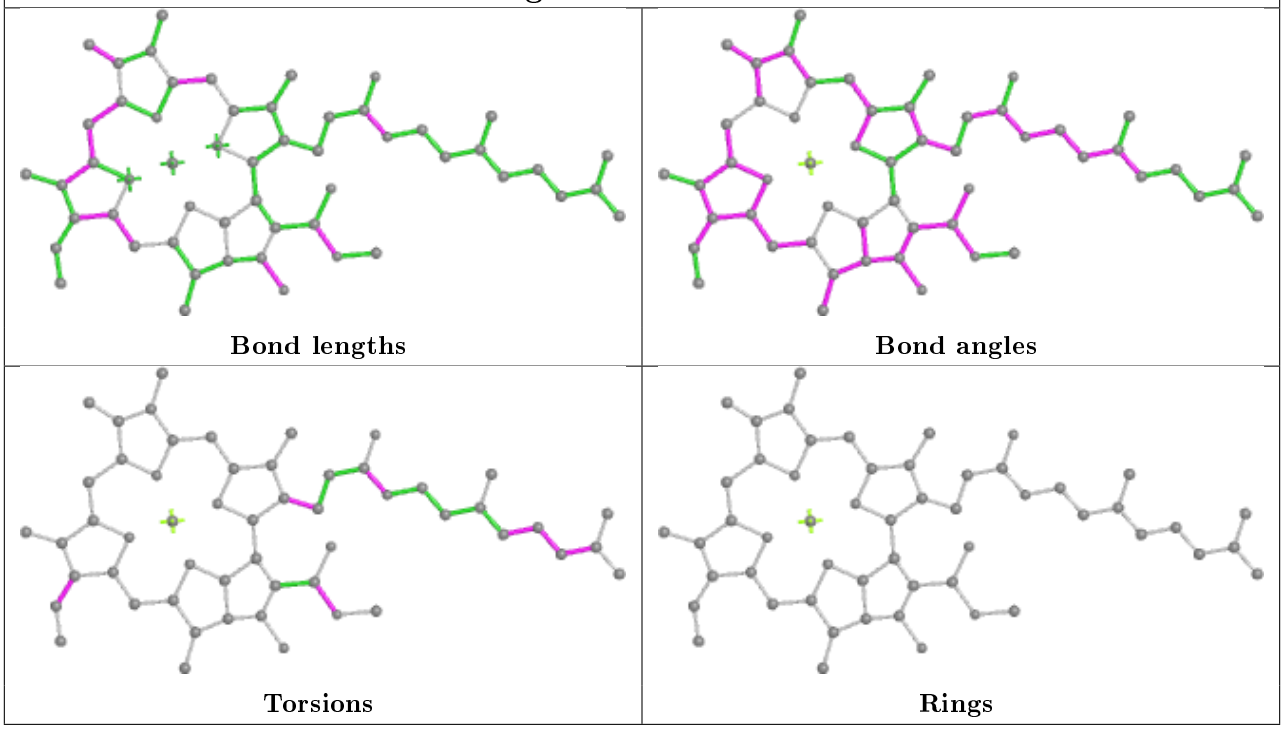
Ligand LMU B 847



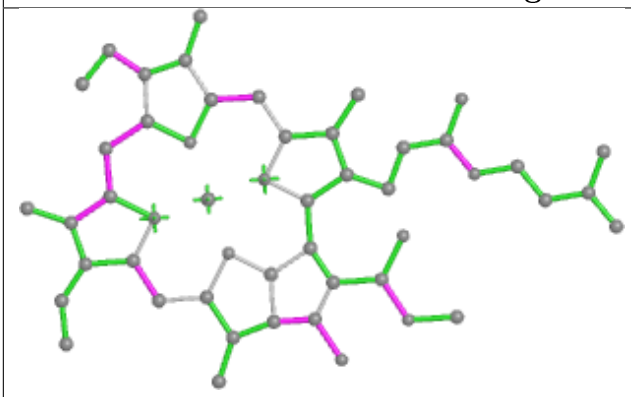
Ligand BCR B 846



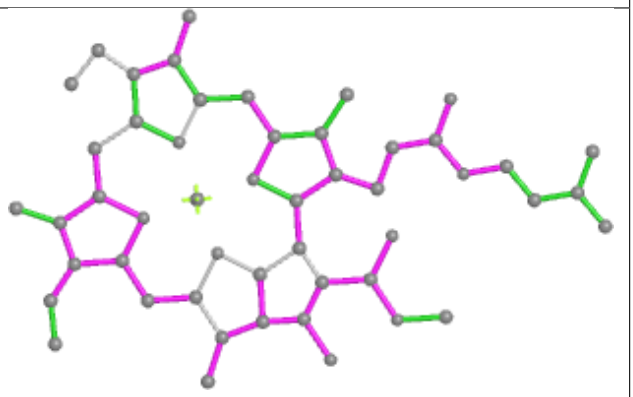
Ligand CLA B 809



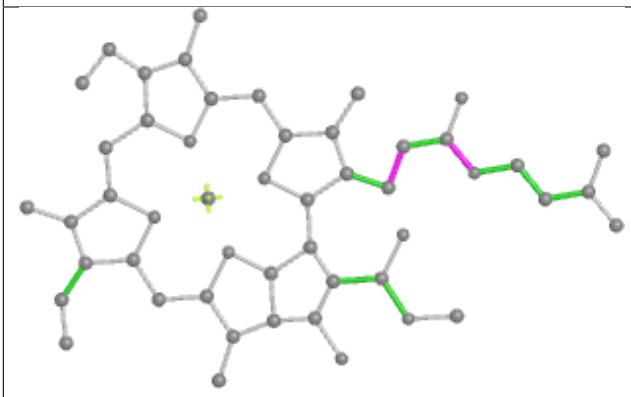
Ligand CLA A 829



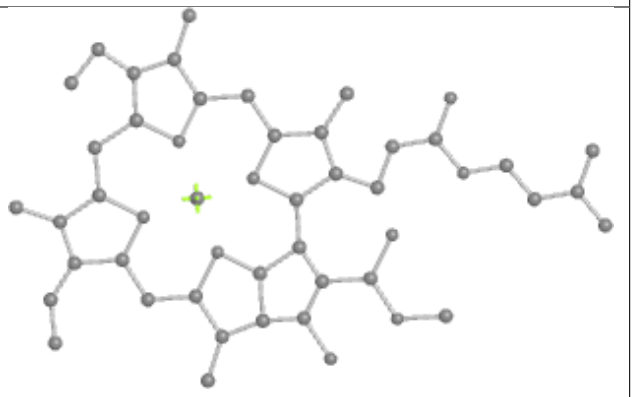
Bond lengths



Bond angles

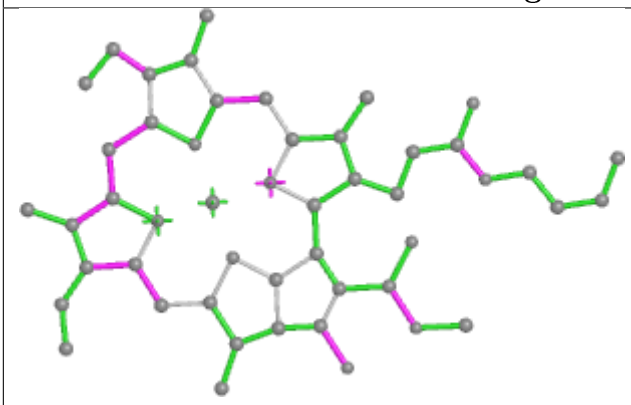


Torsions

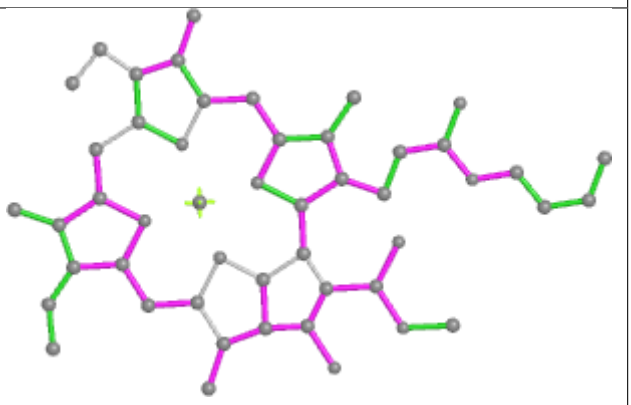


Rings

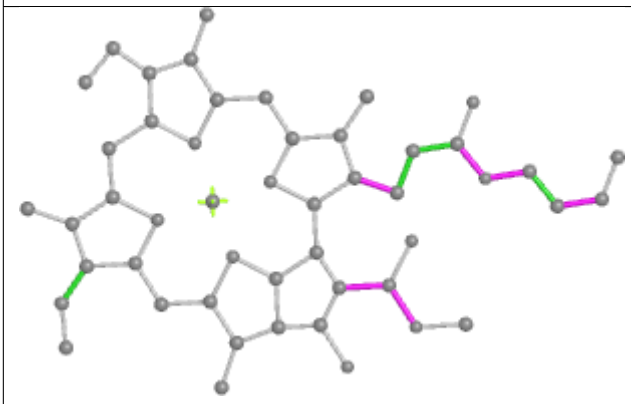
Ligand CLA A 834



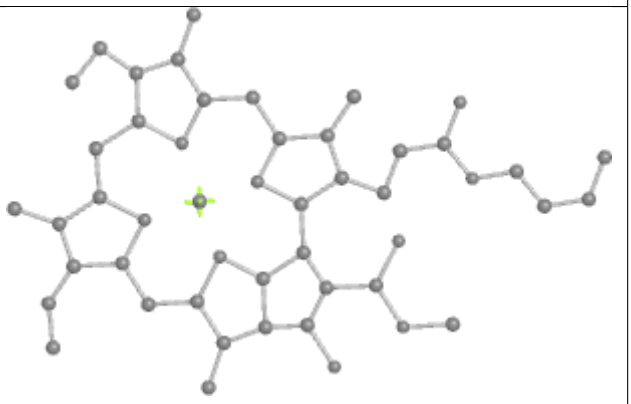
Bond lengths



Bond angles

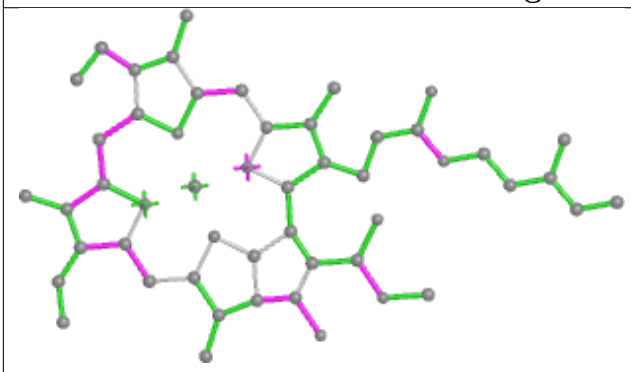


Torsions

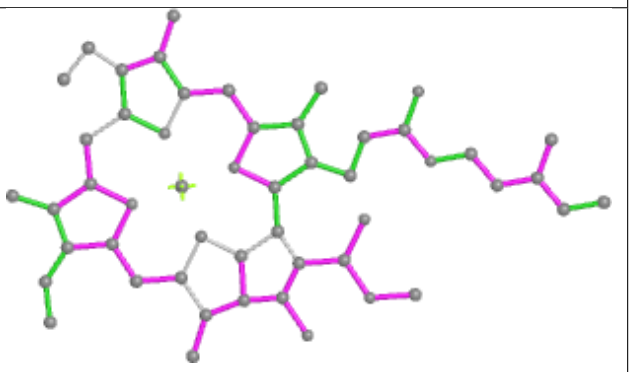


Rings

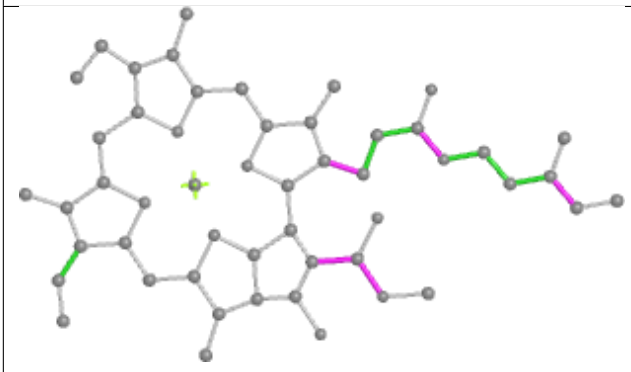
Ligand CLA A 820



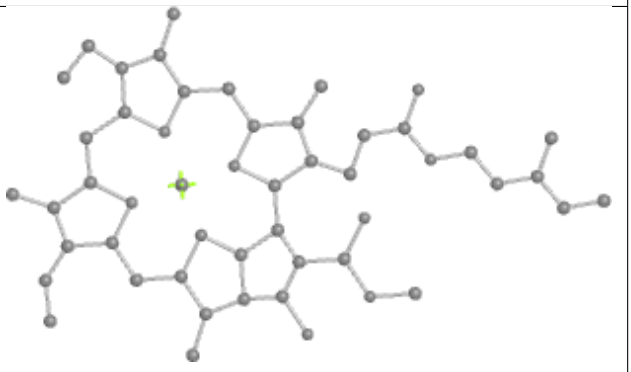
Bond lengths



Bond angles

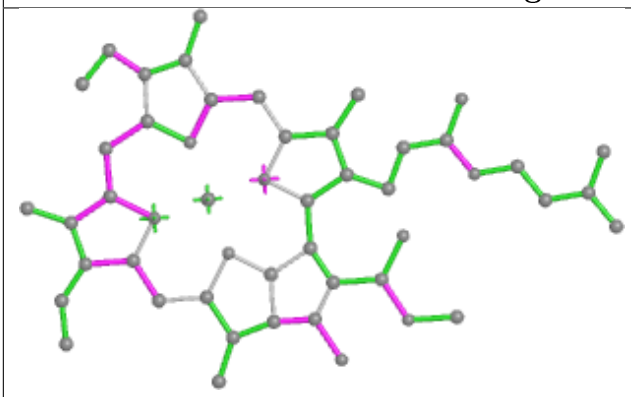


Torsions

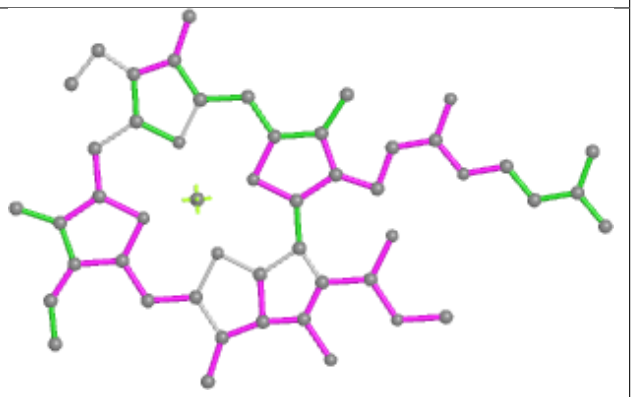


Rings

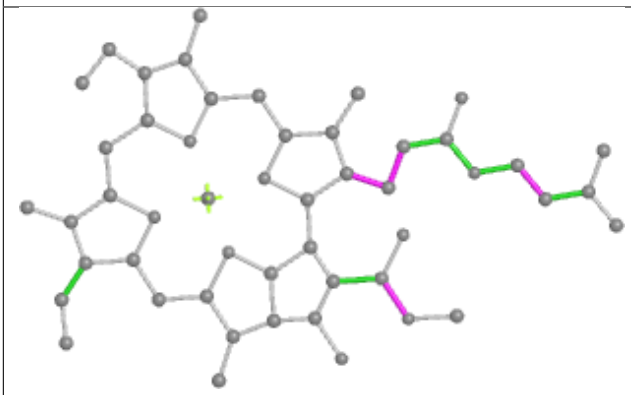
Ligand CLA B 831



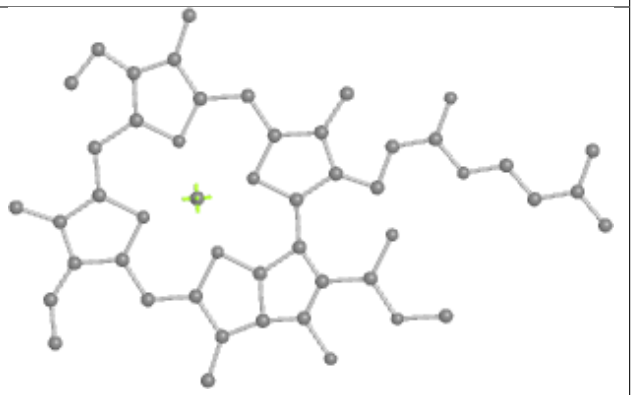
Bond lengths



Bond angles

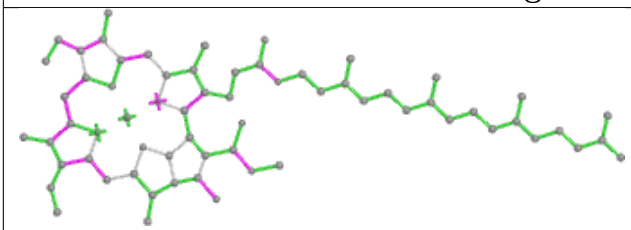


Torsions

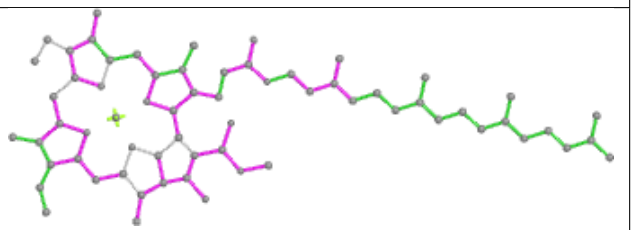


Rings

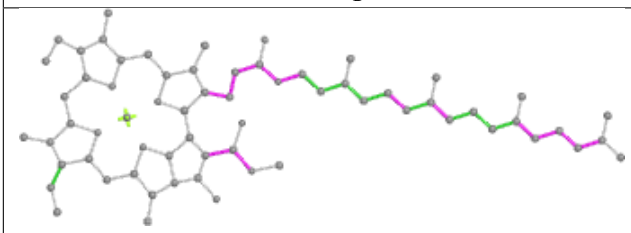
Ligand CLA B 803



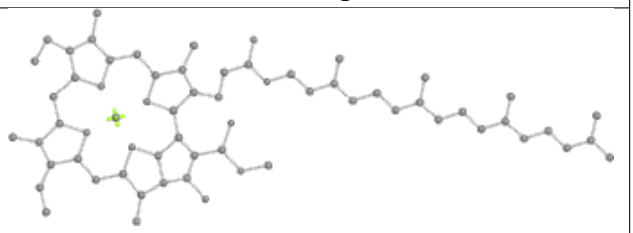
Bond lengths



Bond angles

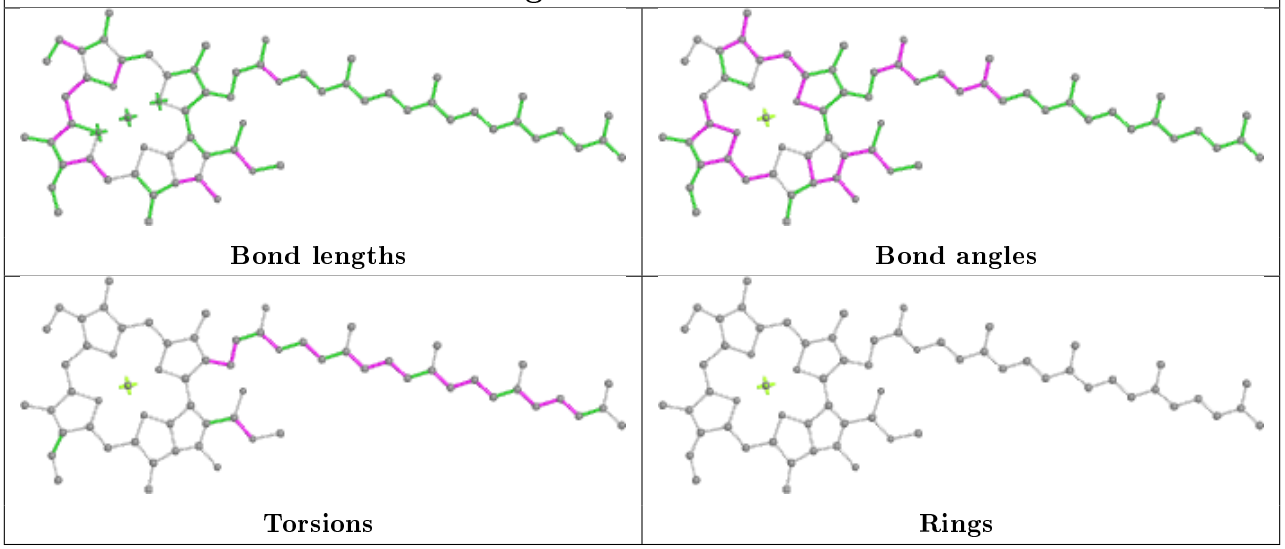


Torsions

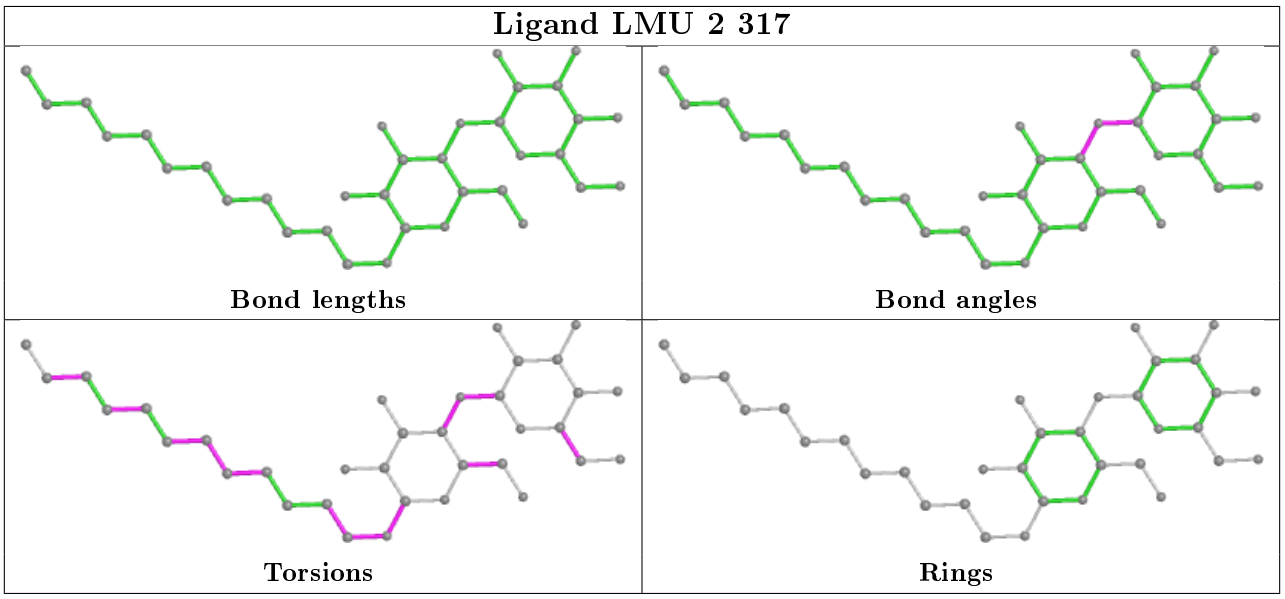


Rings

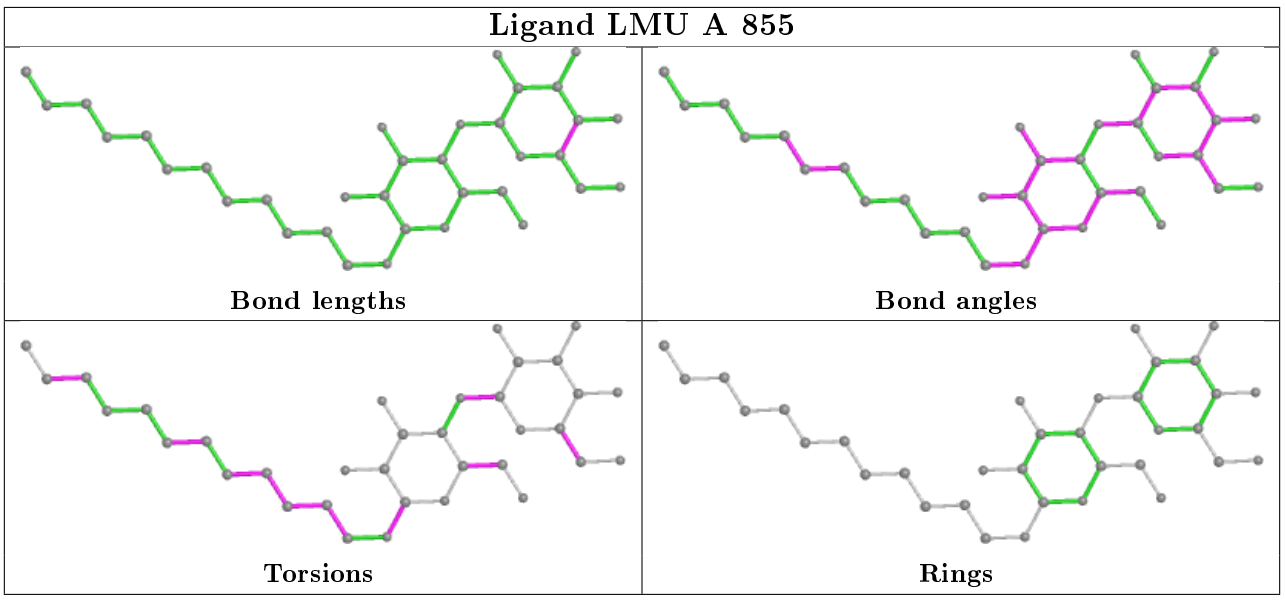
Ligand CLA B 808



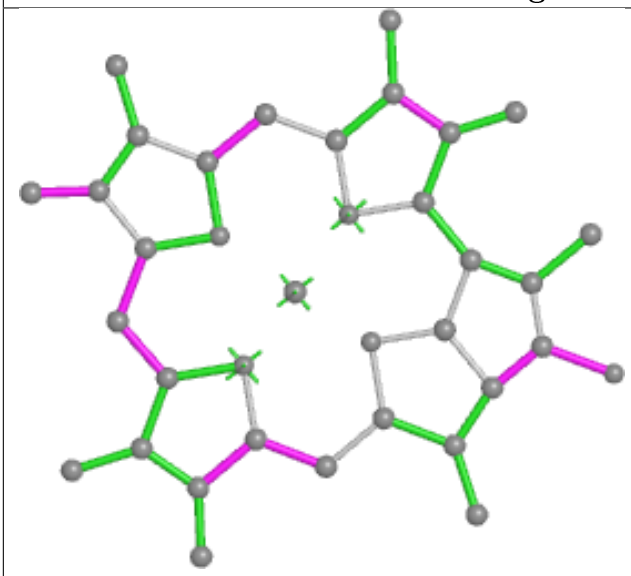
Ligand LMU 2 317



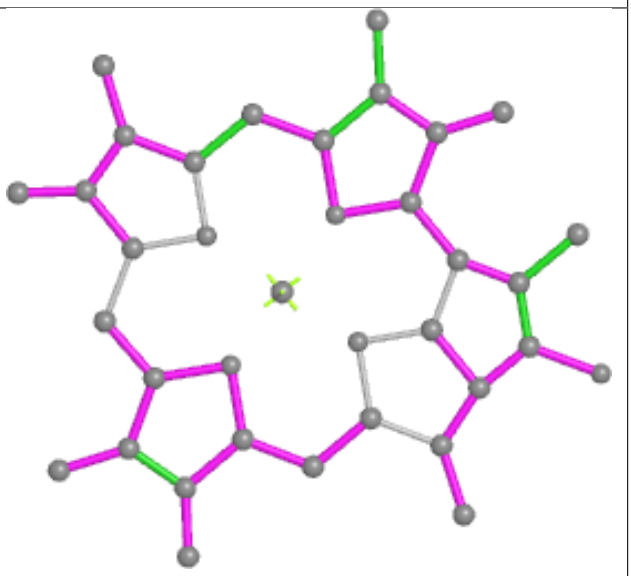
Ligand LMU A 855



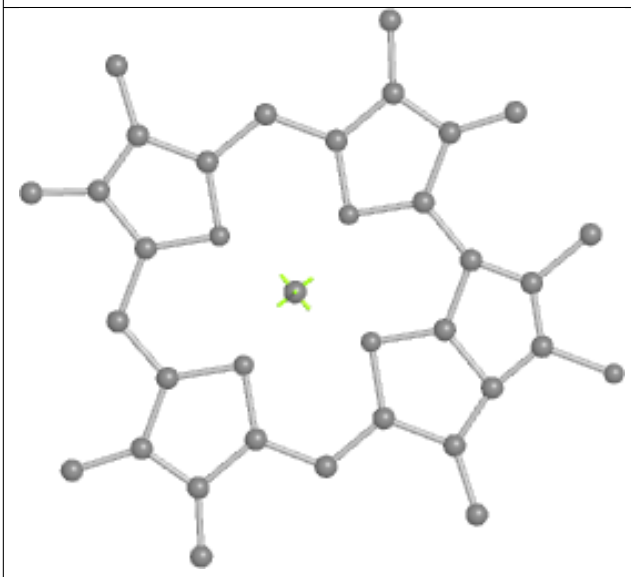
Ligand CLA 3 301



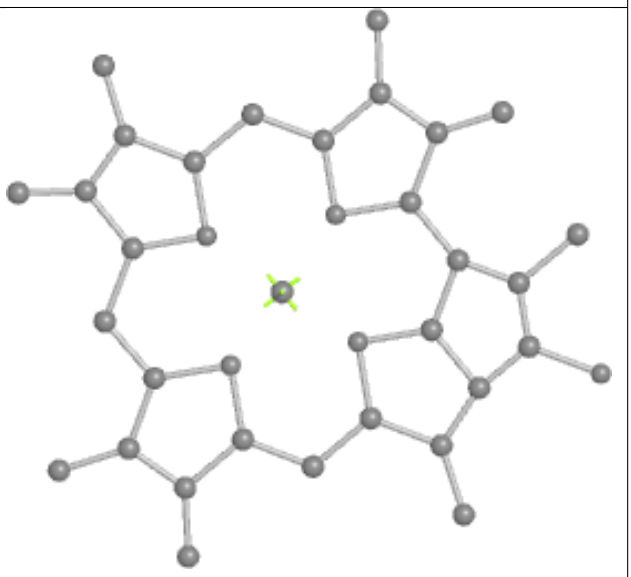
Bond lengths



Bond angles

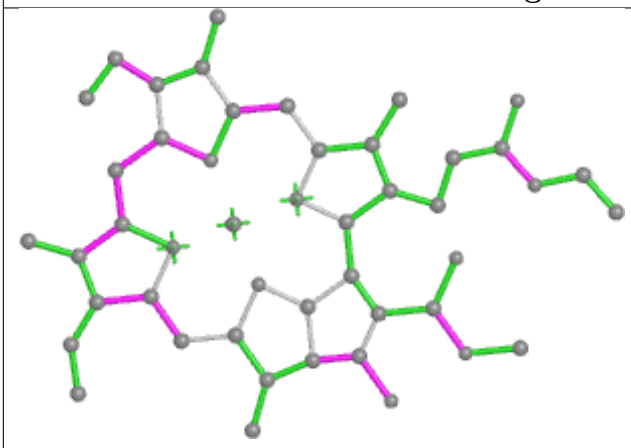


Torsions

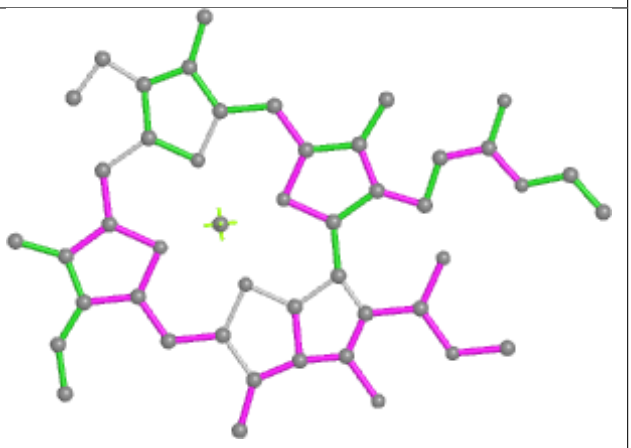


Rings

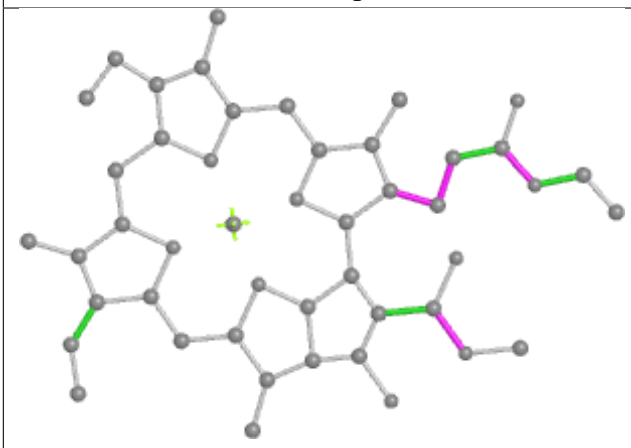
Ligand CLA B 837



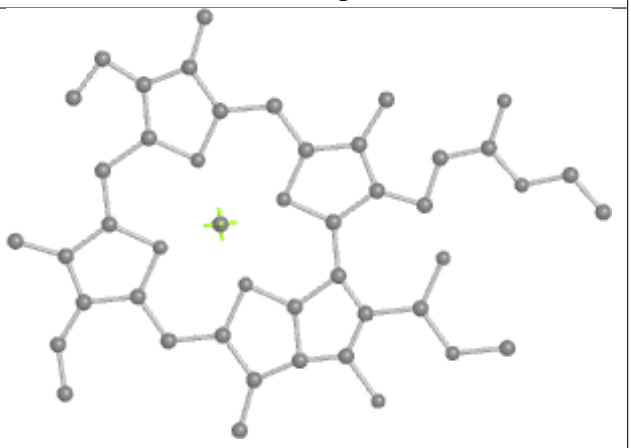
Bond lengths



Bond angles

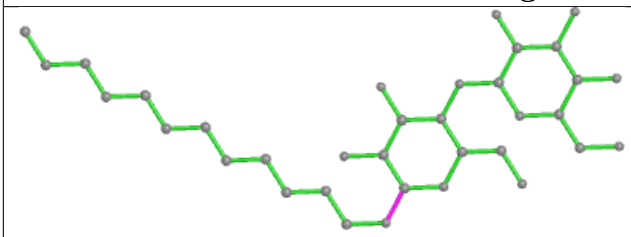


Torsions

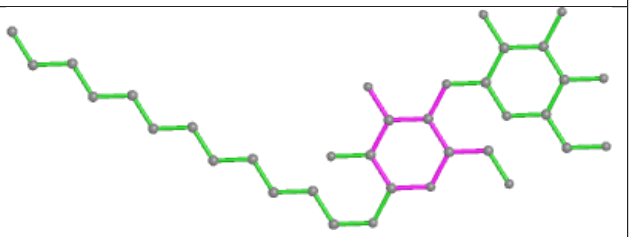


Rings

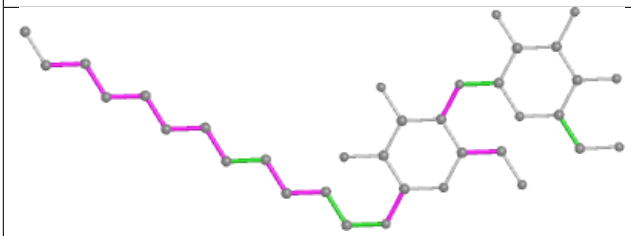
Ligand LMU A 856



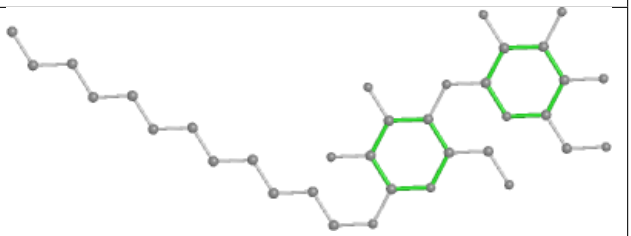
Bond lengths



Bond angles

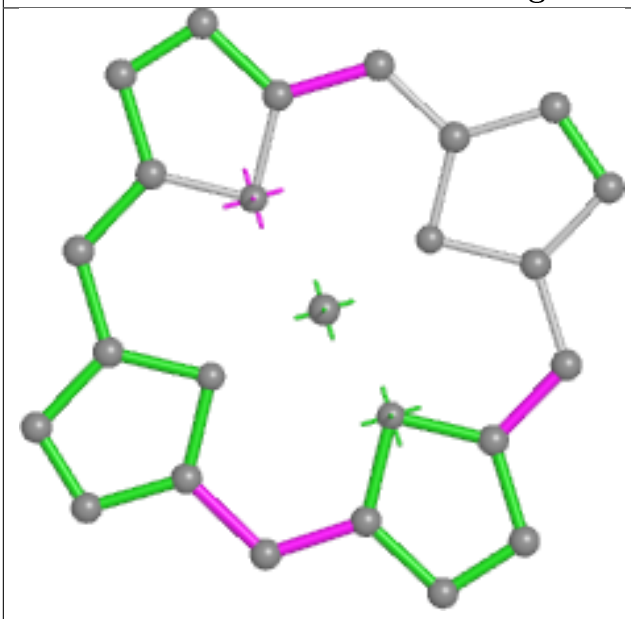


Torsions

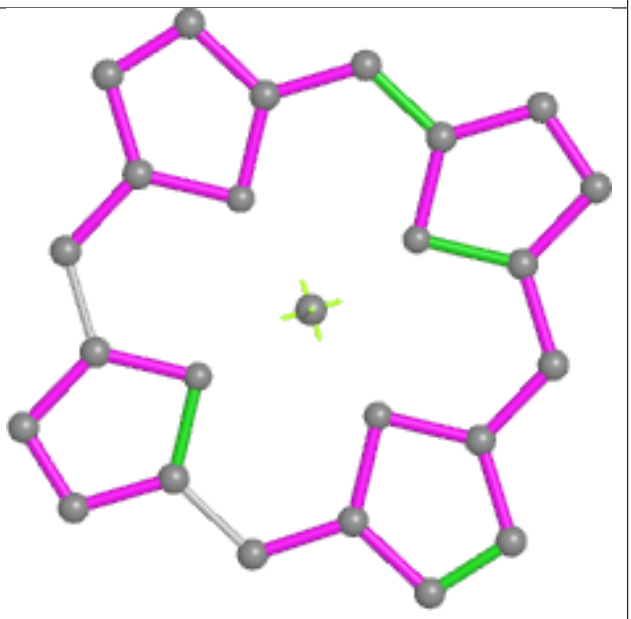


Rings

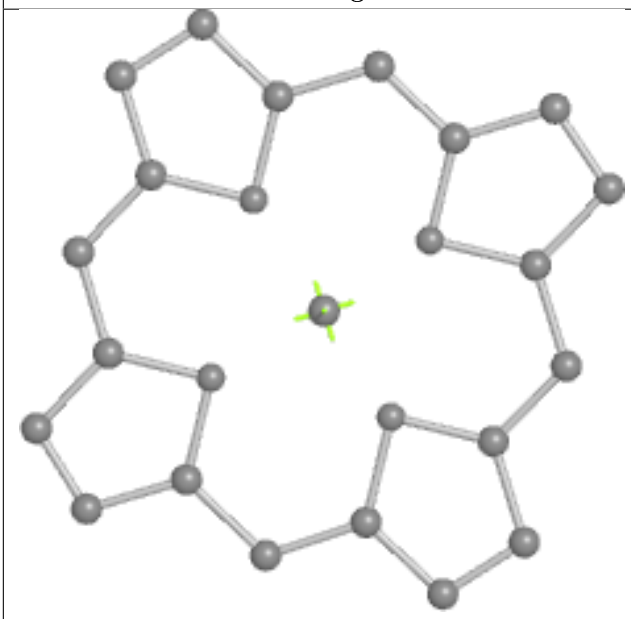
Ligand CLA 1 214



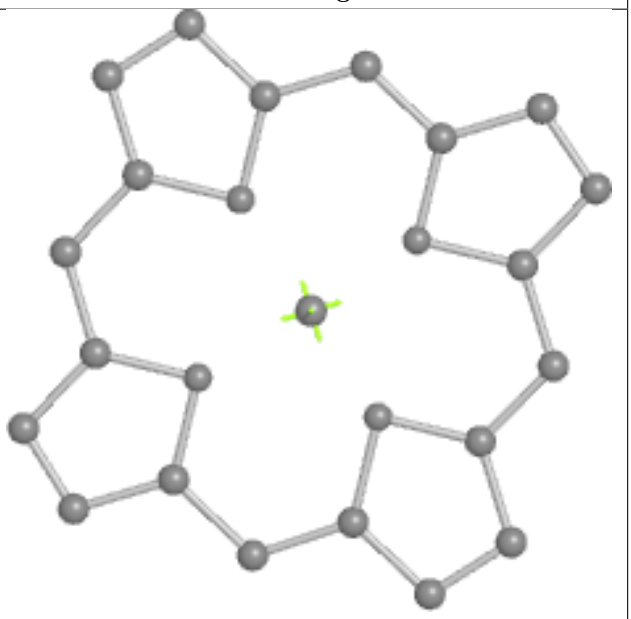
Bond lengths



Bond angles

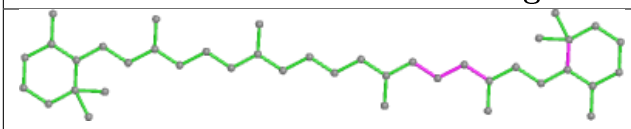


Torsions

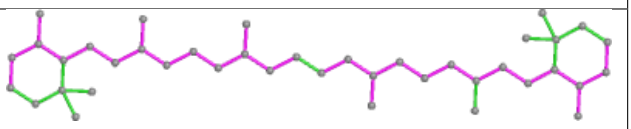


Rings

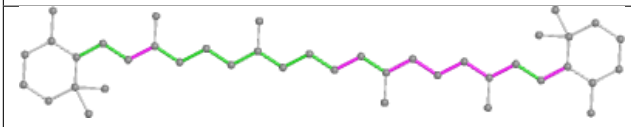
Ligand BCR B 842



Bond lengths



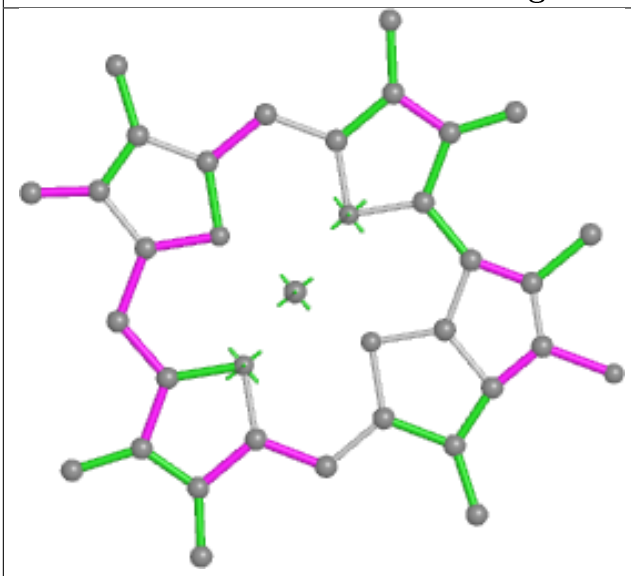
Bond angles



Torsions

Rings

Ligand CLA 4 303



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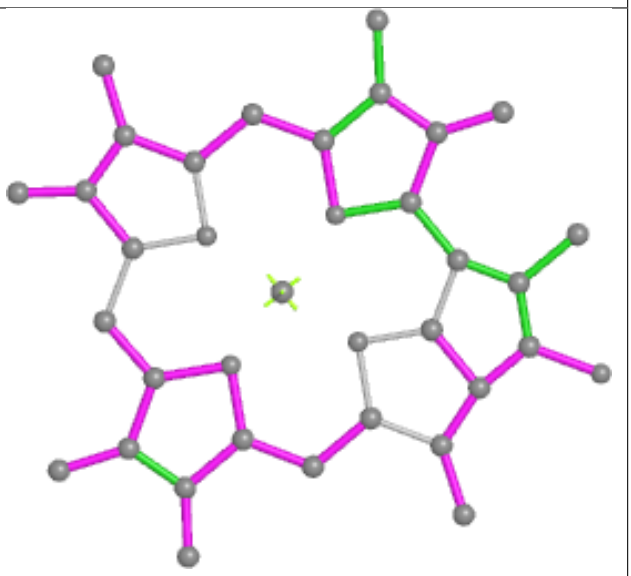
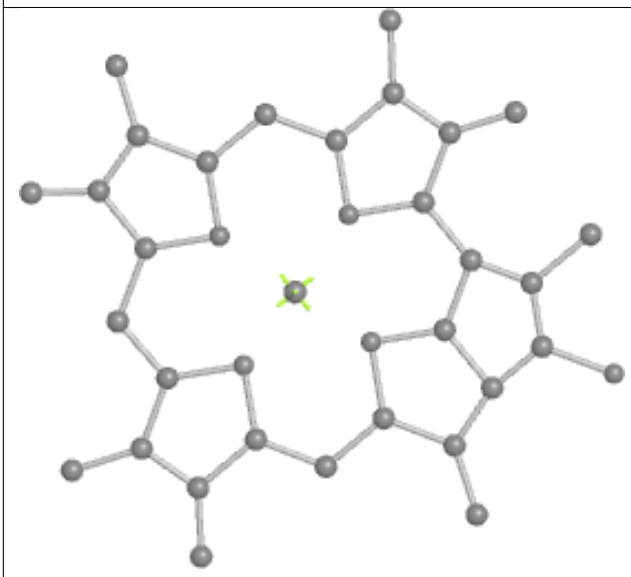
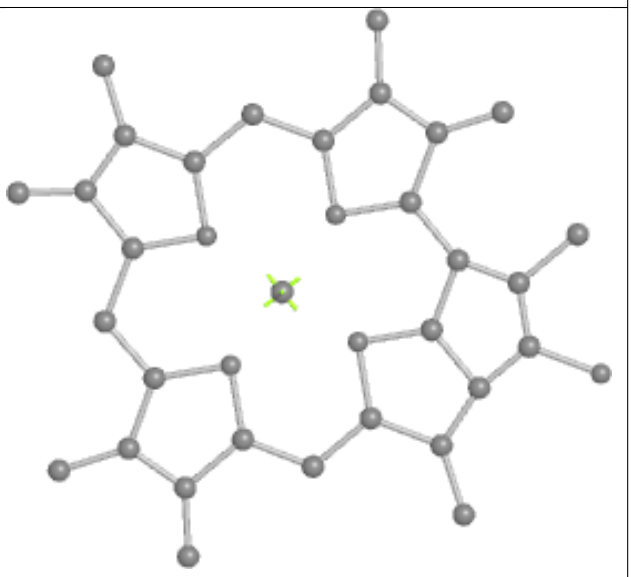


Bond angles

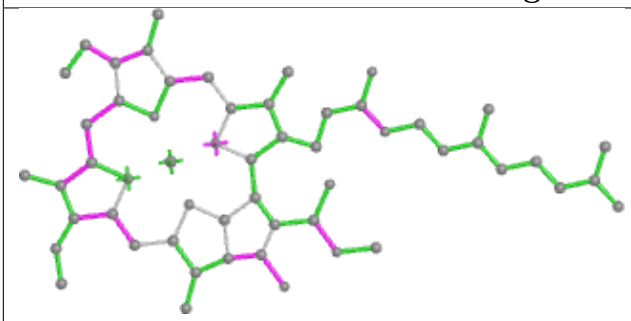


Torsions

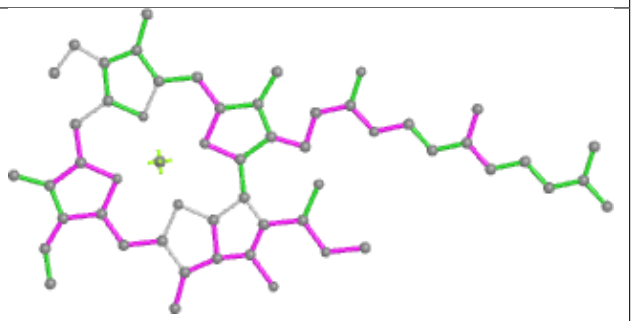


Rings

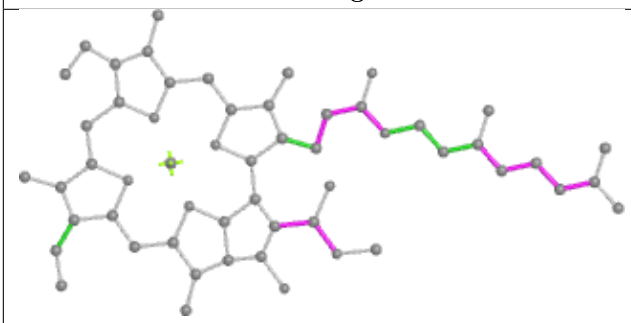
Ligand CLA H 103



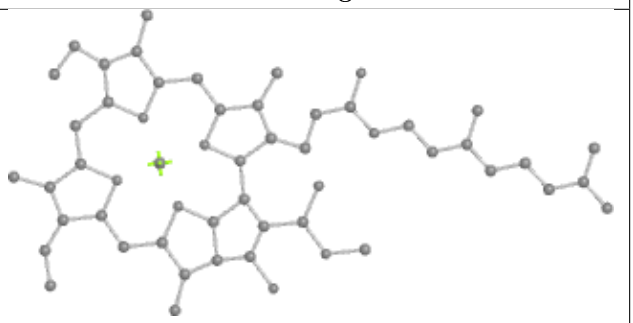
Bond lengths



Bond angles

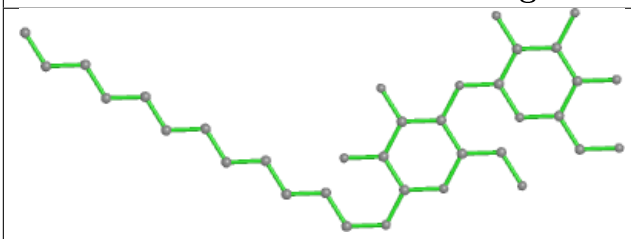


Torsions

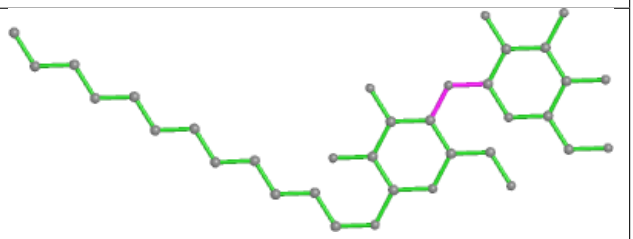


Rings

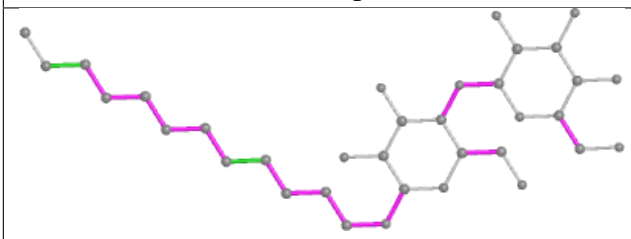
Ligand LMU A 853



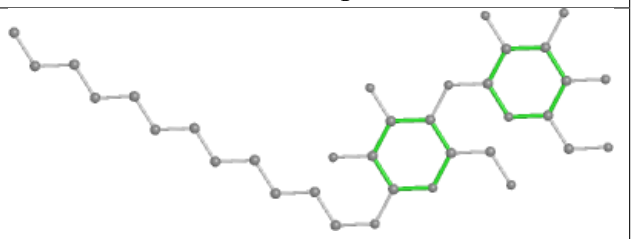
Bond lengths



Bond angles

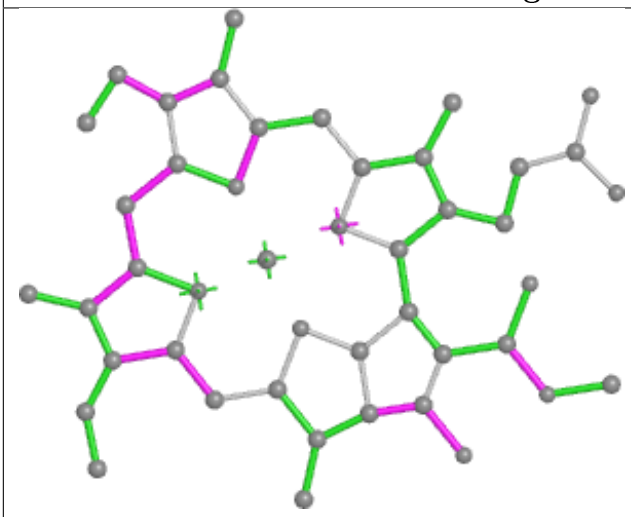


Torsions

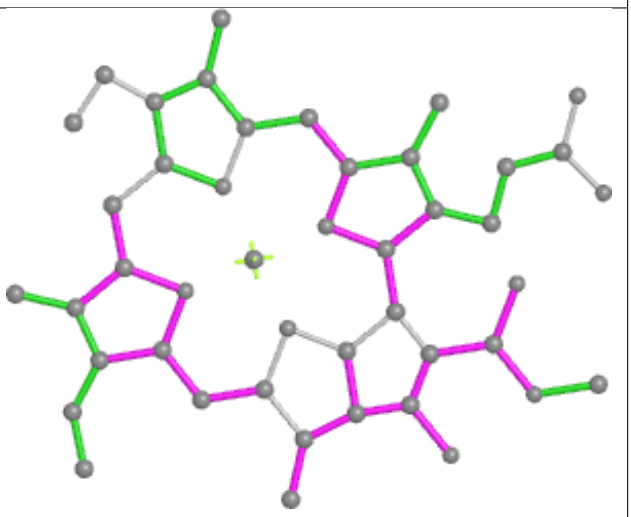


Rings

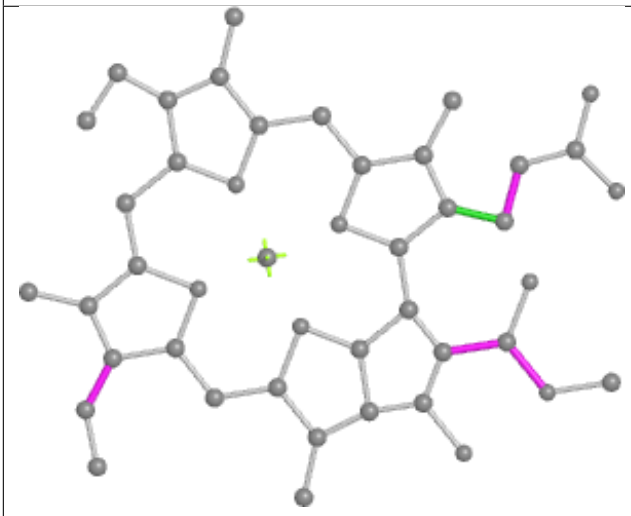
Ligand CLA K 101



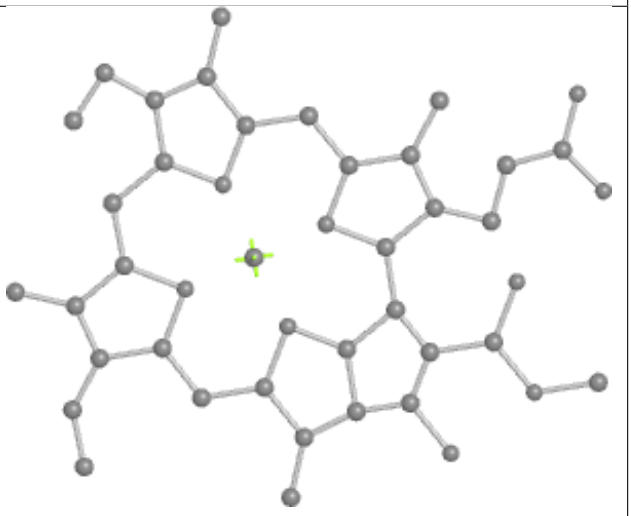
Bond lengths



Bond angles

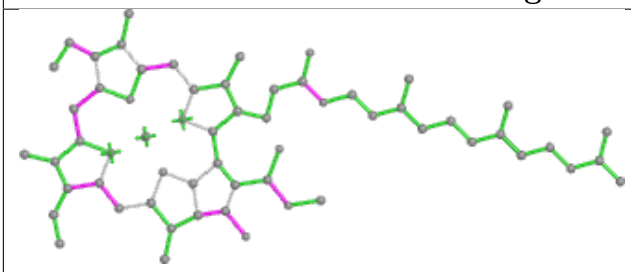


Torsions

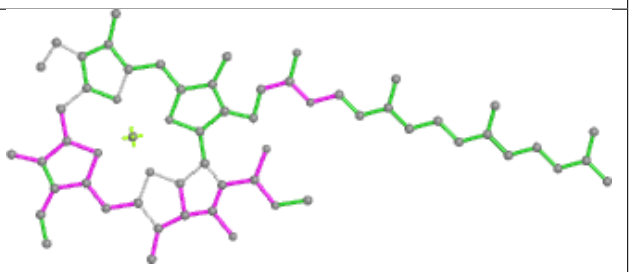


Rings

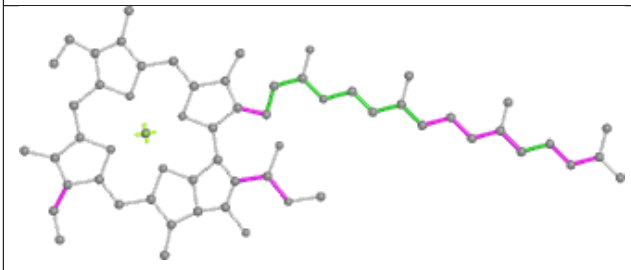
Ligand CLA B 835



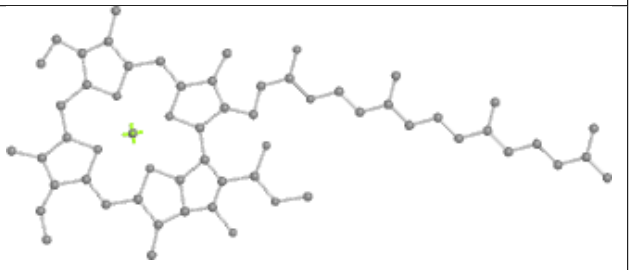
Bond lengths



Bond angles

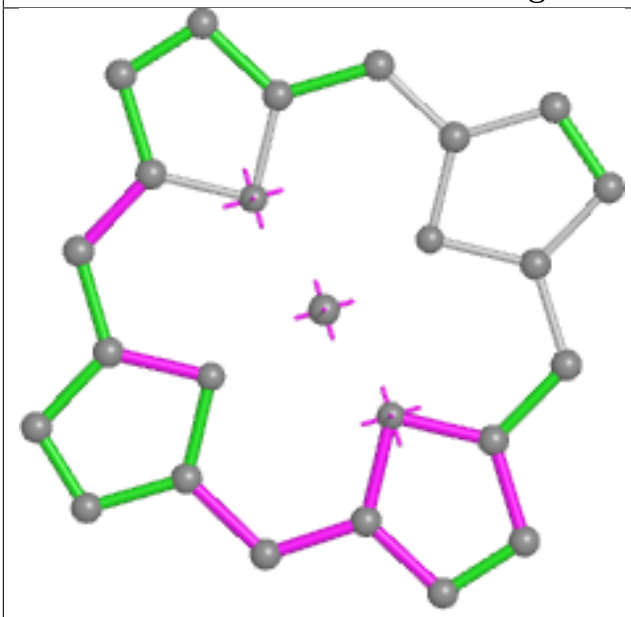


Torsions

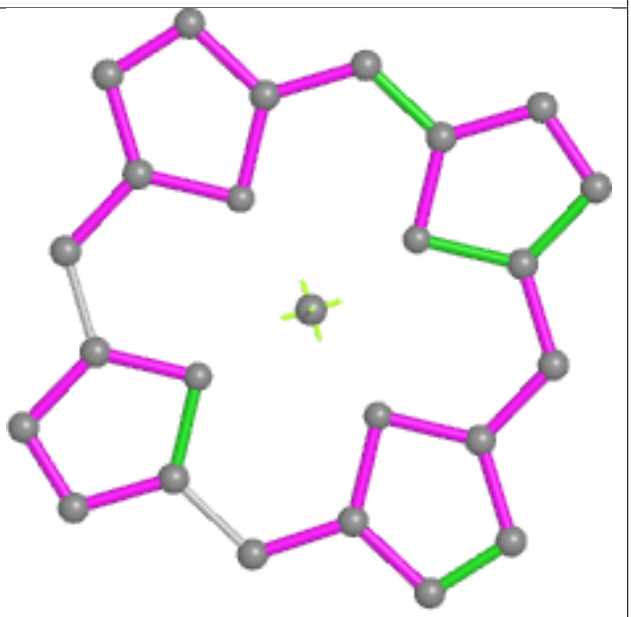


Rings

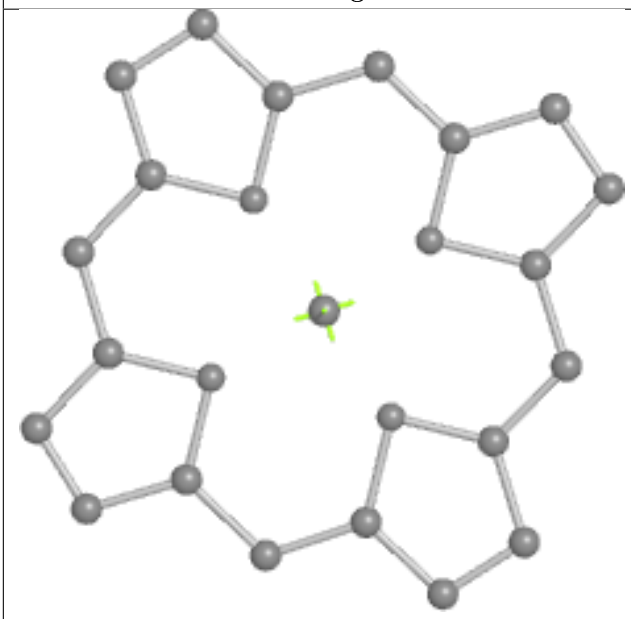
Ligand CLA 3 319



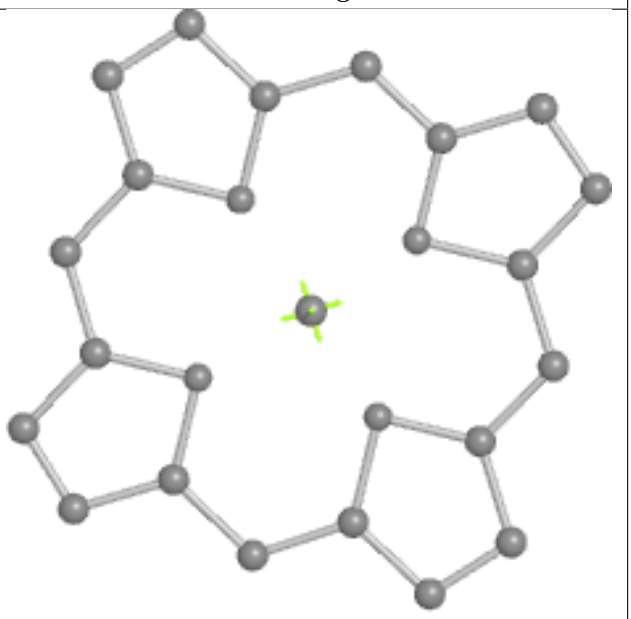
Bond lengths



Bond angles

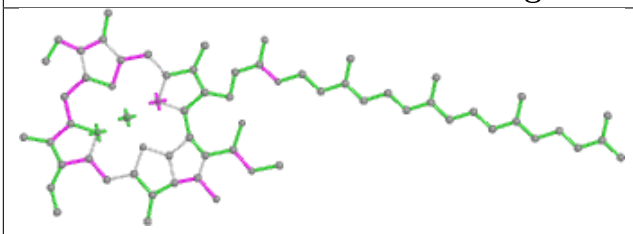


Torsions

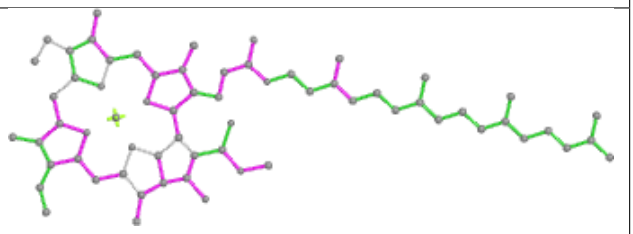


Rings

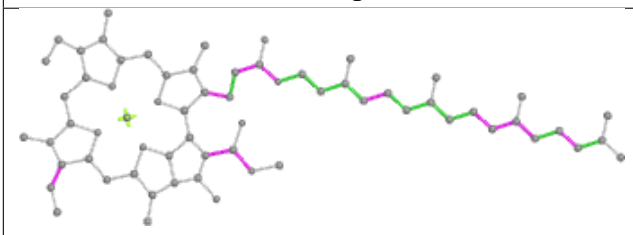
Ligand CLA B 839



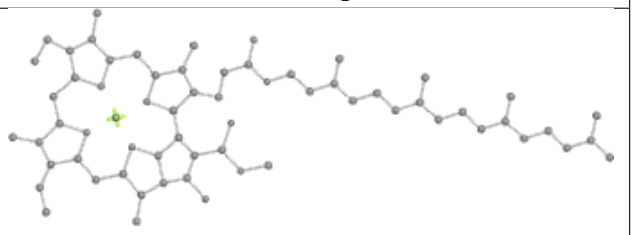
Bond lengths



Bond angles

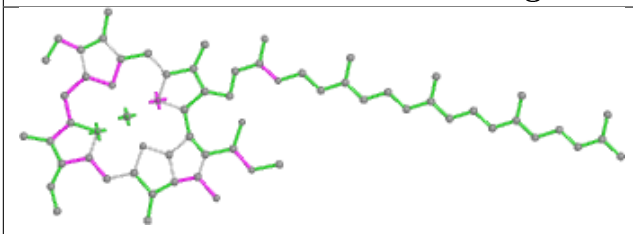


Torsions

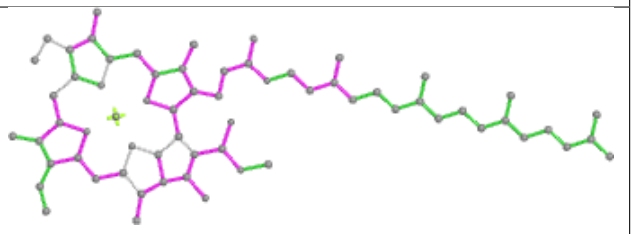


Rings

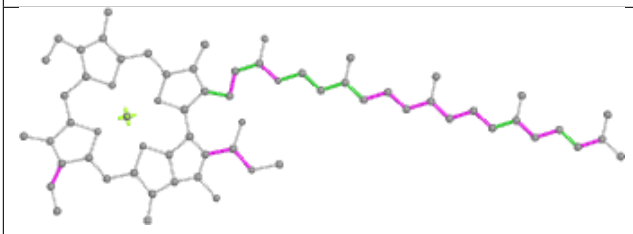
Ligand CLA B 838



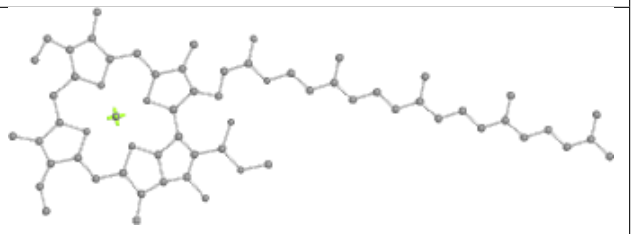
Bond lengths



Bond angles

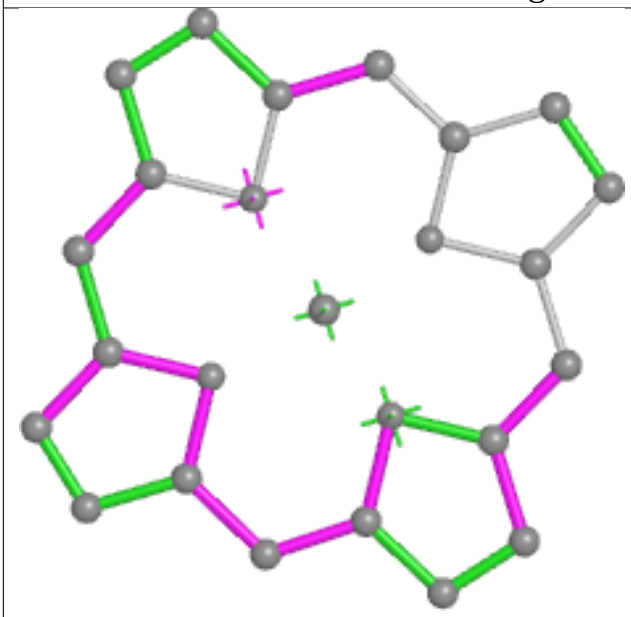


Torsions

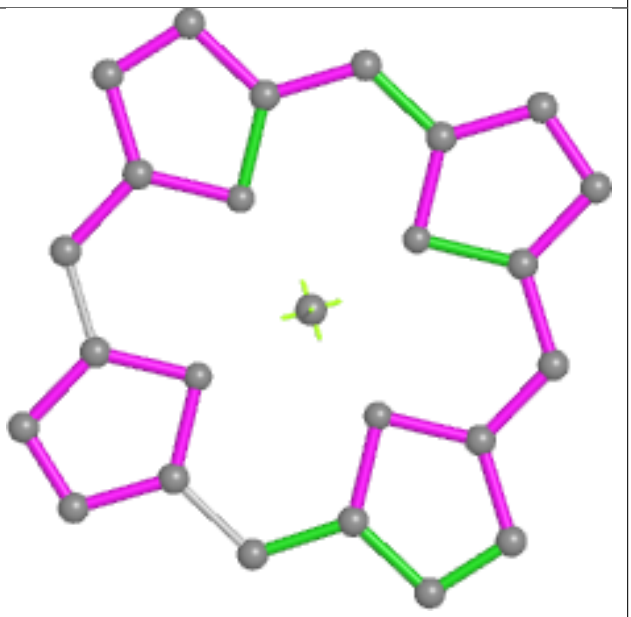


Rings

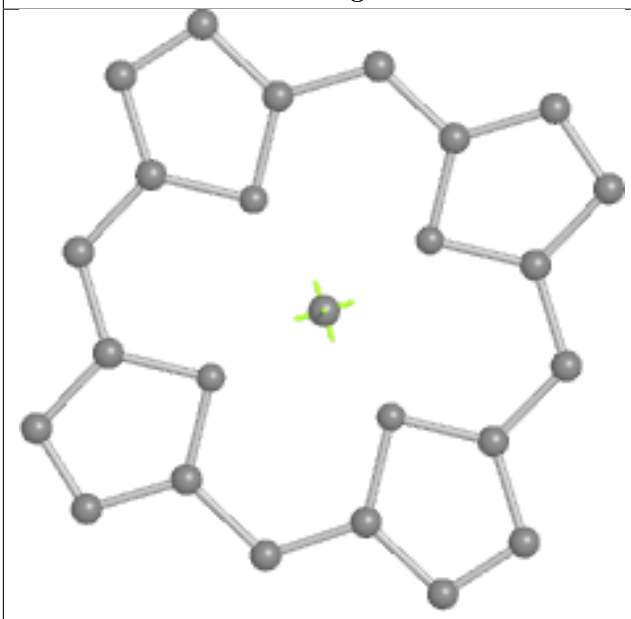
Ligand CLA 2 301



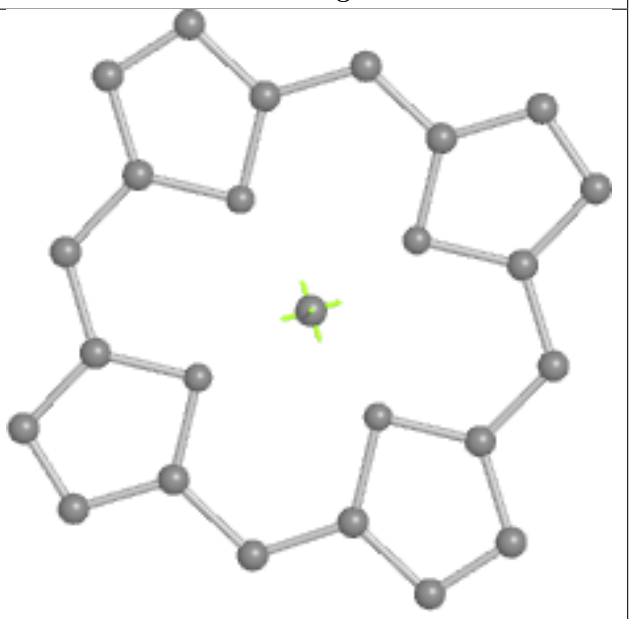
Bond lengths



Bond angles

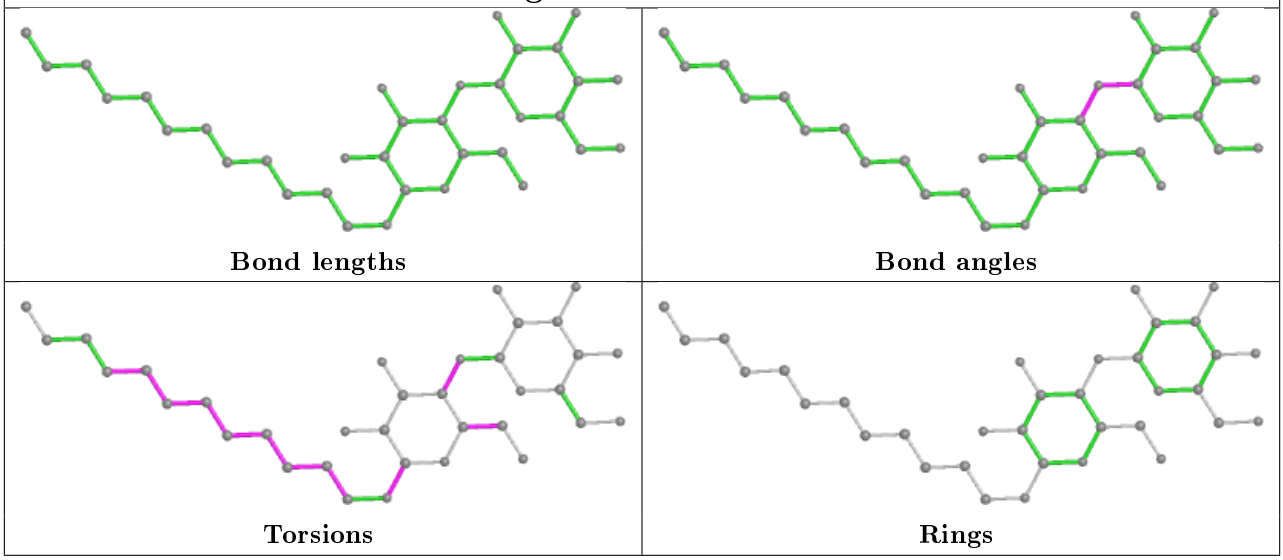


Torsions

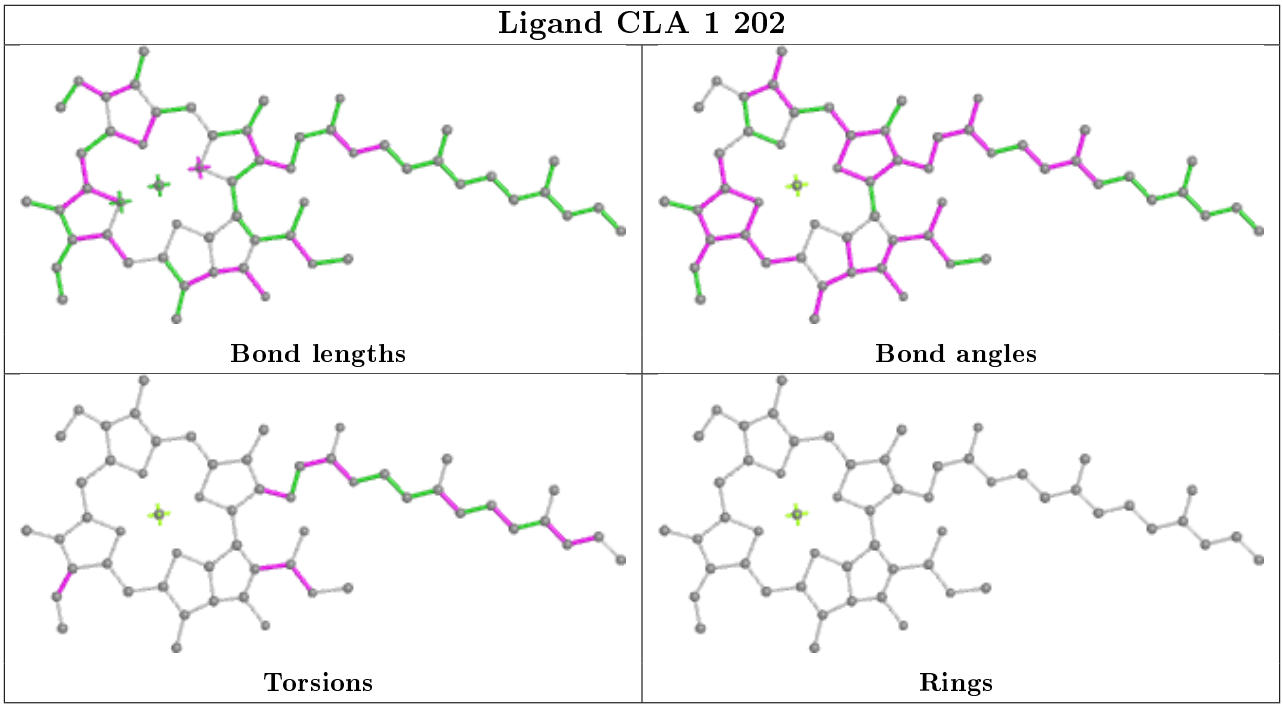


Rings

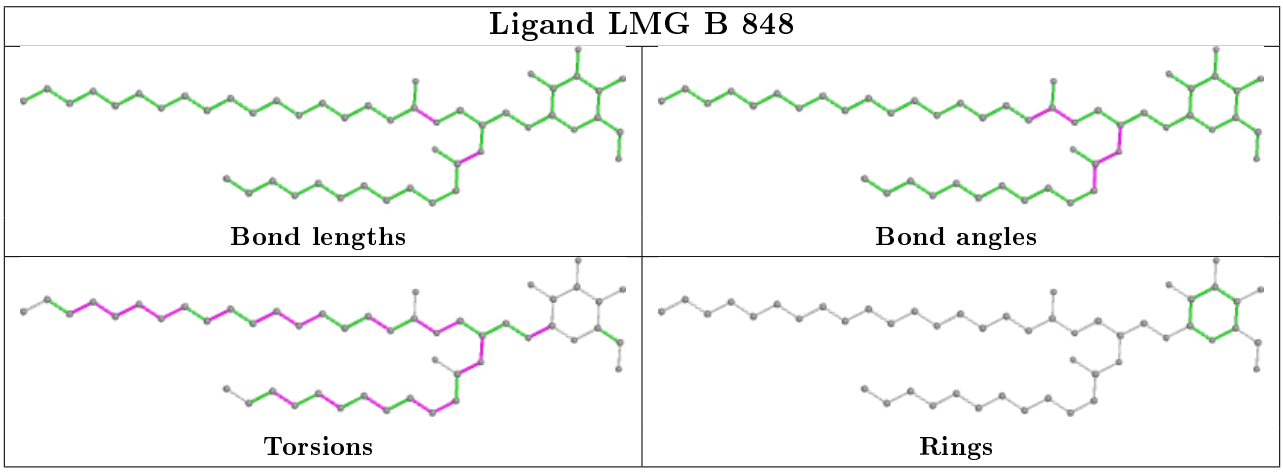
Ligand LMU 4 301



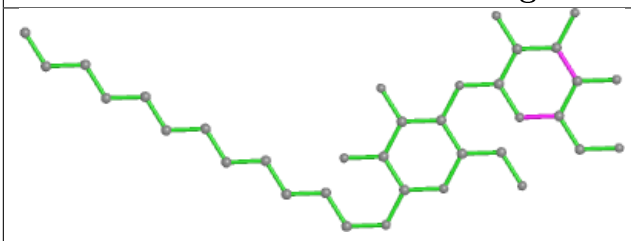
Ligand CLA 1 202



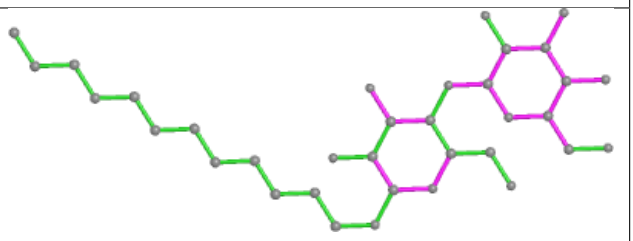
Ligand LMG B 848



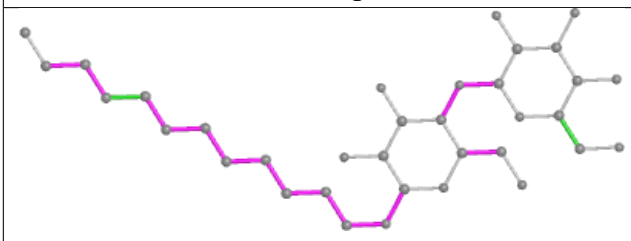
Ligand LMU G 101



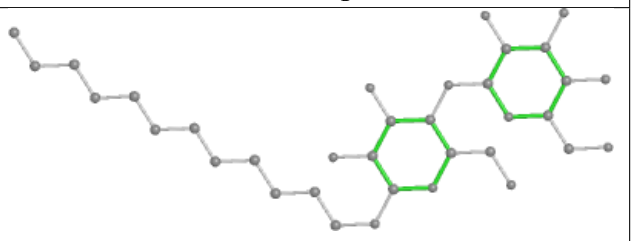
Bond lengths



Bond angles

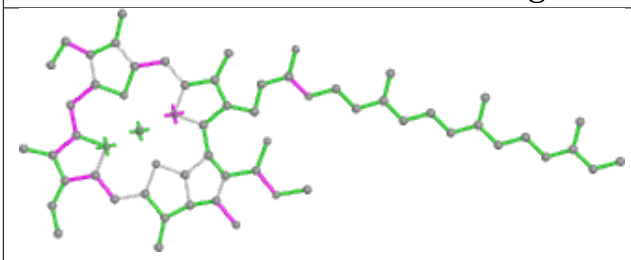


Torsions

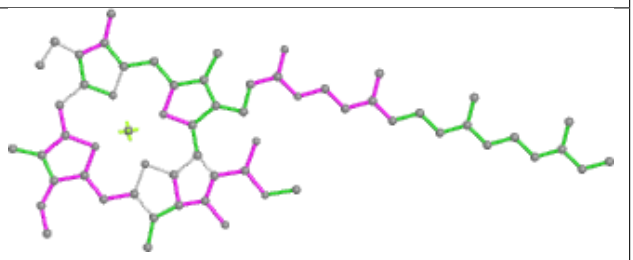


Rings

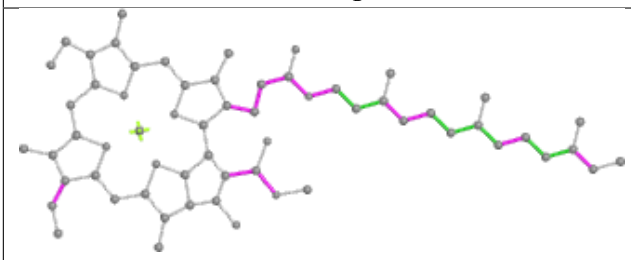
Ligand CLA 1 206



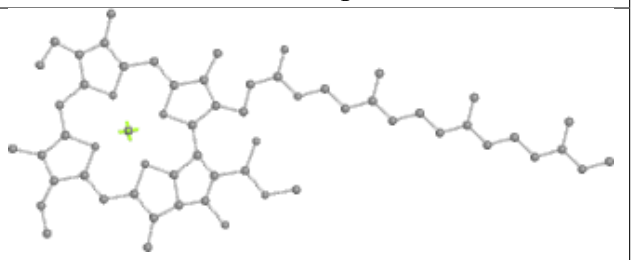
Bond lengths



Bond angles

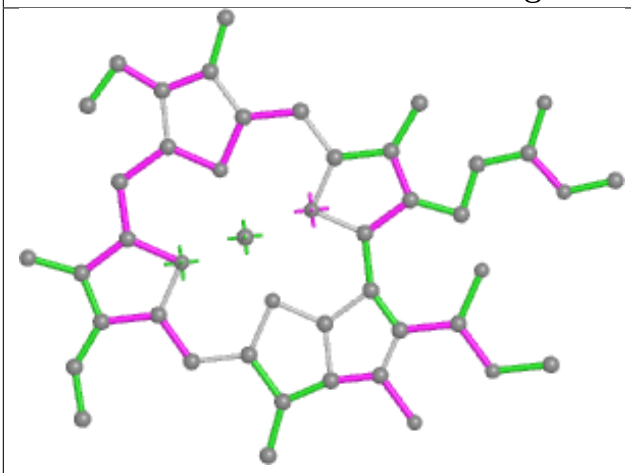


Torsions

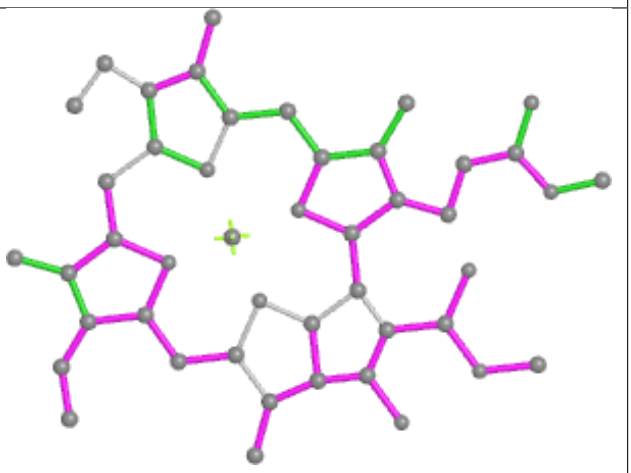


Rings

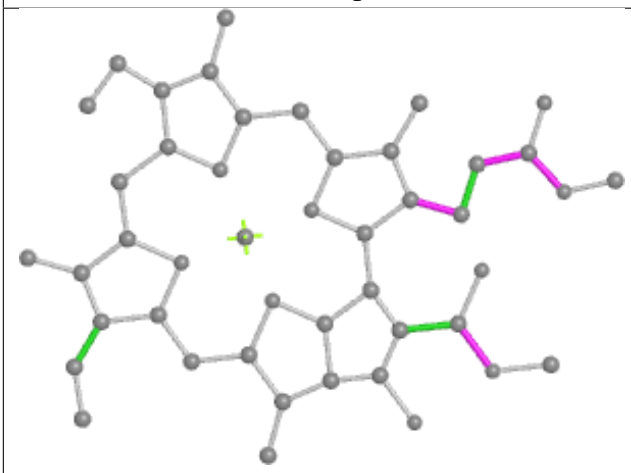
Ligand CLA A 807



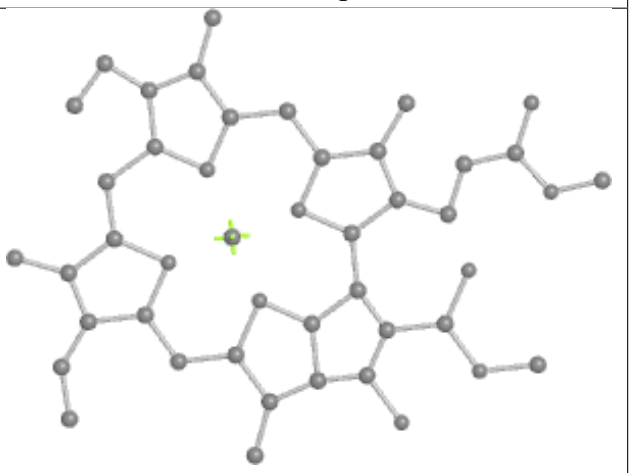
Bond lengths



Bond angles

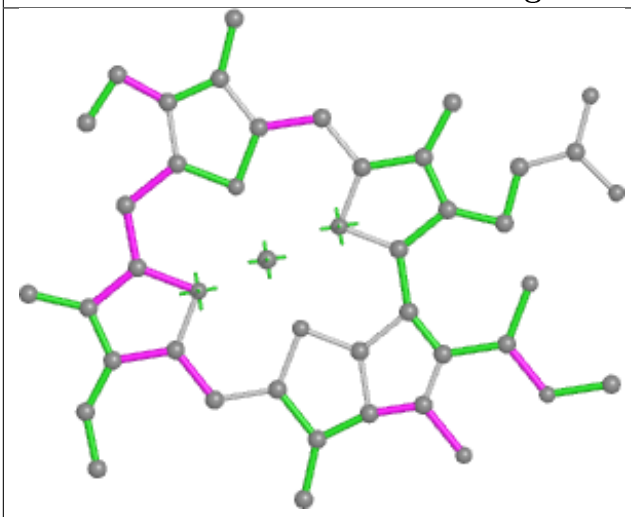


Torsions

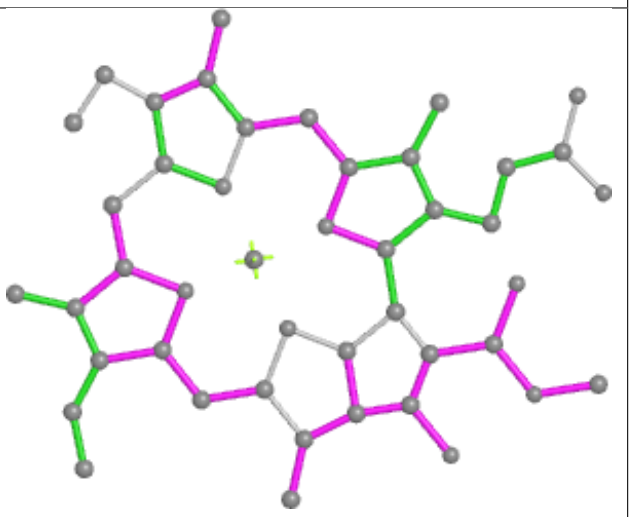


Rings

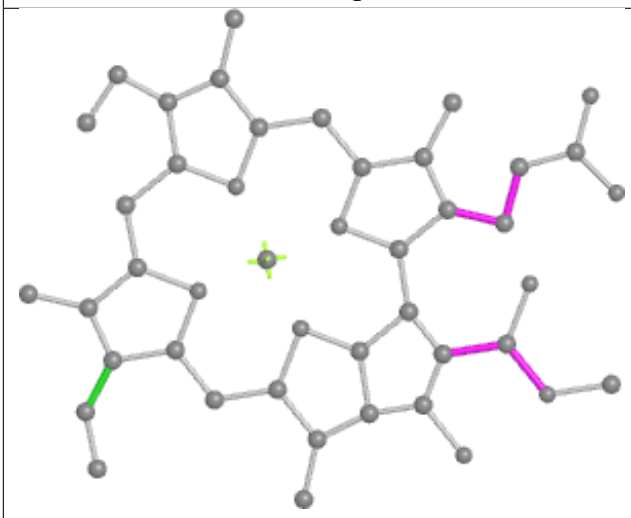
Ligand CLA B 832



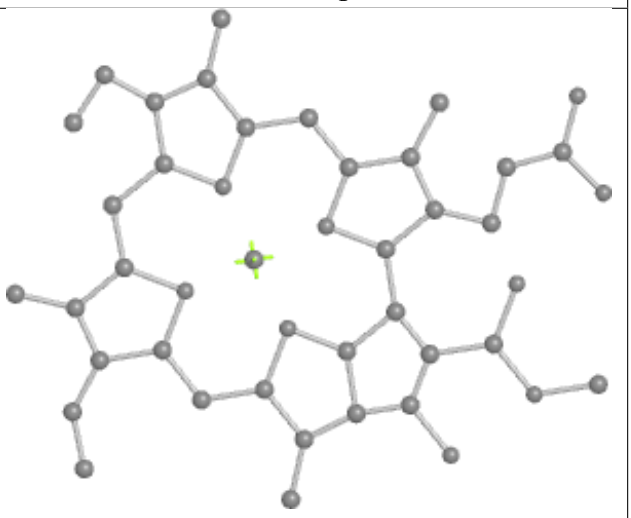
Bond lengths



Bond angles

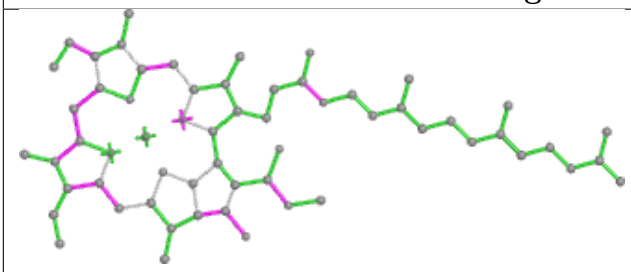


Torsions

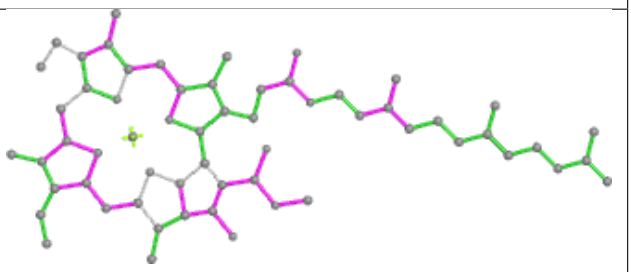


Rings

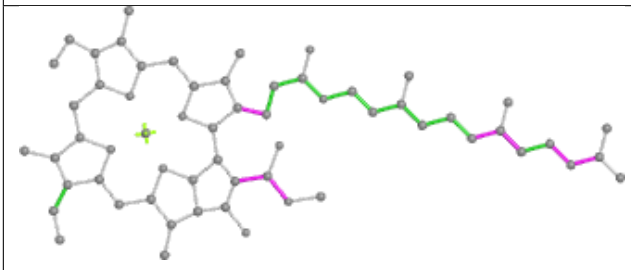
Ligand CLA B 813



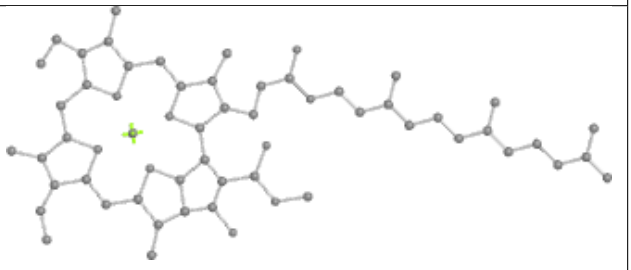
Bond lengths



Bond angles

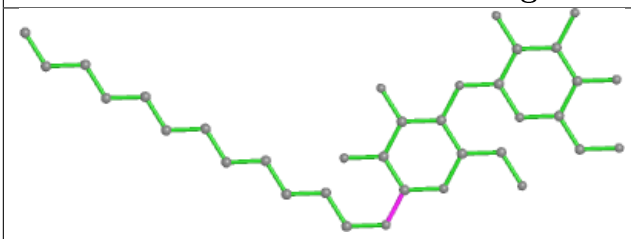


Torsions

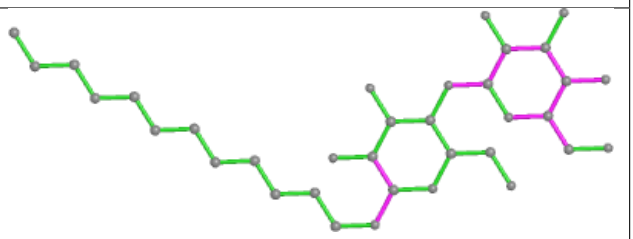


Rings

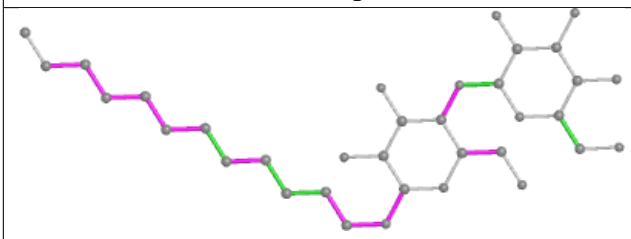
Ligand LMU C 101



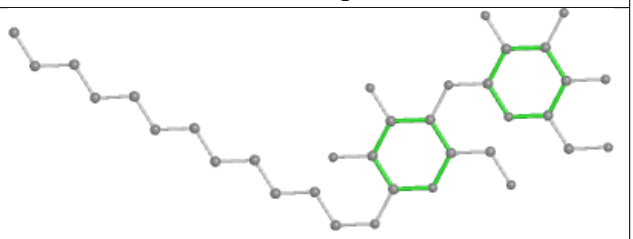
Bond lengths



Bond angles

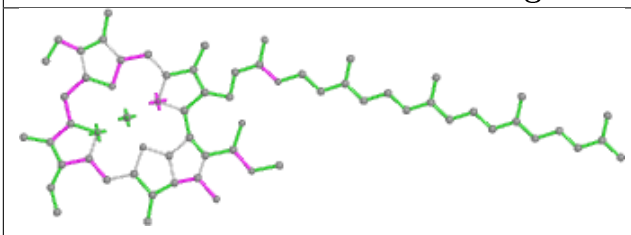


Torsions

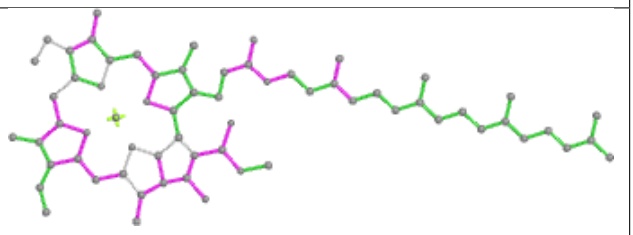


Rings

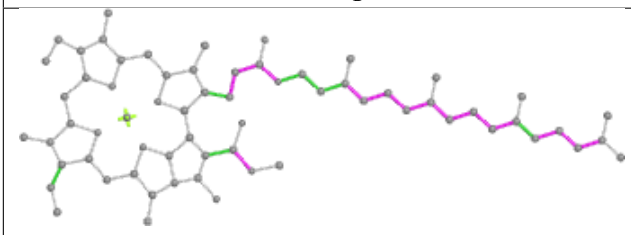
Ligand CLA A 830



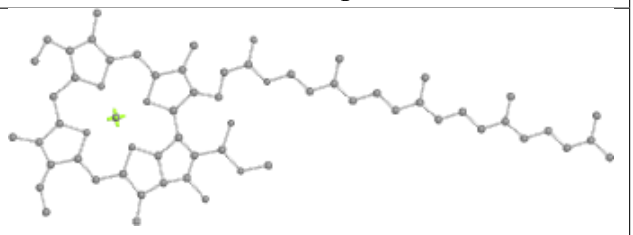
Bond lengths



Bond angles

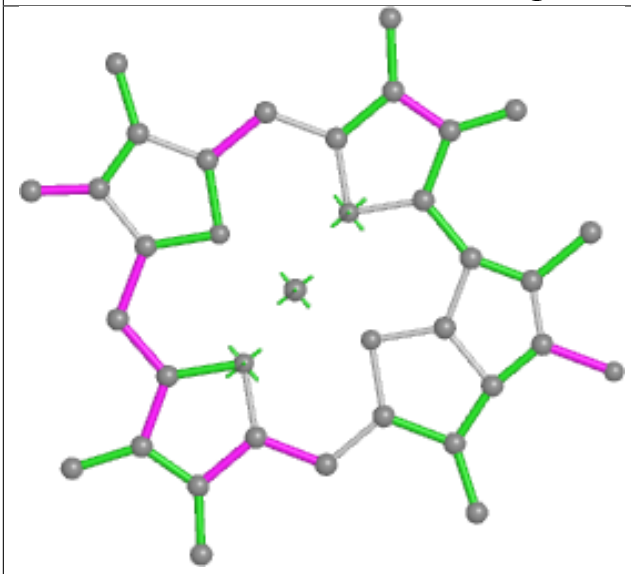


Torsions

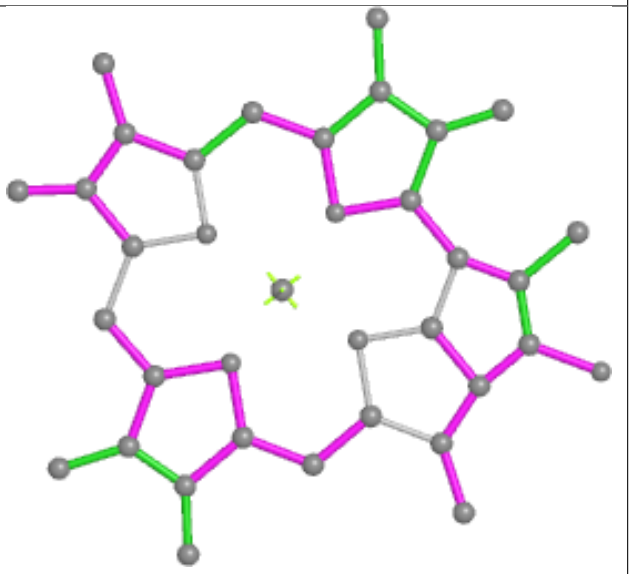


Rings

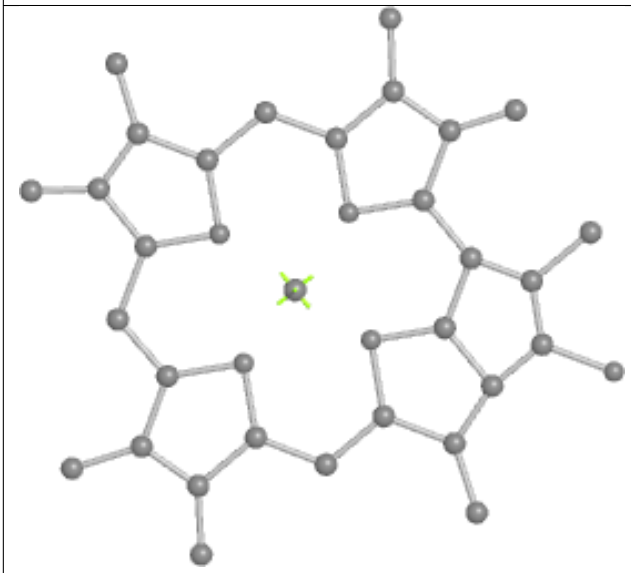
Ligand CLA 3 304



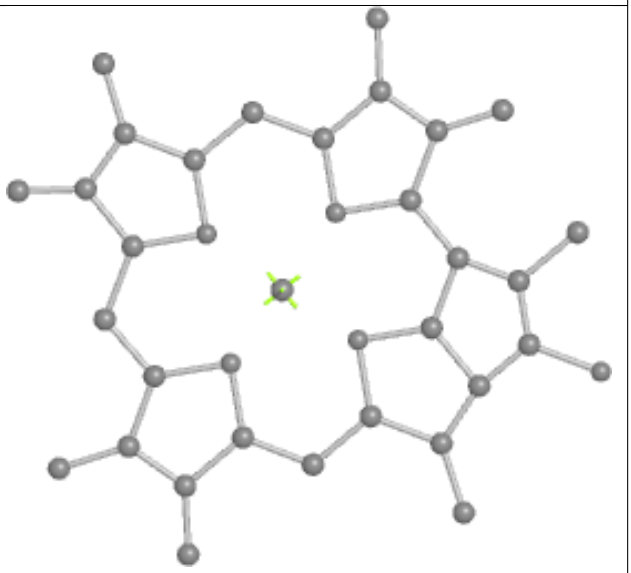
Bond lengths



Bond angles

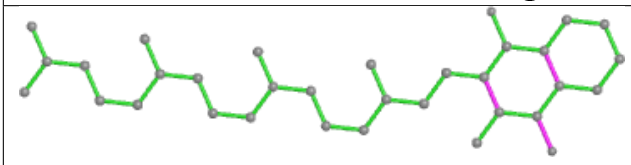


Torsions

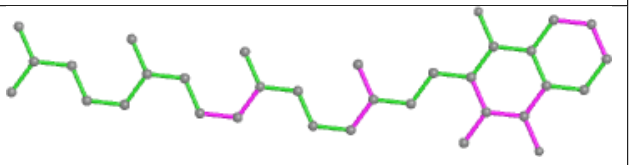


Rings

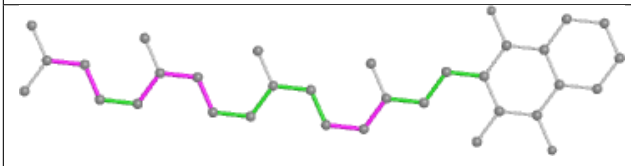
Ligand PQN A 842



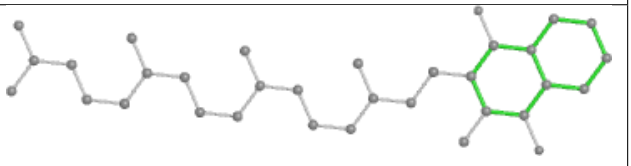
Bond lengths



Bond angles

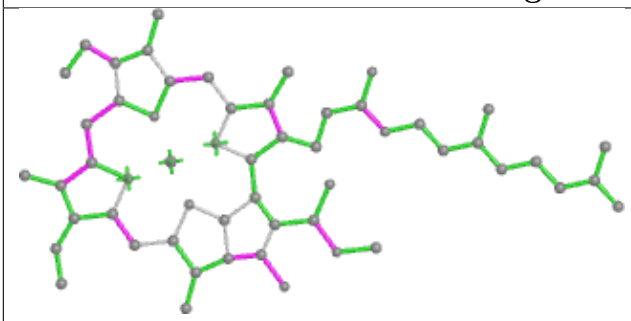


Torsions

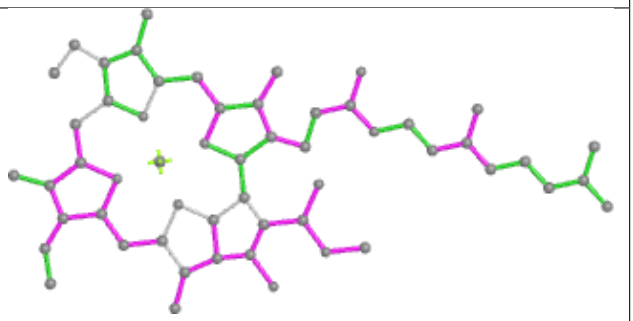


Rings

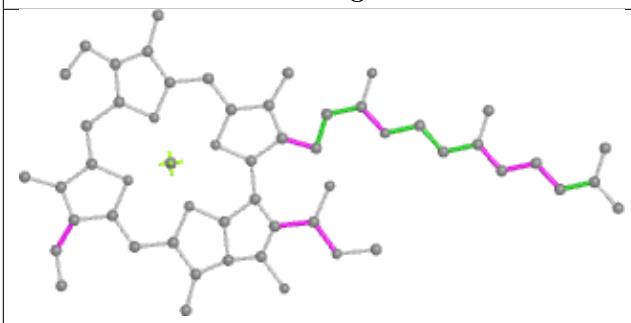
Ligand CLA A 831



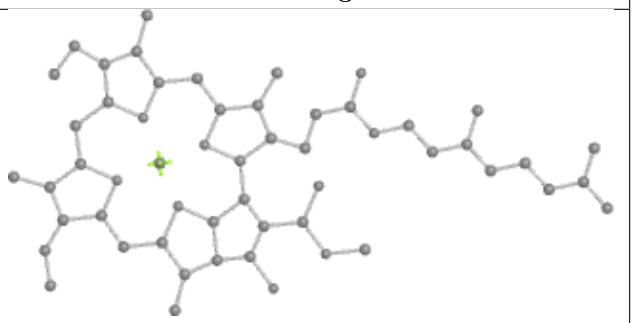
Bond lengths



Bond angles

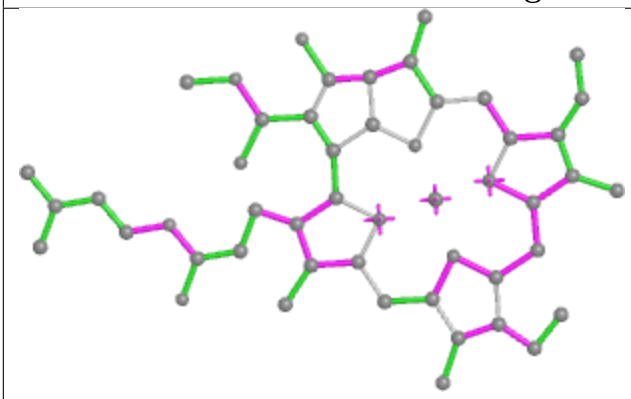


Torsions

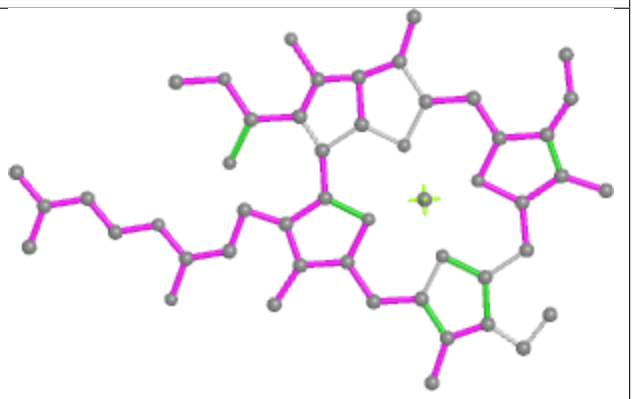


Rings

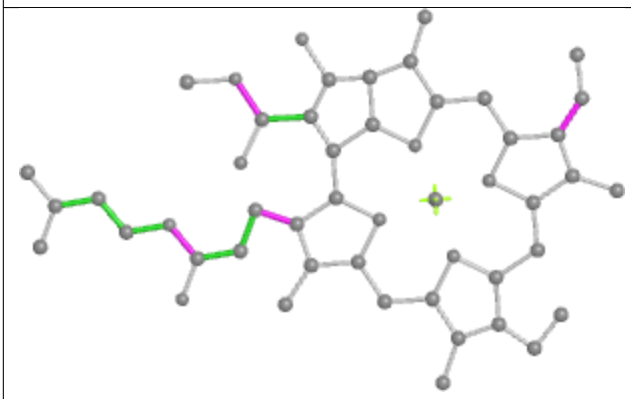
Ligand CLA A 815



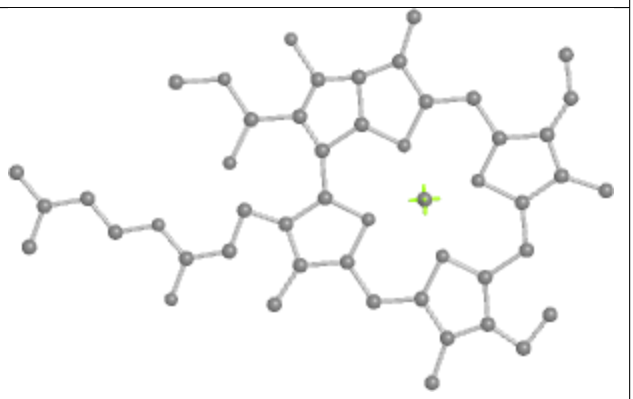
Bond lengths



Bond angles

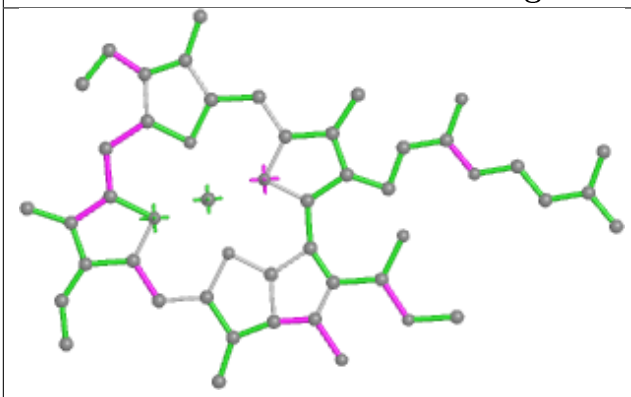


Torsions

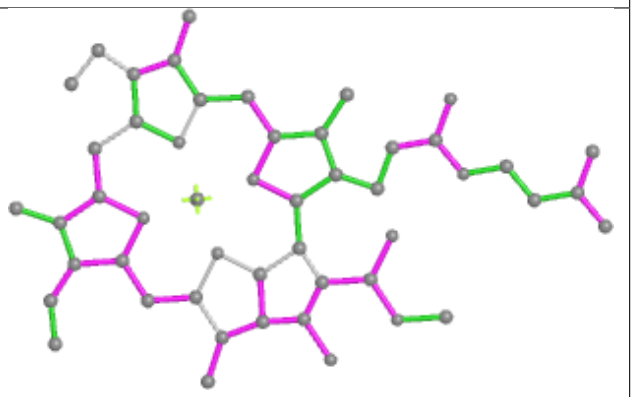


Rings

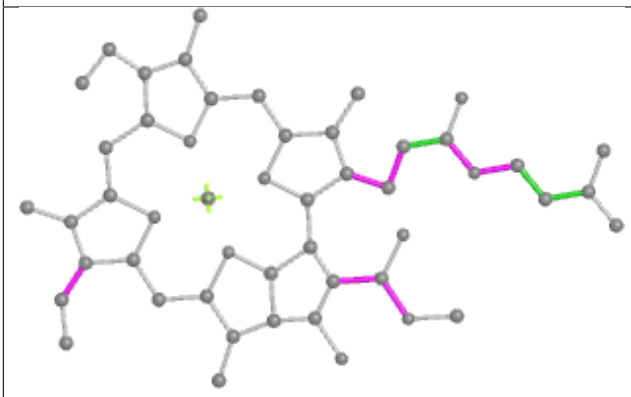
Ligand CLA A 840



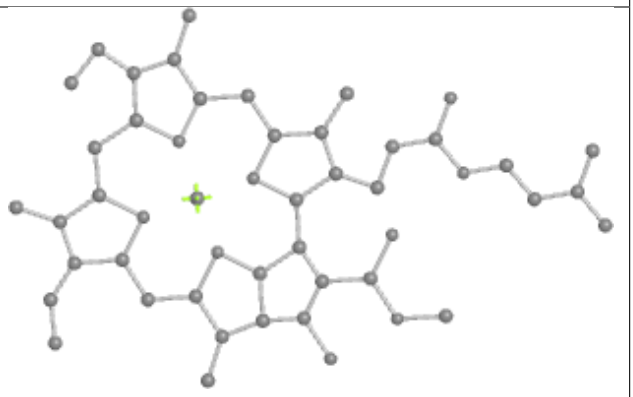
Bond lengths



Bond angles

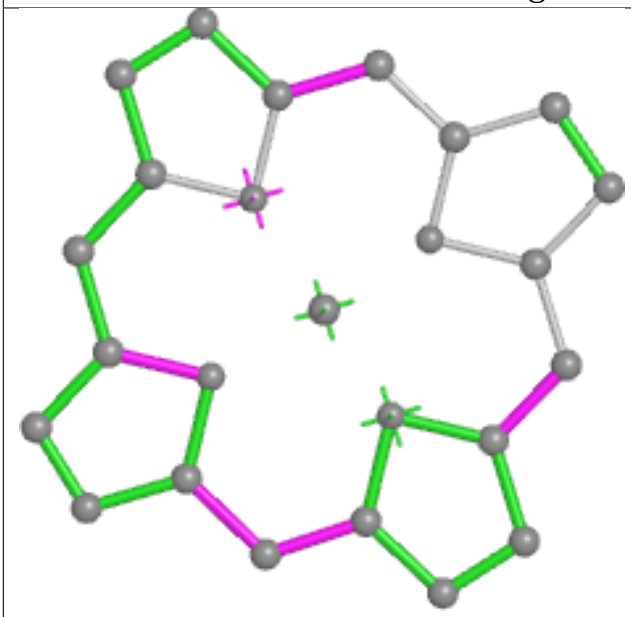


Torsions

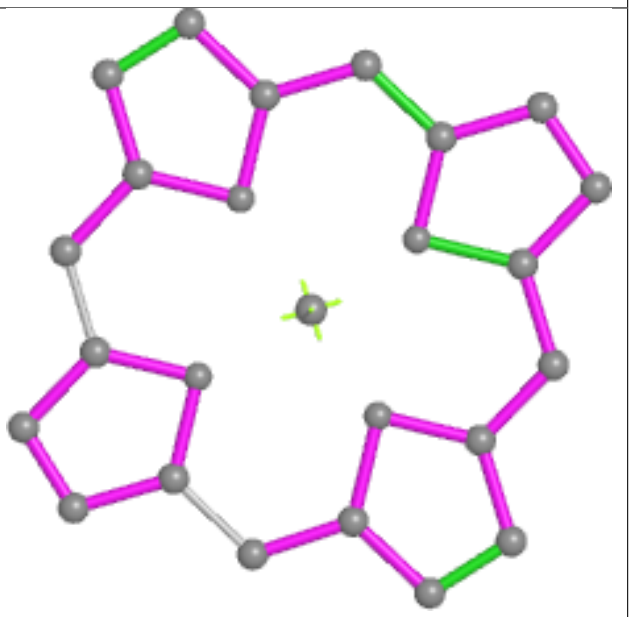


Rings

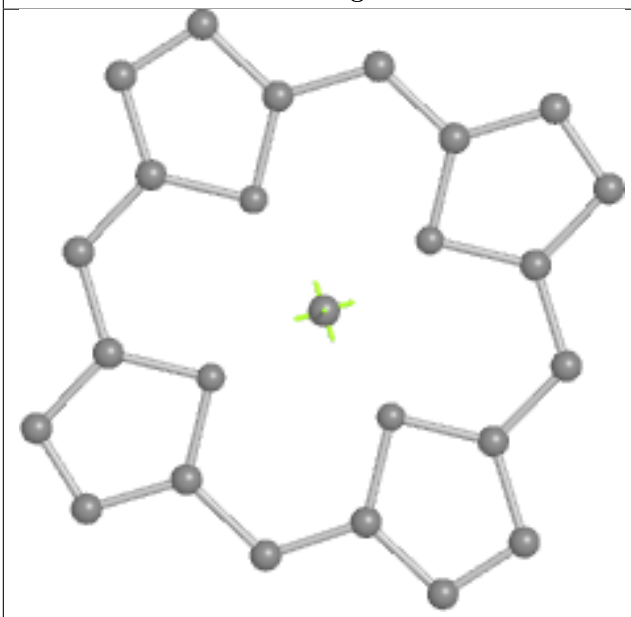
Ligand CLA 2 309



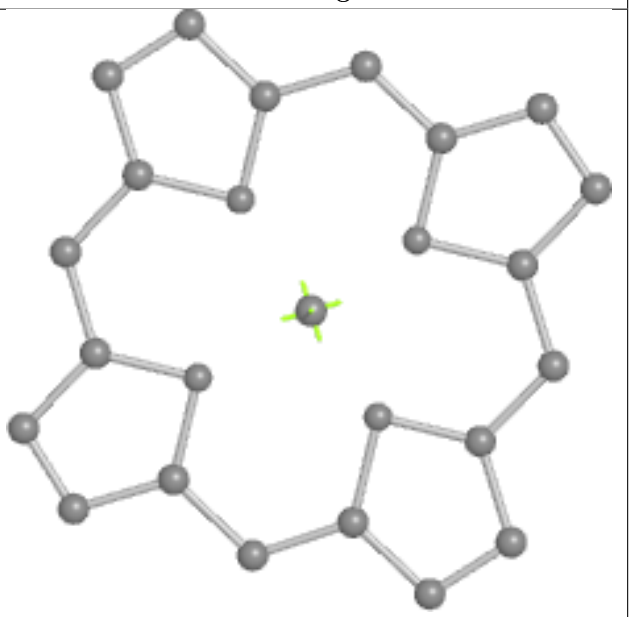
Bond lengths



Bond angles

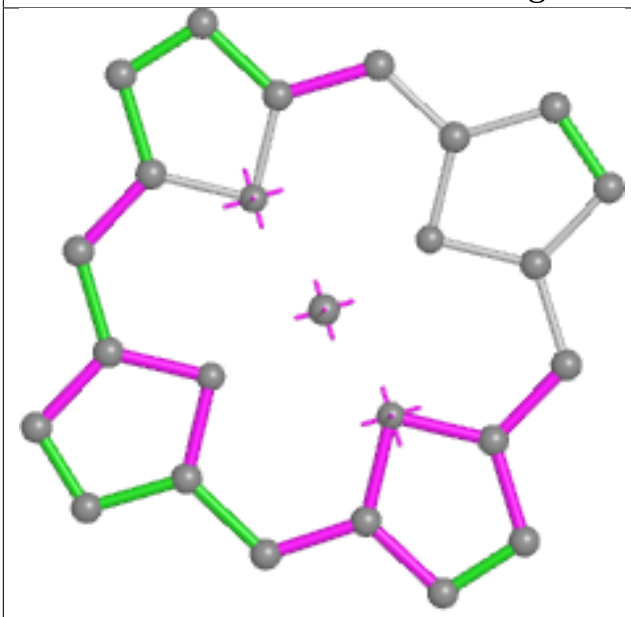


Torsions



Rings

Ligand CLA 4 309



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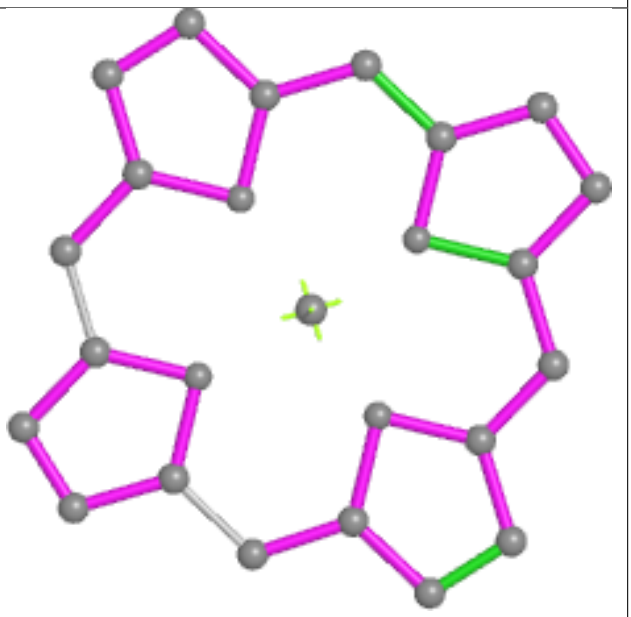
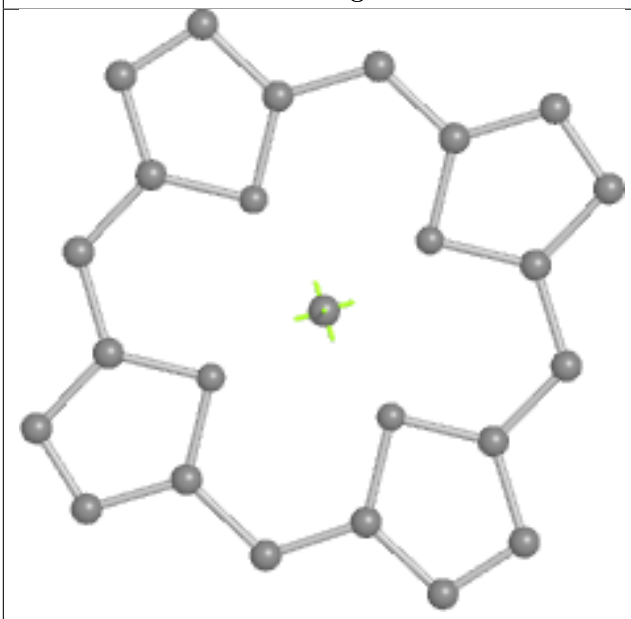
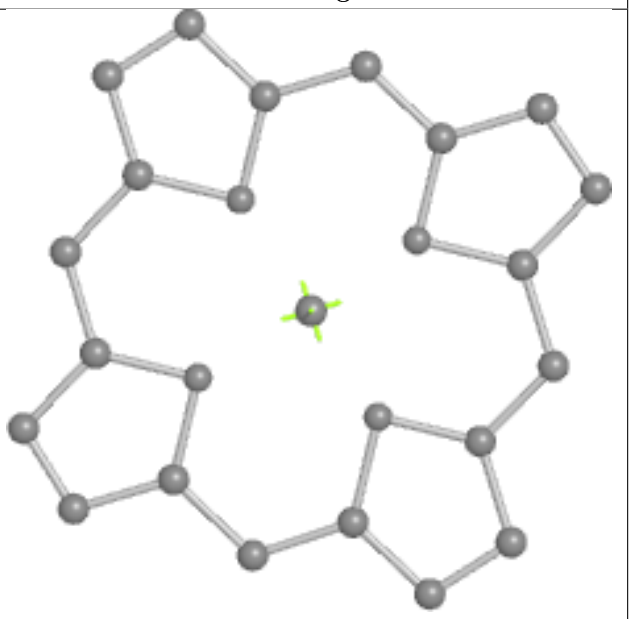


Bond angles

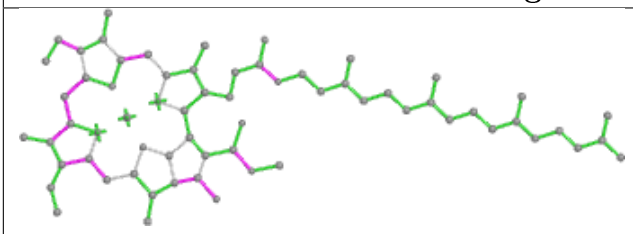


Torsions



Rings

Ligand CLA A 826



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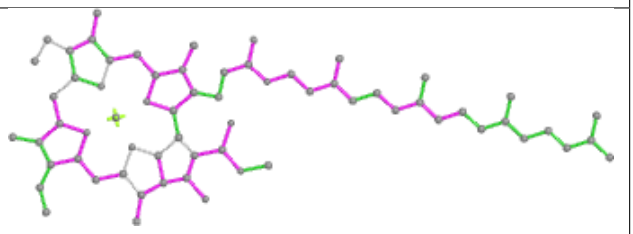
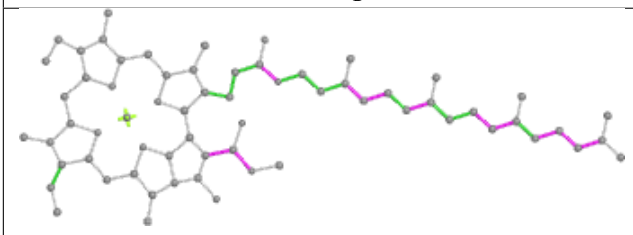
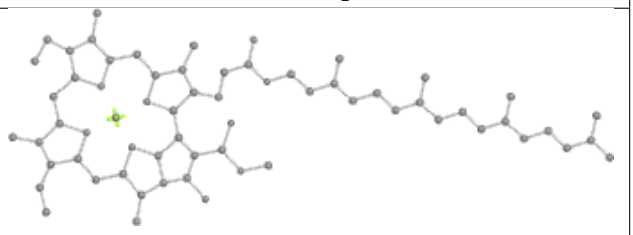


Bond angles

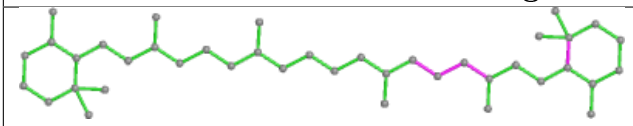


Torsions

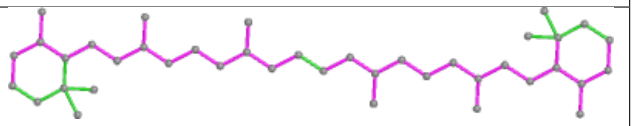


Rings

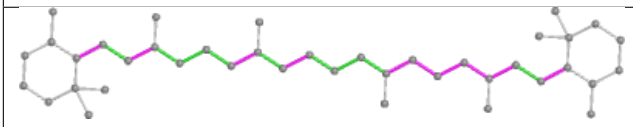
Ligand BCR A 846



Bond lengths



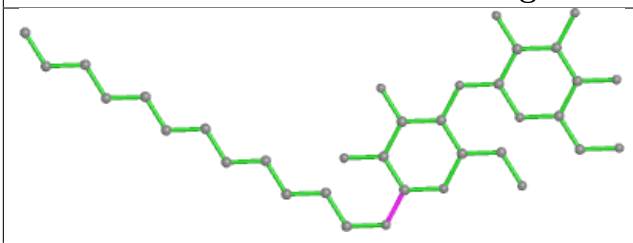
Bond angles



Torsions

Rings

Ligand LMU R 106



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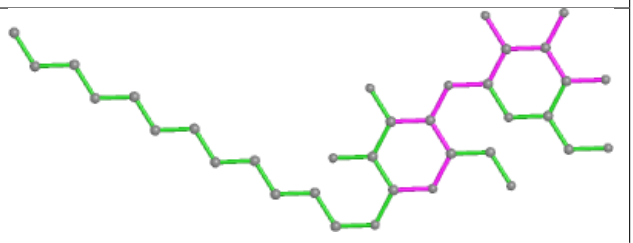
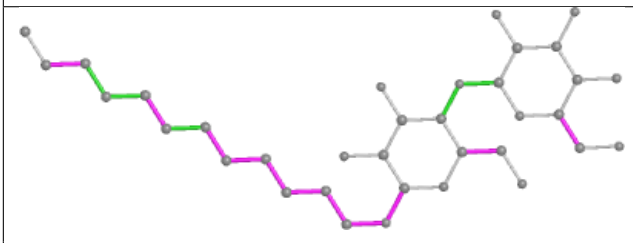
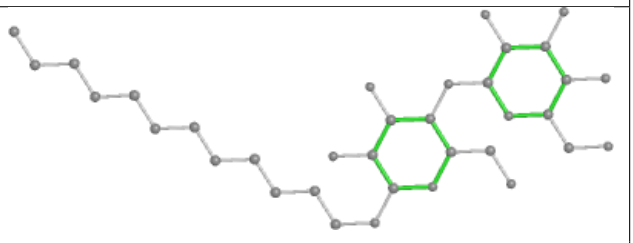


Bond angles

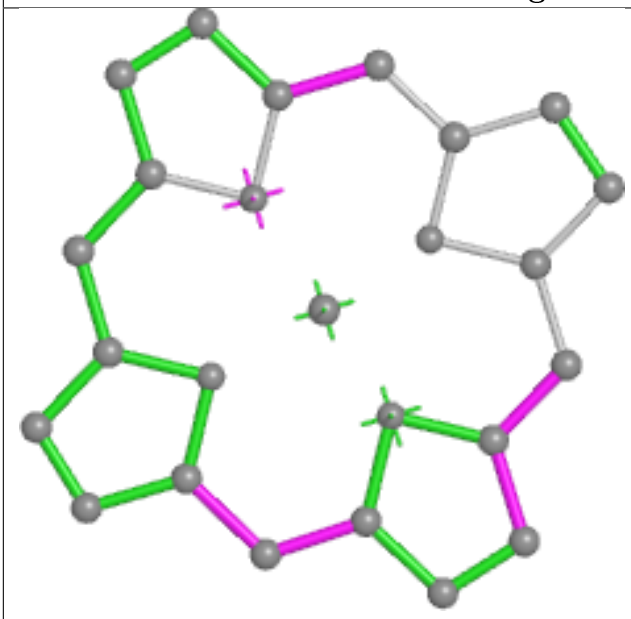


Torsions

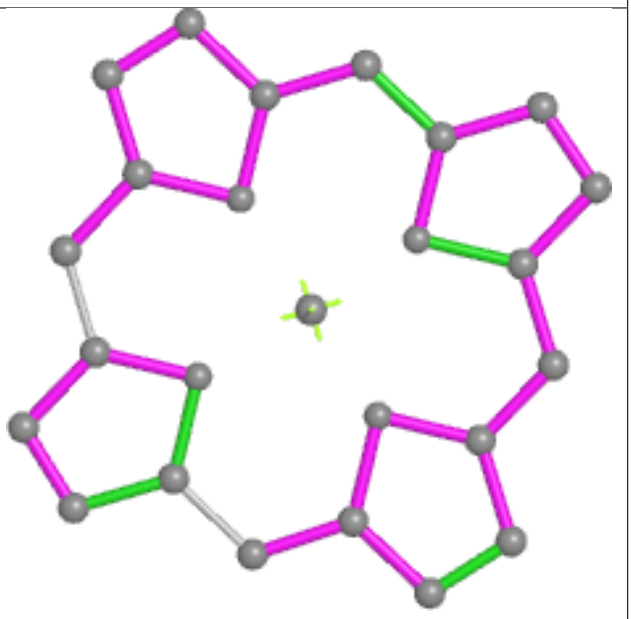


Rings

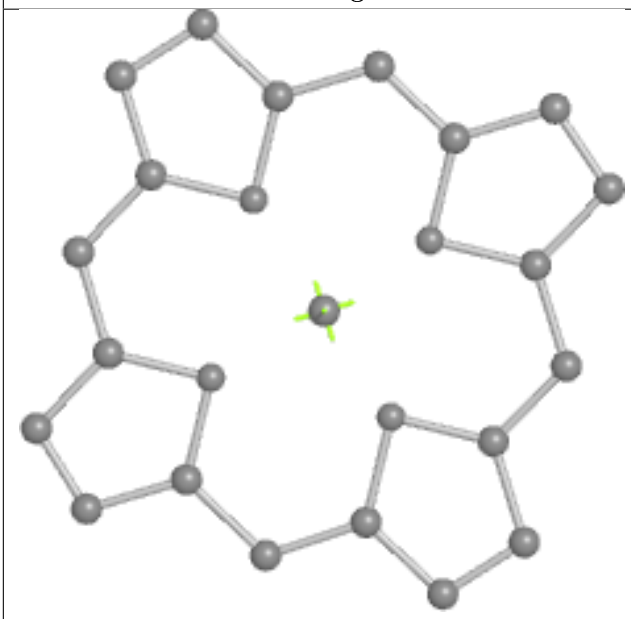
Ligand CLA 4 312



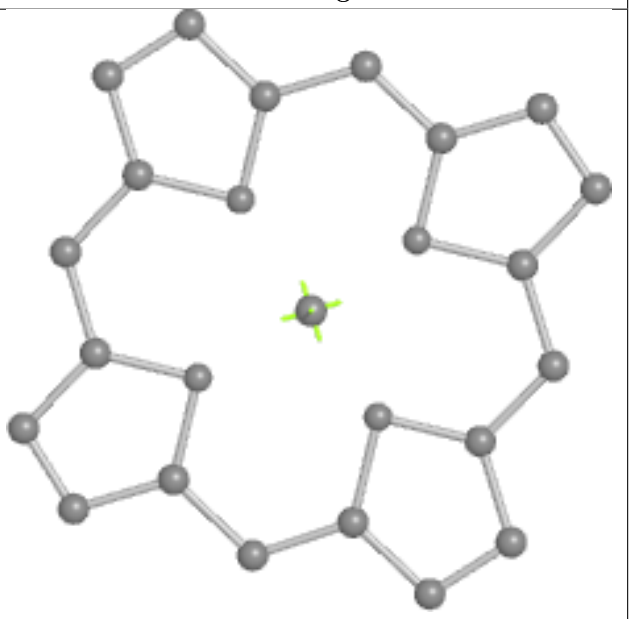
Bond lengths



Bond angles

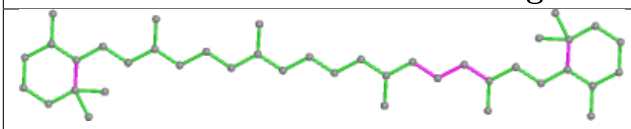


Torsions

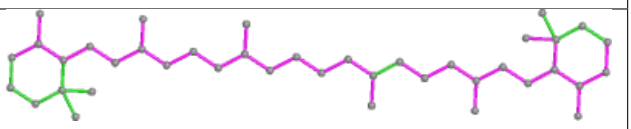


Rings

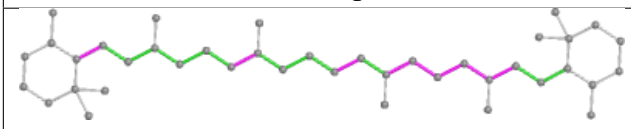
Ligand BCR 3 314



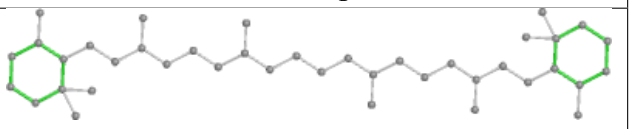
Bond lengths



Bond angles

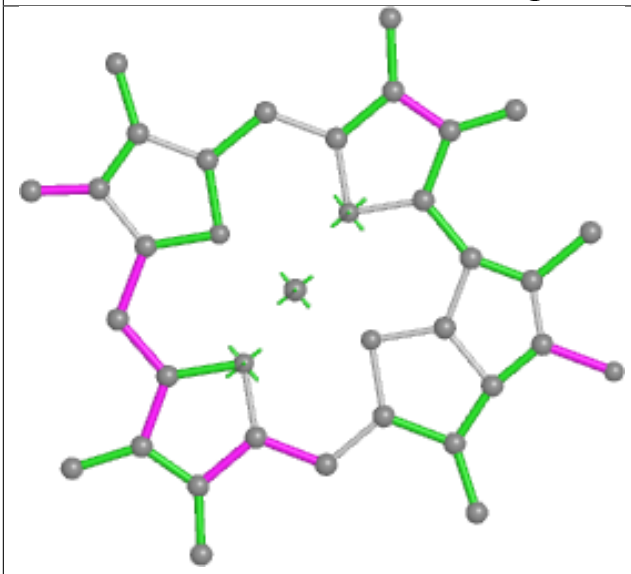


Torsions



Rings

Ligand CLA F 204



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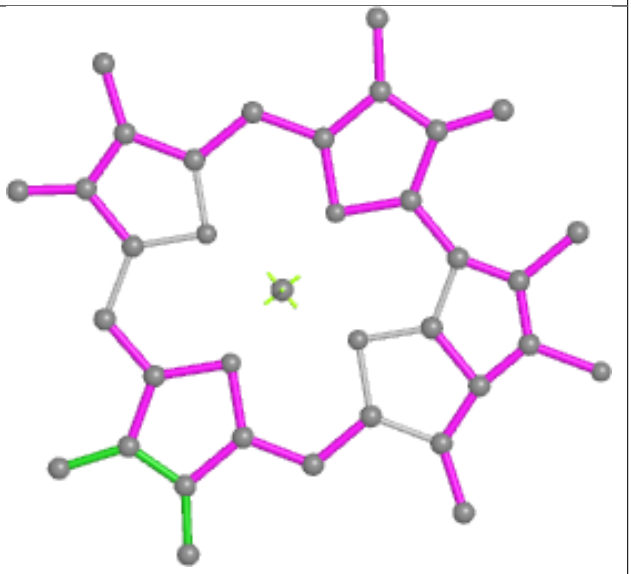
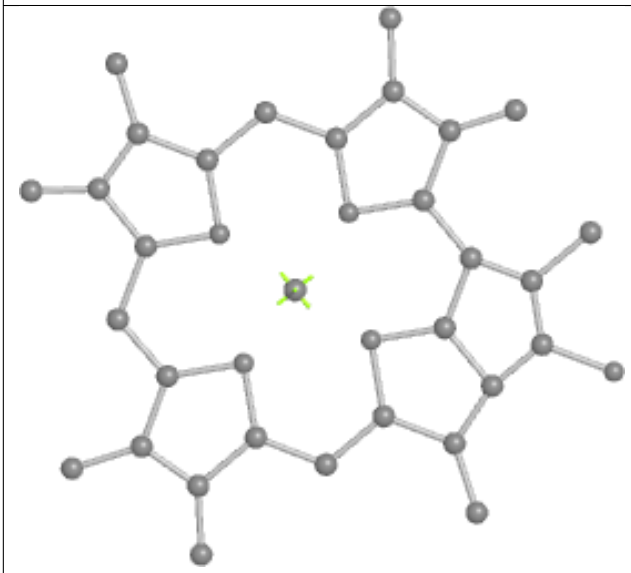
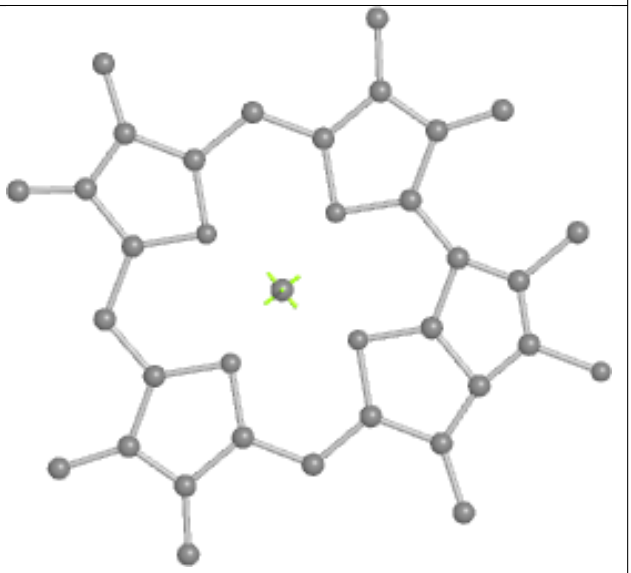


Bond angles

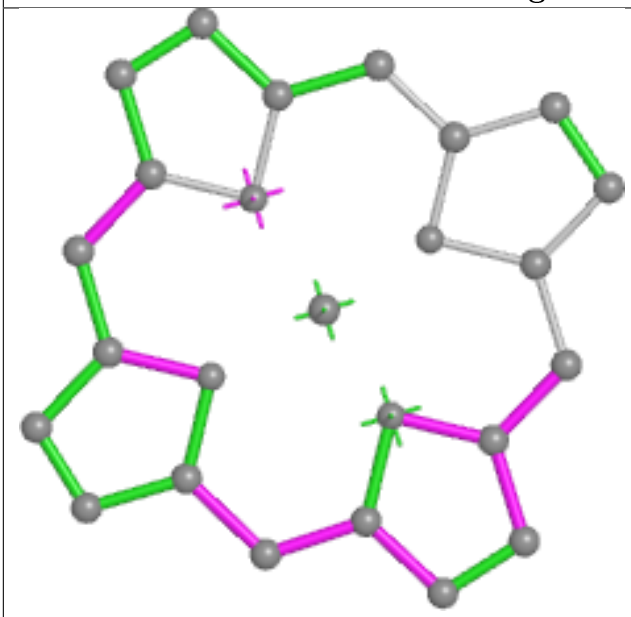


Torsions

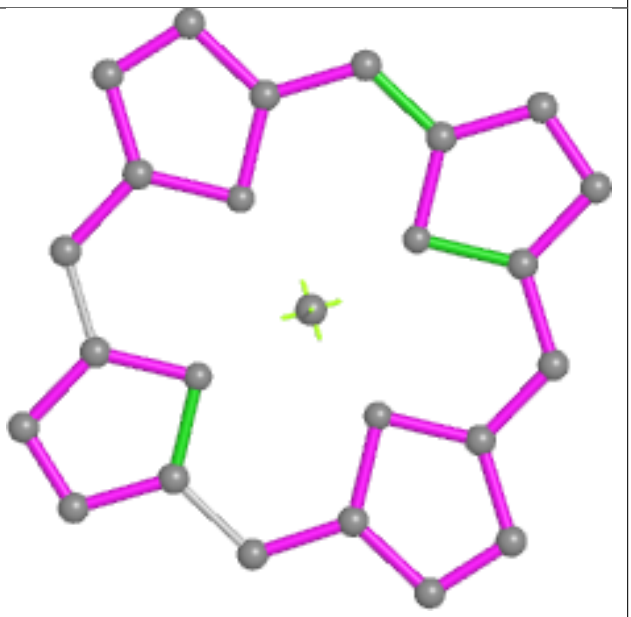


Rings

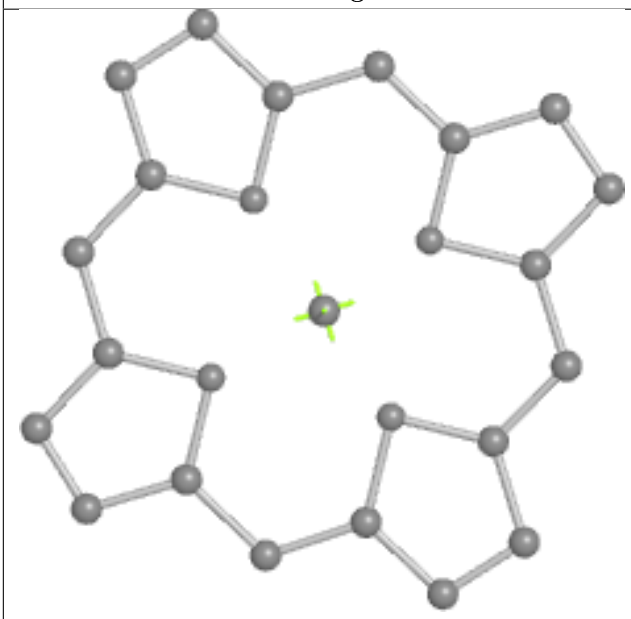
Ligand CLA 3 312



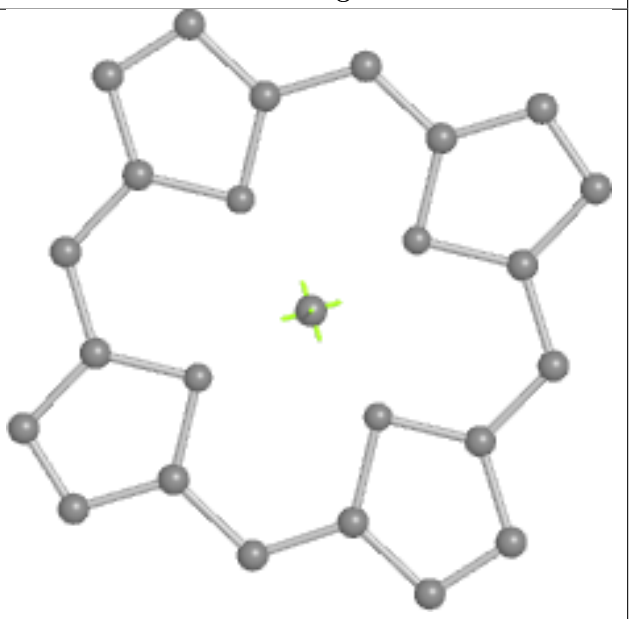
Bond lengths



Bond angles

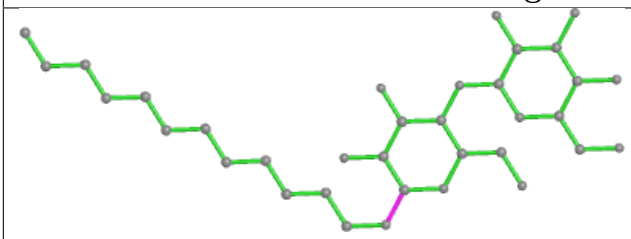


Torsions



Rings

Ligand LMU 1 220



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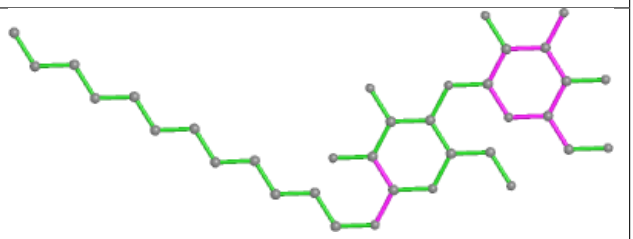
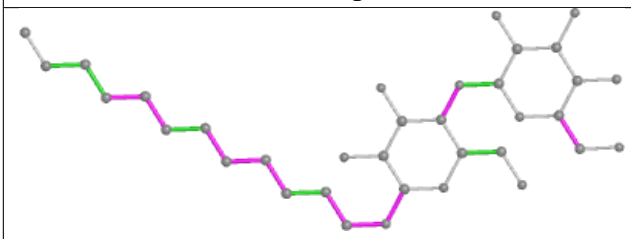
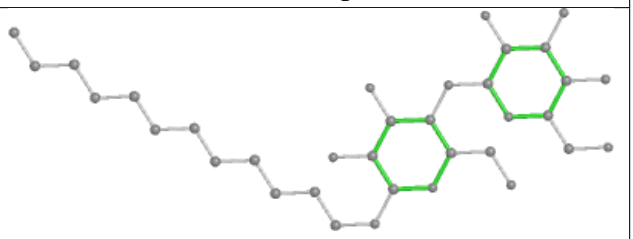


Bond angles

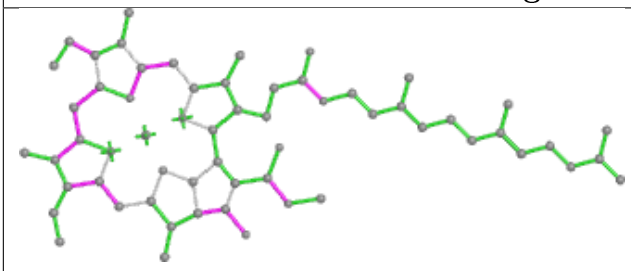


Torsions

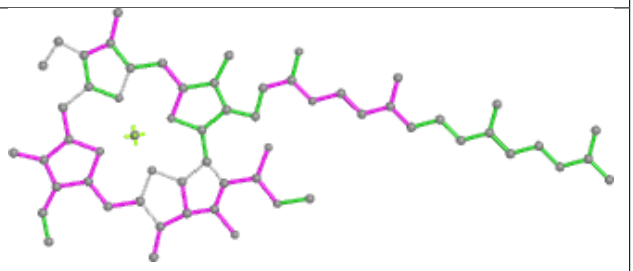


Rings

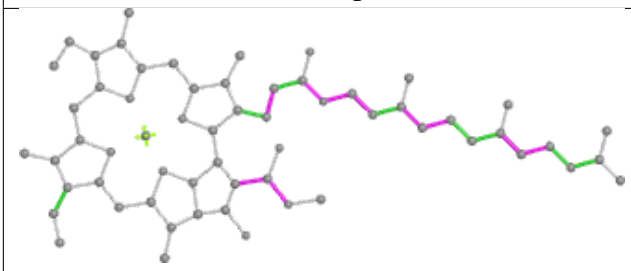
Ligand CLA H 109



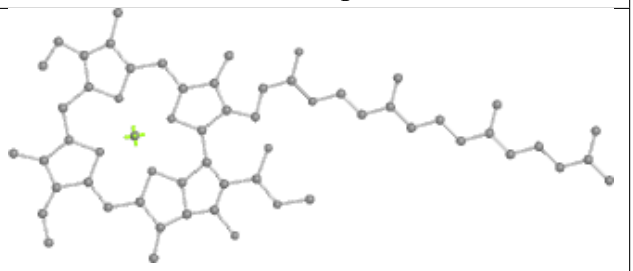
Bond lengths



Bond angles

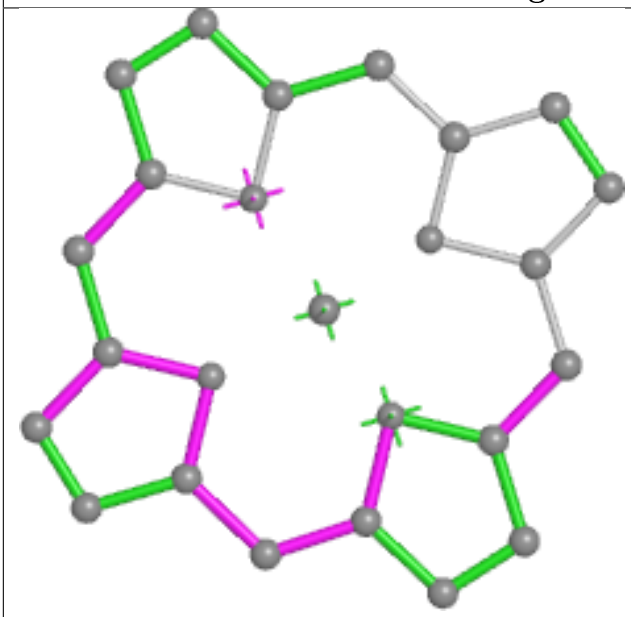


Torsions

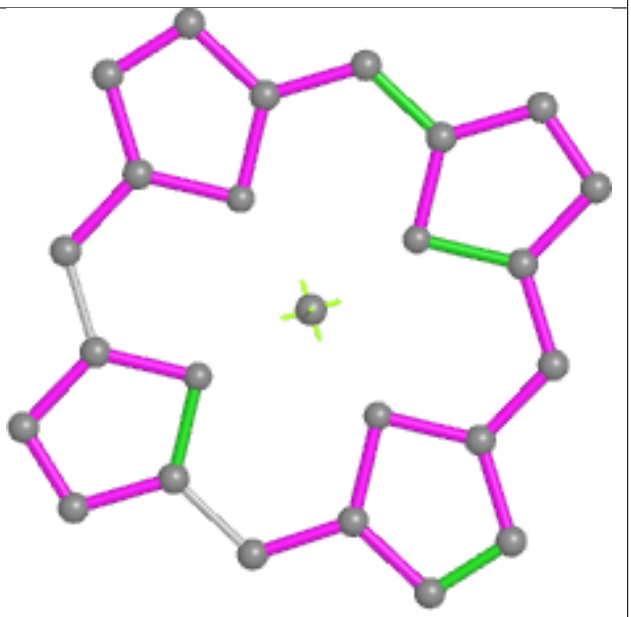


Rings

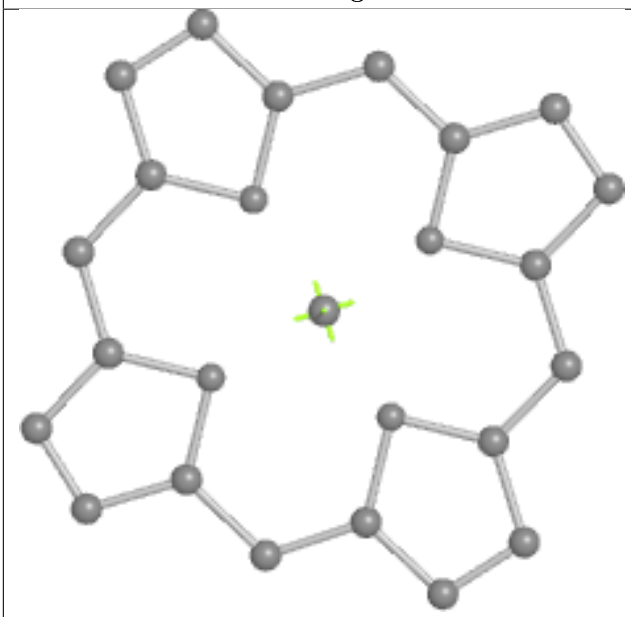
Ligand CLA 1 212



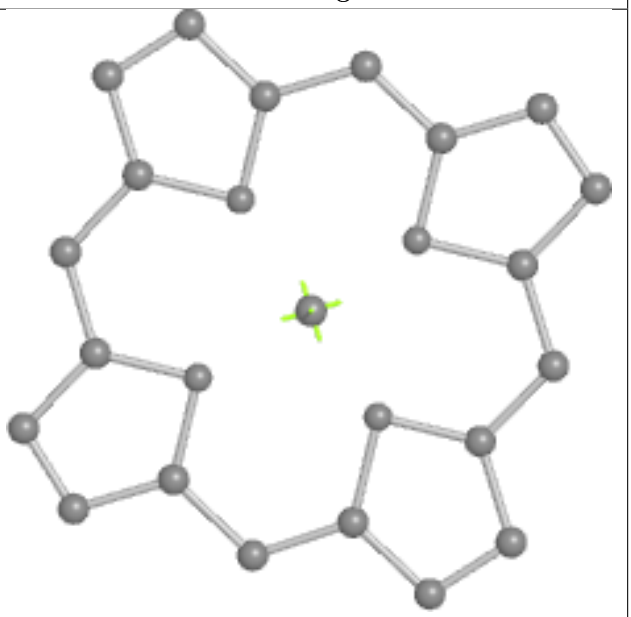
Bond lengths



Bond angles

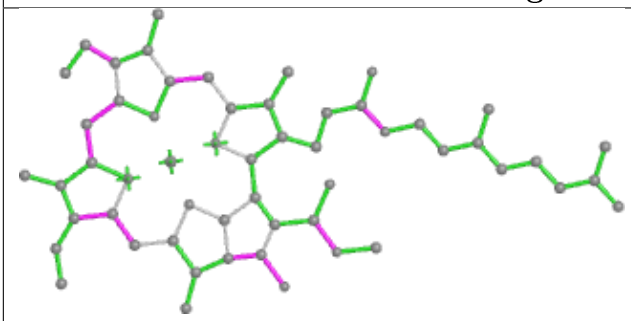


Torsions

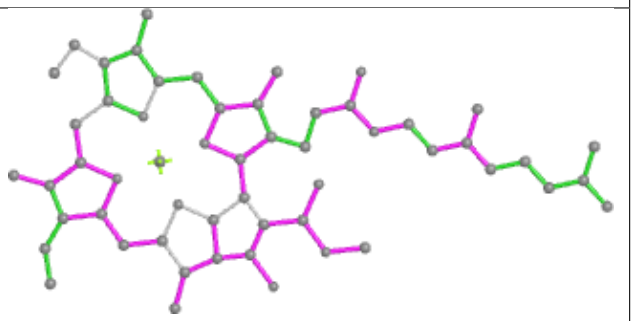


Rings

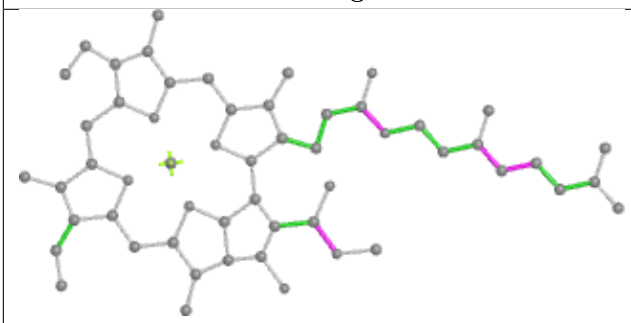
Ligand CLA L 203



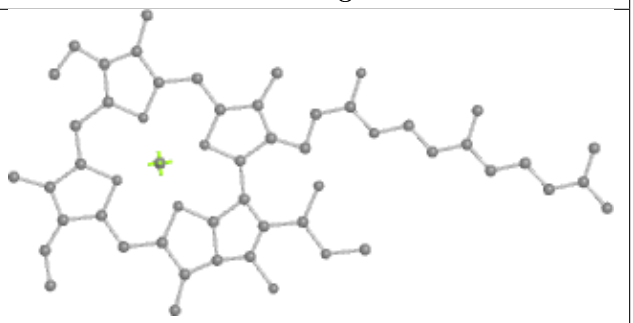
Bond lengths



Bond angles

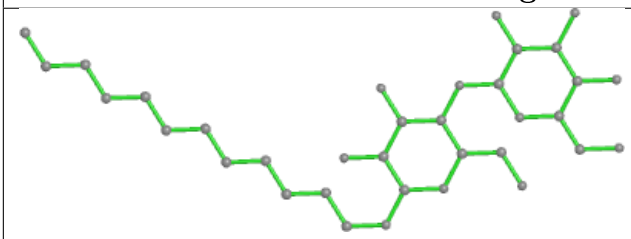


Torsions

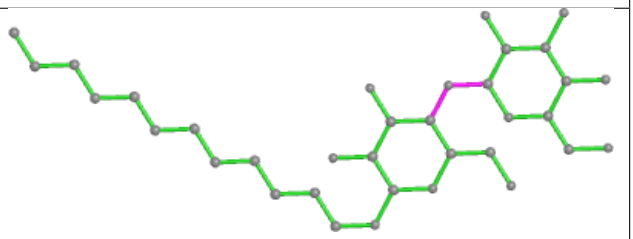


Rings

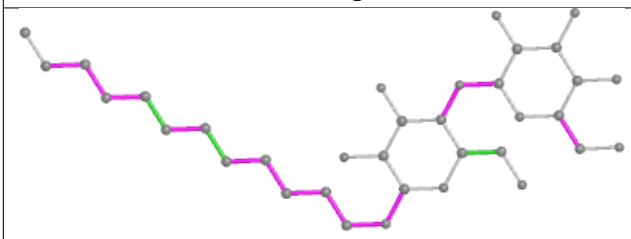
Ligand LMU R 109



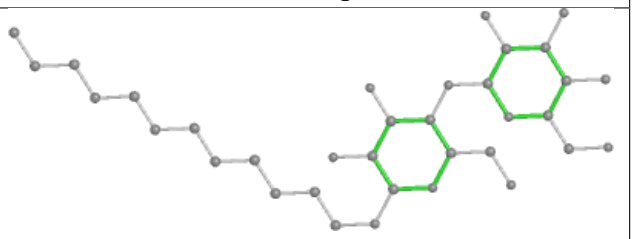
Bond lengths



Bond angles

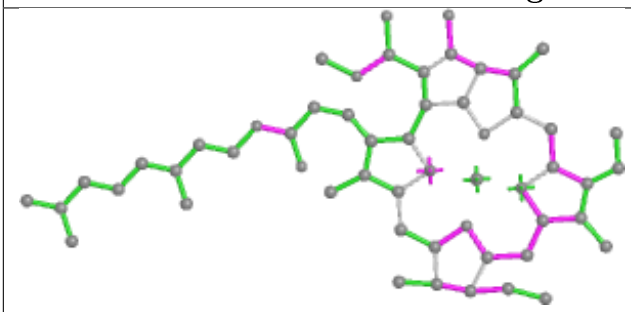


Torsions

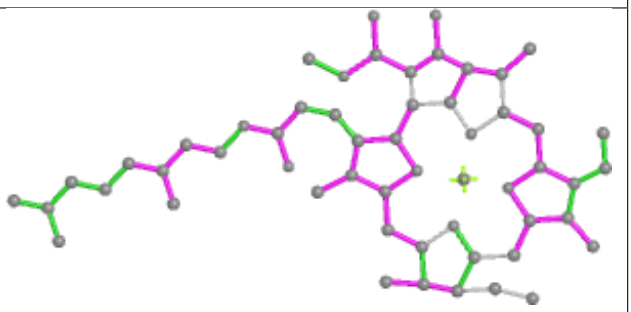


Rings

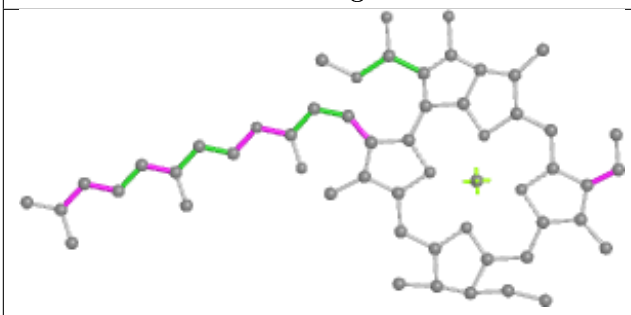
Ligand CLA L 201



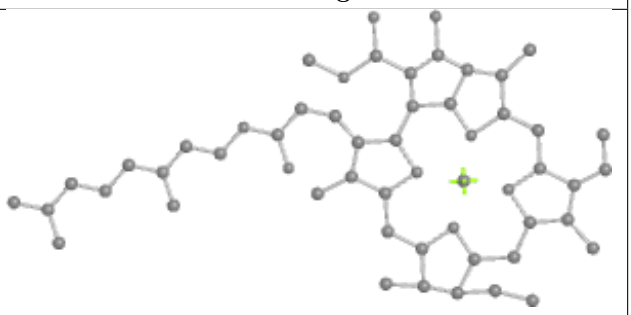
Bond lengths



Bond angles

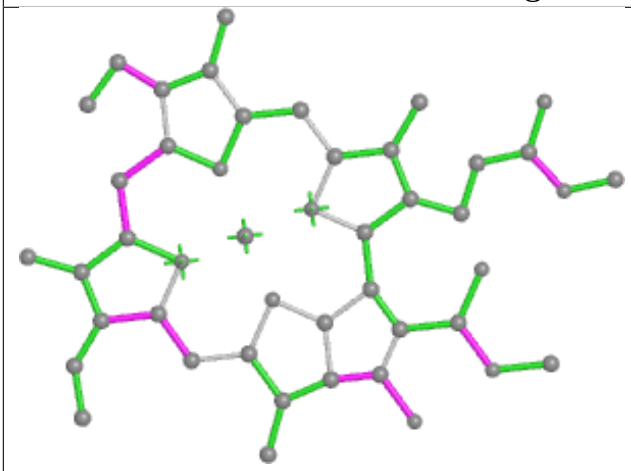


Torsions

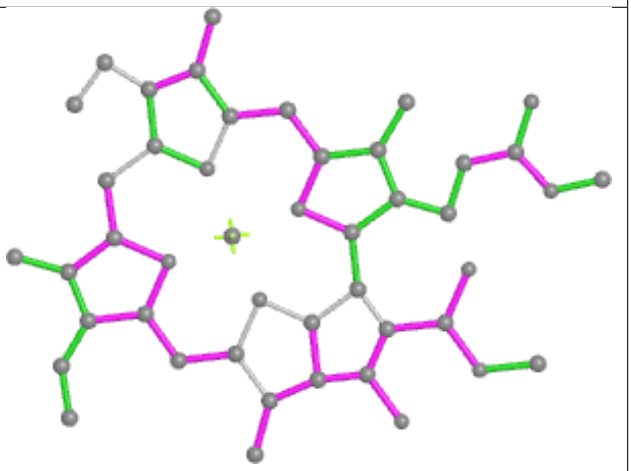


Rings

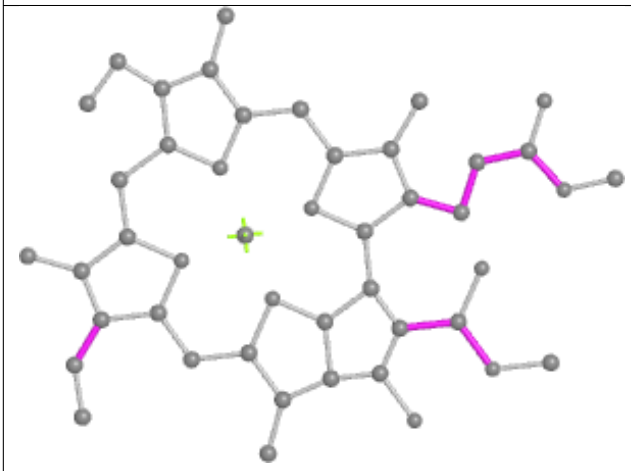
Ligand CLA B 819



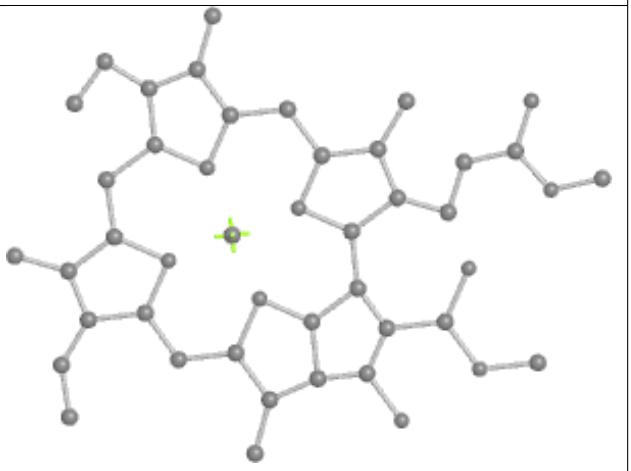
Bond lengths



Bond angles

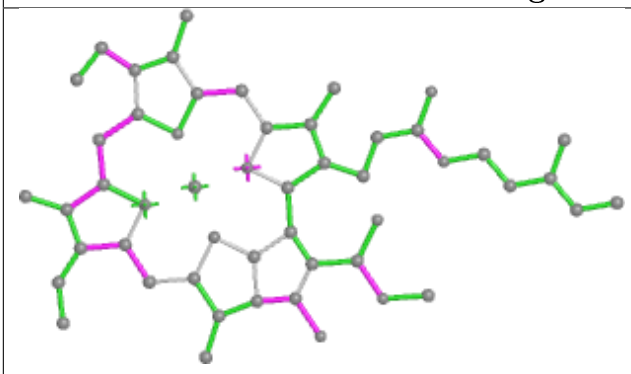


Torsions

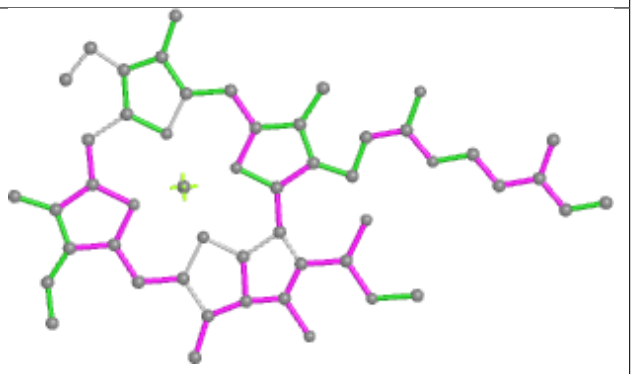


Rings

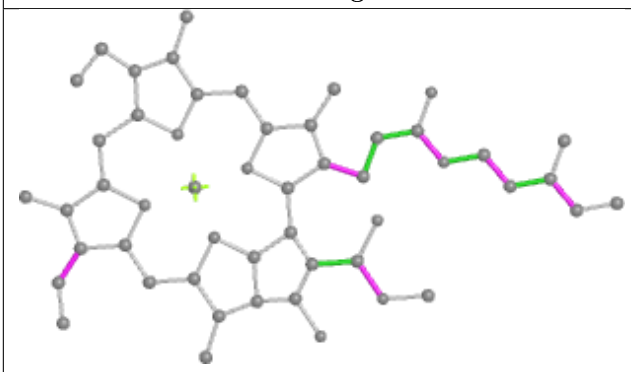
Ligand CLA 2 302



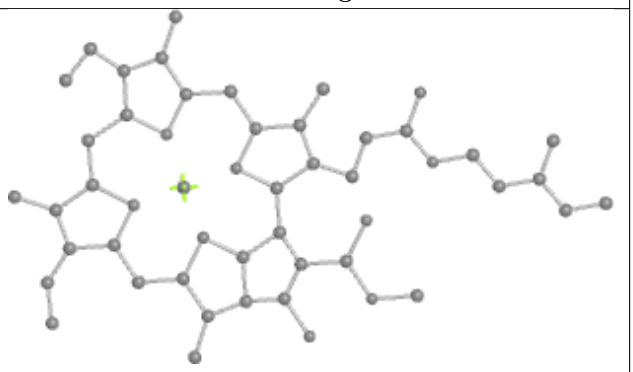
Bond lengths



Bond angles

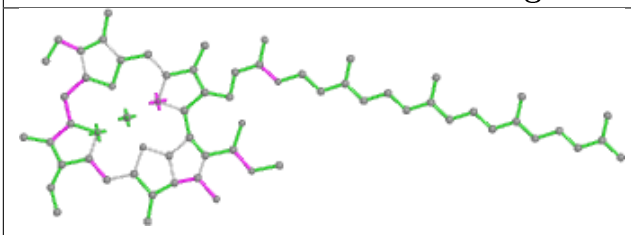


Torsions

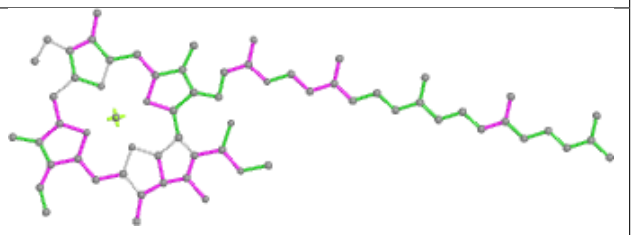


Rings

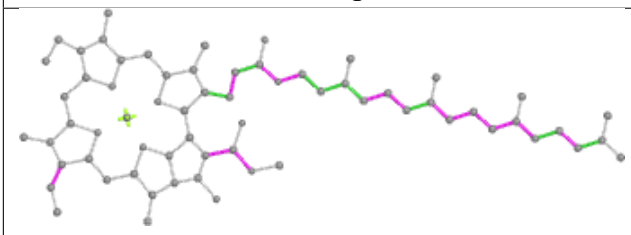
Ligand CLA A 823



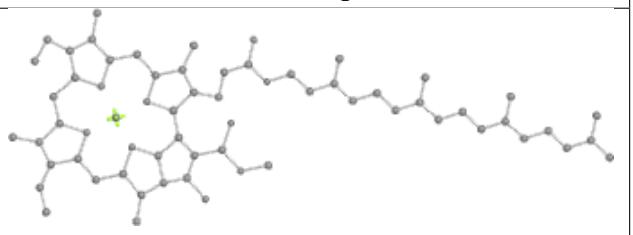
Bond lengths



Bond angles

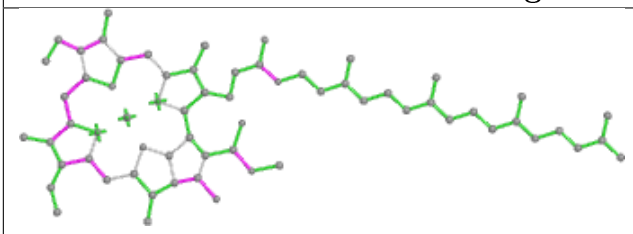


Torsions

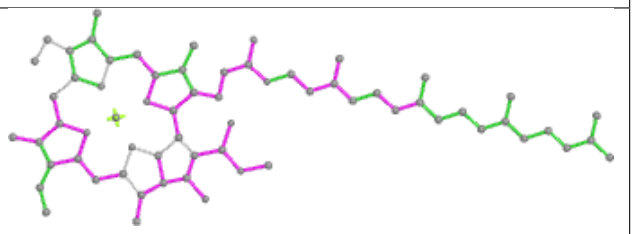


Rings

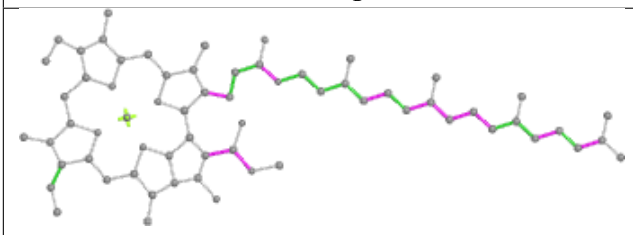
Ligand CLA A 828



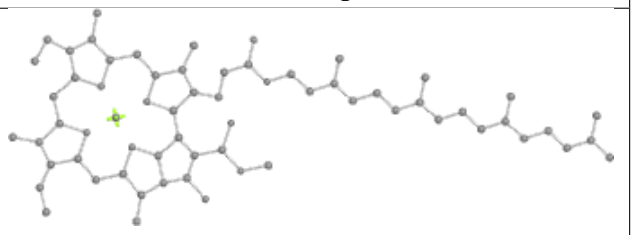
Bond lengths



Bond angles

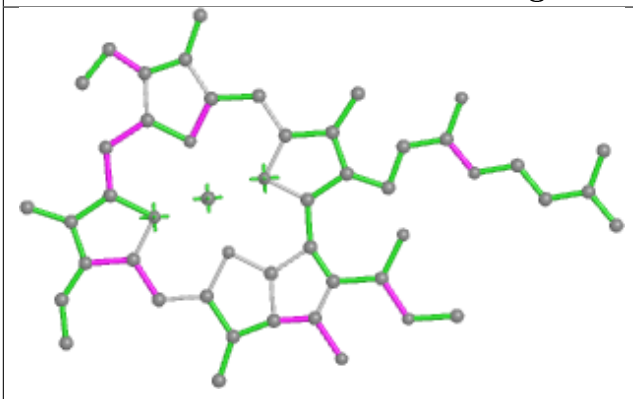


Torsions

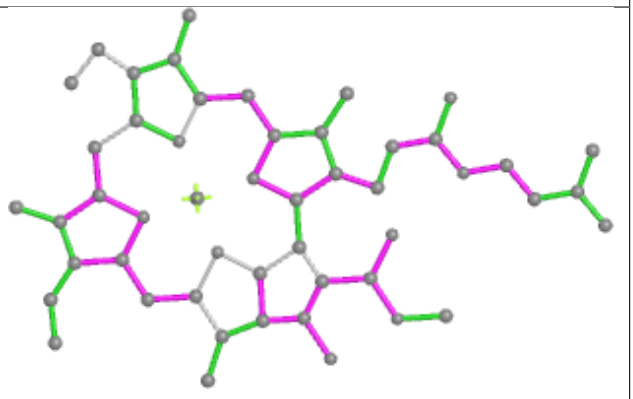


Rings

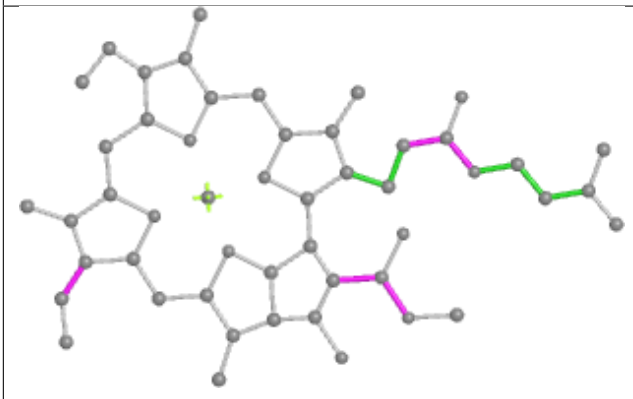
Ligand CLA 2 312



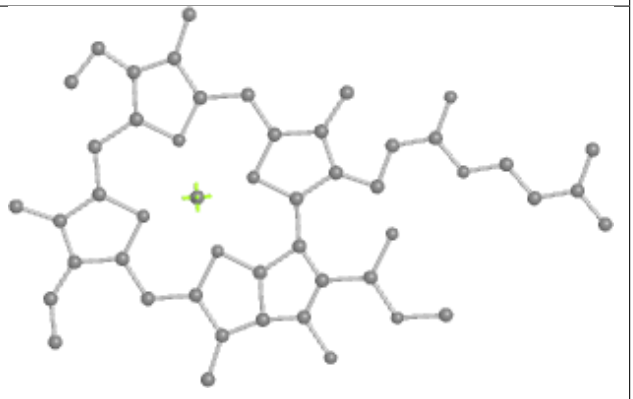
Bond lengths



Bond angles

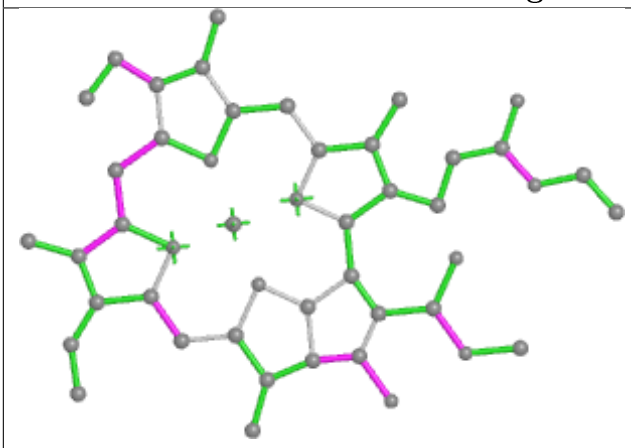


Torsions

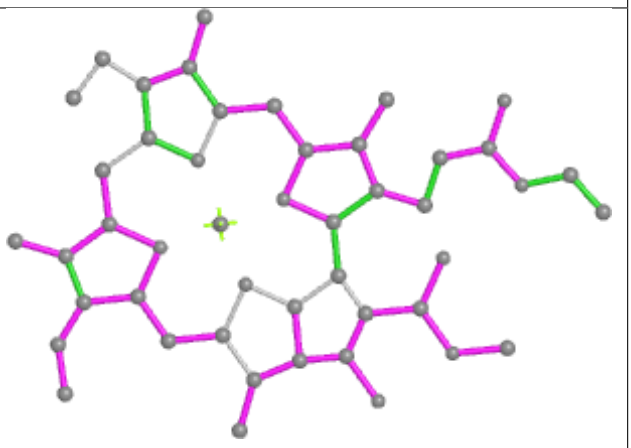


Rings

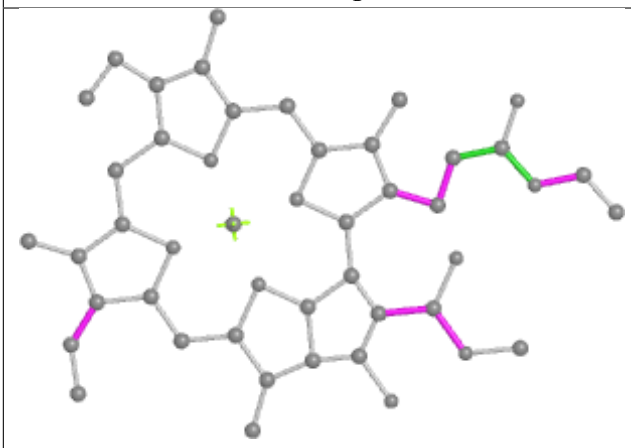
Ligand CLA L 208



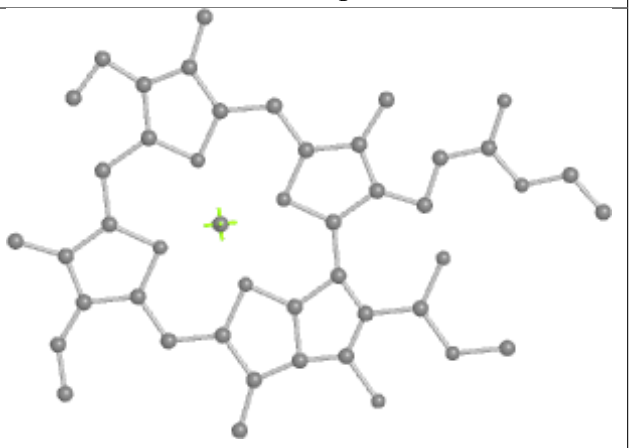
Bond lengths



Bond angles

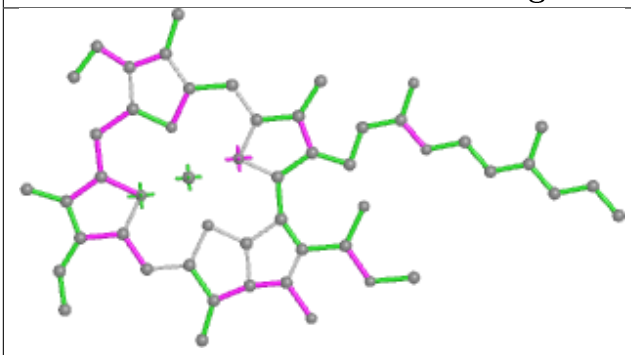


Torsions

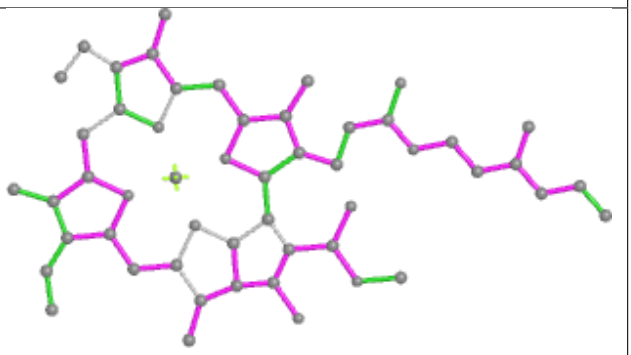


Rings

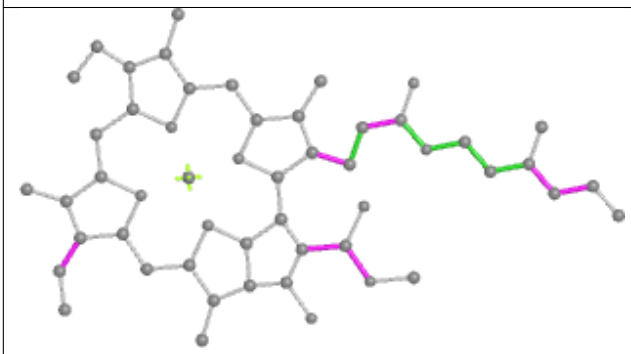
Ligand CLA 4 318



Bond lengths



Bond angles



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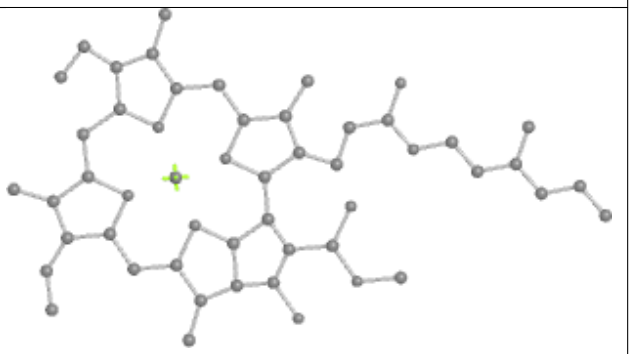
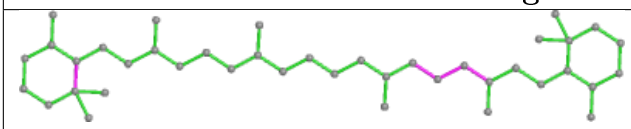
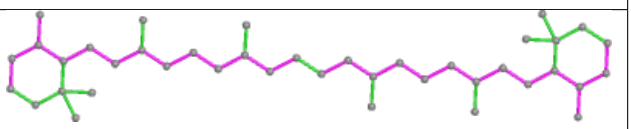


Rings

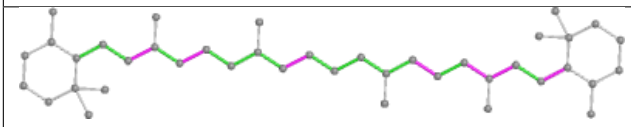
Ligand BCR A 843



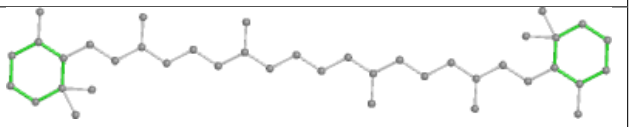
Bond lengths



Bond angles

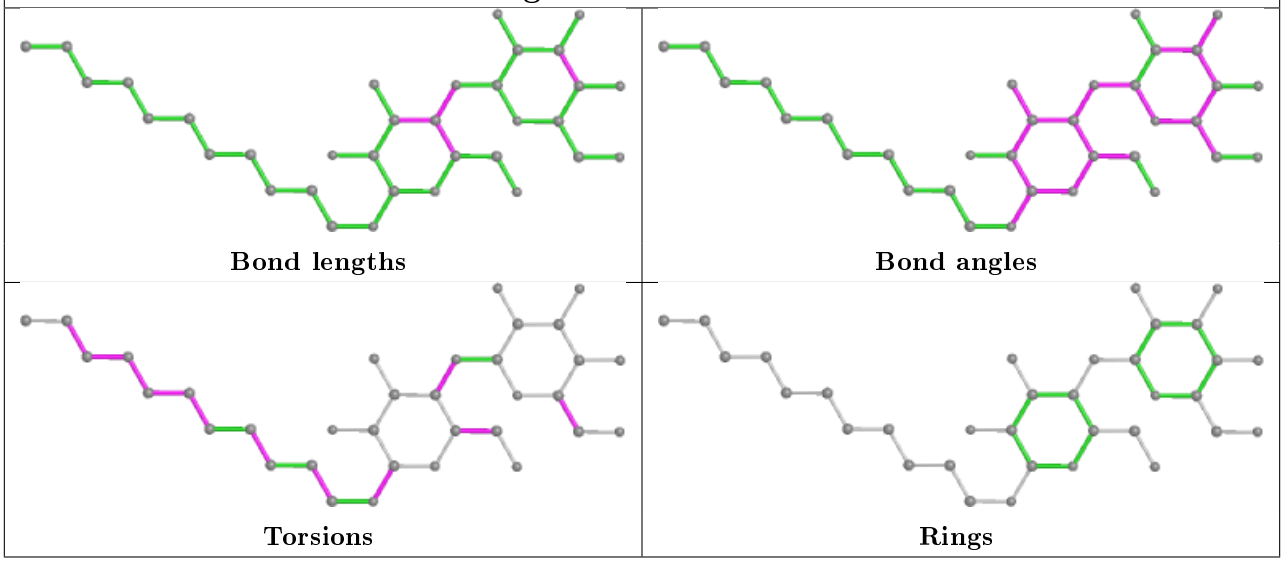


Torsions

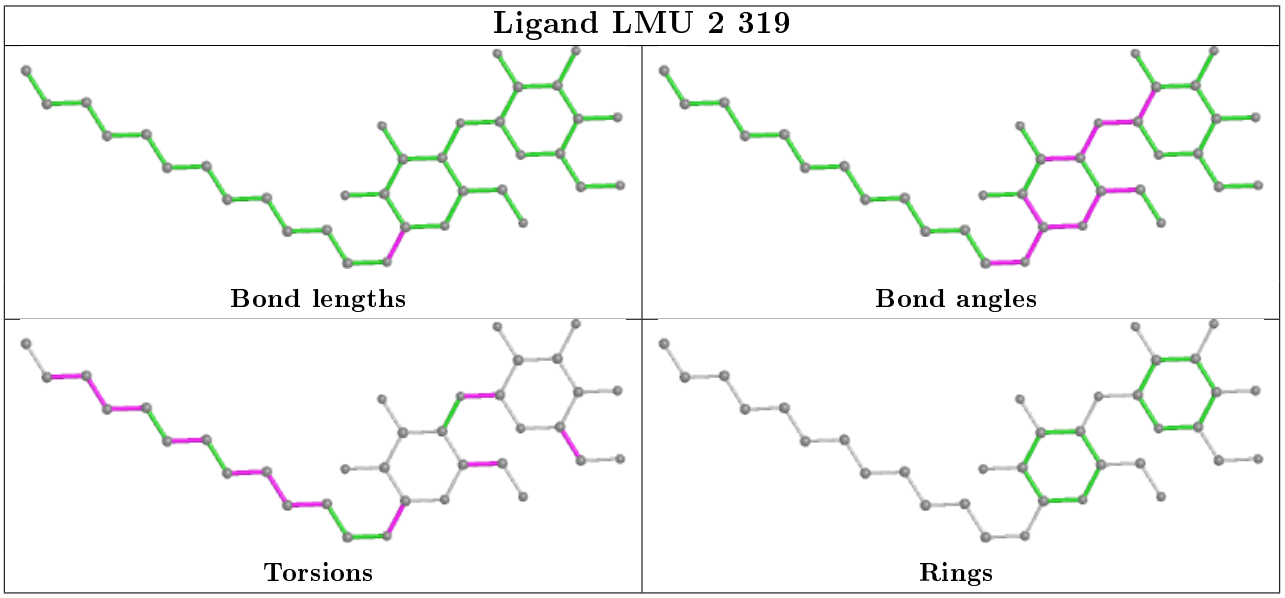


Rings

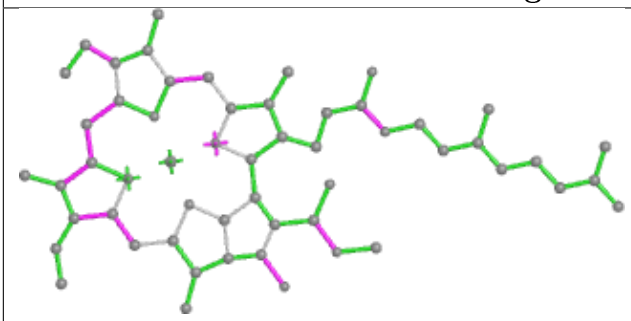
Ligand LMU F 201



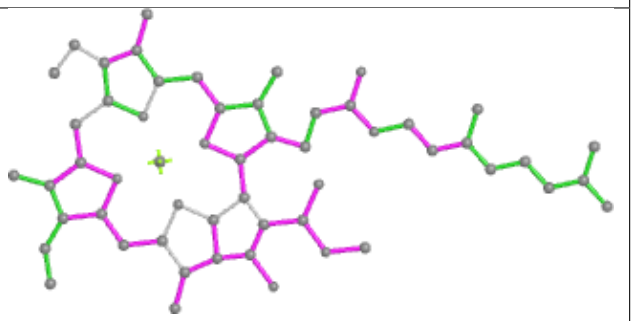
Ligand LMU 2 319



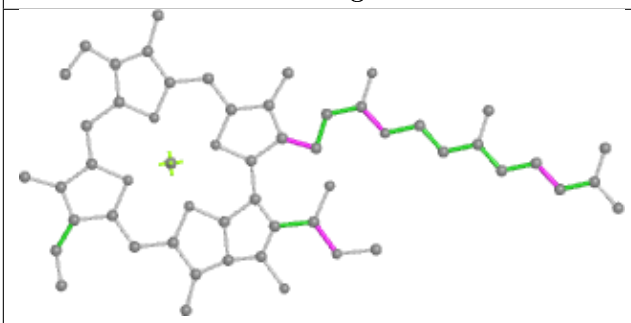
Ligand CLA A 806



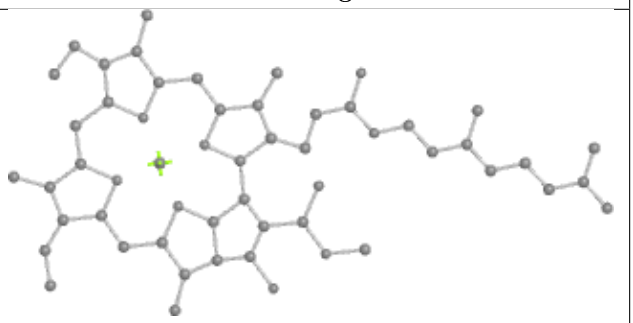
Bond lengths



Bond angles

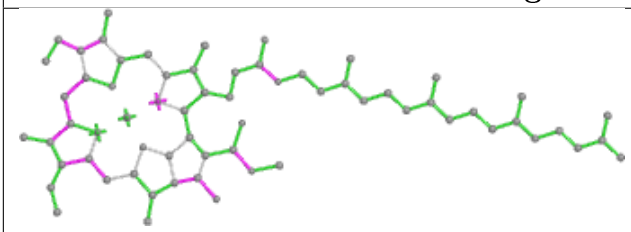


Torsions

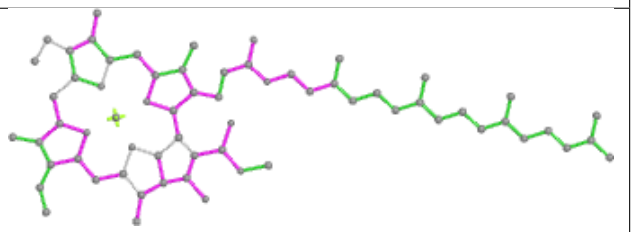


Rings

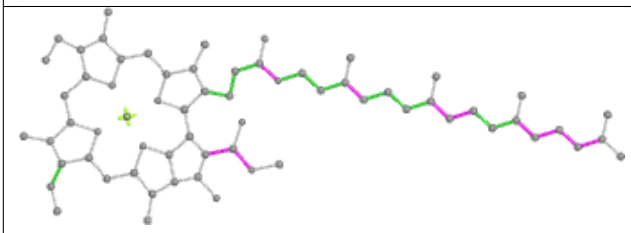
Ligand CLA A 835



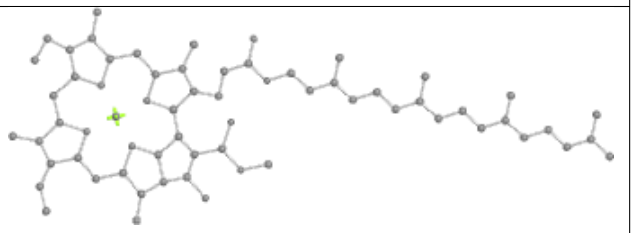
Bond lengths



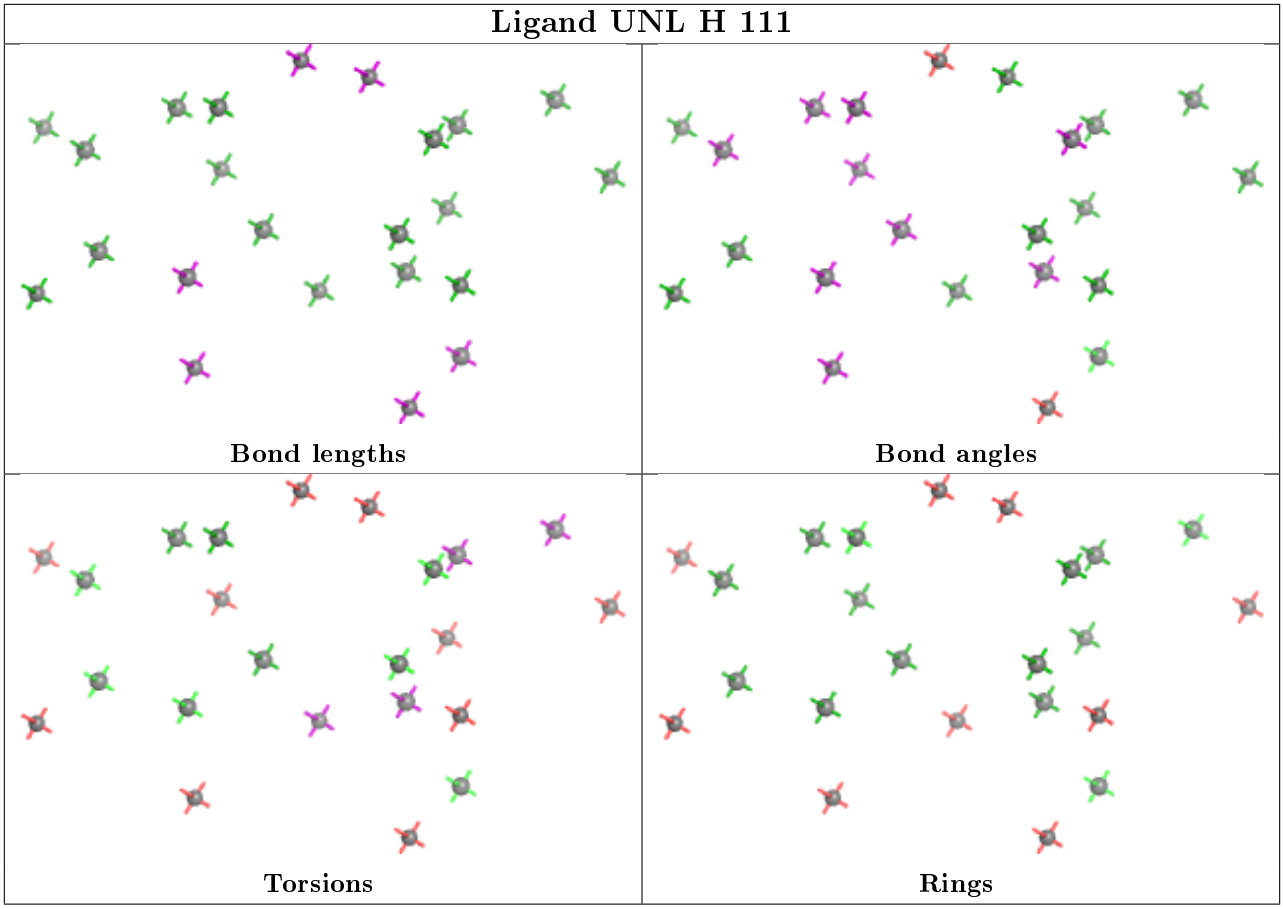
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	164/241 (68%)	1.40	44 (26%) 0 0	32, 62, 71, 73	0
2	2	176/269 (65%)	1.11	38 (21%) 0 1	20, 20, 20, 20	0
3	3	160/276 (57%)	1.92	64 (40%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	0.90	24 (14%) 2 3	20, 20, 20, 20	0
5	A	730/758 (96%)	0.90	87 (11%) 4 5	20, 20, 20, 20	0
6	B	733/734 (99%)	0.77	52 (7%) 16 15	20, 20, 20, 20	0
7	C	81/81 (100%)	1.17	11 (13%) 3 4	20, 20, 20, 20	0
8	D	138/212 (65%)	1.03	25 (18%) 1 1	20, 20, 20, 20	0
9	E	65/143 (45%)	1.17	16 (24%) 0 0	20, 20, 20, 20	0
10	F	154/231 (66%)	0.59	12 (7%) 13 13	20, 20, 20, 20	0
11	G	95/167 (56%)	0.62	10 (10%) 6 7	20, 20, 20, 20	0
12	H	69/144 (47%)	0.79	9 (13%) 3 4	20, 20, 20, 20	0
13	I	30/40 (75%)	0.33	1 (3%) 46 41	20, 20, 20, 20	0
14	J	42/44 (95%)	0.59	4 (9%) 8 8	20, 20, 20, 20	0
15	K	84/131 (64%)	1.95	32 (38%) 0 0	20, 20, 20, 20	0
16	L	161/216 (74%)	0.75	22 (13%) 3 4	20, 20, 20, 20	0
17	N	85/170 (50%)	0.99	15 (17%) 1 1	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3133/4161 (75%)	0.96	466 (14%) 2 3	20, 20, 65, 112	0

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	61	ASN	11.8
1	1	75	ALA	9.9
4	4	67	ILE	9.2

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Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	9.0
5	A	635	THR	8.2
15	K	63	CYS	8.2
3	3	62	GLY	7.3
2	2	116	PRO	7.2
1	1	33	PRO	7.1
4	4	66	SER	7.0
9	E	79	THR	7.0
4	4	68	GLY	6.8
16	L	117	ALA	6.6
3	3	59	ILE	6.6
8	D	125	PRO	6.1
1	1	32	VAL	5.8
2	2	123	PRO	5.8
3	3	165	ASN	5.8
3	3	91	PRO	5.7
5	A	263	ALA	5.7
2	2	140	GLY	5.6
3	3	58	GLU	5.6
3	3	166	PRO	5.6
5	A	124	TRP	5.6
3	3	57	GLY	5.5
2	2	166	ASN	5.5
3	3	55	ALA	5.5
2	2	117	GLY	5.4
2	2	118	CYS	5.4
2	2	139	GLY	5.4
1	1	140	LEU	5.3
2	2	77	PRO	5.3
6	B	470	THR	5.3
10	F	127	SER	5.1
3	3	89	ALA	5.1
1	1	34	ALA	5.1
3	3	199	VAL	5.0
3	3	154	GLY	5.0
15	K	56	THR	5.0
8	D	136	SER	4.9
6	B	259	GLY	4.8
7	C	80	ALA	4.8
4	4	63	VAL	4.8
3	3	207	GLY	4.7
10	F	124	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
6	B	258	LEU	4.7
9	E	80	ASN	4.7
5	A	264	GLU	4.6
5	A	105	ASN	4.6
6	B	69	ALA	4.6
15	K	50	GLY	4.6
2	2	53	ARG	4.6
3	3	90	LEU	4.6
3	3	150	LEU	4.6
1	1	43	GLU	4.6
2	2	92	THR	4.6
1	1	87	ASN	4.5
8	D	32	SER	4.5
6	B	256	THR	4.5
3	3	173	GLU	4.5
9	E	82	TYR	4.5
16	L	118	LEU	4.5
15	K	67	GLY	4.4
1	1	47	CYS	4.4
11	G	59	LYS	4.4
1	1	76	ALA	4.4
3	3	204	THR	4.4
1	1	113	SER	4.3
15	K	49	THR	4.3
1	1	94	LEU	4.3
15	K	45	SER	4.3
1	1	41	GLU	4.3
2	2	141	LEU	4.3
3	3	84	ILE	4.3
11	G	74	TRP	4.2
9	E	28	ILE	4.2
5	A	185	HIS	4.2
3	3	83	LEU	4.2
12	H	26	SER	4.2
5	A	123	VAL	4.2
2	2	134	ASP	4.2
1	1	175	GLU	4.1
1	1	39	TYR	4.1
1	1	129	ASP	4.1
17	N	64	ASP	4.1
6	B	734	GLY	4.1
14	J	9	SER	4.1

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Mol	Chain	Res	Type	RSRZ
15	K	62	ALA	4.1
2	2	136	GLY	4.1
5	A	662	SER	4.0
9	E	34	SER	4.0
3	3	73	ILE	4.0
3	3	143	PHE	4.0
4	4	177	PRO	4.0
1	1	80	GLY	4.0
7	C	34	CYS	4.0
6	B	260	GLY	4.0
2	2	76	THR	4.0
9	E	36	VAL	3.9
15	K	15	THR	3.9
5	A	505	PRO	3.9
8	D	141	VAL	3.9
8	D	149	THR	3.9
5	A	100	GLY	3.9
15	K	27	ALA	3.9
1	1	95	PRO	3.8
2	2	138	PRO	3.8
15	K	46	GLY	3.8
5	A	292	GLY	3.8
15	K	44	GLU	3.7
1	1	92	GLY	3.7
3	3	110	SER	3.7
1	1	88	PRO	3.7
5	A	500	PRO	3.7
17	N	30	ALA	3.7
17	N	56	LYS	3.7
15	K	1	ASP	3.7
2	2	119	VAL	3.7
5	A	634	VAL	3.6
10	F	125	LEU	3.6
4	4	134	PRO	3.6
15	K	26	LEU	3.6
1	1	120	LYS	3.6
1	1	28	GLY	3.6
5	A	329	ASP	3.6
5	A	291	THR	3.6
15	K	64	GLY	3.6
5	A	340	GLY	3.6
1	1	17	SER	3.6

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Mol	Chain	Res	Type	RSRZ
7	C	60	THR	3.6
6	B	492	ILE	3.5
5	A	344	LYS	3.5
11	G	7	VAL	3.5
17	N	82	PHE	3.5
5	A	191	PRO	3.5
15	K	16	THR	3.5
15	K	35	THR	3.5
5	A	752	ALA	3.5
3	3	131	ASP	3.5
5	A	501	GLY	3.5
15	K	28	PRO	3.4
8	D	51	GLU	3.4
3	3	68	GLY	3.4
4	4	136	GLY	3.4
9	E	67	VAL	3.4
7	C	61	ASP	3.4
3	3	142	TYR	3.4
5	A	277	TYR	3.4
2	2	181	HIS	3.4
3	3	85	PRO	3.4
9	E	51	SER	3.3
1	1	74	TRP	3.3
4	4	135	GLY	3.3
5	A	483	GLN	3.3
10	F	137	PRO	3.3
3	3	153	SER	3.3
5	A	79	PHE	3.3
5	A	433	ASP	3.3
3	3	116	PHE	3.3
6	B	493	TRP	3.3
3	3	72	ALA	3.3
5	A	520	LEU	3.3
3	3	54	LEU	3.2
8	D	116	ASP	3.2
15	K	71	GLY	3.2
4	4	191	ASN	3.2
15	K	14	THR	3.2
1	1	174	LEU	3.2
3	3	191	MET	3.2
15	K	21	ALA	3.2
15	K	22	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
15	K	29	SER	3.2
5	A	631	GLN	3.2
6	B	292	ARG	3.2
10	F	66	ASP	3.2
5	A	104	SER	3.2
15	K	58	ALA	3.1
5	A	182	GLY	3.1
5	A	535	GLY	3.1
6	B	568	CYS	3.1
4	4	114	SER	3.1
10	F	138	VAL	3.1
5	A	99	HIS	3.1
3	3	196	GLY	3.1
17	N	40	CYS	3.1
6	B	6	PRO	3.1
1	1	24	PHE	3.1
12	H	17	THR	3.1
6	B	562	PRO	3.1
1	1	57	ILE	3.1
12	H	25	GLY	3.1
2	2	61	GLY	3.0
16	L	134	ASP	3.0
8	D	99	GLN	3.0
3	3	174	LYS	3.0
7	C	37	LYS	3.0
8	D	150	GLY	3.0
4	4	125	SER	3.0
6	B	366	THR	3.0
5	A	485	GLN	3.0
2	2	161	THR	3.0
14	J	38	THR	3.0
3	3	123	PHE	3.0
14	J	8	LEU	3.0
5	A	122	VAL	3.0
10	F	1	ASP	3.0
3	3	182	LYS	3.0
3	3	184	VAL	3.0
17	N	18	ASP	3.0
17	N	13	ASN	2.9
2	2	112	ASP	2.9
6	B	509	PHE	2.9
6	B	469	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
5	A	31	PHE	2.9
5	A	266	ALA	2.9
5	A	726	SER	2.9
5	A	493	GLN	2.9
3	3	151	GLY	2.9
3	3	160	GLY	2.9
16	L	9	GLN	2.9
11	G	76	SER	2.9
1	1	173	PRO	2.9
5	A	108	ALA	2.9
3	3	140	LYS	2.8
5	A	45	ALA	2.8
17	N	55	GLN	2.8
15	K	61	LEU	2.8
3	3	208	PRO	2.8
5	A	398	HIS	2.8
2	2	122	ASP	2.8
5	A	582	ASP	2.8
5	A	497	ALA	2.8
4	4	86	SER	2.8
1	1	122	LYS	2.8
4	4	83	TYR	2.8
1	1	42	SER	2.8
5	A	430	ASP	2.8
2	2	75	ASN	2.8
4	4	34	PRO	2.8
15	K	17	LEU	2.8
6	B	630	GLN	2.8
5	A	378	SER	2.8
6	B	569	ASP	2.8
16	L	141	GLY	2.8
3	3	148	LYS	2.8
4	4	115	VAL	2.8
6	B	629	SER	2.8
2	2	165	LYS	2.8
3	3	112	THR	2.8
6	B	312	GLY	2.8
3	3	88	THR	2.7
6	B	495	PRO	2.7
7	C	9	ASP	2.7
9	E	92	ALA	2.7
5	A	342	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
13	I	6	SER	2.7
1	1	141	GLU	2.7
3	3	66	MET	2.7
7	C	62	PHE	2.7
4	4	145	PRO	2.7
1	1	79	GLY	2.7
9	E	61	THR	2.7
16	L	120	LEU	2.7
11	G	27	GLN	2.7
15	K	55	PHE	2.7
6	B	242	HIS	2.7
12	H	22	ASP	2.6
5	A	369	THR	2.6
12	H	28	ALA	2.6
5	A	514	THR	2.6
7	C	54	CYS	2.6
1	1	78	PRO	2.6
6	B	449	PRO	2.6
17	N	17	ASN	2.6
12	H	29	PRO	2.6
1	1	38	ARG	2.6
6	B	298	GLY	2.6
6	B	435	GLY	2.6
16	L	159	TYR	2.6
6	B	311	PRO	2.6
2	2	93	THR	2.6
1	1	164	GLN	2.6
6	B	299	HIS	2.6
9	E	65	VAL	2.6
3	3	77	ILE	2.6
8	D	97	LYS	2.6
2	2	78	SER	2.6
9	E	39	LEU	2.6
8	D	67	ILE	2.6
2	2	194	ALA	2.5
4	4	38	ARG	2.5
3	3	40	SER	2.5
3	3	167	LEU	2.5
5	A	265	GLY	2.5
6	B	212	PHE	2.5
12	H	20	GLN	2.5
1	1	111	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
5	A	195	TRP	2.5
5	A	536	THR	2.5
10	F	38	PRO	2.5
16	L	17	ASP	2.5
8	D	71	GLY	2.5
1	1	29	LEU	2.5
2	2	210	PRO	2.5
11	G	96	SER	2.5
5	A	111	ASN	2.5
3	3	79	GLY	2.5
8	D	146	VAL	2.5
16	L	81	GLY	2.5
16	L	116	PRO	2.5
1	1	176	ASN	2.5
5	A	484	LEU	2.5
6	B	342	GLY	2.5
11	G	32	ALA	2.5
3	3	42	PRO	2.5
5	A	186	TYR	2.5
5	A	368	LEU	2.5
17	N	35	VAL	2.4
15	K	48	GLN	2.4
2	2	163	GLU	2.4
5	A	388	ASP	2.4
2	2	137	TYR	2.4
5	A	339	THR	2.4
15	K	43	ARG	2.4
7	C	32	GLY	2.4
6	B	468	GLY	2.4
6	B	566	GLY	2.4
5	A	695	SER	2.4
16	L	133	ALA	2.4
16	L	153	TRP	2.4
5	A	659	ALA	2.4
16	L	84	GLY	2.4
4	4	62	GLU	2.4
7	C	2	SER	2.4
12	H	71	ASN	2.4
17	N	37	PHE	2.4
3	3	64	TYR	2.4
5	A	181	ALA	2.4
3	3	92	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	2	135	VAL	2.4
9	E	78	SER	2.4
6	B	667	TRP	2.4
2	2	58	GLY	2.4
16	L	29	SER	2.4
8	D	72	PRO	2.4
15	K	72	VAL	2.4
5	A	257	GLN	2.4
1	1	27	LEU	2.4
5	A	272	LEU	2.4
5	A	627	THR	2.4
3	3	119	ALA	2.3
10	F	16	LYS	2.3
16	L	85	SER	2.3
6	B	373	THR	2.3
3	3	67	LEU	2.3
6	B	171	ALA	2.3
3	3	130	GLN	2.3
5	A	271	THR	2.3
8	D	62	THR	2.3
3	3	209	TYR	2.3
5	A	83	PHE	2.3
5	A	153	TRP	2.3
17	N	65	LEU	2.3
16	L	46	ALA	2.3
16	L	65	VAL	2.3
5	A	334	HIS	2.3
10	F	126	ALA	2.3
1	1	169	PRO	2.3
1	1	46	HIS	2.3
2	2	110	TRP	2.3
8	D	50	TRP	2.3
16	L	24	GLU	2.3
8	D	22	PRO	2.3
17	N	14	LYS	2.3
6	B	346	SER	2.3
17	N	81	VAL	2.3
5	A	404	GLY	2.2
2	2	65	PRO	2.2
5	A	121	GLN	2.2
2	2	54	TRP	2.2
6	B	300	SER	2.2

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Mol	Chain	Res	Type	RSRZ
6	B	704	GLN	2.2
6	B	549	ASP	2.2
6	B	438	VAL	2.2
17	N	12	THR	2.2
1	1	177	LEU	2.2
11	G	75	GLY	2.2
5	A	150	PHE	2.2
6	B	345	THR	2.2
6	B	530	THR	2.2
8	D	156	LEU	2.2
4	4	132	GLY	2.2
10	F	122	ASP	2.2
5	A	371	VAL	2.2
5	A	628	ILE	2.2
14	J	37	LEU	2.2
8	D	151	LYS	2.2
5	A	749	PHE	2.2
2	2	133	THR	2.2
12	H	24	TYR	2.2
6	B	205	GLU	2.1
9	E	56	ASP	2.1
4	4	139	ASN	2.1
5	A	568	LEU	2.1
3	3	53	TRP	2.1
6	B	472	TYR	2.1
5	A	750	PHE	2.1
9	E	58	ASP	2.1
5	A	744	ALA	2.1
6	B	31	PHE	2.1
6	B	271	THR	2.1
5	A	341	GLN	2.1
3	3	181	LEU	2.1
4	4	56	ALA	2.1
5	A	516	GLY	2.1
5	A	63	ASP	2.1
5	A	394	SER	2.1
3	3	63	ARG	2.1
4	4	107	GLN	2.1
15	K	38	LEU	2.1
9	E	64	PRO	2.1
1	1	73	GLU	2.1
5	A	80	SER	2.1

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Mol	Chain	Res	Type	RSRZ
5	A	87	SER	2.1
7	C	20	ALA	2.1
2	2	155	LYS	2.1
5	A	372	VAL	2.1
10	F	99	TRP	2.1
2	2	125	PHE	2.1
3	3	105	ASN	2.1
2	2	170	ALA	2.1
6	B	490	ARG	2.1
1	1	77	LEU	2.1
15	K	40	LEU	2.1
8	D	120	PRO	2.1
1	1	183	ASP	2.1
5	A	506	GLY	2.1
6	B	340	SER	2.1
4	4	193	ILE	2.1
4	4	190	HIS	2.1
5	A	745	THR	2.0
6	B	84	VAL	2.0
6	B	131	THR	2.0
16	L	15	ASN	2.0
6	B	297	ILE	2.0
8	D	34	GLY	2.0
5	A	359	SER	2.0
15	K	59	ASP	2.0
16	L	101	MET	2.0
16	L	82	ALA	2.0
5	A	287	LEU	2.0
6	B	543	GLY	2.0
3	3	126	HIS	2.0
5	A	33	GLN	2.0
3	3	190	ALA	2.0
11	G	82	ALA	2.0
3	3	168	GLY	2.0
8	D	68	MET	2.0
5	A	610	SER	2.0
8	D	115	LYS	2.0
16	L	37	LEU	2.0
3	3	96	GLY	2.0
8	D	33	THR	2.0
3	3	127	ARG	2.0
8	D	130	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
11	G	6	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

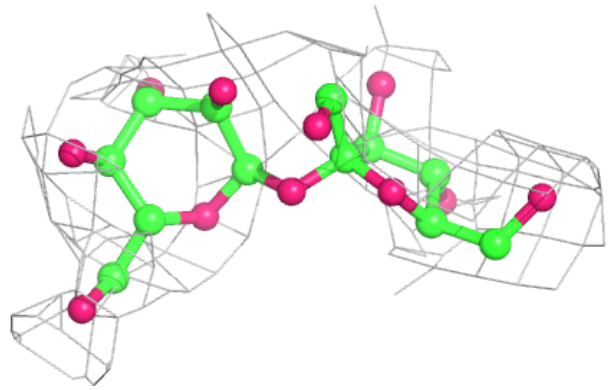
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

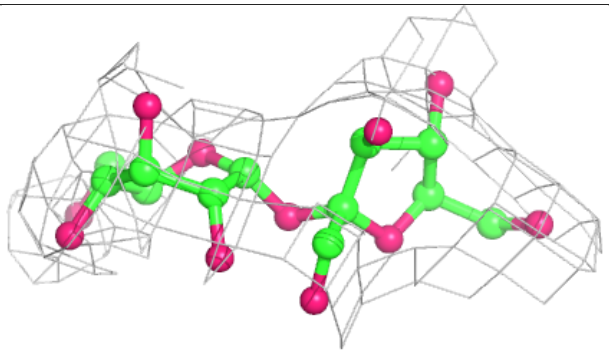
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	GLC	Q	1	11/12	0.43	0.79	20,20,20,20	0
19	FRU	a	2	12/12	0.62	0.35	20,20,20,20	0
19	FRU	M	2	12/12	0.64	0.49	20,20,20,20	0
19	FRU	O	2	12/12	0.64	0.49	20,20,20,20	0
19	FRU	Q	2	12/12	0.65	0.56	20,20,20,20	0
19	FRU	X	2	12/12	0.66	0.43	20,20,20,20	0
19	FRU	P	2	12/12	0.66	0.42	20,20,20,20	0
19	GLC	M	1	11/12	0.67	0.42	20,20,20,20	0
19	GLC	Y	1	11/12	0.67	0.32	20,20,20,20	0
19	GLC	W	1	11/12	0.69	0.32	20,20,20,20	0
19	GLC	a	1	11/12	0.69	0.40	20,20,20,20	0
19	FRU	S	2	12/12	0.70	0.25	20,20,20,20	0
19	GLC	S	1	11/12	0.71	0.34	20,20,20,20	0
19	GLC	O	1	10/12	0.72	0.23	20,20,20,20	0
19	FRU	V	2	12/12	0.73	0.21	20,20,20,20	0
19	FRU	U	2	12/12	0.74	0.31	2,36,60,60	0
19	FRU	Z	2	12/12	0.75	0.23	2,33,60,60	0
19	FRU	Y	2	12/12	0.76	0.29	20,20,20,20	0
19	GLC	P	1	11/12	0.77	0.32	20,20,20,20	0
19	GLC	T	1	11/12	0.77	0.23	20,20,20,20	0
19	GLC	V	1	11/12	0.78	0.38	20,20,20,20	0
19	FRU	W	2	12/12	0.80	0.20	20,20,20,20	0
19	GLC	X	1	11/12	0.82	0.53	20,20,20,20	0
19	GLC	Z	1	11/12	0.83	0.17	2,57,60,60	0
19	FRU	T	2	12/12	0.84	0.21	20,20,20,20	0
19	GLC	U	1	11/12	0.85	0.27	2,13,57,60	0

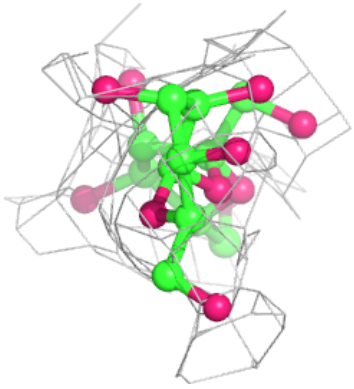
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

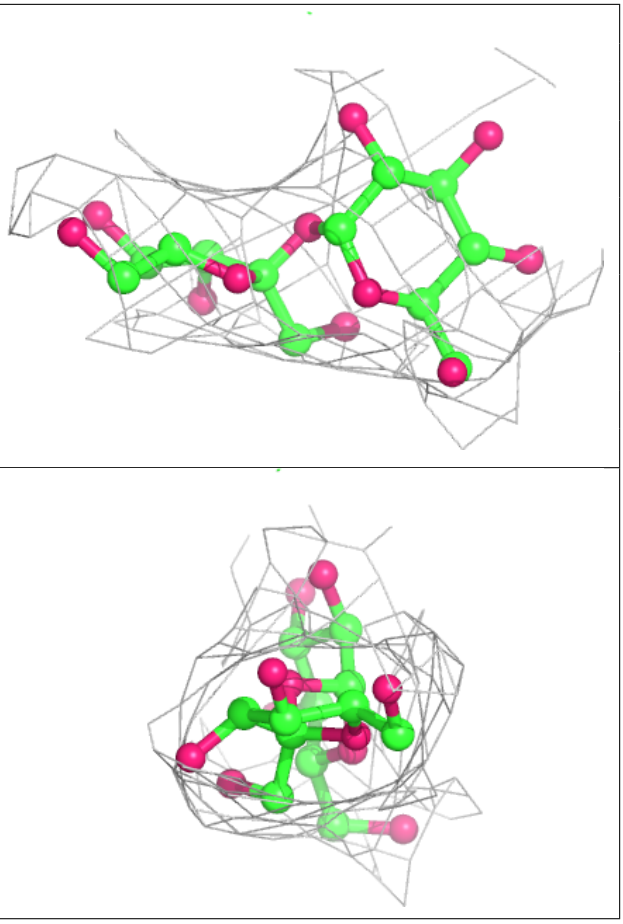


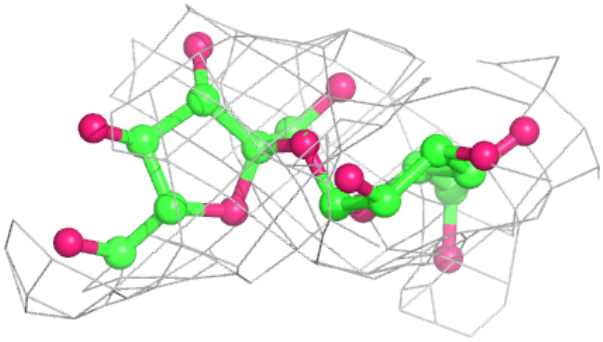




Electron density around Chain T:

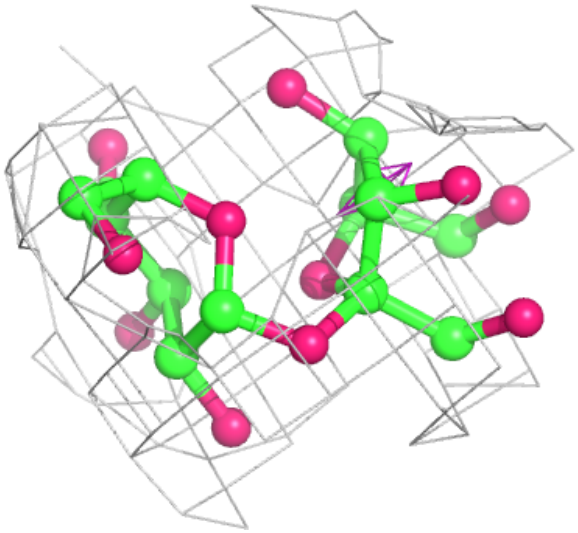
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

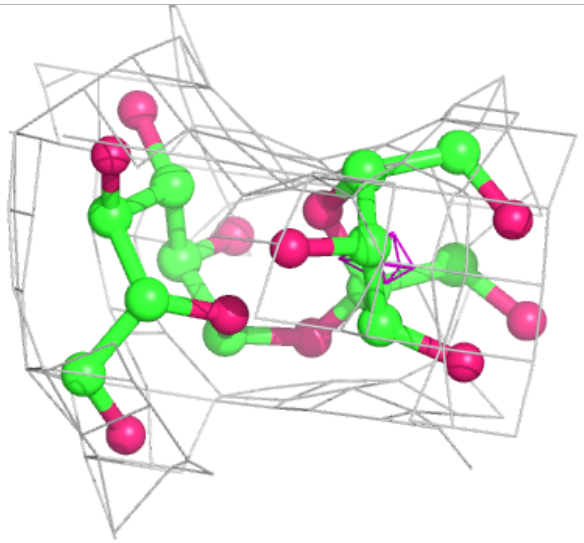


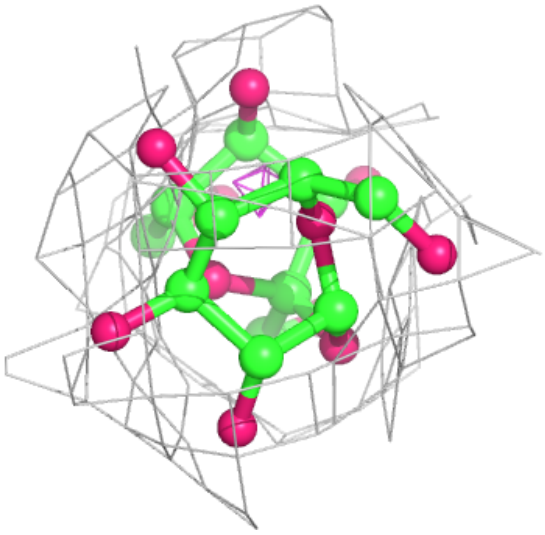


Electron density around Chain U:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

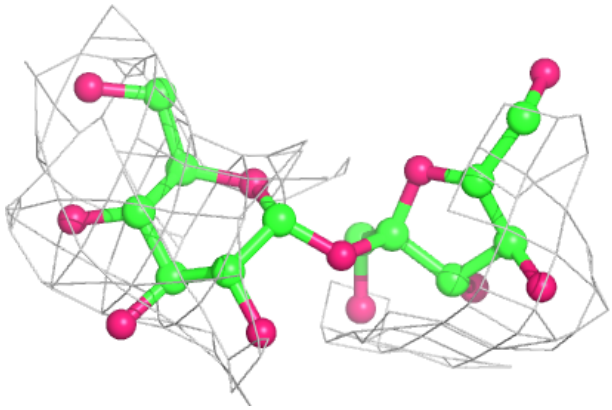


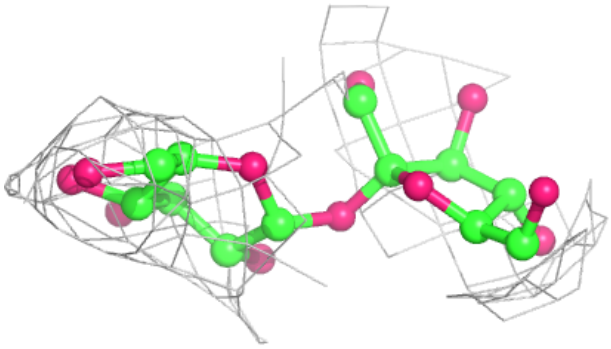


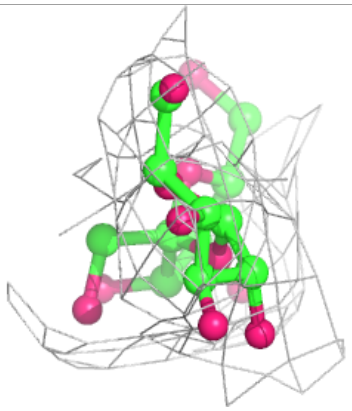


Electron density around Chain V:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

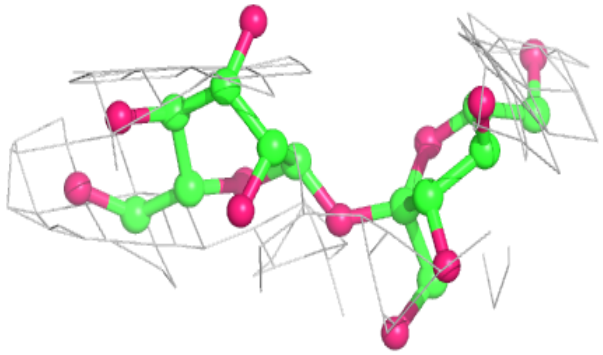


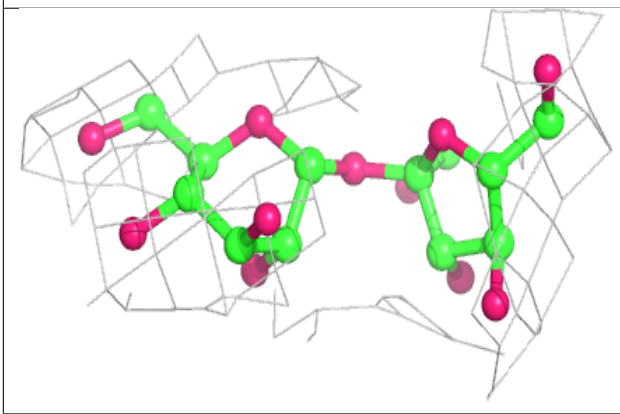


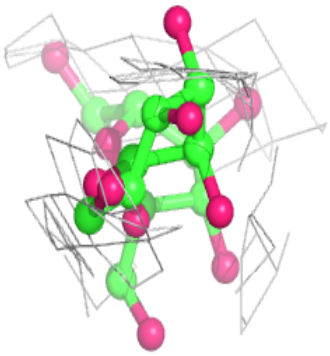


Electron density around Chain W:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

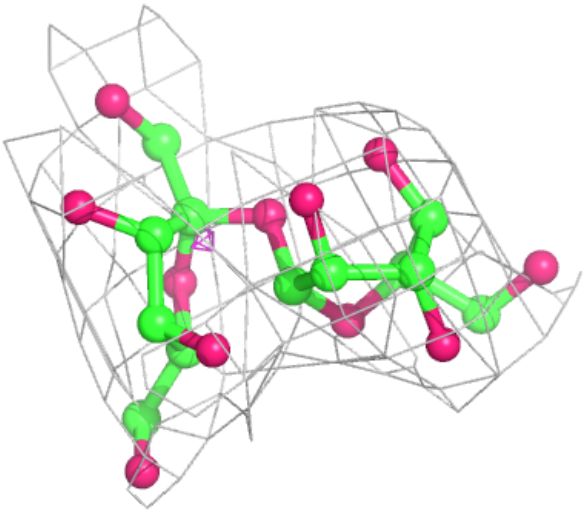


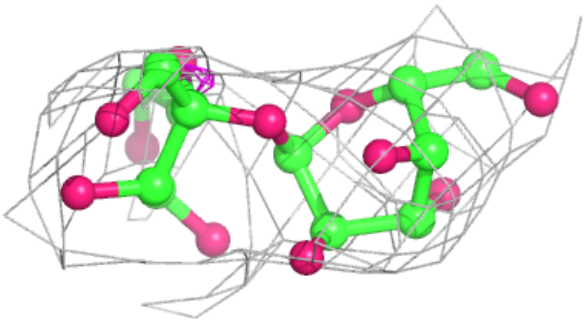


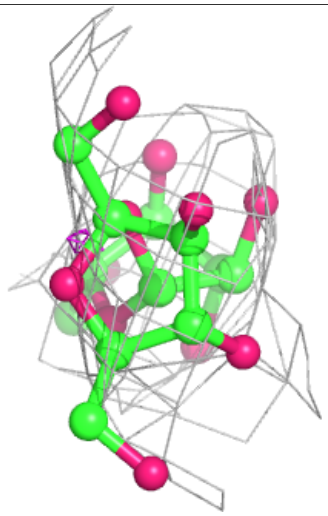


Electron density around Chain X:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

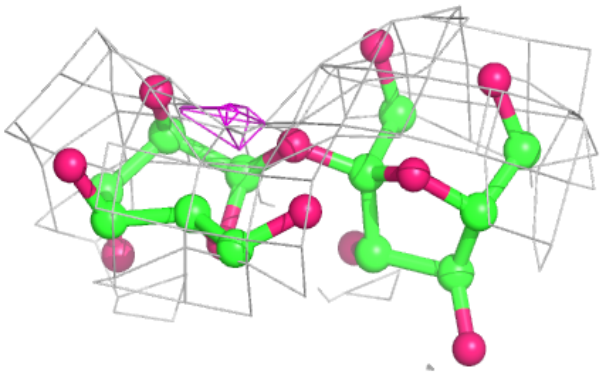


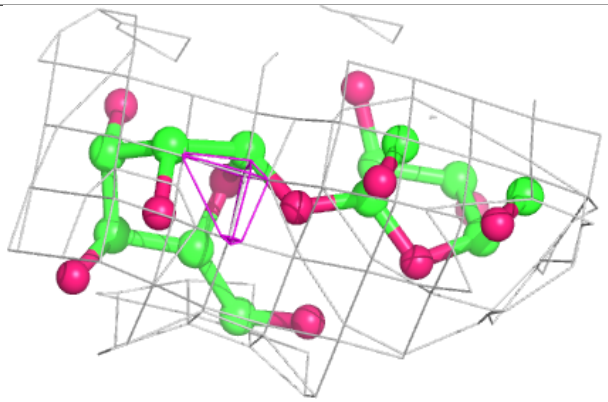


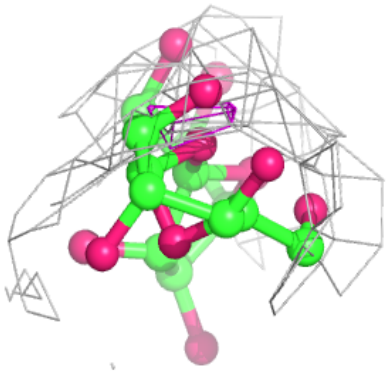


Electron density around Chain Y:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

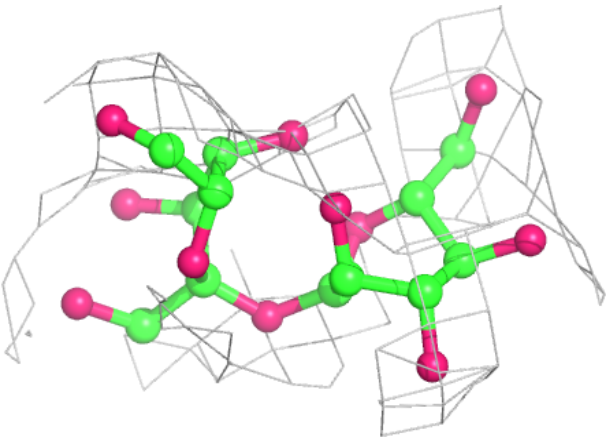


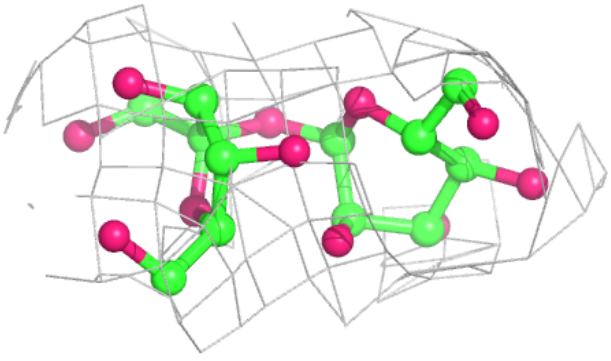


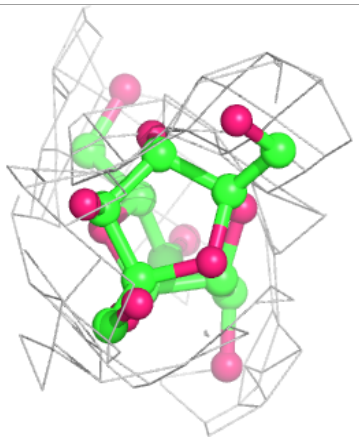


Electron density around Chain Z:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	3	310	25/65	0.46	0.43	20,20,20,20	0
21	LMU	1	218	35/35	0.46	0.42	20,20,20,20	0
21	LMU	R	102	35/35	0.51	0.48	20,20,20,20	0
21	LMU	R	106	35/35	0.53	0.37	20,20,20,20	0
21	LMU	L	204	35/35	0.53	0.51	20,20,20,20	0
21	LMU	A	853	35/35	0.54	0.51	20,20,20,20	0
20	CLA	3	306	25/65	0.55	0.40	20,20,20,20	0
20	CLA	B	834	51/65	0.55	0.47	20,20,20,20	0
20	CLA	A	839	65/65	0.55	0.47	20,20,20,20	0
20	CLA	H	102	55/65	0.55	0.38	20,20,20,20	0
21	LMU	B	801	35/35	0.56	0.48	20,20,20,20	0
21	LMU	4	301	35/35	0.56	0.36	20,20,20,20	0
20	CLA	2	322	61/65	0.57	0.36	20,20,20,20	0
20	CLA	3	301	36/65	0.58	0.48	20,20,20,20	0
22	BCR	A	843	40/40	0.58	0.45	20,20,20,20	0
20	CLA	B	833	45/65	0.59	0.42	20,20,20,20	0
20	CLA	2	302	51/65	0.59	0.37	20,20,20,20	0
21	LMU	2	320	35/35	0.59	0.54	20,20,20,20	0
22	BCR	J	102	40/40	0.60	0.46	20,20,20,20	0
20	CLA	K	102	50/65	0.60	0.49	20,20,20,20	0
20	CLA	H	103	55/65	0.60	0.49	20,20,20,20	0
20	CLA	K	101	45/65	0.60	0.37	20,20,20,20	0
21	LMU	H	108	35/35	0.60	0.36	2,41,60,60	0
21	LMU	R	101	35/35	0.60	0.33	20,20,20,20	0
20	CLA	A	814	45/65	0.60	0.53	20,20,20,20	0
21	LMU	A	848	35/35	0.61	0.45	20,20,20,20	0
20	CLA	2	308	65/65	0.61	0.42	20,20,20,20	0
20	CLA	2	301	25/65	0.61	0.67	20,20,20,20	0
20	CLA	3	311	65/65	0.62	0.39	20,20,20,20	0
20	CLA	3	313	65/65	0.62	0.55	20,20,20,20	0
21	LMU	2	313	35/35	0.62	0.40	20,20,20,20	0
20	CLA	A	802	25/65	0.62	0.43	20,20,20,20	0
21	LMU	H	105	35/35	0.62	0.30	20,20,20,20	0
20	CLA	3	309	25/65	0.62	0.44	20,20,20,20	0
21	LMU	D	201	35/35	0.62	0.31	2,30,60,60	0
21	LMU	3	321	35/35	0.63	0.33	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	3	308	42/65	0.63	0.37	20,20,20,20	0
20	CLA	A	840	50/65	0.63	0.32	20,20,20,20	0
21	LMU	4	317	35/35	0.63	0.31	20,20,20,20	0
20	CLA	3	317	50/65	0.63	0.37	20,20,20,20	0
21	LMU	H	107	35/35	0.64	0.33	20,20,20,20	0
20	CLA	2	306	25/65	0.64	0.36	20,20,20,20	0
20	CLA	B	814	46/65	0.64	0.51	20,20,20,20	0
20	CLA	4	306	50/65	0.65	0.41	20,20,20,20	0
20	CLA	4	308	36/65	0.65	0.39	20,20,20,20	0
20	CLA	4	302	55/65	0.65	0.35	20,20,20,20	0
21	LMU	1	213	35/35	0.65	0.35	2,45,60,60	0
22	BCR	3	314	40/40	0.65	0.37	20,20,20,20	0
21	LMU	1	220	35/35	0.65	0.28	2,51,60,60	0
21	LMU	R	109	35/35	0.65	0.31	20,20,20,20	0
21	LMU	1	217	35/35	0.65	0.47	20,20,20,20	0
20	CLA	A	810	45/65	0.65	0.56	20,20,20,20	0
21	LMU	2	317	35/35	0.66	0.32	20,20,20,20	0
20	CLA	L	201	55/65	0.66	0.38	20,20,20,20	0
21	LMU	A	849	35/35	0.66	0.41	20,20,20,20	0
20	CLA	3	307	25/65	0.66	0.37	20,20,20,20	0
21	LMU	4	320	34/35	0.67	0.40	20,20,20,20	0
21	LMU	K	104	35/35	0.67	0.42	20,20,20,20	0
21	LMU	R	105	35/35	0.67	0.26	20,20,20,20	0
20	CLA	B	838	65/65	0.67	0.47	20,20,20,20	0
20	CLA	K	108	50/65	0.67	0.59	20,20,20,20	0
20	CLA	1	211	25/65	0.67	0.36	20,20,20,20	0
21	LMU	K	106	35/35	0.67	0.36	2,38,60,60	0
21	LMU	K	109	35/35	0.67	0.39	20,20,20,20	0
21	LMU	H	104	35/35	0.67	0.37	20,20,20,20	0
20	CLA	3	302	50/65	0.68	0.34	20,20,20,20	0
20	CLA	3	319	25/65	0.68	0.30	20,20,20,20	0
20	CLA	R	107	57/65	0.68	0.49	20,20,20,20	0
21	LMU	R	103	35/35	0.68	0.29	20,20,20,20	0
20	CLA	B	840	36/65	0.68	0.46	20,20,20,20	0
20	CLA	1	215	61/65	0.68	0.29	2,35,60,60	0
20	CLA	1	210	51/65	0.68	0.39	20,20,20,20	0
20	CLA	4	305	55/65	0.68	0.35	20,20,20,20	0
21	LMU	4	322	35/35	0.68	0.26	20,20,20,20	0
21	LMU	L	211	35/35	0.68	0.32	20,20,20,20	0
21	LMU	2	318	35/35	0.68	0.26	20,20,20,20	0
22	BCR	A	844	40/40	0.69	0.41	20,20,20,20	0
22	BCR	A	845	40/40	0.69	0.38	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	1	201	46/65	0.69	0.31	20,20,20,20	0
22	BCR	B	846	40/40	0.69	0.46	20,20,20,20	0
20	CLA	4	304	65/65	0.69	0.31	20,20,20,20	0
20	CLA	L	203	55/65	0.69	0.43	20,20,20,20	0
20	CLA	4	319	47/65	0.69	0.29	20,20,20,20	0
20	CLA	J	103	61/65	0.69	0.29	20,20,20,20	0
21	LMU	N	101	35/35	0.69	0.32	2,39,60,60	0
22	BCR	L	210	40/40	0.69	0.47	20,20,20,20	0
20	CLA	2	310	25/65	0.70	0.40	20,20,20,20	0
21	LMU	1	219	35/35	0.70	0.30	20,20,20,20	0
22	BCR	I	103	40/40	0.70	0.47	20,20,20,20	0
20	CLA	2	307	65/65	0.70	0.38	20,20,20,20	0
20	CLA	4	311	55/65	0.70	0.36	20,20,20,20	0
20	CLA	R	108	58/65	0.70	0.34	20,20,20,20	0
20	CLA	2	303	65/65	0.70	0.35	20,20,20,20	0
20	CLA	K	103	65/65	0.70	0.49	20,20,20,20	0
21	LMU	R	104	35/35	0.70	0.36	20,20,20,20	0
20	CLA	A	833	45/65	0.70	0.40	20,20,20,20	0
20	CLA	F	206	53/65	0.70	0.34	20,20,20,20	0
20	CLA	A	820	51/65	0.70	0.48	20,20,20,20	0
20	CLA	A	818	65/65	0.70	0.42	20,20,20,20	0
20	CLA	4	318	52/65	0.70	0.31	20,20,20,20	0
20	CLA	A	811	65/65	0.70	0.43	20,20,20,20	0
20	CLA	A	816	54/65	0.71	0.39	20,20,20,20	0
20	CLA	2	304	25/65	0.71	0.35	20,20,20,20	0
20	CLA	A	823	65/65	0.71	0.41	20,20,20,20	0
25	LMG	B	848	49/55	0.71	0.42	20,20,20,20	0
20	CLA	H	101	55/65	0.71	0.39	20,20,20,20	0
20	CLA	B	824	65/65	0.72	0.38	20,20,20,20	0
20	CLA	B	813	60/65	0.72	0.36	20,20,20,20	0
20	CLA	3	318	65/65	0.72	0.32	20,20,20,20	0
21	LMU	3	322	35/35	0.72	0.28	20,20,20,20	0
21	LMU	A	856	35/35	0.72	0.29	20,20,20,20	0
20	CLA	1	216	25/65	0.72	0.36	20,20,20,20	0
20	CLA	A	829	50/65	0.73	0.41	20,20,20,20	0
22	BCR	A	847	40/40	0.73	0.47	20,20,20,20	0
22	BCR	B	844	40/40	0.73	0.39	20,20,20,20	0
20	CLA	A	801	46/65	0.73	0.24	20,20,20,20	0
21	LMU	4	321	35/35	0.73	0.21	20,20,20,20	0
20	CLA	A	821	42/65	0.73	0.36	20,20,20,20	0
21	LMU	C	101	35/35	0.73	0.26	20,20,20,20	0
23	PQN	A	842	33/33	0.73	0.46	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	3	305	25/65	0.73	0.34	20,20,20,20	0
21	LMU	F	201	34/35	0.73	0.26	20,20,20,20	0
20	CLA	A	805	65/65	0.74	0.37	20,20,20,20	0
20	CLA	2	305	50/65	0.74	0.34	20,20,20,20	0
20	CLA	3	312	25/65	0.74	0.26	20,20,20,20	0
23	PQN	B	841	33/33	0.74	0.42	20,20,20,20	0
20	CLA	H	109	60/65	0.74	0.35	20,20,20,20	0
20	CLA	F	205	41/65	0.74	0.29	20,20,20,20	0
21	LMU	B	802	35/35	0.74	0.23	20,20,20,20	0
20	CLA	A	819	65/65	0.74	0.40	20,20,20,20	0
20	CLA	B	819	46/65	0.74	0.38	20,20,20,20	0
20	CLA	1	205	25/65	0.74	0.29	20,20,20,20	0
20	CLA	A	813	54/65	0.74	0.39	20,20,20,20	0
20	CLA	B	803	65/65	0.74	0.40	20,20,20,20	0
20	CLA	G	102	51/65	0.74	0.31	20,20,20,20	0
20	CLA	A	817	52/65	0.74	0.38	20,20,20,20	0
21	LMU	2	319	35/35	0.74	0.23	20,20,20,20	0
20	CLA	A	806	55/65	0.74	0.39	20,20,20,20	0
20	CLA	L	207	50/65	0.75	0.34	20,20,20,20	0
20	CLA	4	309	25/65	0.75	0.33	20,20,20,20	0
20	CLA	A	826	65/65	0.75	0.45	20,20,20,20	0
22	BCR	F	202	40/40	0.75	0.45	20,20,20,20	0
20	CLA	A	828	65/65	0.75	0.38	20,20,20,20	0
20	CLA	3	320	25/65	0.75	0.28	20,20,20,20	0
20	CLA	B	831	50/65	0.75	0.39	20,20,20,20	0
20	CLA	1	207	51/65	0.75	0.33	20,20,20,20	0
20	CLA	3	304	36/65	0.75	0.35	20,20,20,20	0
20	CLA	L	209	50/65	0.75	0.30	20,20,20,20	0
20	CLA	A	812	54/65	0.76	0.34	20,20,20,20	0
21	LMU	B	847	35/35	0.76	0.29	2,35,60,60	0
20	CLA	B	849	65/65	0.76	0.39	20,20,20,20	0
20	CLA	2	312	50/65	0.76	0.31	20,20,20,20	0
21	LMU	L	205	35/35	0.76	0.24	20,20,20,20	0
20	CLA	A	804	55/65	0.76	0.33	20,20,20,20	0
21	LMU	A	854	35/35	0.76	0.27	20,20,20,20	0
20	CLA	A	832	50/65	0.76	0.36	20,20,20,20	0
20	CLA	1	203	47/65	0.76	0.27	20,20,20,20	0
20	CLA	3	303	25/65	0.77	0.36	20,20,20,20	0
20	CLA	B	823	58/65	0.77	0.37	20,20,20,20	0
22	BCR	B	845	40/40	0.77	0.40	20,20,20,20	0
20	CLA	2	315	25/65	0.77	0.32	20,20,20,20	0
20	CLA	3	316	25/65	0.77	0.38	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	LMU	G	101	35/35	0.77	0.24	20,20,20,20	0
20	CLA	2	316	65/65	0.77	0.29	20,20,20,20	0
20	CLA	F	204	36/65	0.77	0.35	20,20,20,20	0
20	CLA	A	807	46/65	0.78	0.48	20,20,20,20	0
20	CLA	B	832	45/65	0.78	0.32	20,20,20,20	0
20	CLA	L	202	65/65	0.78	0.36	20,20,20,20	0
21	LMU	K	105	35/35	0.78	0.28	20,20,20,20	0
22	BCR	F	203	40/40	0.78	0.31	20,20,20,20	0
20	CLA	4	310	25/65	0.78	0.27	20,20,20,20	0
20	CLA	A	851	65/65	0.78	0.36	20,20,20,20	0
20	CLA	A	824	65/65	0.78	0.36	20,20,20,20	0
20	CLA	1	206	61/65	0.78	0.32	20,20,20,20	0
21	LMU	A	855	35/35	0.79	0.30	20,20,20,20	0
20	CLA	A	822	55/65	0.79	0.35	20,20,20,20	0
20	CLA	4	307	52/65	0.79	0.25	20,20,20,20	0
20	CLA	B	817	61/65	0.79	0.34	20,20,20,20	0
20	CLA	B	815	59/65	0.79	0.37	20,20,20,20	0
20	CLA	4	316	46/65	0.79	0.25	20,20,20,20	0
20	CLA	A	815	50/65	0.79	0.31	20,20,20,20	0
21	LMU	H	106	35/35	0.79	0.33	20,20,20,20	0
20	CLA	2	309	25/65	0.79	0.30	20,20,20,20	0
20	CLA	A	825	65/65	0.79	0.35	20,20,20,20	0
20	CLA	B	829	50/65	0.79	0.36	20,20,20,20	0
20	CLA	B	851	65/65	0.79	0.35	20,20,20,20	0
26	UNL	H	111	23/-	0.79	0.24	20,20,20,20	0
20	CLA	B	808	65/65	0.79	0.37	20,20,20,20	0
20	CLA	A	852	65/65	0.79	0.36	20,20,20,20	0
20	CLA	A	835	65/65	0.79	0.34	20,20,20,20	0
20	CLA	A	809	52/65	0.80	0.34	20,20,20,20	0
20	CLA	B	835	60/65	0.80	0.34	20,20,20,20	0
20	CLA	A	827	55/65	0.80	0.40	20,20,20,20	0
20	CLA	A	836	47/65	0.80	0.35	20,20,20,20	0
21	LMU	E	101	35/35	0.80	0.24	20,20,20,20	0
20	CLA	1	202	57/65	0.80	0.22	2,38,60,60	0
20	CLA	1	214	25/65	0.80	0.20	20,20,20,20	0
20	CLA	4	312	25/65	0.80	0.27	20,20,20,20	0
22	BCR	B	843	40/40	0.80	0.37	20,20,20,20	0
20	CLA	B	804	45/65	0.80	0.33	20,20,20,20	0
22	BCR	B	852	40/40	0.80	0.35	20,20,20,20	0
22	BCR	B	842	40/40	0.80	0.39	20,20,20,20	0
20	CLA	B	812	65/65	0.80	0.33	20,20,20,20	0
20	CLA	2	311	50/65	0.80	0.28	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	1	204	46/65	0.81	0.27	20,20,20,20	0
20	CLA	B	805	60/65	0.81	0.33	20,20,20,20	0
20	CLA	B	810	55/65	0.81	0.29	20,20,20,20	0
20	CLA	A	838	65/65	0.81	0.34	20,20,20,20	0
20	CLA	B	809	54/65	0.81	0.30	20,20,20,20	0
20	CLA	4	314	36/65	0.81	0.29	20,20,20,20	0
20	CLA	B	830	65/65	0.81	0.33	20,20,20,20	0
22	BCR	I	101	40/40	0.81	0.38	20,20,20,20	0
20	CLA	A	830	65/65	0.81	0.35	20,20,20,20	0
20	CLA	A	841	65/65	0.81	0.37	20,20,20,20	0
20	CLA	B	827	65/65	0.81	0.36	20,20,20,20	0
20	CLA	1	212	25/65	0.81	0.44	20,20,20,20	0
20	CLA	A	837	47/65	0.81	0.33	20,20,20,20	0
20	CLA	A	803	50/65	0.82	0.32	20,20,20,20	0
20	CLA	L	208	47/65	0.82	0.31	20,20,20,20	0
20	CLA	B	821	65/65	0.82	0.28	20,20,20,20	0
20	CLA	B	850	65/65	0.82	0.34	20,20,20,20	0
20	CLA	B	822	54/65	0.82	0.32	20,20,20,20	0
20	CLA	J	101	48/65	0.82	0.25	20,20,20,20	0
20	CLA	A	850	65/65	0.82	0.35	20,20,20,20	0
20	CLA	B	818	50/65	0.82	0.35	20,20,20,20	0
20	CLA	A	834	49/65	0.83	0.30	20,20,20,20	0
22	BCR	A	846	40/40	0.83	0.32	20,20,20,20	0
20	CLA	1	208	25/65	0.83	0.34	20,20,20,20	0
20	CLA	I	102	60/65	0.83	0.29	20,20,20,20	0
20	CLA	B	806	65/65	0.83	0.36	20,20,20,20	0
20	CLA	A	831	55/65	0.84	0.33	20,20,20,20	0
20	CLA	B	825	65/65	0.84	0.36	20,20,20,20	0
20	CLA	1	209	36/65	0.84	0.27	20,20,20,20	0
20	CLA	B	811	58/65	0.85	0.27	20,20,20,20	0
20	CLA	B	837	47/65	0.85	0.31	20,20,20,20	0
20	CLA	B	828	50/65	0.85	0.30	20,20,20,20	0
20	CLA	B	820	55/65	0.85	0.29	20,20,20,20	0
20	CLA	B	839	65/65	0.86	0.40	20,20,20,20	0
20	CLA	4	303	36/65	0.86	0.33	20,20,20,20	0
20	CLA	A	808	65/65	0.86	0.35	20,20,20,20	0
20	CLA	4	313	25/65	0.86	0.30	20,20,20,20	0
24	SF4	C	102	8/8	0.87	0.16	20,20,20,20	0
20	CLA	B	816	60/65	0.87	0.32	20,20,20,20	0
20	CLA	B	826	65/65	0.87	0.32	20,20,20,20	0
20	CLA	B	836	65/65	0.88	0.28	20,20,20,20	0
20	CLA	B	807	65/65	0.88	0.33	20,20,20,20	0

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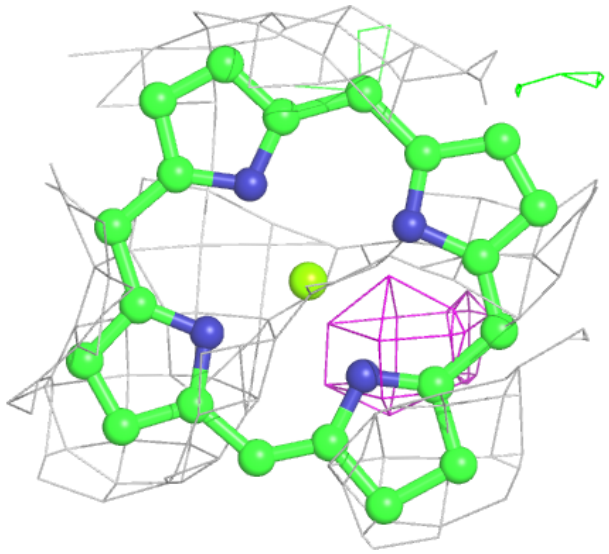
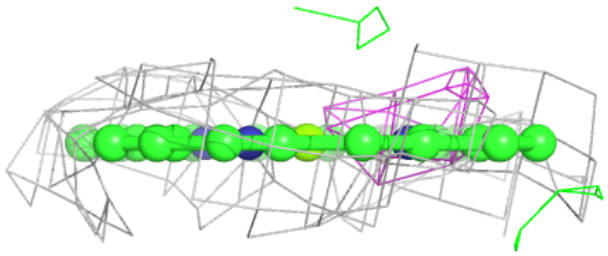
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	4	315	25/65	0.90	0.21	20,20,20,20	0
24	SF4	C	103	8/8	0.91	0.14	20,20,20,20	0
24	SF4	A	857	8/8	0.93	0.14	20,20,20,20	0

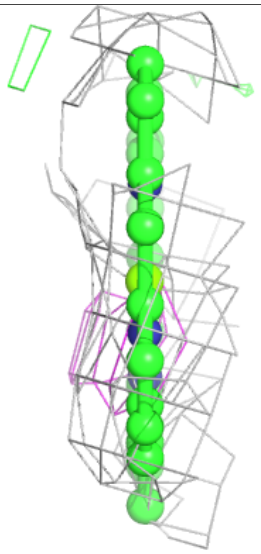
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLA 3 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

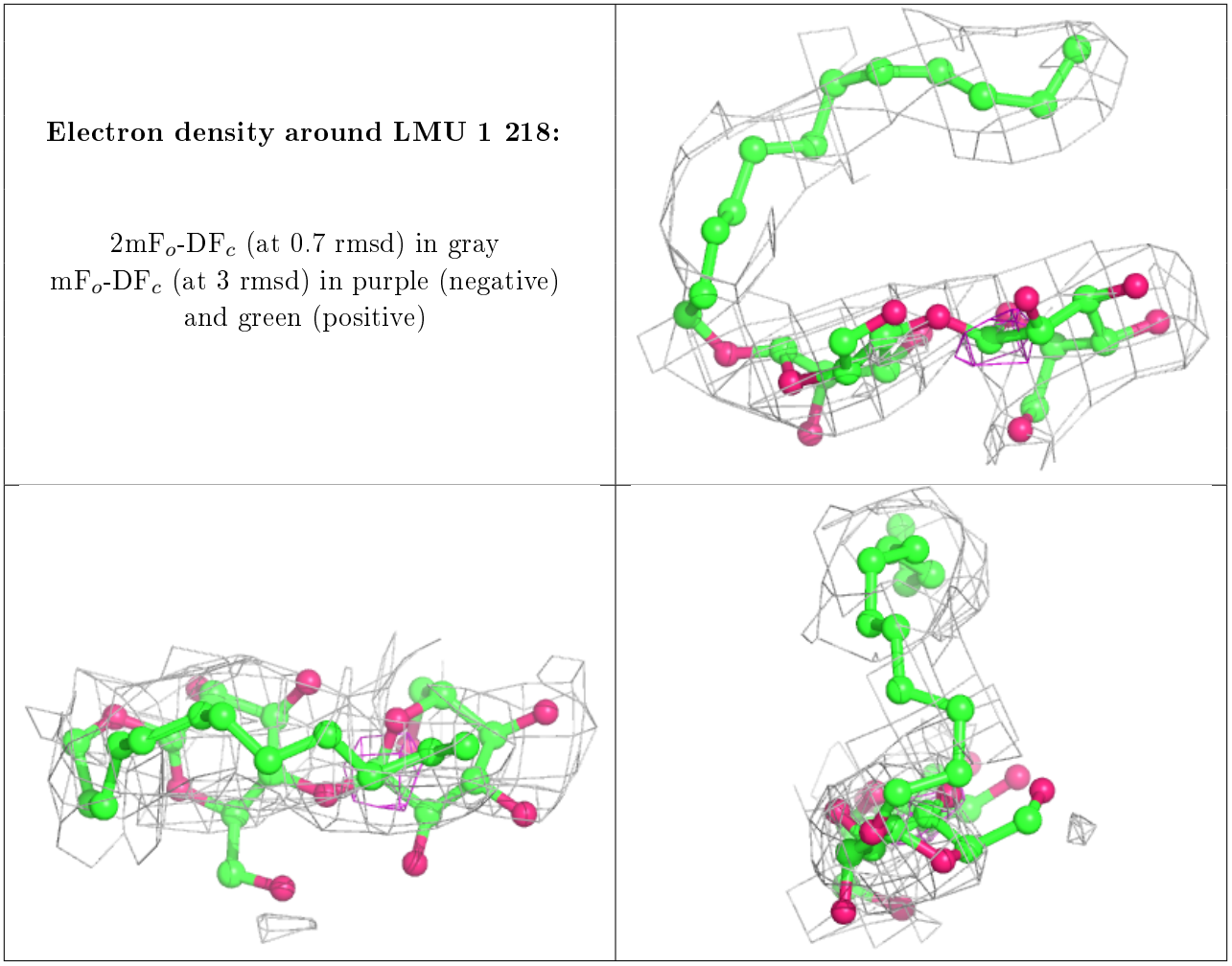






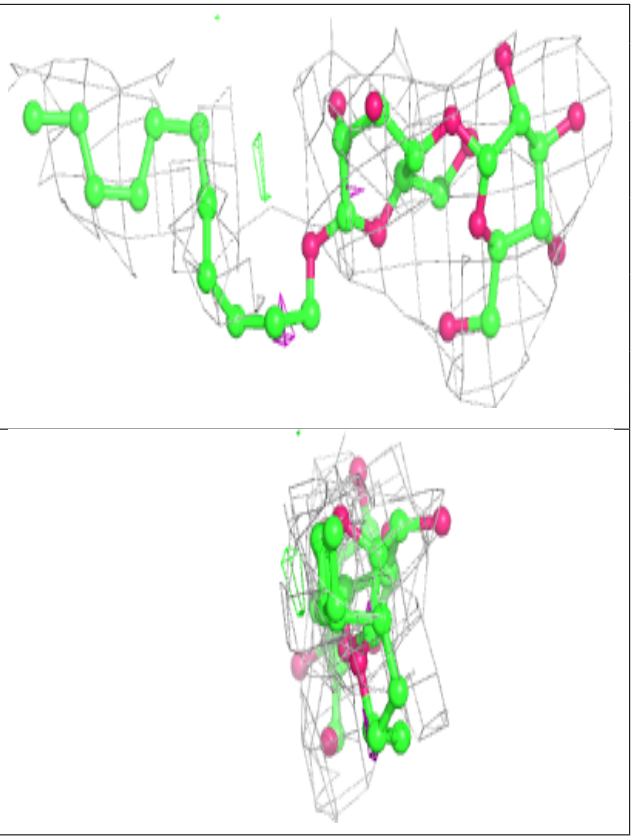
Electron density around LMU 1 218:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



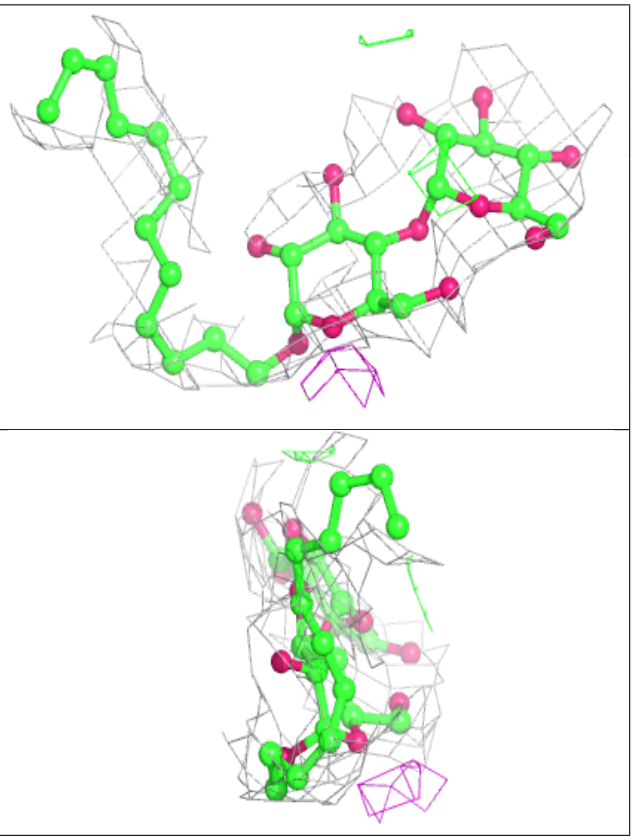
Electron density around LMU R 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



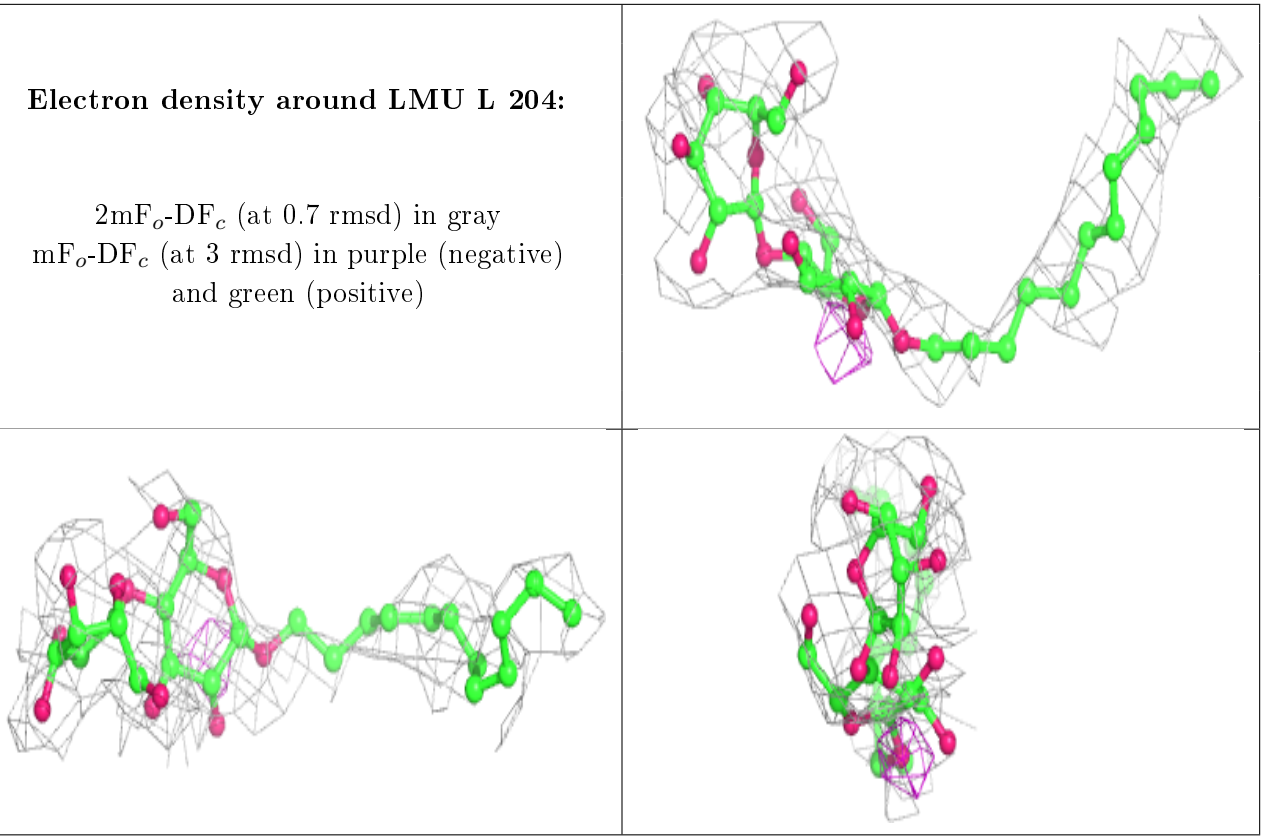
Electron density around LMU R 106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



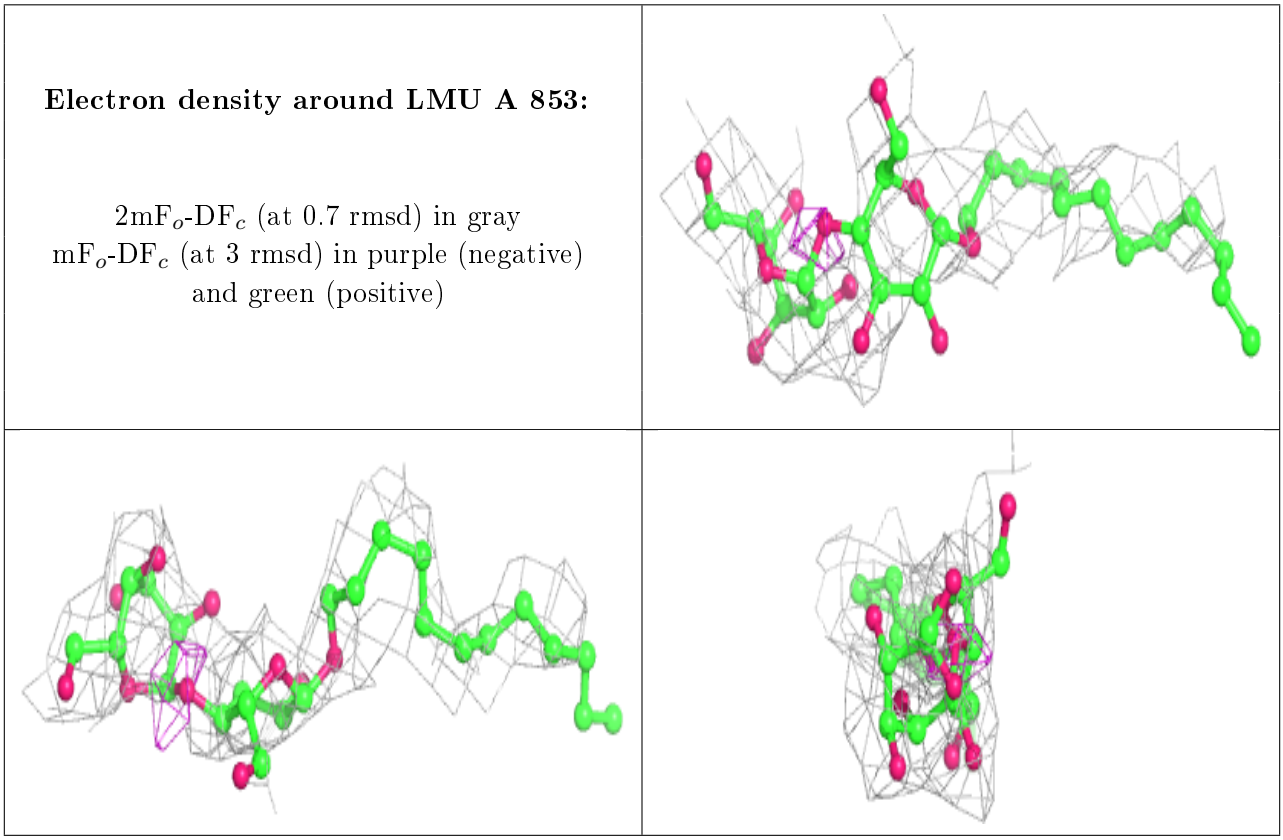
Electron density around LMU L 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



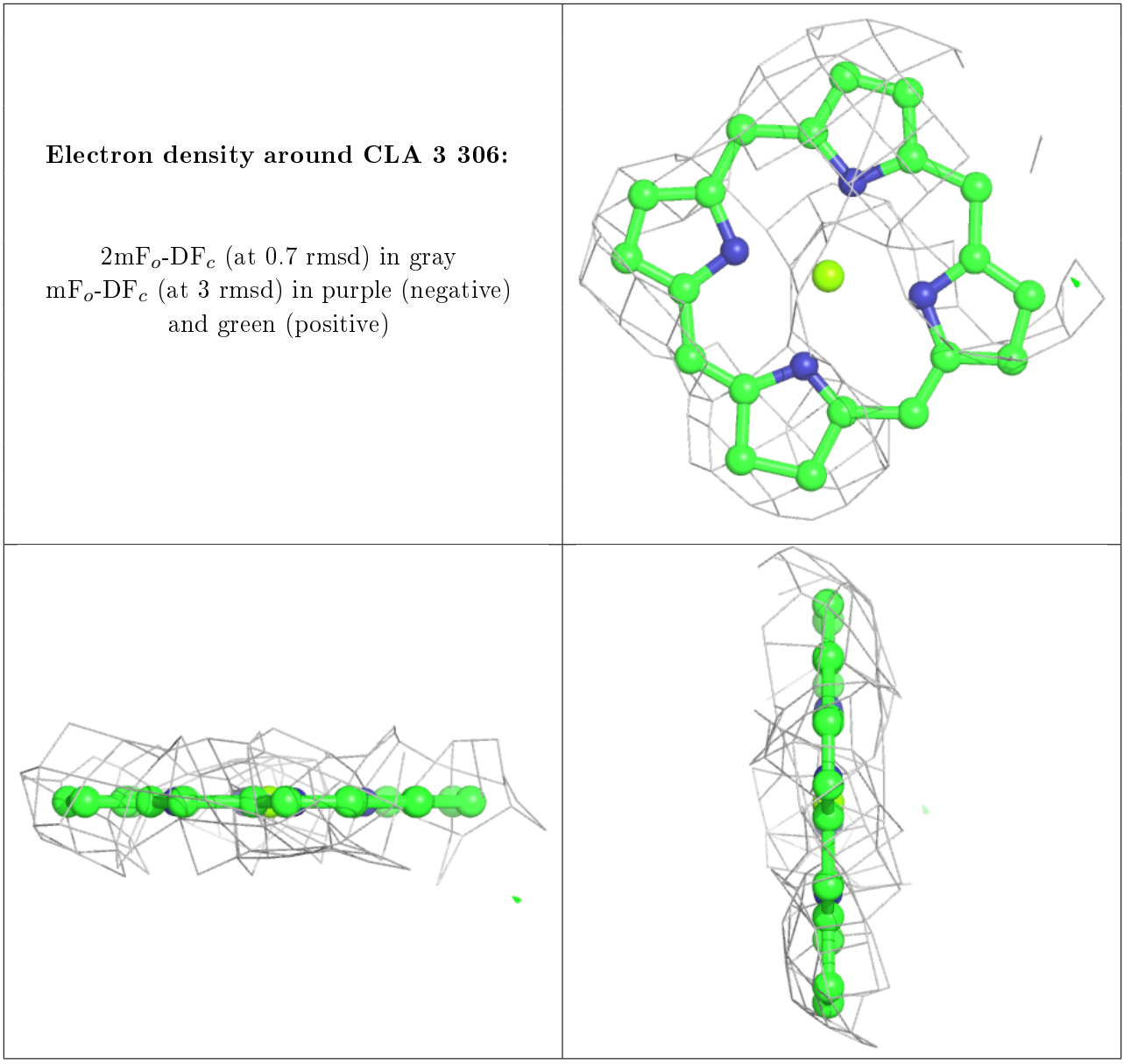
Electron density around LMU A 853:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



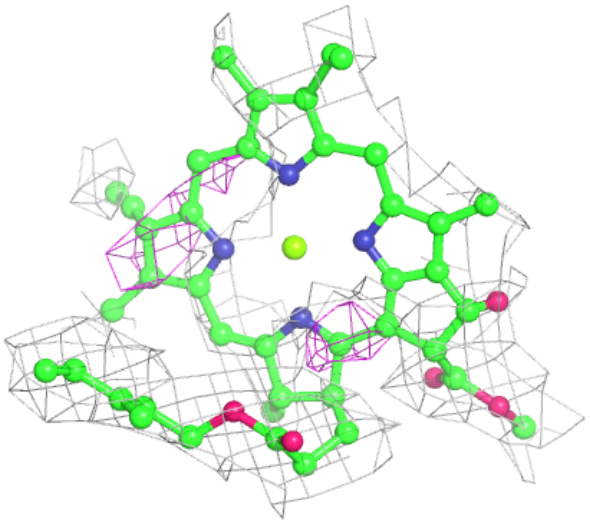
Electron density around CLA 3 306:

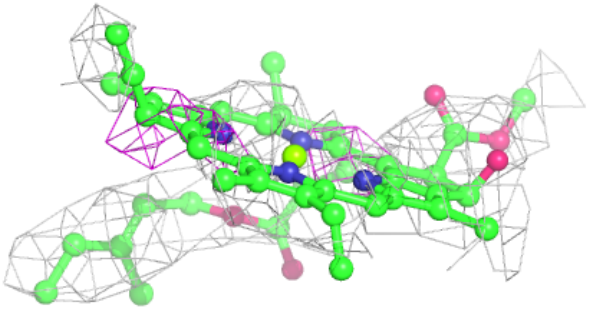
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

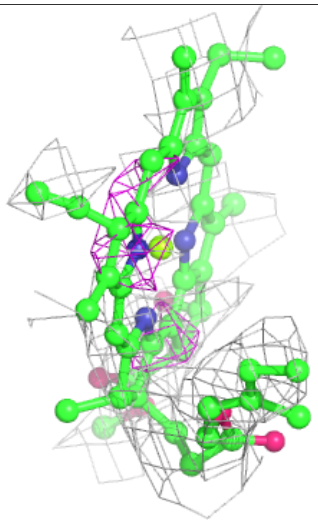


Electron density around CLA B 834:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

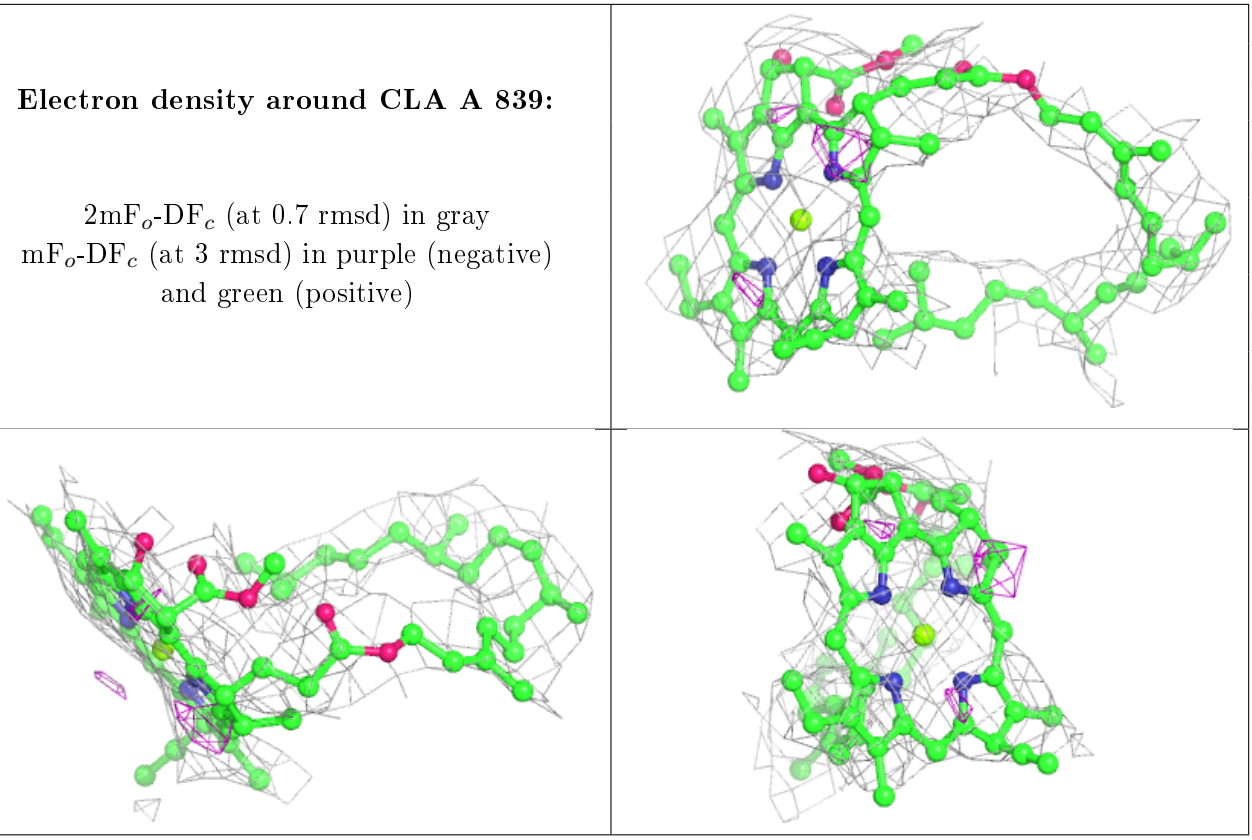






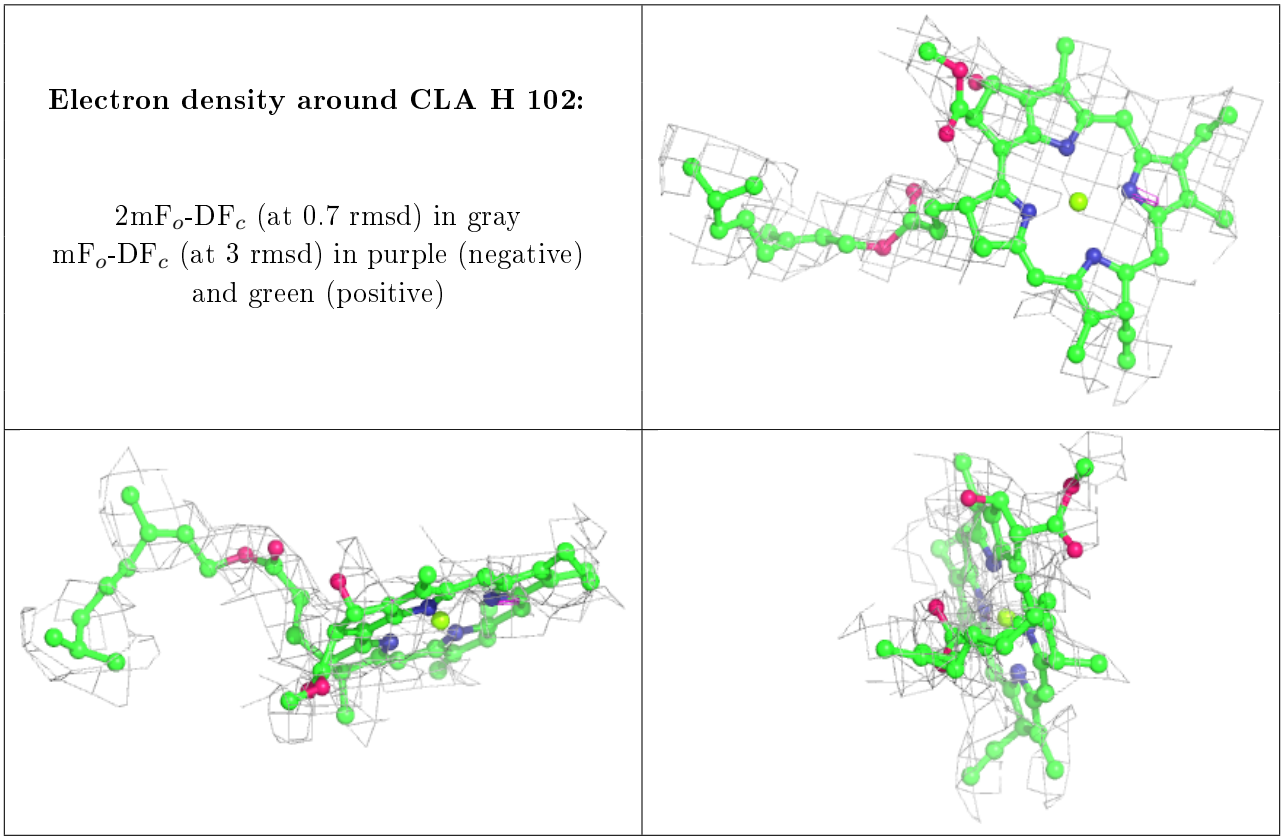
Electron density around CLA A 839:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



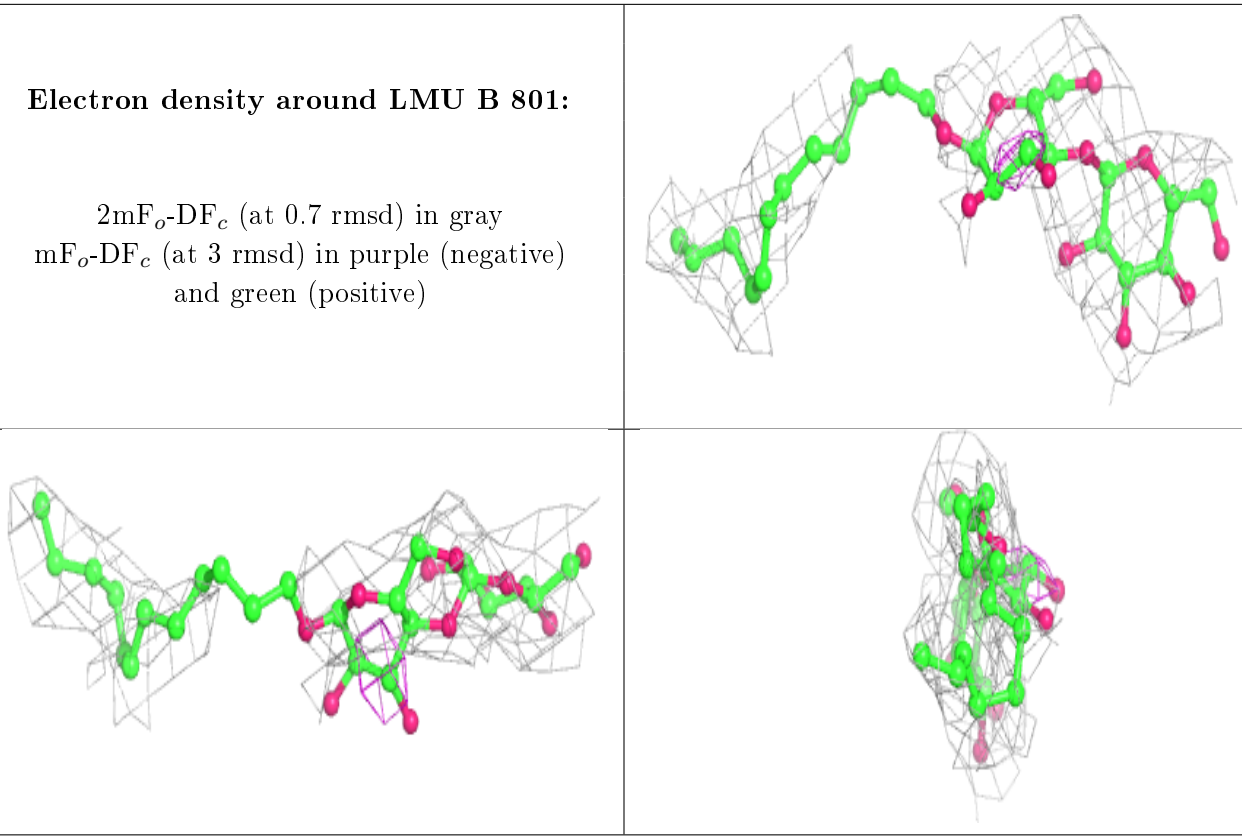
Electron density around CLA H 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



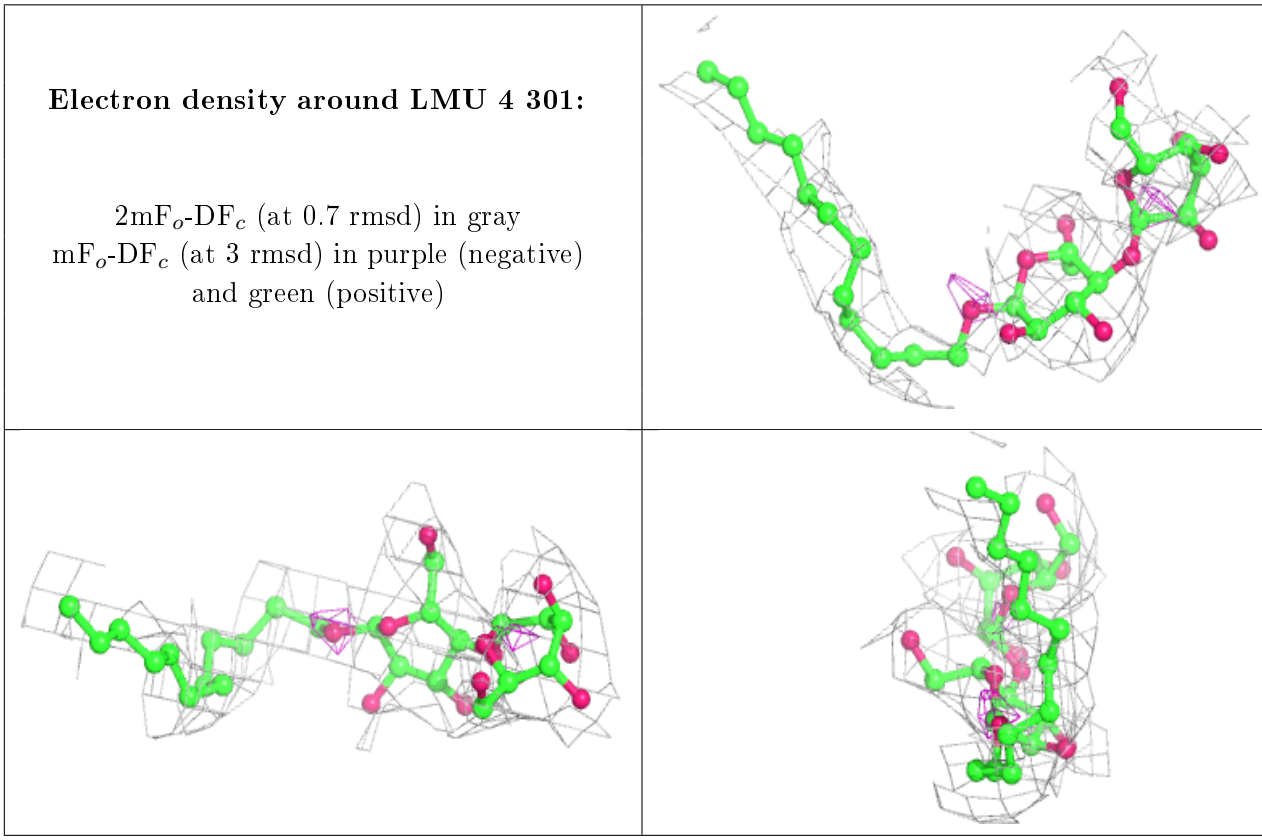
Electron density around LMU B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



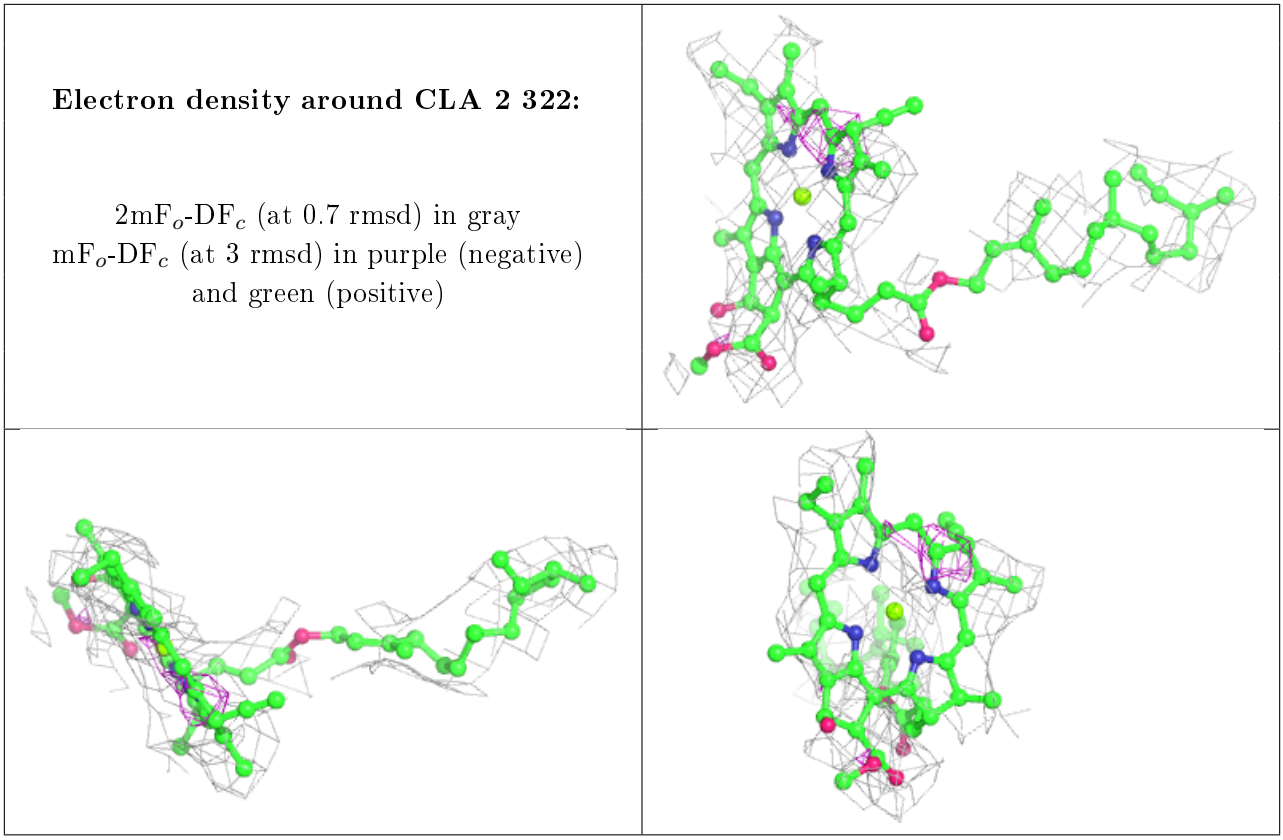
Electron density around LMU 4 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



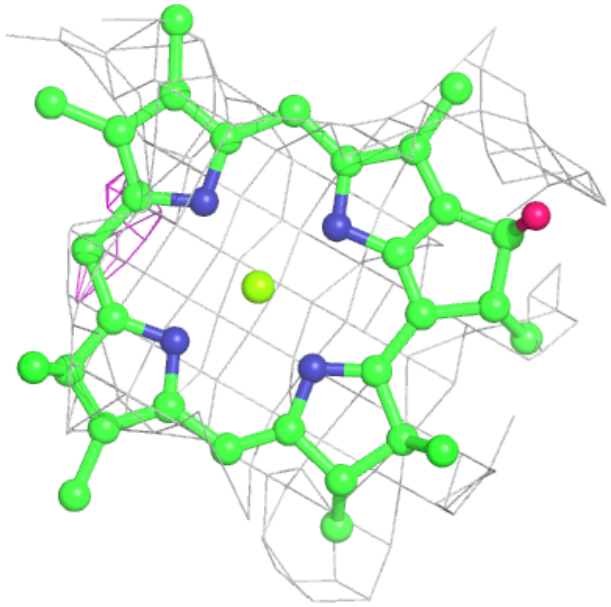
Electron density around CLA 2 322:

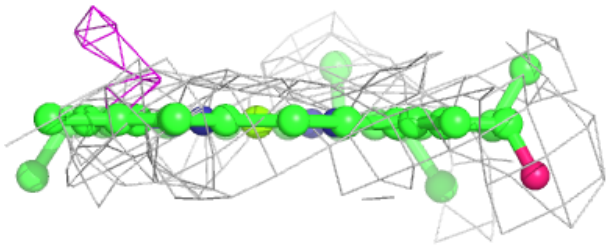
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

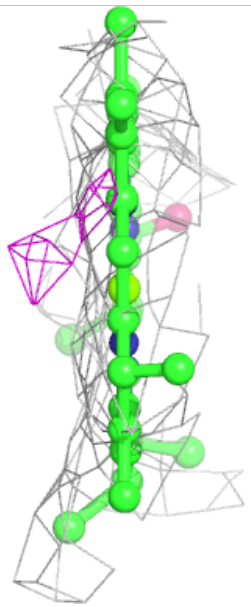


Electron density around CLA 3 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

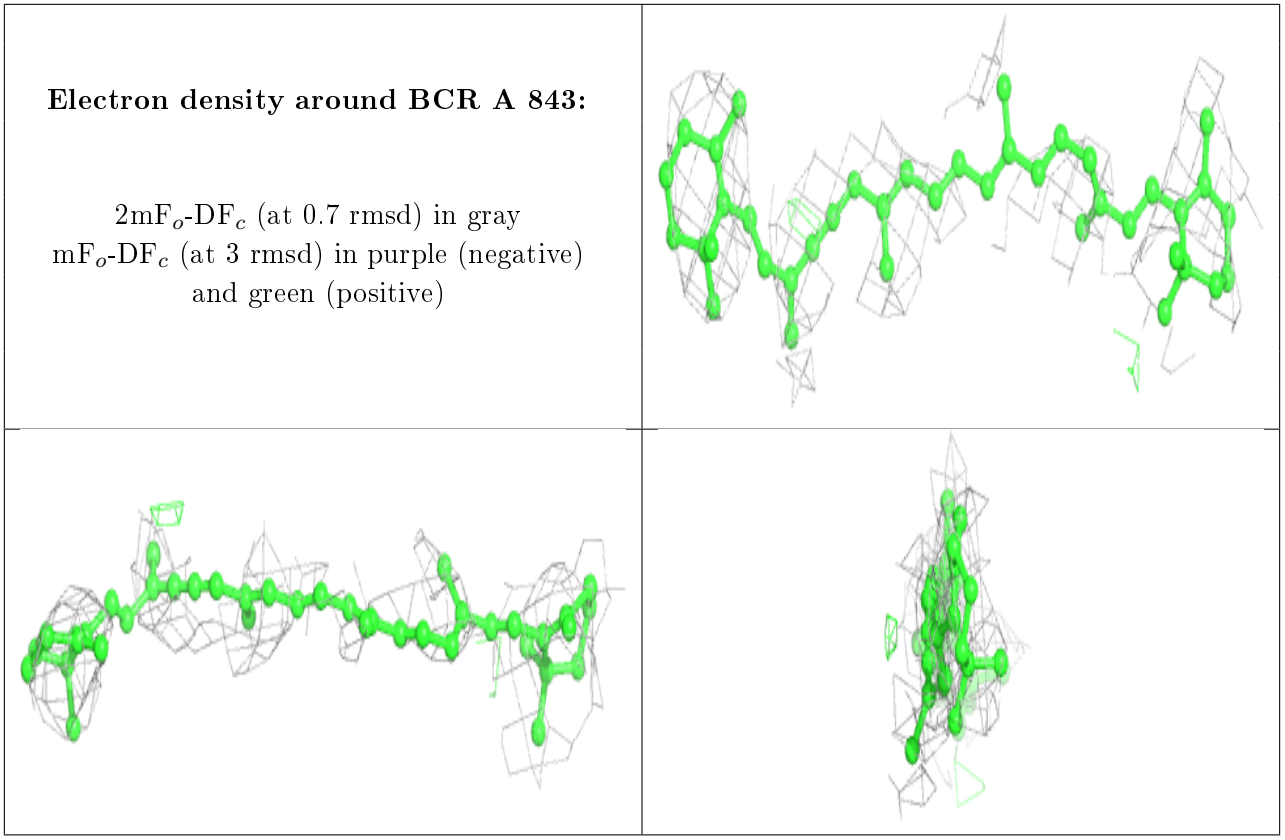






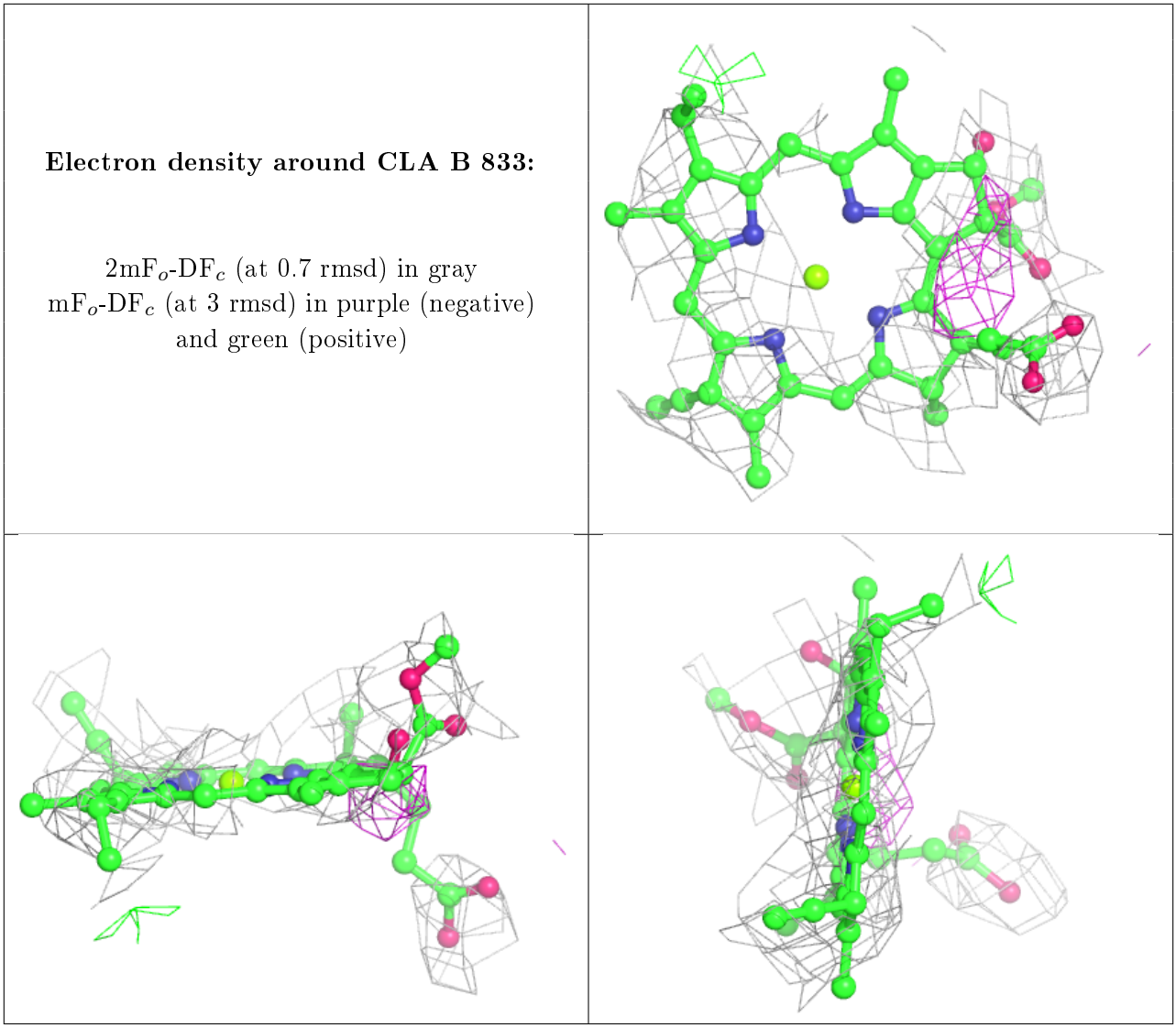
Electron density around BCR A 843:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



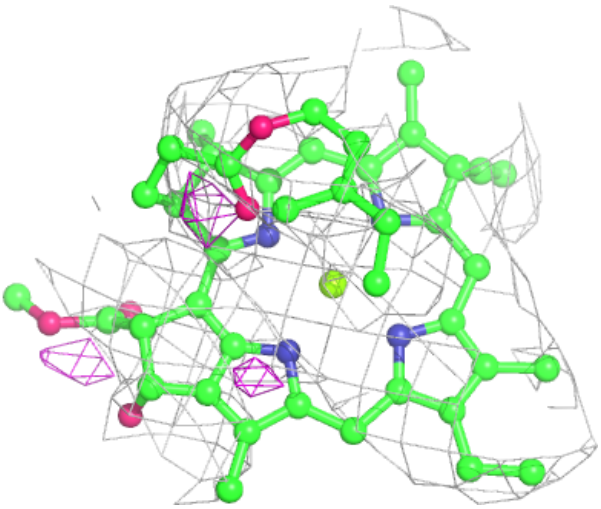
Electron density around CLA B 833:

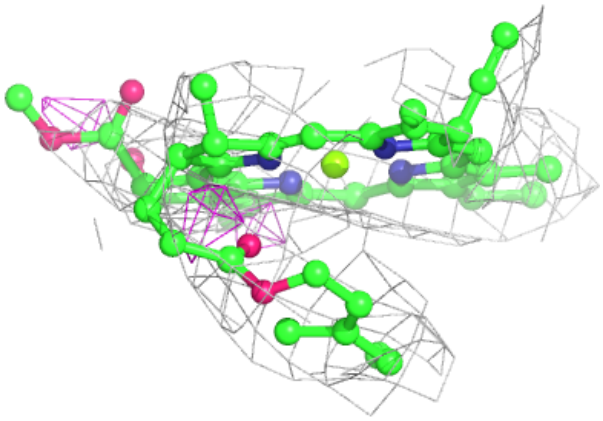
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

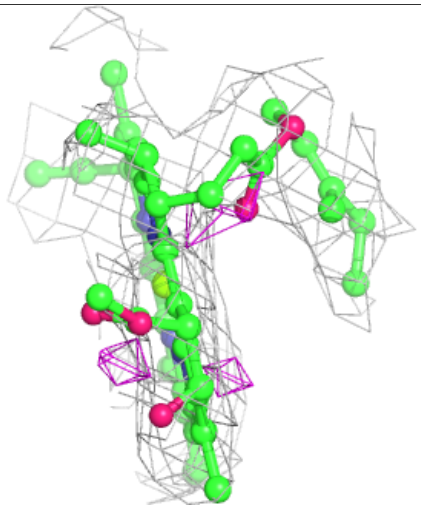


Electron density around CLA 2 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

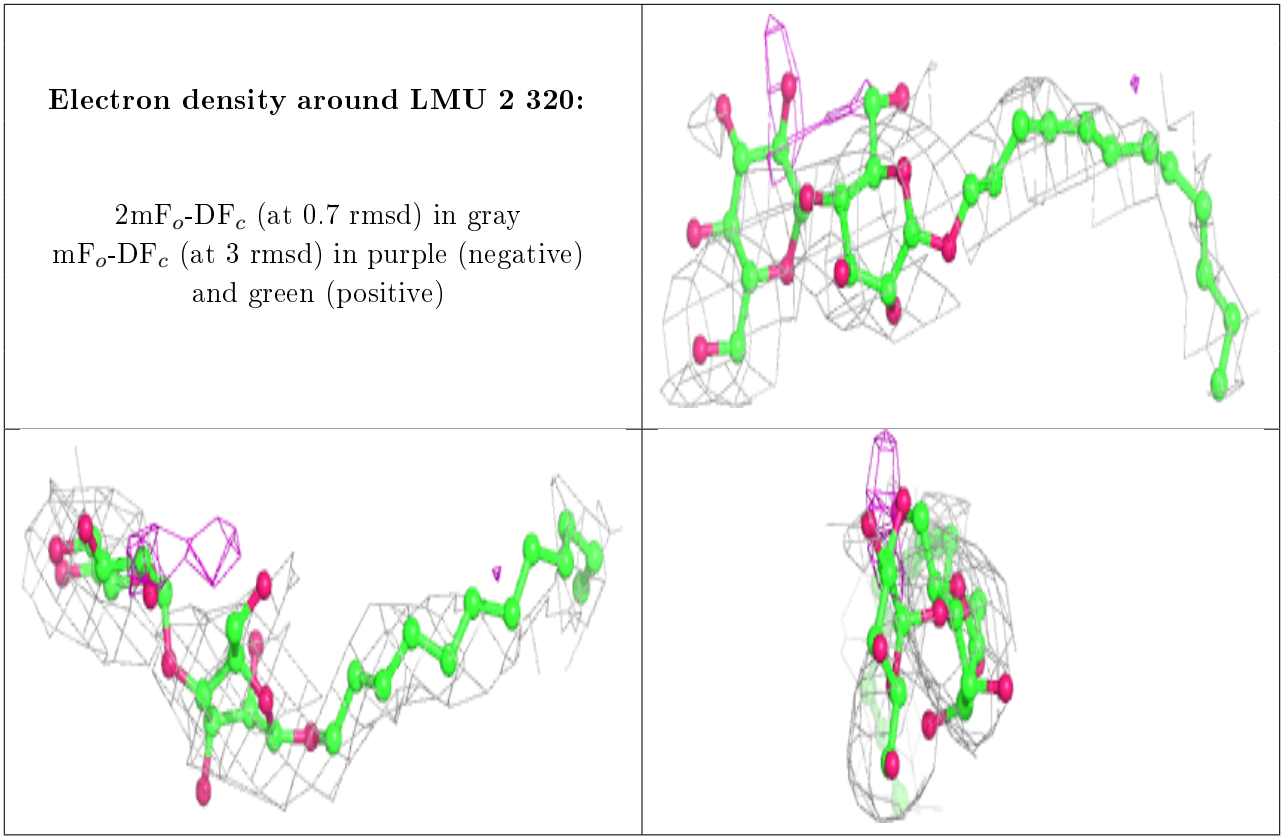






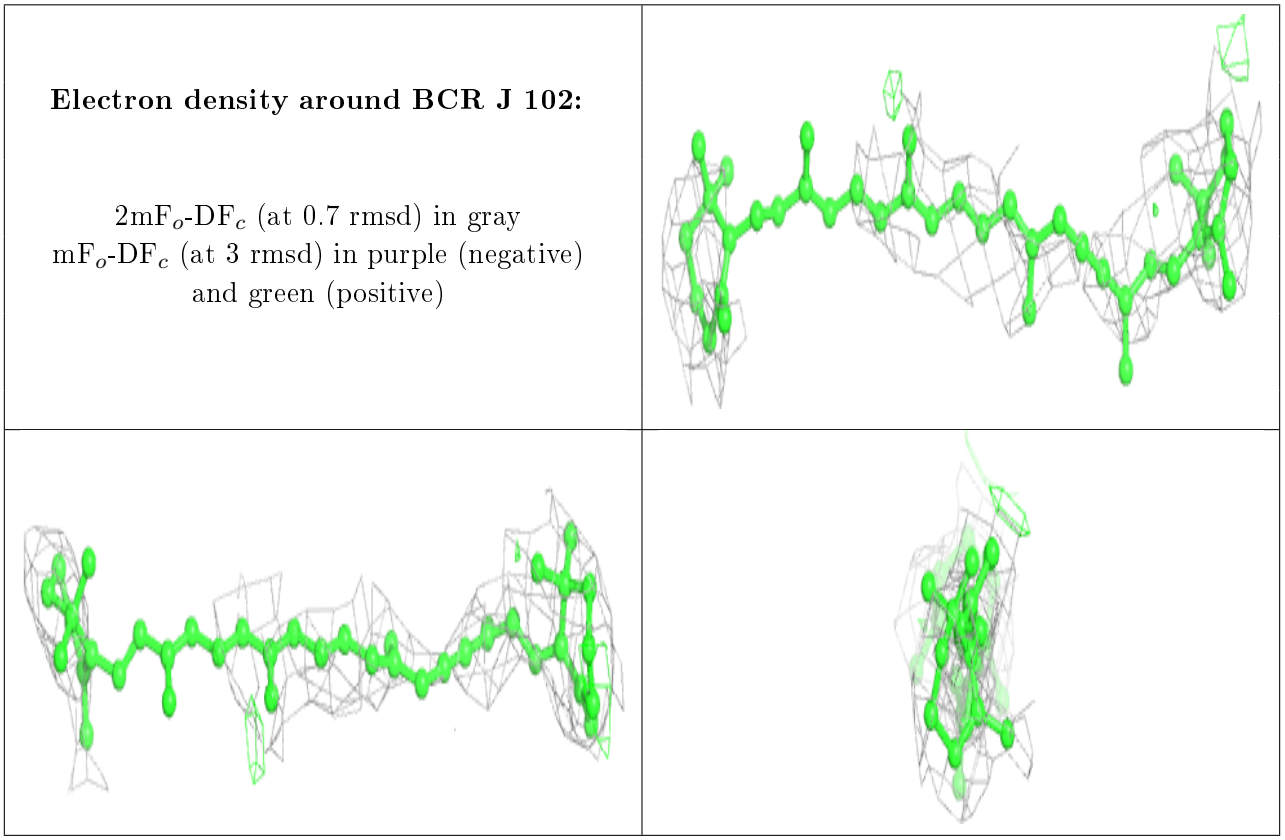
Electron density around LMU 2 320:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



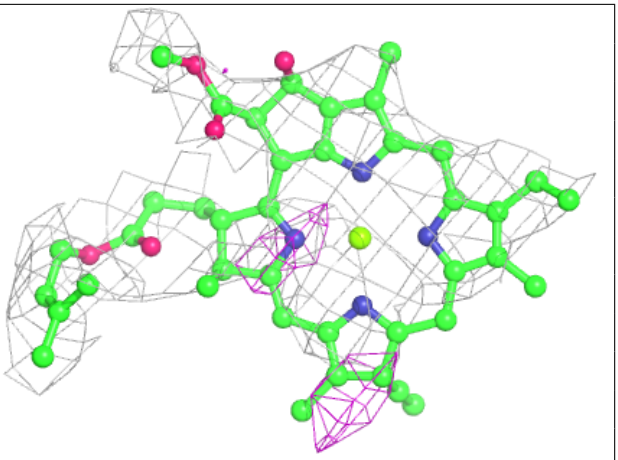
Electron density around BCR J 102:

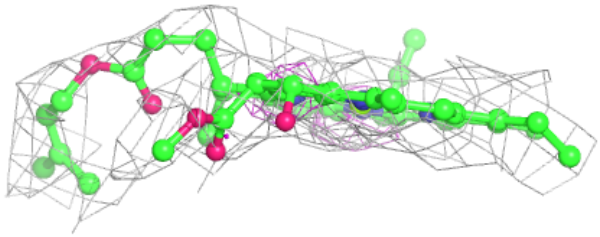
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

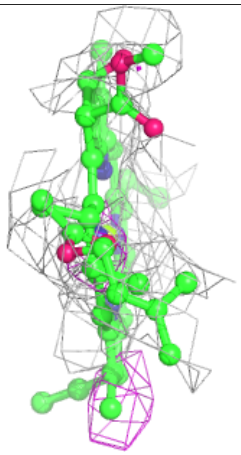


Electron density around CLA K 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

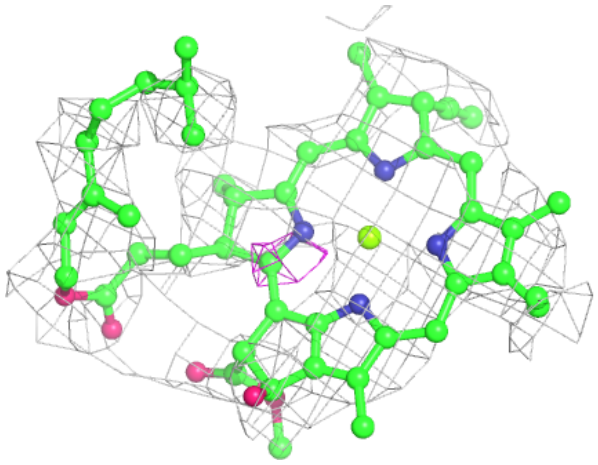


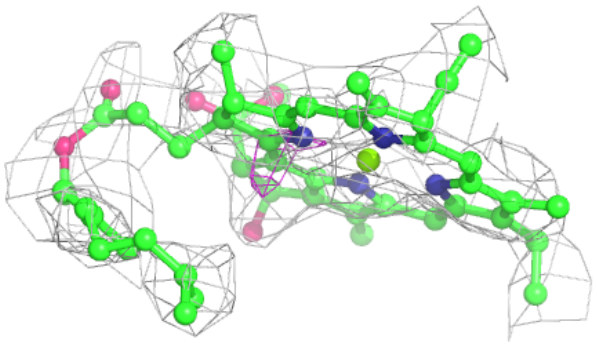


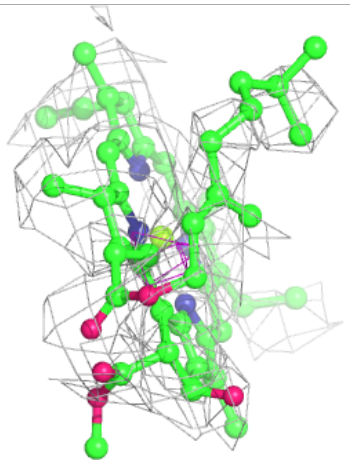


Electron density around CLA H 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

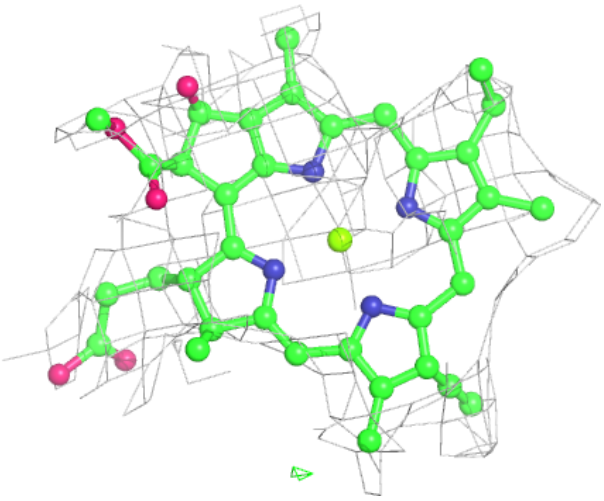


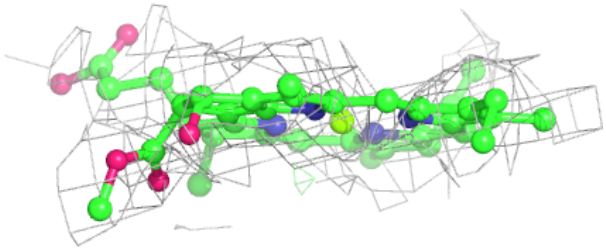


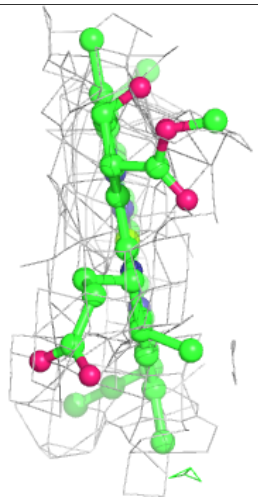


Electron density around CLA K 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

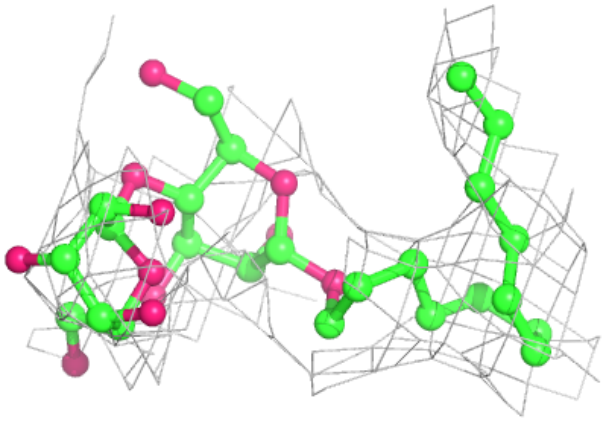


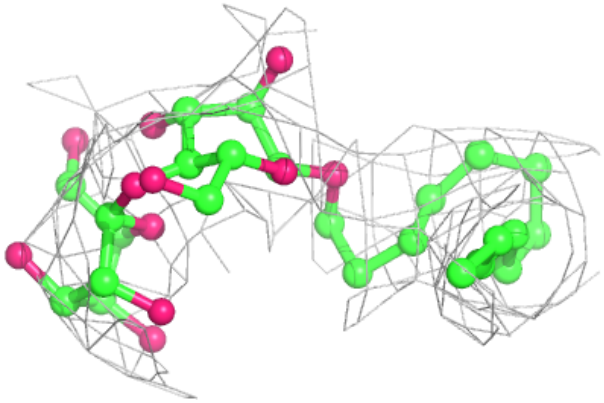


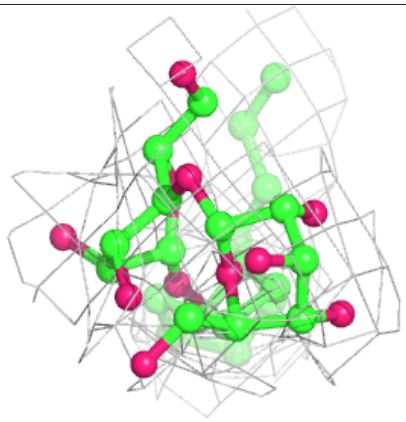


Electron density around LMU H 108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

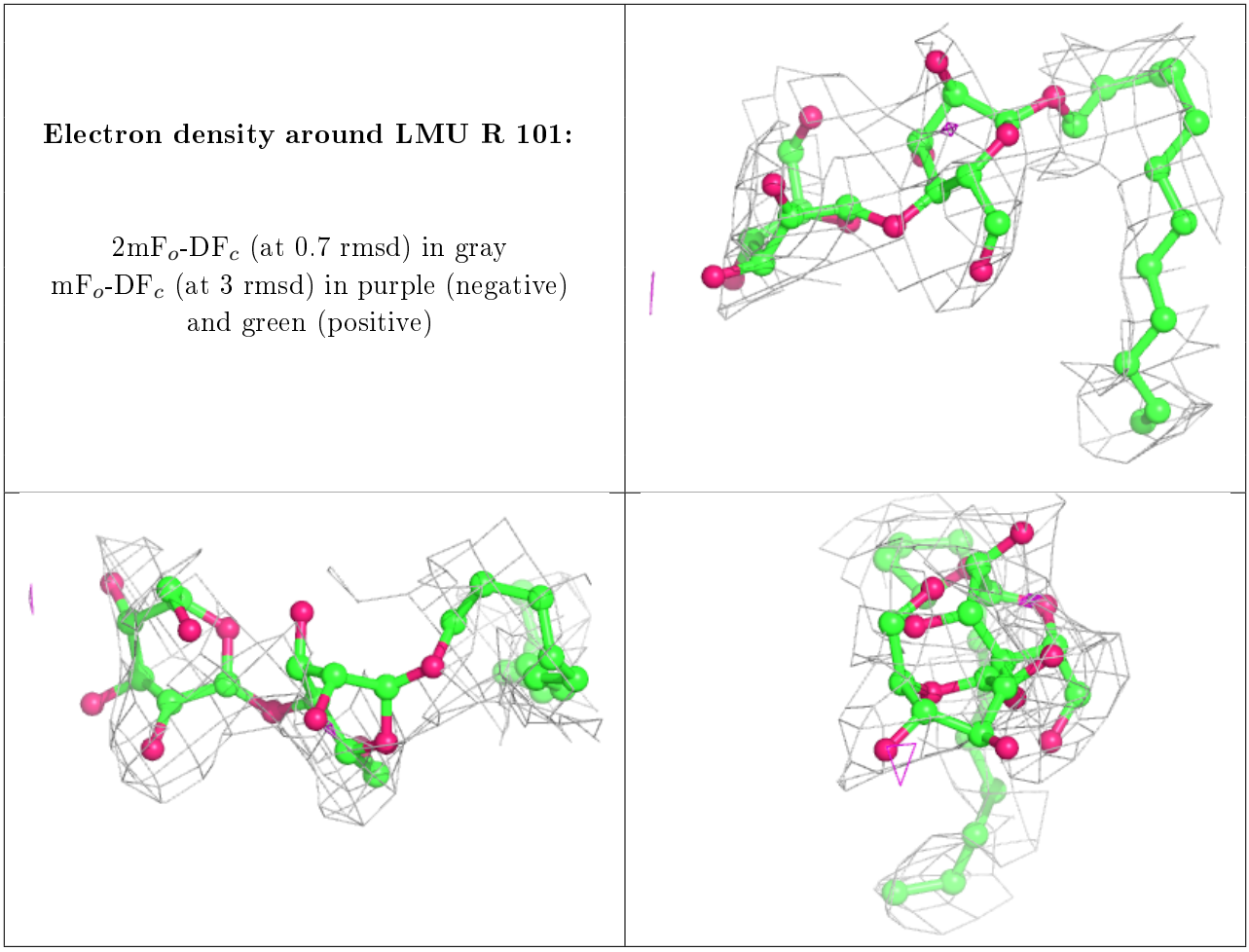






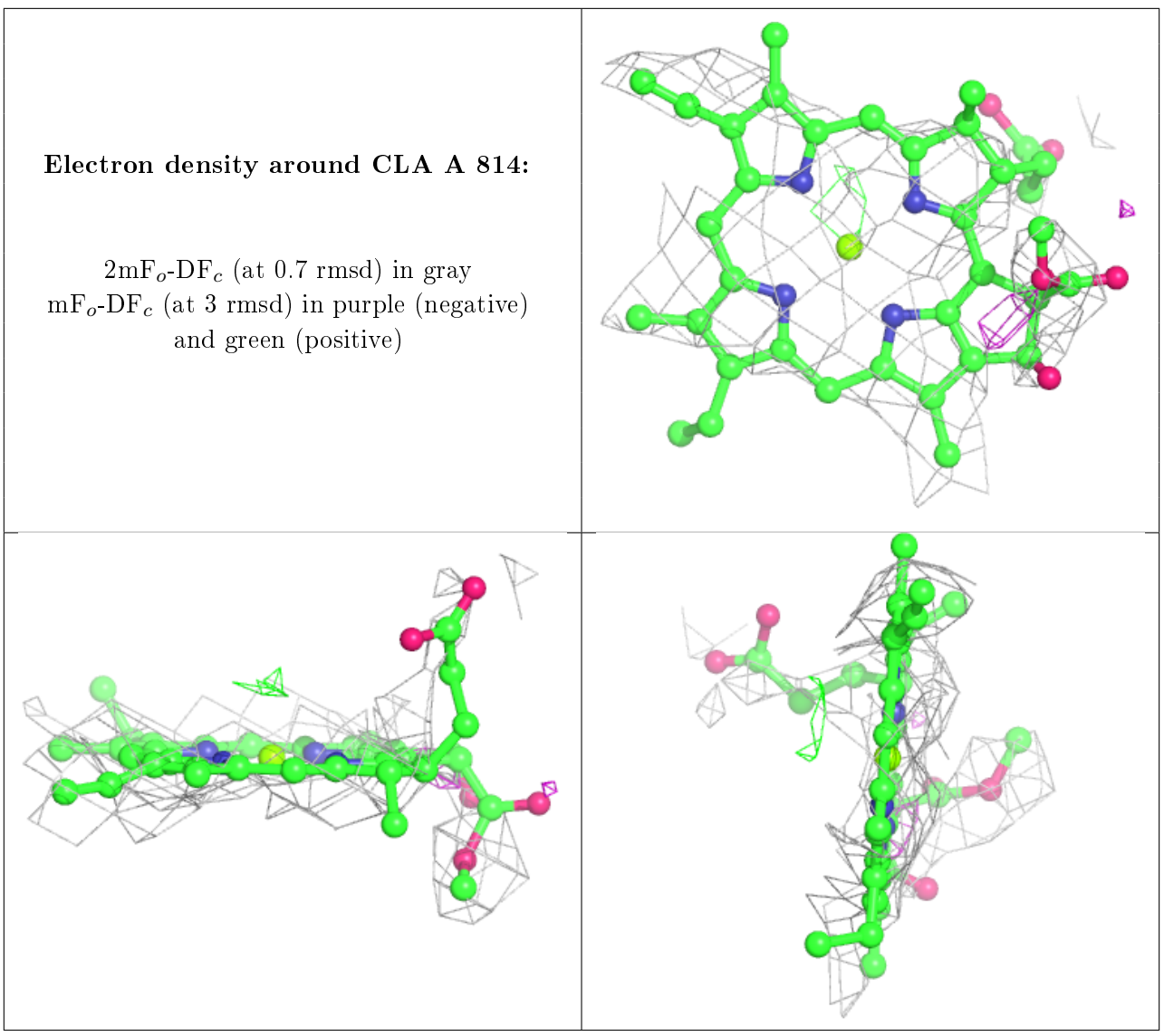
Electron density around LMU R 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



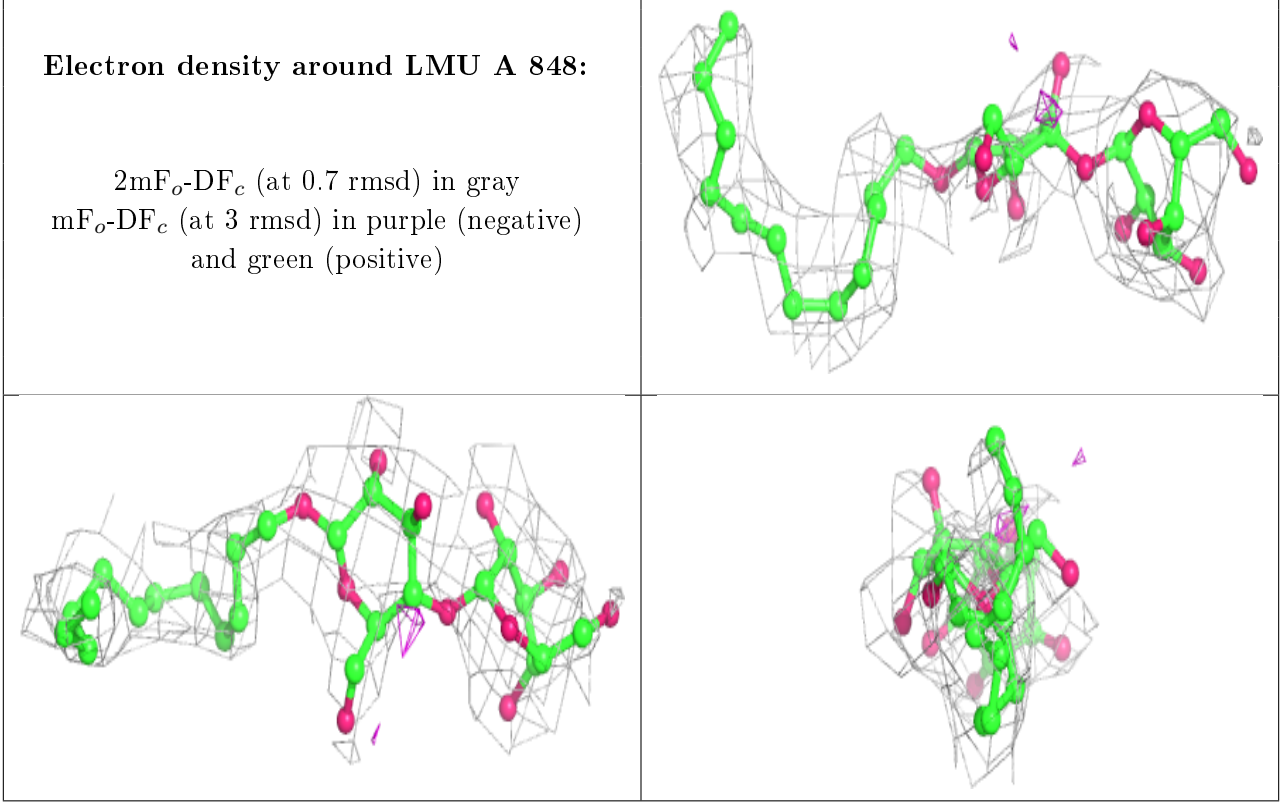
Electron density around CLA A 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



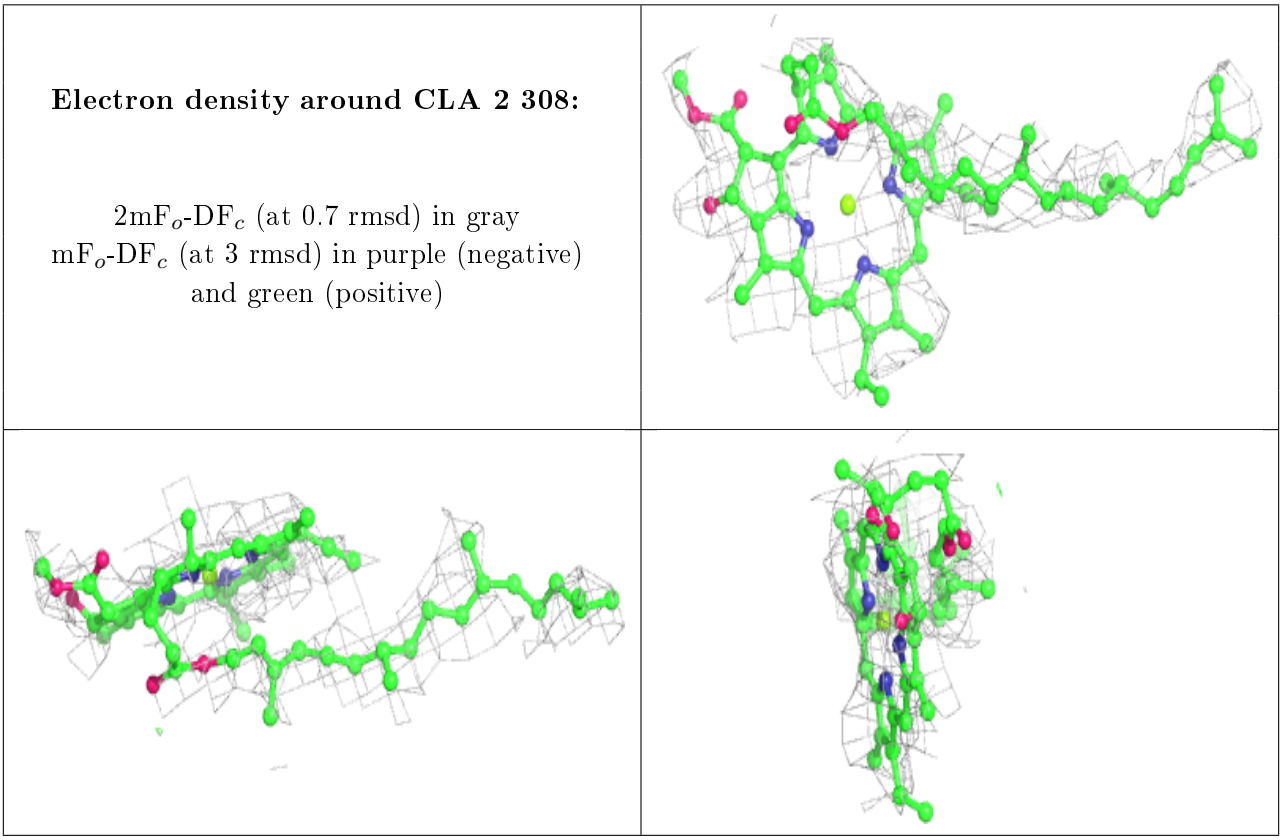
Electron density around LMU A 848:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



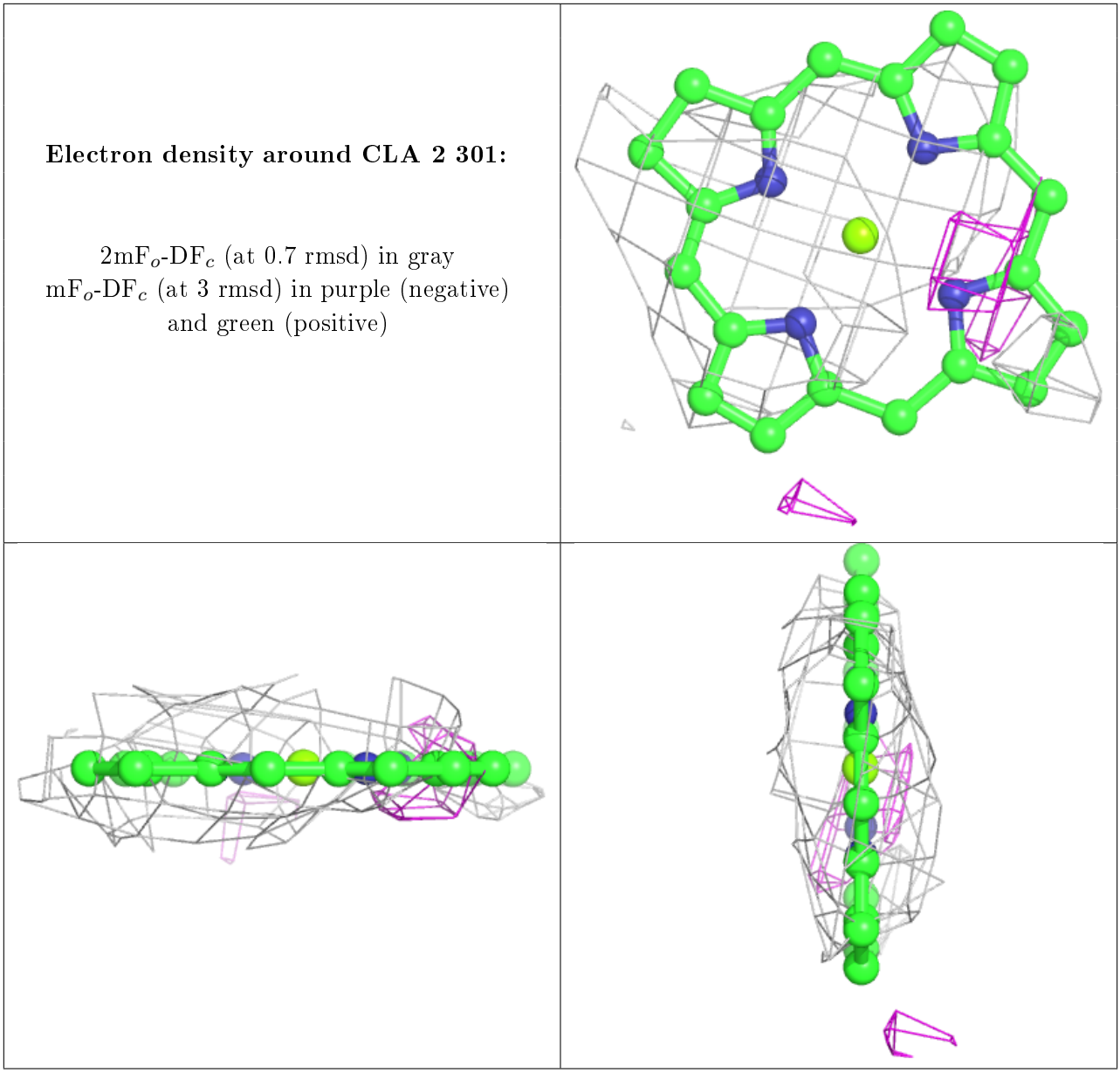
Electron density around CLA 2 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



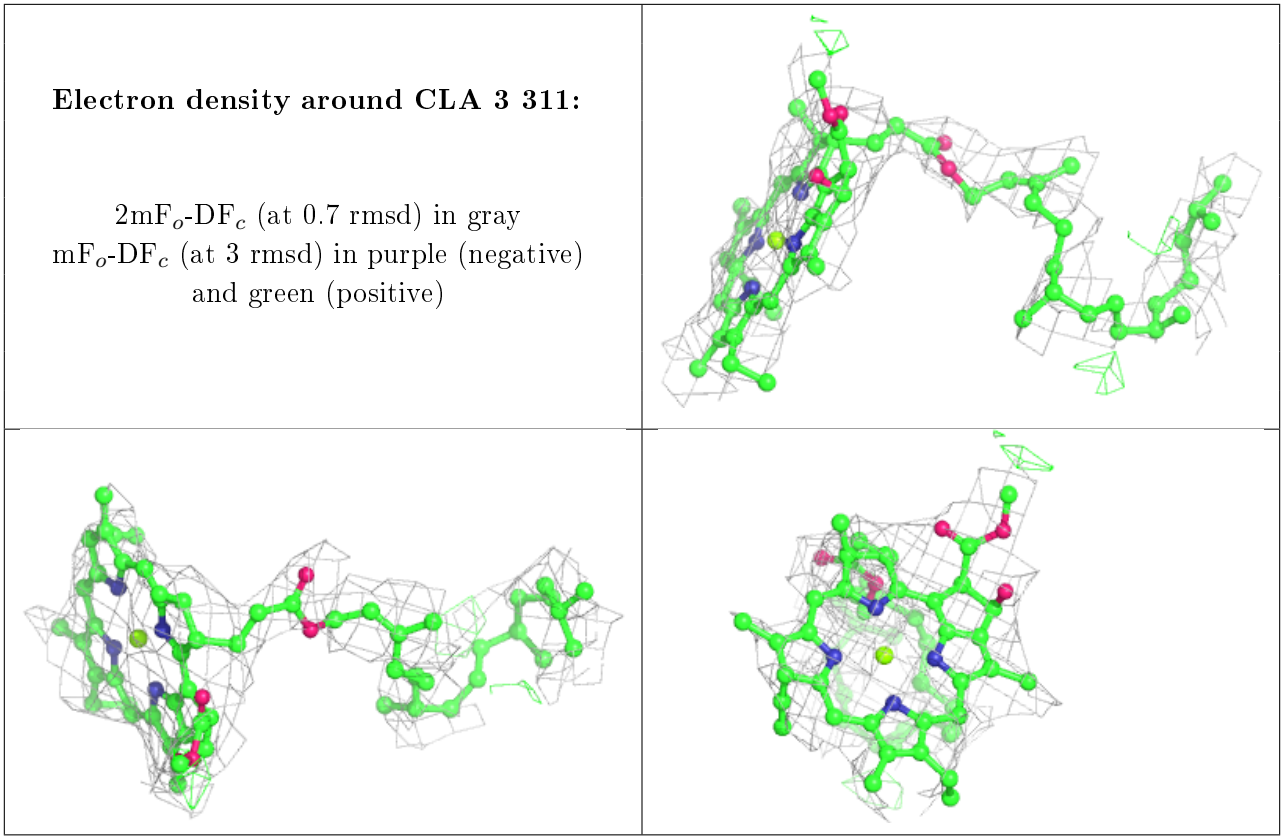
Electron density around CLA 2 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



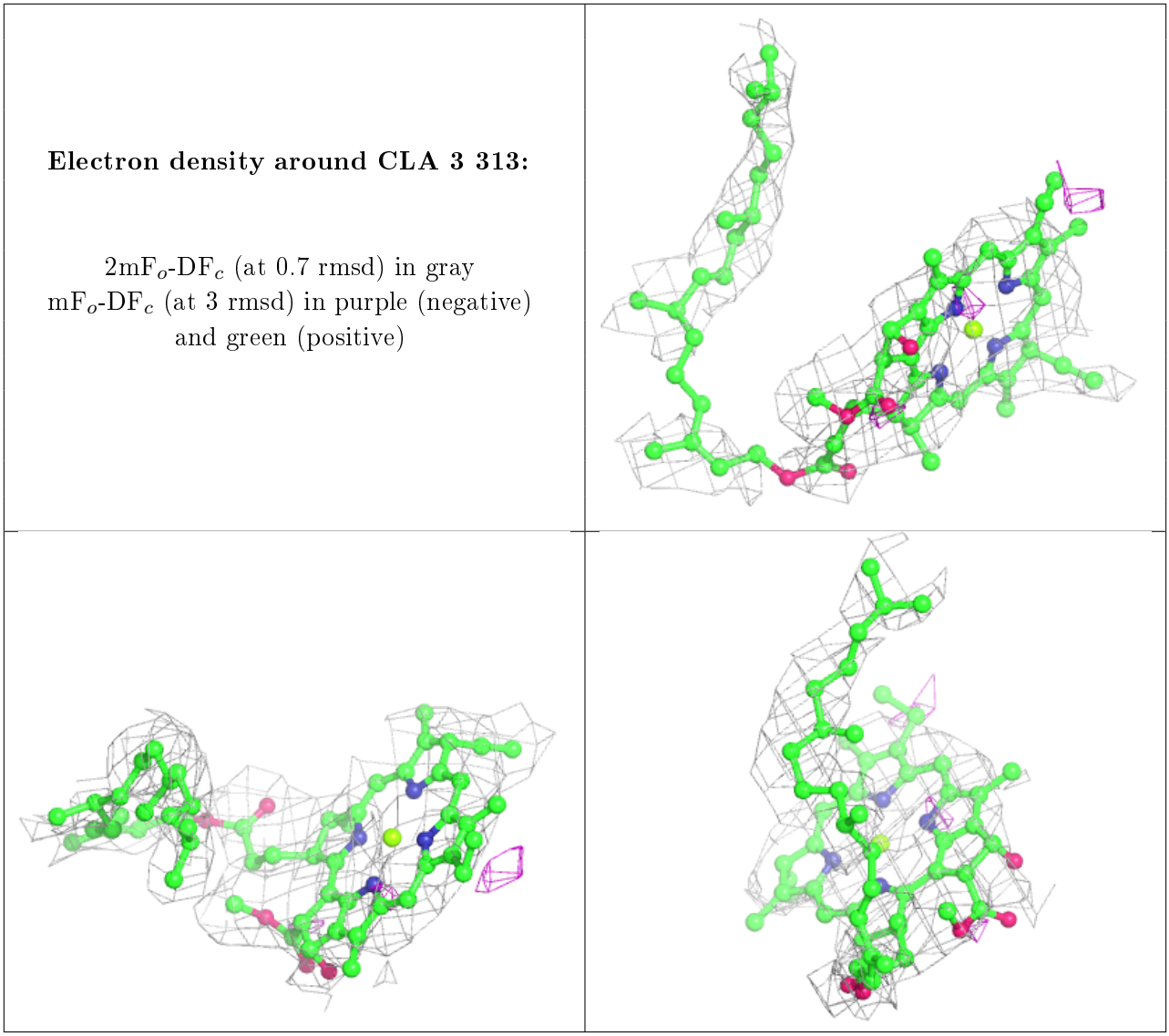
Electron density around CLA 3 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



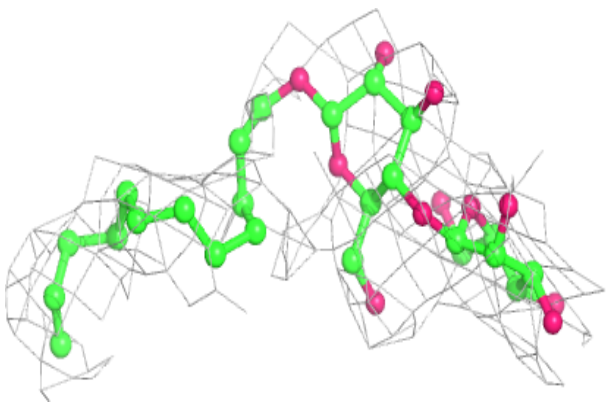
Electron density around CLA 3 313:

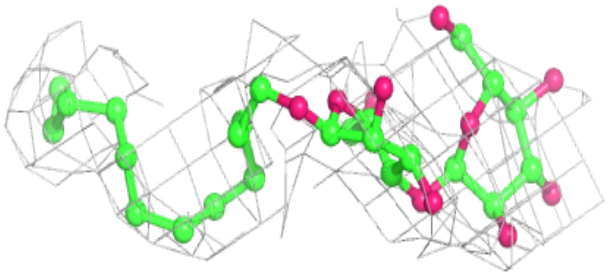
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

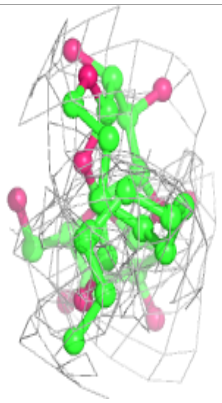


Electron density around LMU 2 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

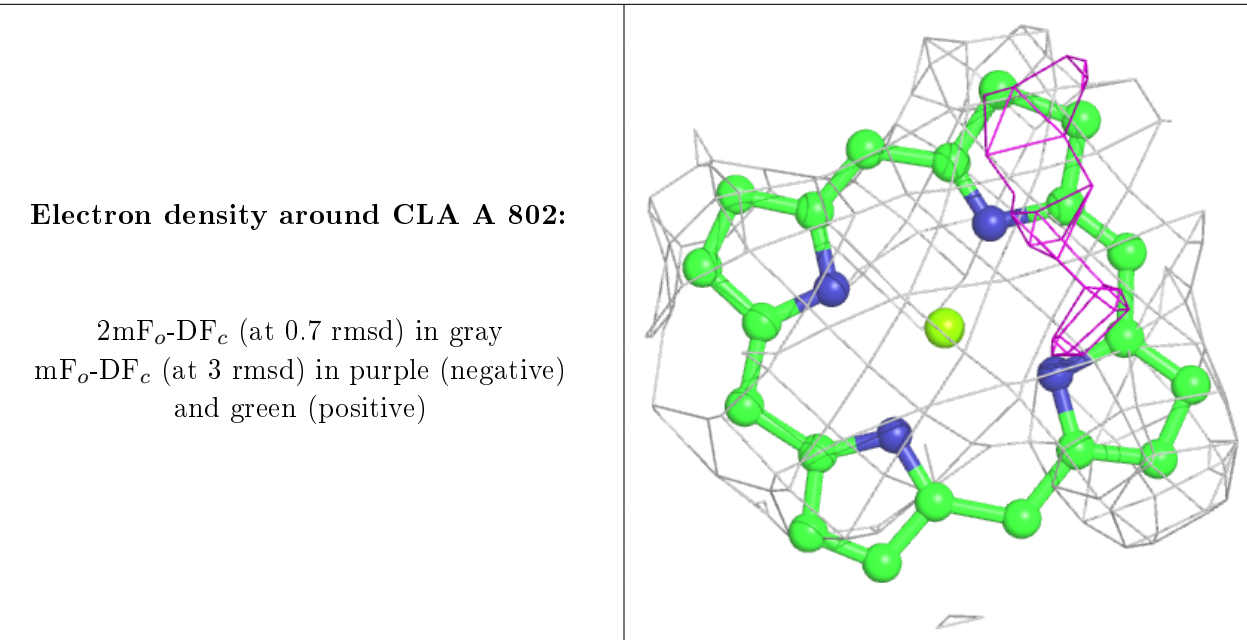


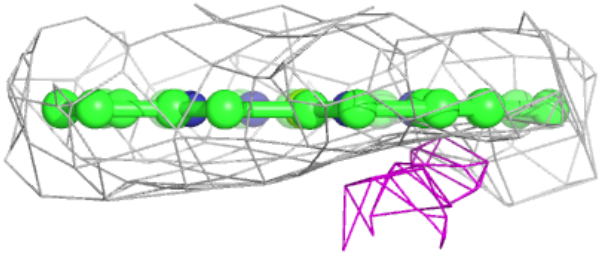


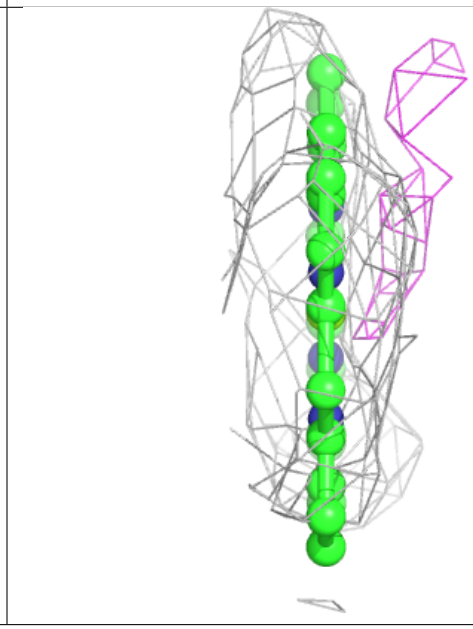


Electron density around CLA A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

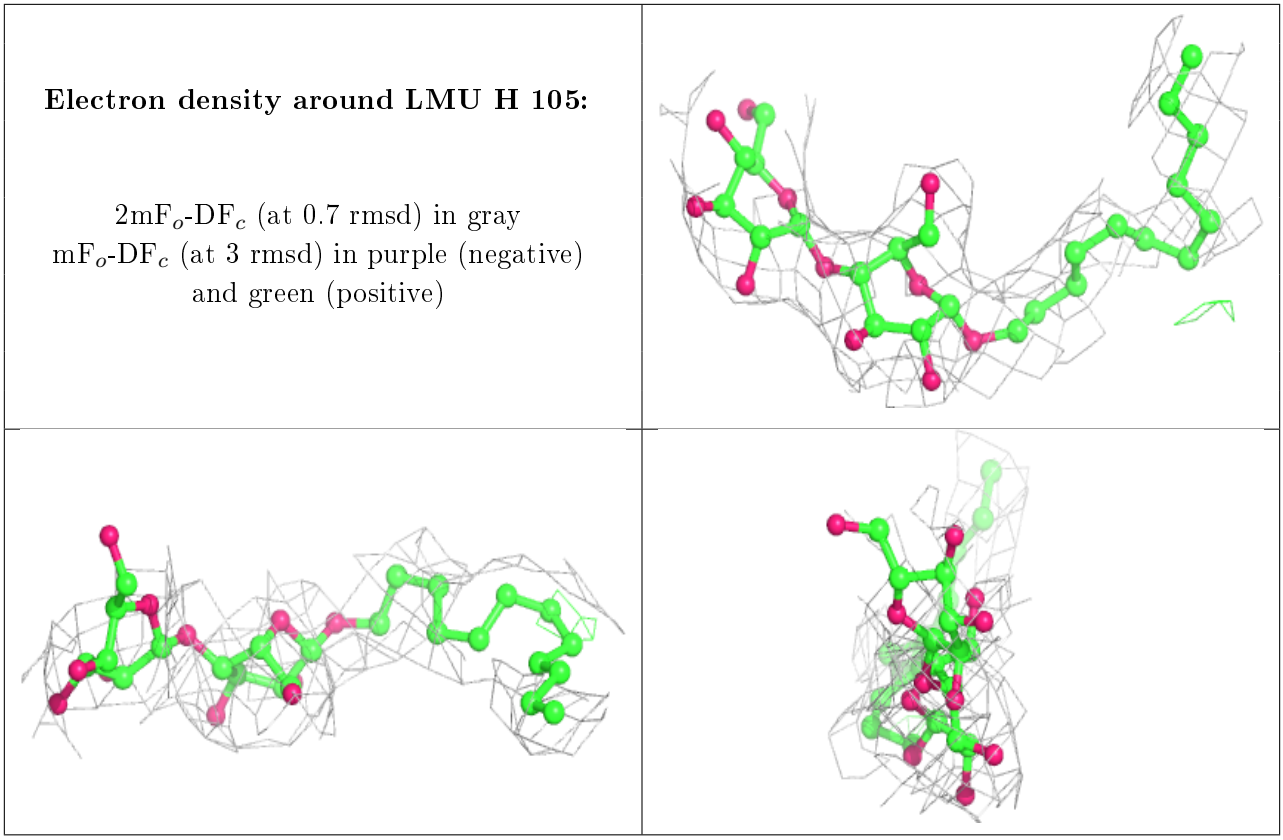






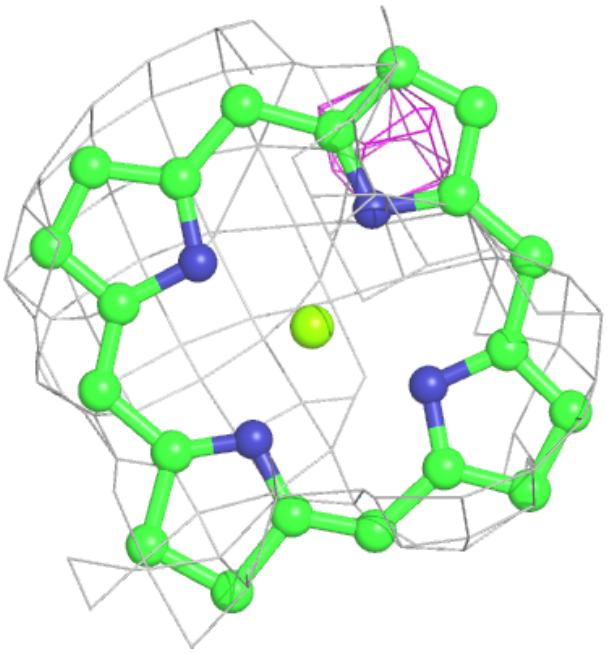
Electron density around LMU H 105:

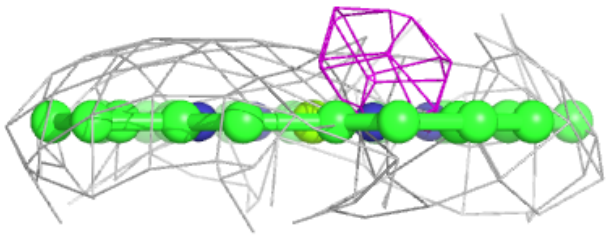
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

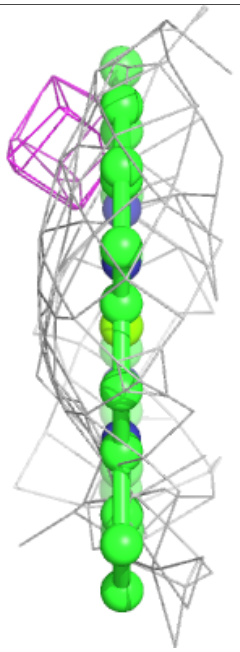


Electron density around CLA 3 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

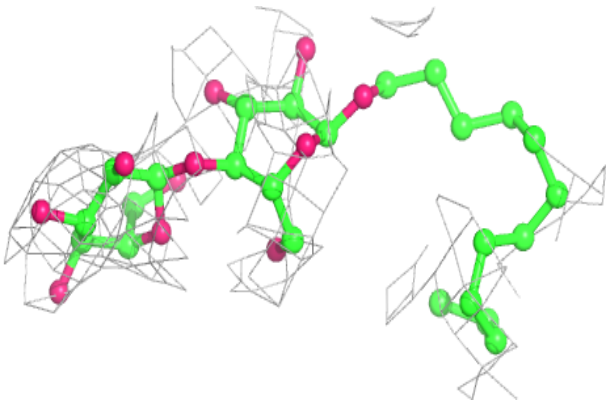


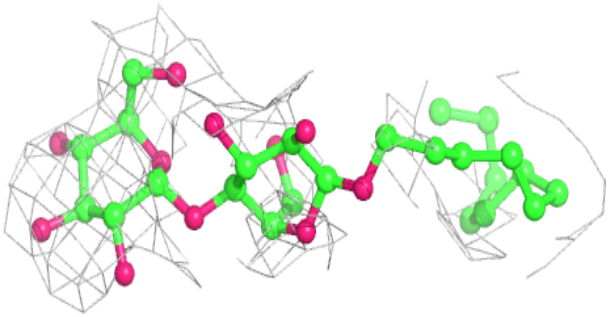


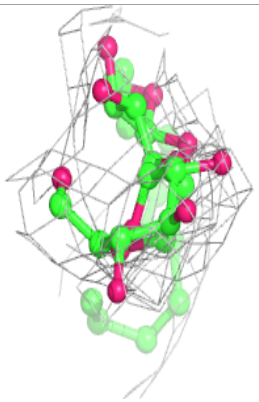


Electron density around LMU D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

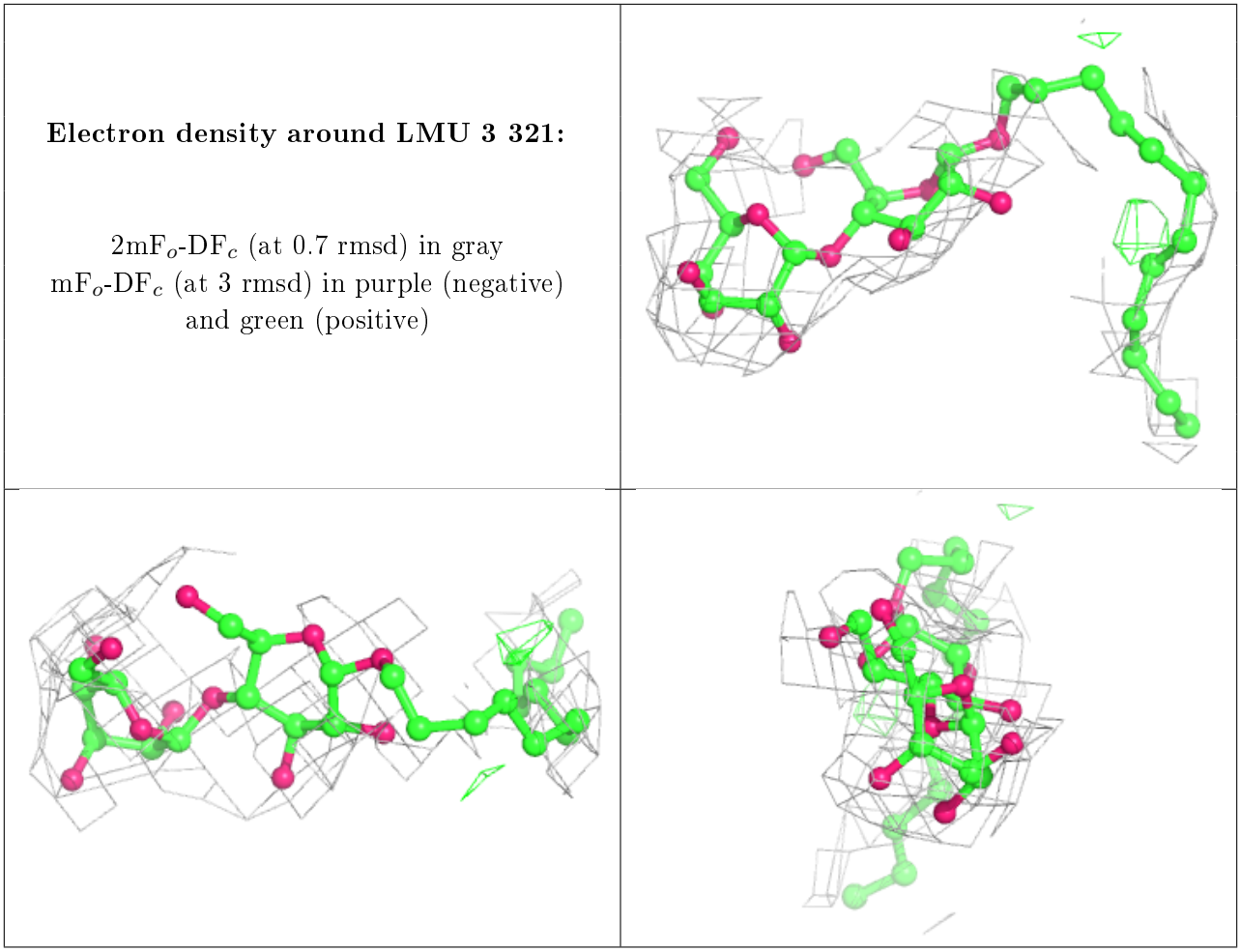






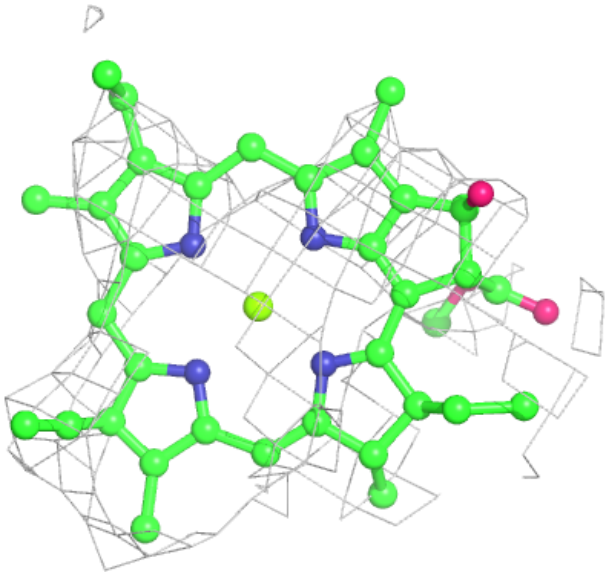
Electron density around LMU 3 321:

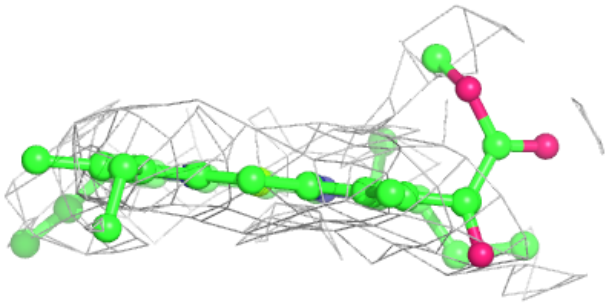
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

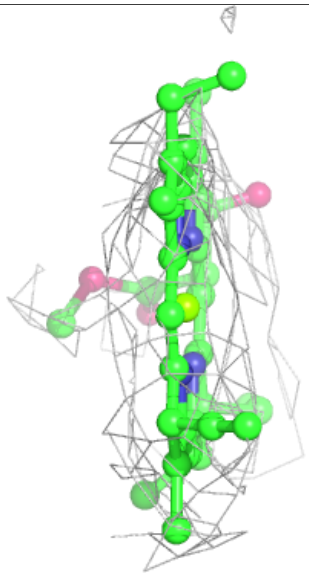


Electron density around CLA 3 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

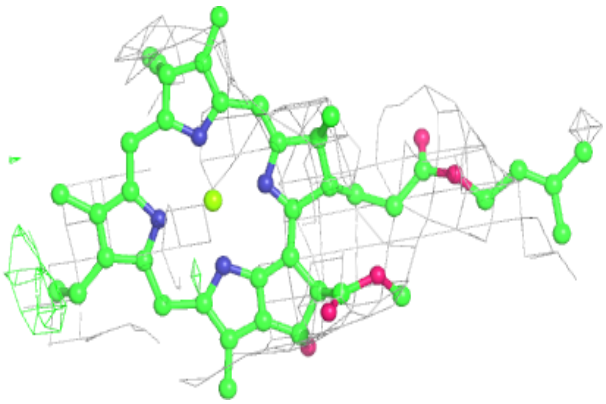


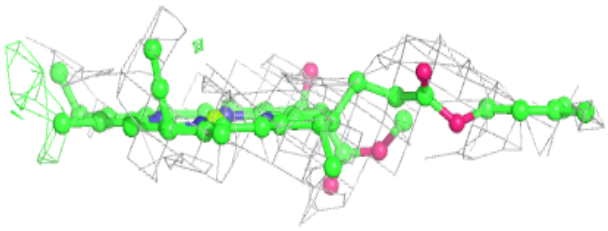


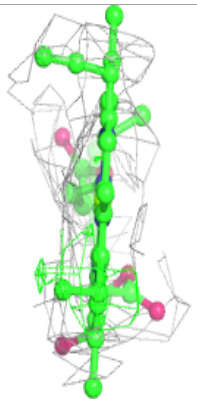


Electron density around CLA A 840:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

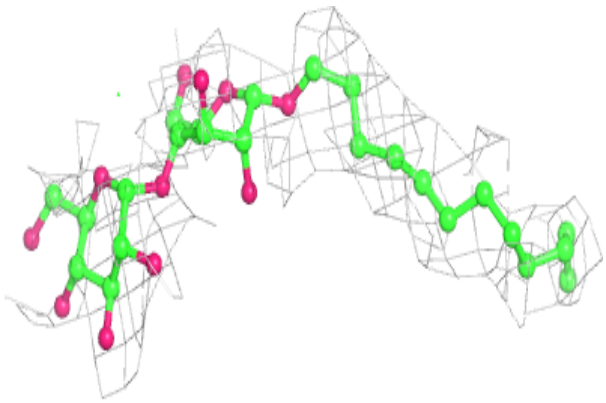


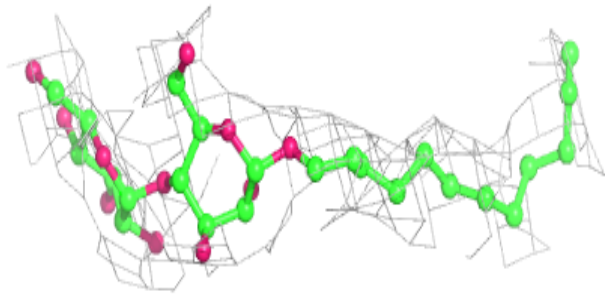




Electron density around LMU 4 317:

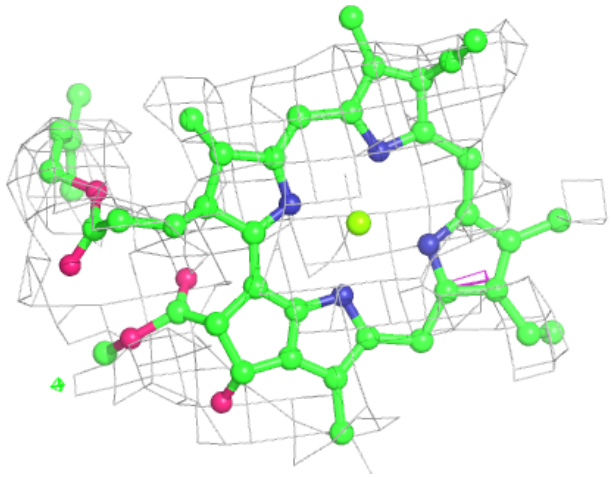
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

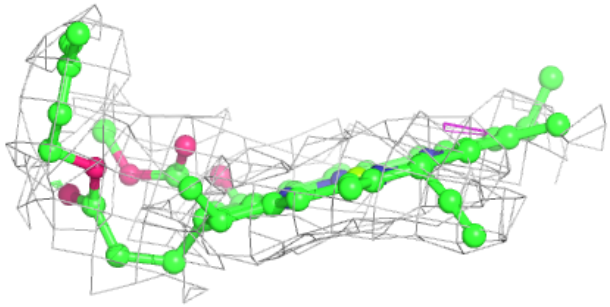


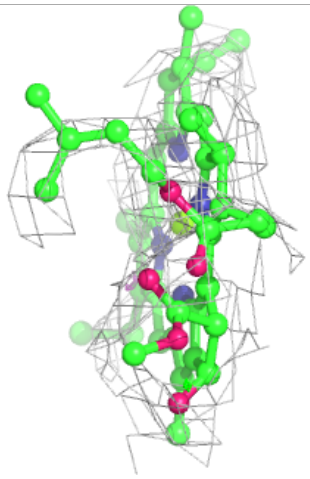


Electron density around CLA 3 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

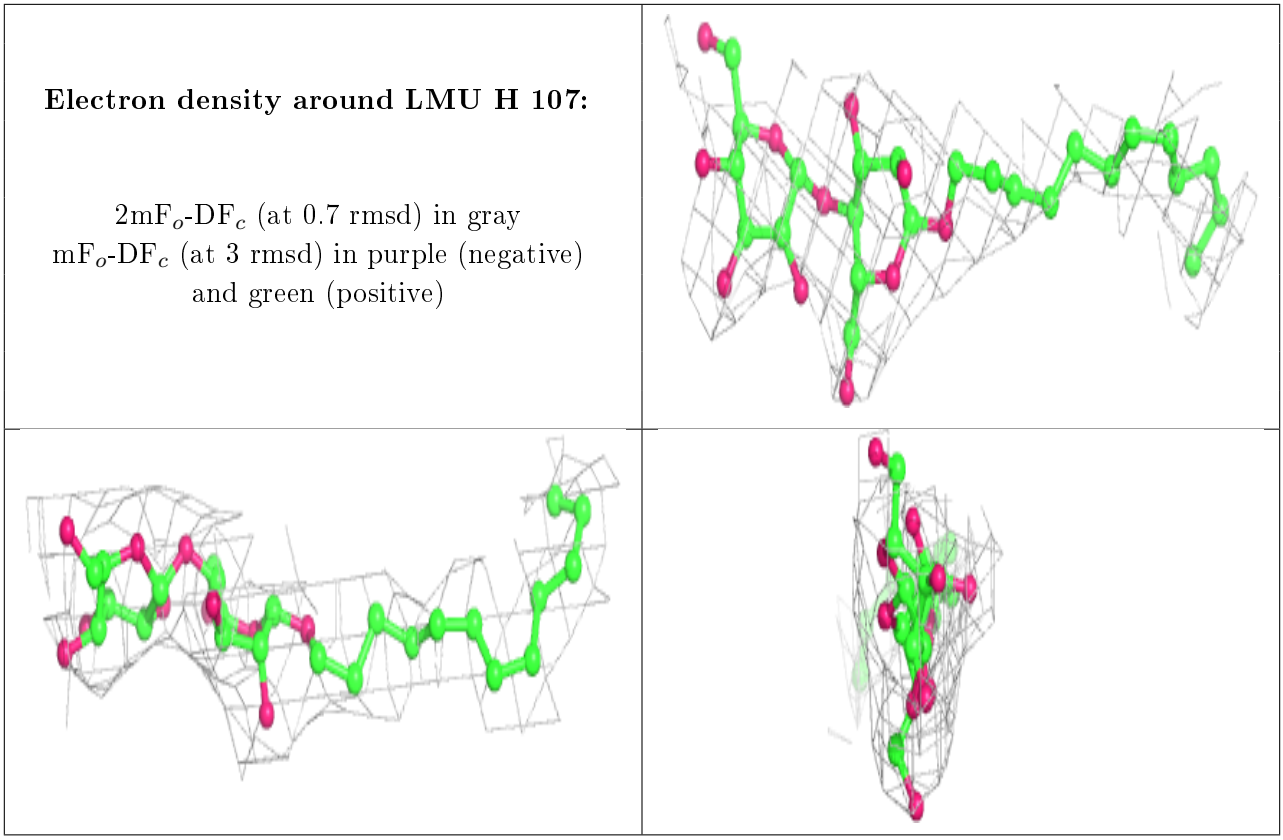






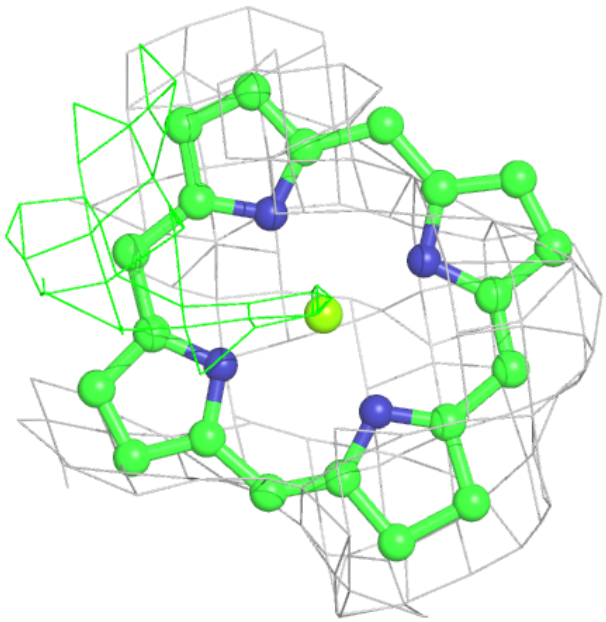
Electron density around LMU H 107:

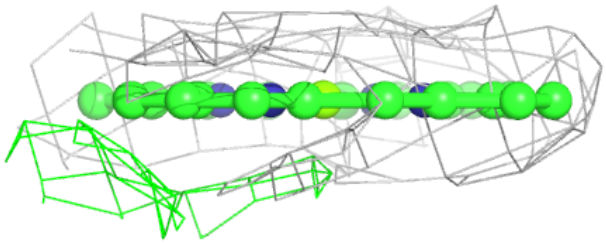
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

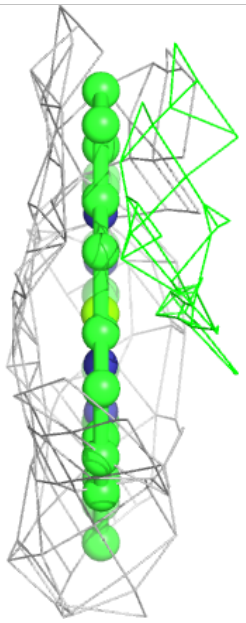


Electron density around CLA 2 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

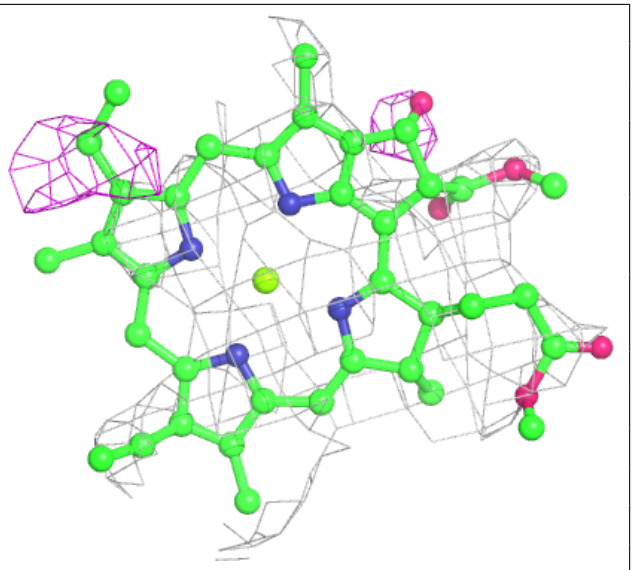


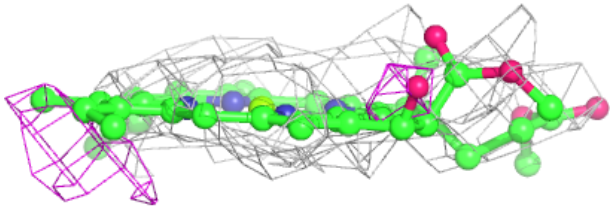


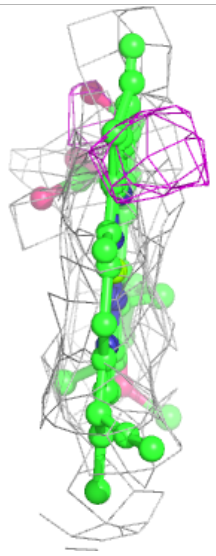


Electron density around CLA B 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

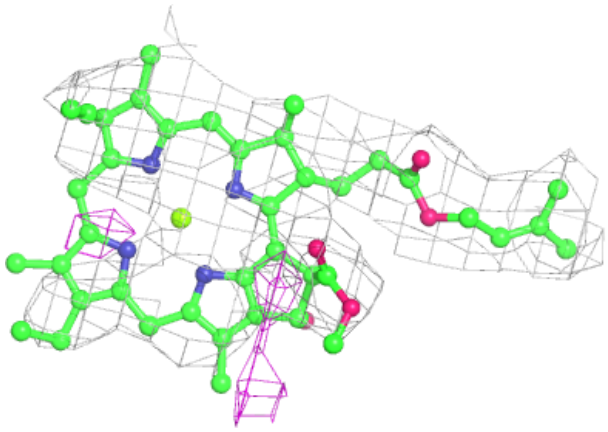


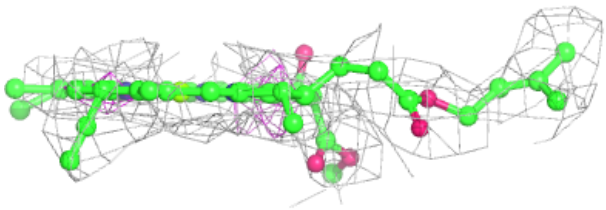


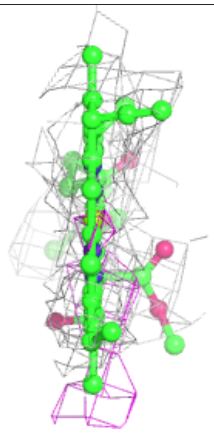


Electron density around CLA 4 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

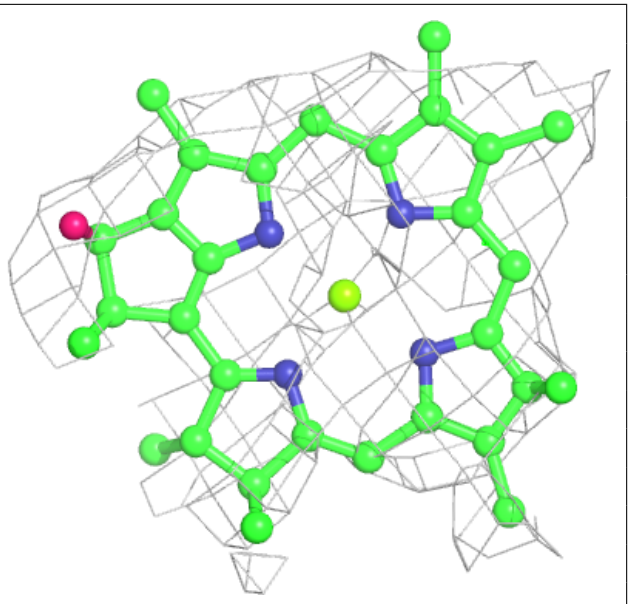


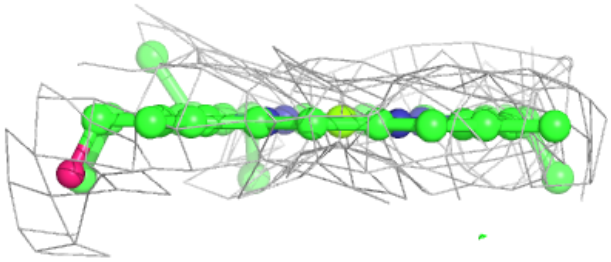


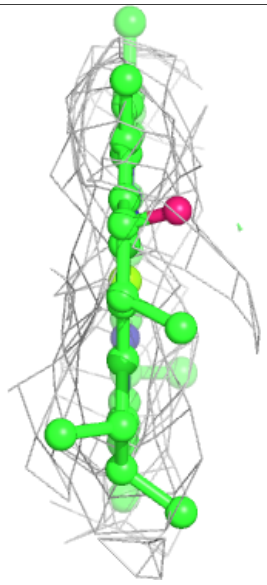


Electron density around CLA 4 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

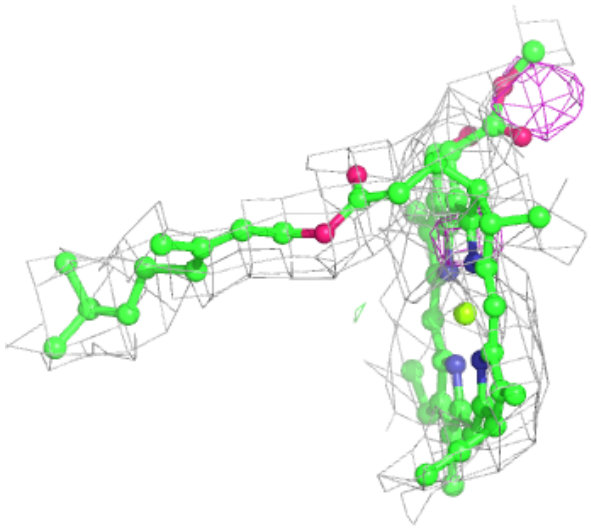


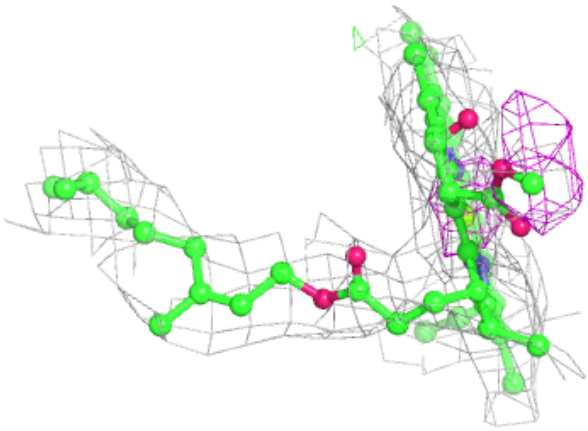


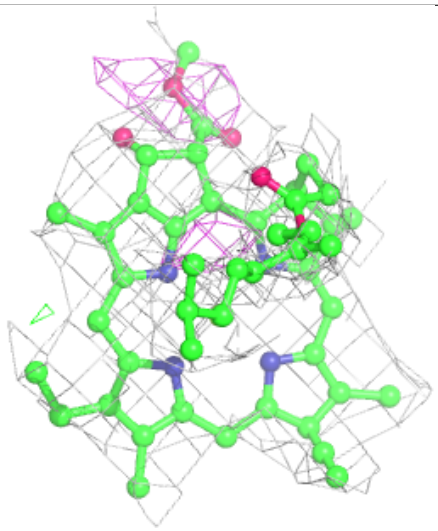


Electron density around CLA 4 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

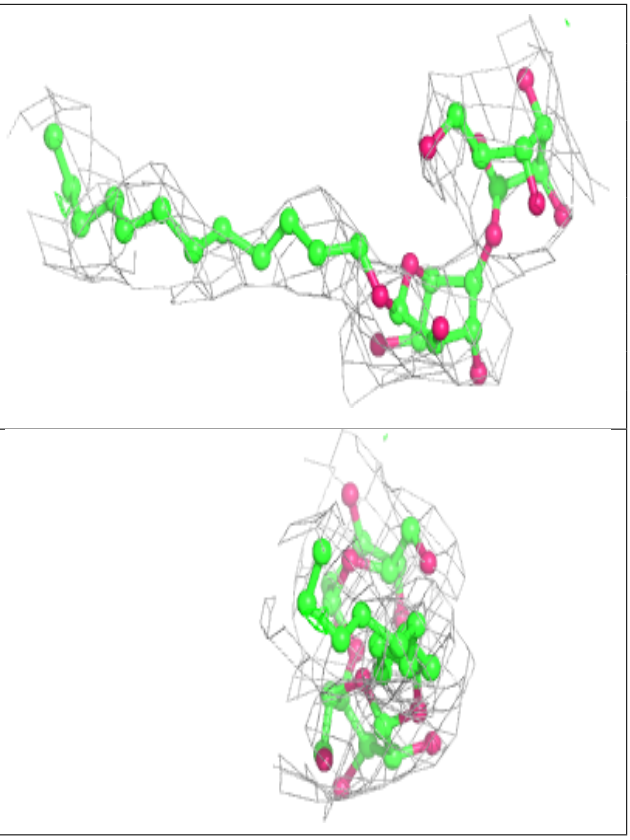






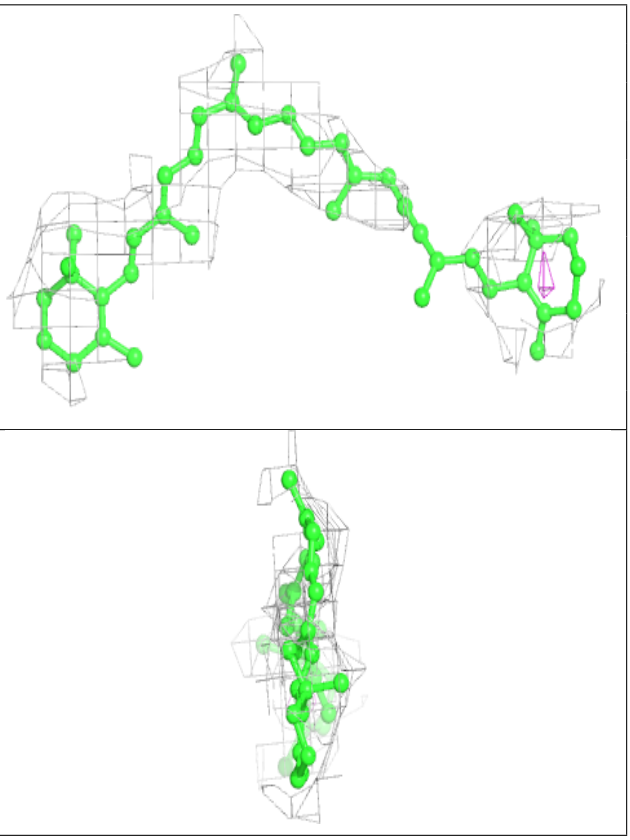
Electron density around LMU 1 213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



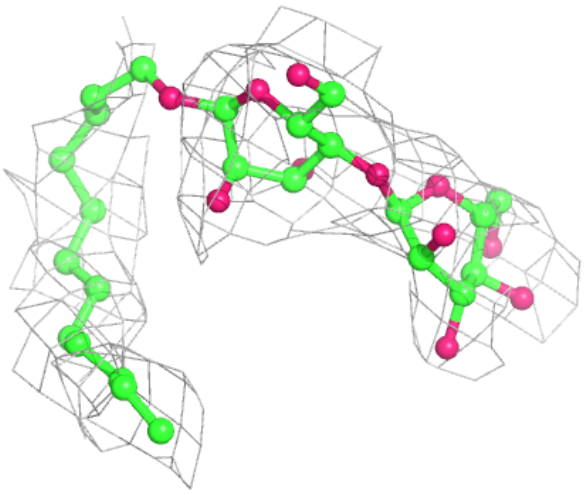
Electron density around BCR 3 314:

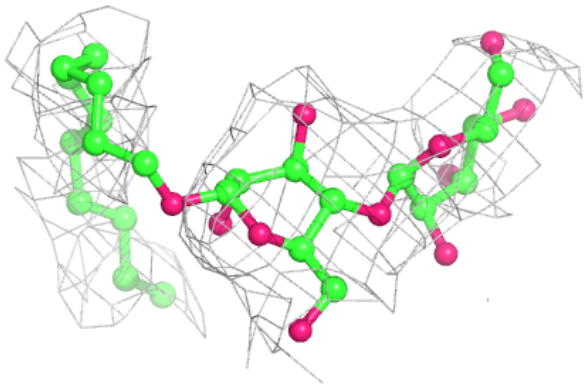
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

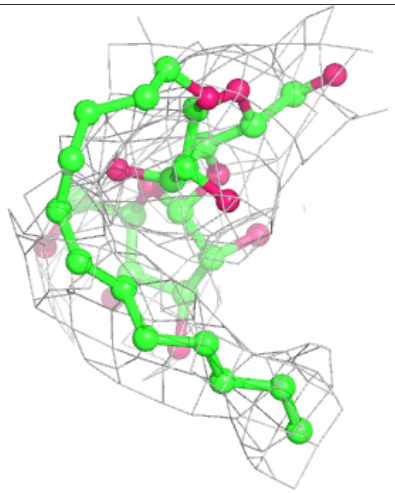


Electron density around LMU 1 220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

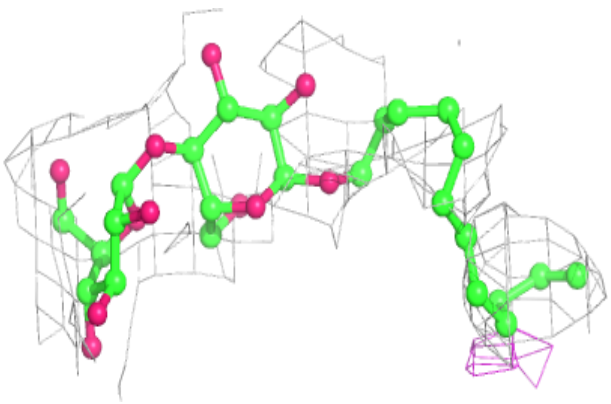


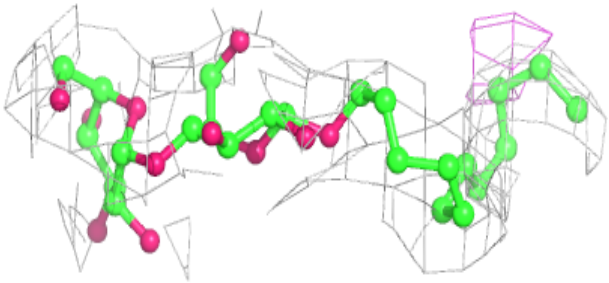


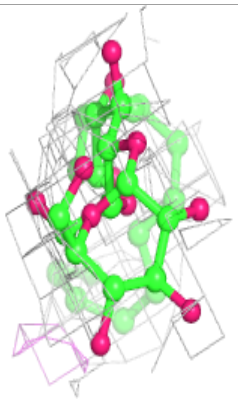


Electron density around LMU R 109:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

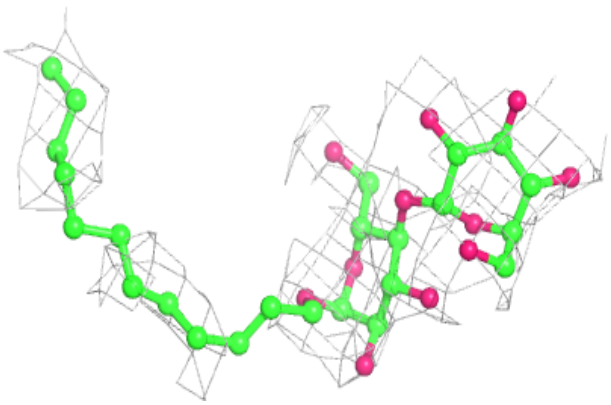


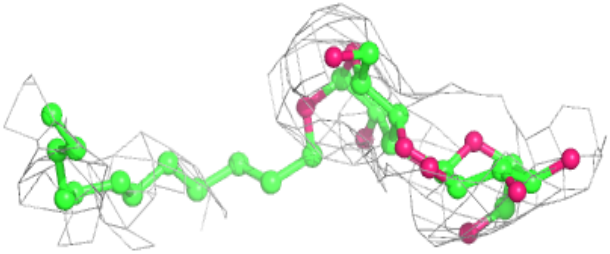


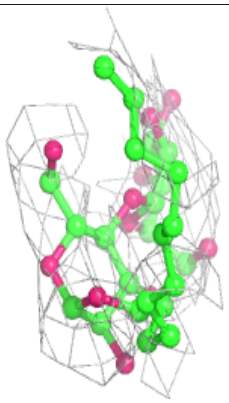


Electron density around LMU 1 217:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

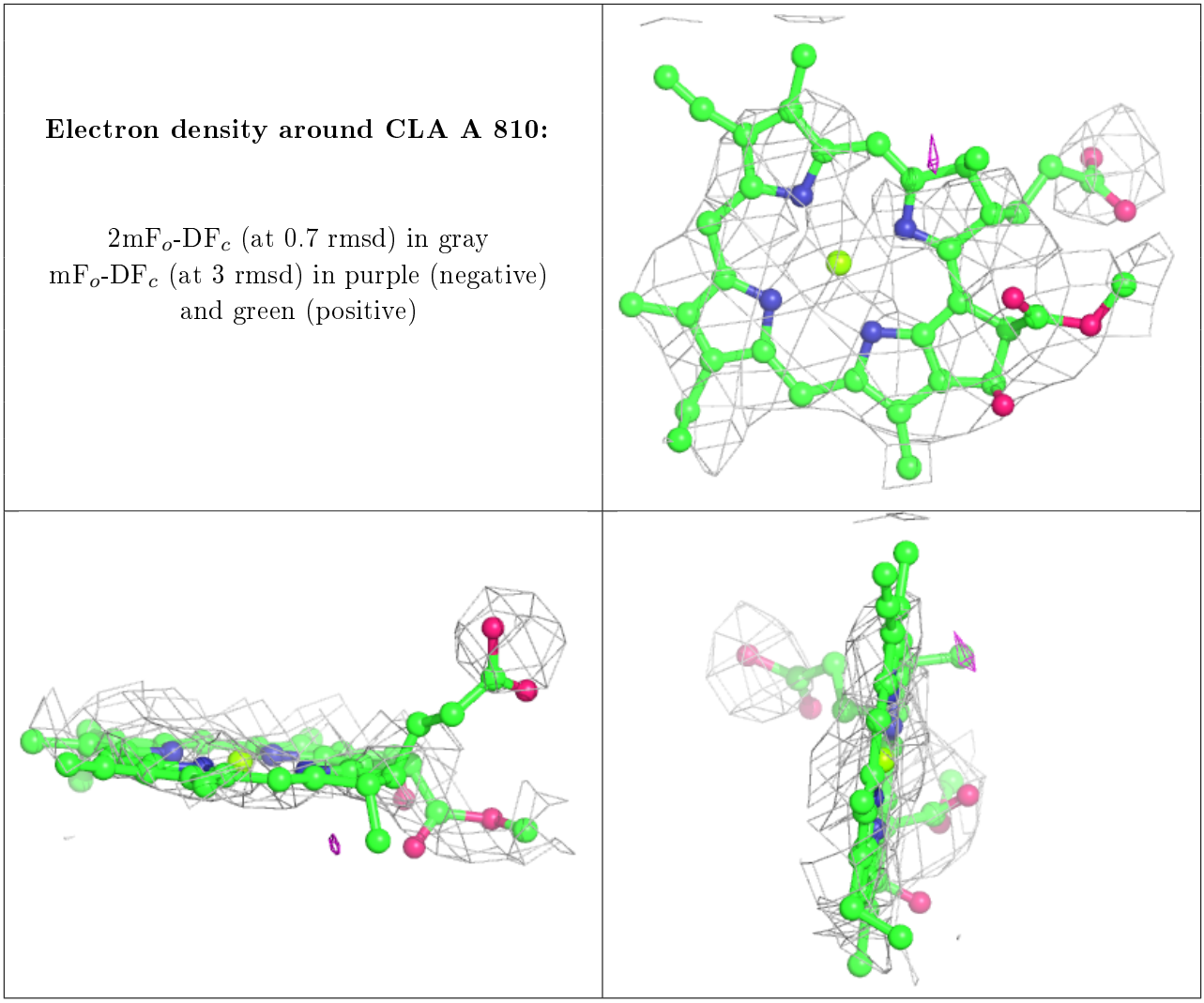






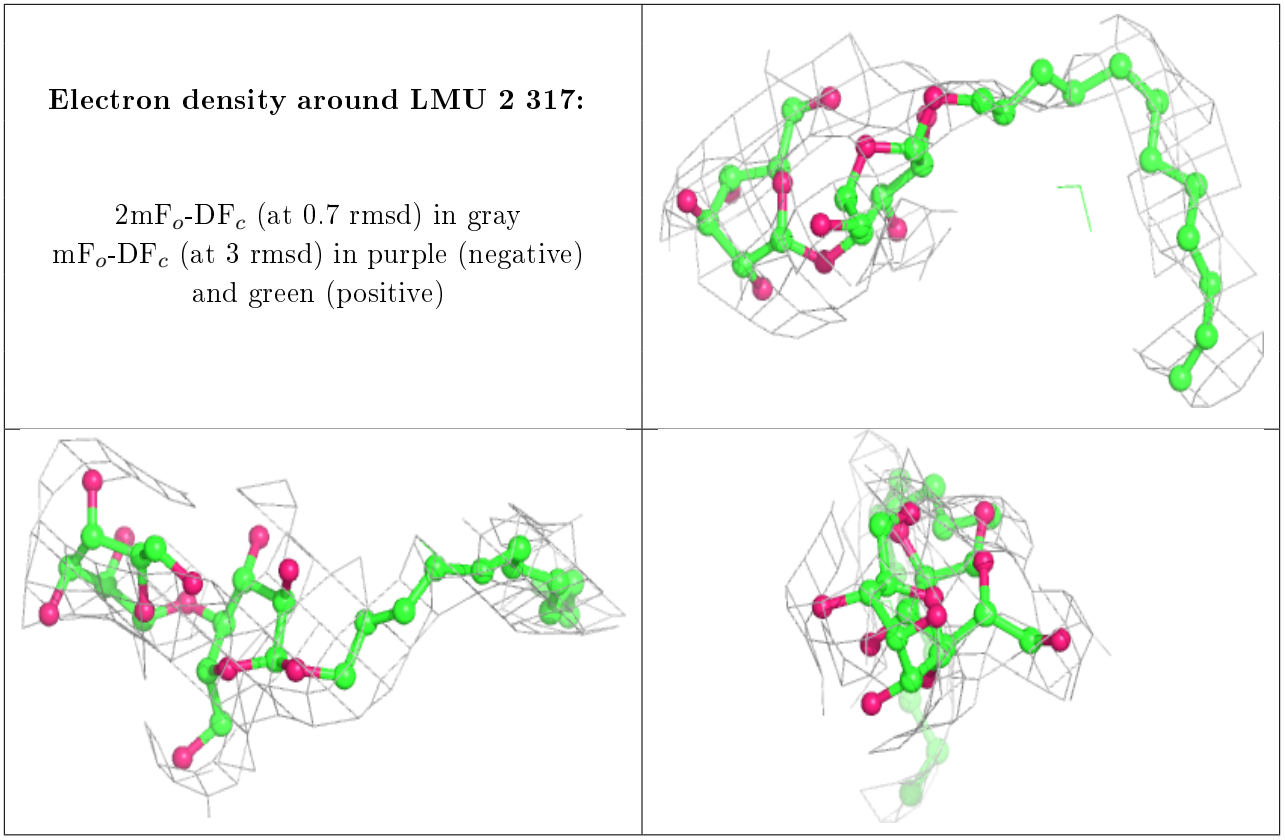
Electron density around CLA A 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



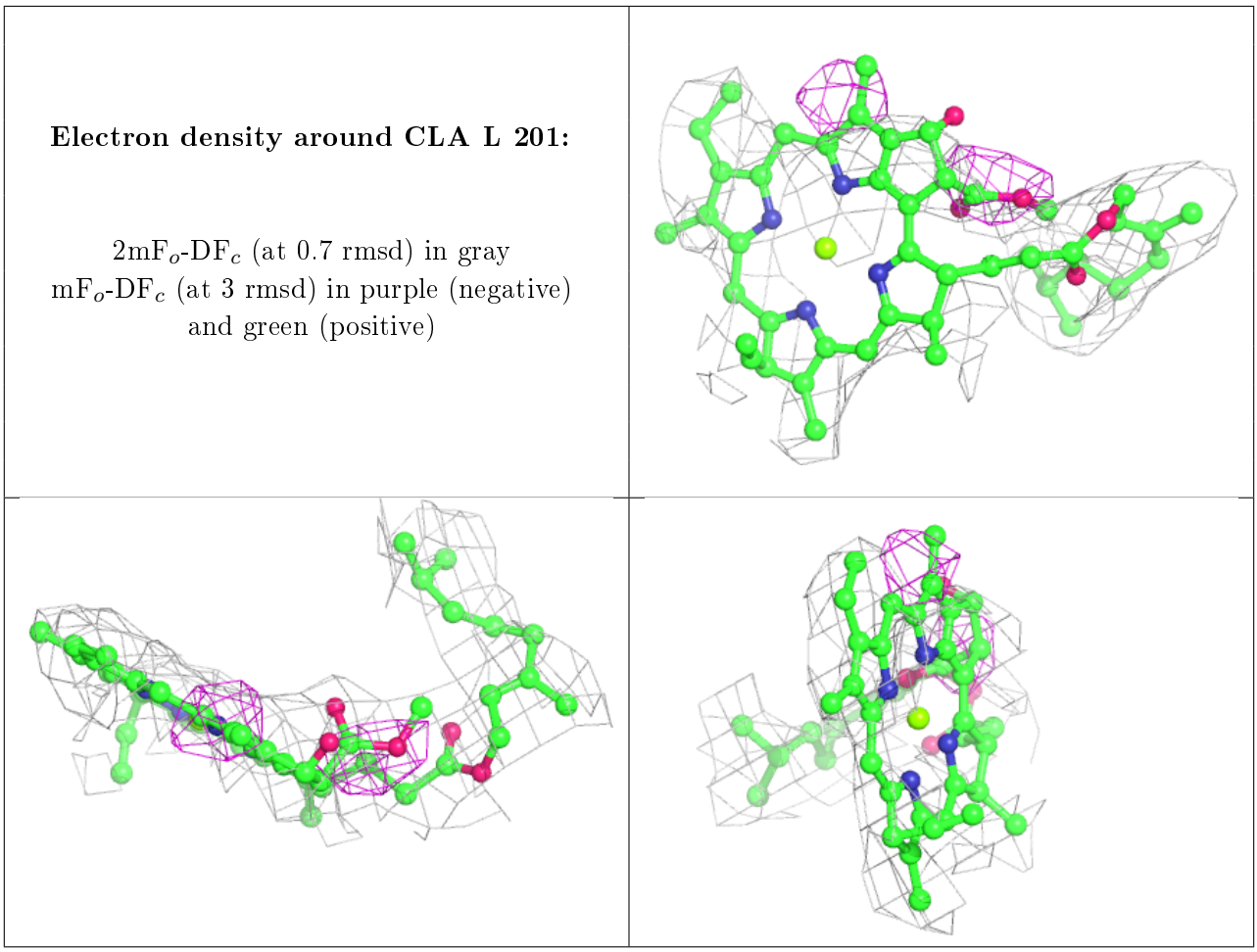
Electron density around LMU 2 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



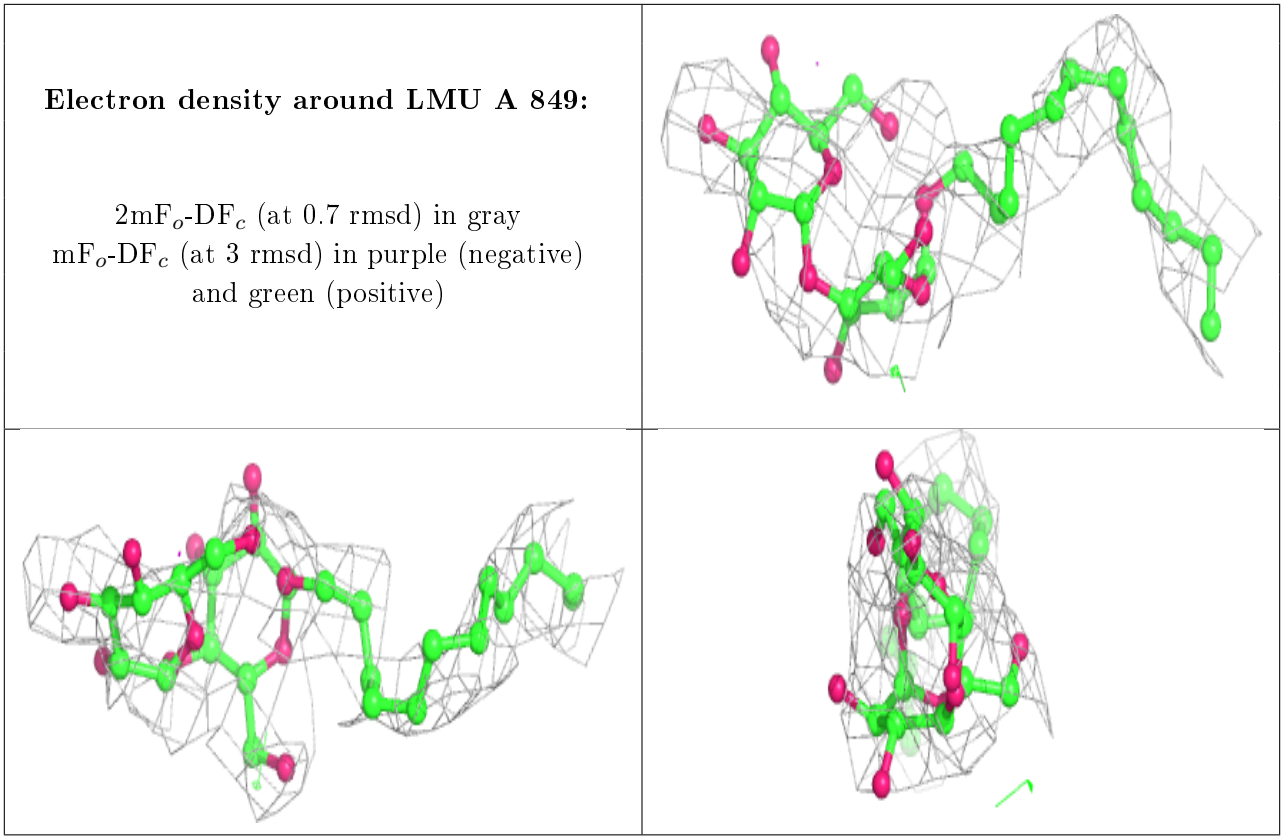
Electron density around CLA L 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



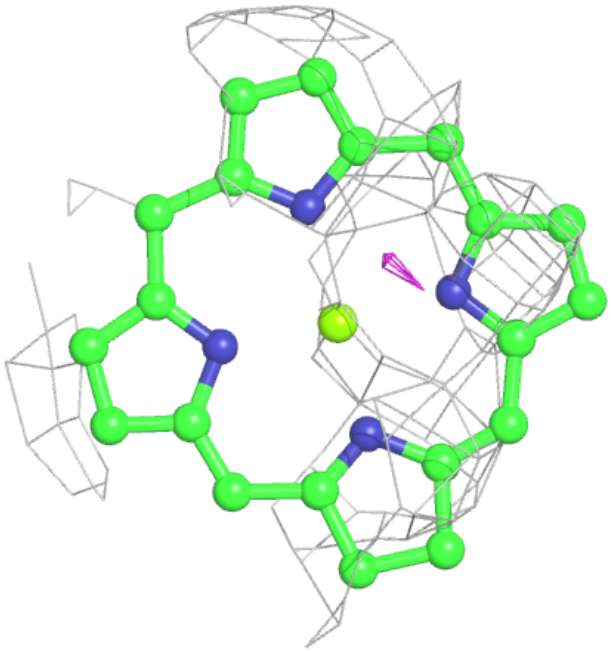
Electron density around LMU A 849:

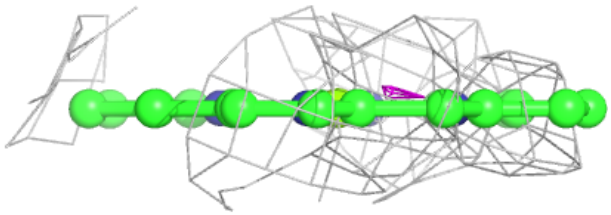
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

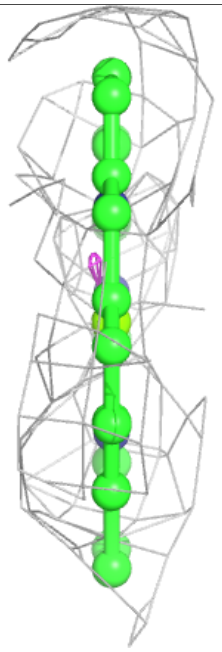


Electron density around CLA 3 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

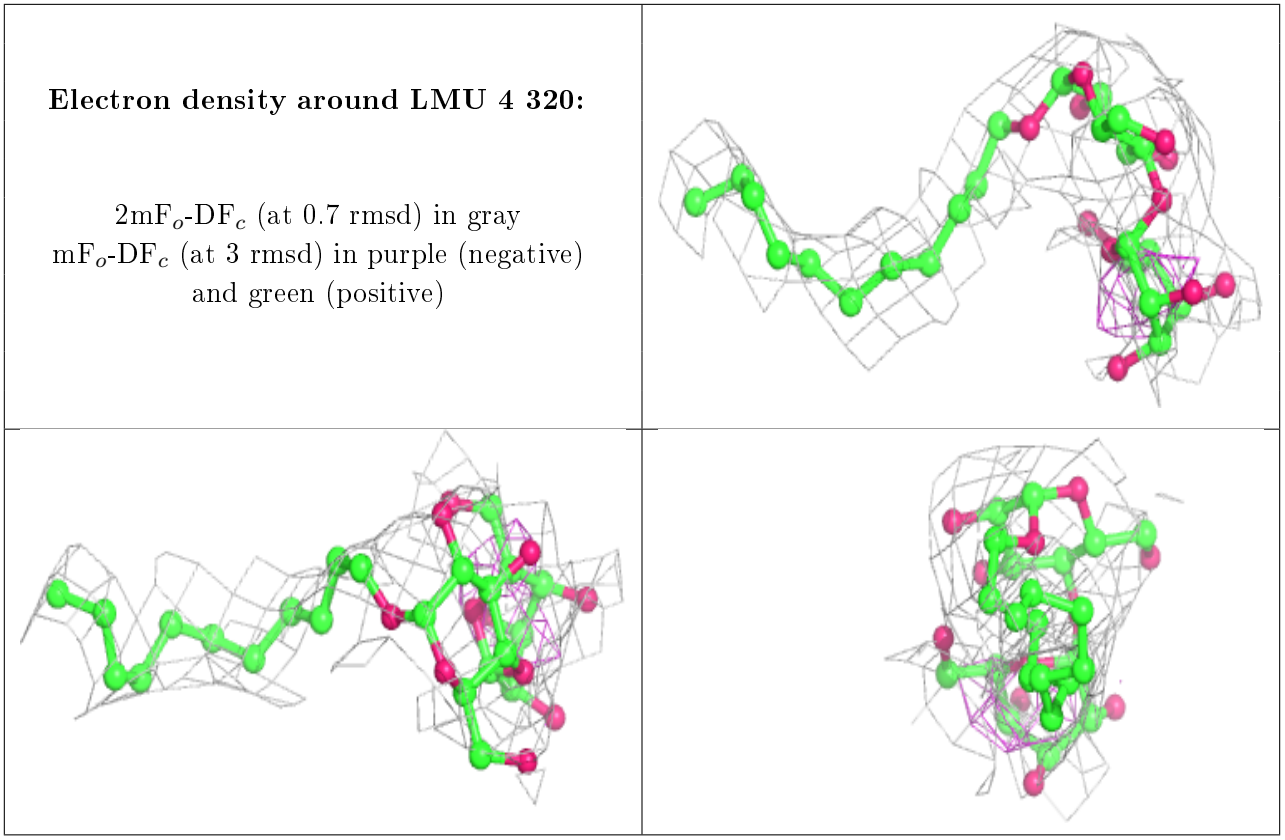






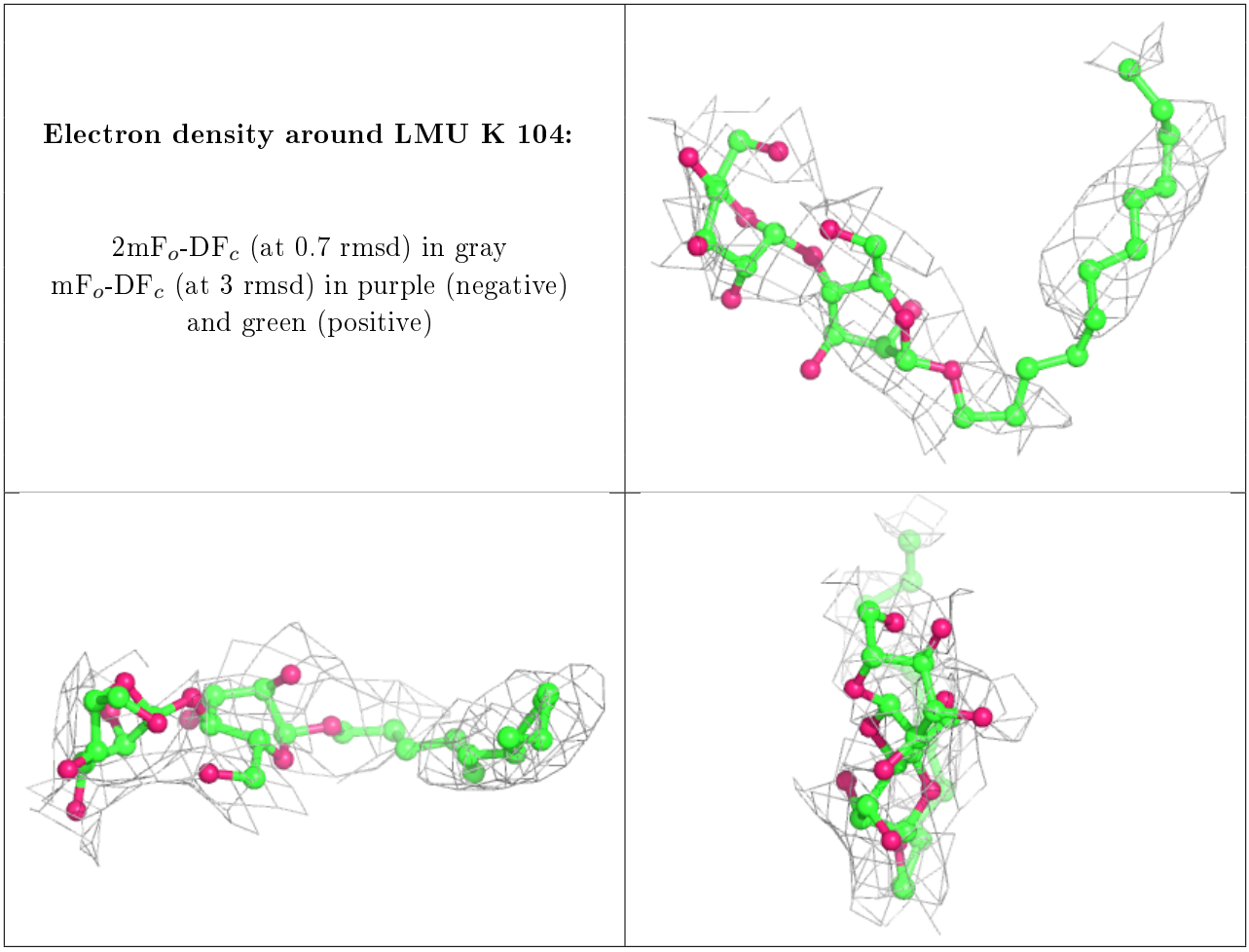
Electron density around LMU 4 320:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



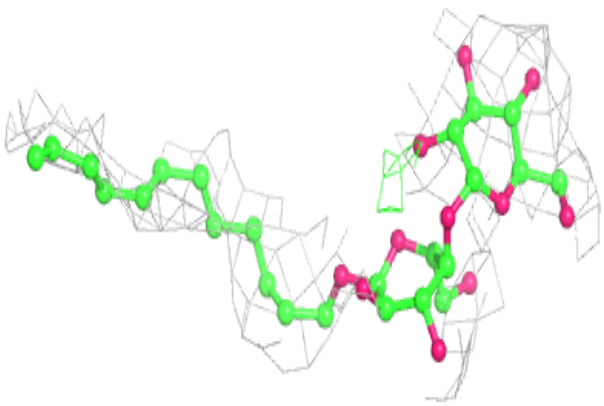
Electron density around LMU K 104:

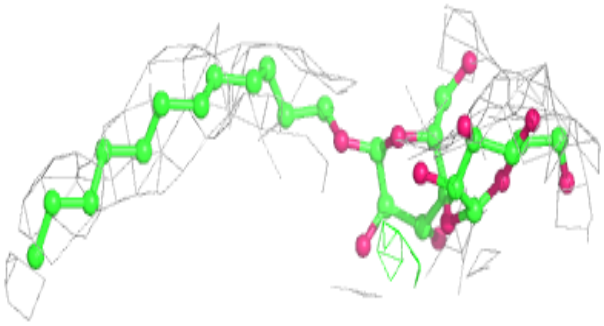
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMU R 105:

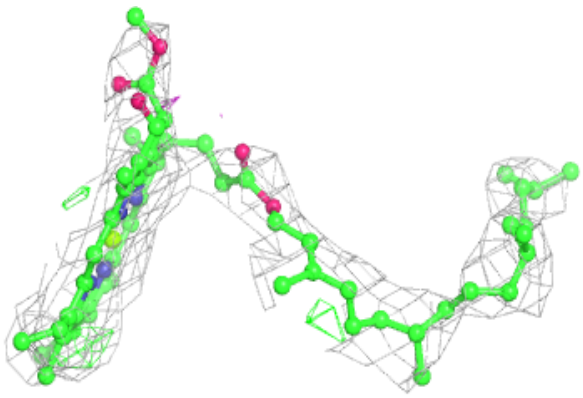
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

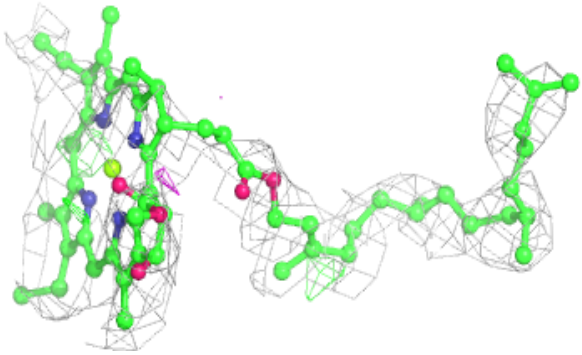


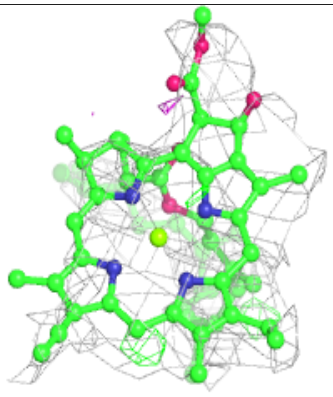


Electron density around CLA B 838:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

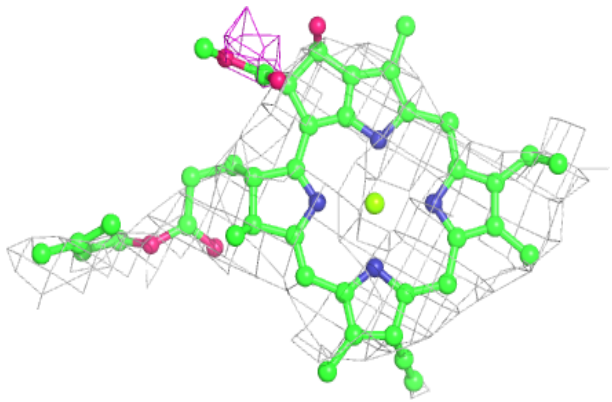


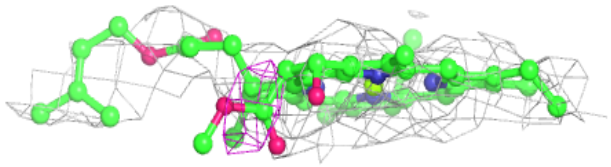


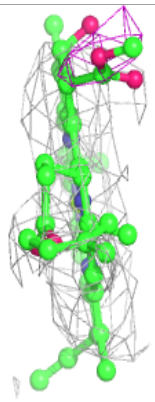


Electron density around CLA K 108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

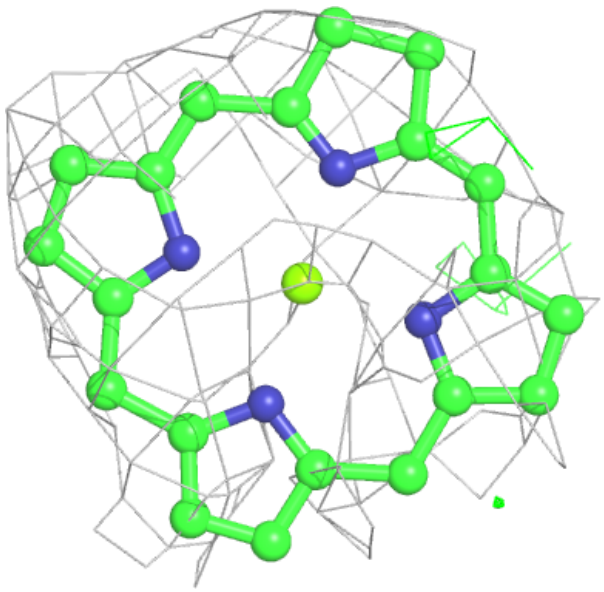


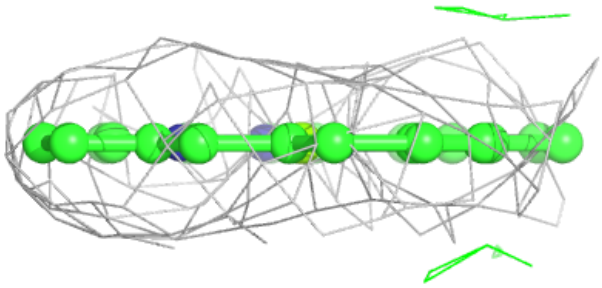


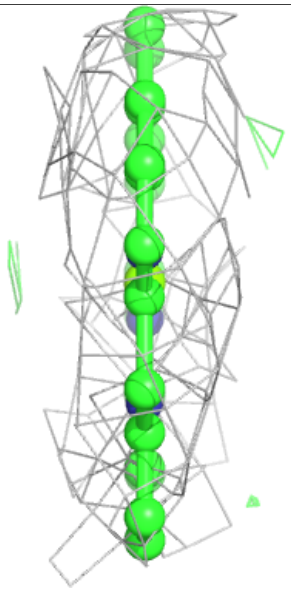


Electron density around CLA 1 211:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

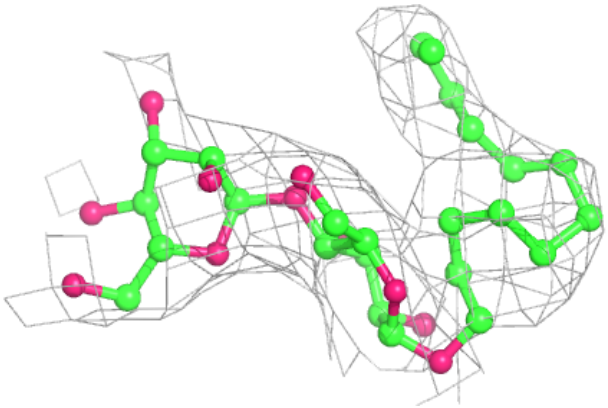


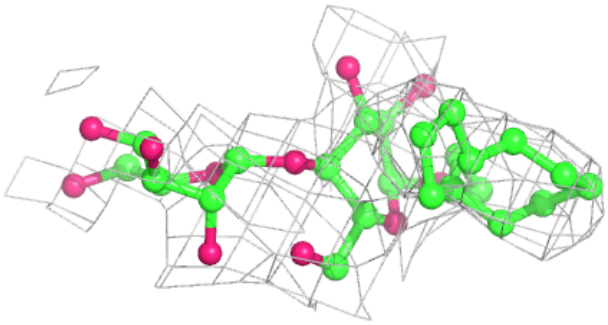


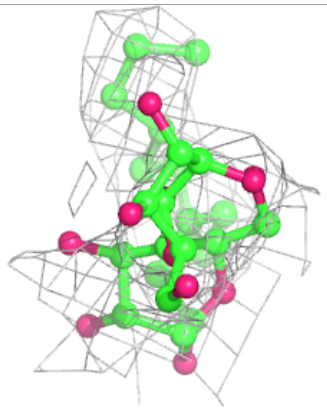


Electron density around LMU K 106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

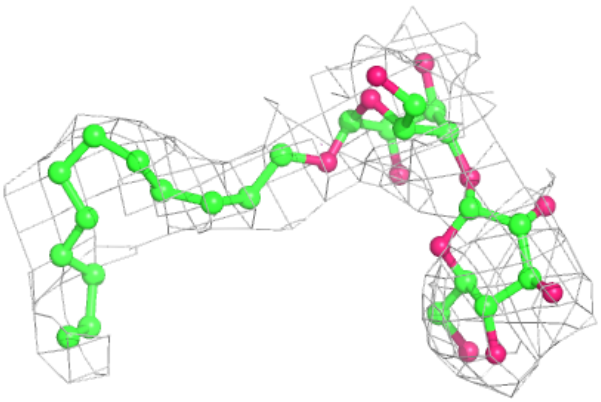


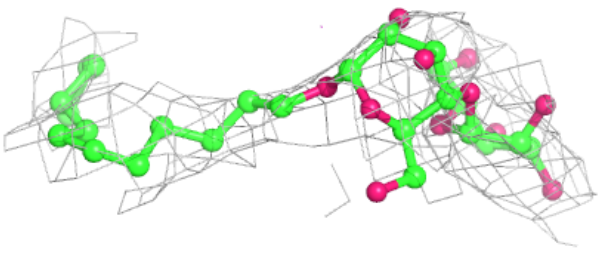


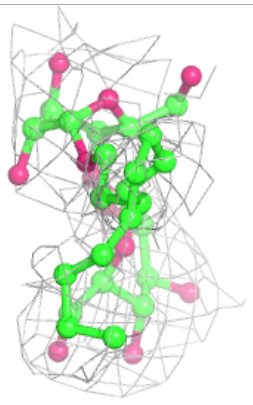


Electron density around LMU K 109:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

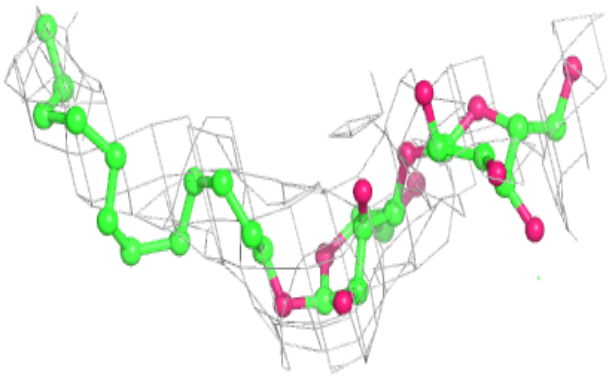


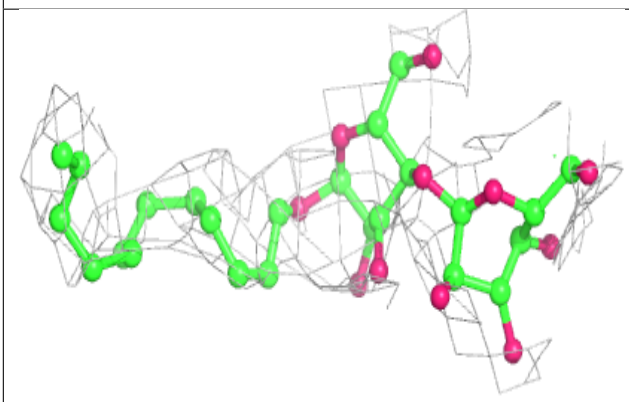


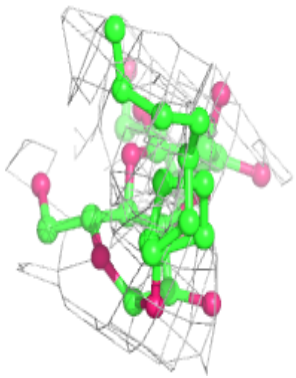


Electron density around LMU H 104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

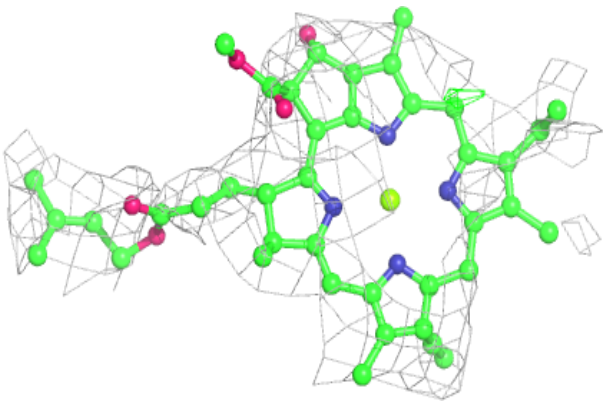


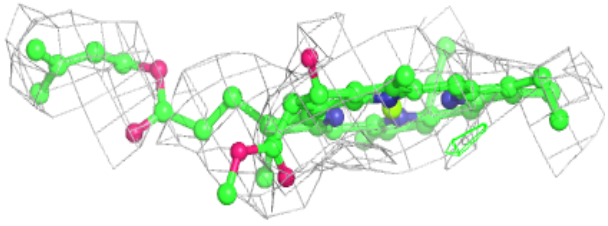


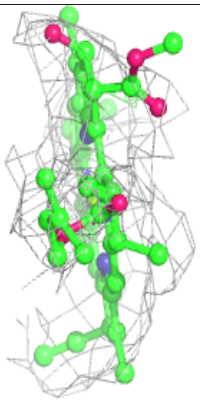


Electron density around CLA 3 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

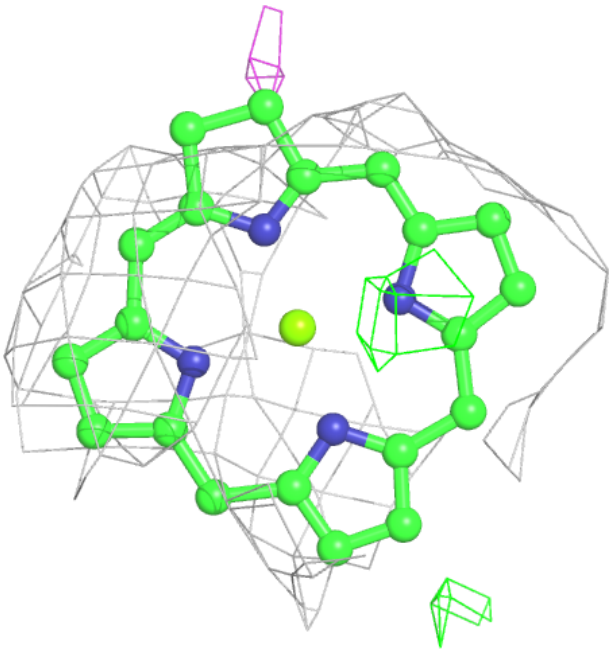


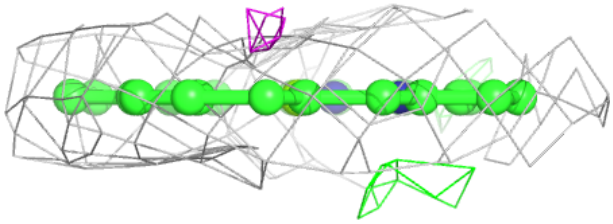


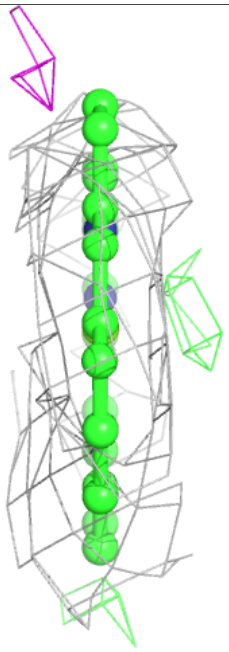


Electron density around CLA 3 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

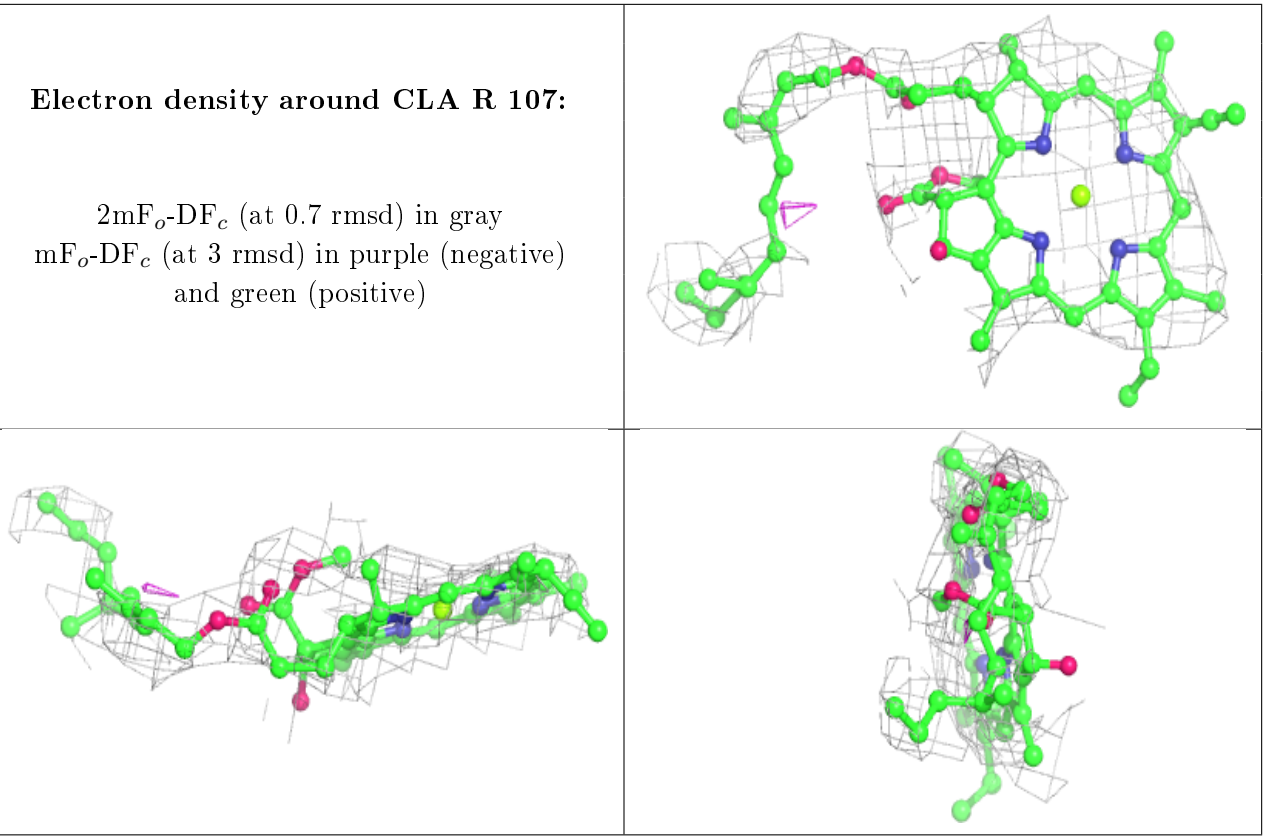






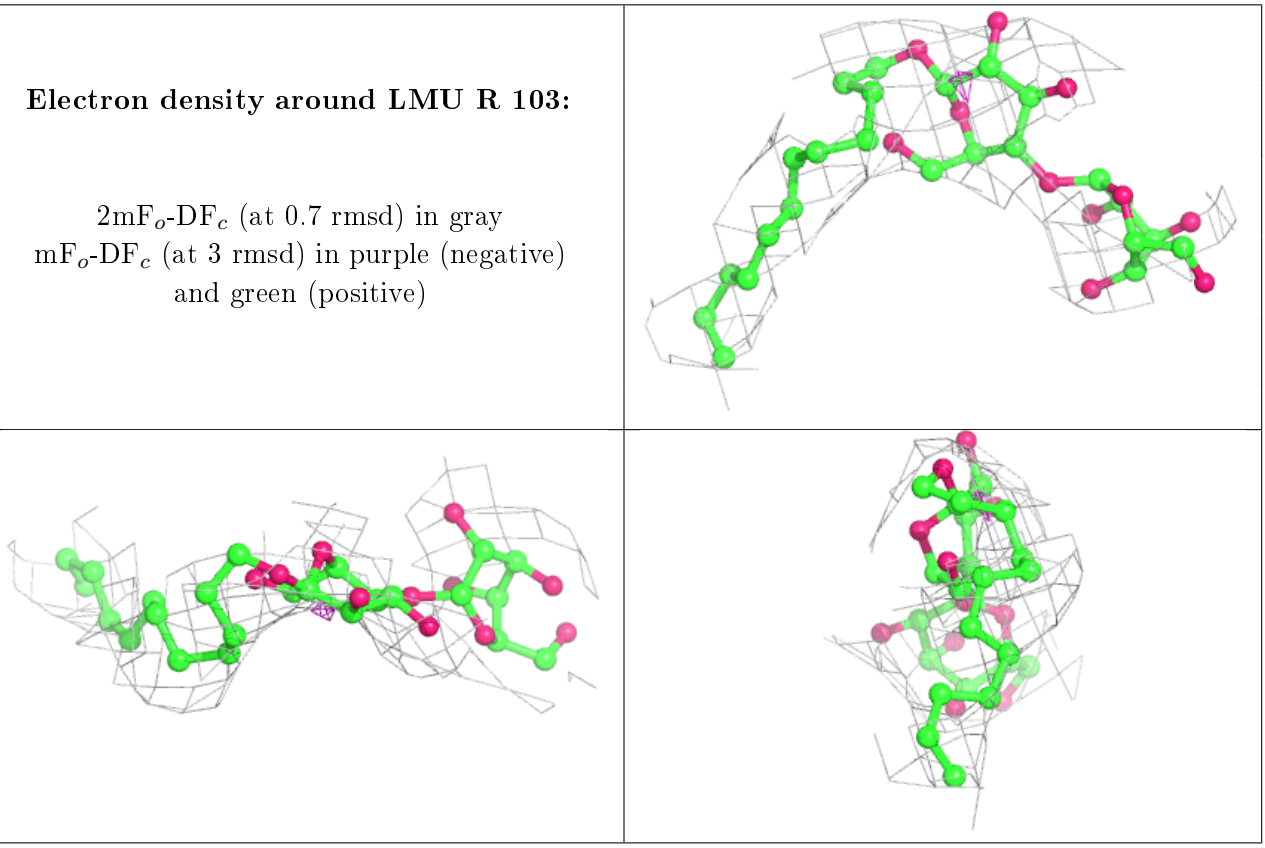
Electron density around CLA R 107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



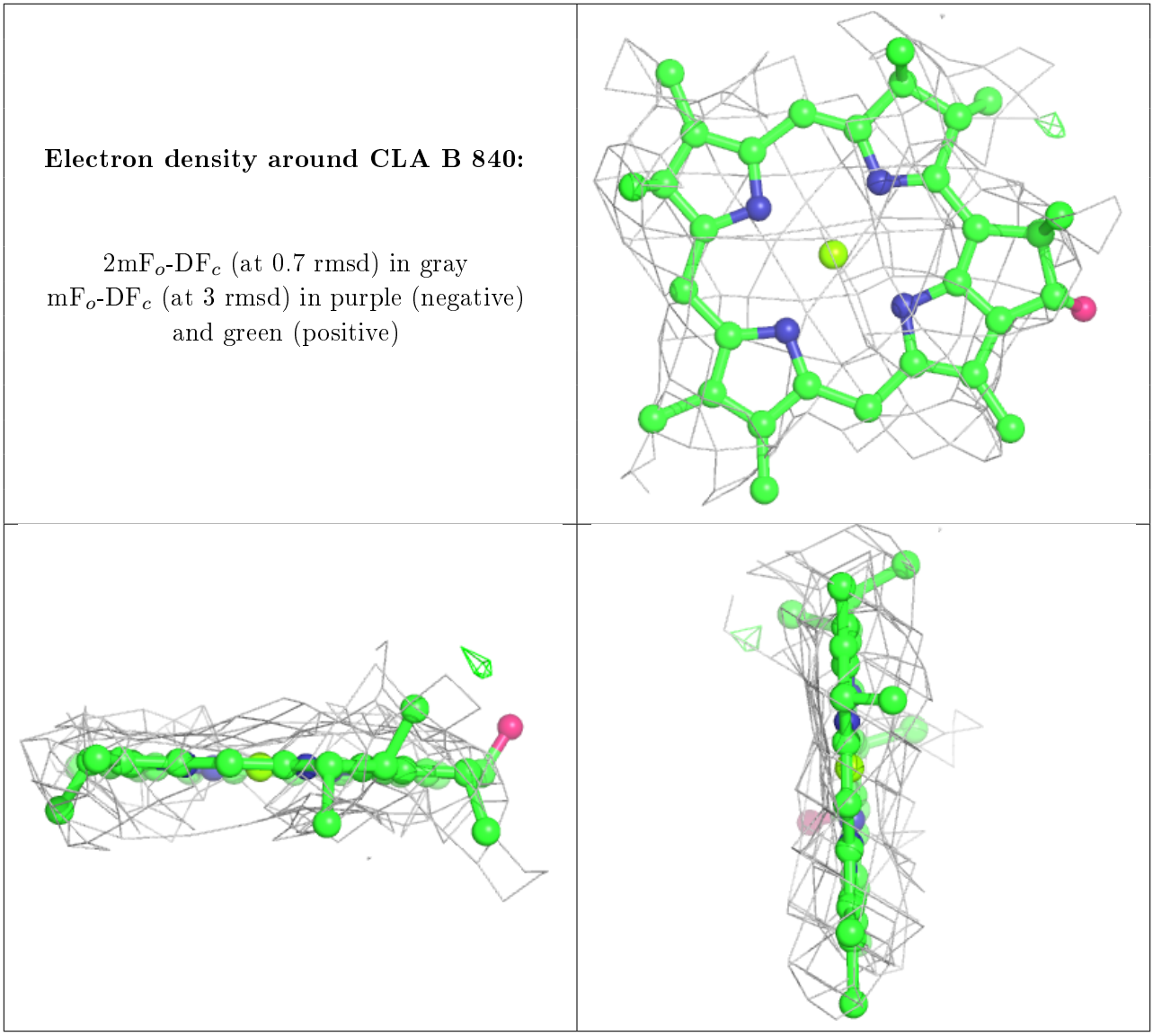
Electron density around LMU R 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



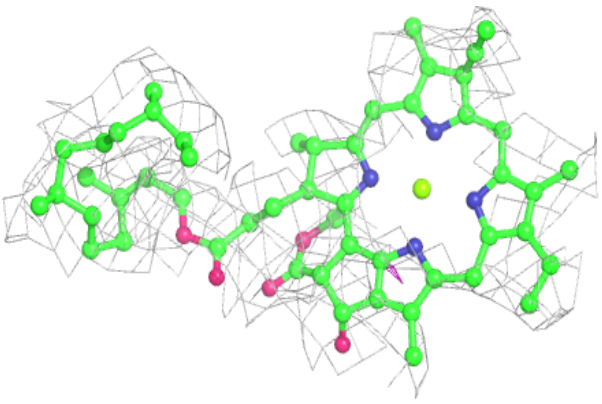
Electron density around CLA B 840:

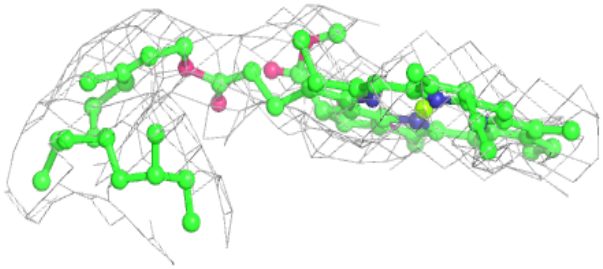
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

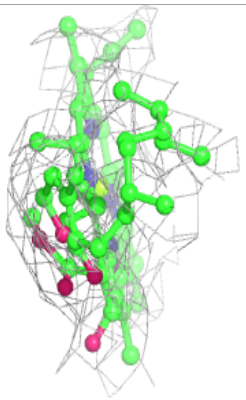


Electron density around CLA 1 215:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

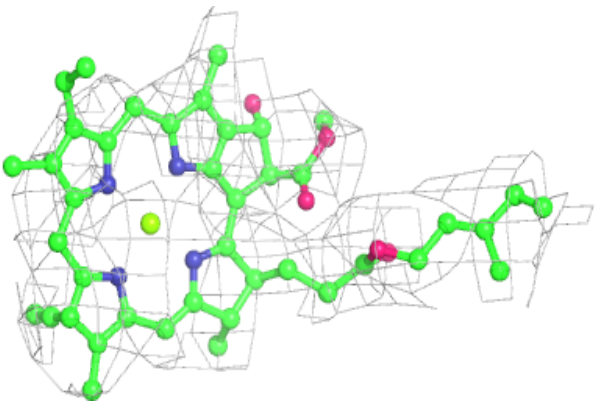


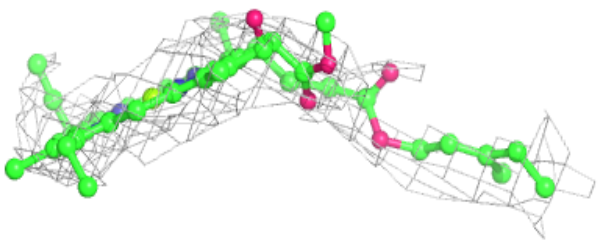


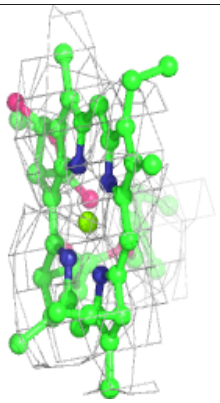


Electron density around CLA 1 210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

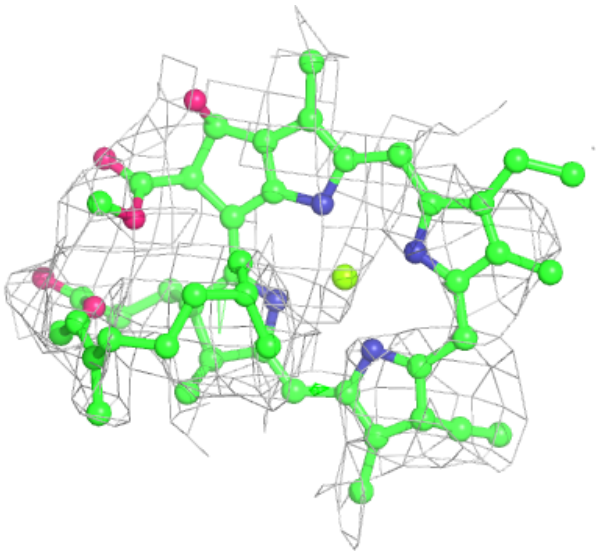


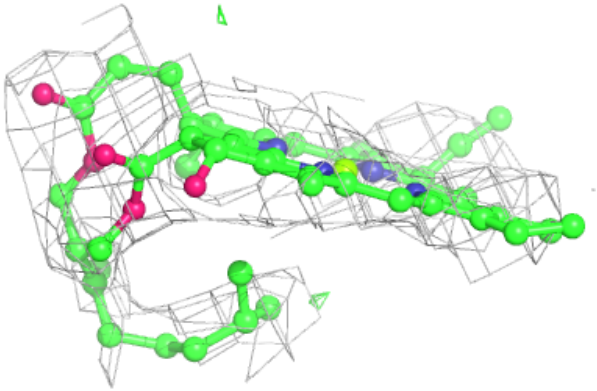


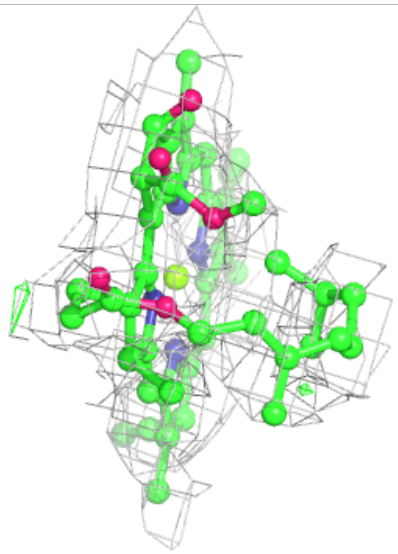


Electron density around CLA 4 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

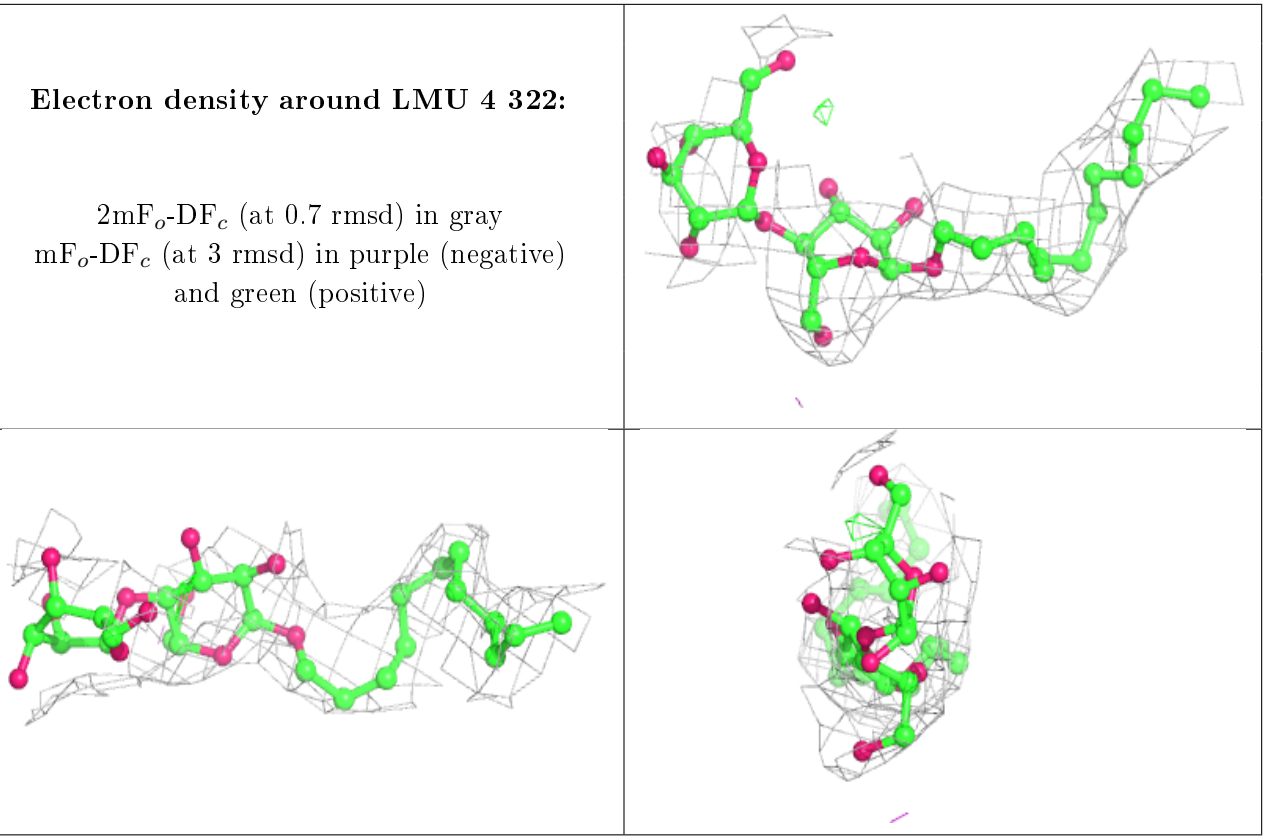






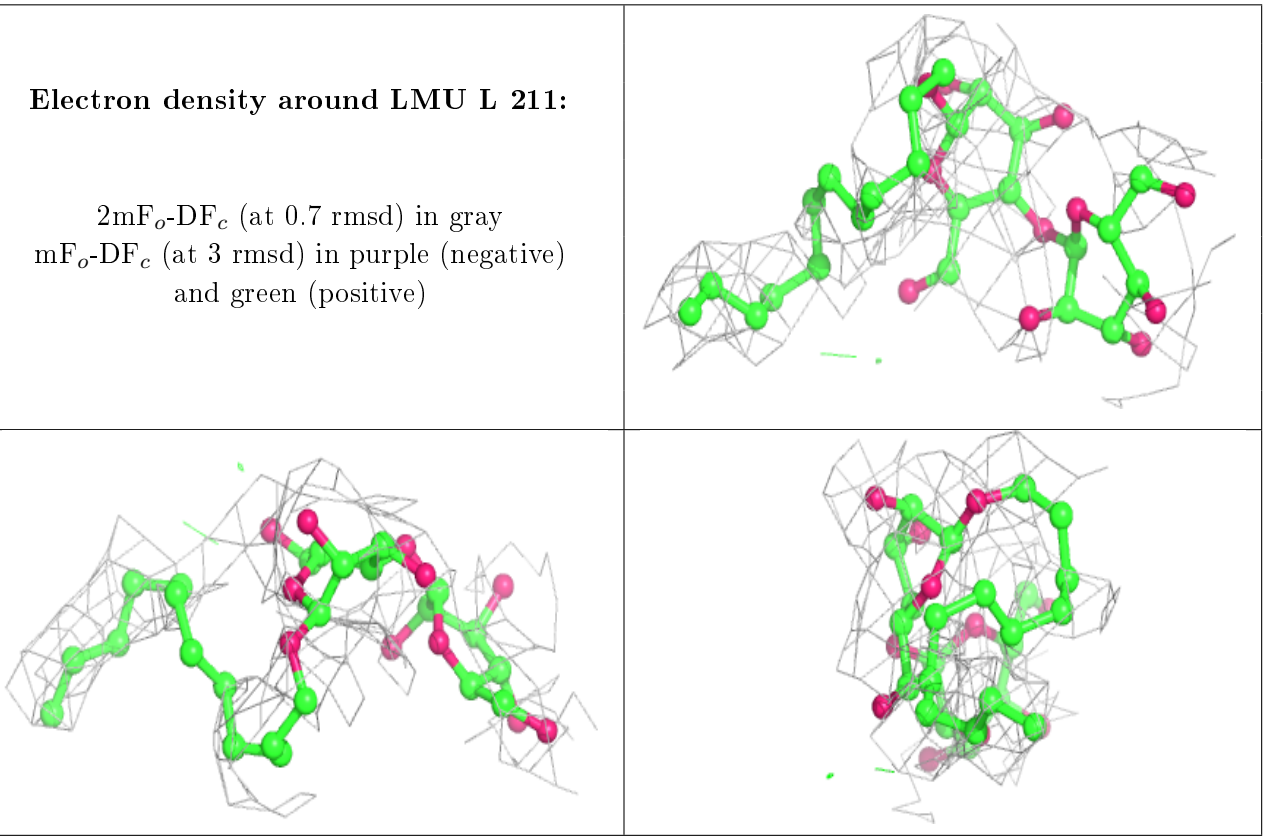
Electron density around LMU 4 322:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



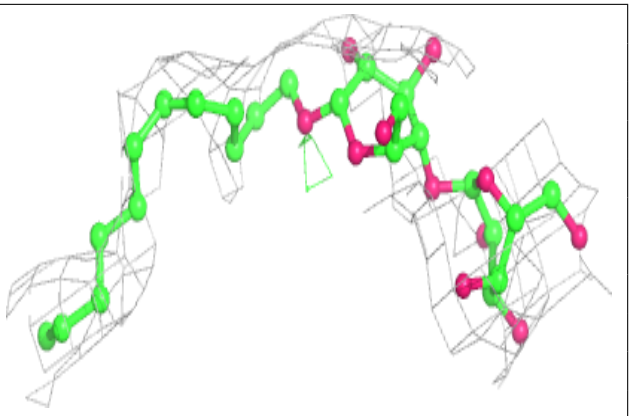
Electron density around LMU L 211:

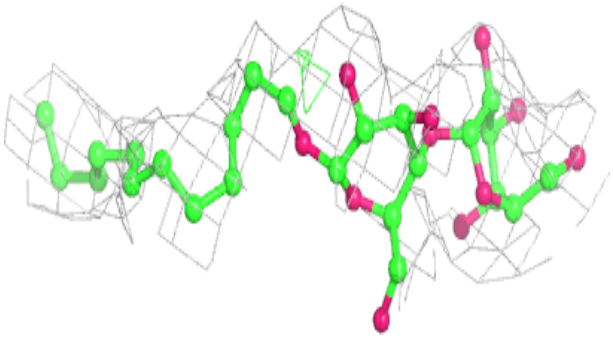
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMU 2 318:

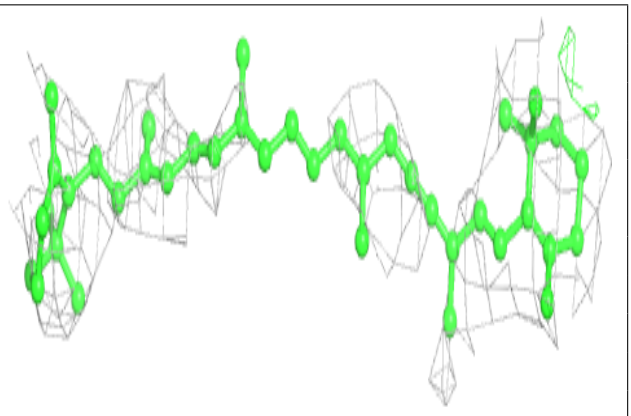
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

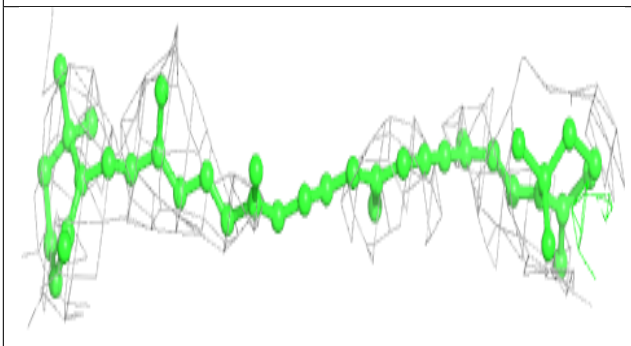


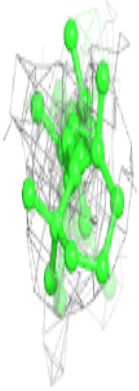


Electron density around BCR A 844:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

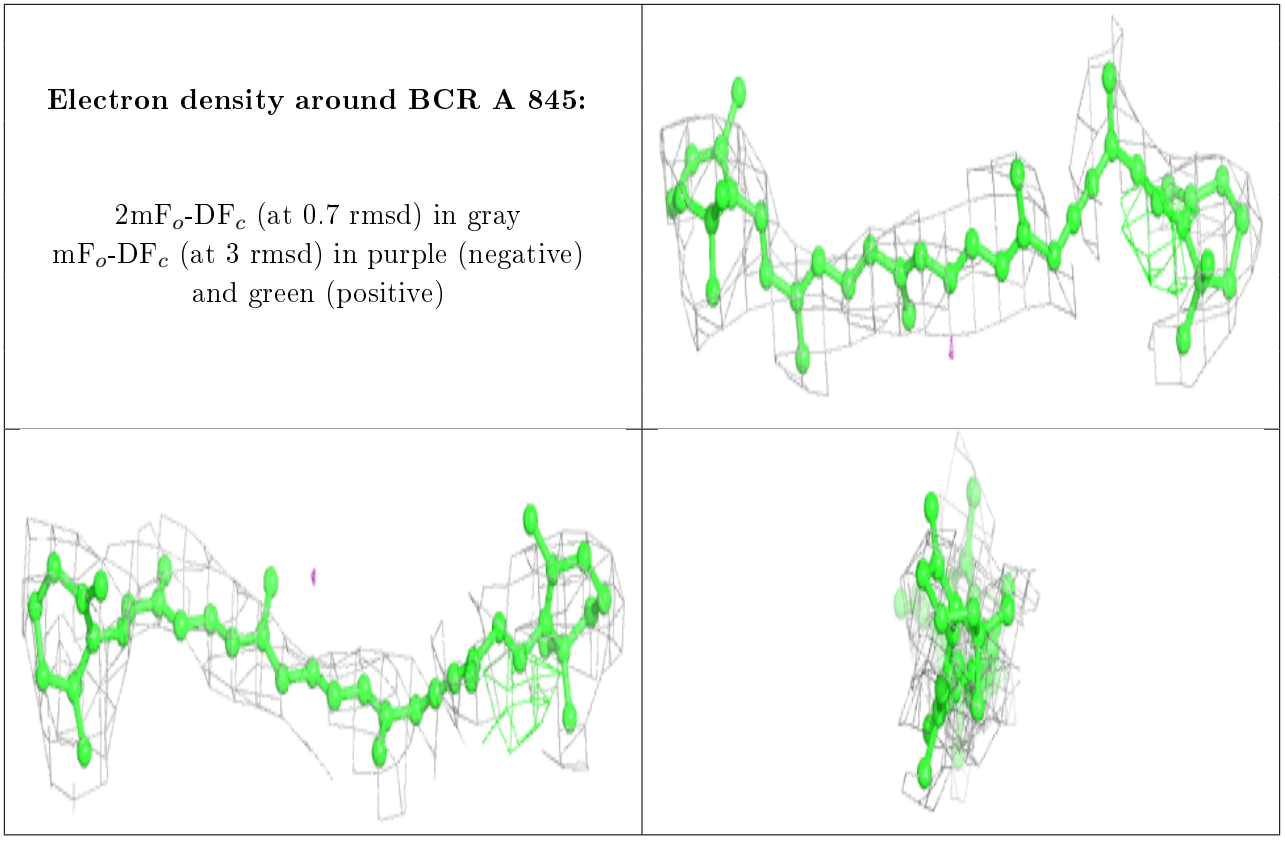






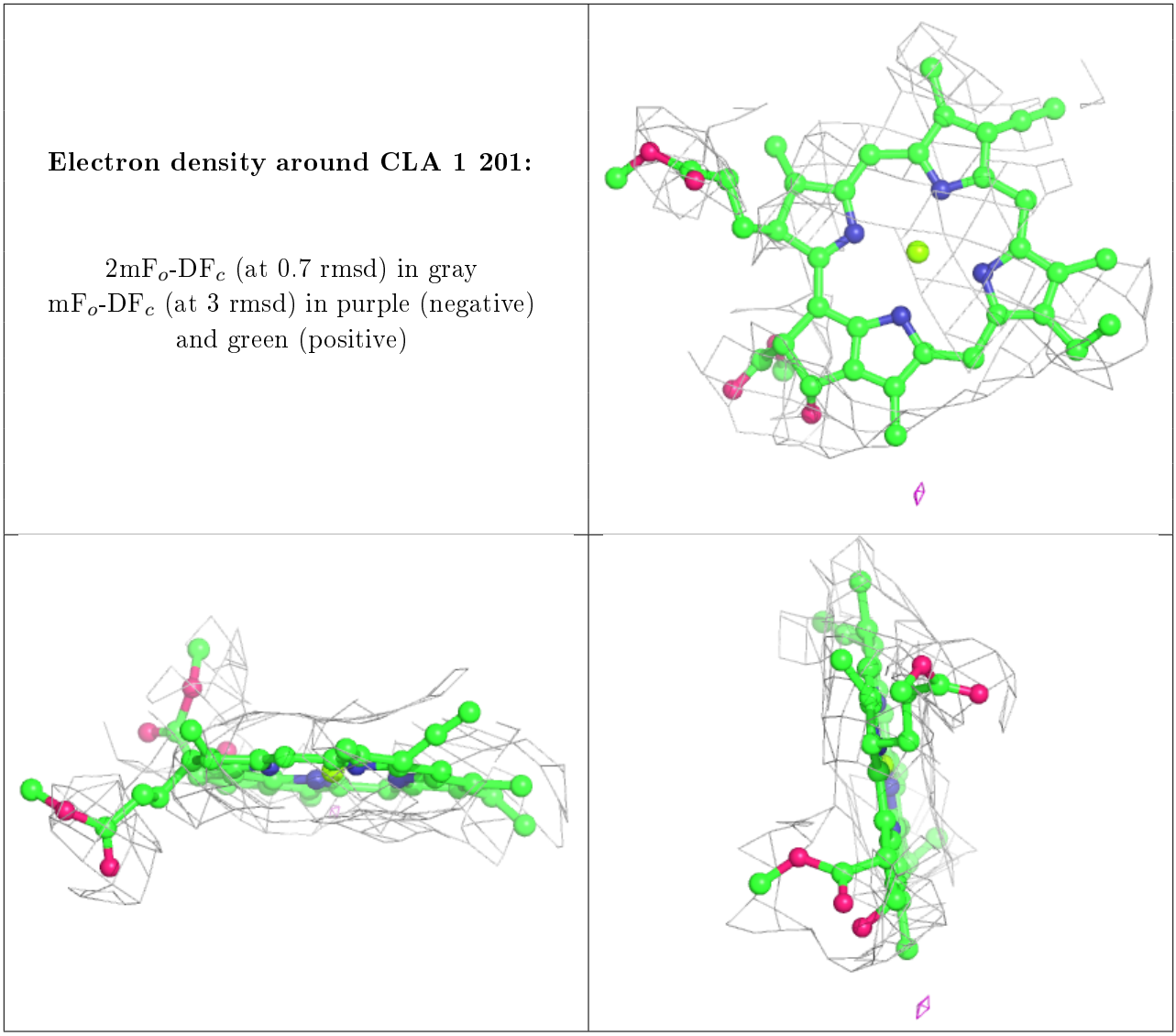
Electron density around BCR A 845:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



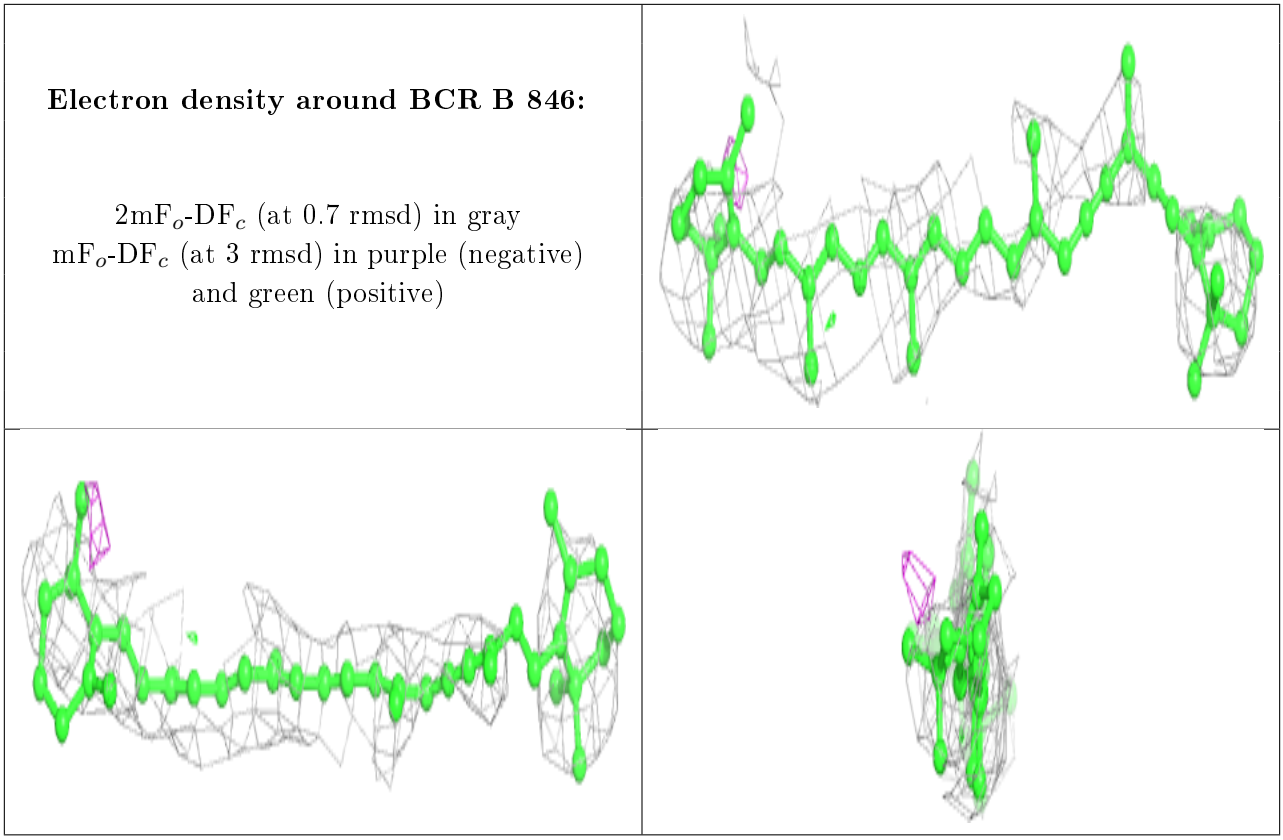
Electron density around CLA 1 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



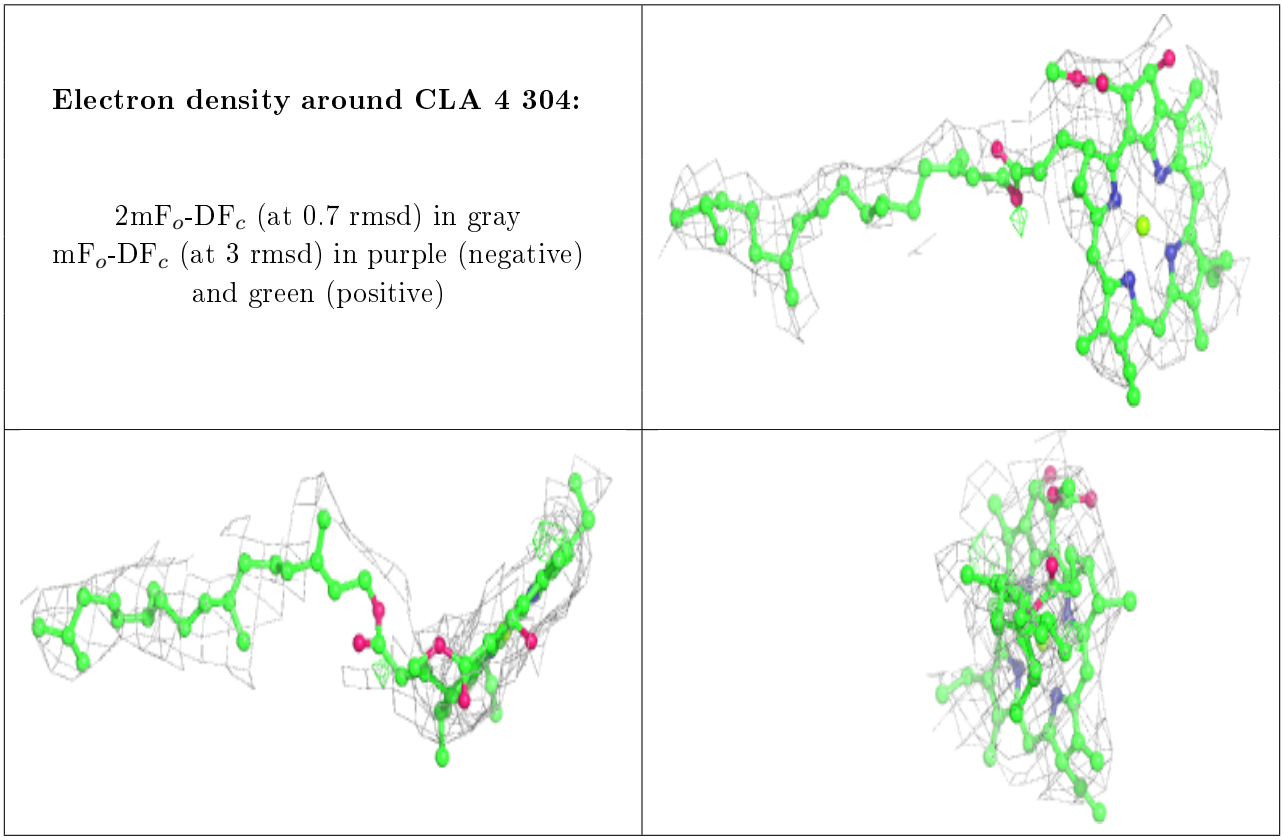
Electron density around BCR B 846:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



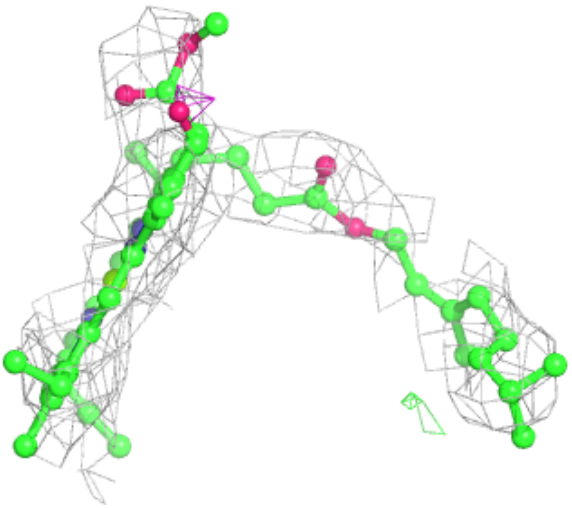
Electron density around CLA 4 304:

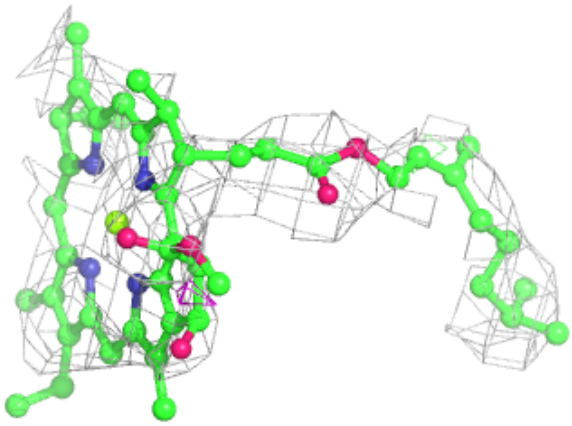
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

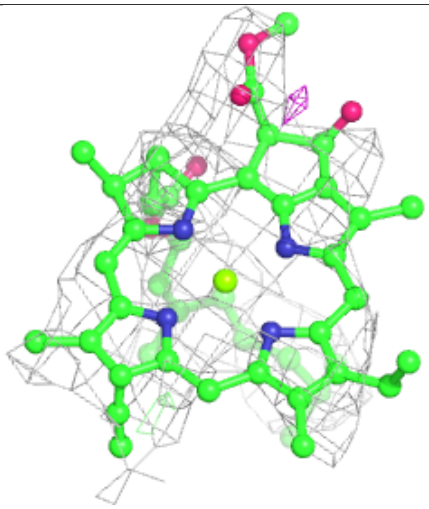


Electron density around CLA L 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

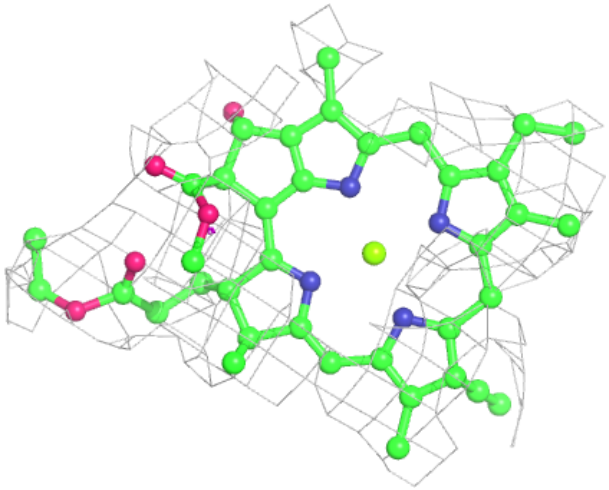


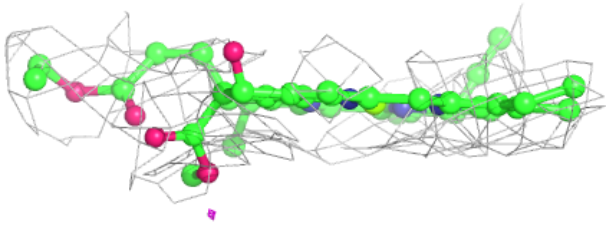


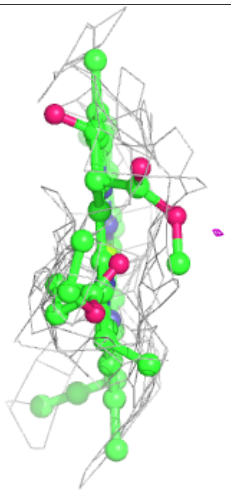


Electron density around CLA 4 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

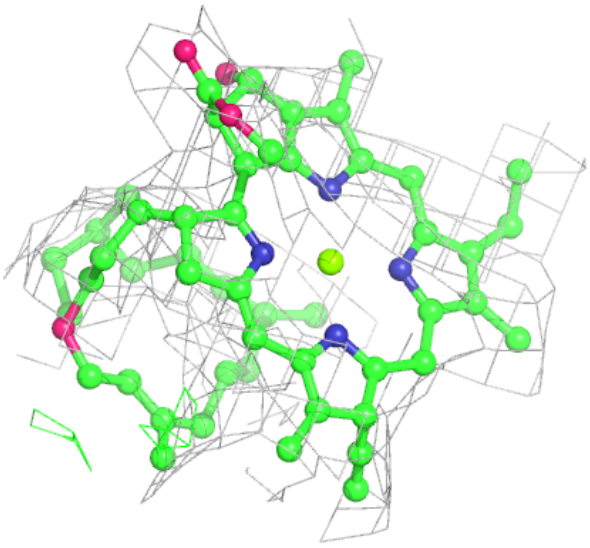


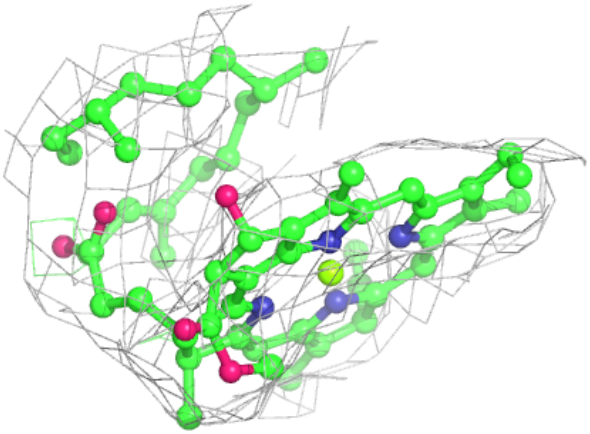


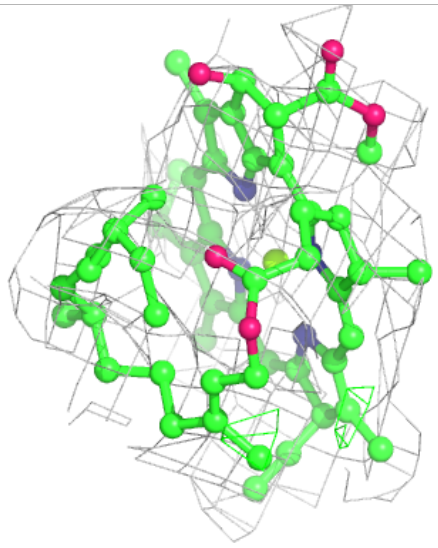


Electron density around CLA J 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

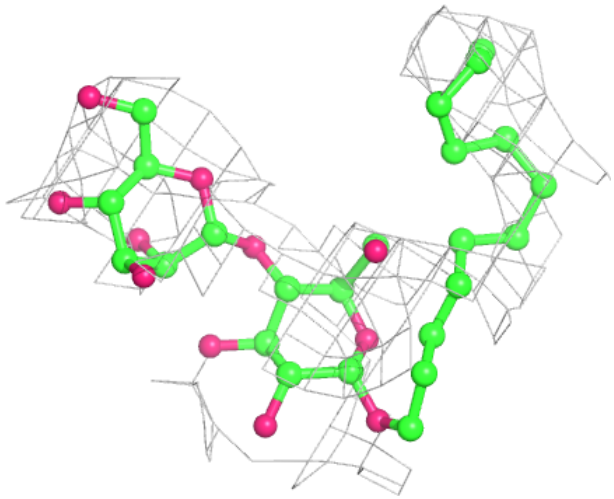


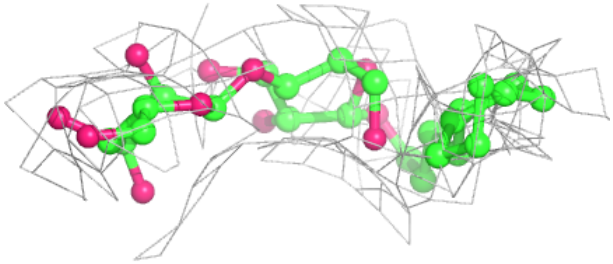


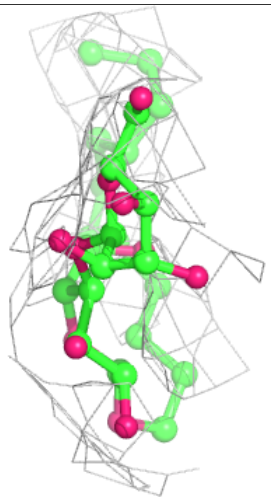


Electron density around LMU N 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

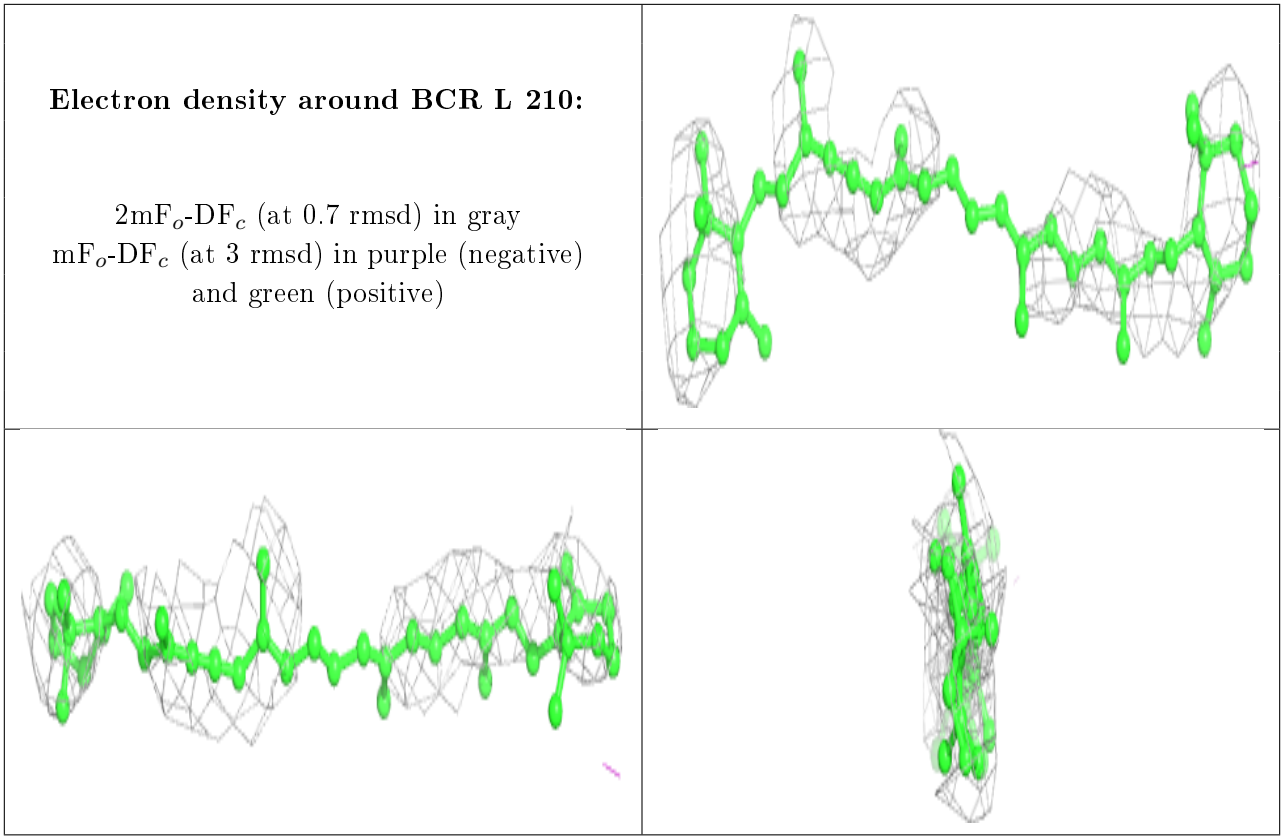






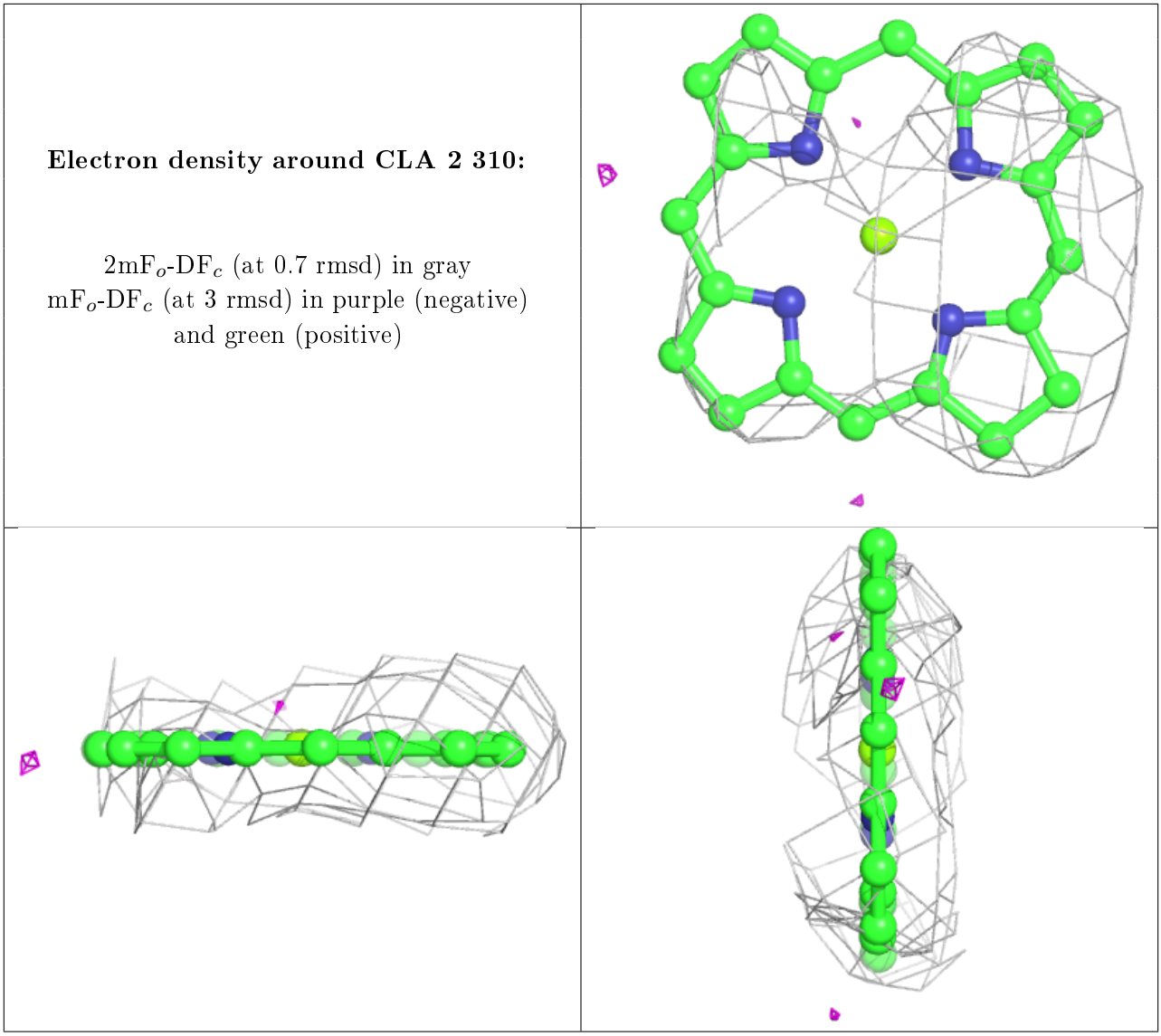
Electron density around BCR L 210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



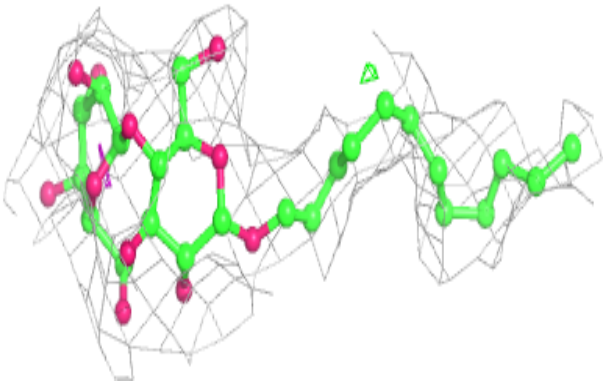
Electron density around CLA 2 310:

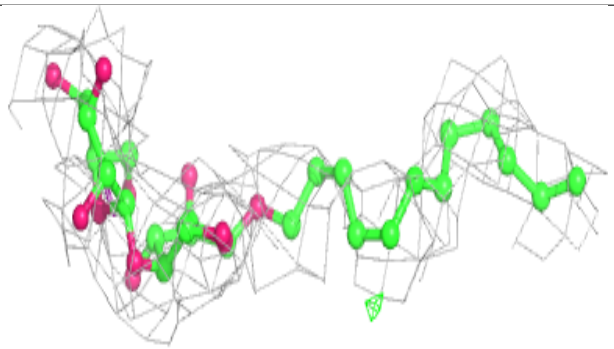
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

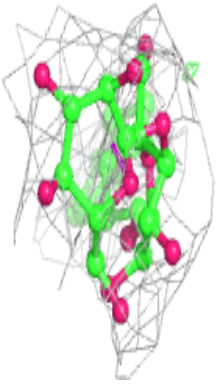


Electron density around LMU 1 219:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

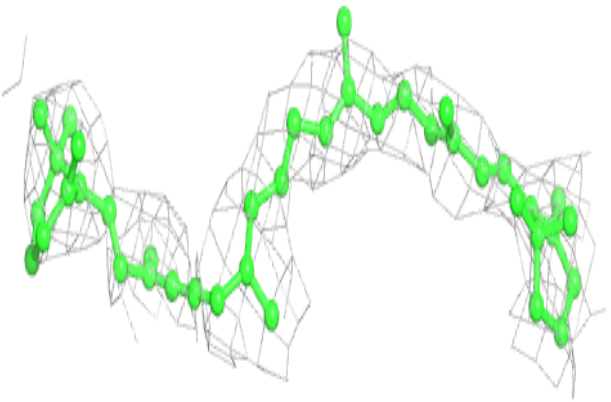


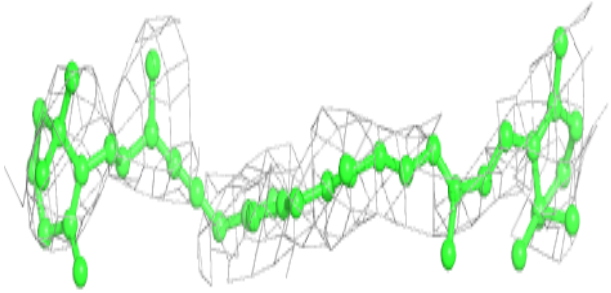


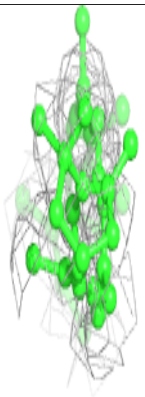


Electron density around BCR I 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

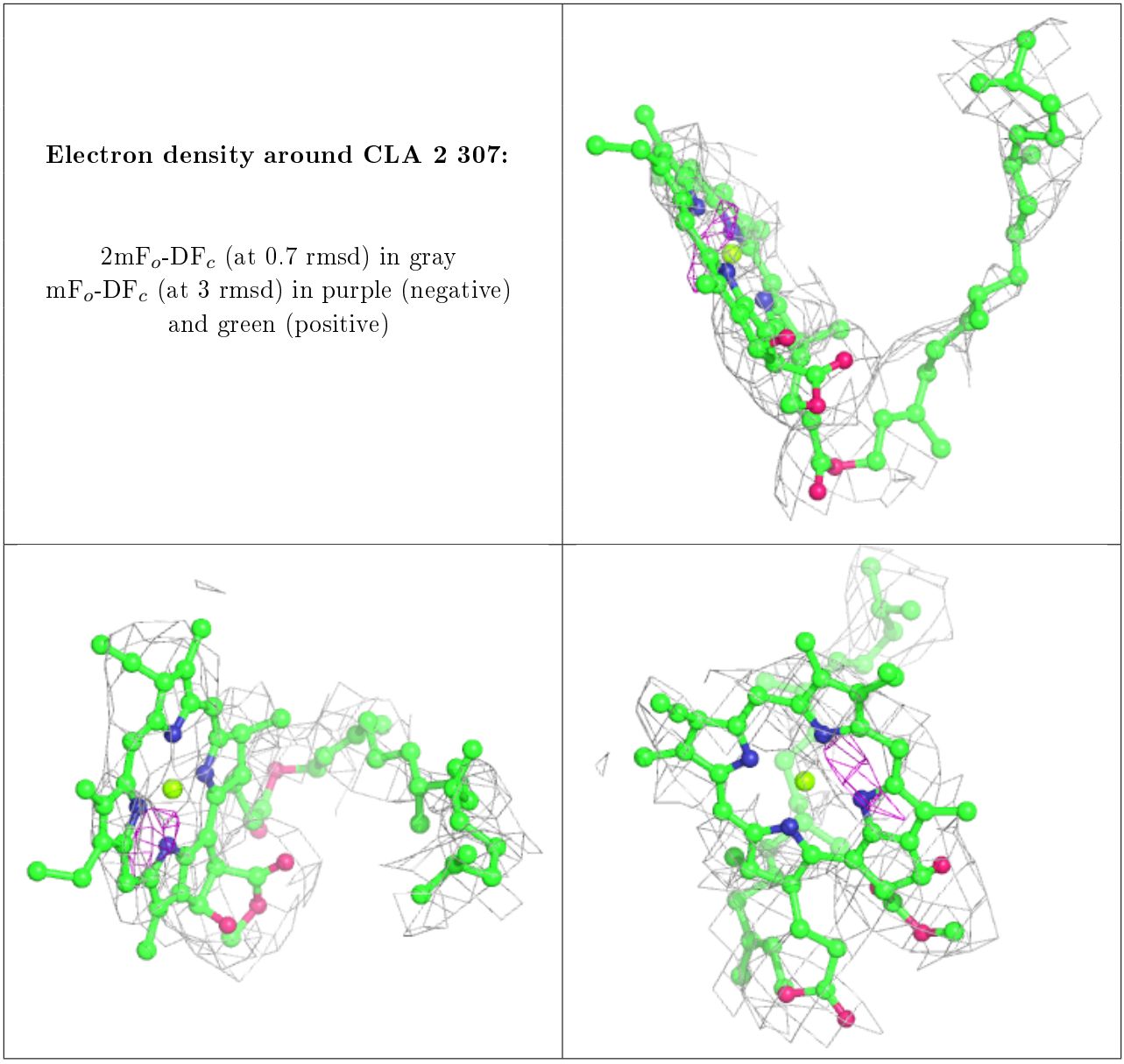






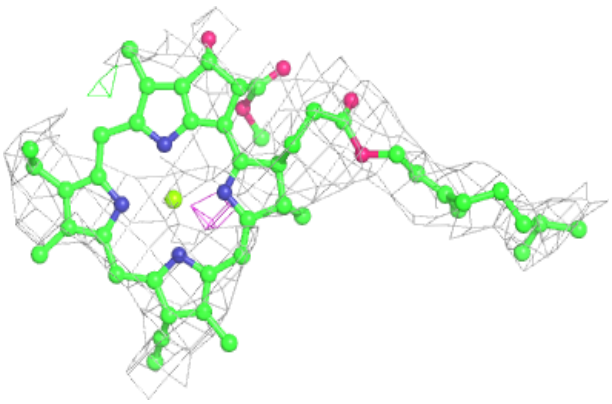
Electron density around CLA 2 307:

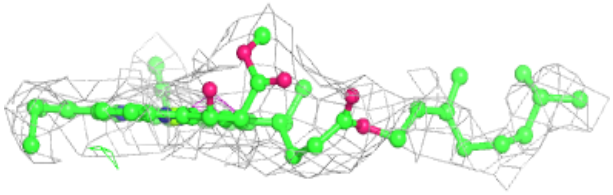
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

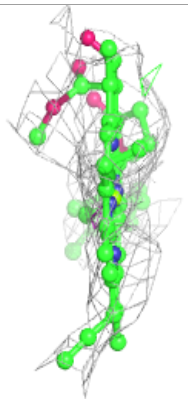


Electron density around CLA 4 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

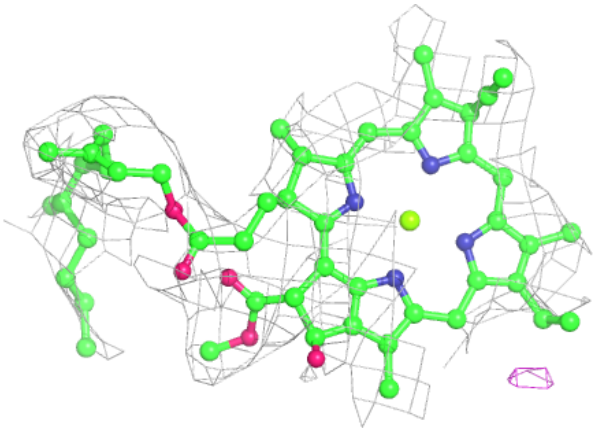


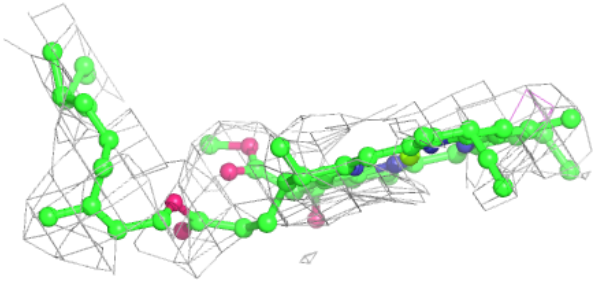


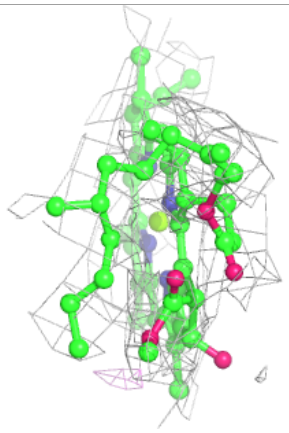


Electron density around CLA R 108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

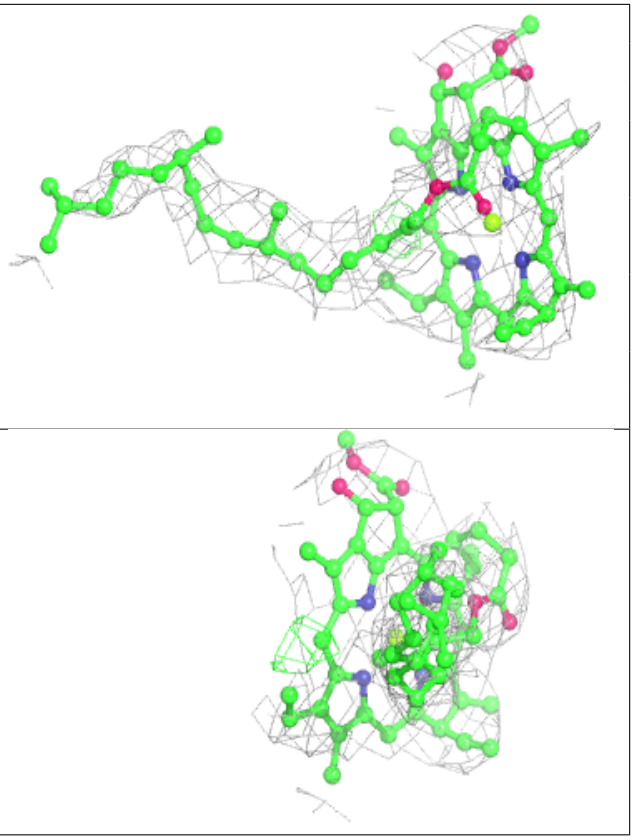






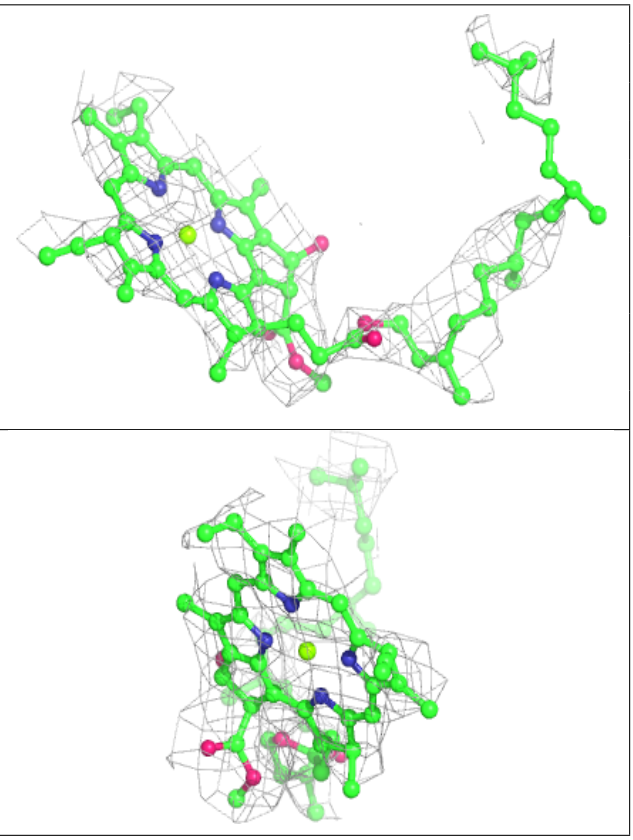
Electron density around CLA 2 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



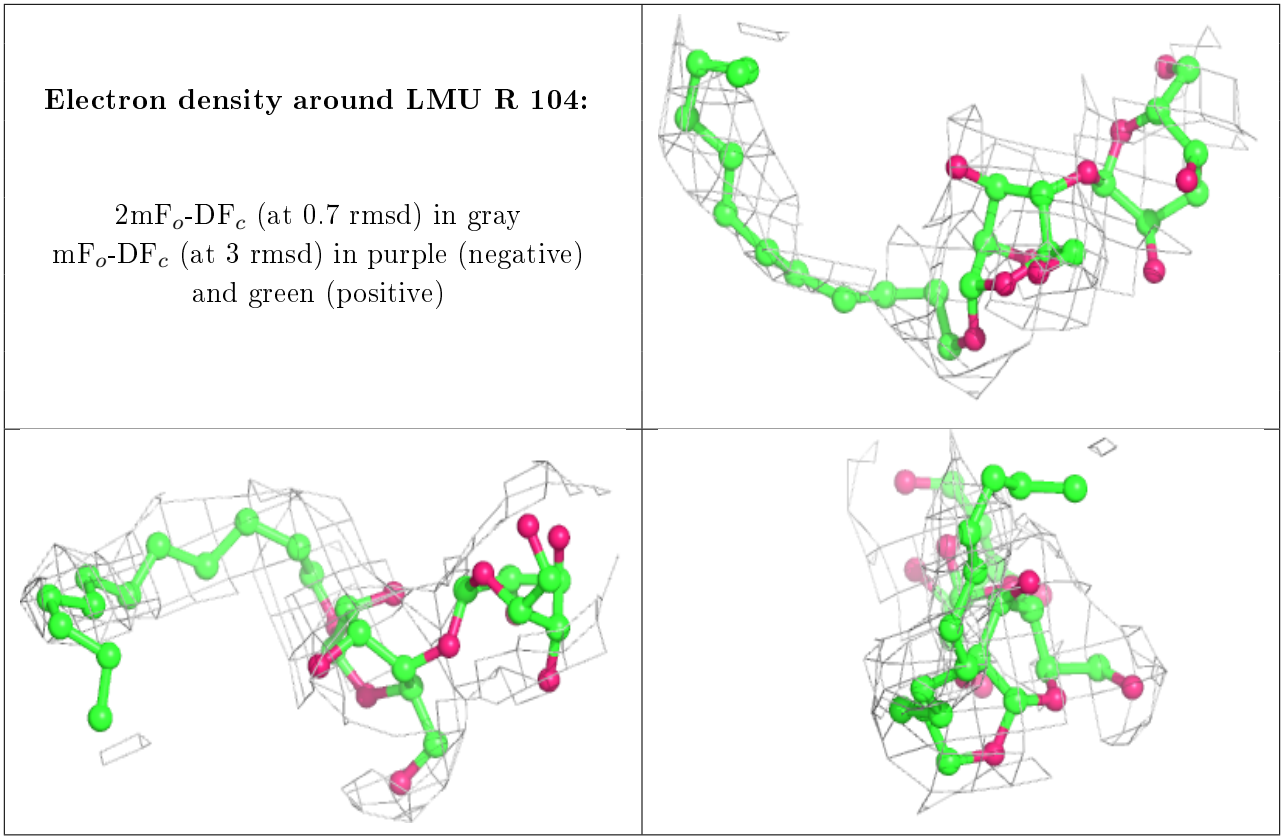
Electron density around CLA K 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



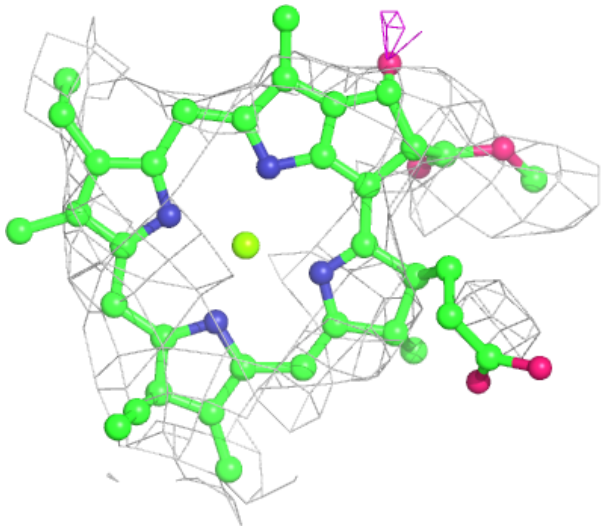
Electron density around LMU R 104:

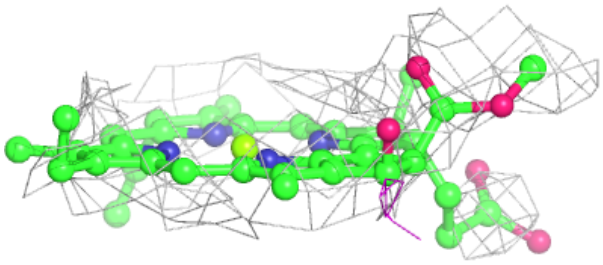
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

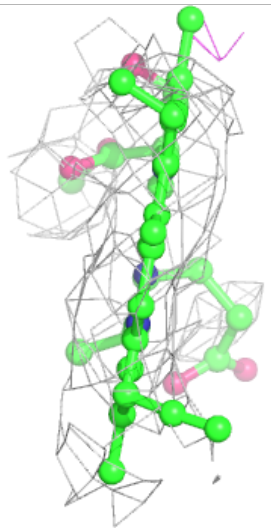


Electron density around CLA A 833:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

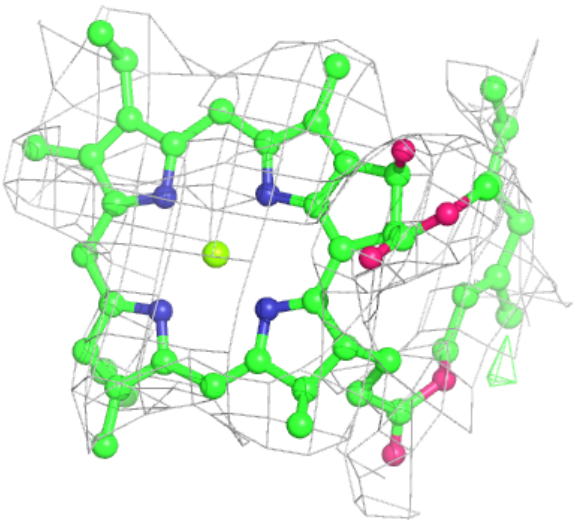


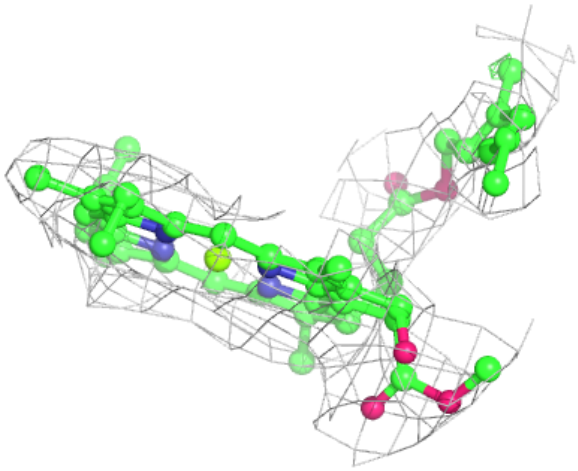


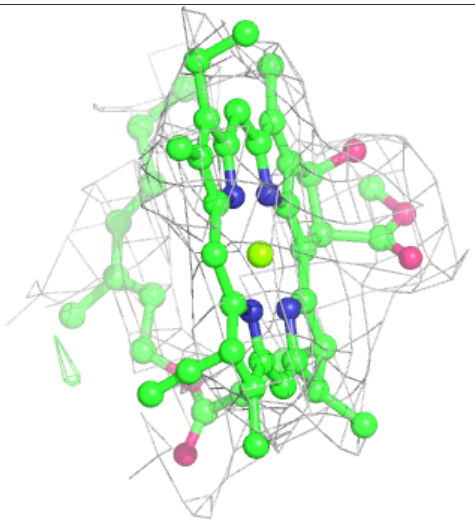


Electron density around CLA F 206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

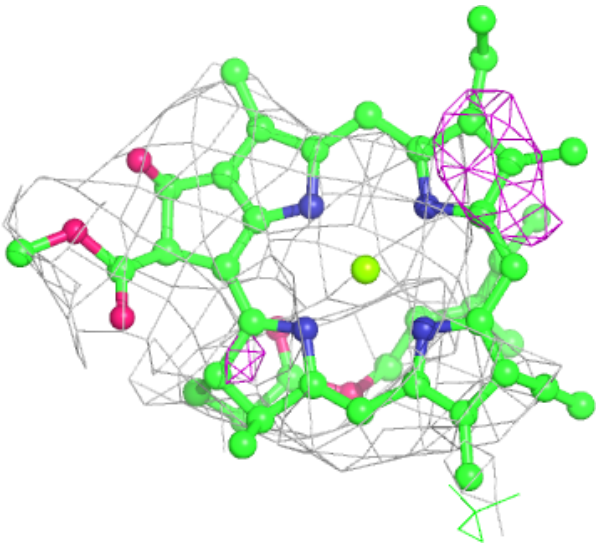


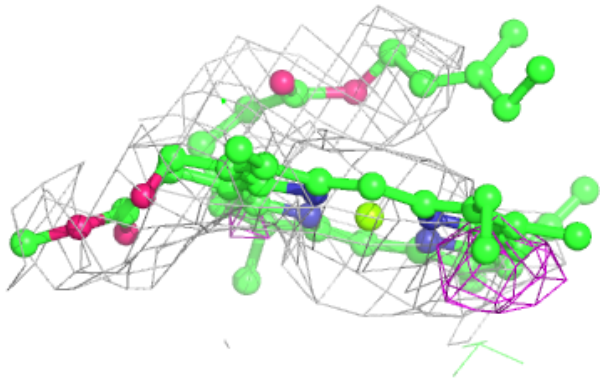




Electron density around CLA A 820:

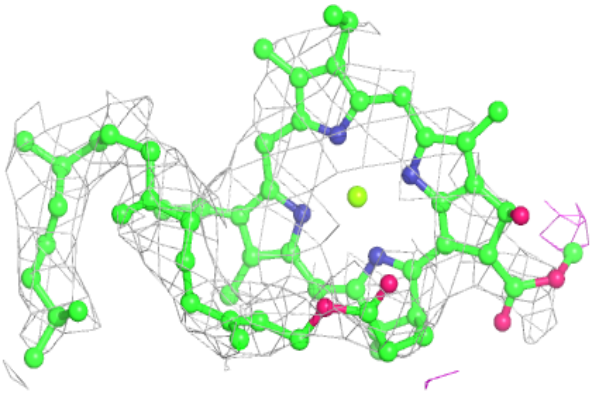
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

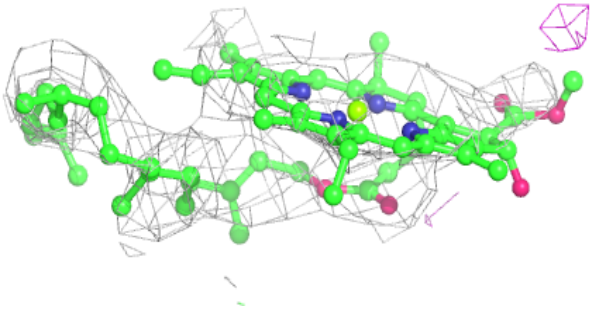


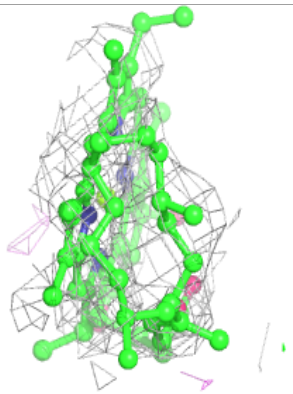


Electron density around CLA A 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

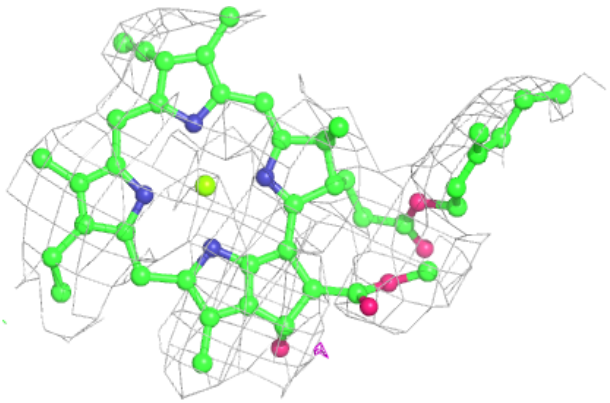


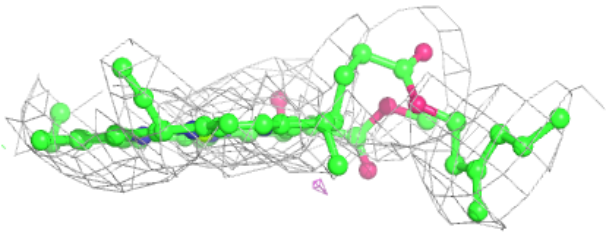


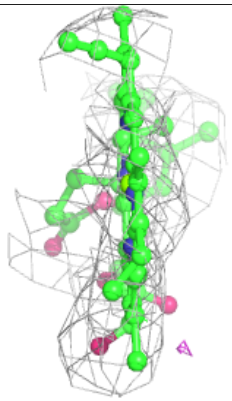


Electron density around CLA 4 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

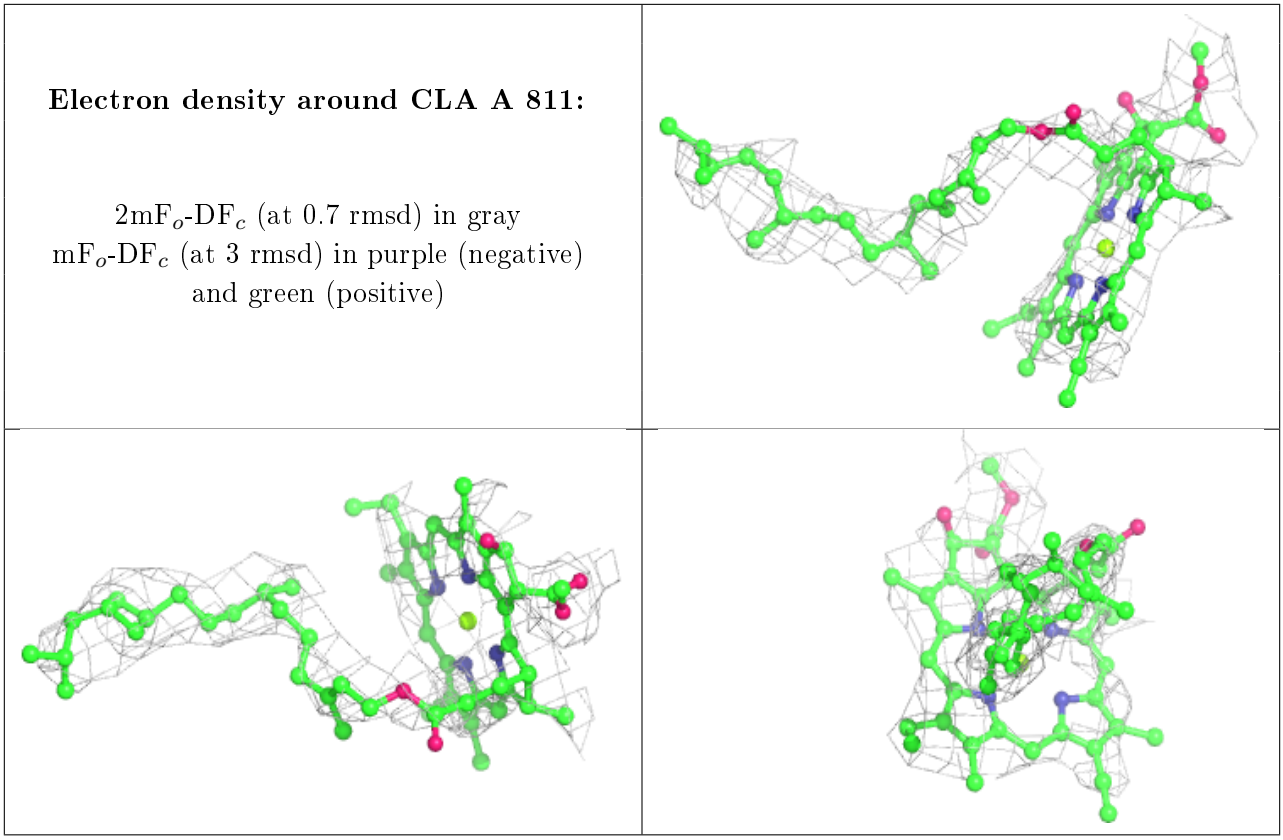






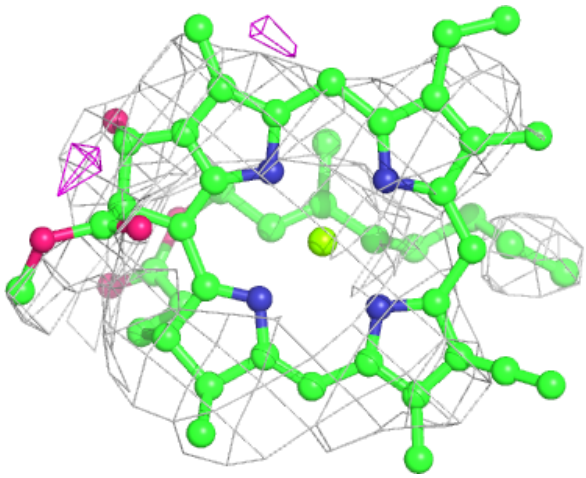
Electron density around CLA A 811:

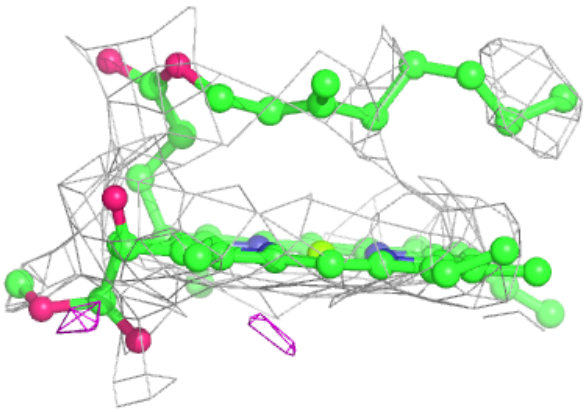
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

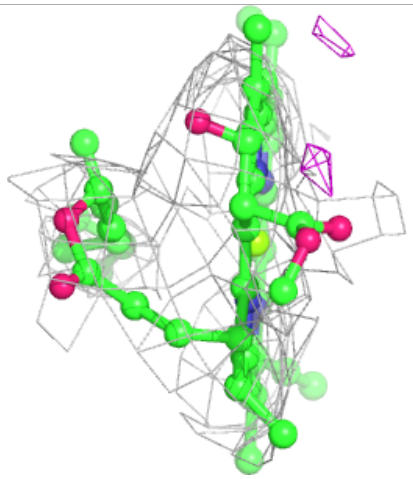


Electron density around CLA A 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

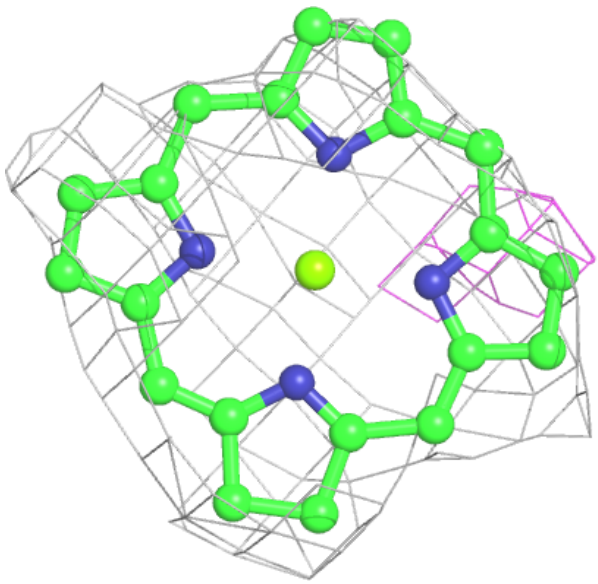


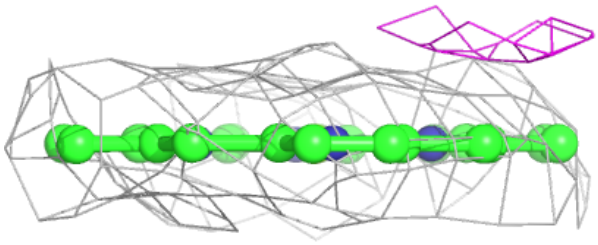


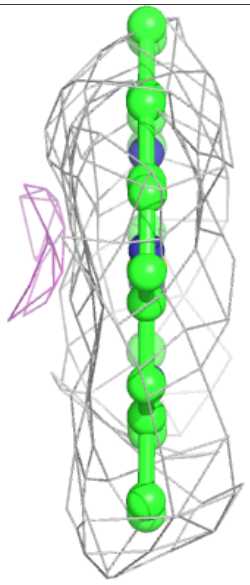


Electron density around CLA 2 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

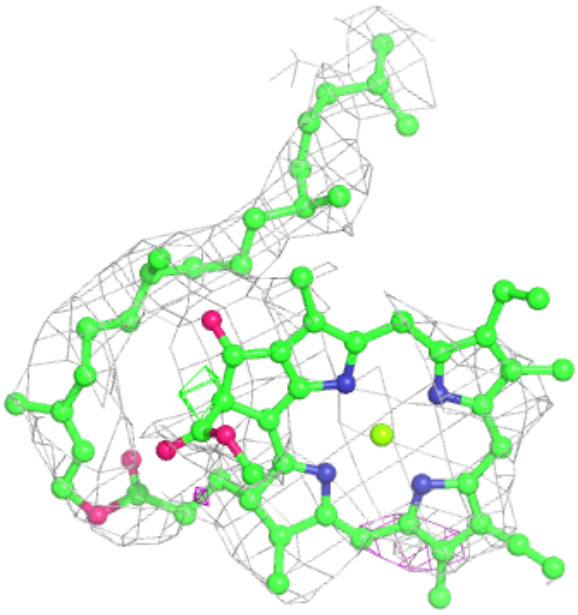


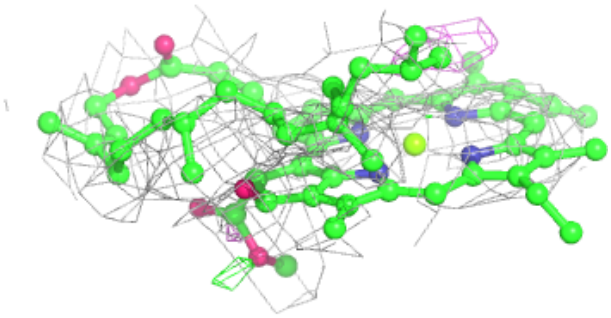


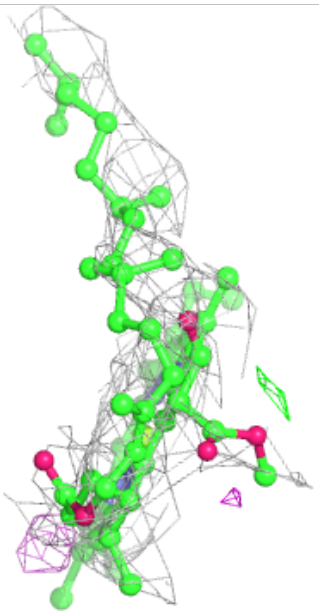


Electron density around CLA A 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

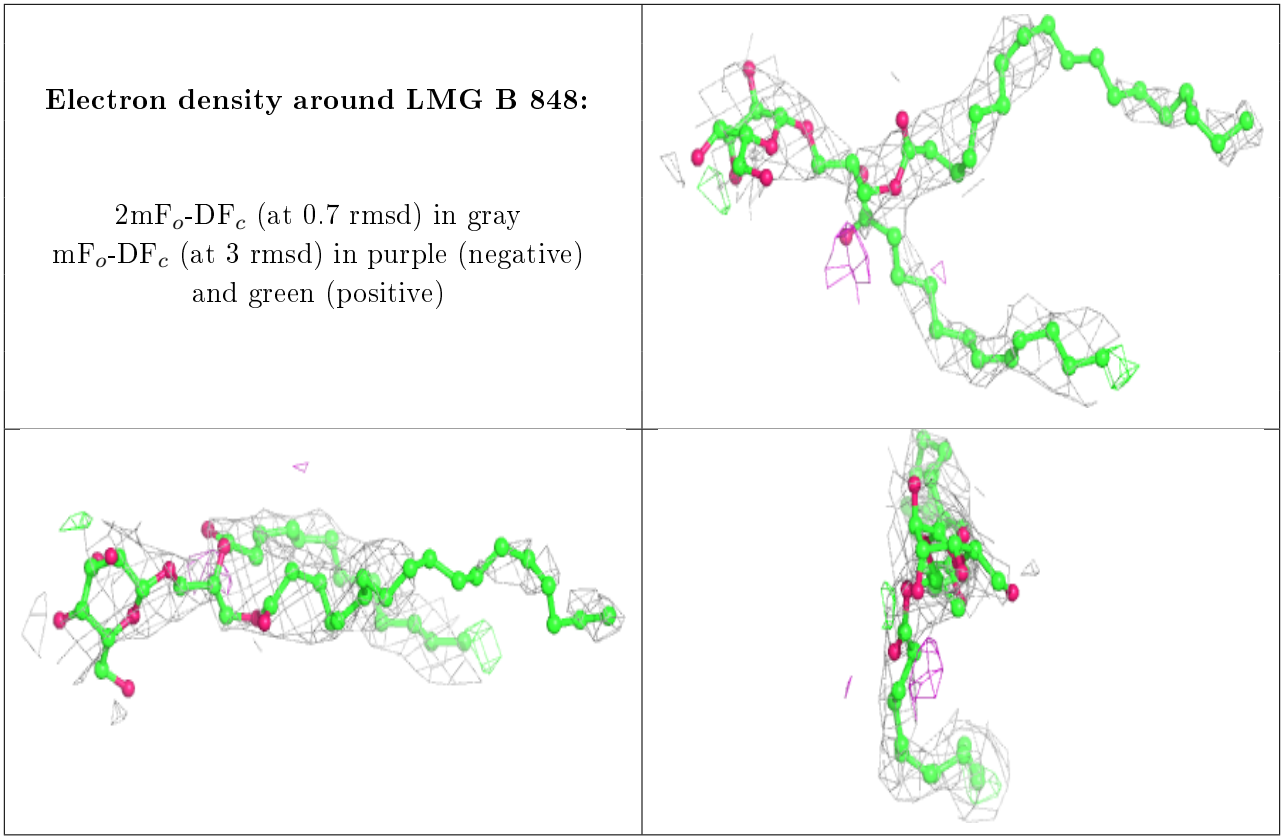






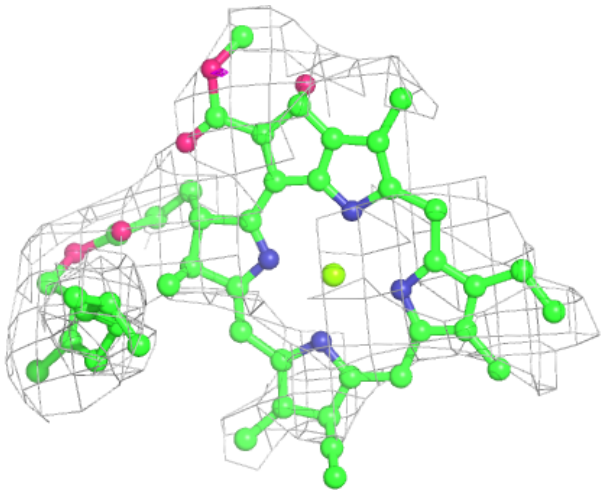
Electron density around LMG B 848:

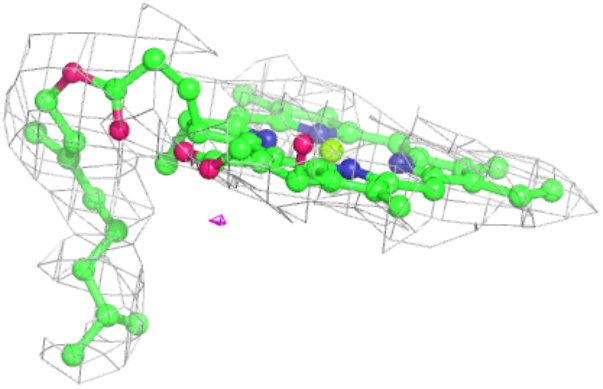
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

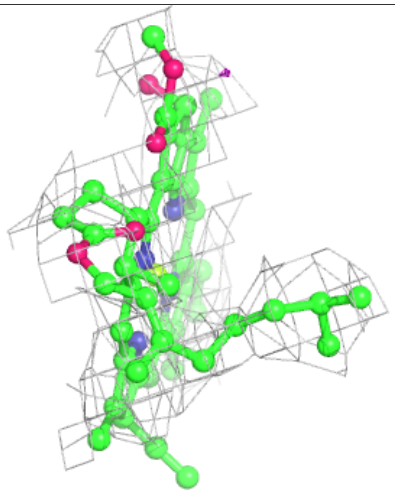


Electron density around CLA H 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

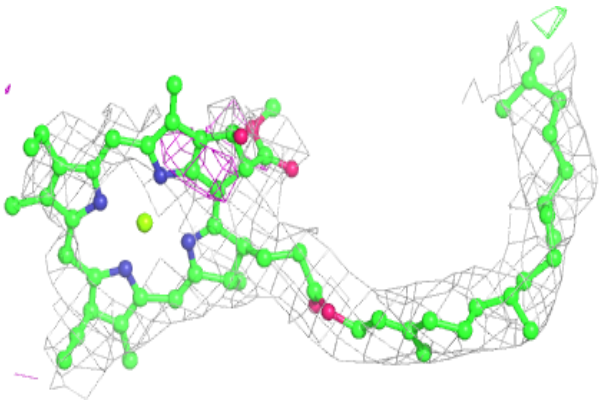


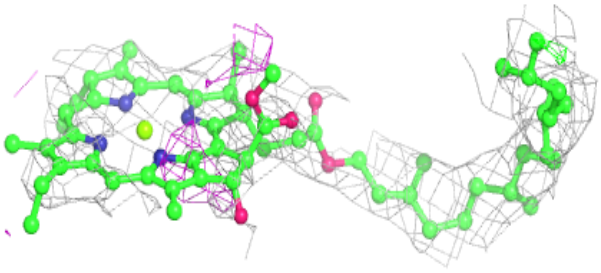


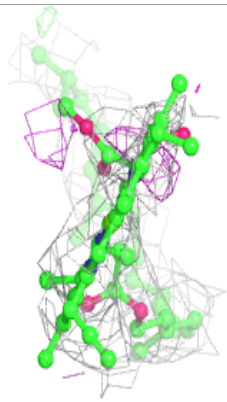


Electron density around CLA B 824:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

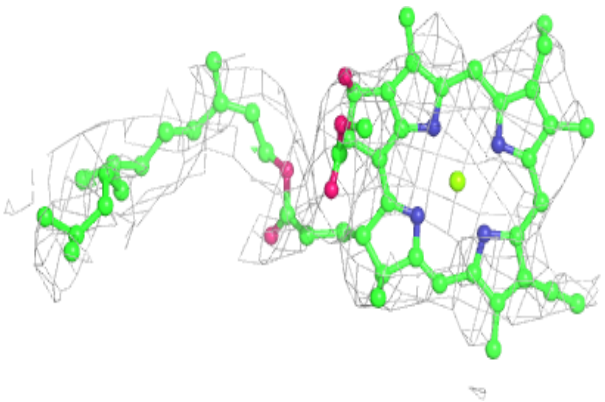


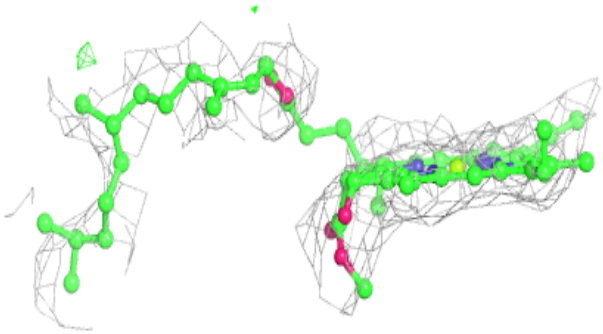


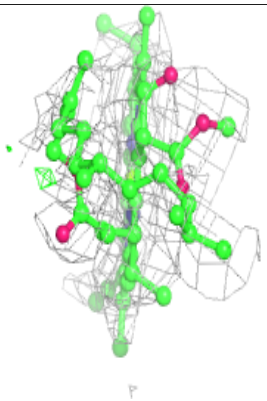


Electron density around CLA B 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

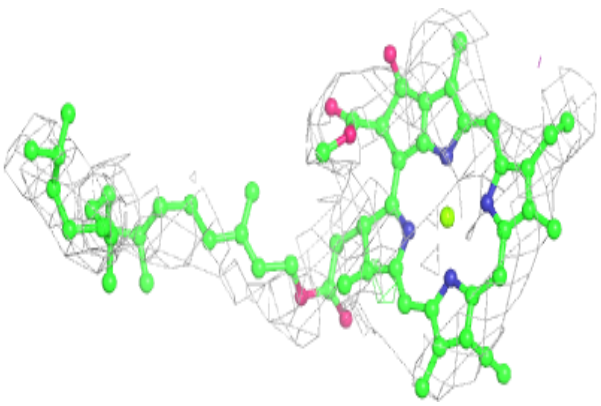


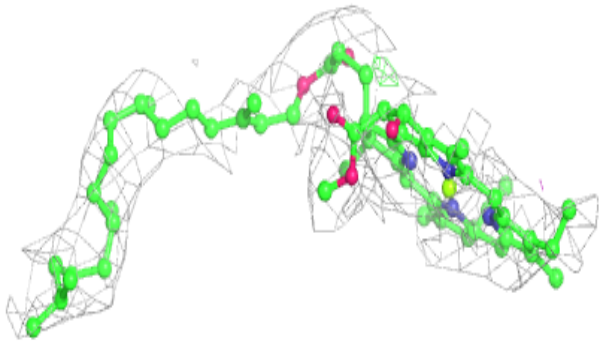


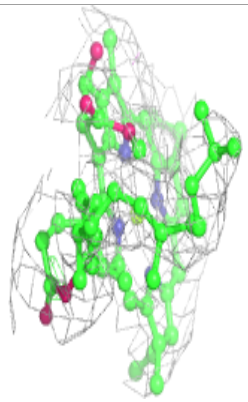


Electron density around CLA 3 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

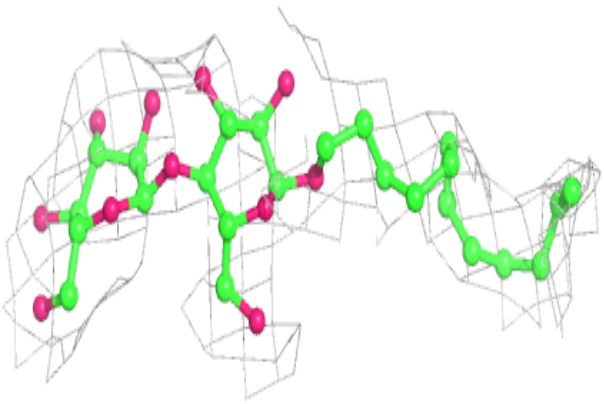


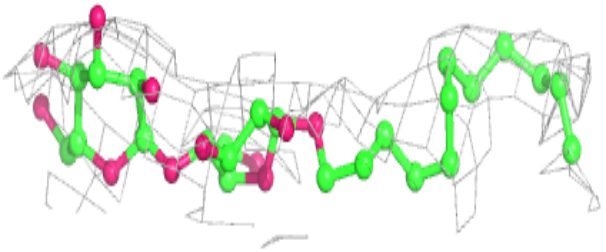




Electron density around LMU 3 322:

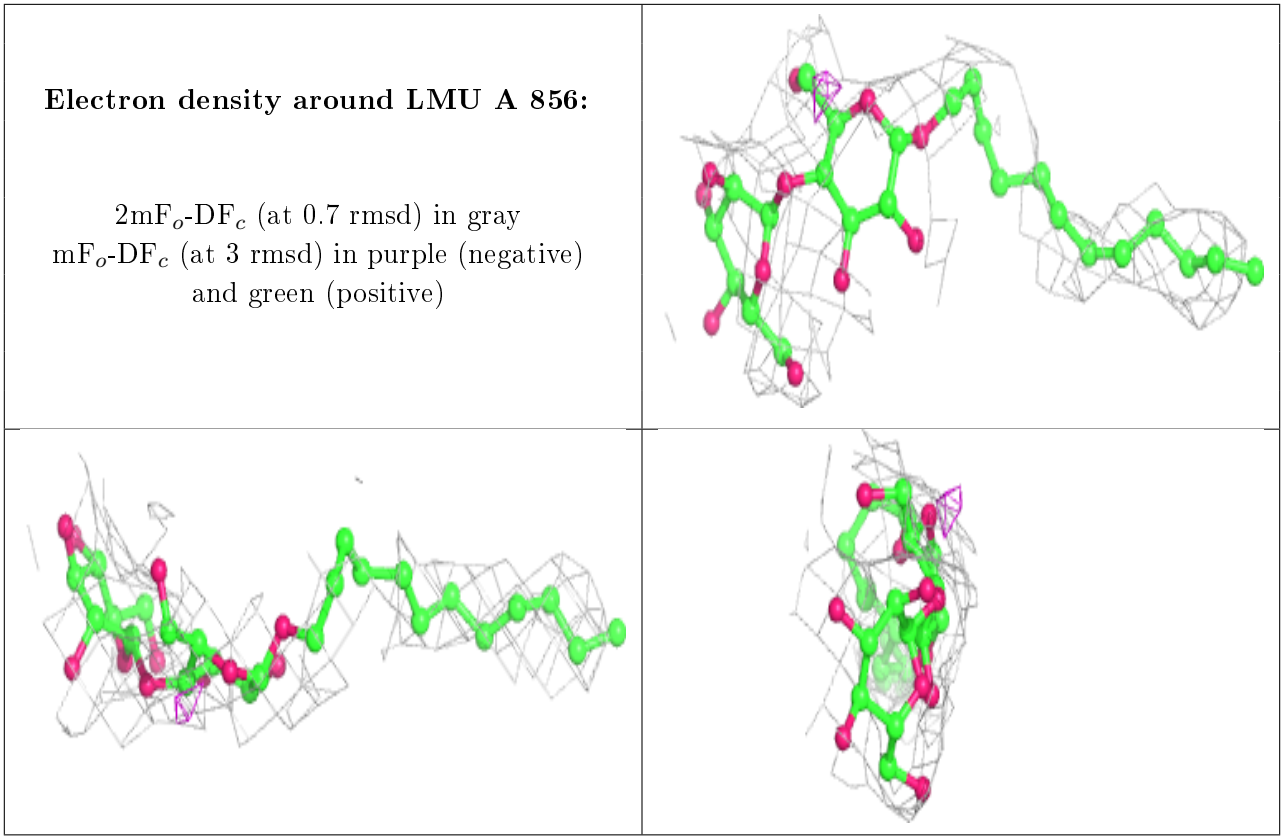
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





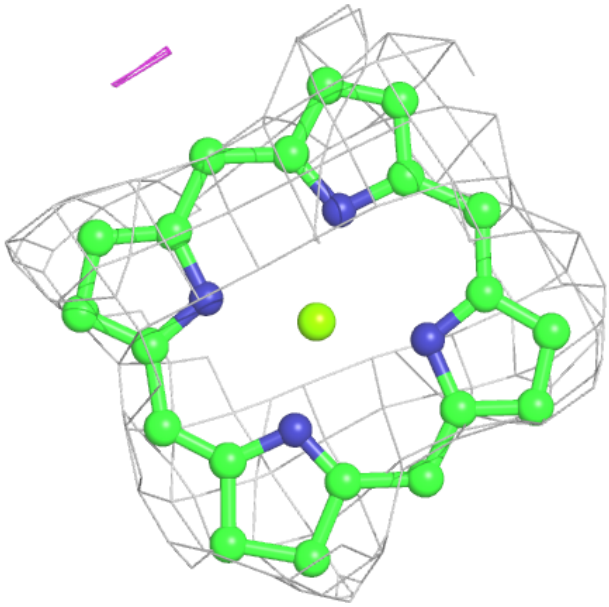
Electron density around LMU A 856:

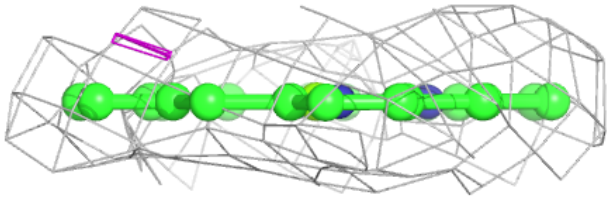
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

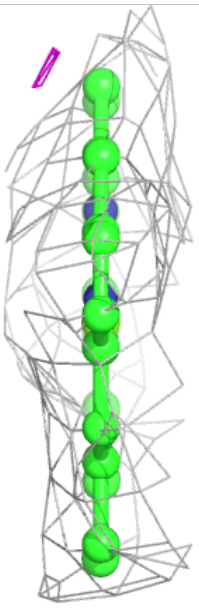


Electron density around CLA 1 216:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

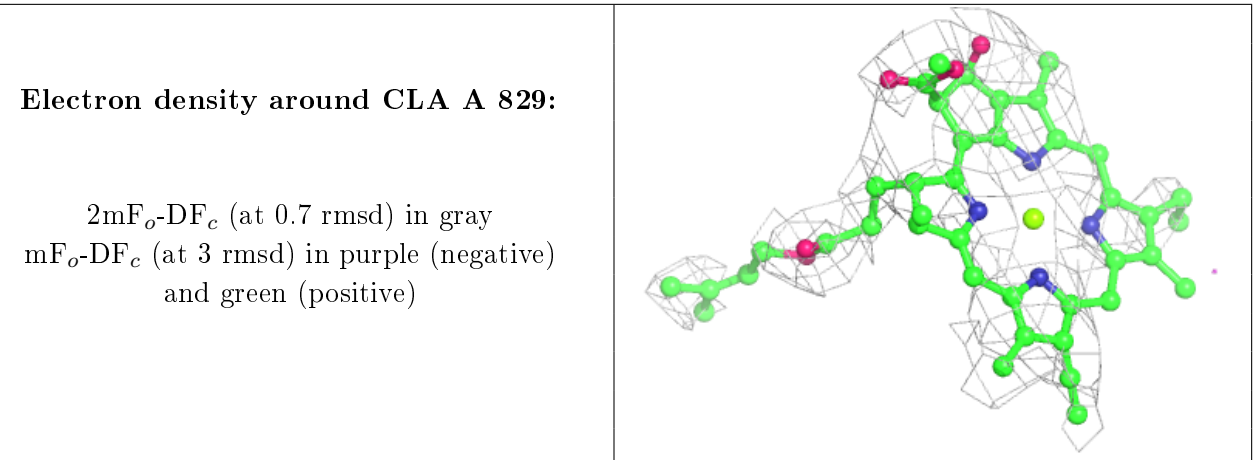


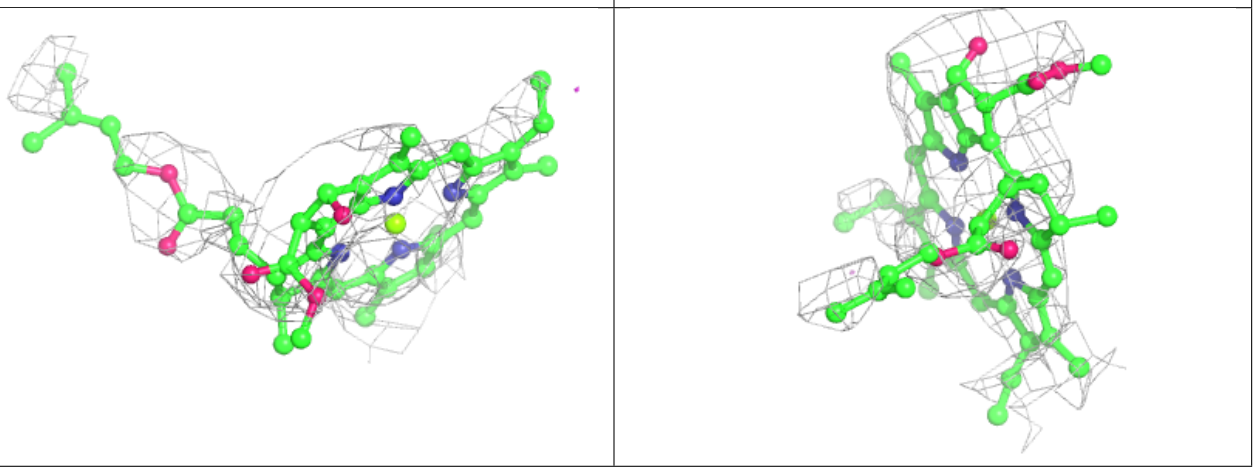




Electron density around CLA A 829:

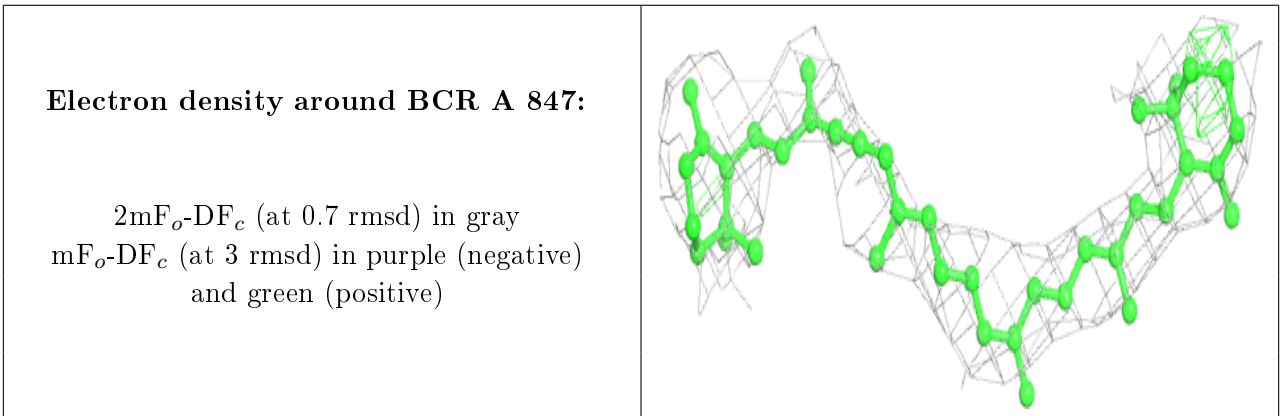
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

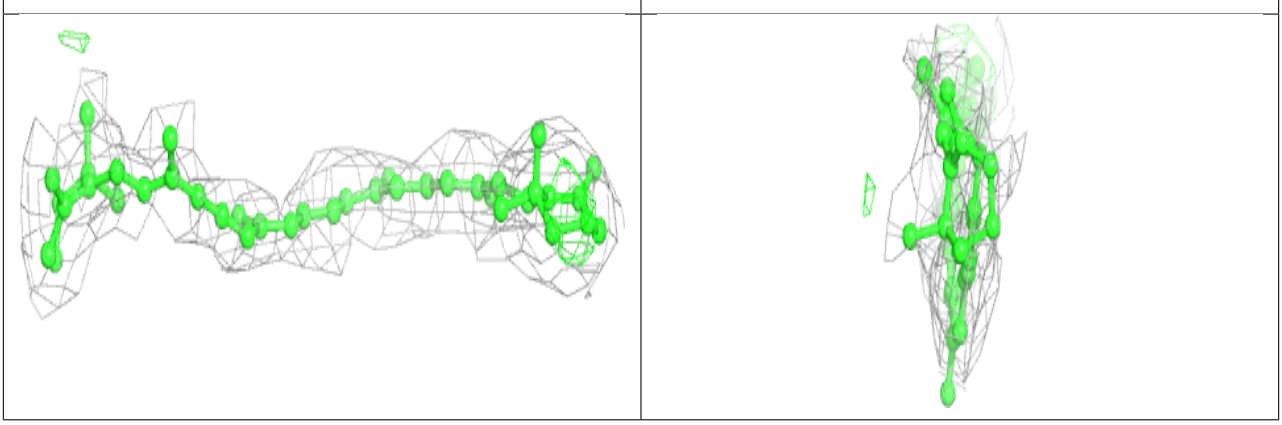




Electron density around BCR A 847:

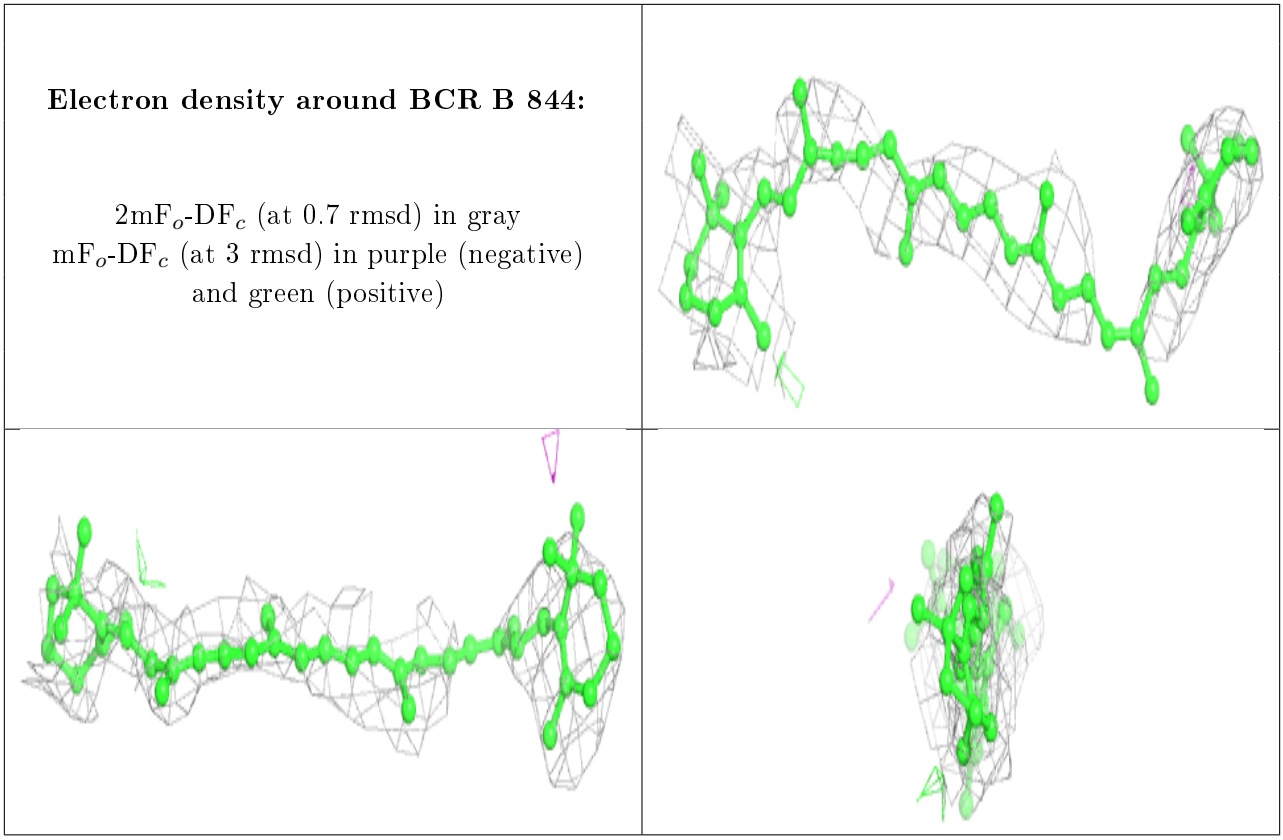
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





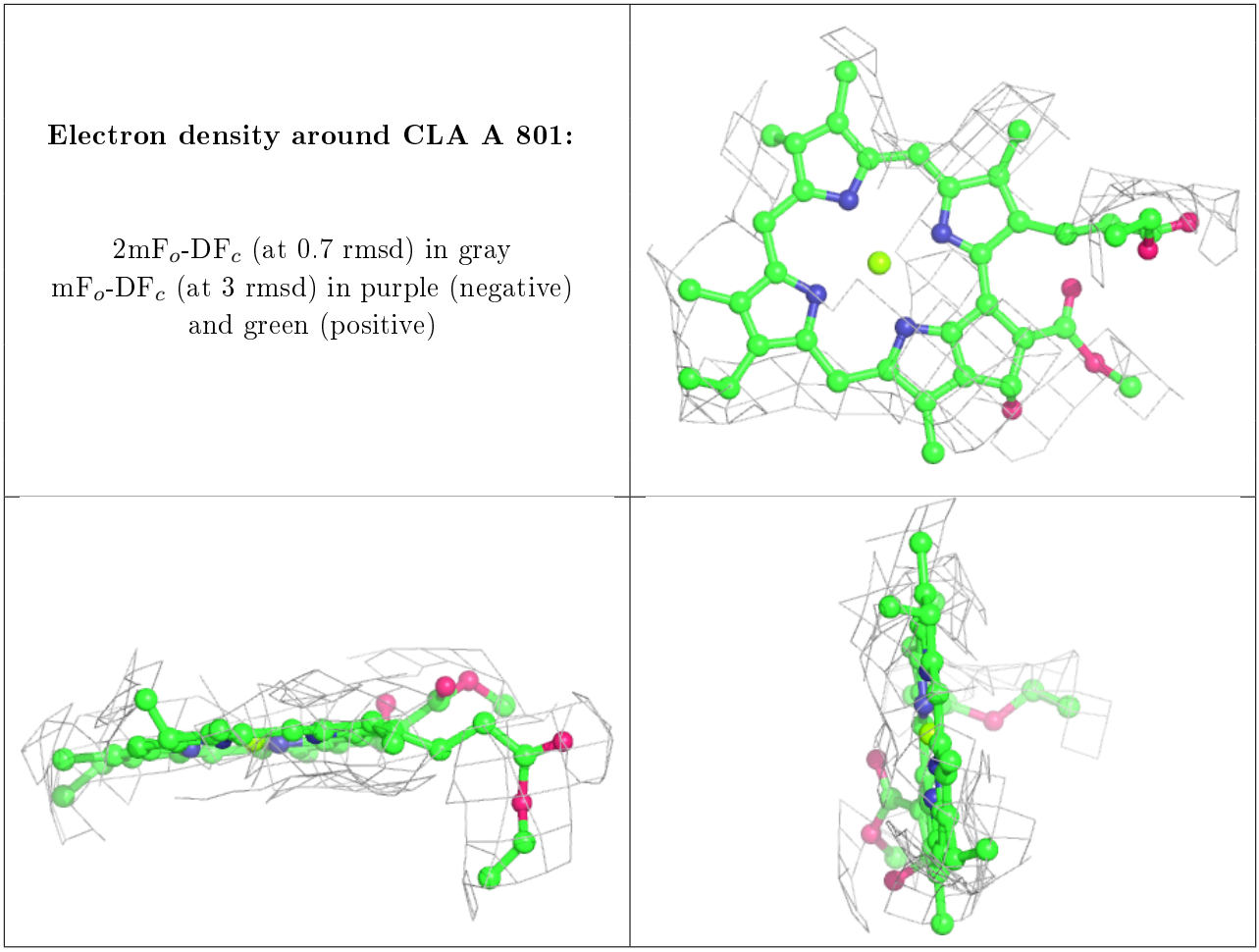
Electron density around BCR B 844:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



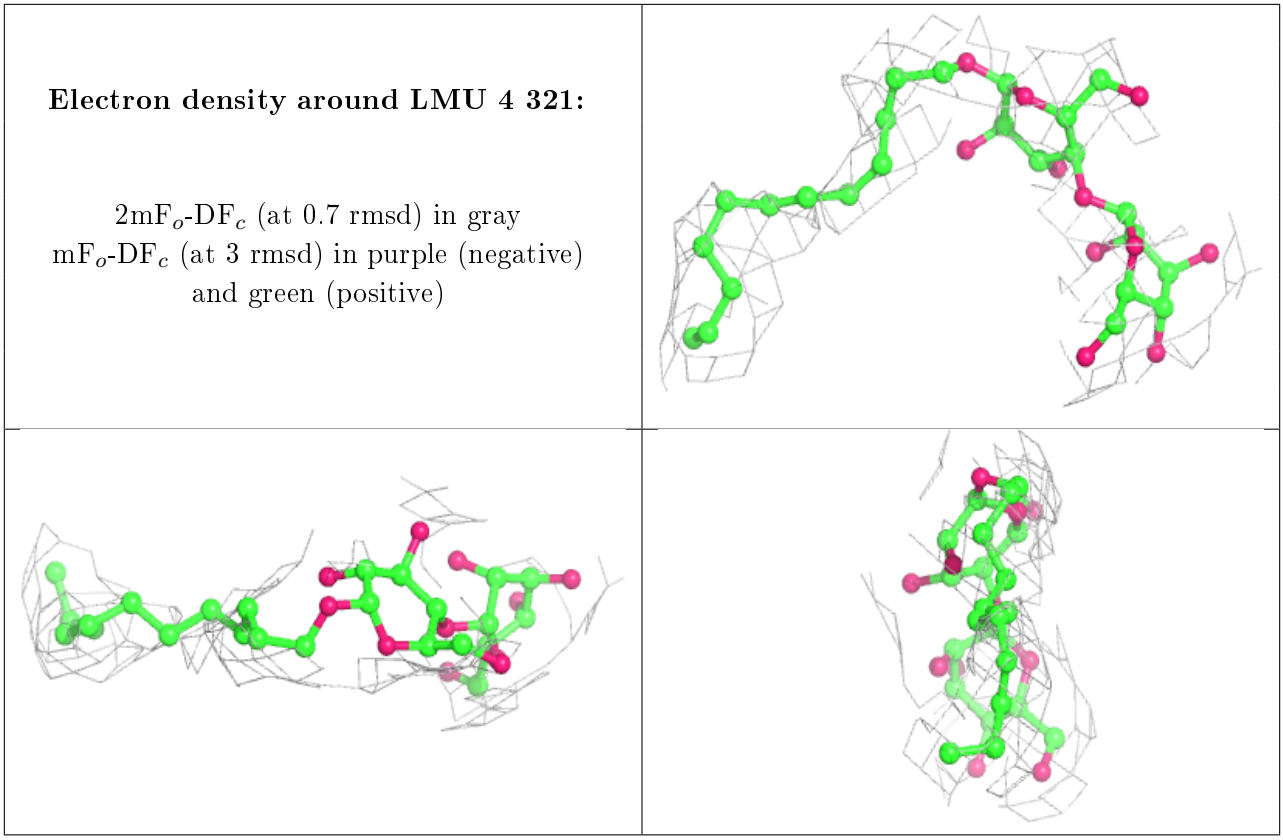
Electron density around CLA A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



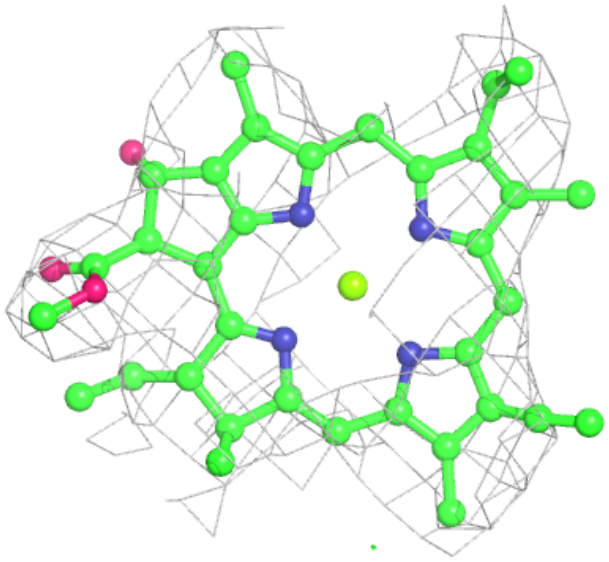
Electron density around LMU 4 321:

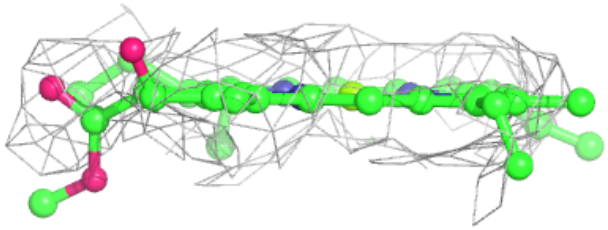
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

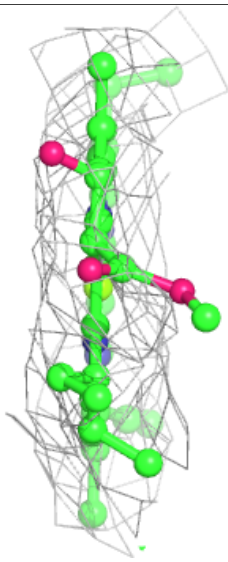


Electron density around CLA A 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

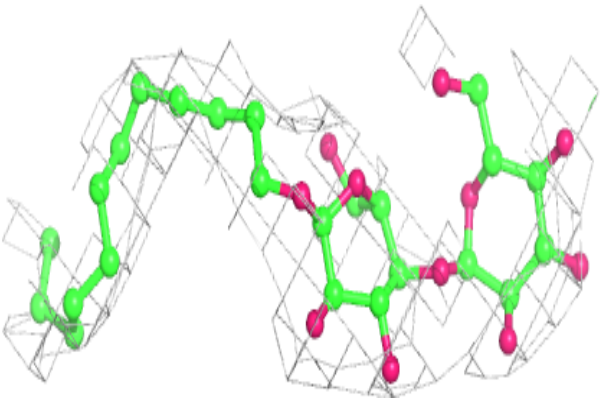


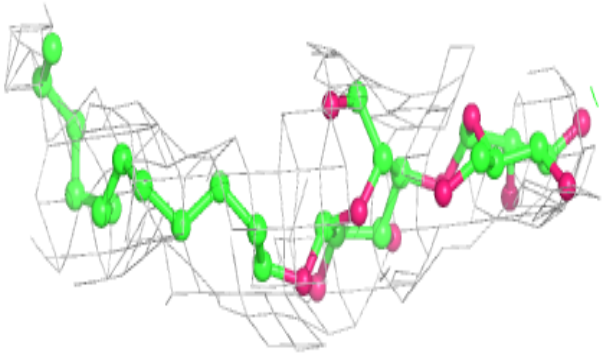


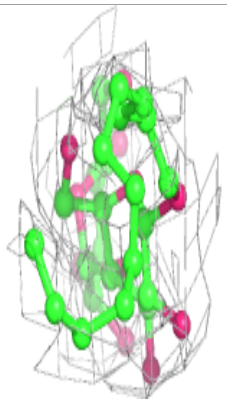


Electron density around LMU C 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

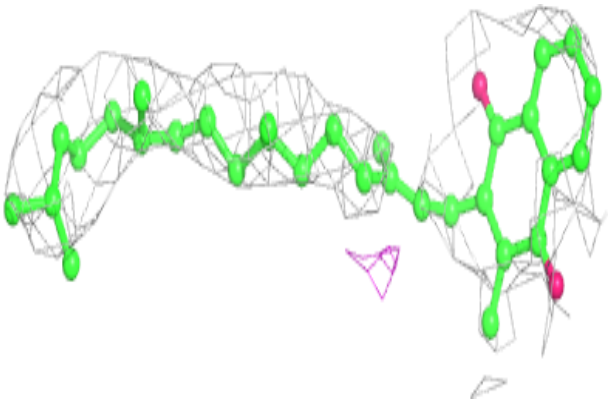


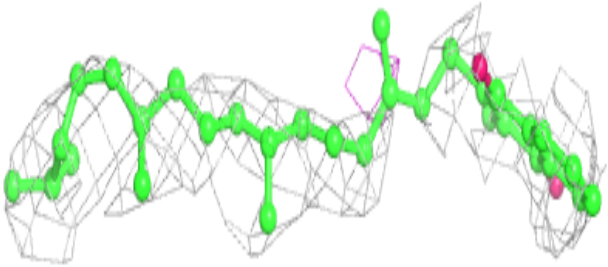


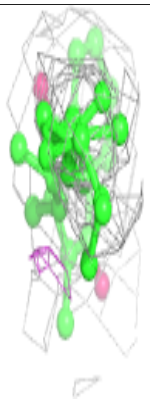


Electron density around PQN A 842:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

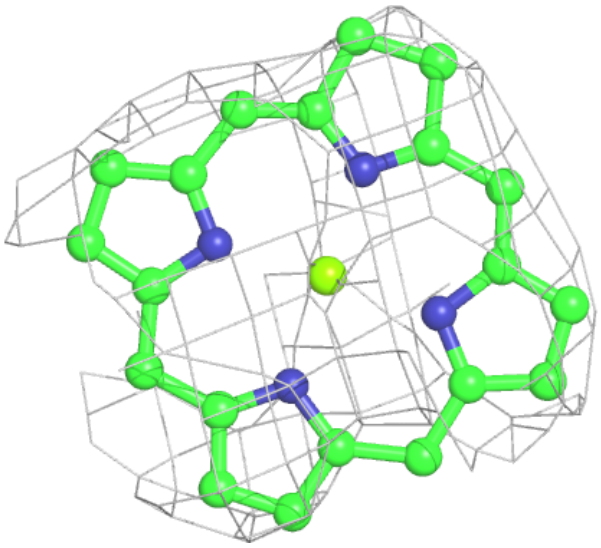


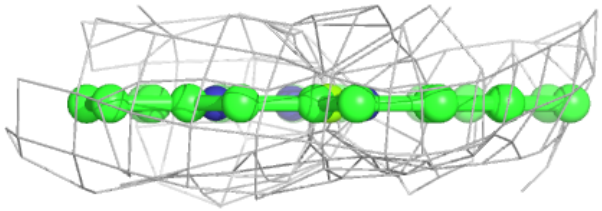


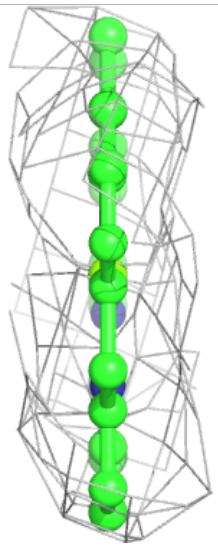


Electron density around CLA 3 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

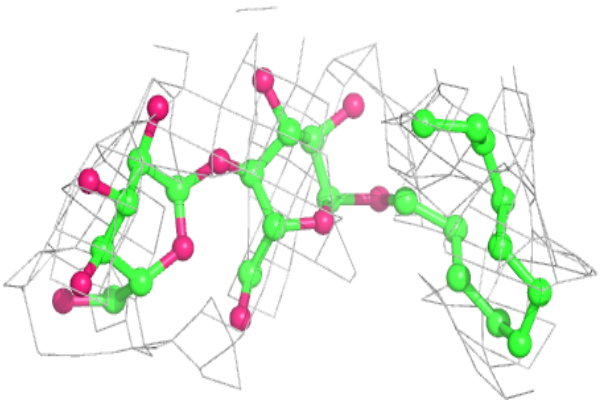


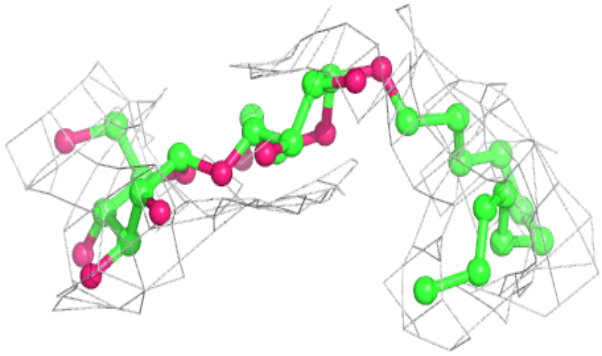


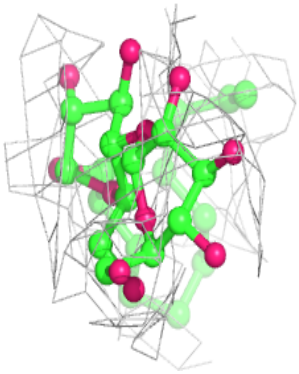


Electron density around LMU F 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

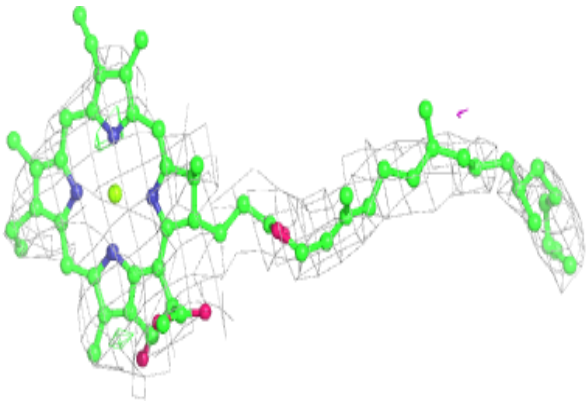


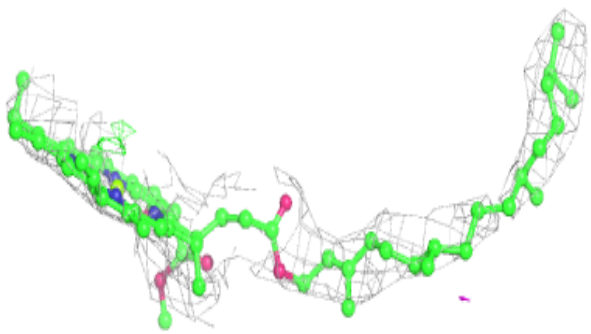


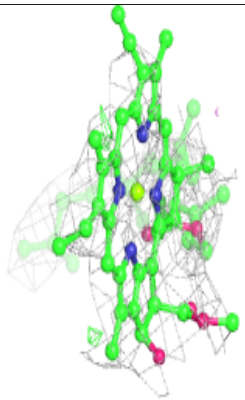


Electron density around CLA A 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

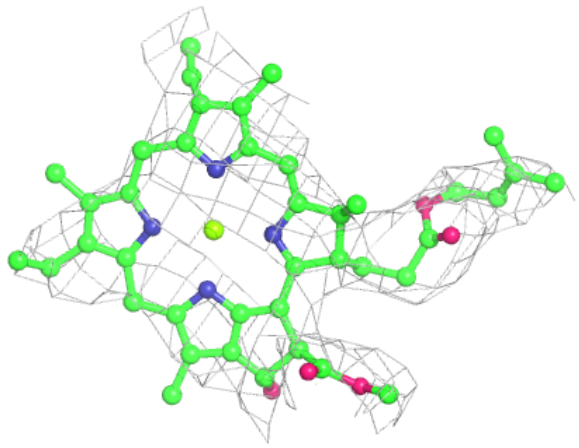


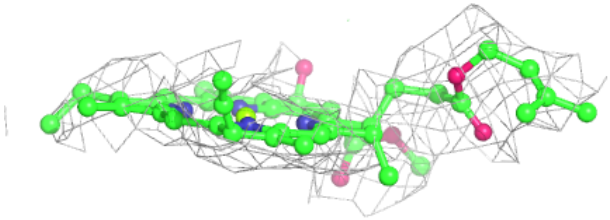


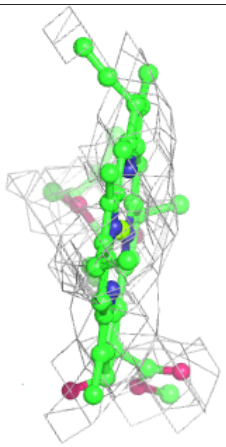


Electron density around CLA 2 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

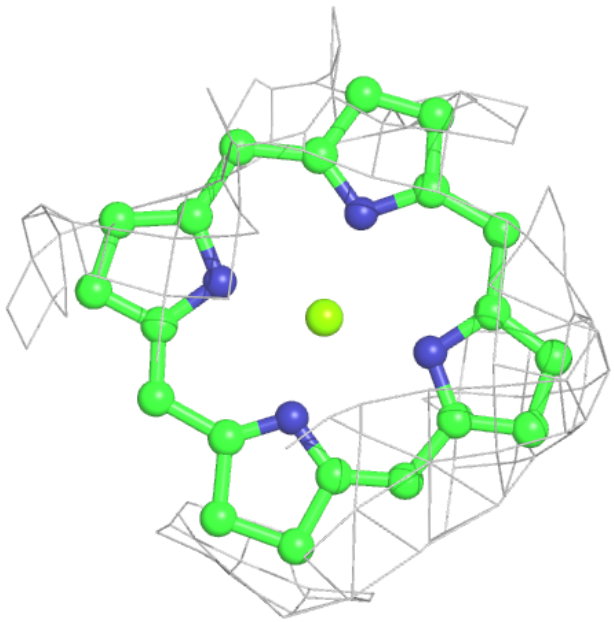


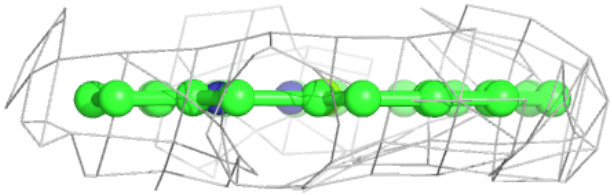


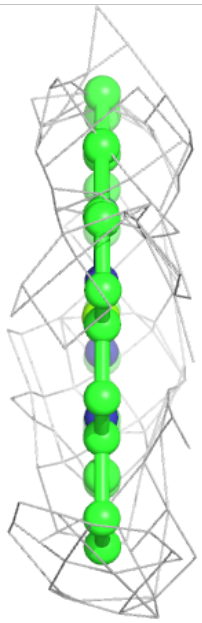


Electron density around CLA 3 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

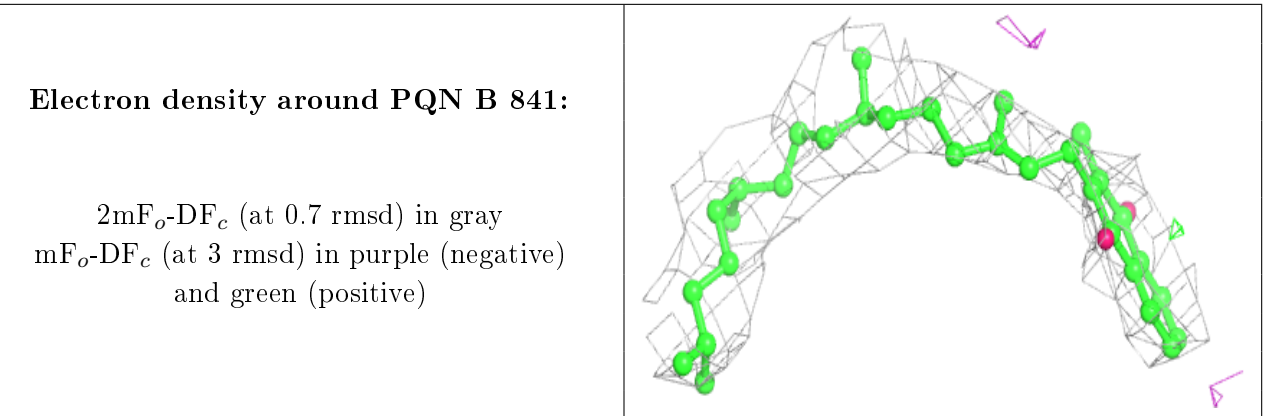


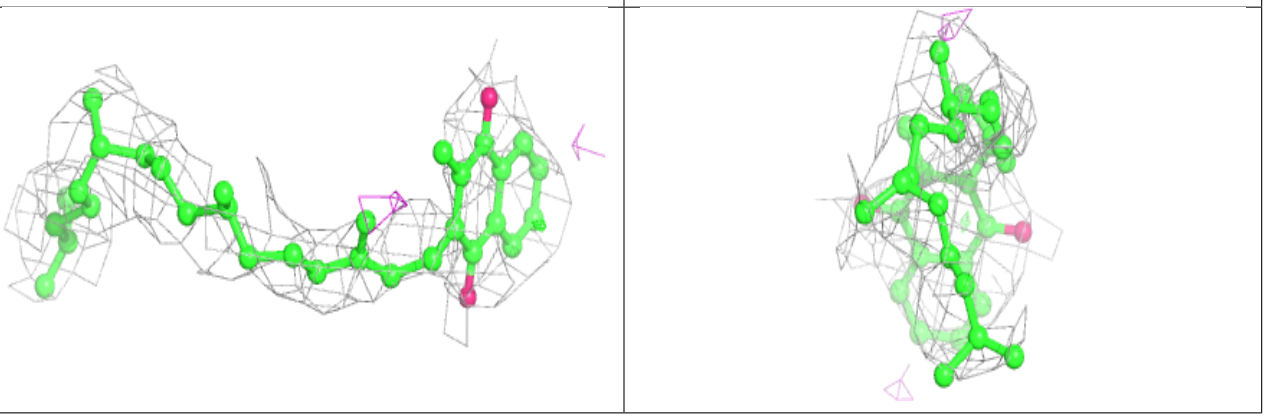




Electron density around PQN B 841:

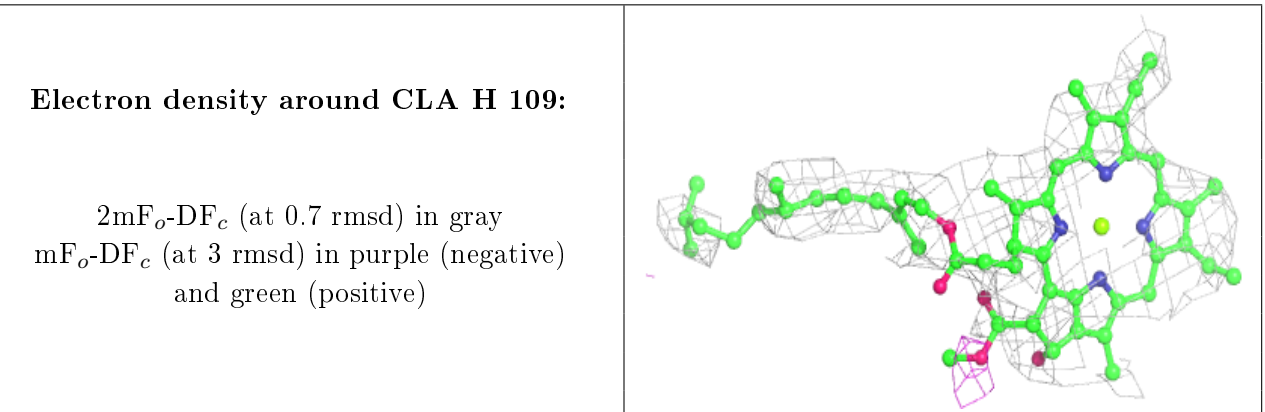
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

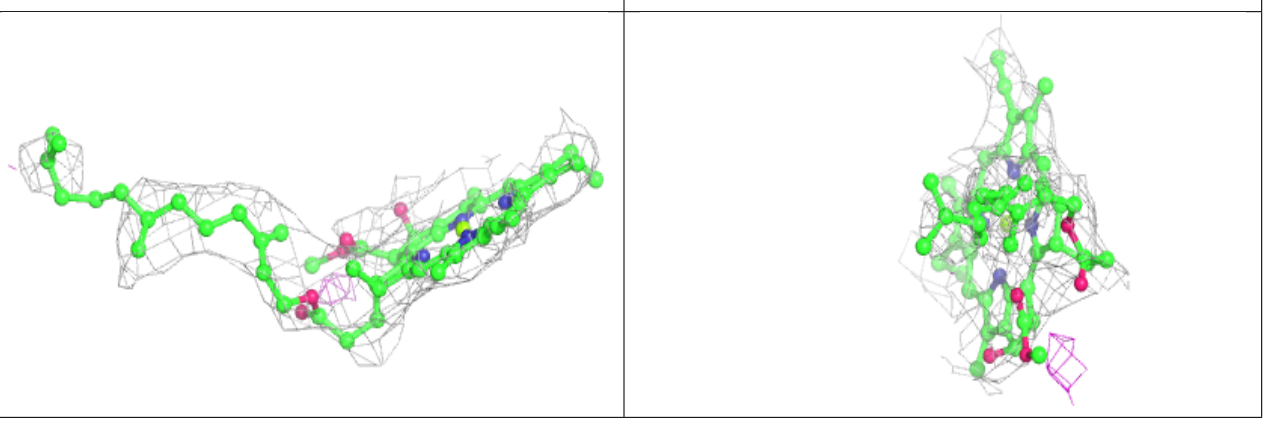




Electron density around CLA H 109:

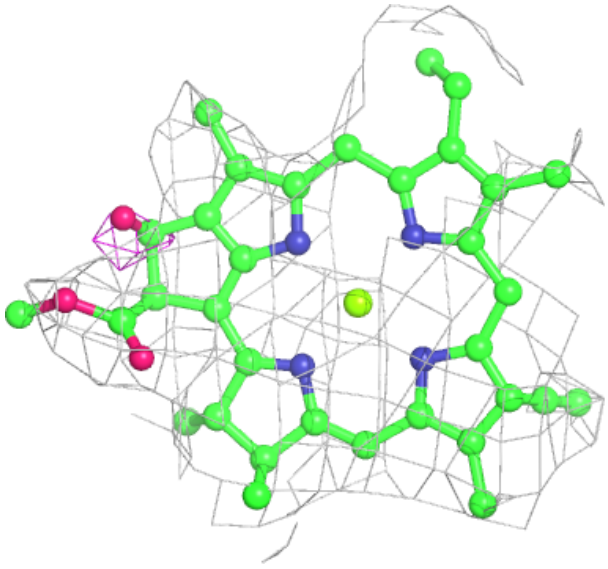
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

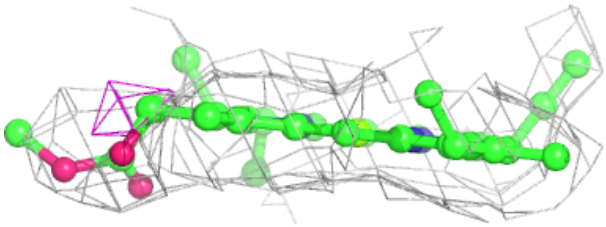


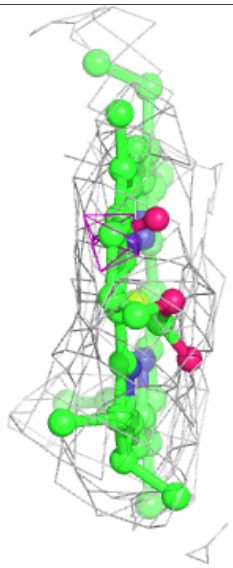


Electron density around CLA F 205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

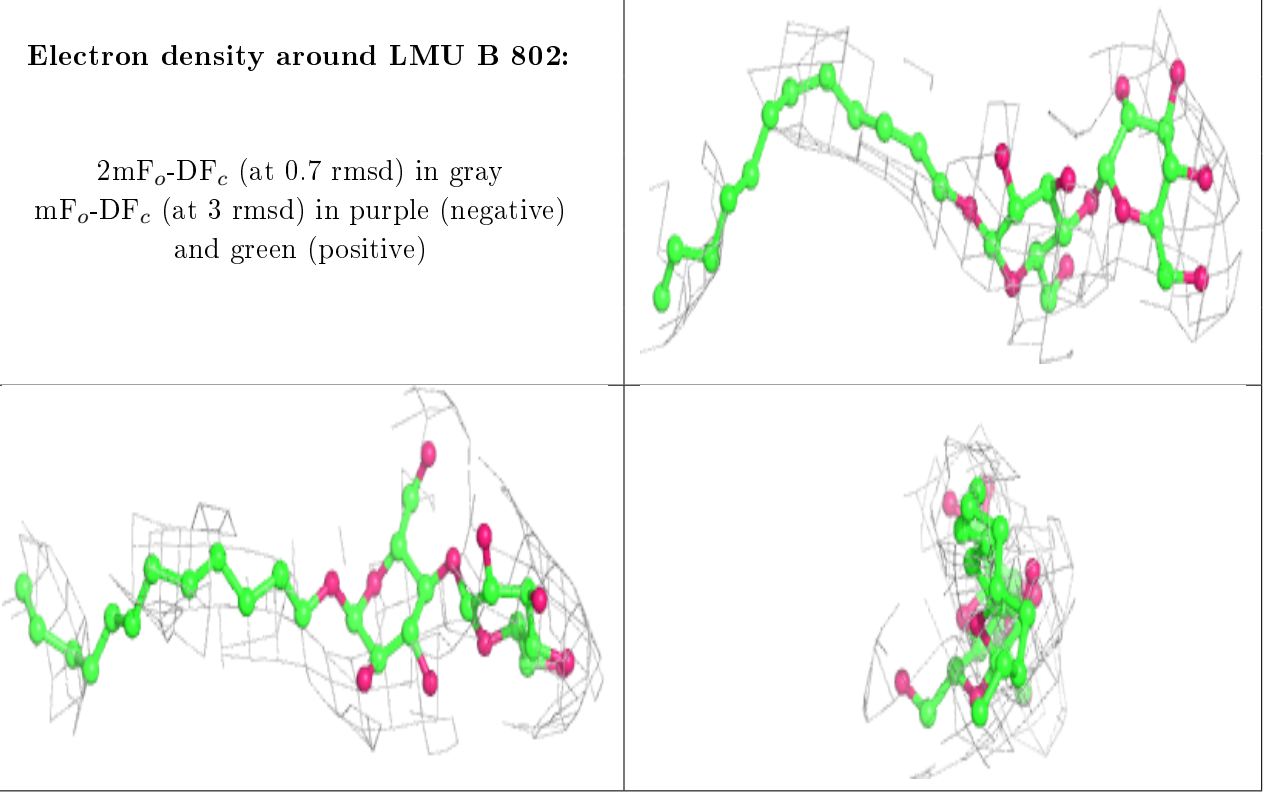






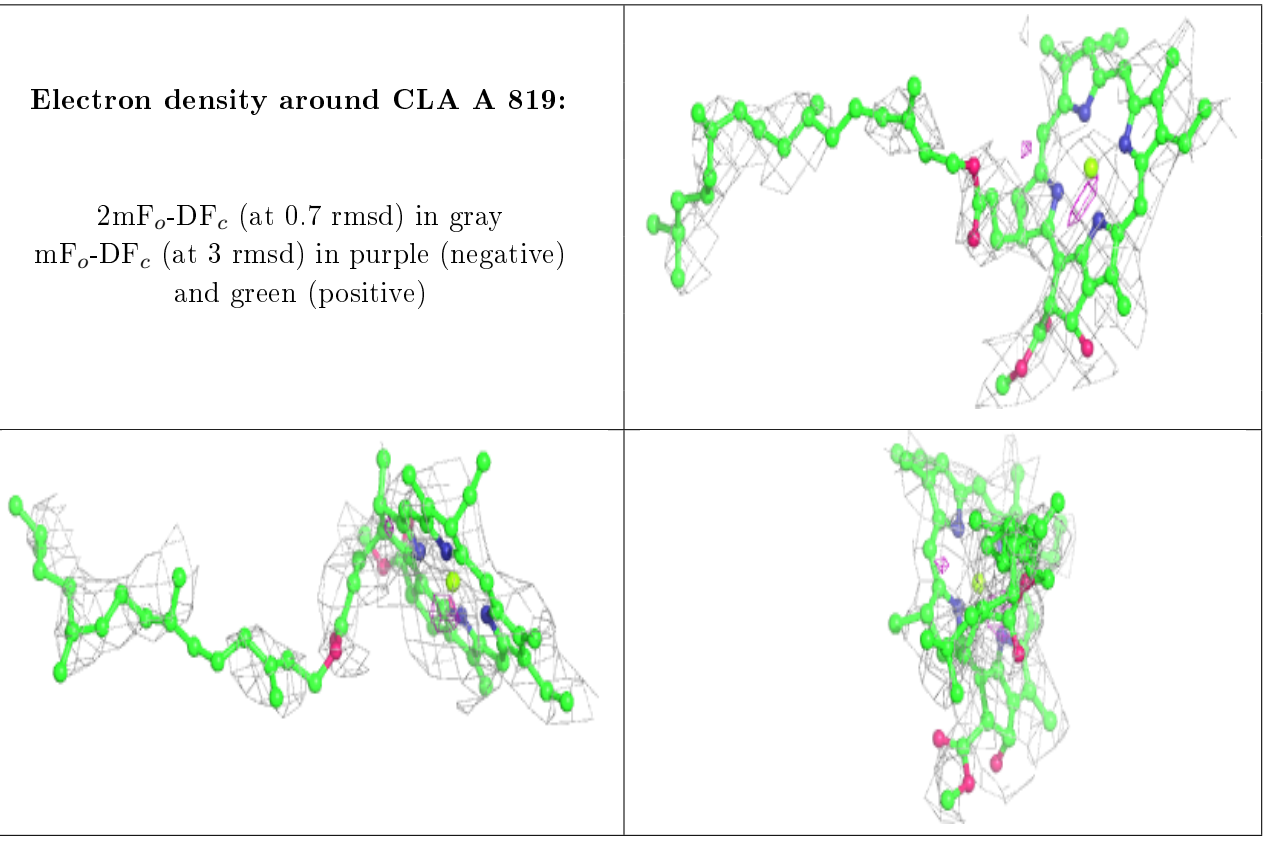
Electron density around LMU B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



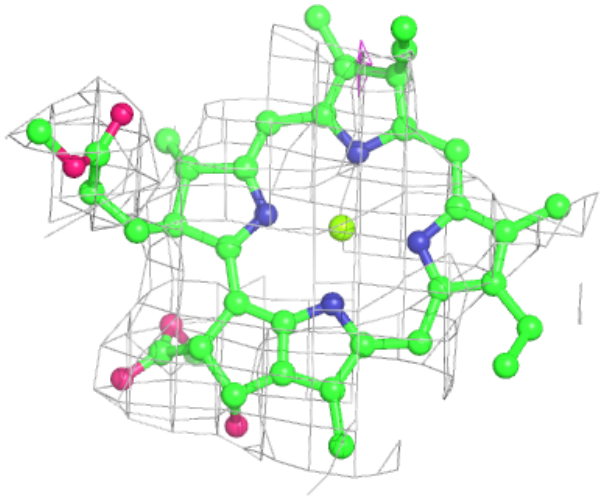
Electron density around CLA A 819:

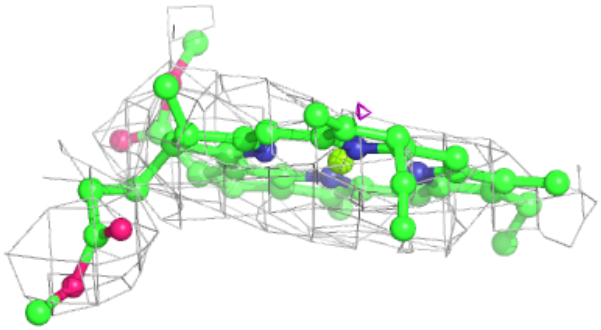
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

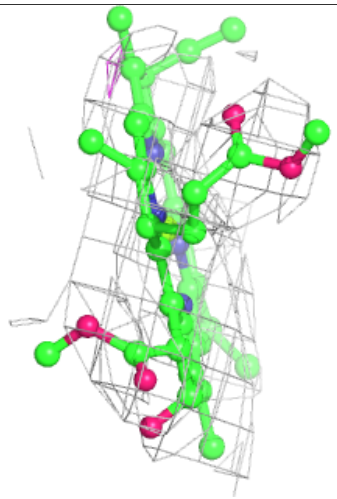


Electron density around CLA B 819:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

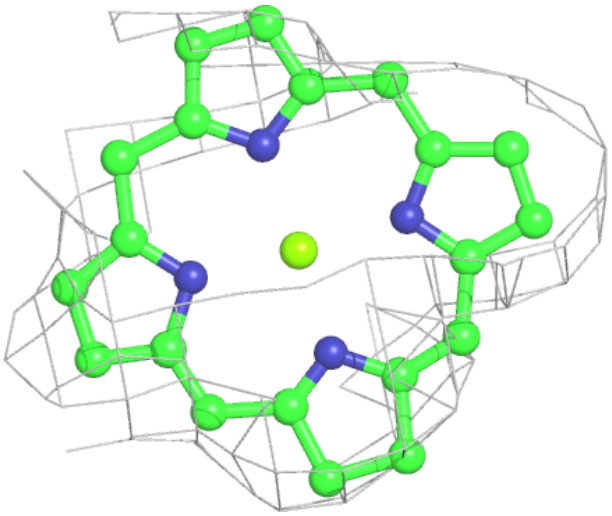


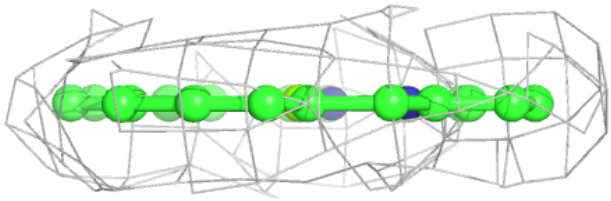


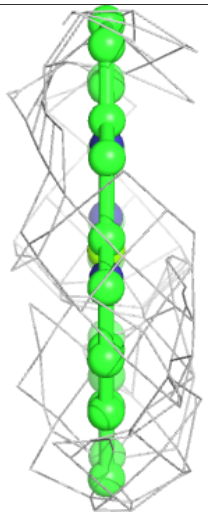


Electron density around CLA 1 205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

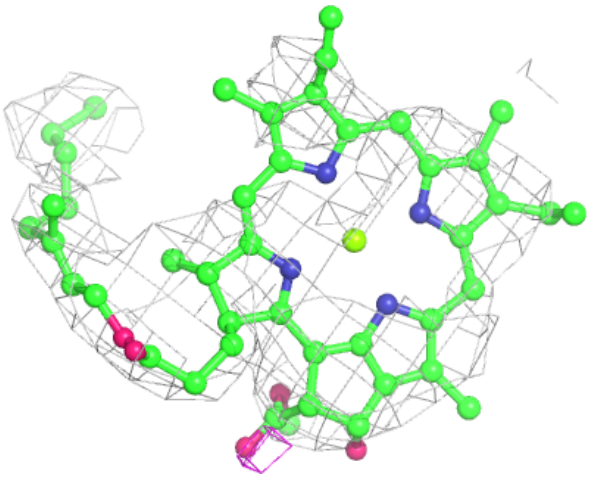


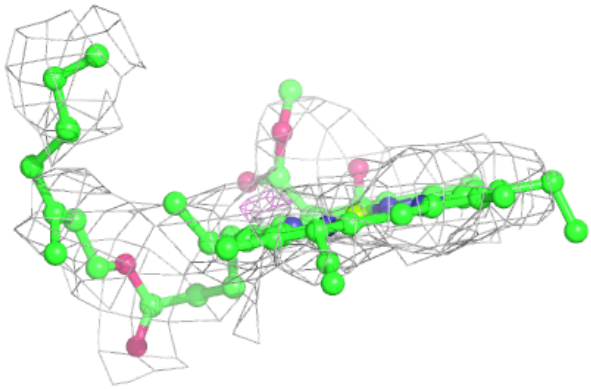


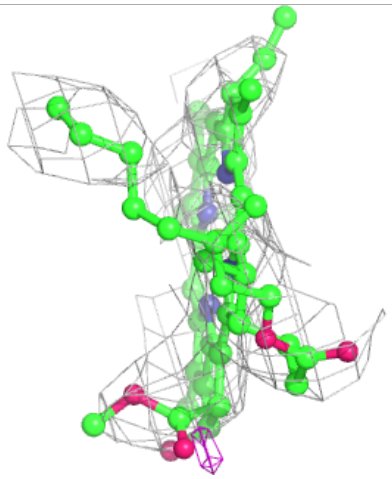


Electron density around CLA A 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

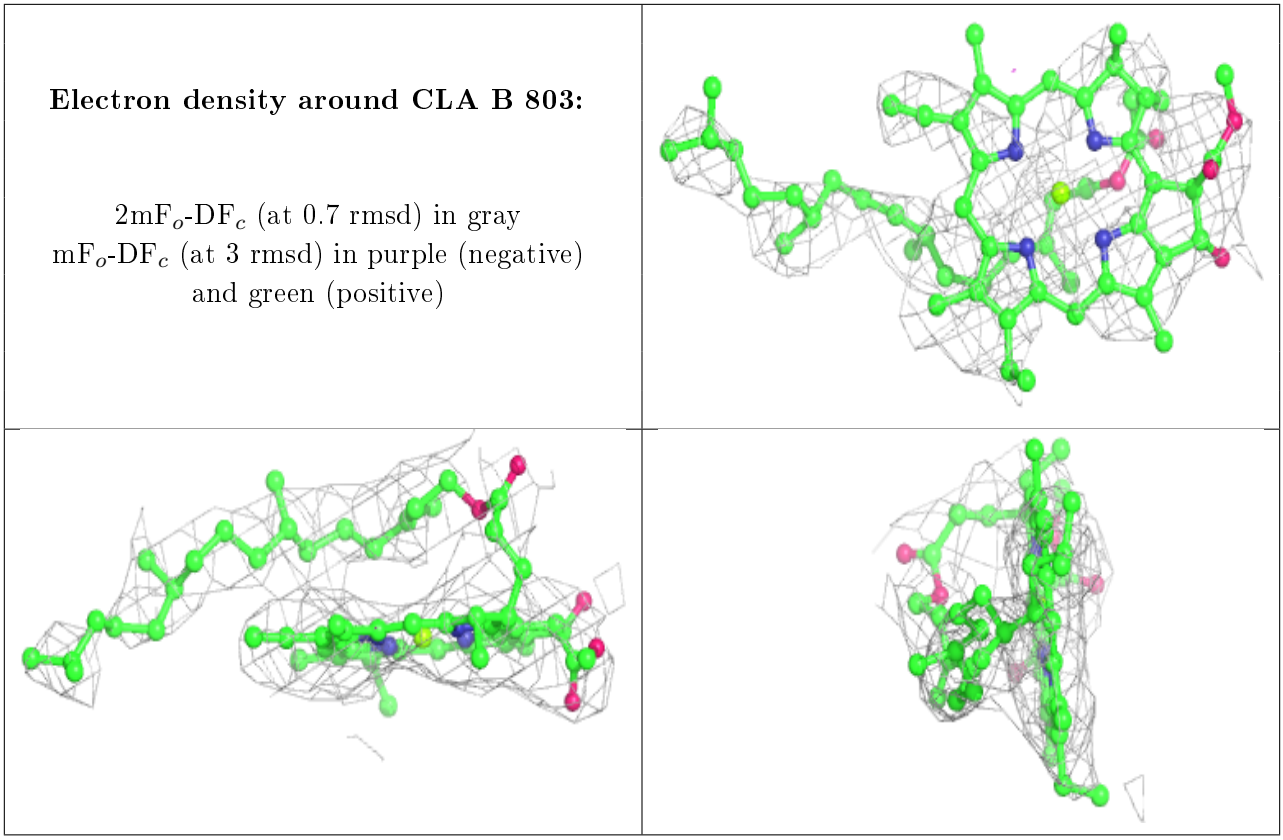






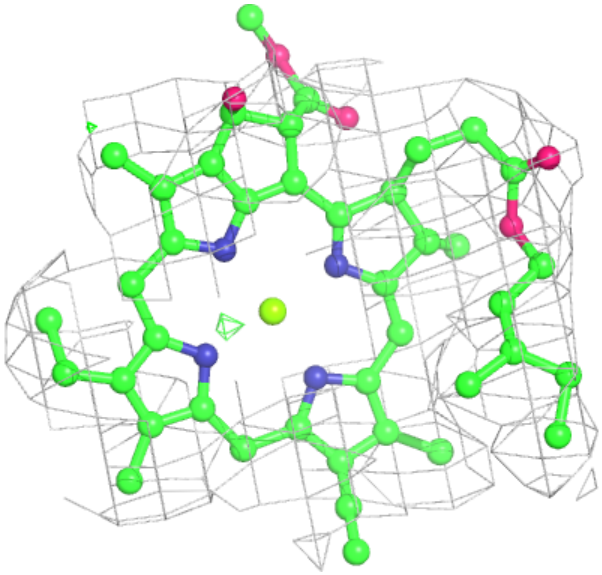
Electron density around CLA B 803:

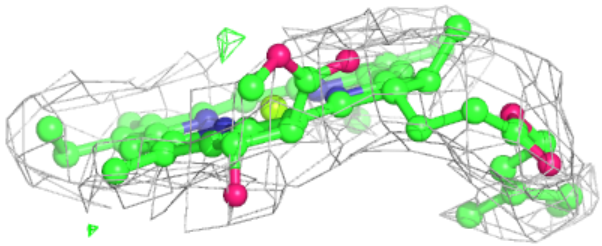
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

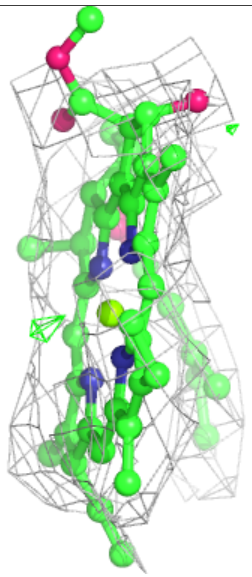


Electron density around CLA G 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

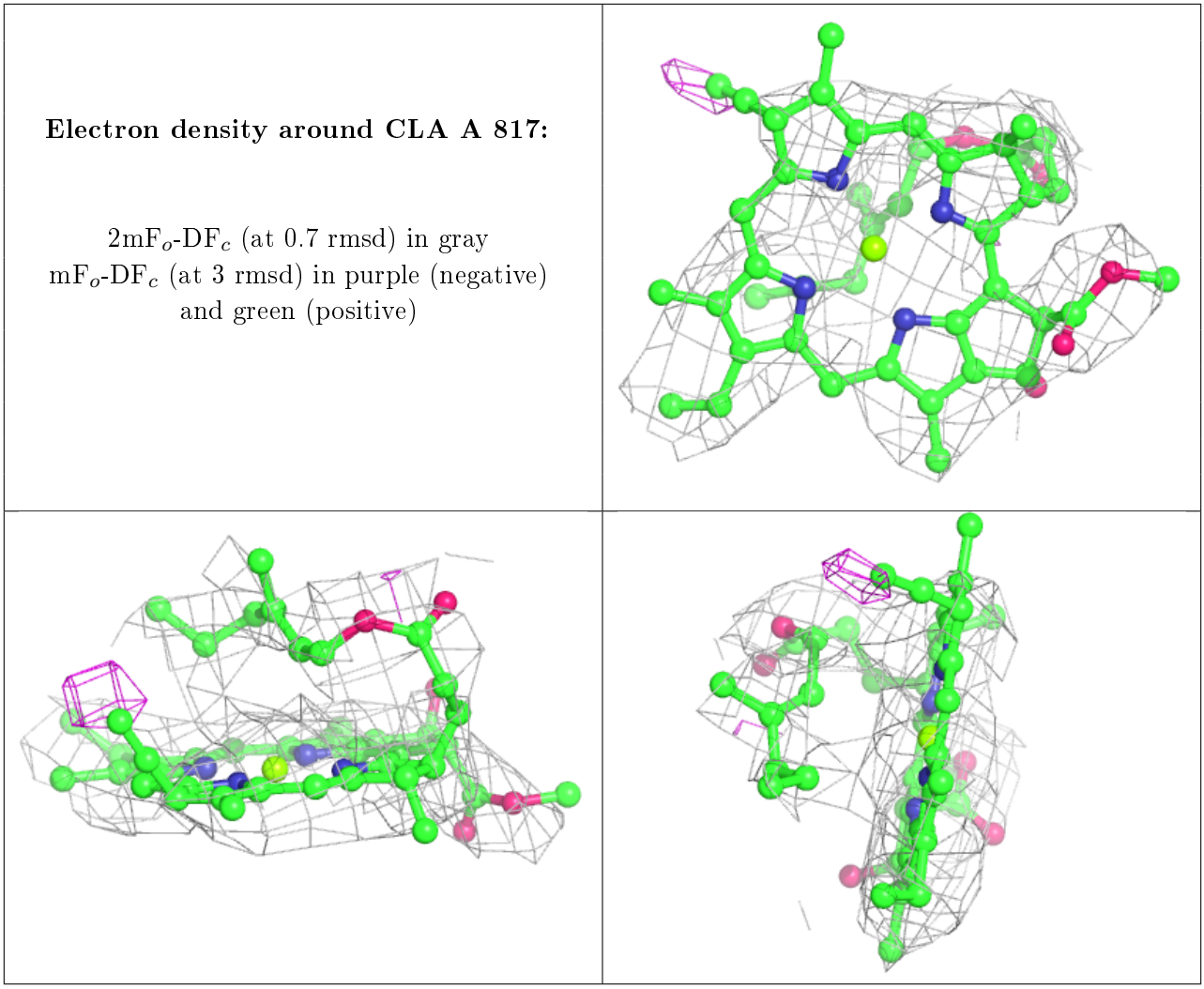






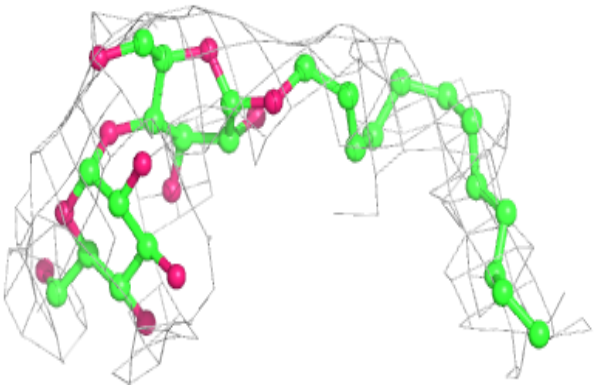
Electron density around CLA A 817:

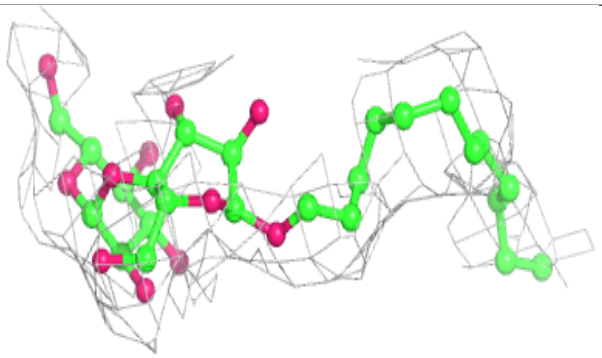
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

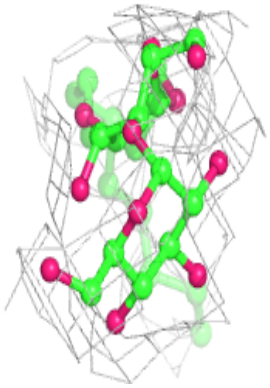


Electron density around LMU 2 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

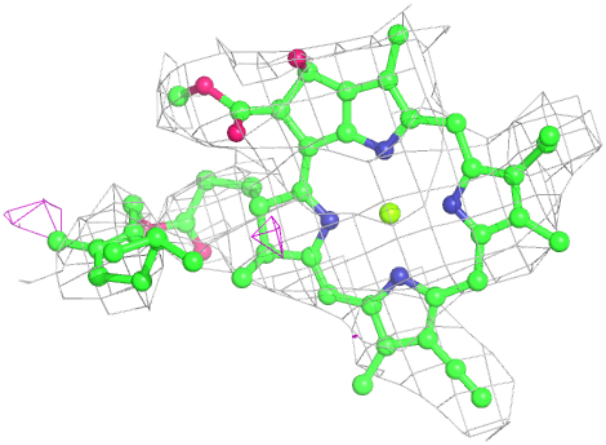


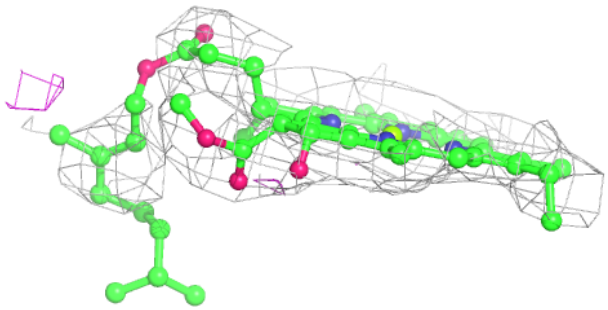


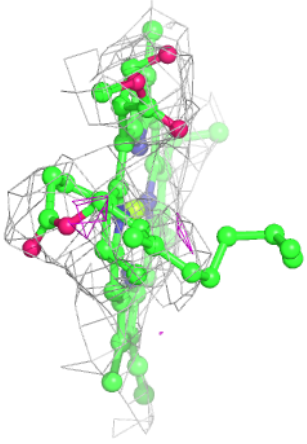


Electron density around CLA A 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

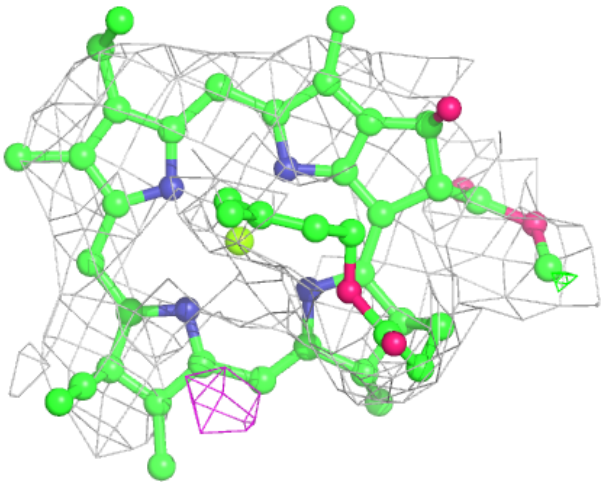


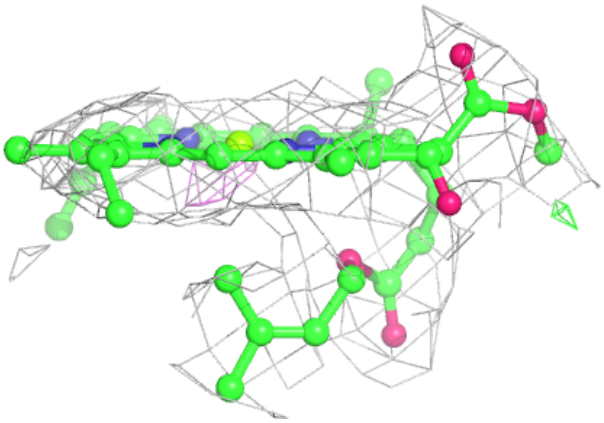


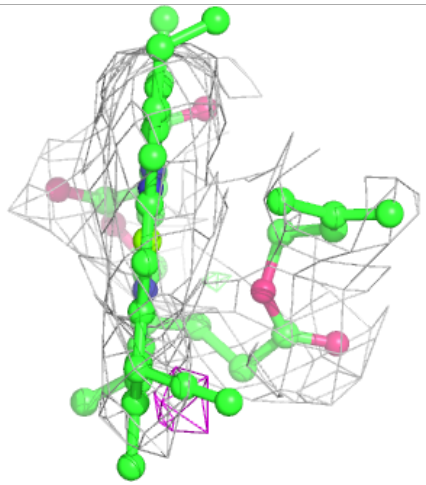


Electron density around CLA L 207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

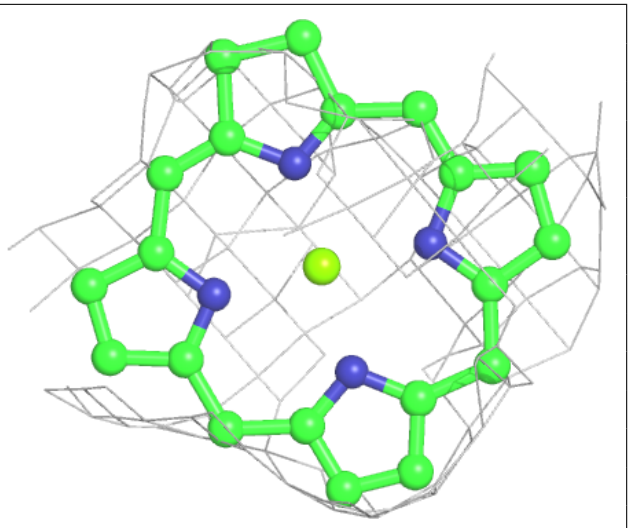


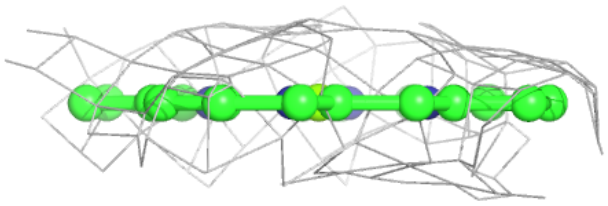


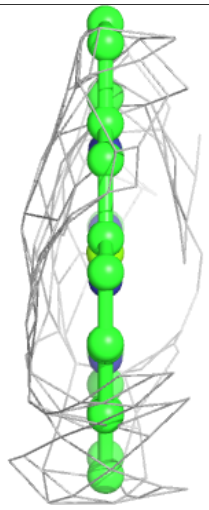


Electron density around CLA 4 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

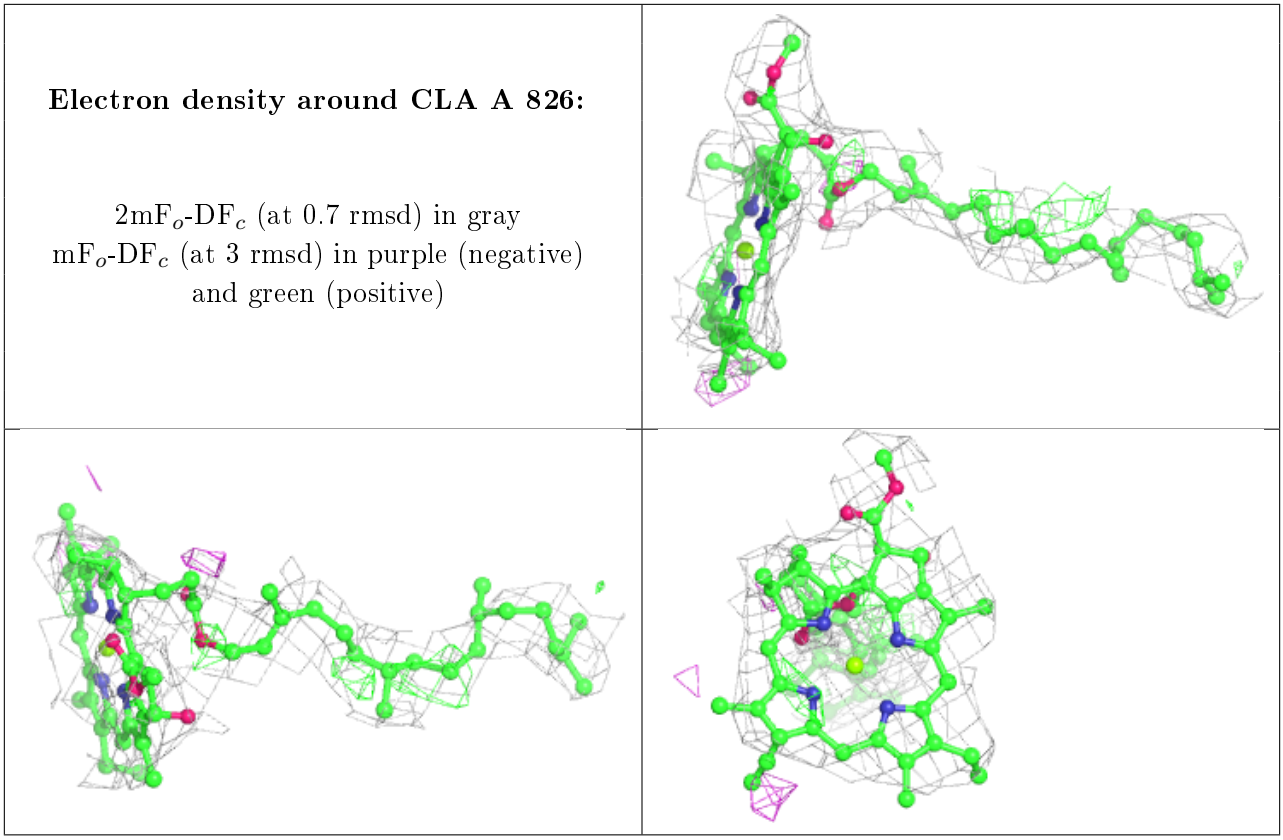






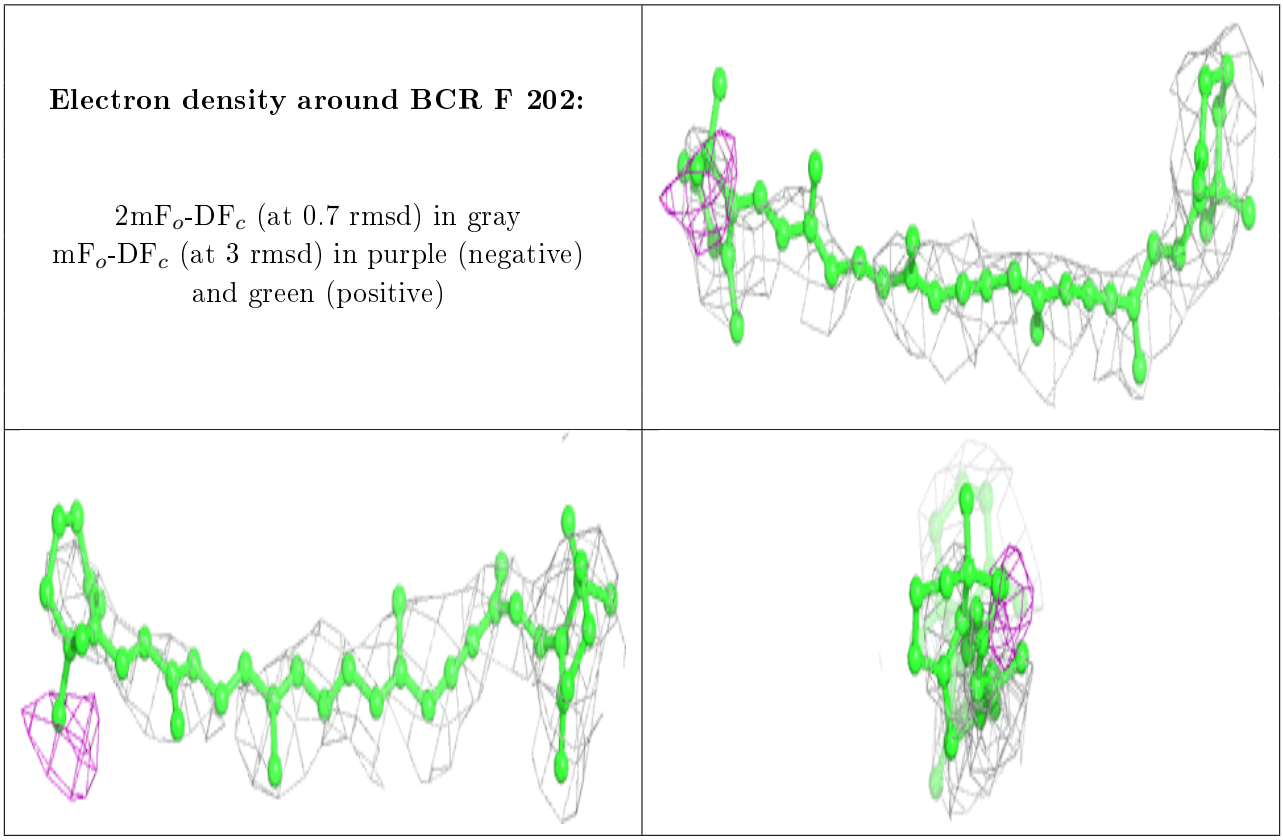
Electron density around CLA A 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



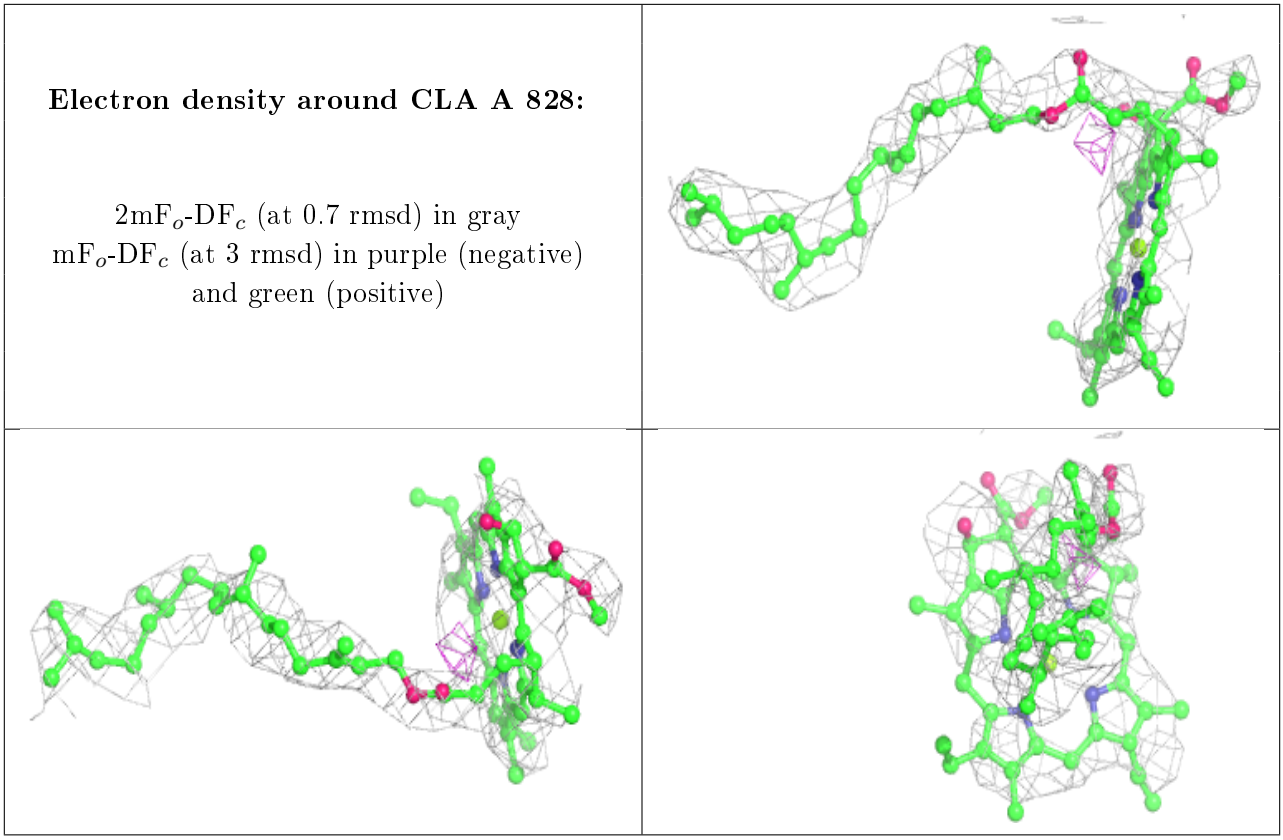
Electron density around BCR F 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



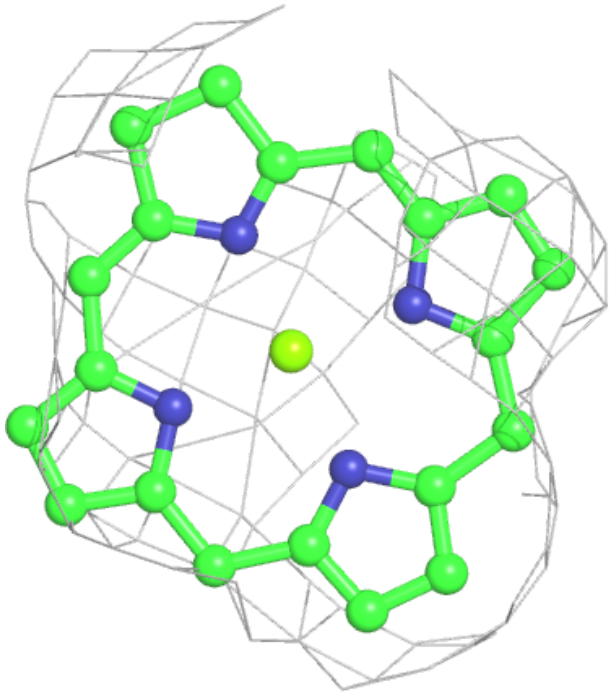
Electron density around CLA A 828:

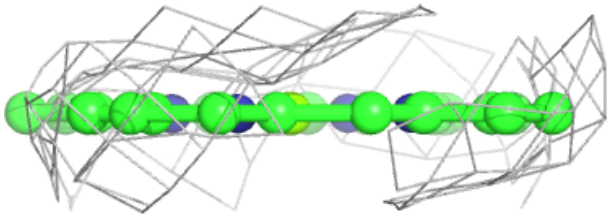
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

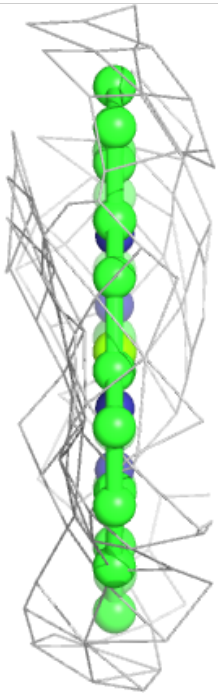


Electron density around CLA 3 320:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

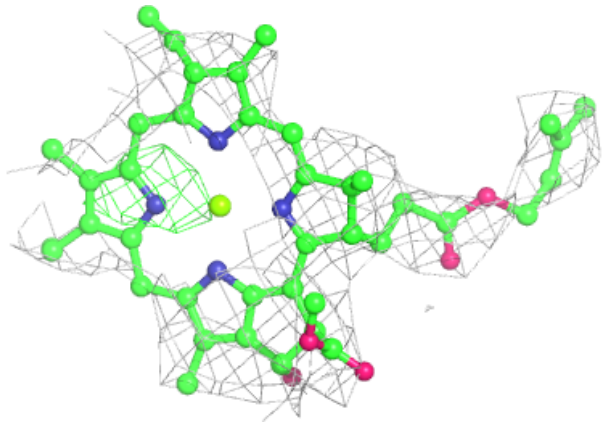


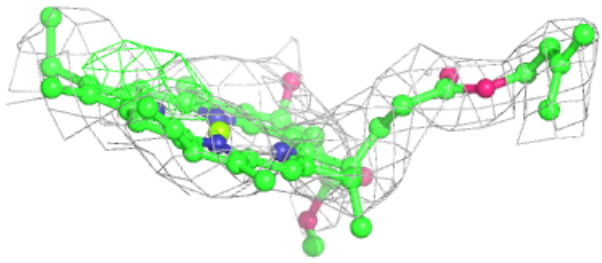


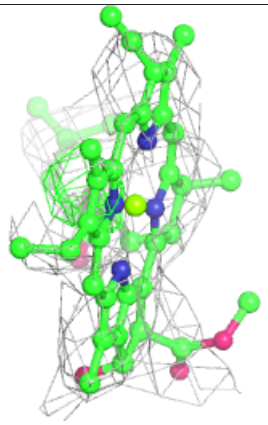


Electron density around CLA B 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

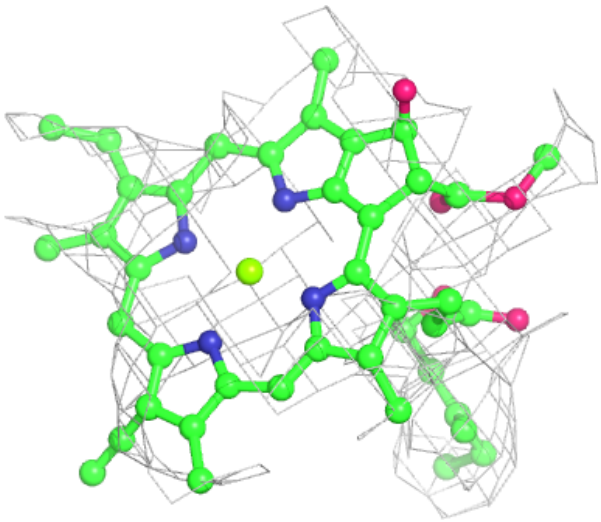


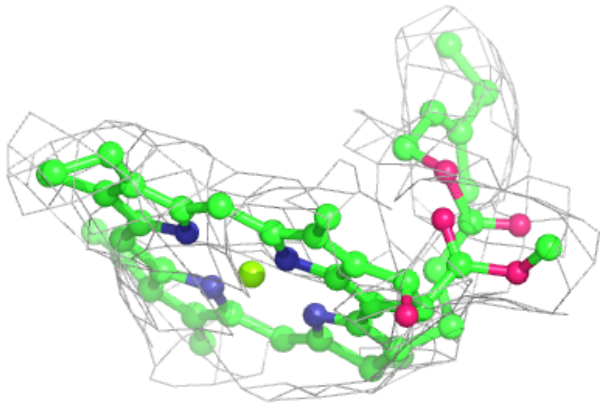


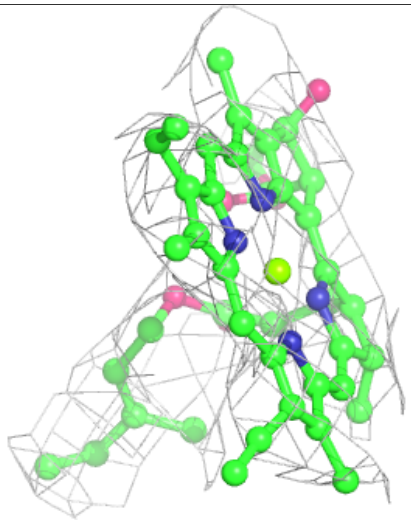


Electron density around CLA 1 207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

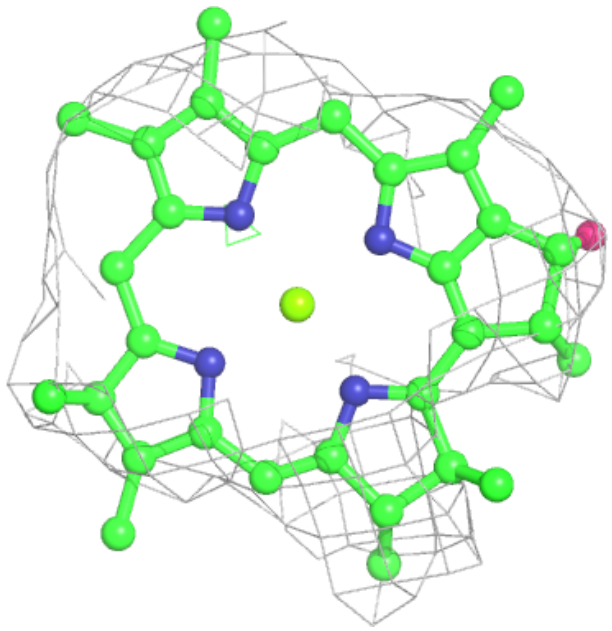


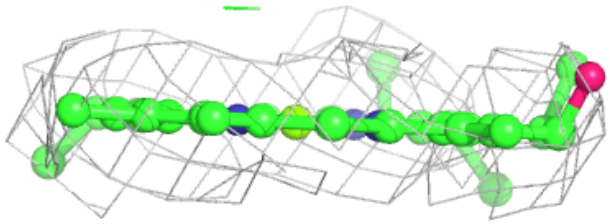




Electron density around CLA 3 304:

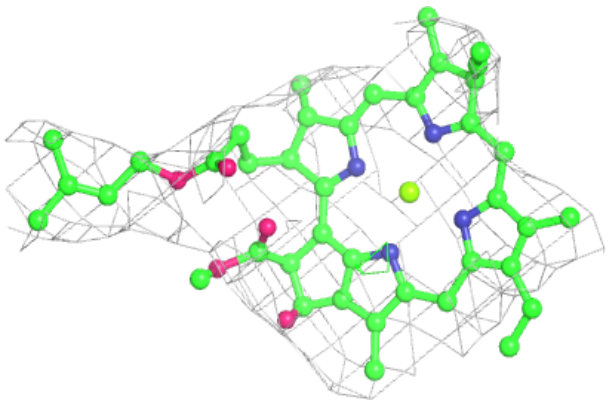
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

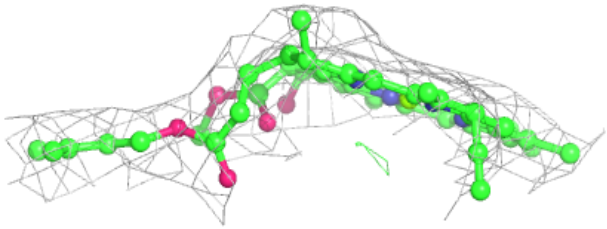


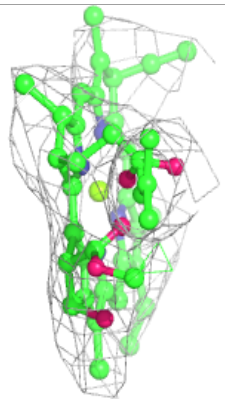


Electron density around CLA L 209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

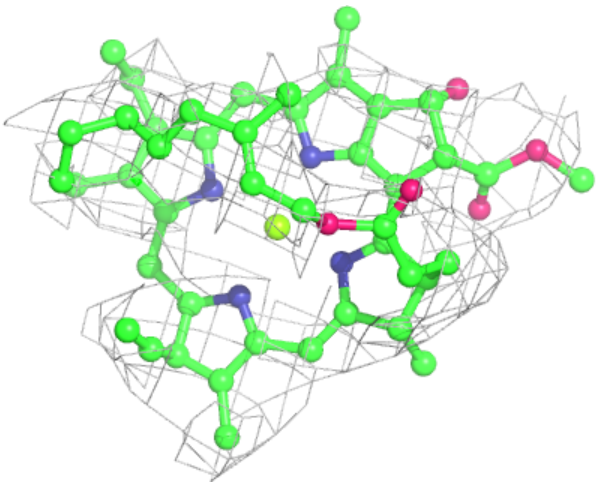


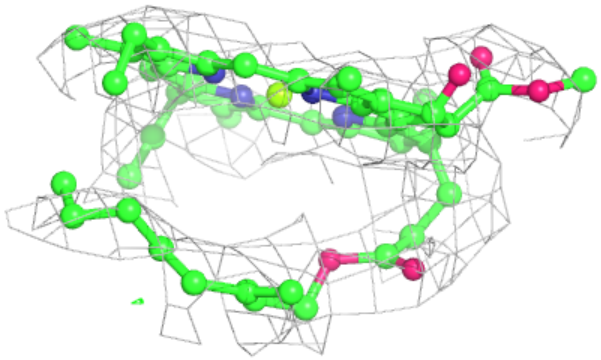


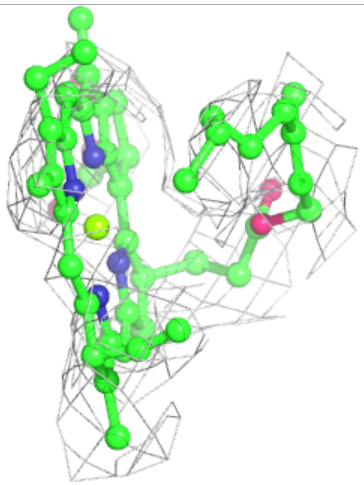


Electron density around CLA A 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

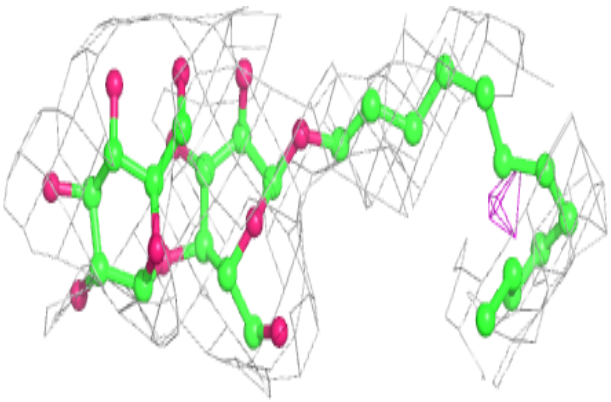


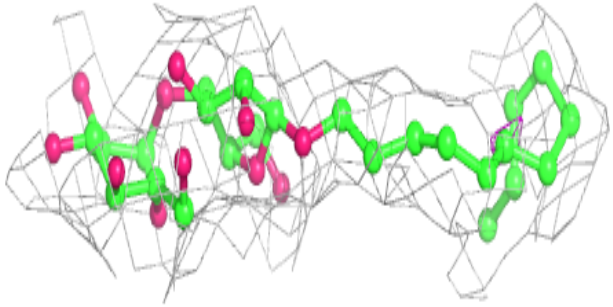


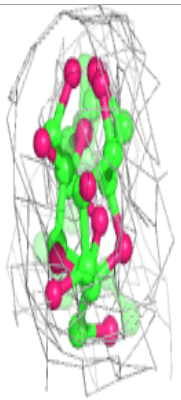


Electron density around LMU B 847:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

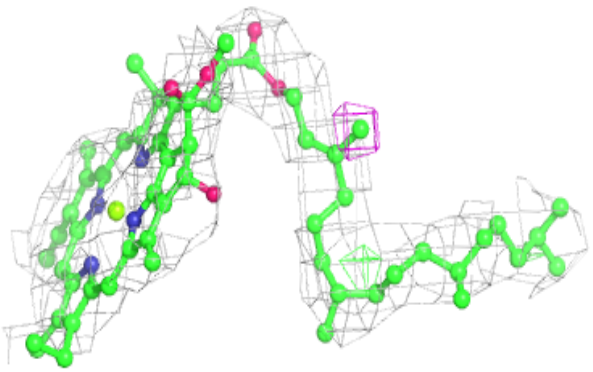


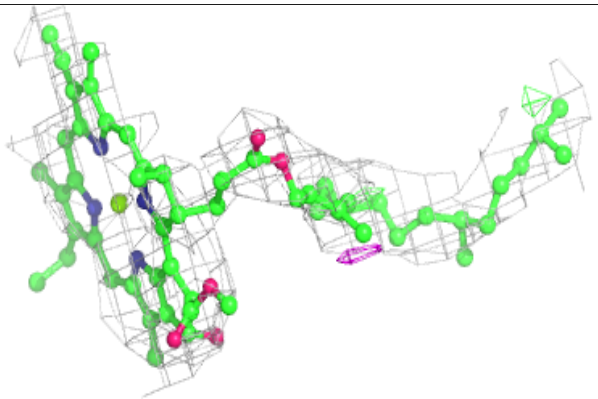


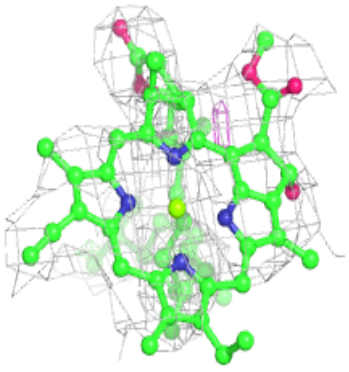


Electron density around CLA B 849:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

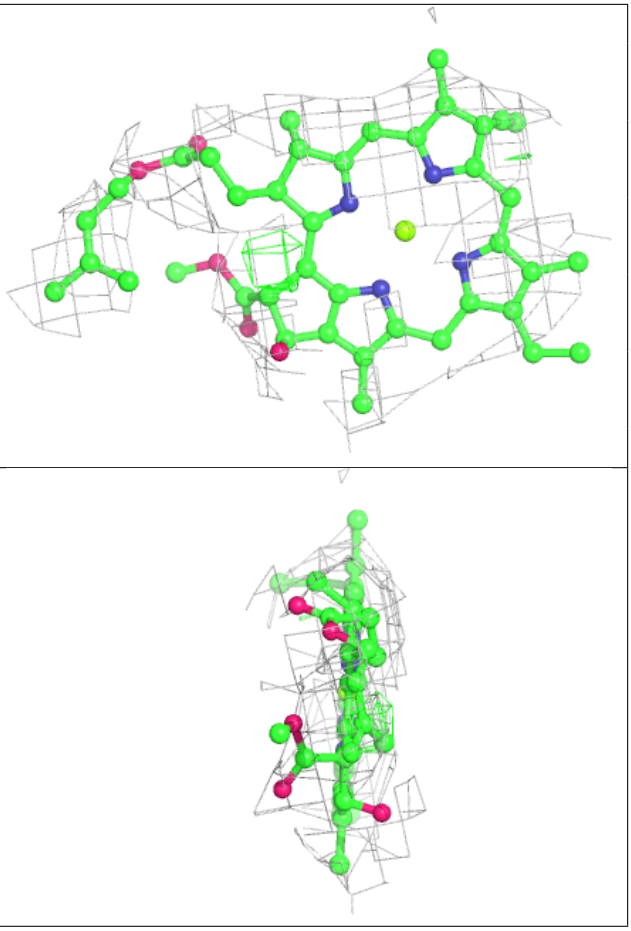






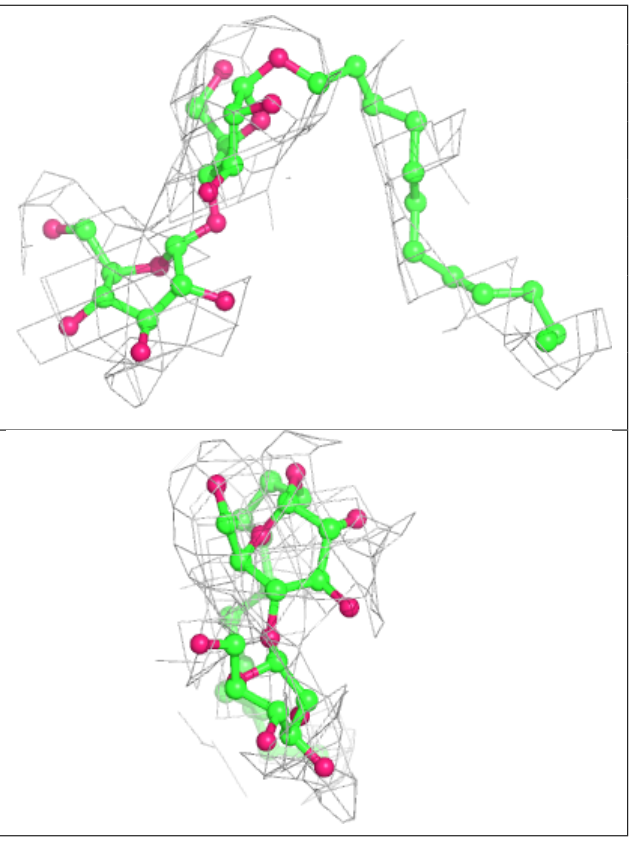
Electron density around CLA 2 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



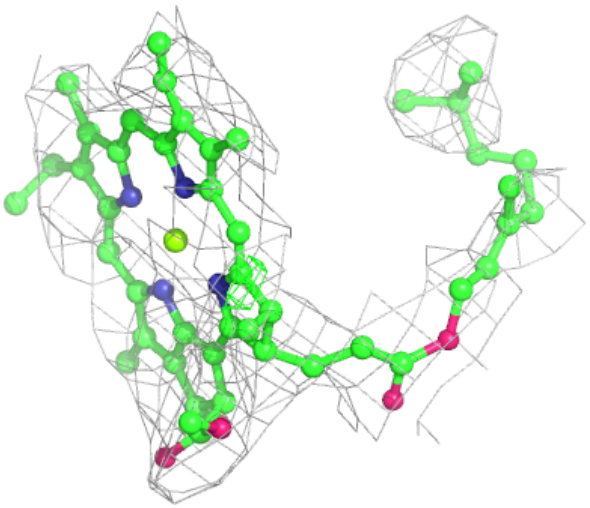
Electron density around LMU L 205:

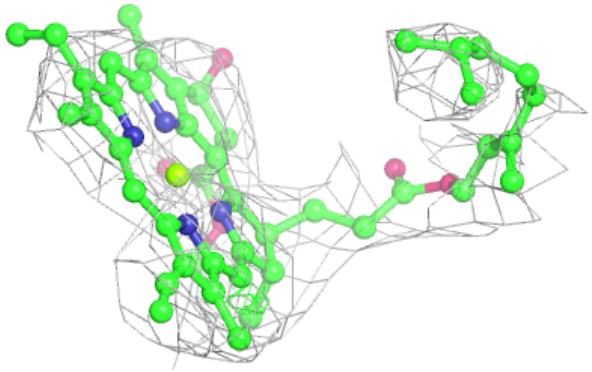
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

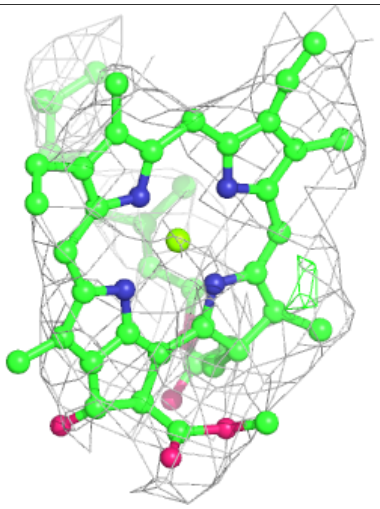


Electron density around CLA A 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

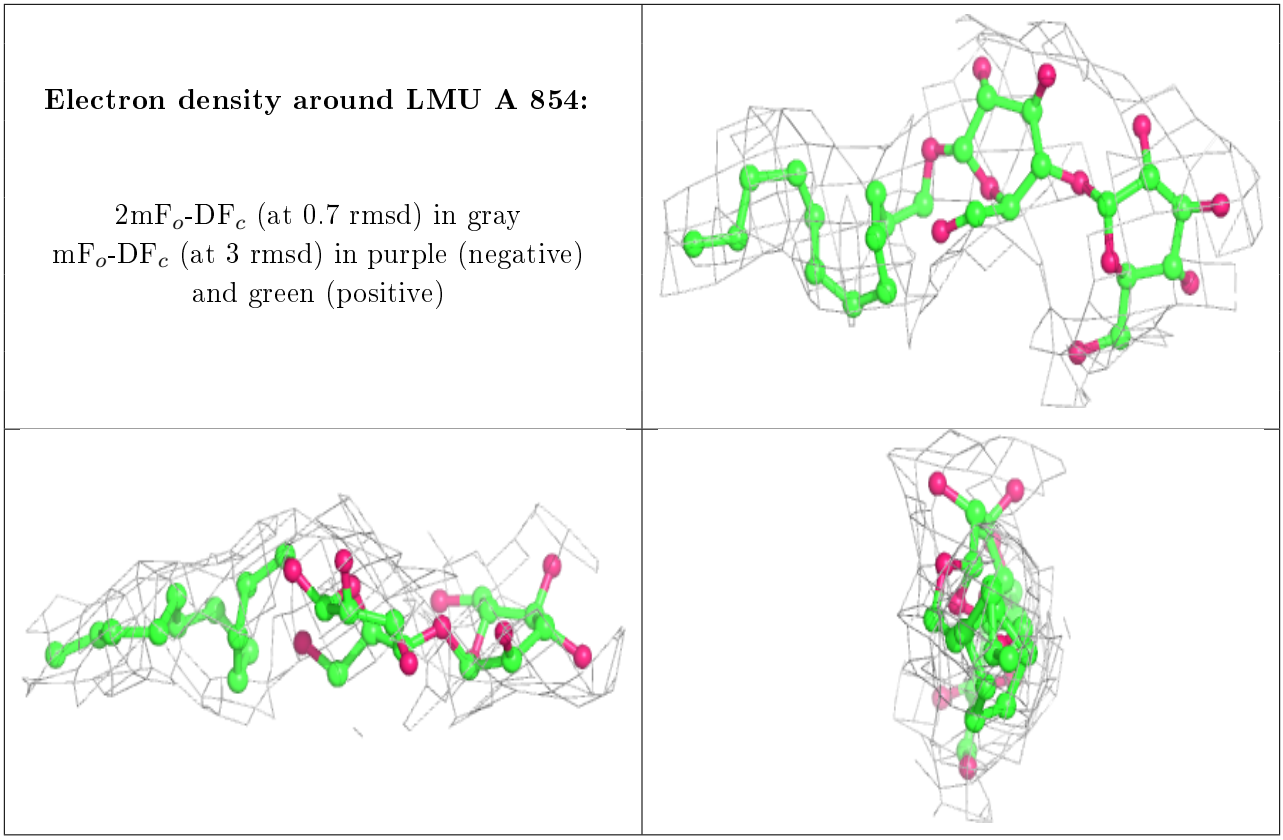






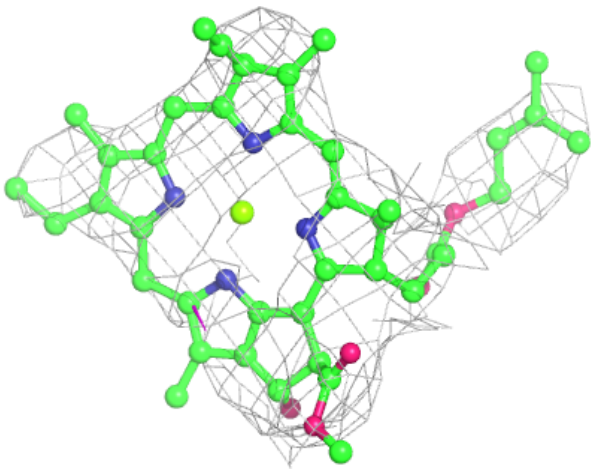
Electron density around LMU A 854:

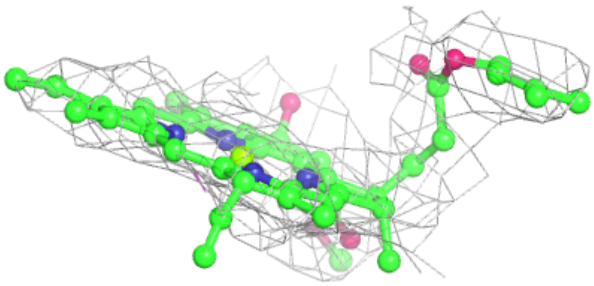
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

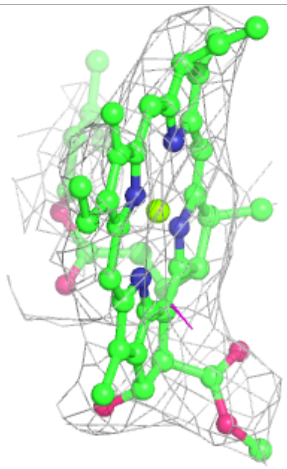


Electron density around CLA A 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

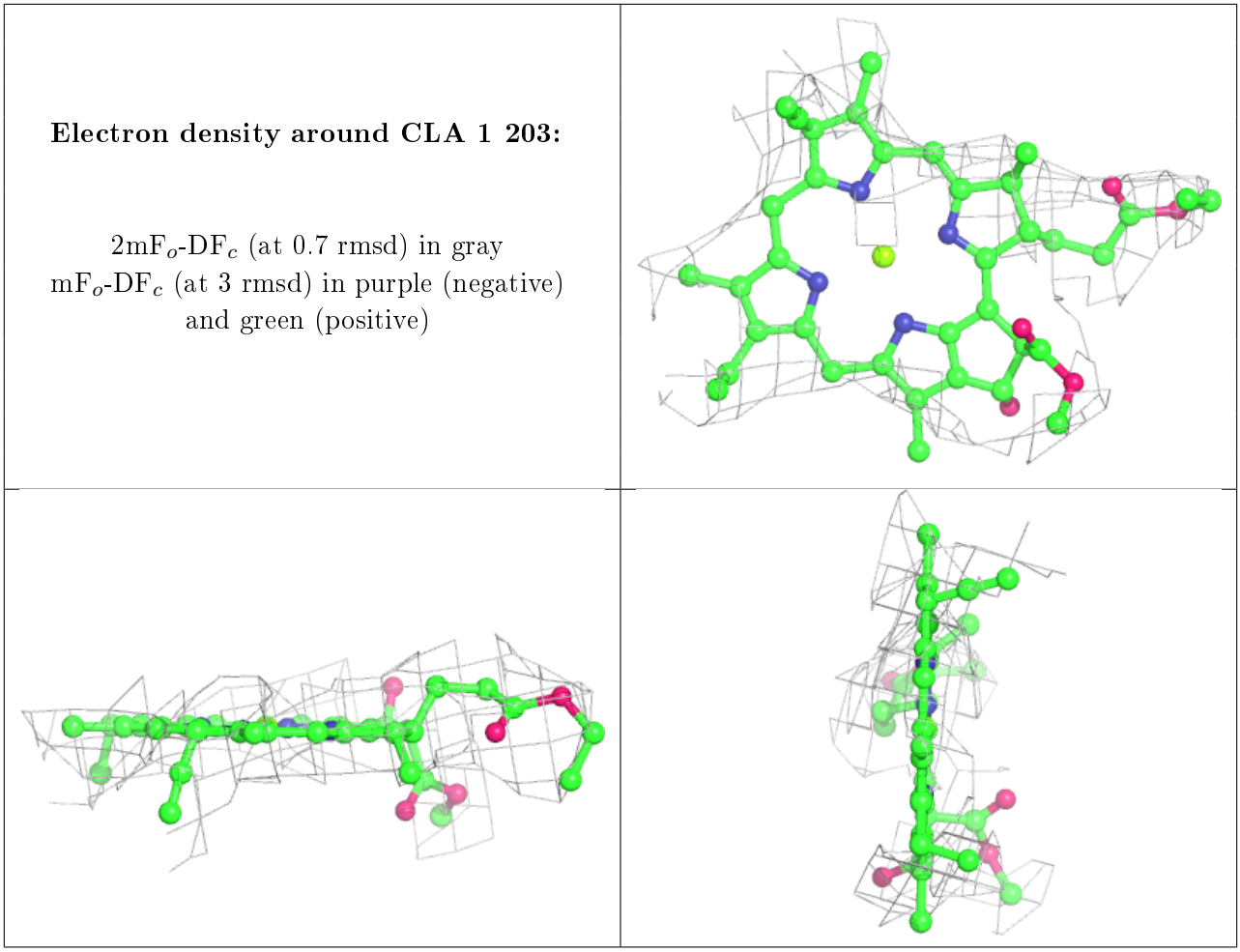






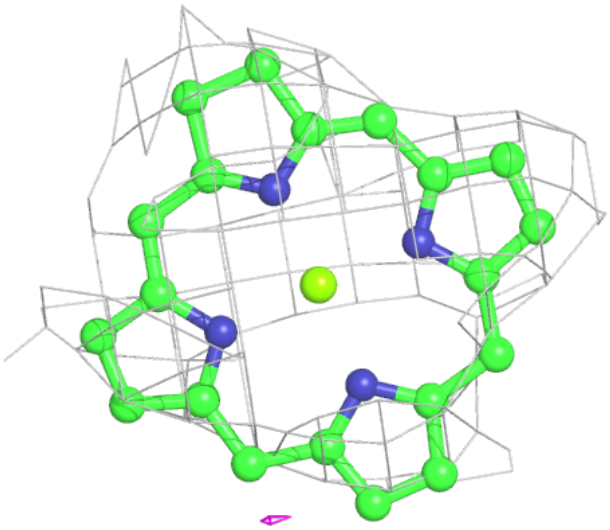
Electron density around CLA 1 203:

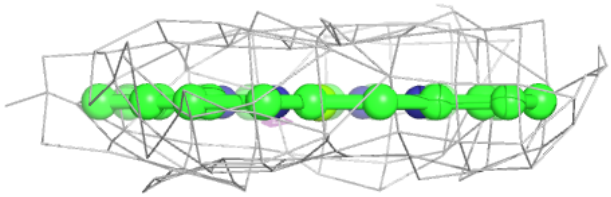
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

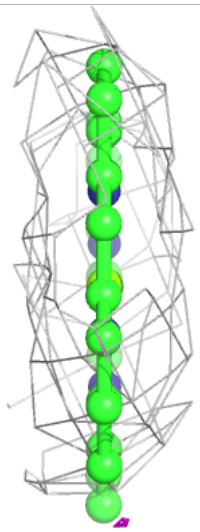


Electron density around CLA 3 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

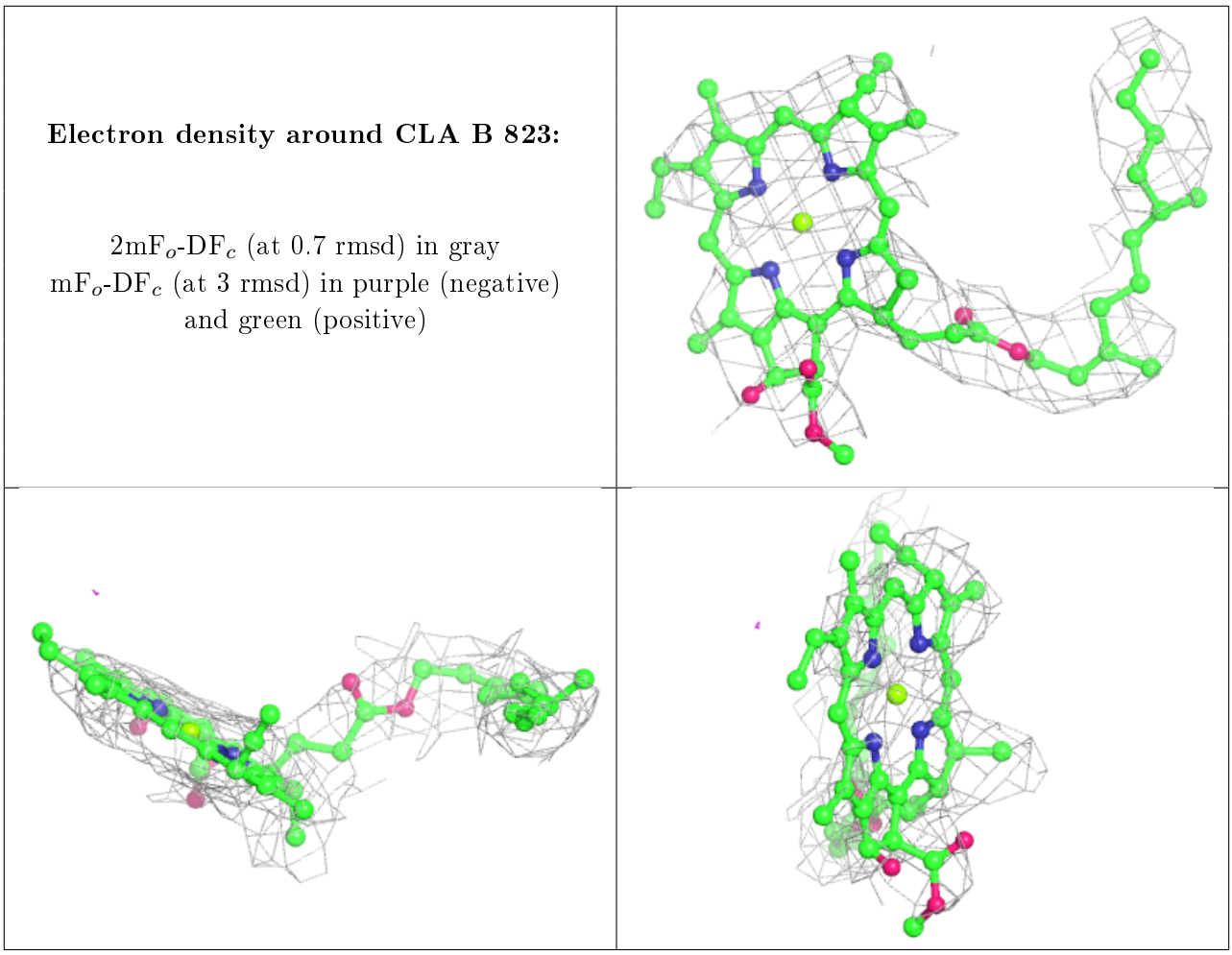






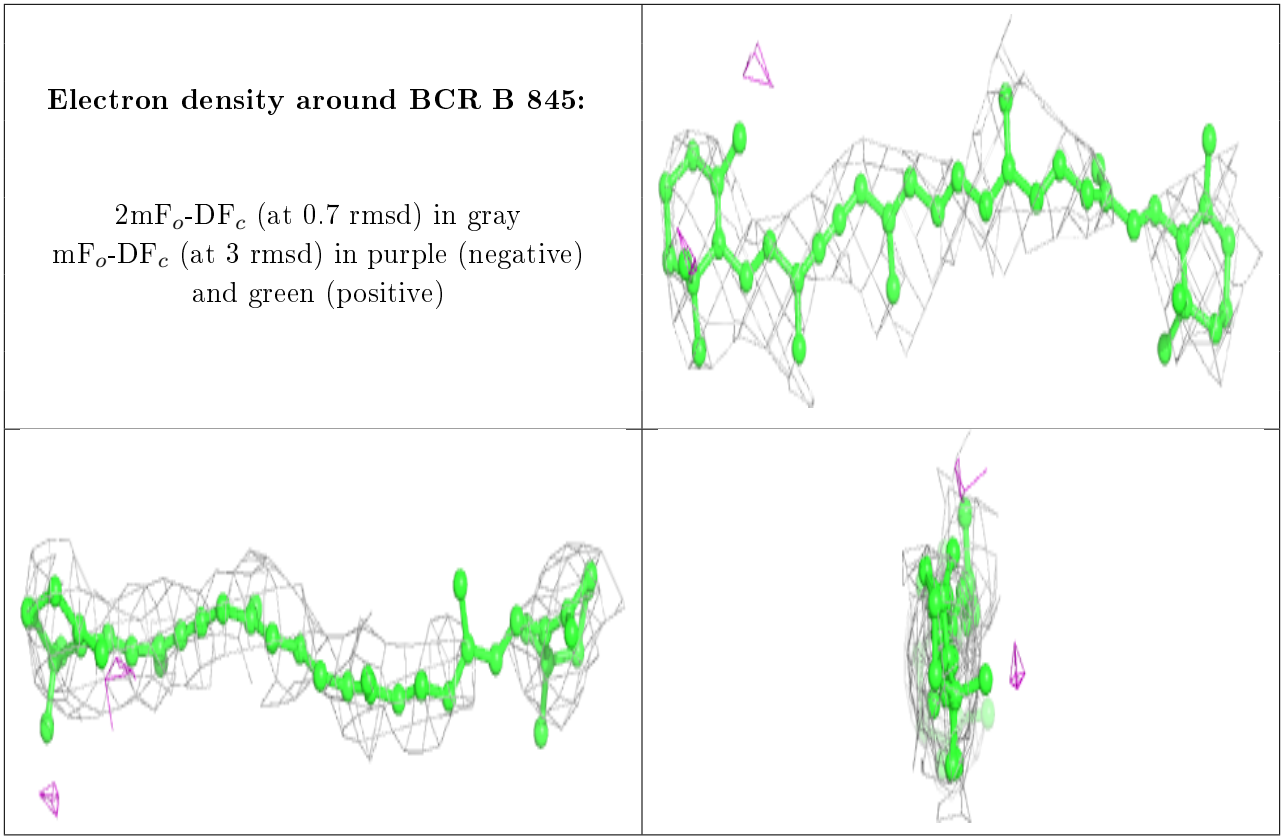
Electron density around CLA B 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



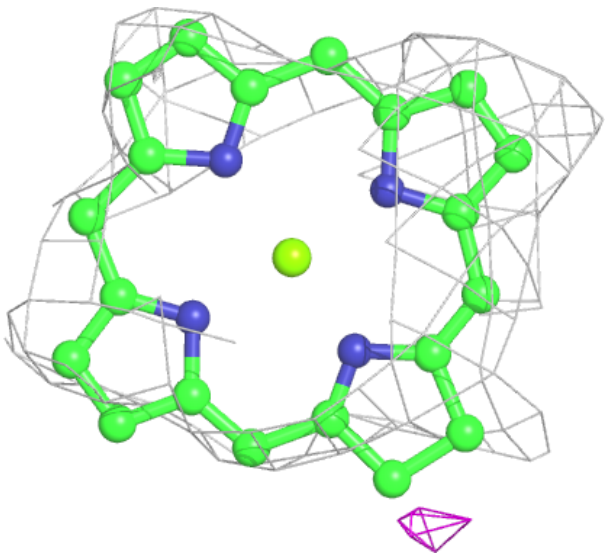
Electron density around BCR B 845:

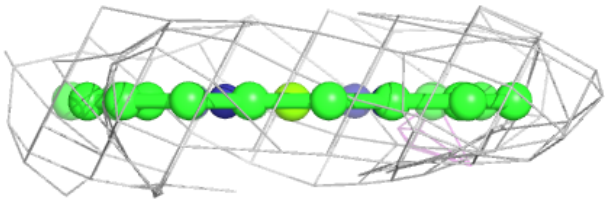
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

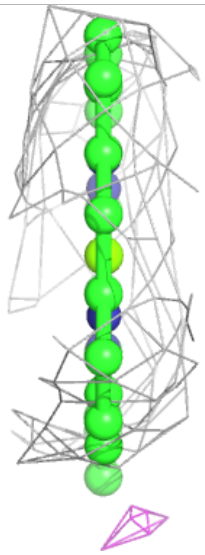


Electron density around CLA 2 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

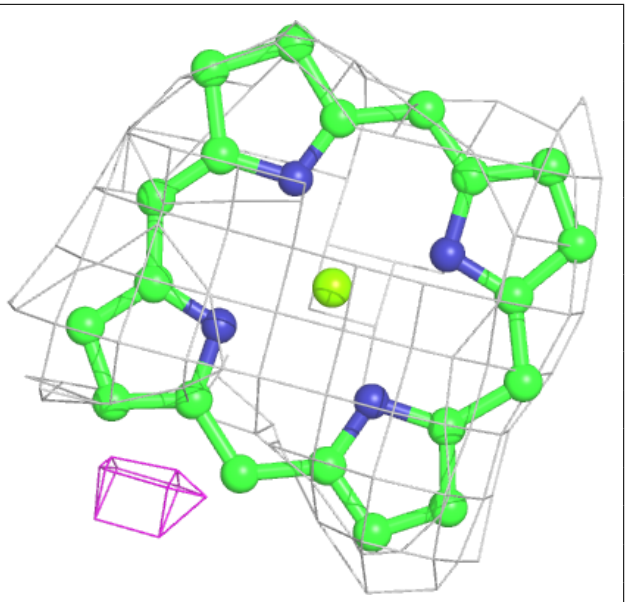


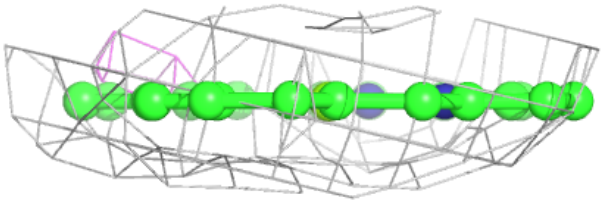


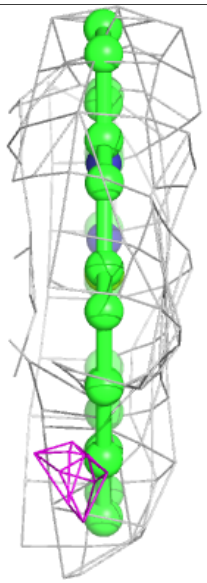


Electron density around CLA 3 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

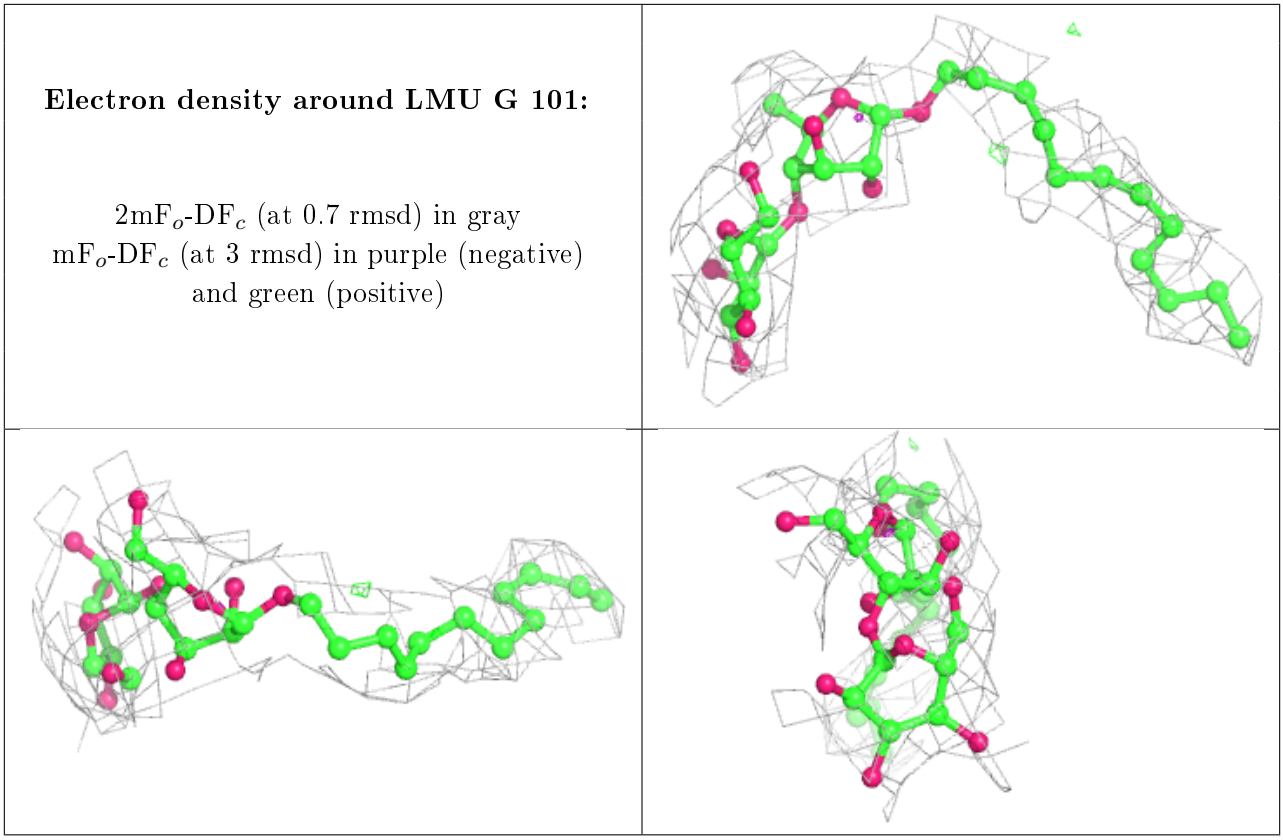






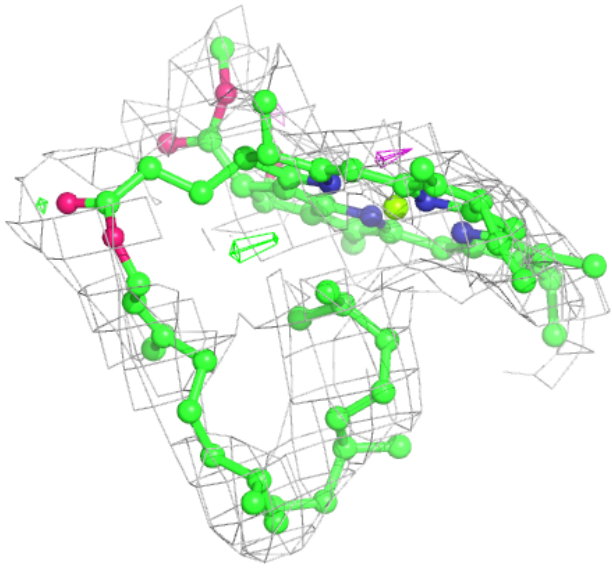
Electron density around LMU G 101:

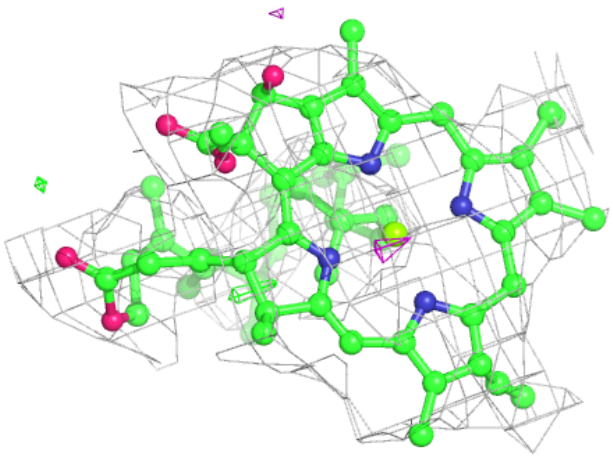
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

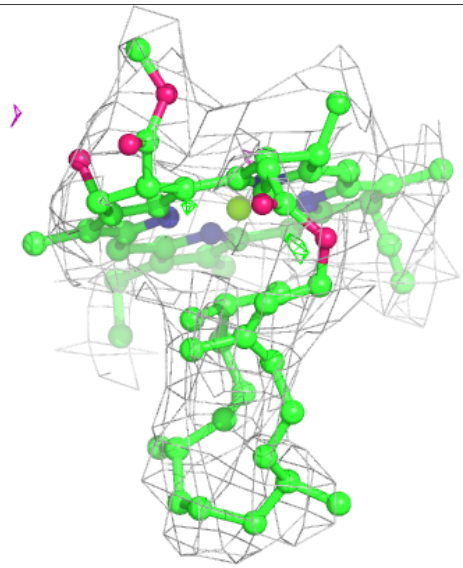


Electron density around CLA 2 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

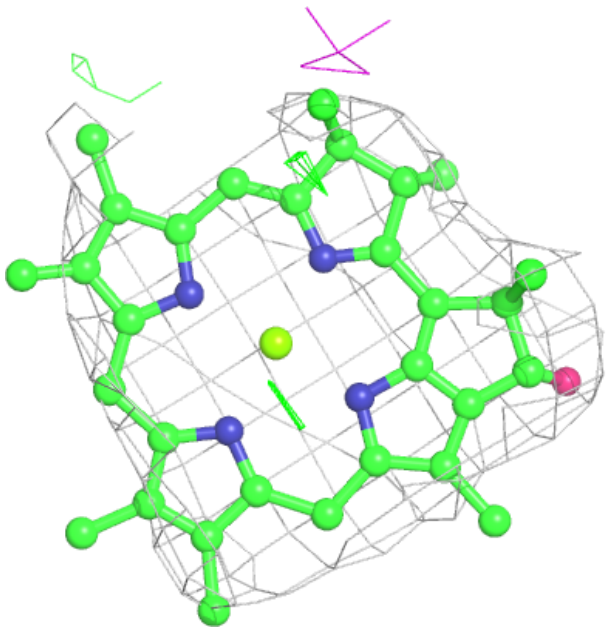


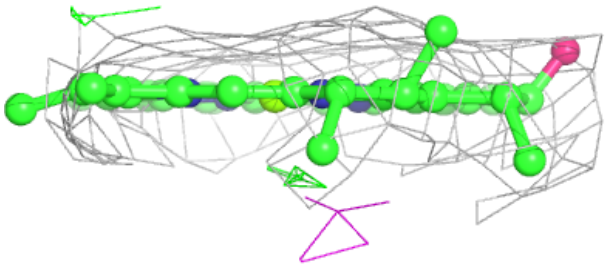


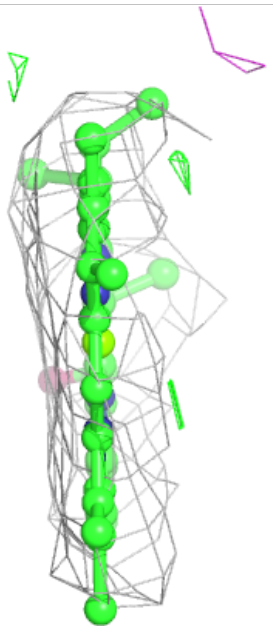


Electron density around CLA F 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

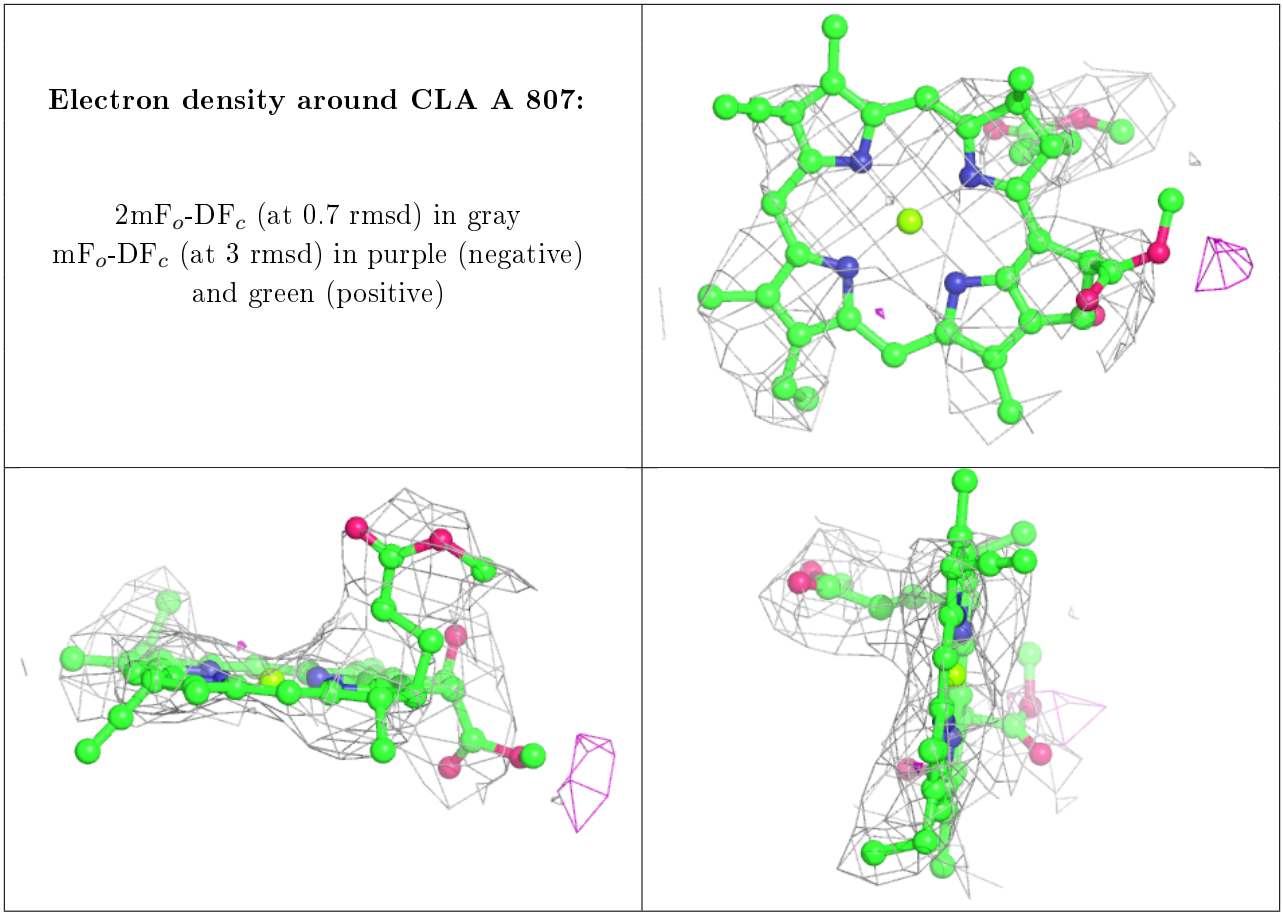






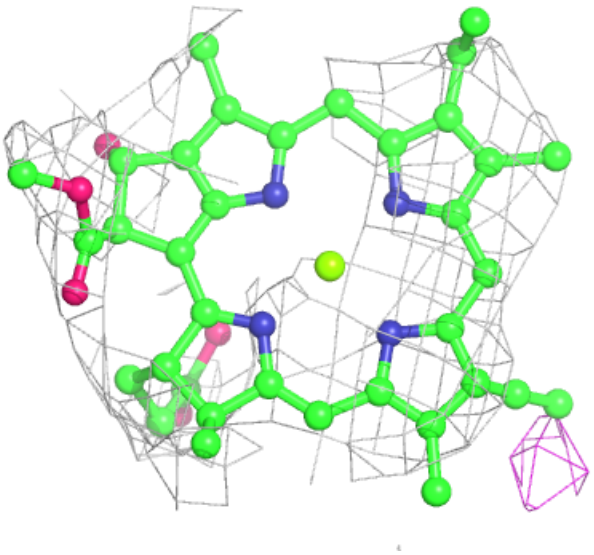
Electron density around CLA A 807:

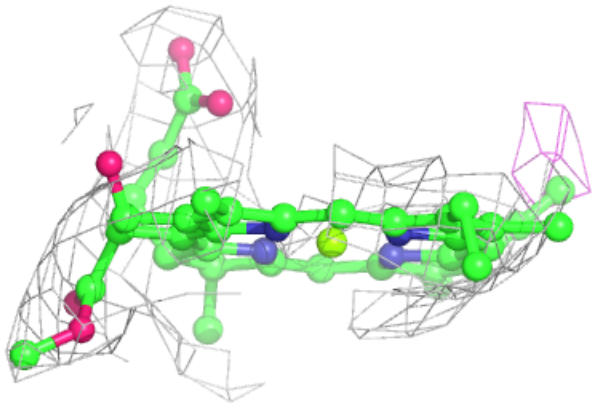
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

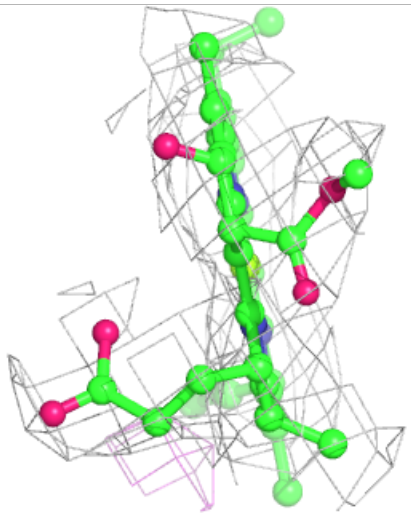


Electron density around CLA B 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

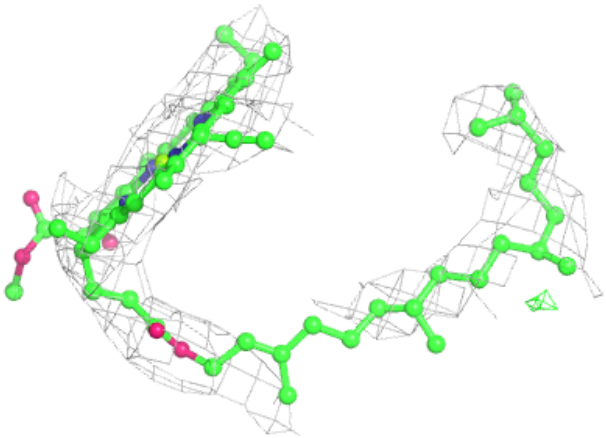


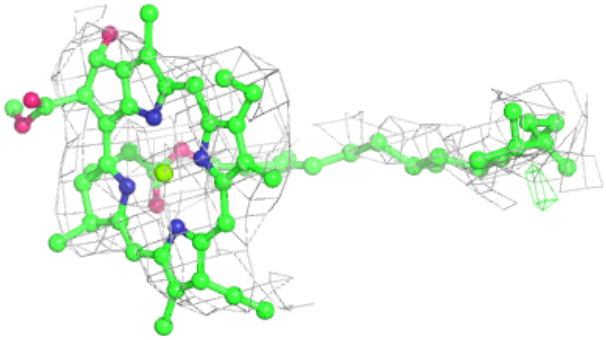


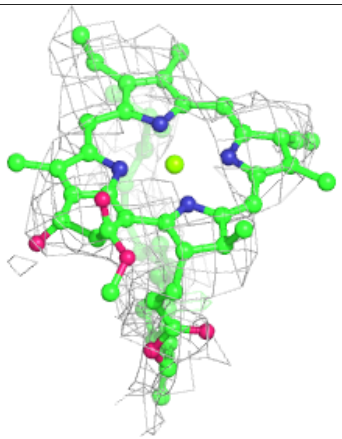


Electron density around CLA L 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

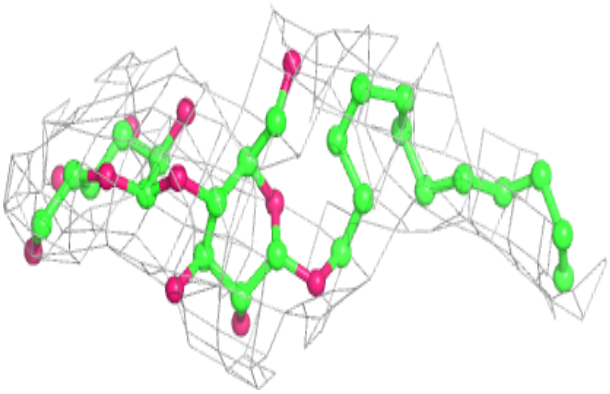


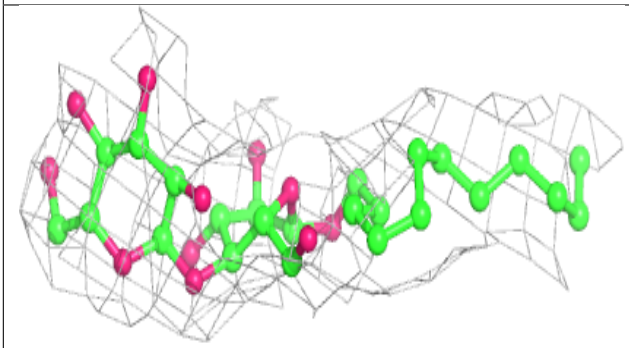


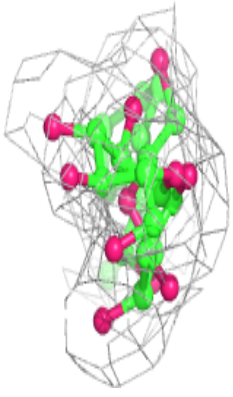


Electron density around LMU K 105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

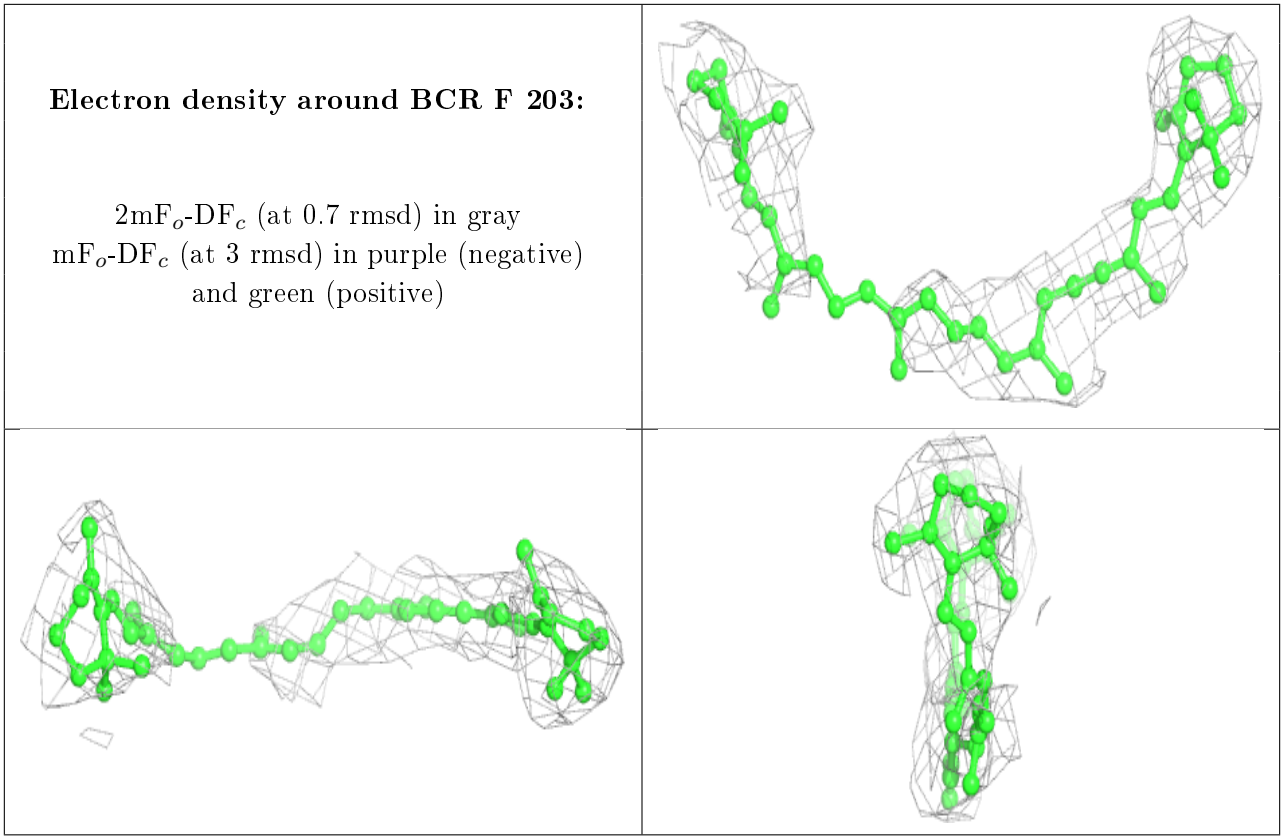






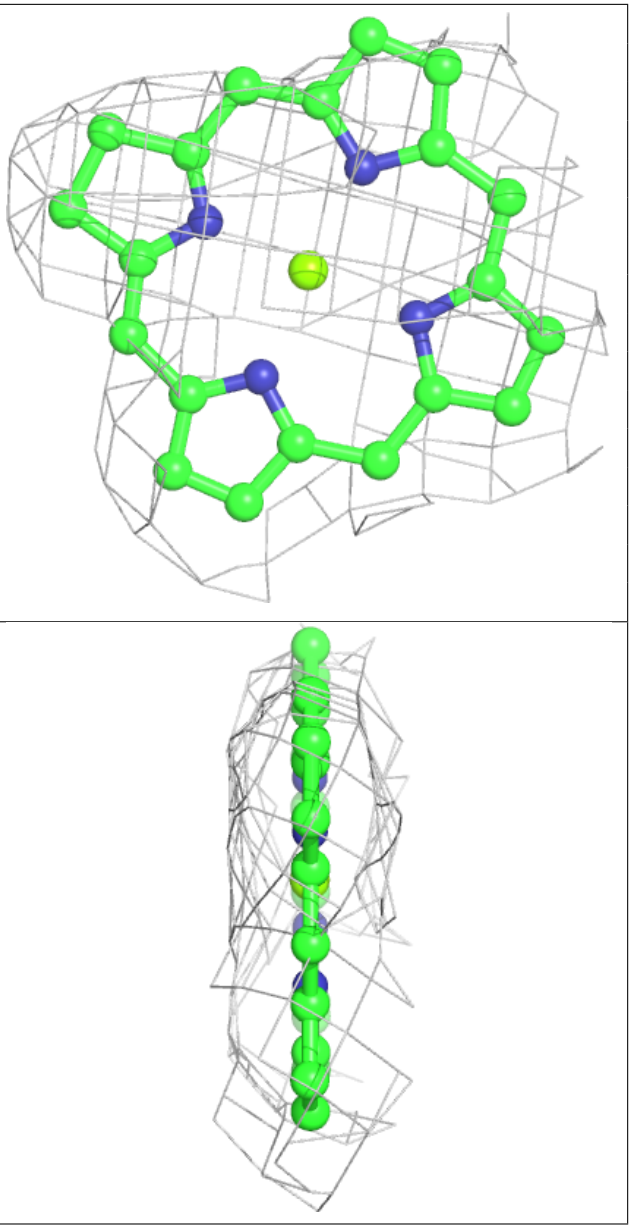
Electron density around BCR F 203:

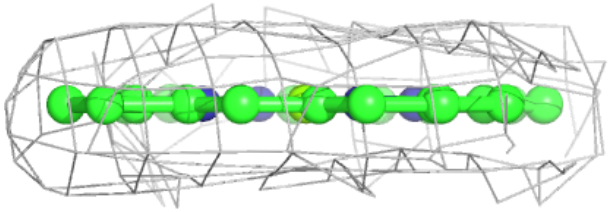
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 4 310:

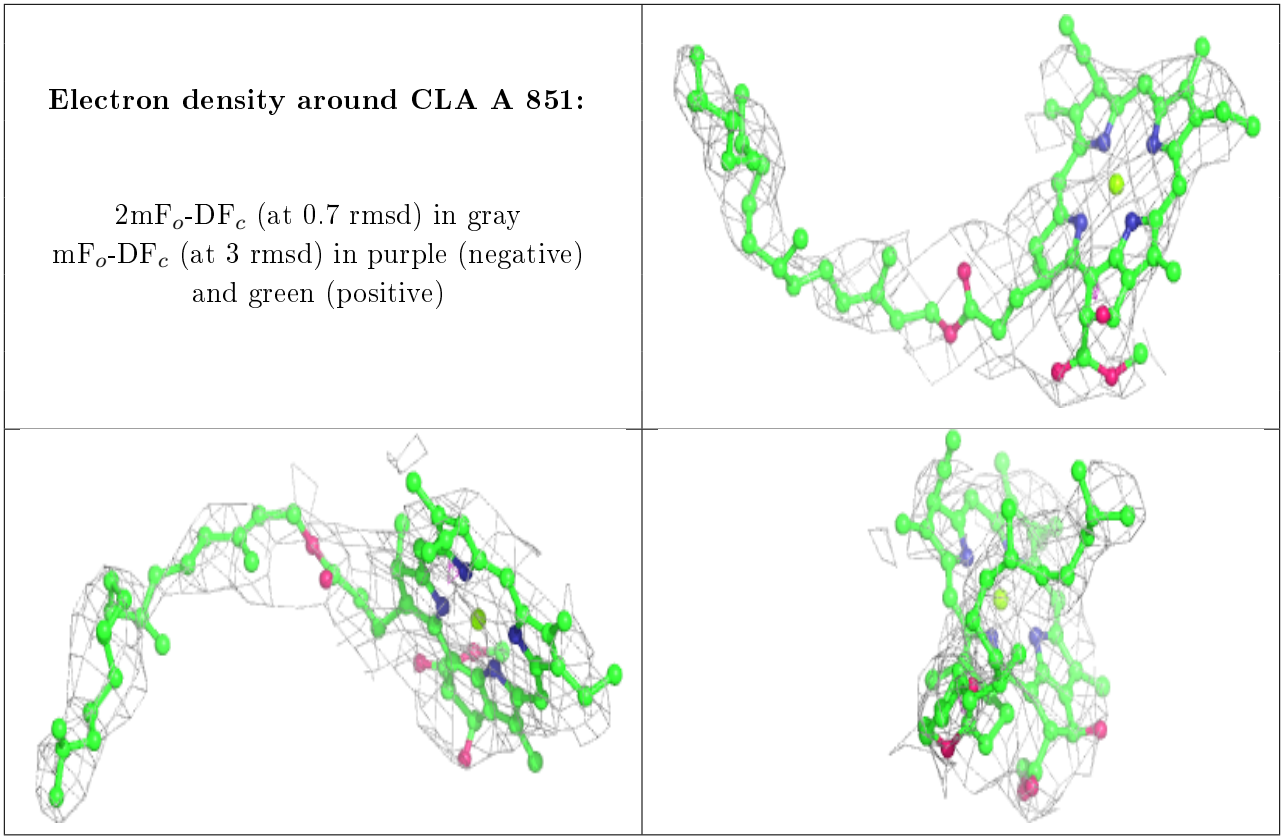
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





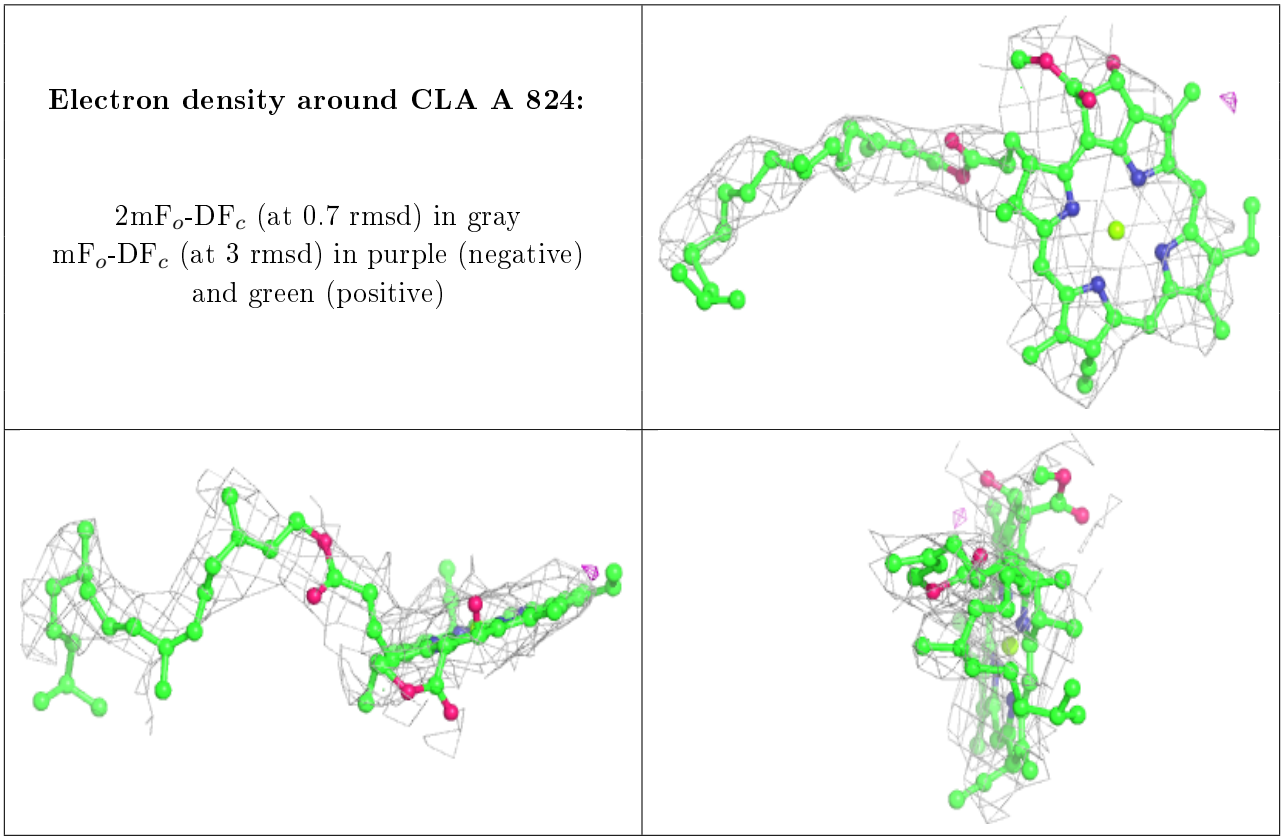
Electron density around CLA A 851:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



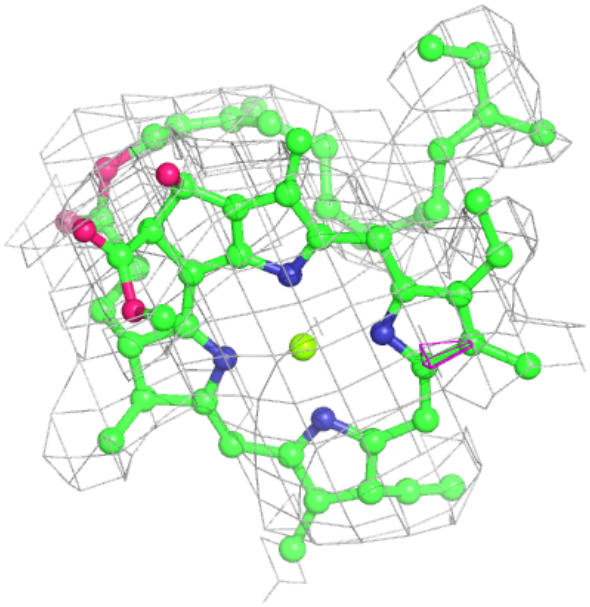
Electron density around CLA A 824:

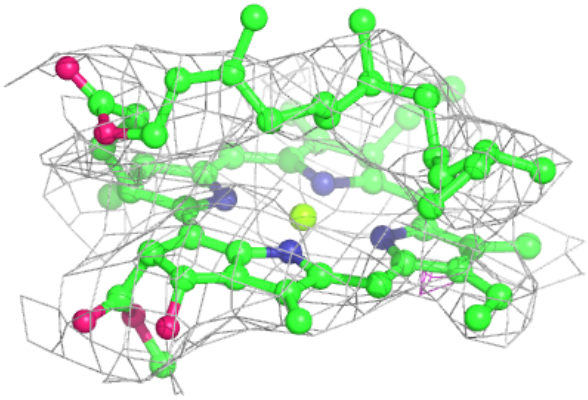
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

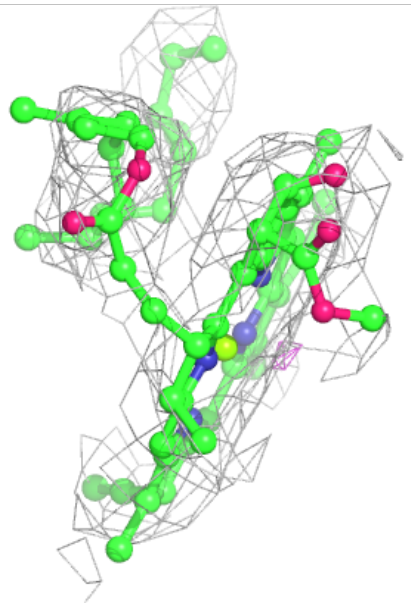


Electron density around CLA 1 206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

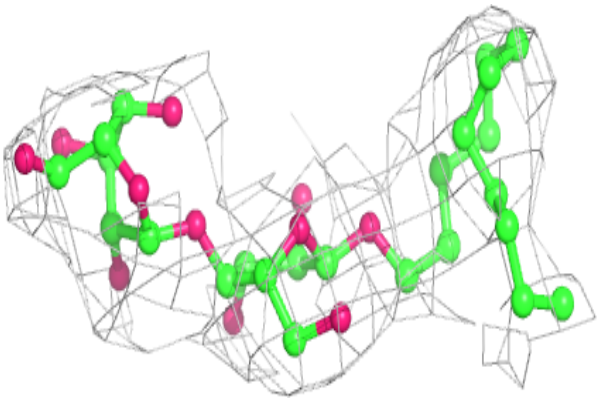


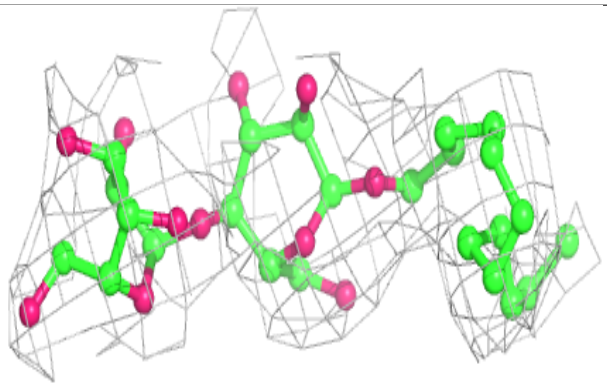


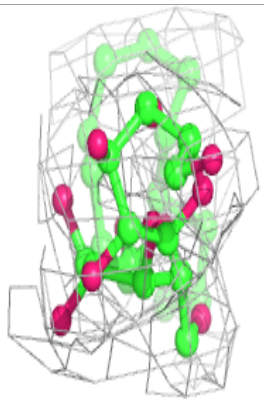


Electron density around LMU A 855:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

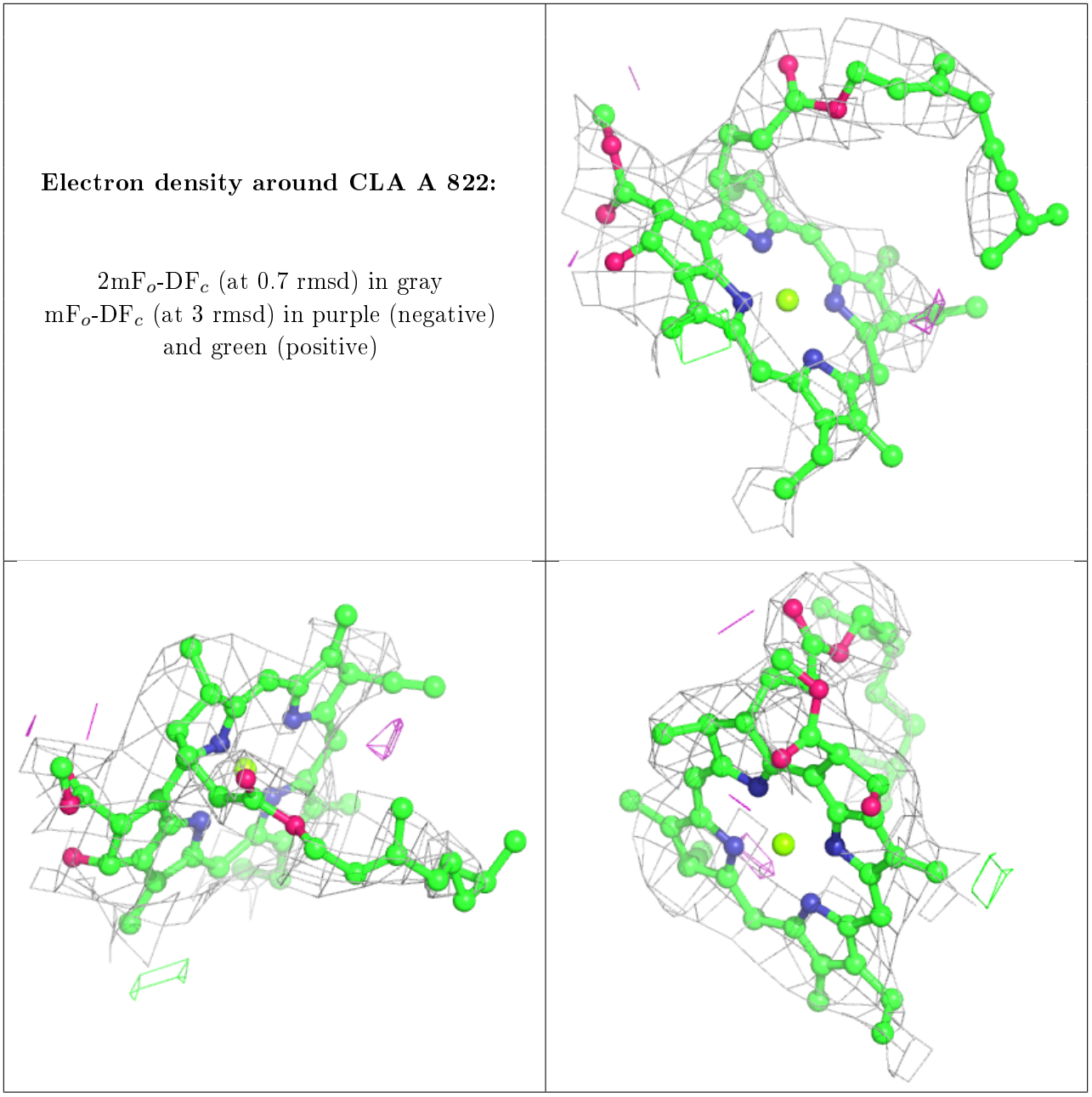






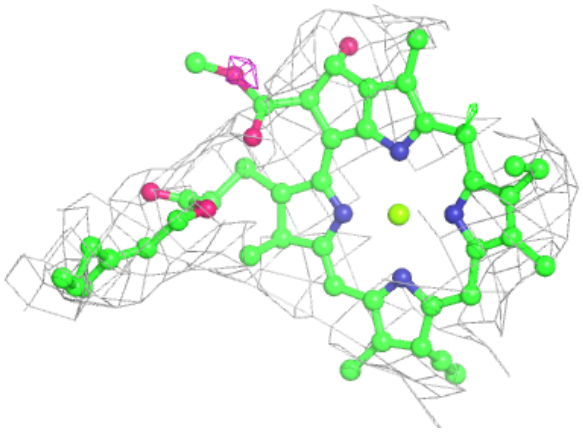
Electron density around CLA A 822:

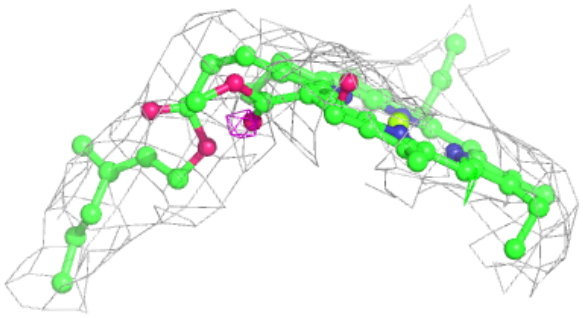
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

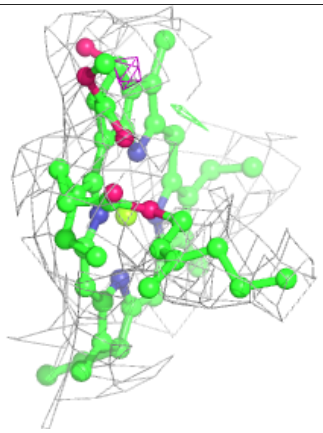


Electron density around CLA 4 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

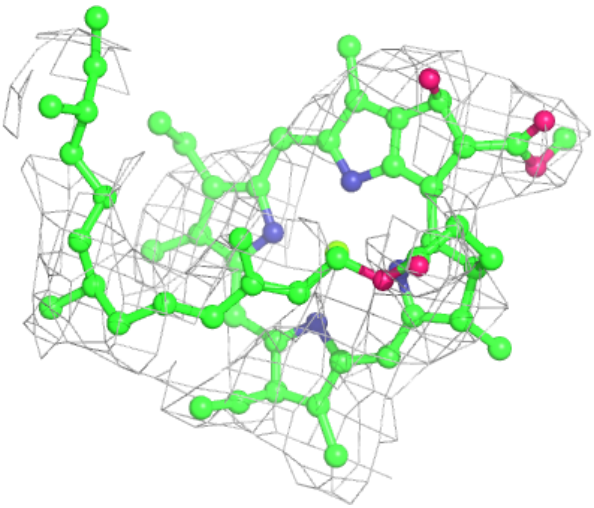


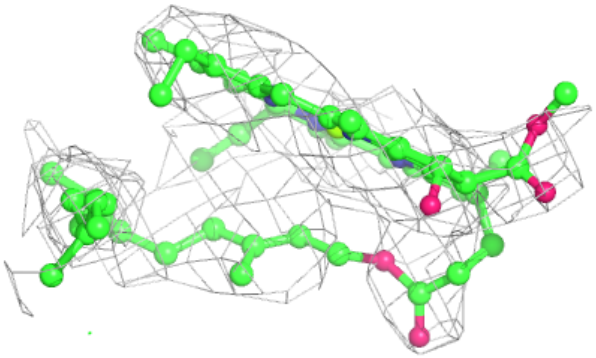


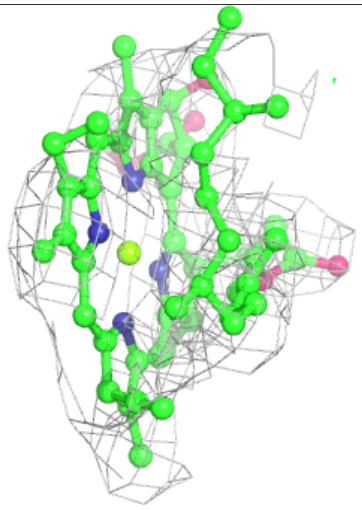


Electron density around CLA B 817:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

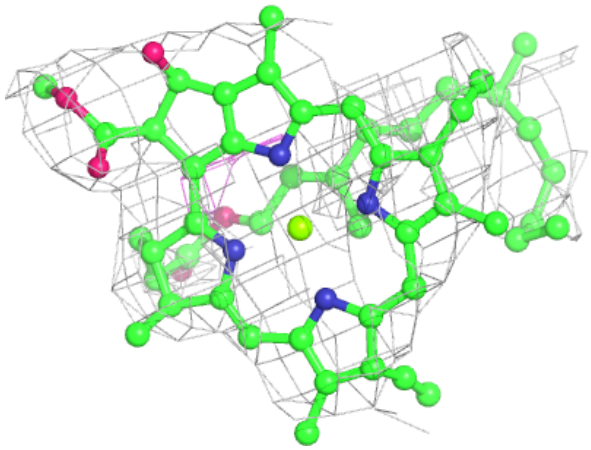


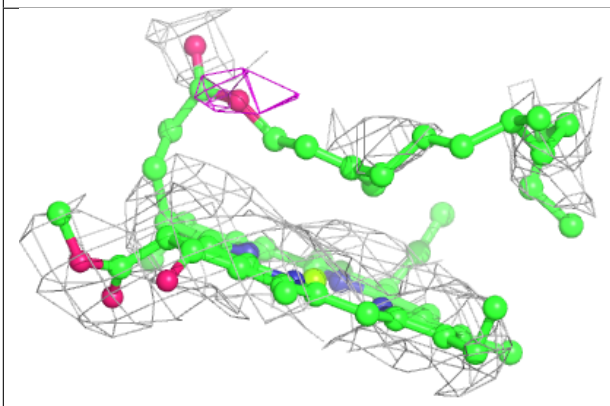


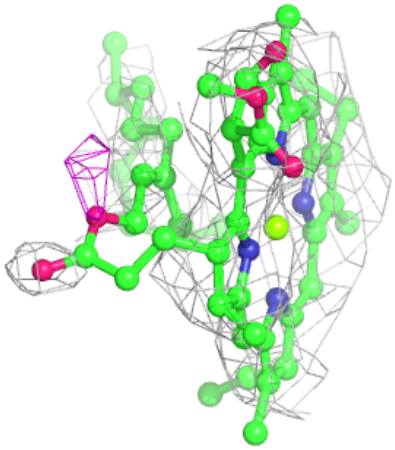


Electron density around CLA B 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

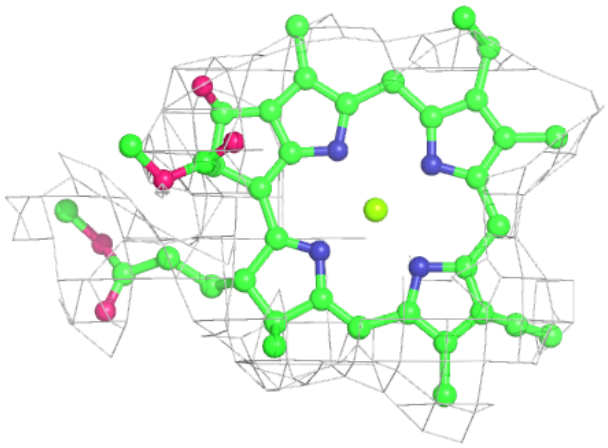


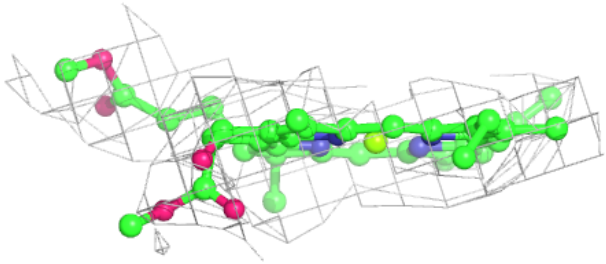


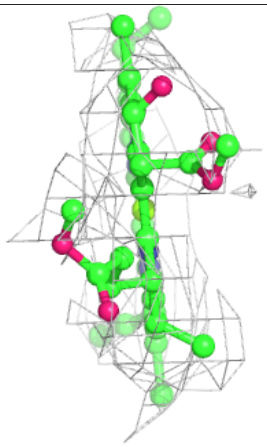


Electron density around CLA 4 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

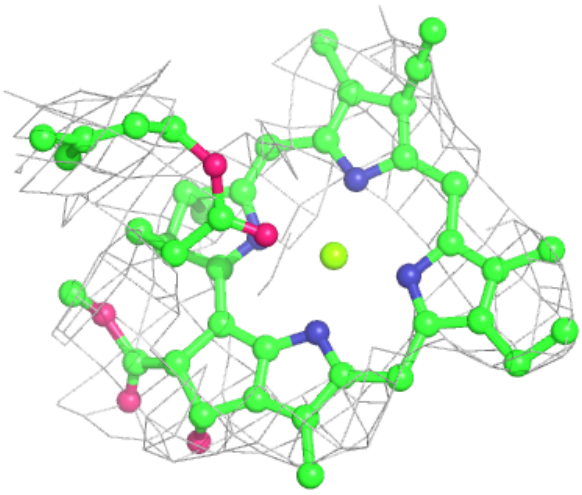


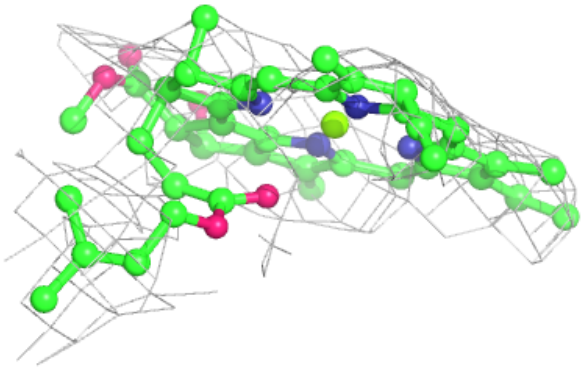


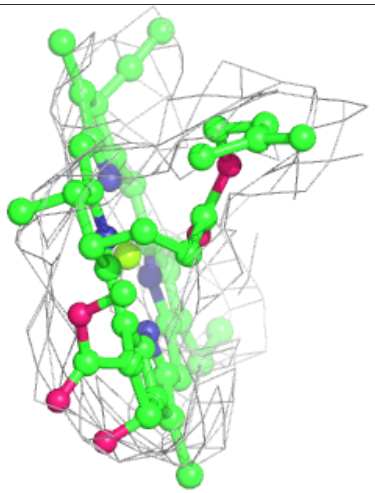


Electron density around CLA A 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

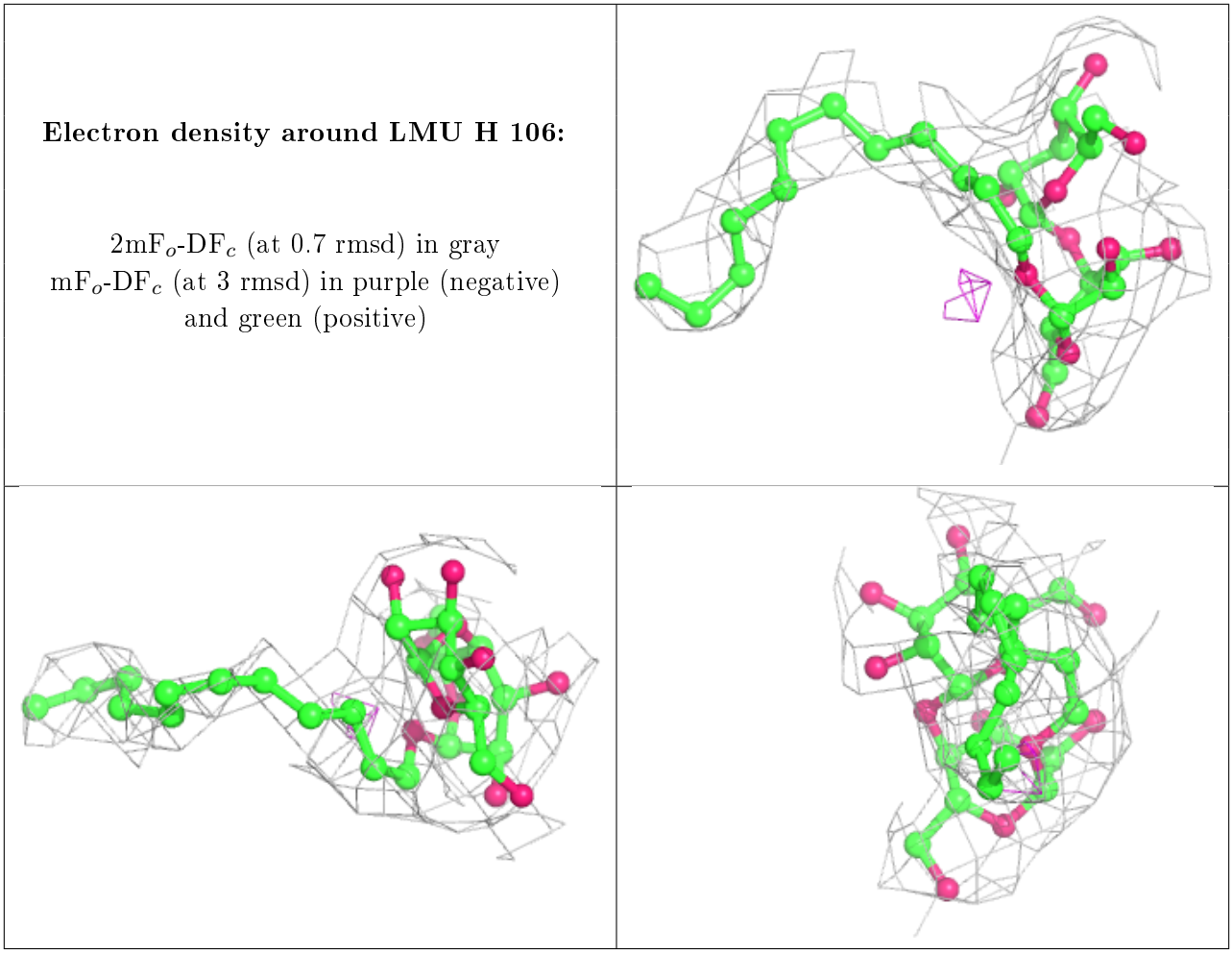






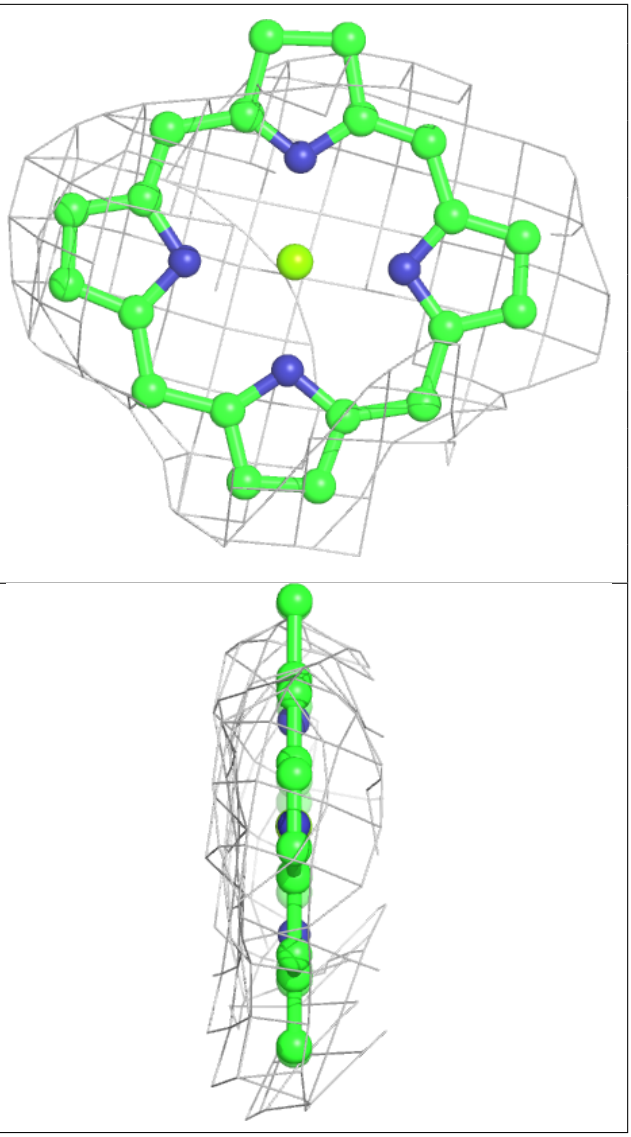
Electron density around LMU H 106:

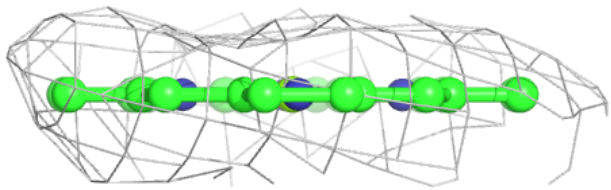
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 2 309:

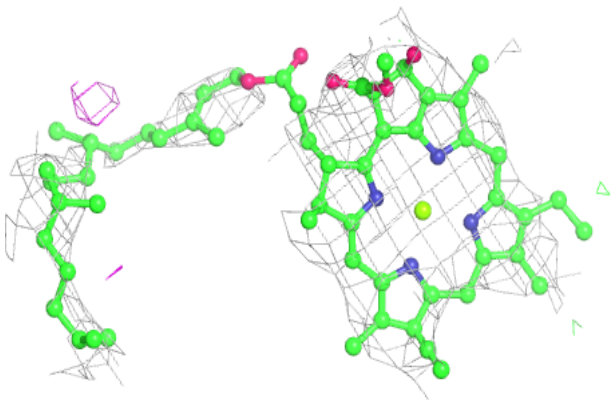
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

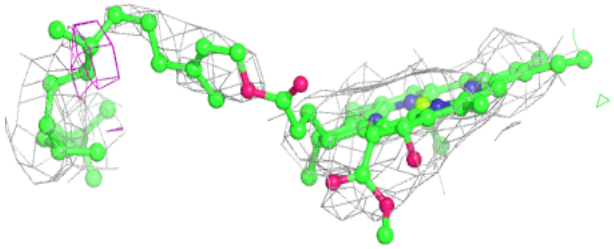


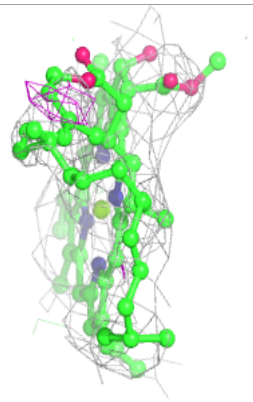


Electron density around CLA A 825:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

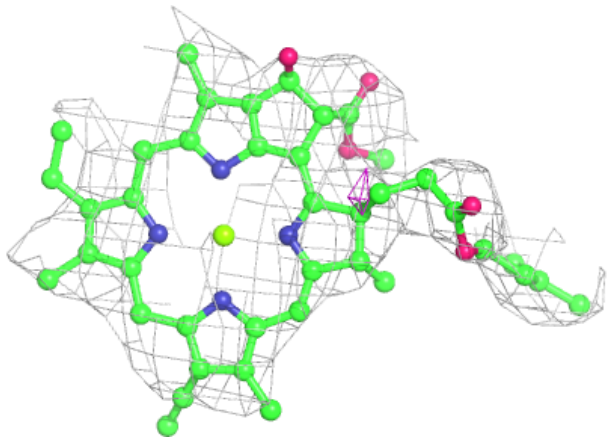


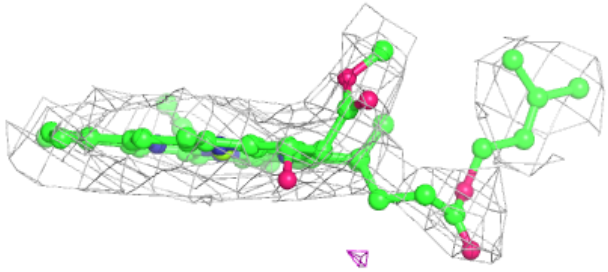




Electron density around CLA B 829:

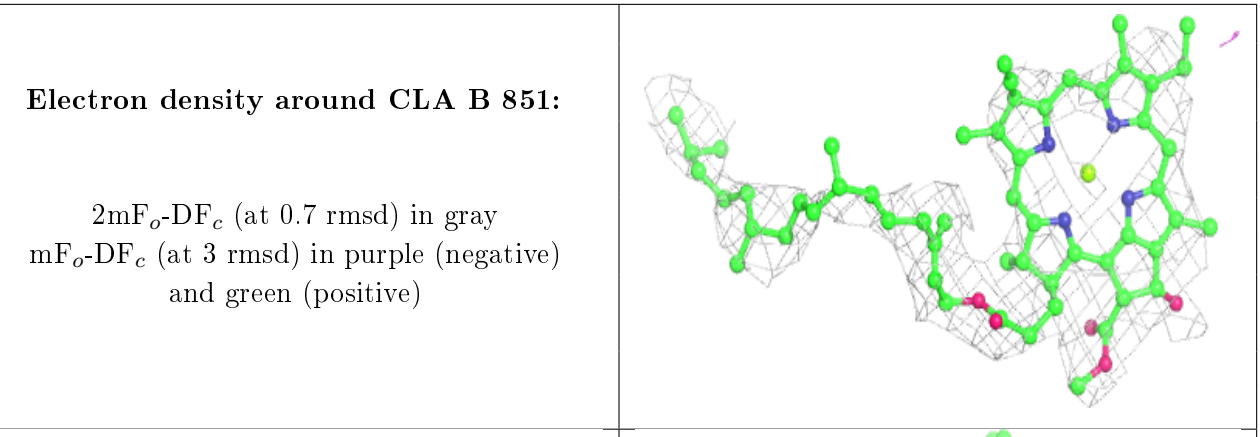
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





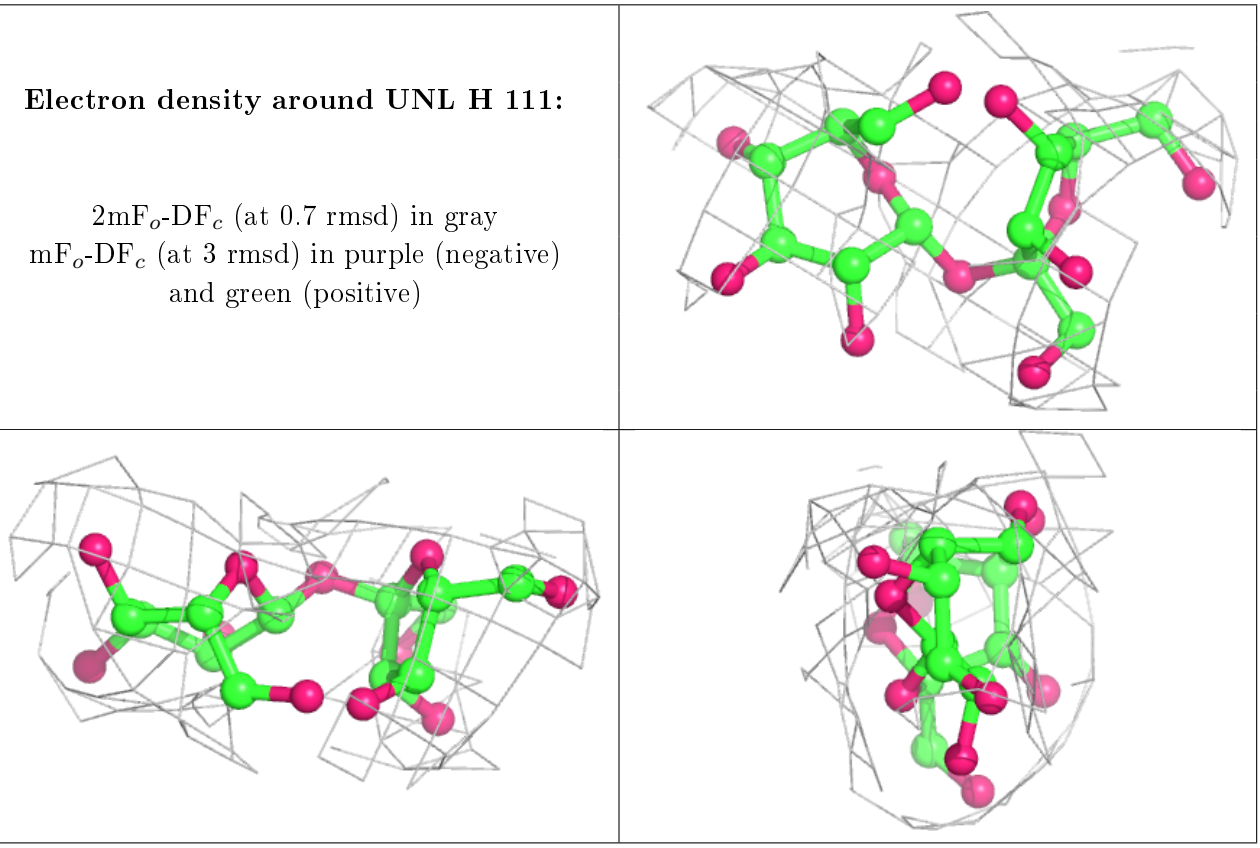
Electron density around CLA B 851:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



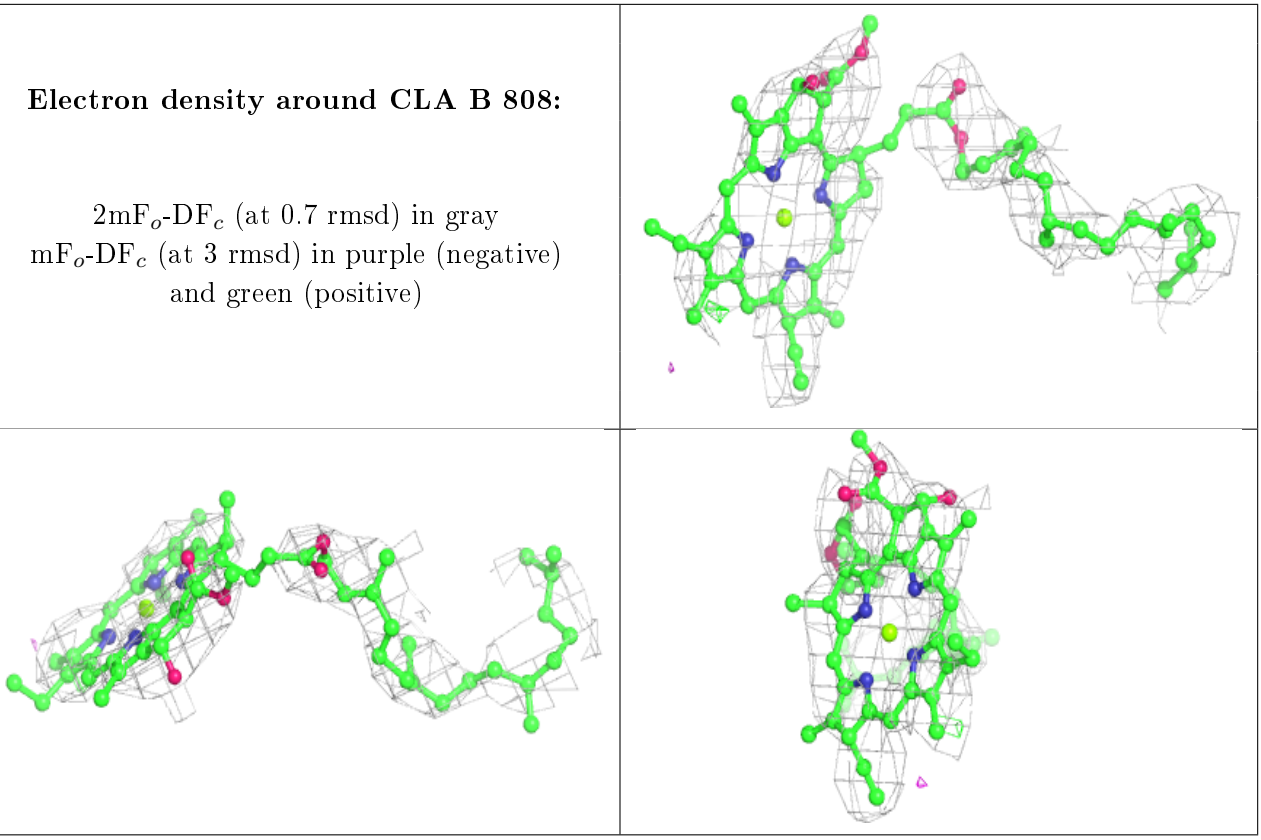
Electron density around UNL H 111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



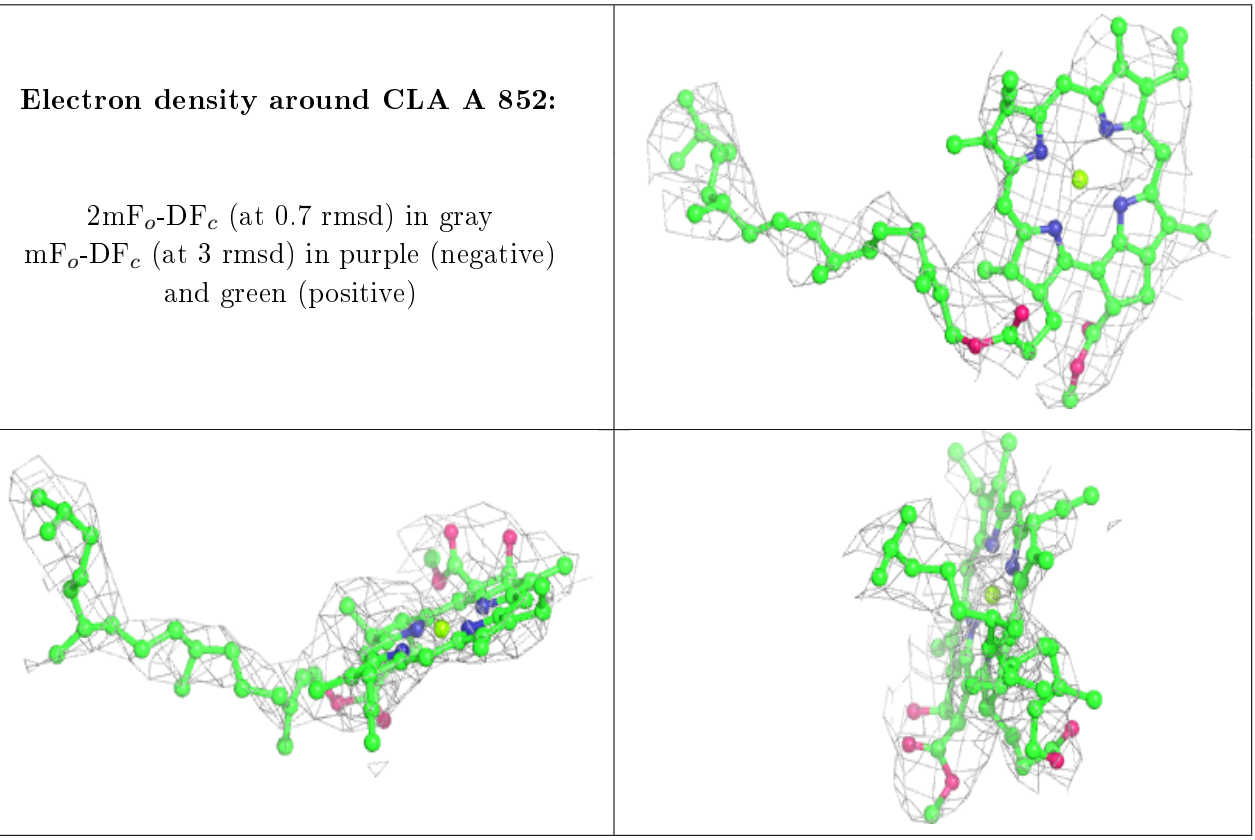
Electron density around CLA B 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



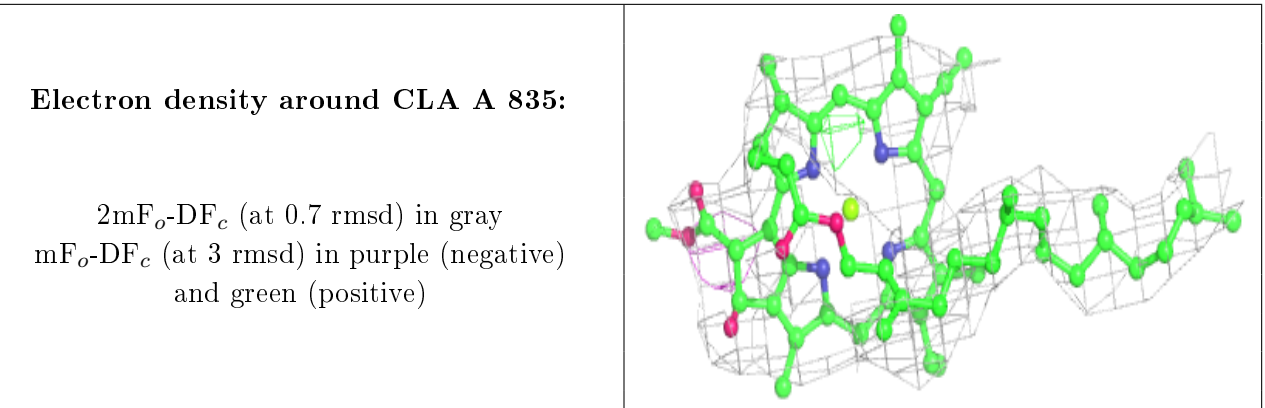
Electron density around CLA A 852:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



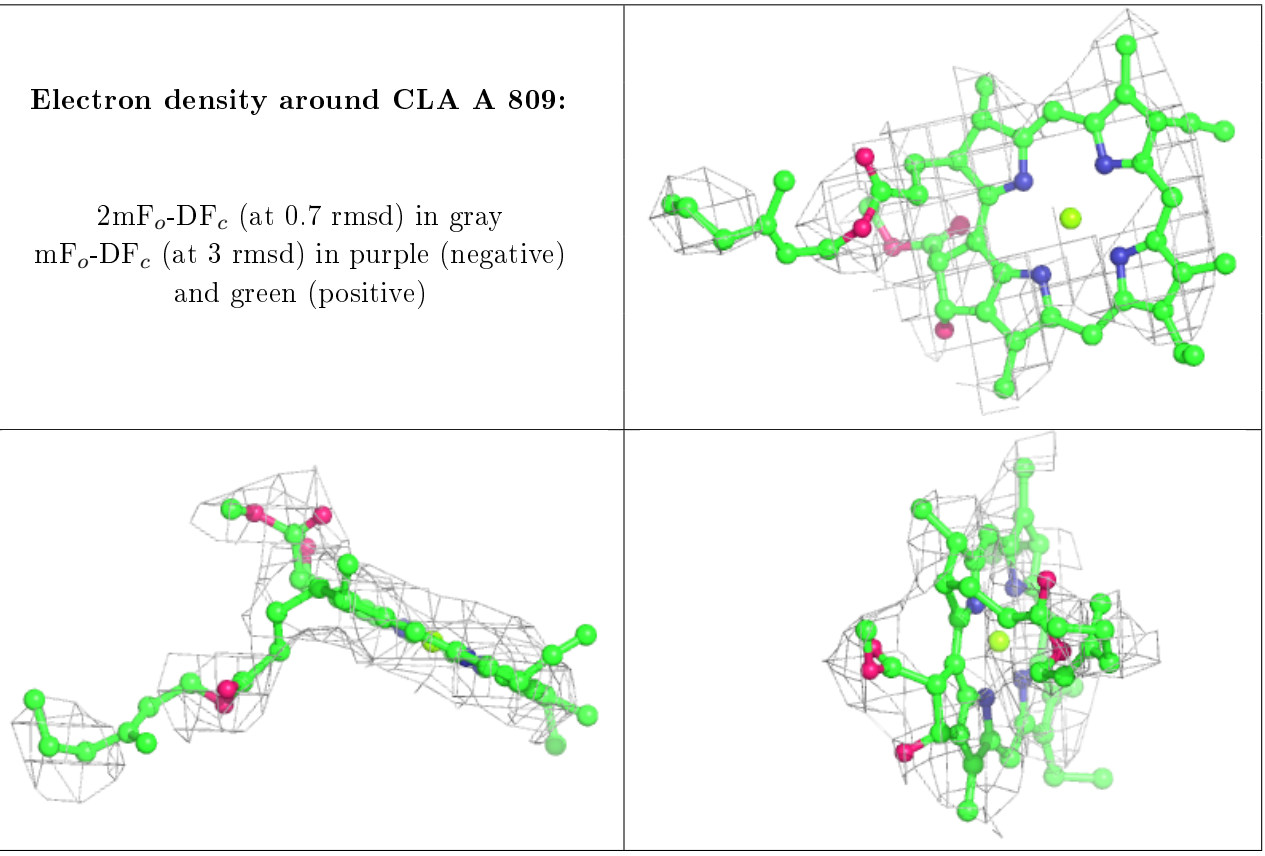
Electron density around CLA A 835:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



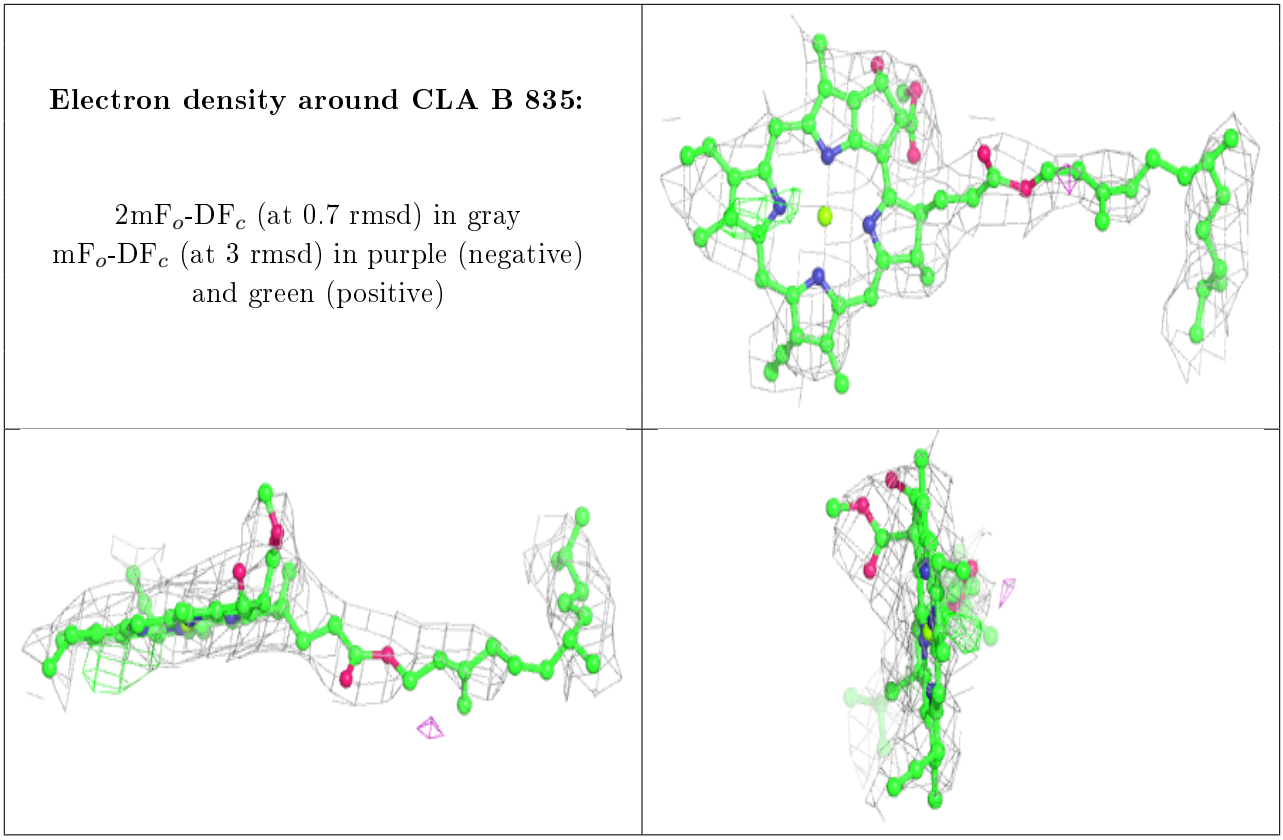
Electron density around CLA A 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



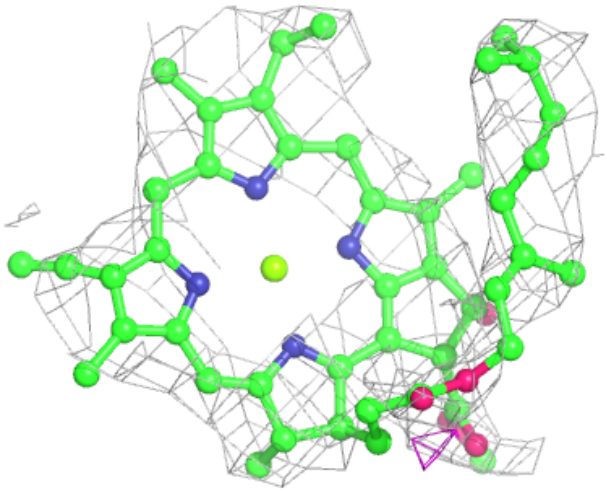
Electron density around CLA B 835:

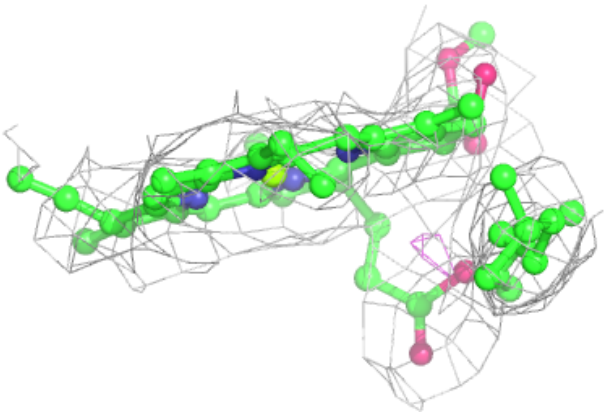
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

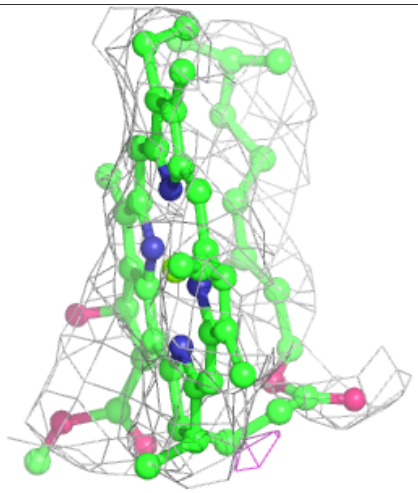


Electron density around CLA A 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

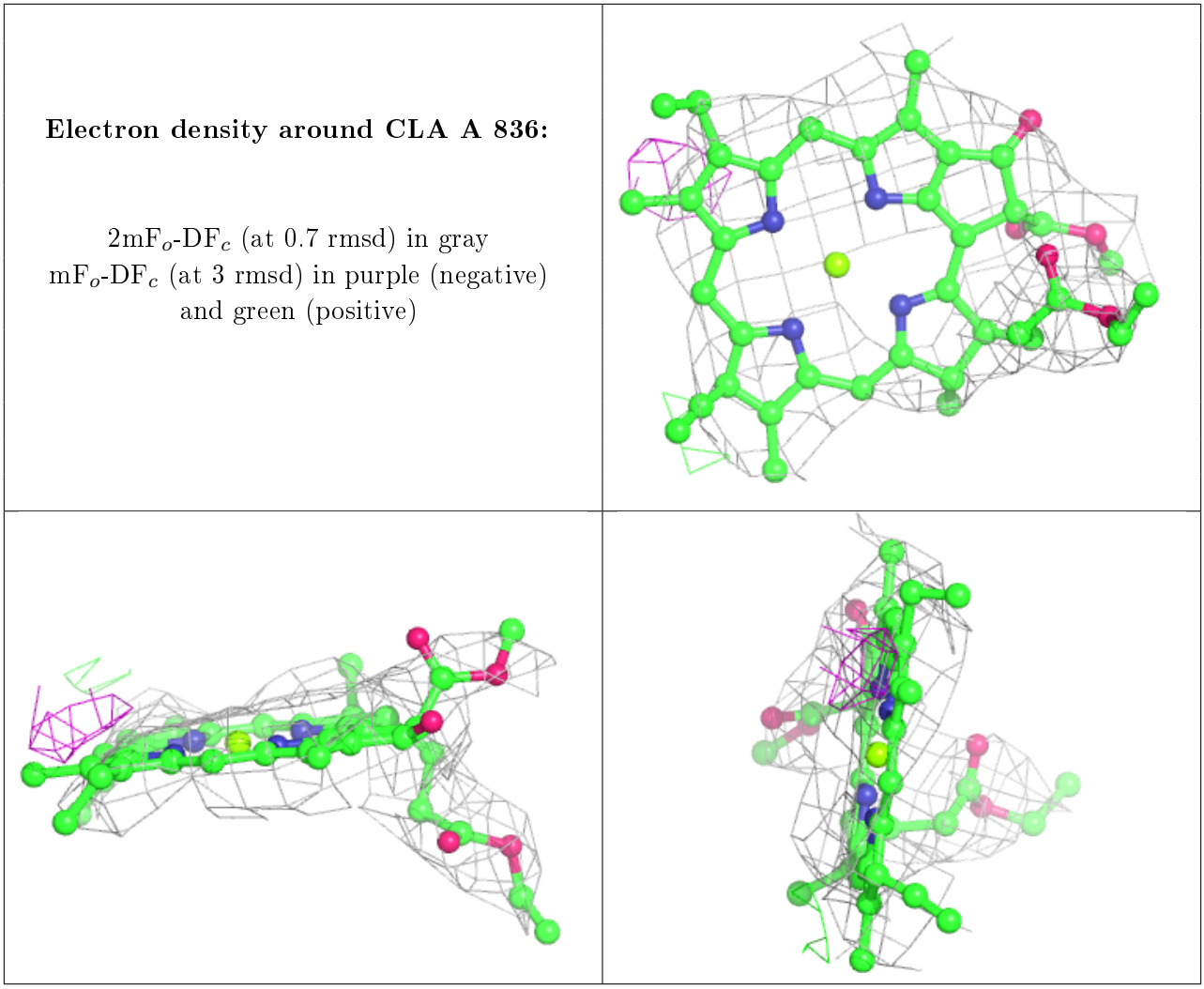






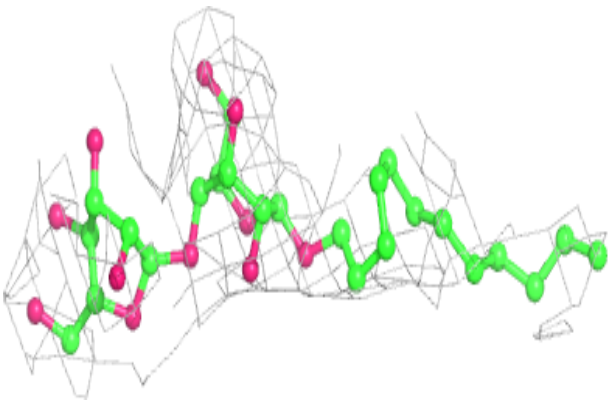
Electron density around CLA A 836:

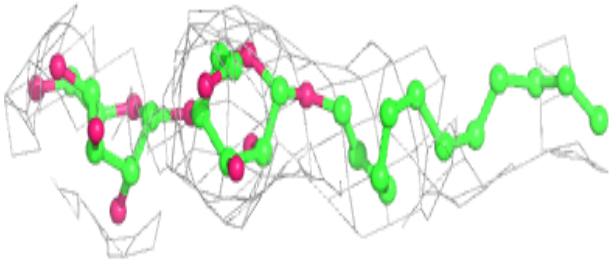
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

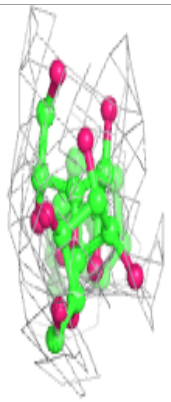


Electron density around LMU E 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

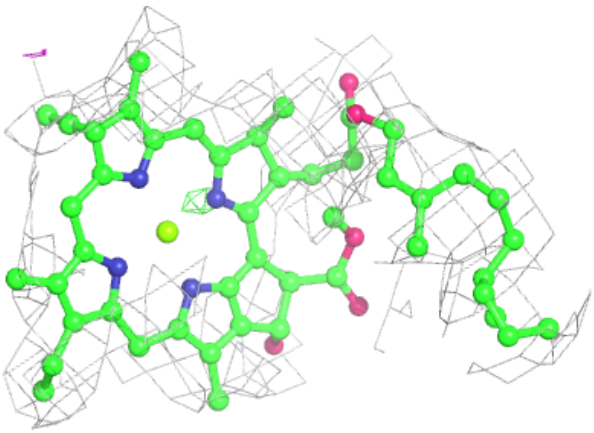


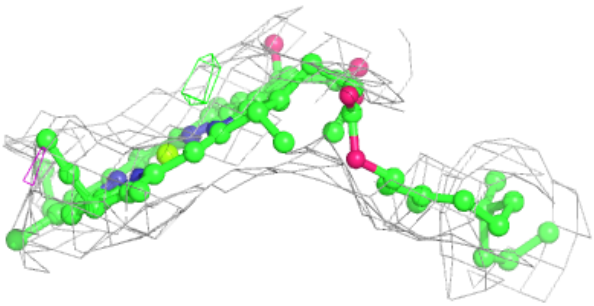


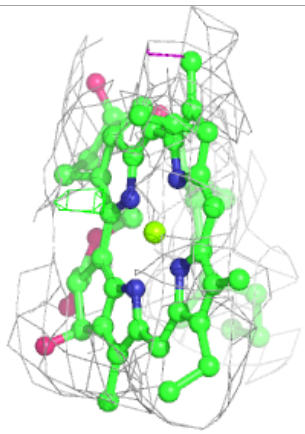


Electron density around CLA 1 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

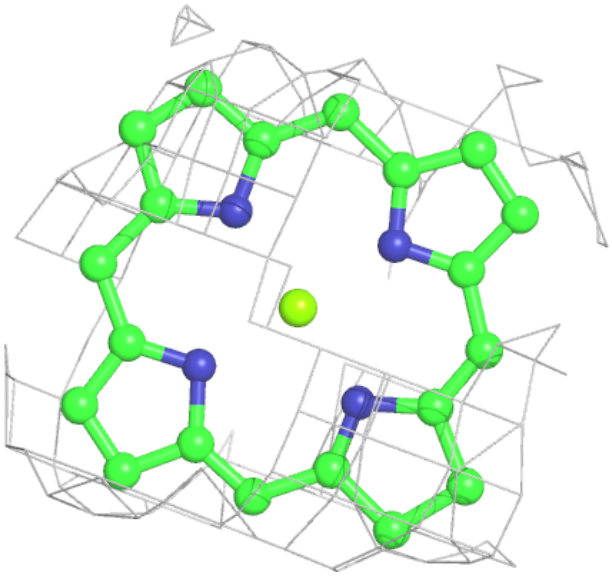


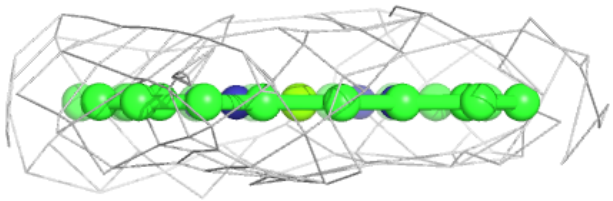


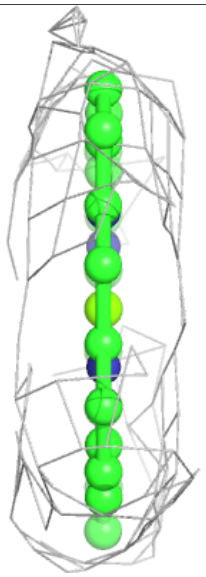


Electron density around CLA 1 214:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

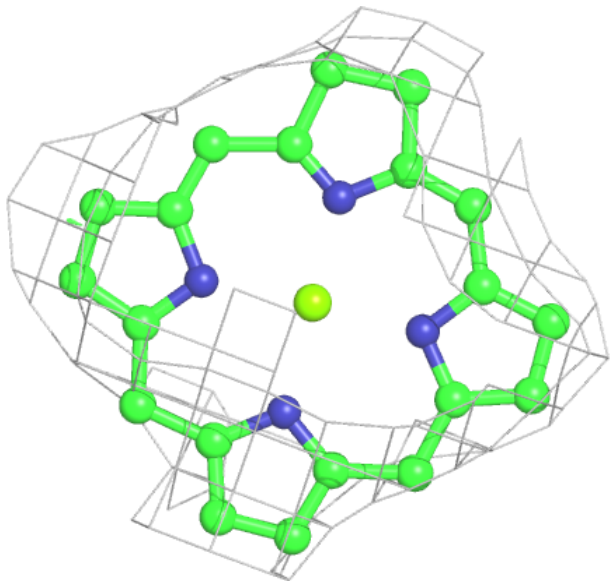


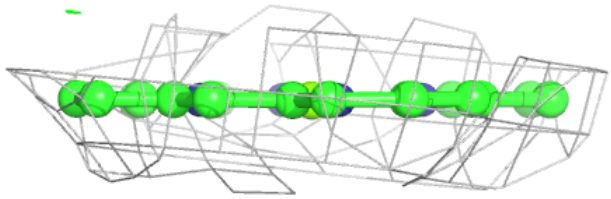


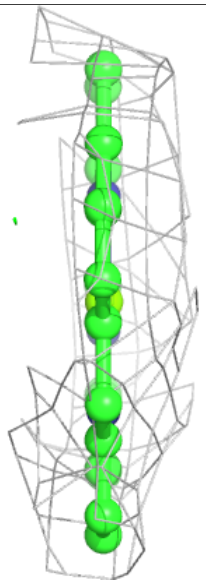


Electron density around CLA 4 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

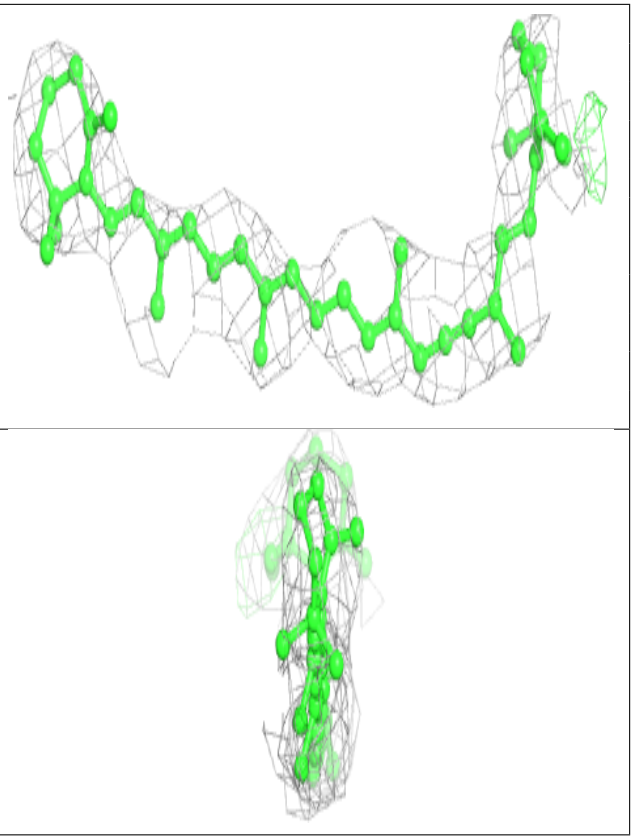






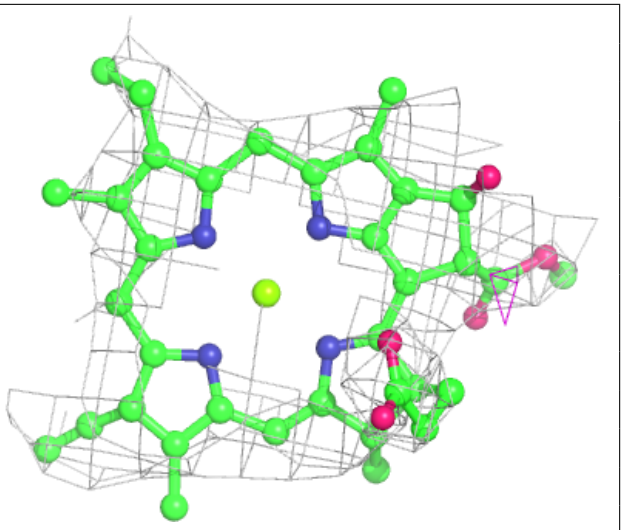
Electron density around BCR B 843:

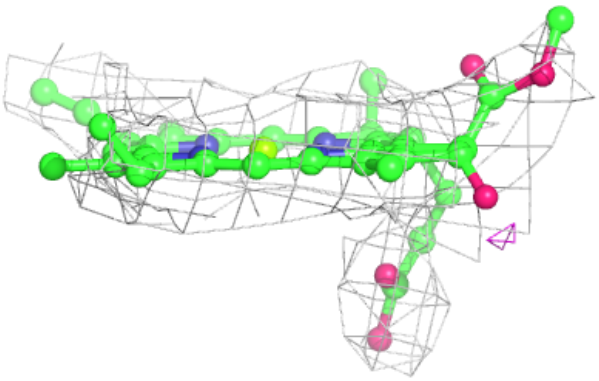
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

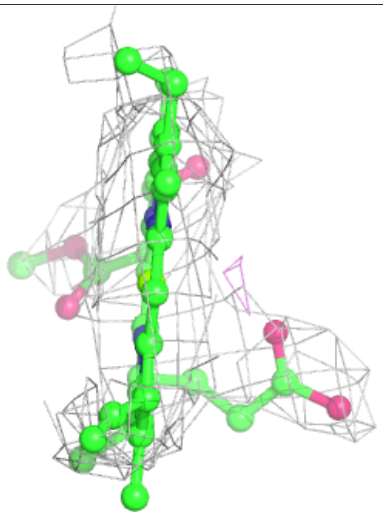


Electron density around CLA B 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

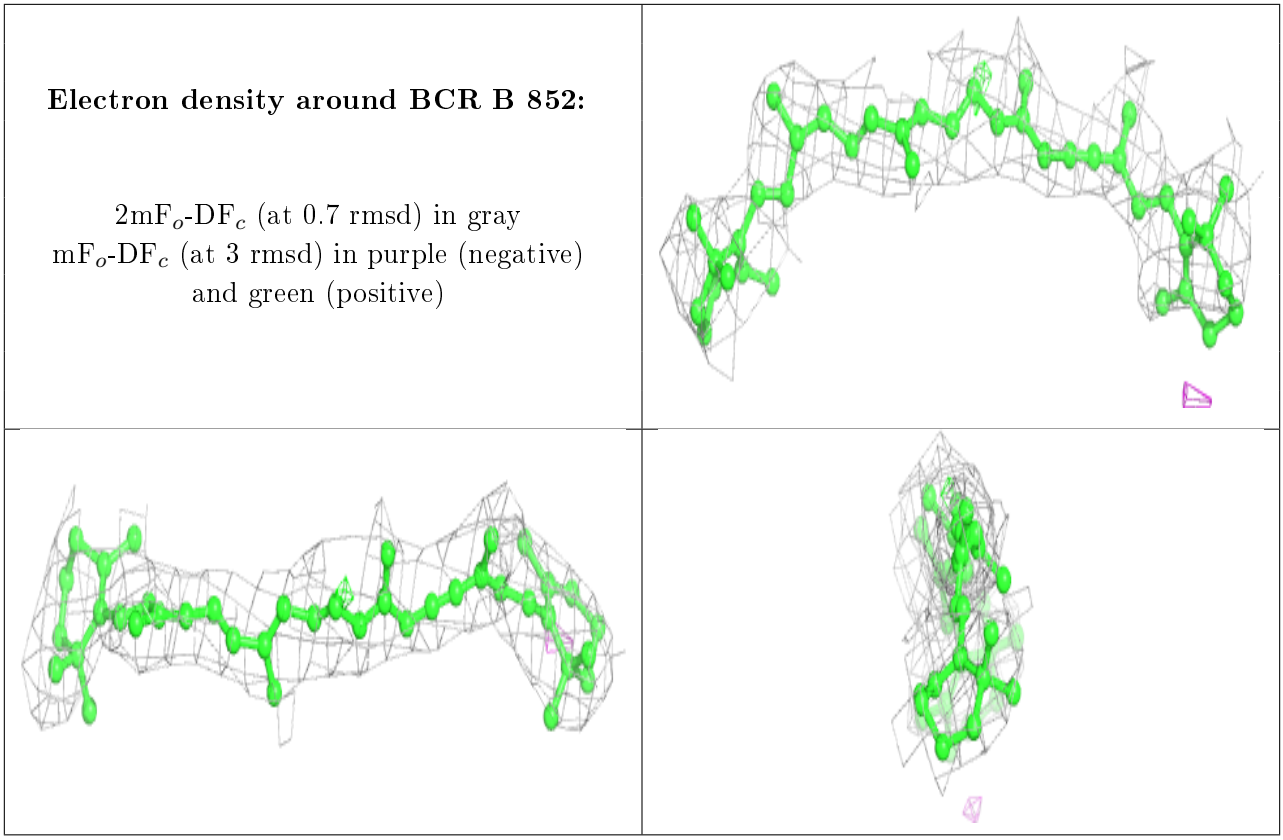






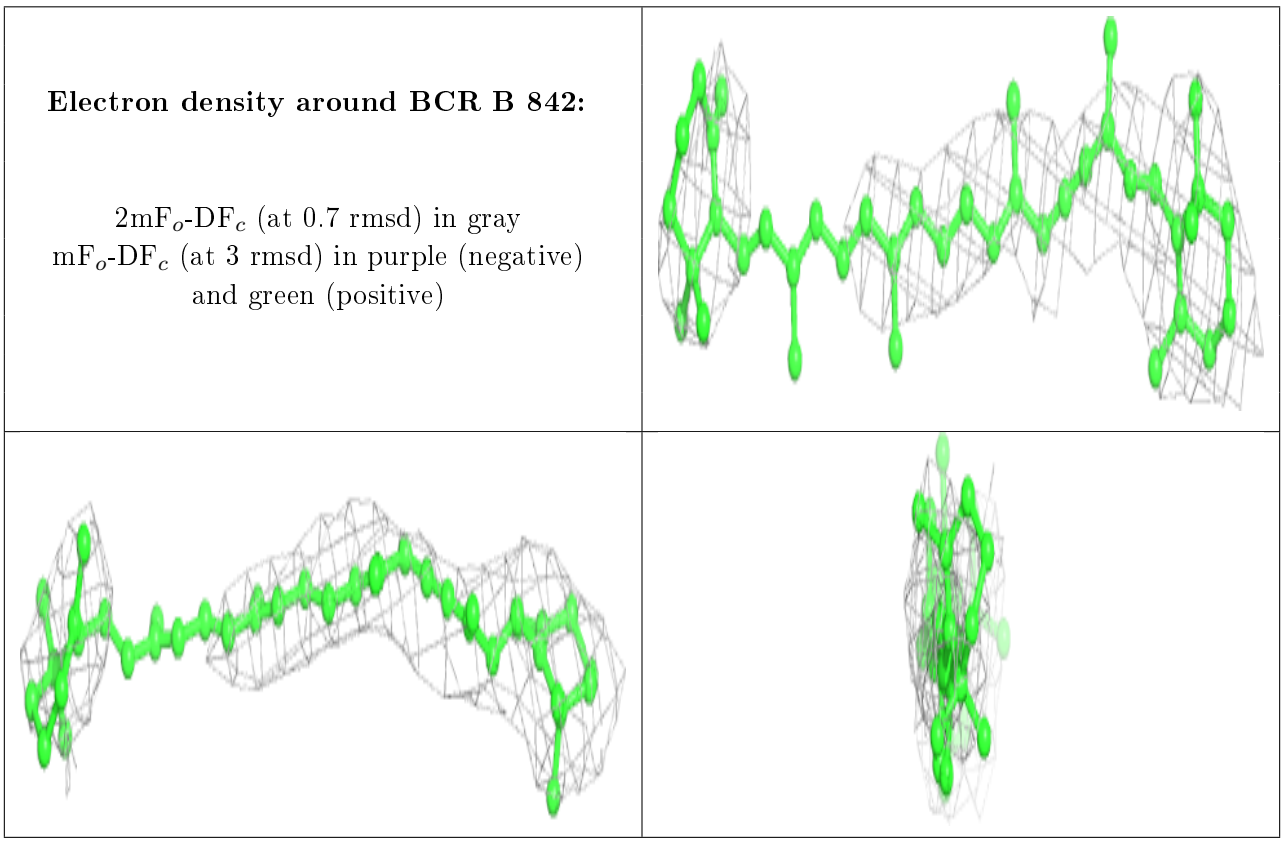
Electron density around BCR B 852:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



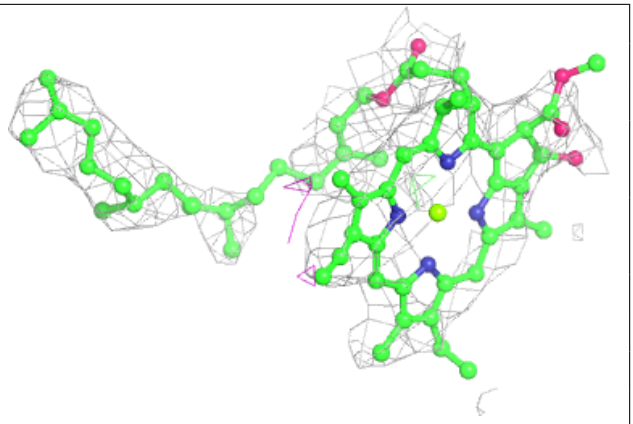
Electron density around BCR B 842:

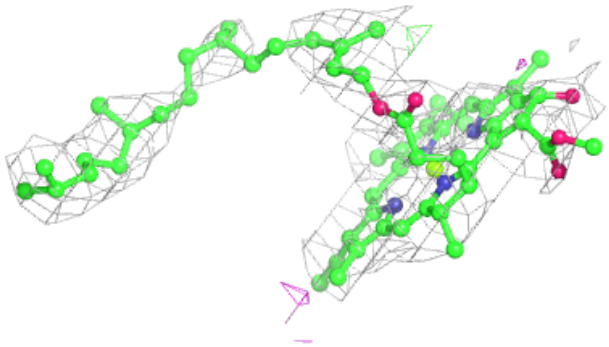
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

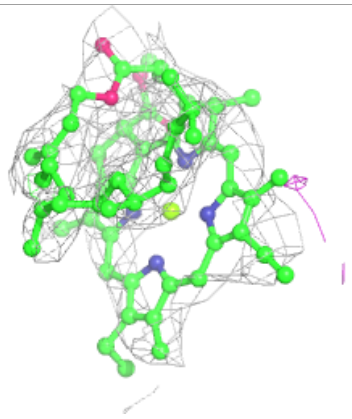


Electron density around CLA B 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

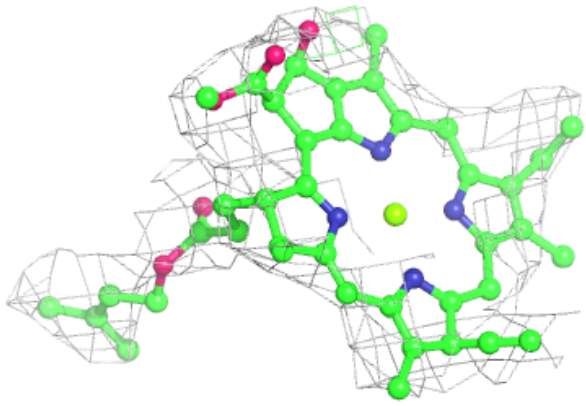


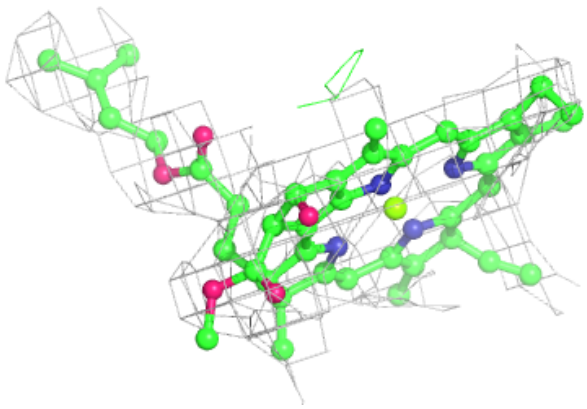


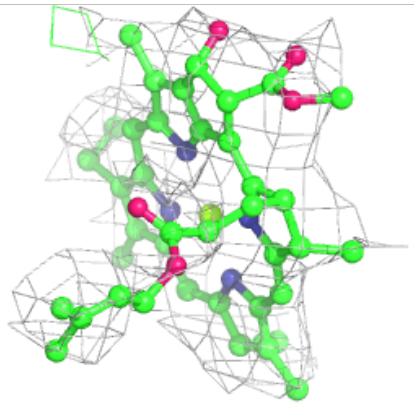


Electron density around CLA 2 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

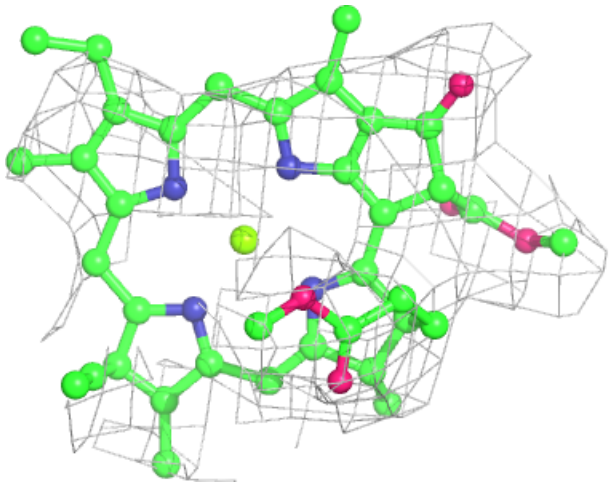


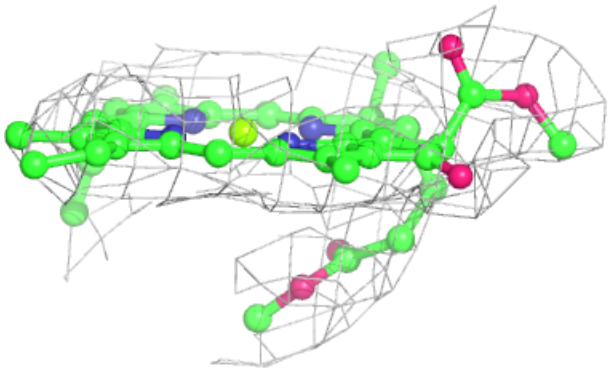


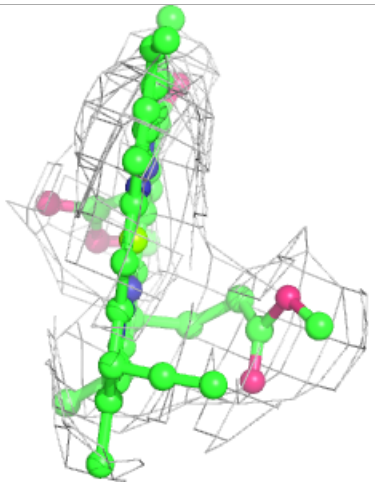


Electron density around CLA 1 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

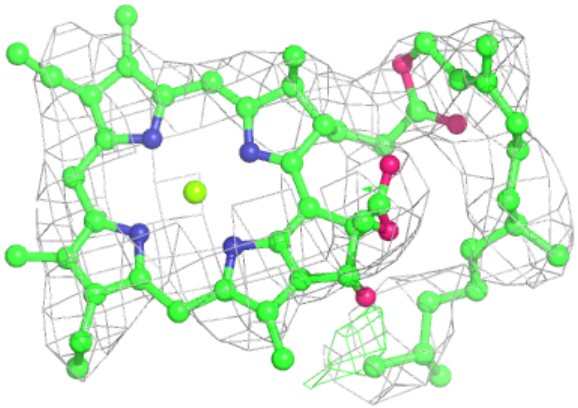


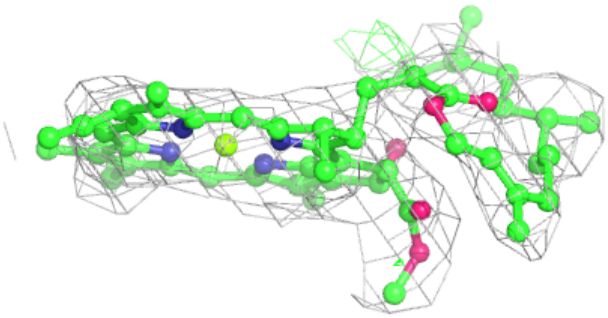


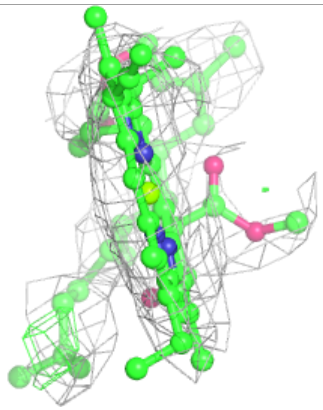


Electron density around CLA B 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

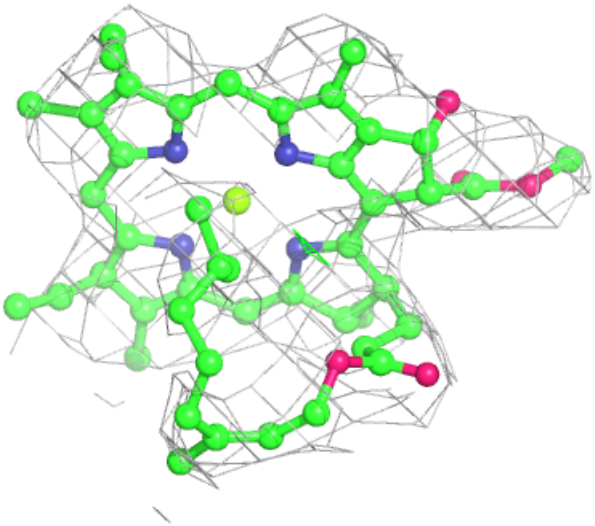


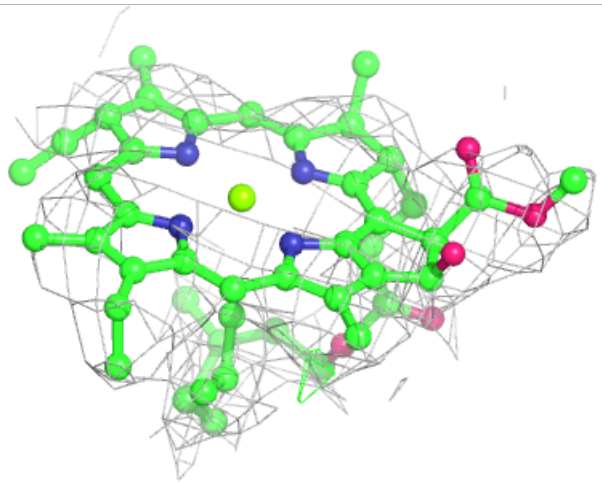


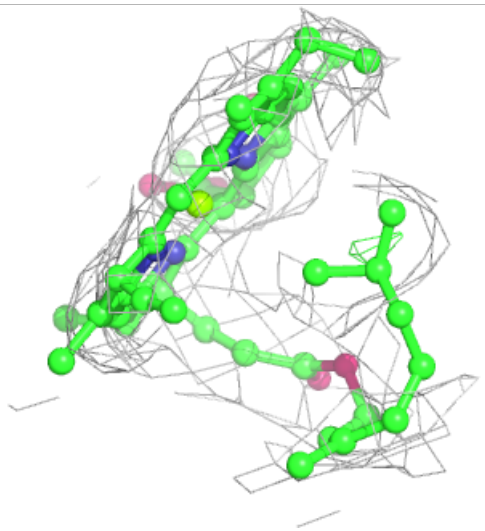


Electron density around CLA B 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

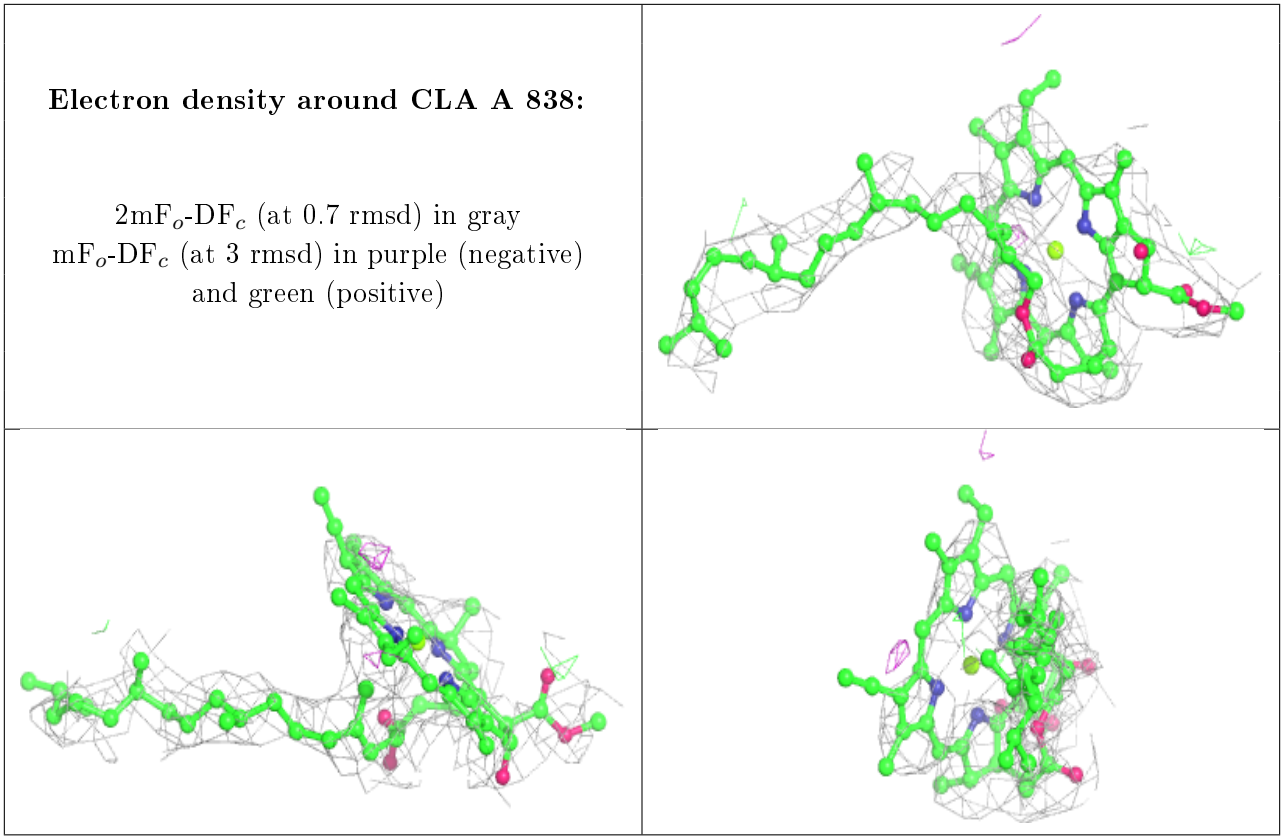






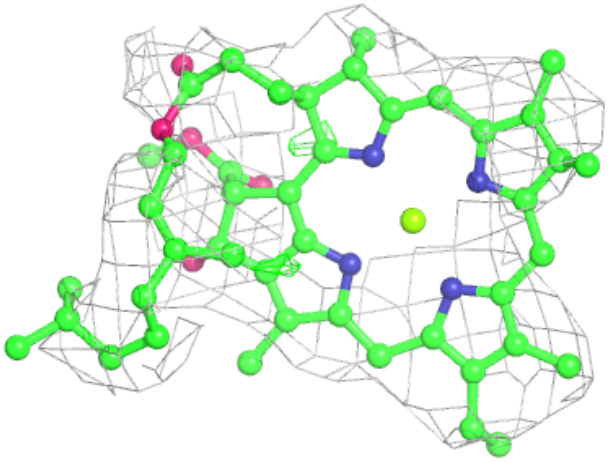
Electron density around CLA A 838:

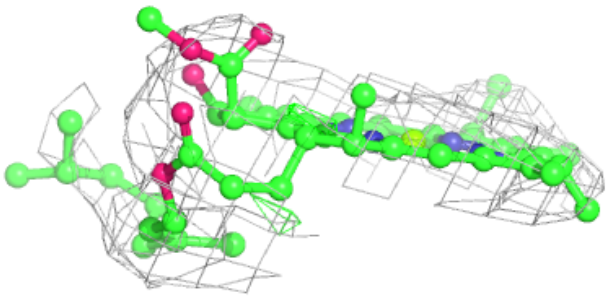
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

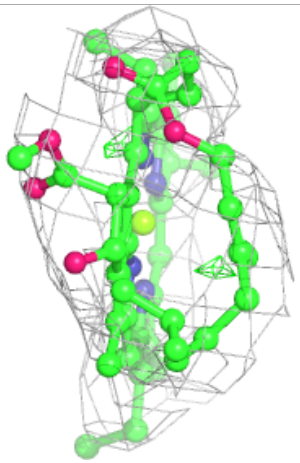


Electron density around CLA B 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

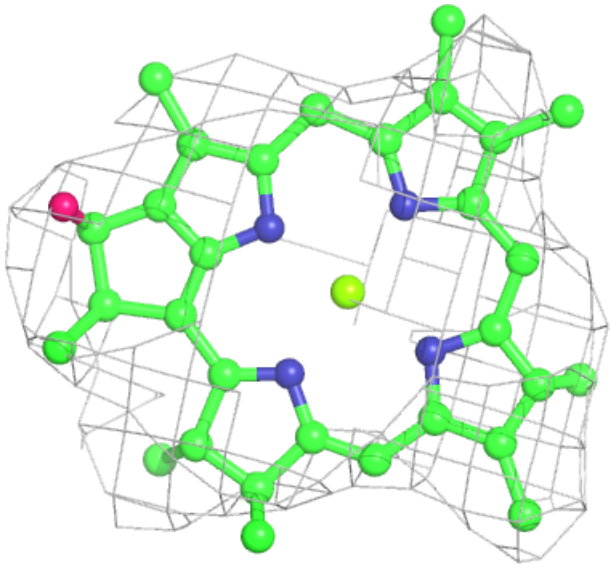


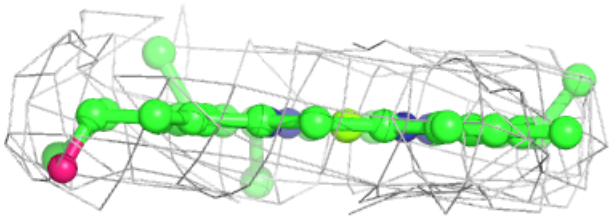


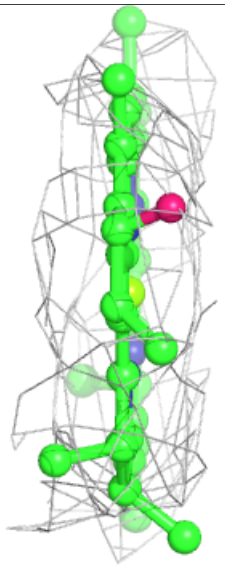


Electron density around CLA 4 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

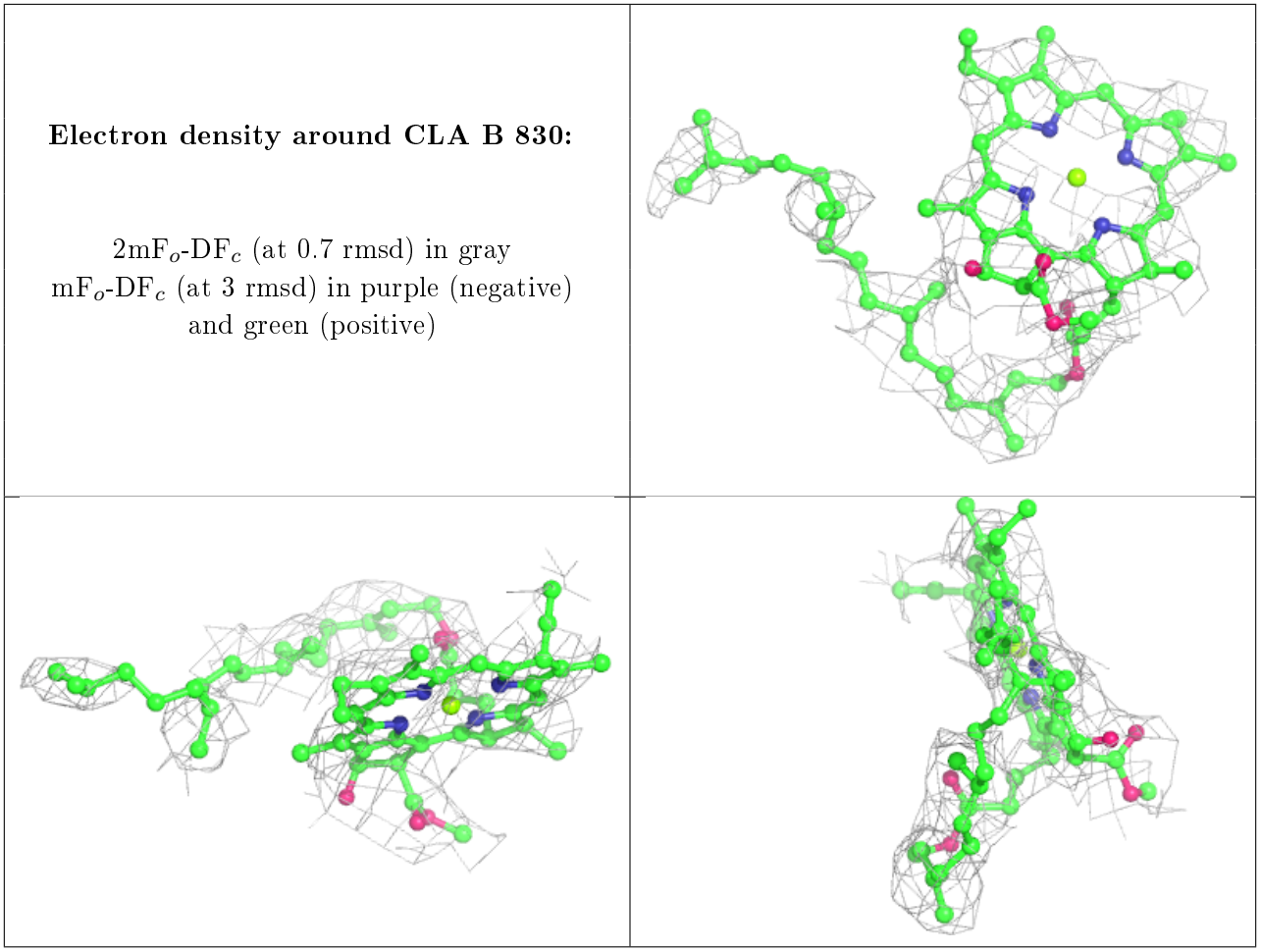






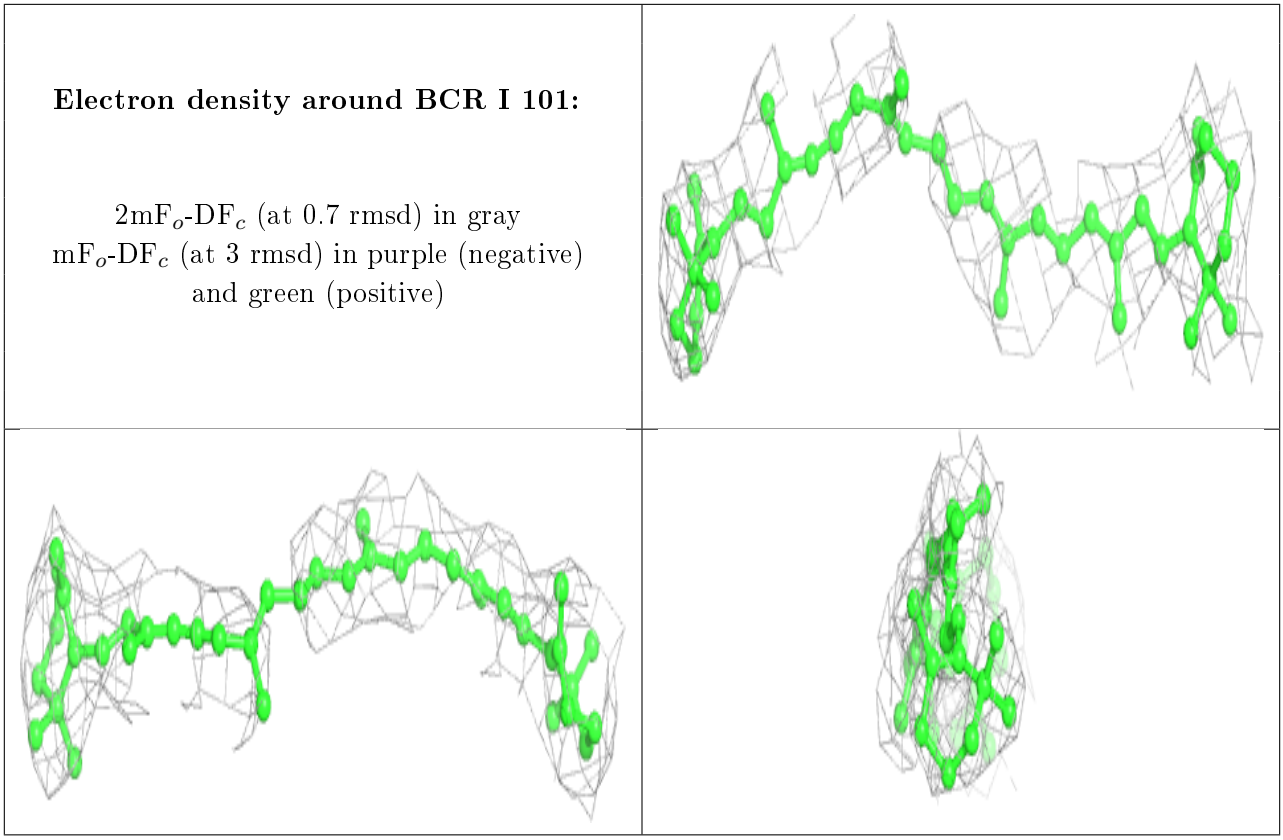
Electron density around CLA B 830:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



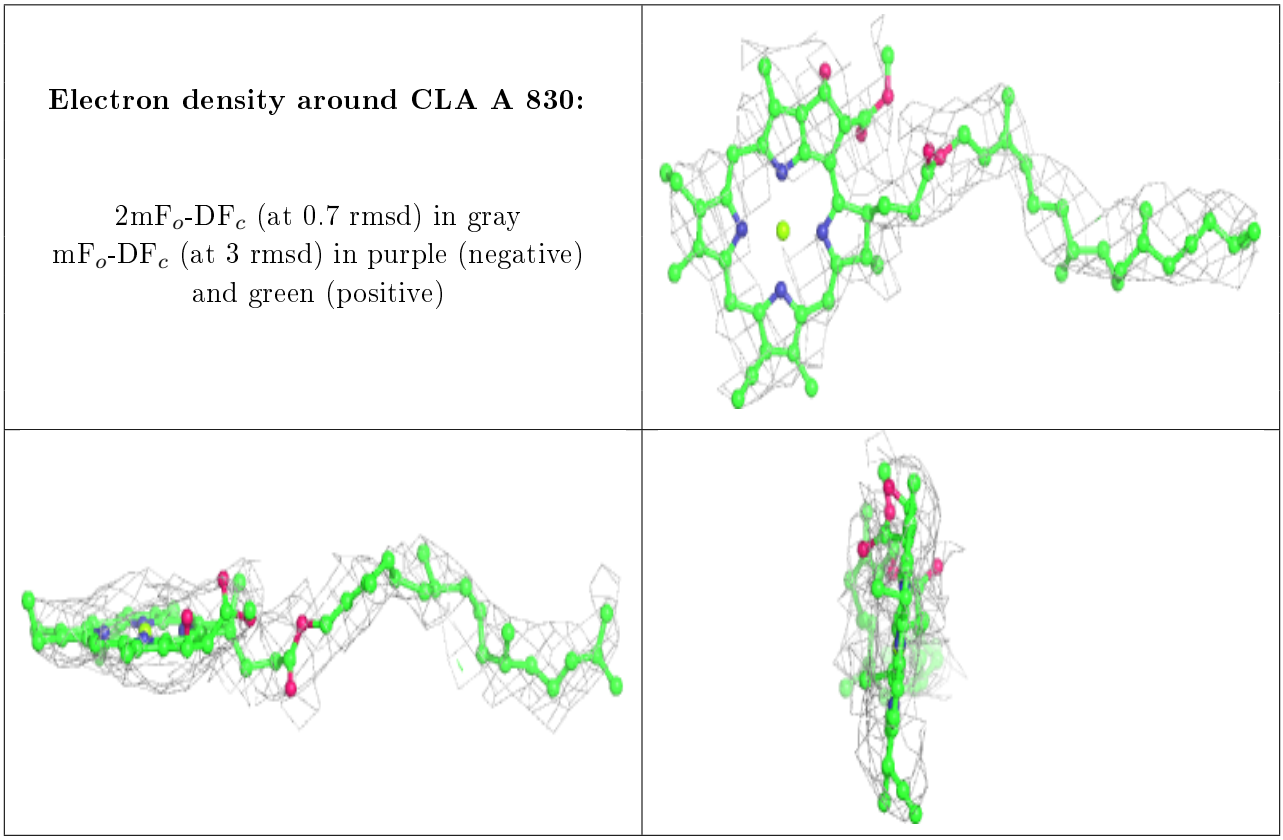
Electron density around BCR I 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



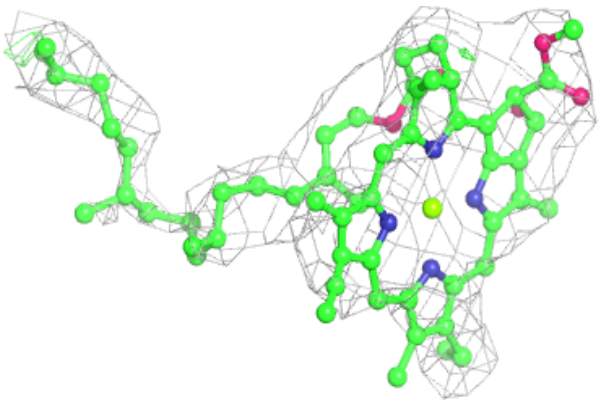
Electron density around CLA A 830:

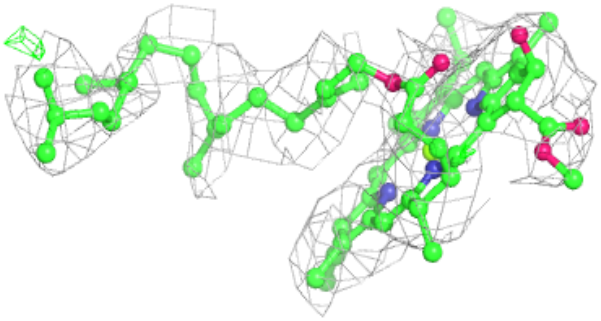
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

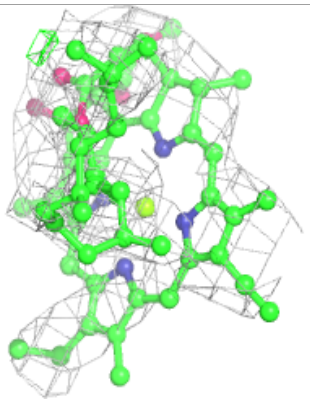


Electron density around CLA A 841:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

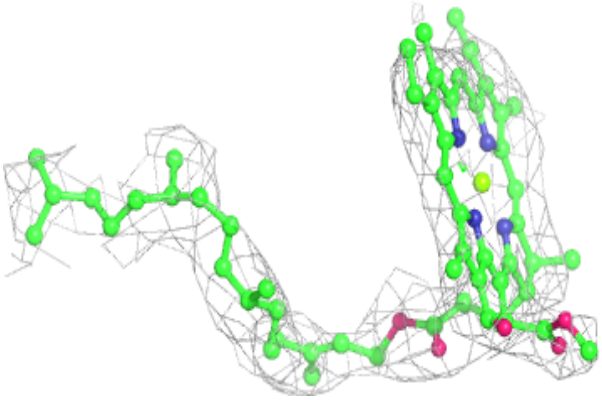


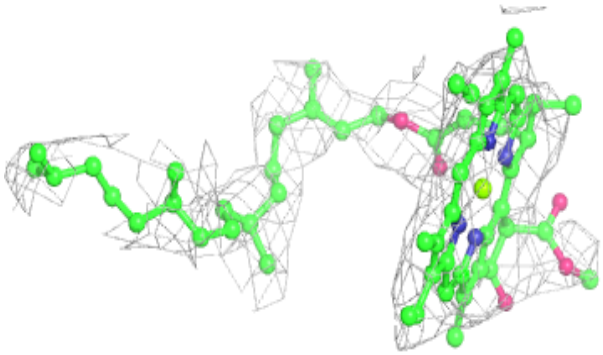


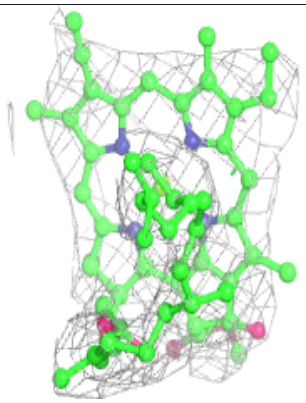


Electron density around CLA B 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

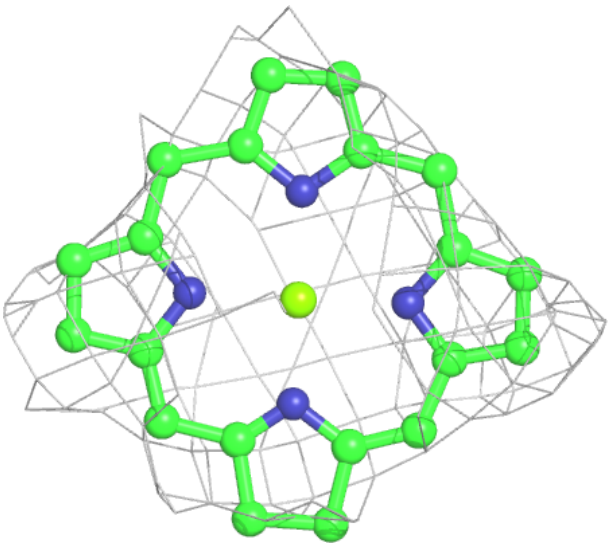


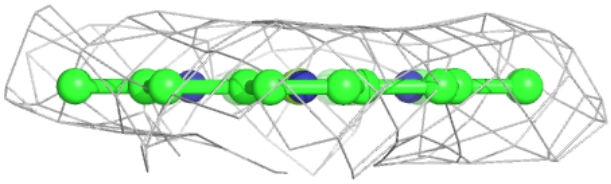


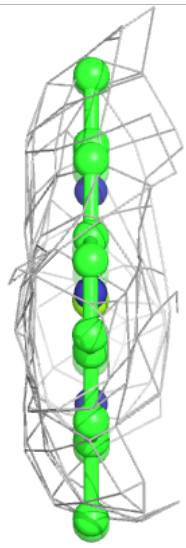


Electron density around CLA 1 212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

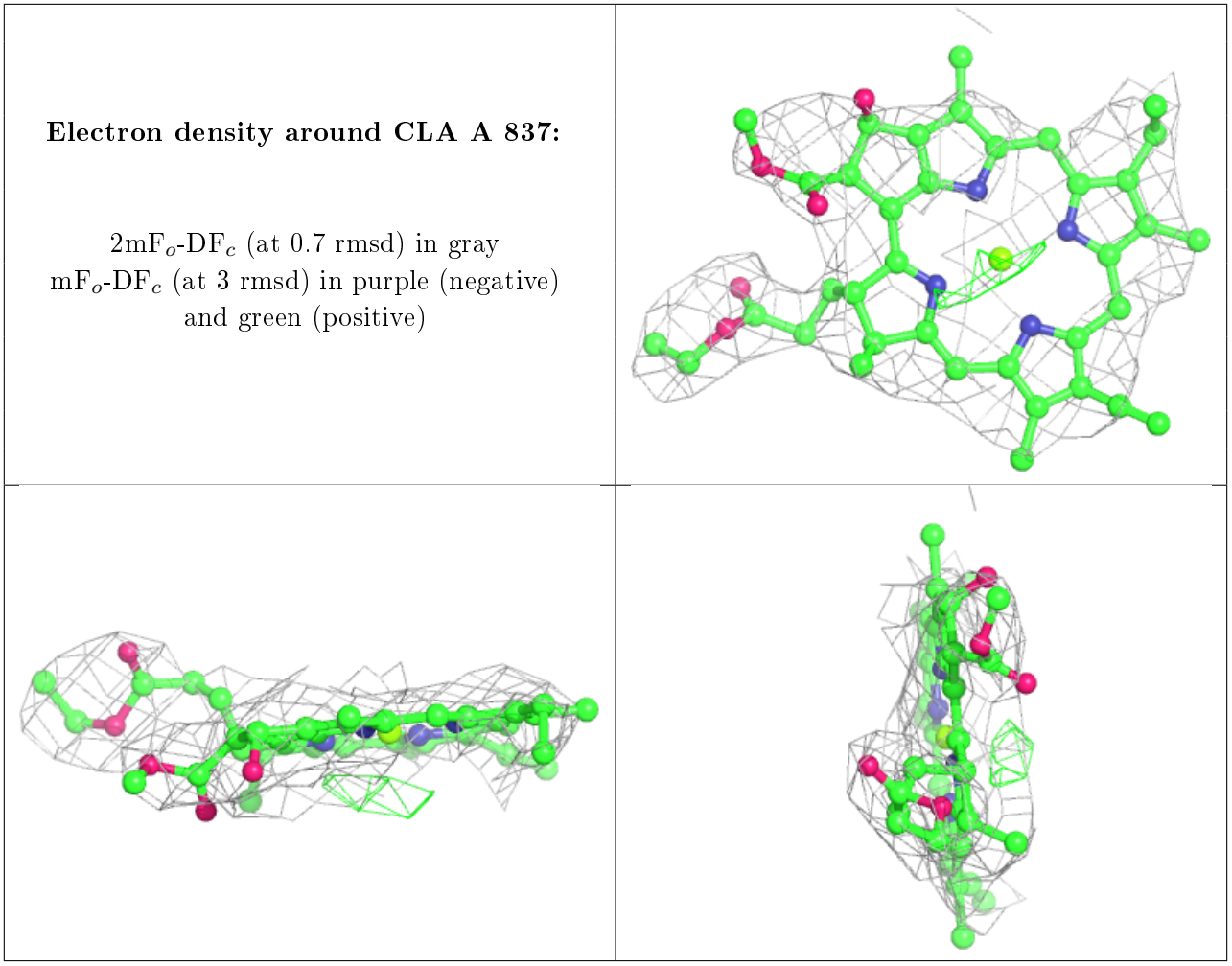






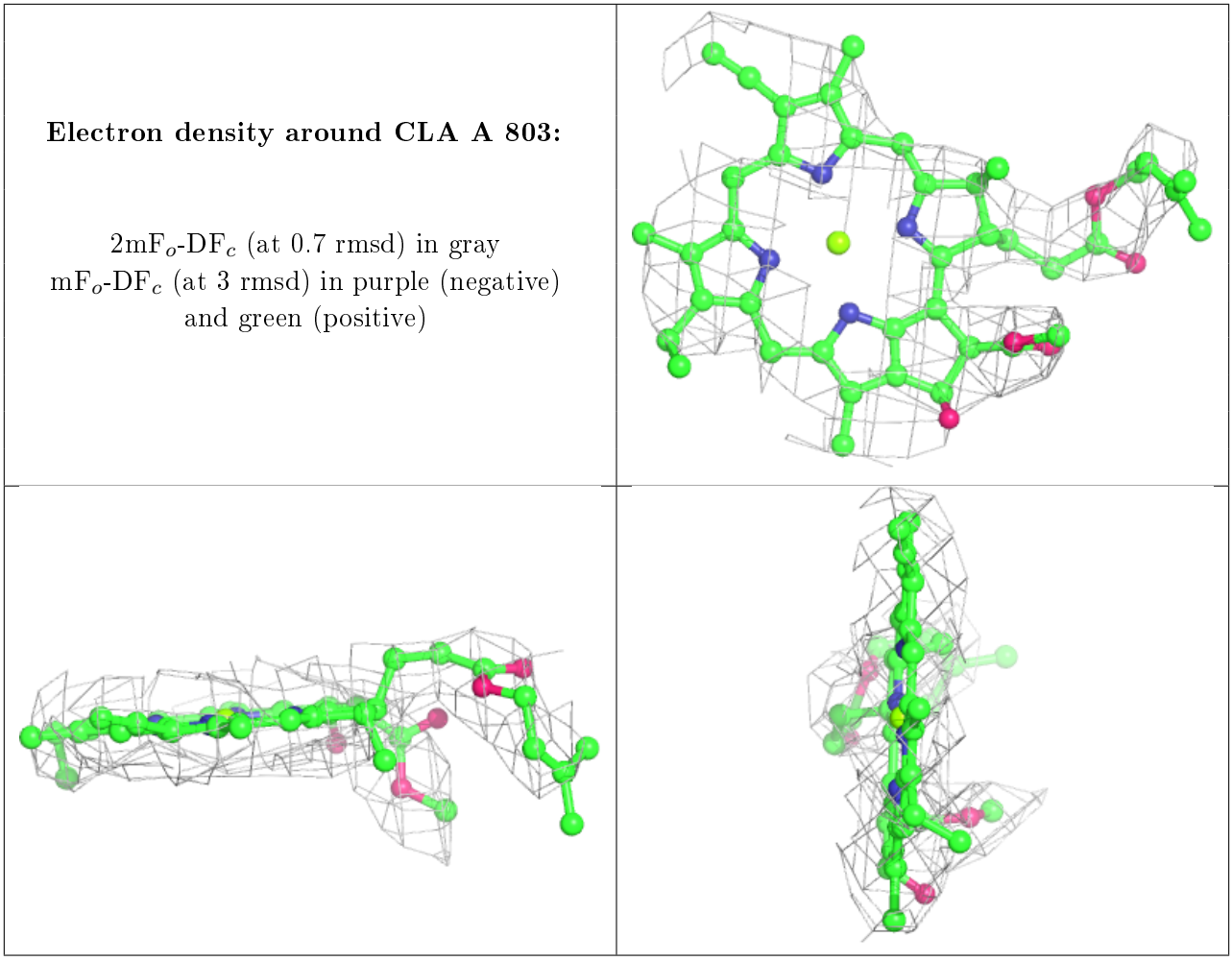
Electron density around CLA A 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



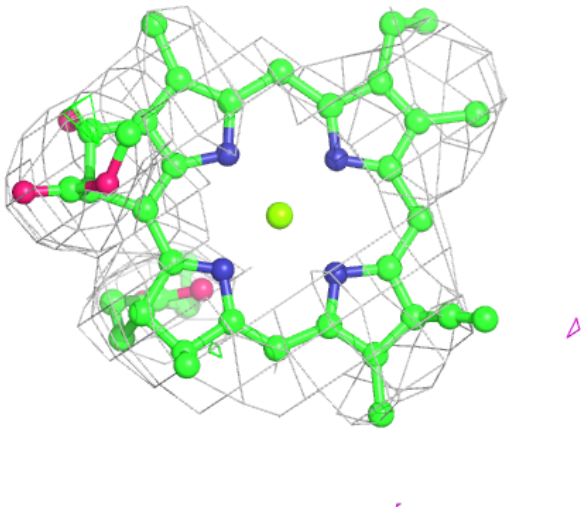
Electron density around CLA A 803:

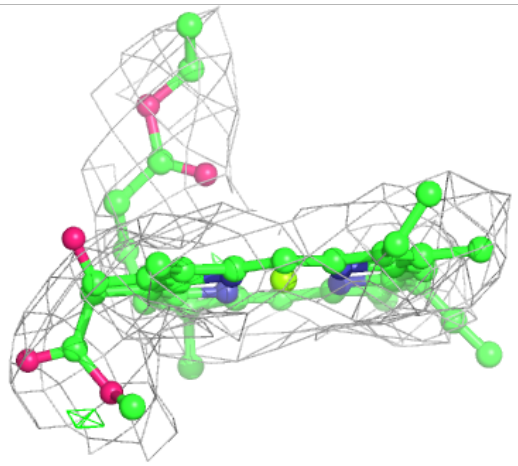
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

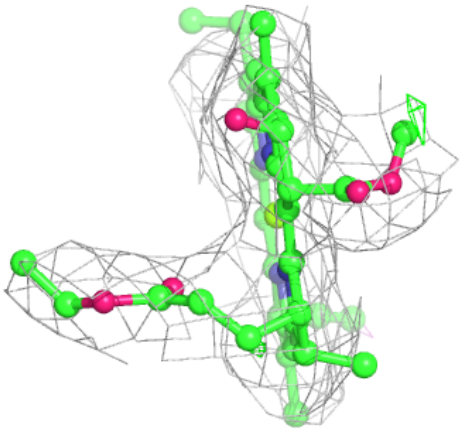


Electron density around CLA L 208:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

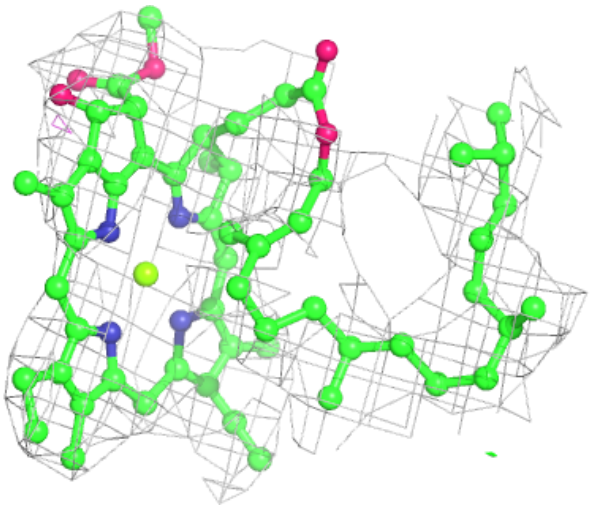


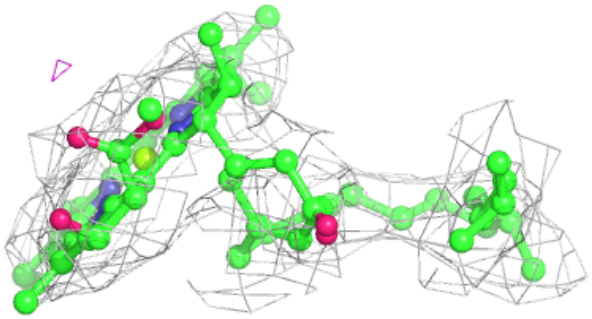


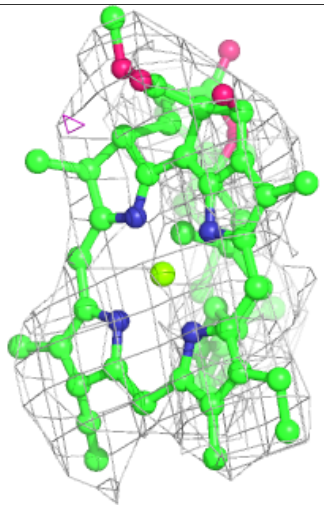


Electron density around CLA B 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

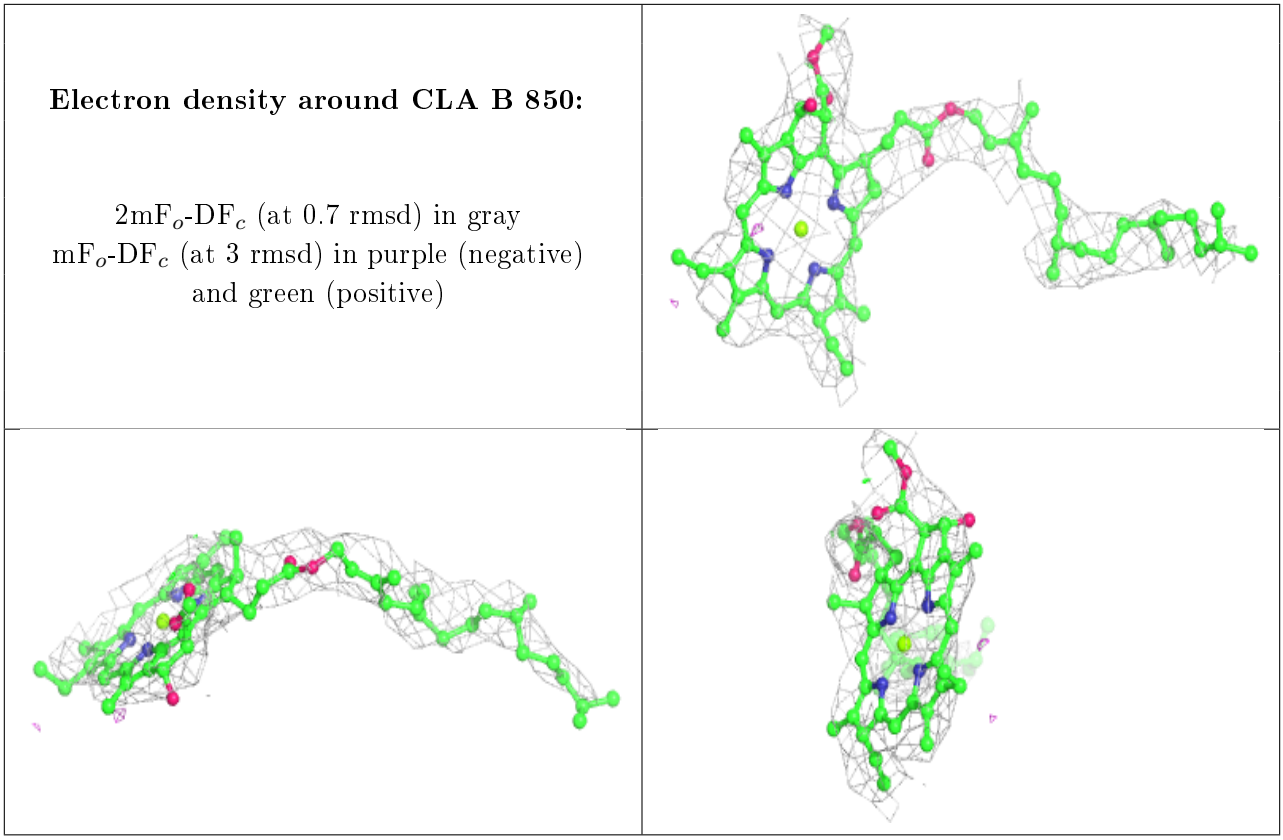






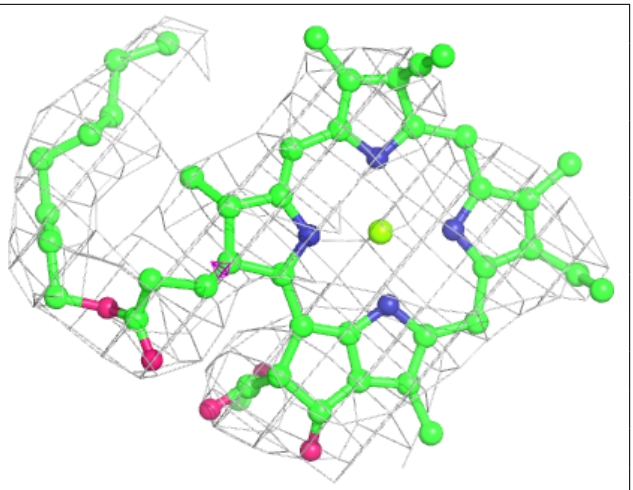
Electron density around CLA B 850:

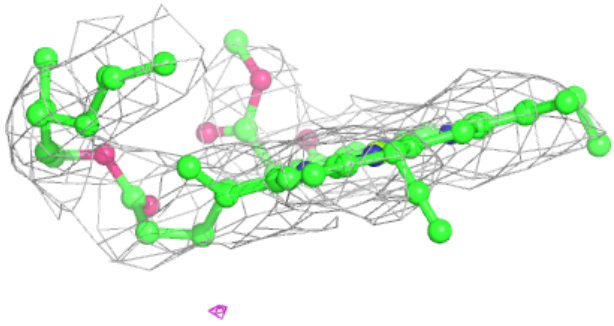
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

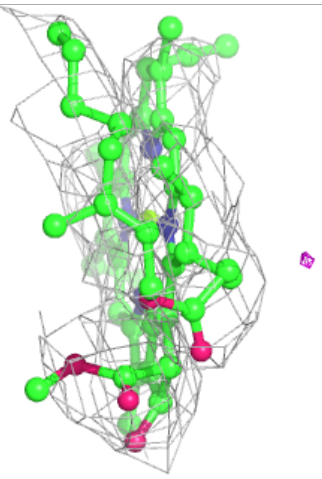


Electron density around CLA B 822:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

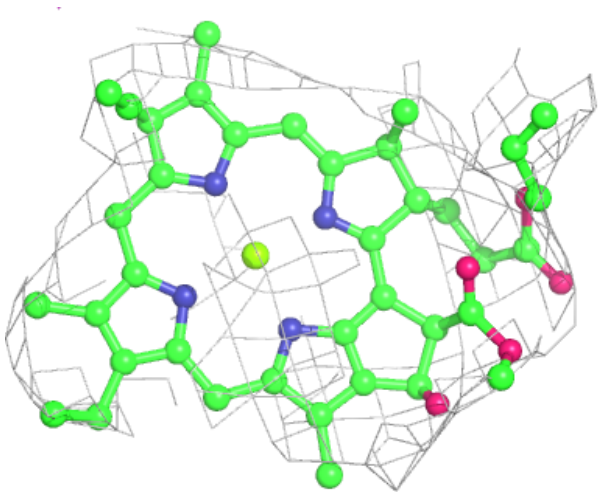


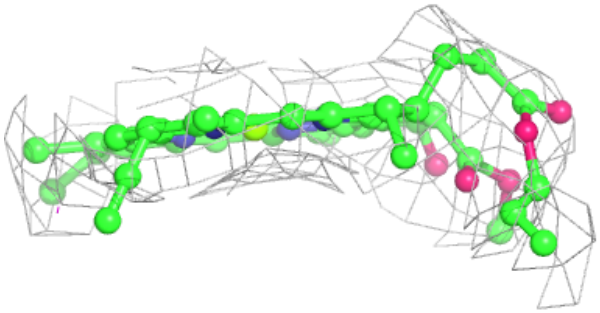


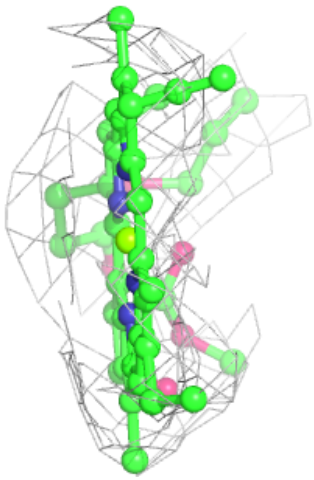


Electron density around CLA J 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

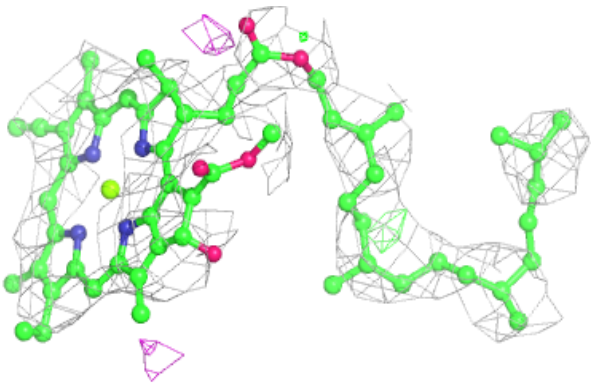


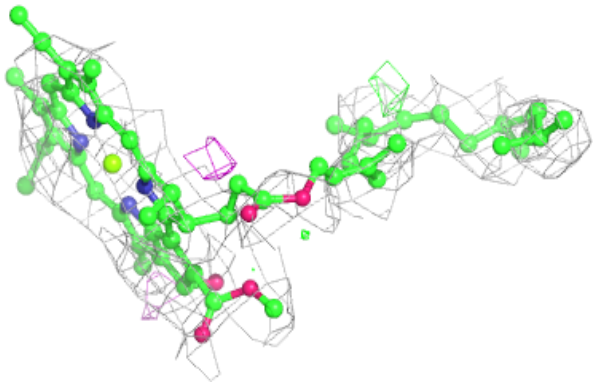


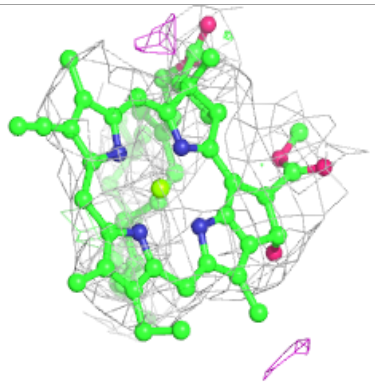


Electron density around CLA A 850:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

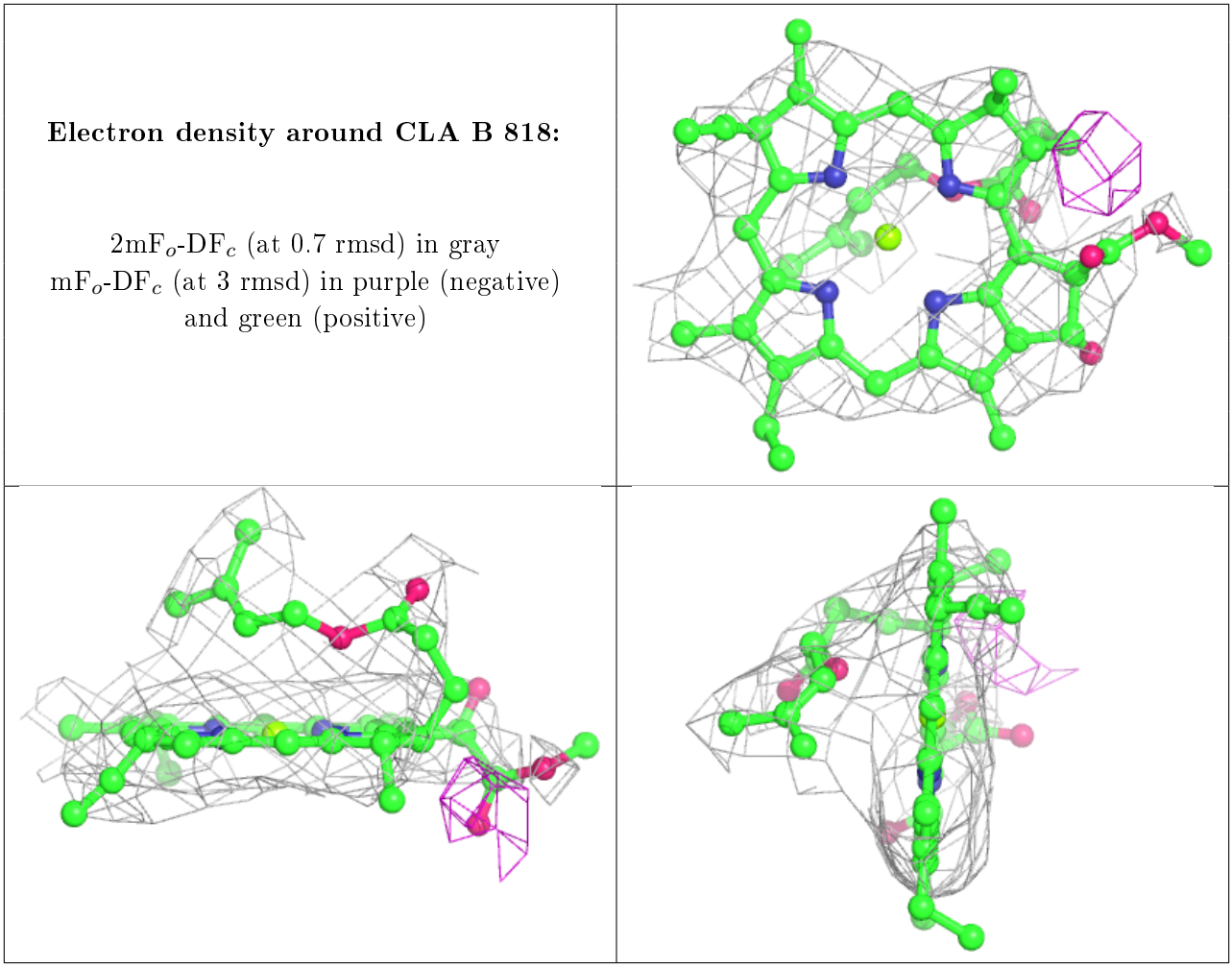






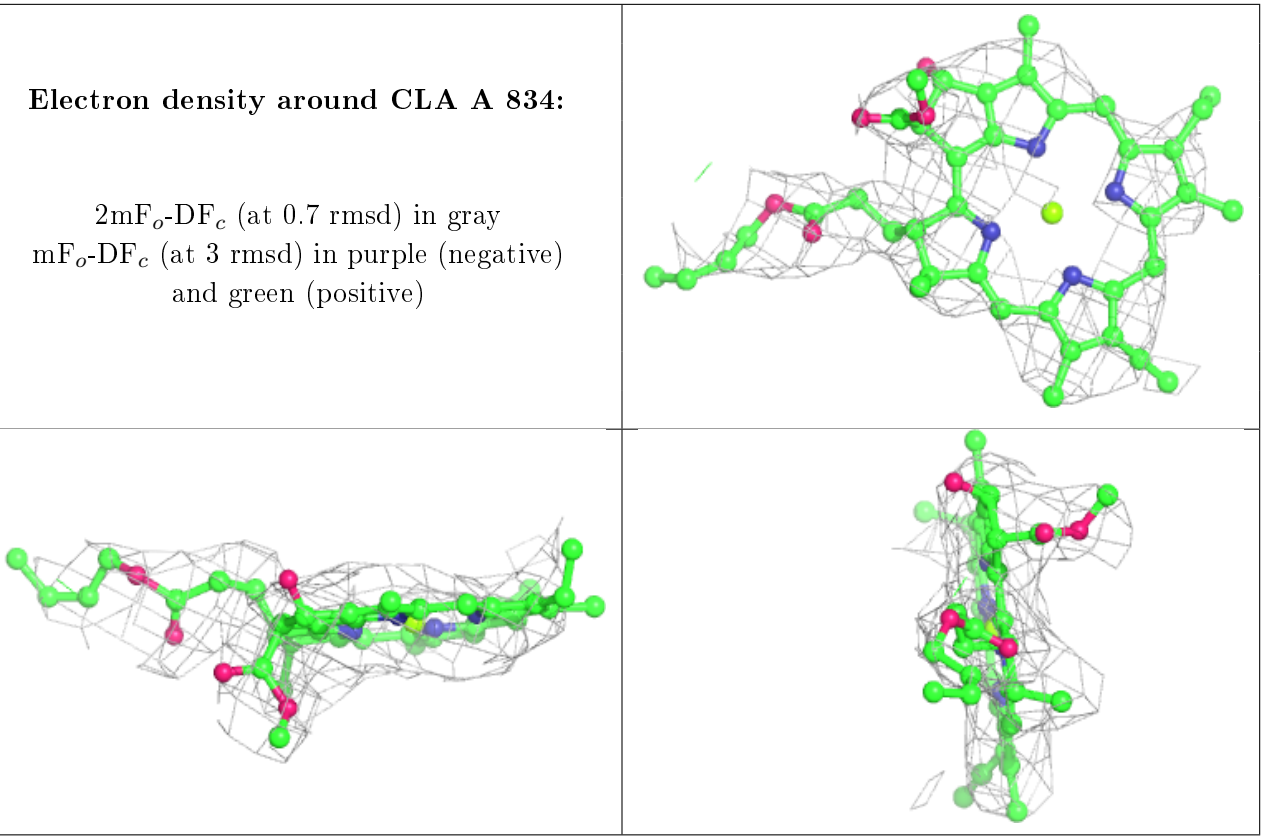
Electron density around CLA B 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



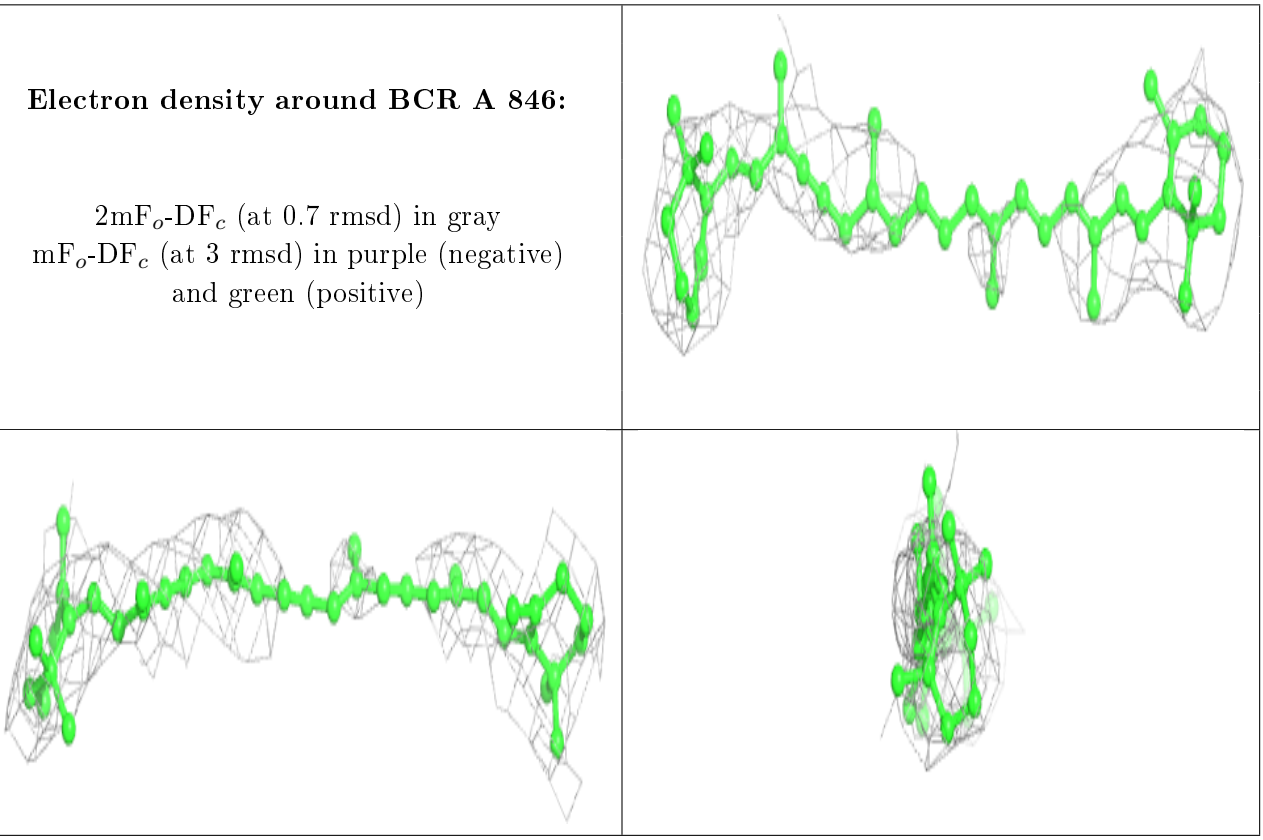
Electron density around CLA A 834:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



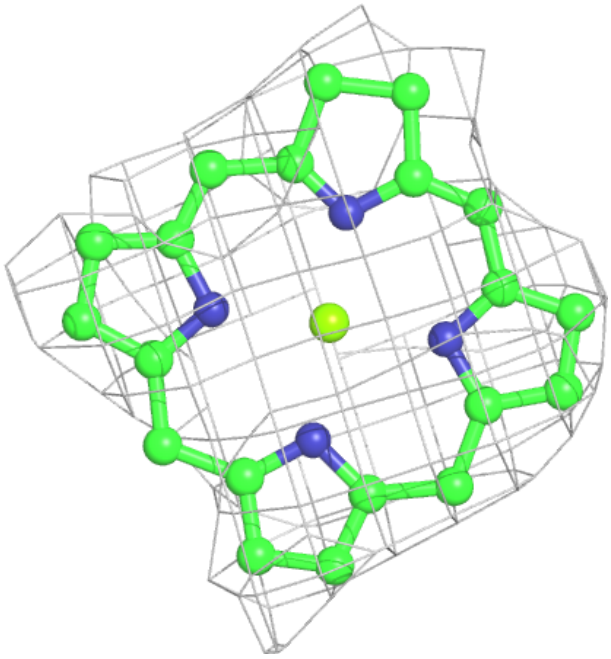
Electron density around BCR A 846:

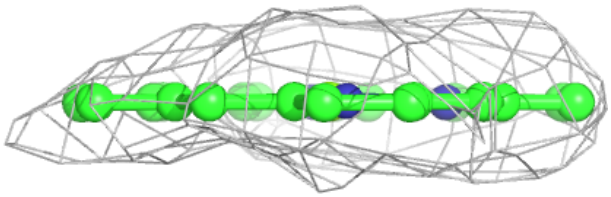
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

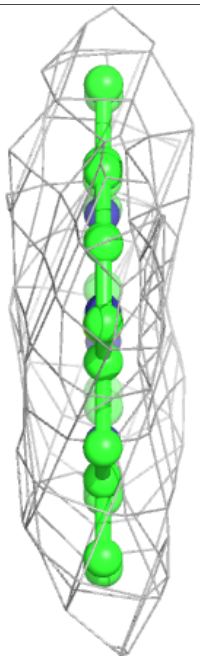


Electron density around CLA 1 208:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

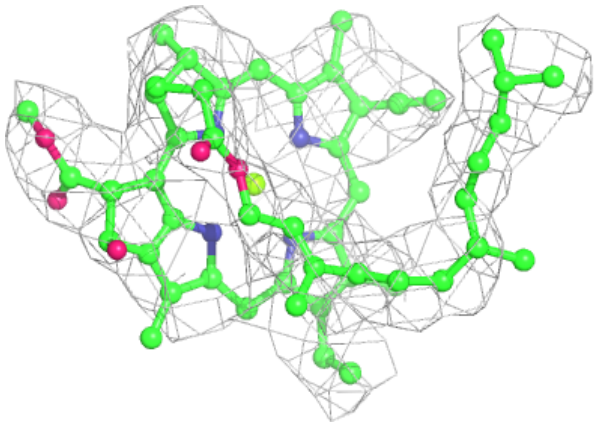


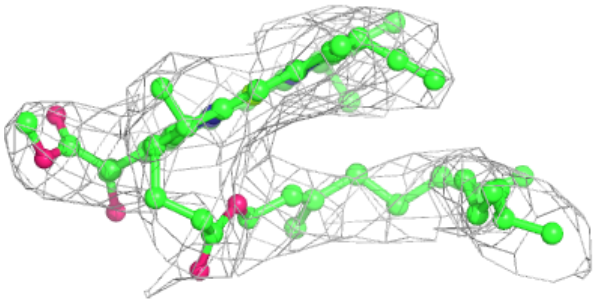


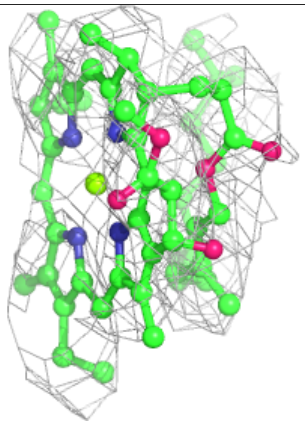


Electron density around CLA I 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

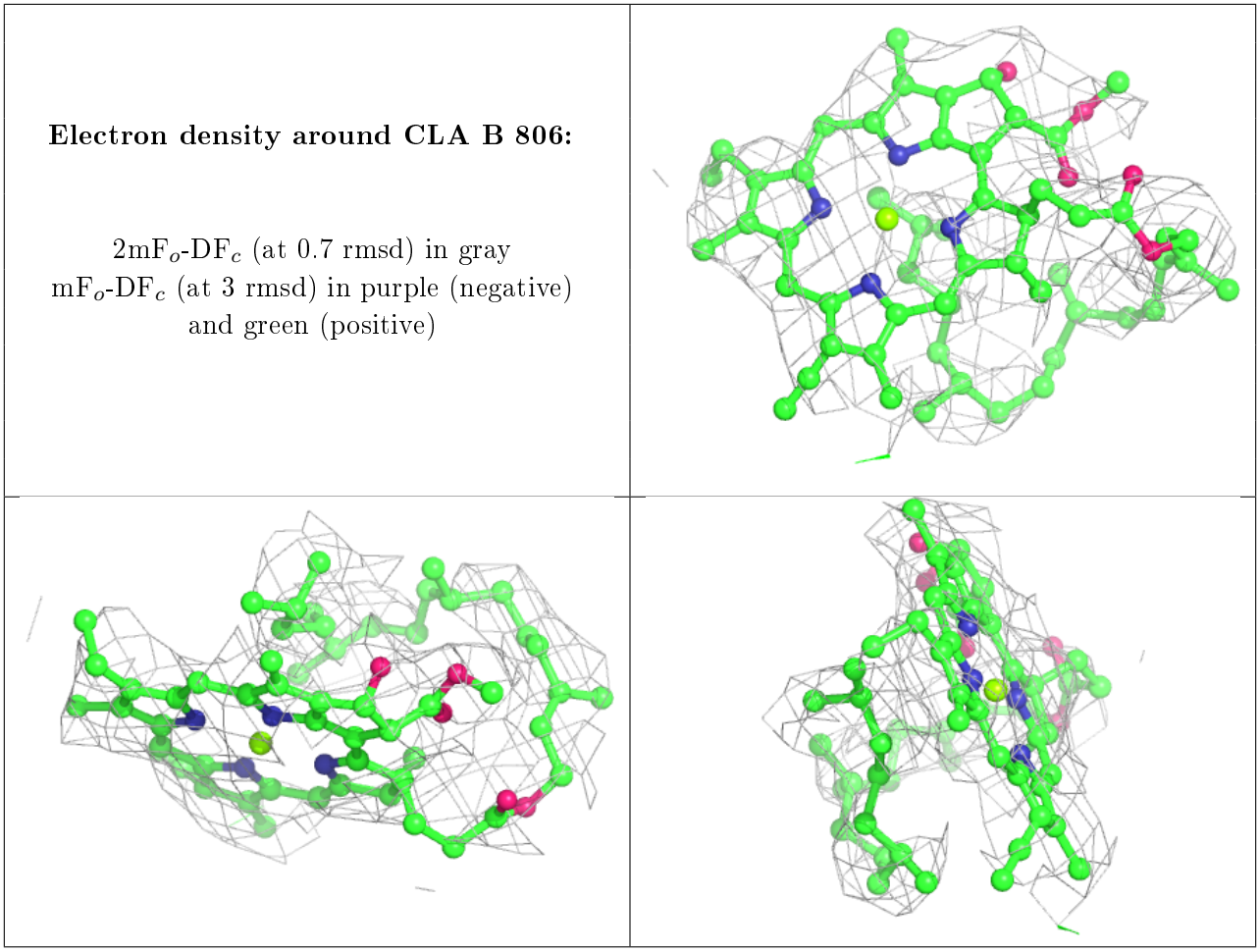






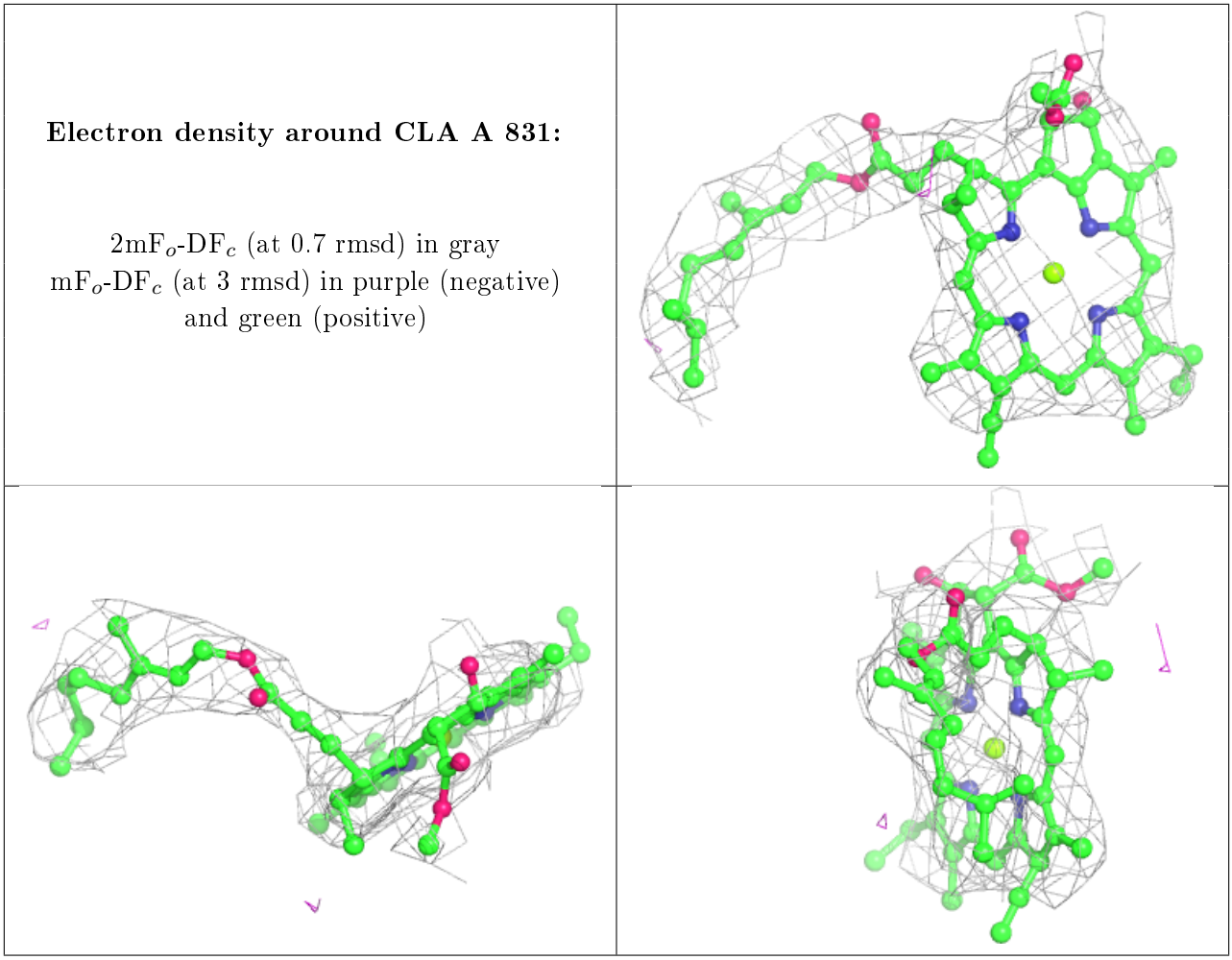
Electron density around CLA B 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



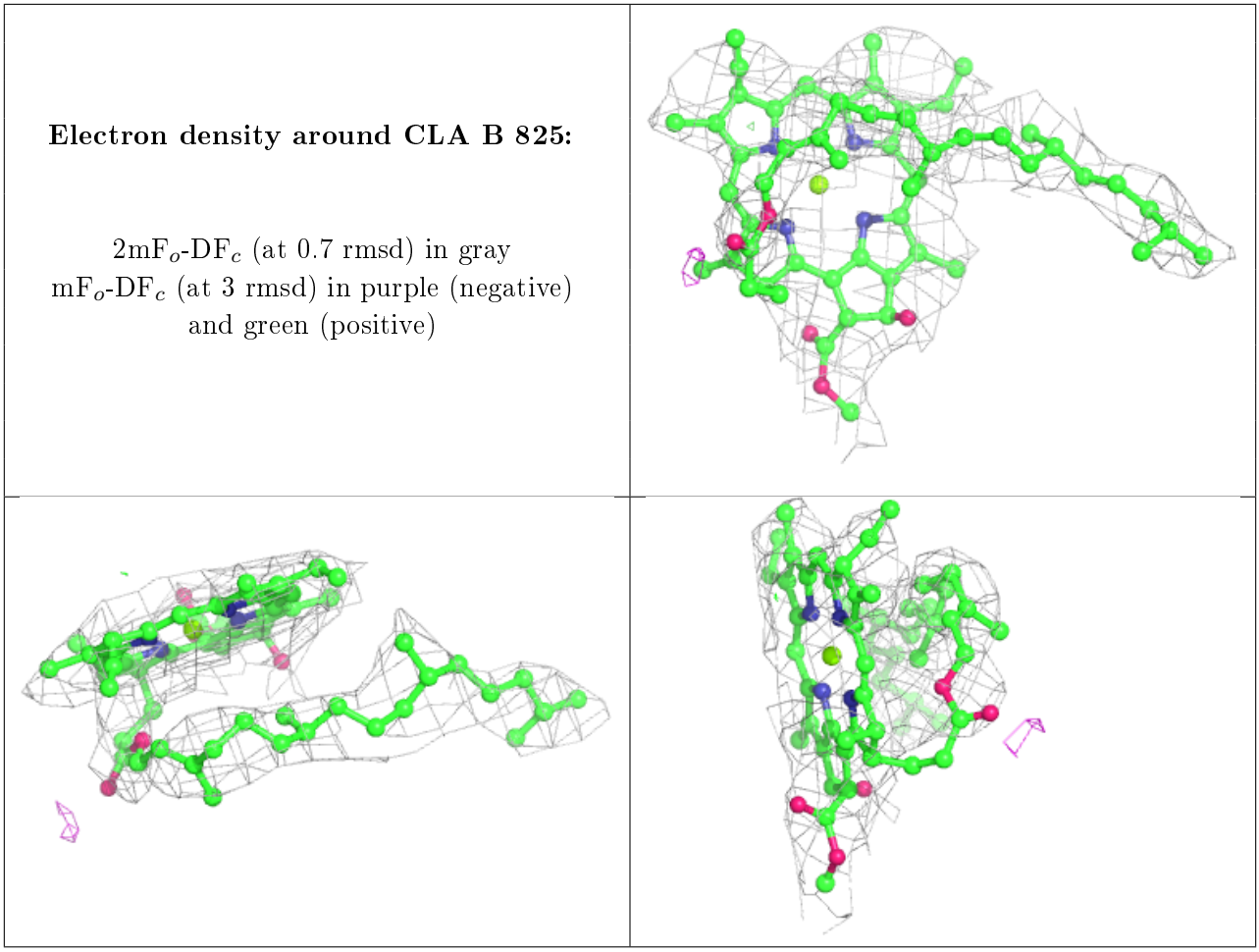
Electron density around CLA A 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



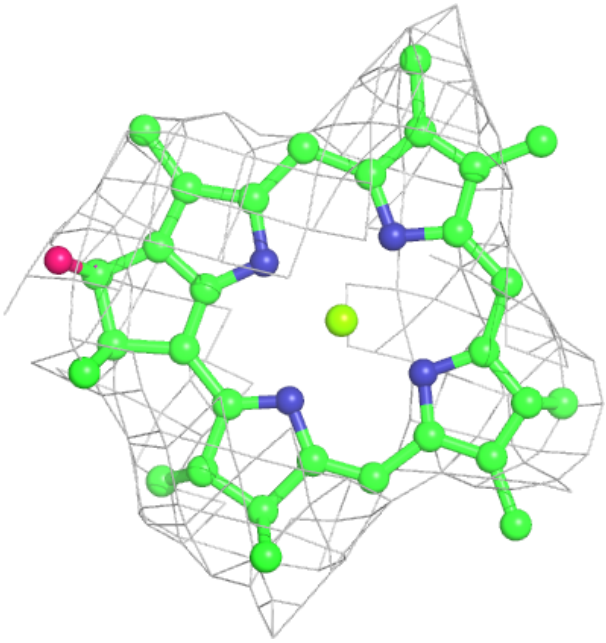
Electron density around CLA B 825:

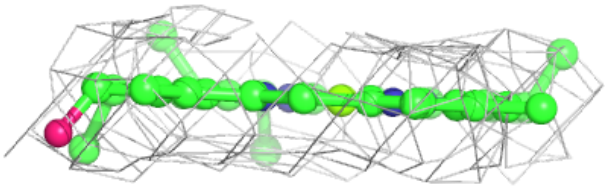
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

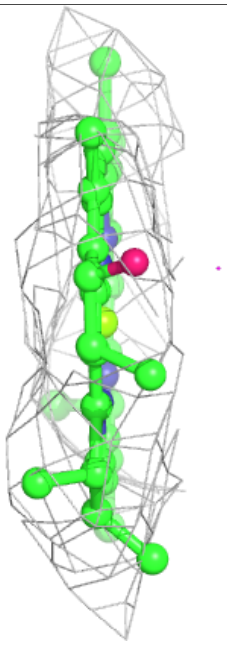


Electron density around CLA 1 209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

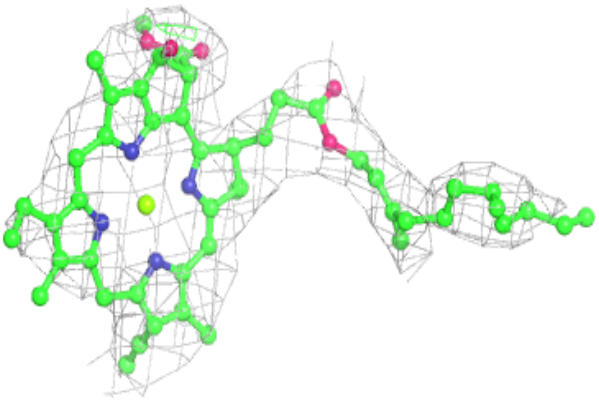


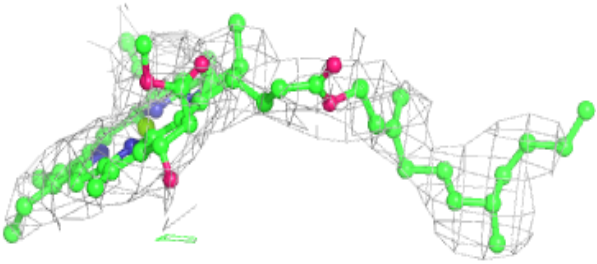


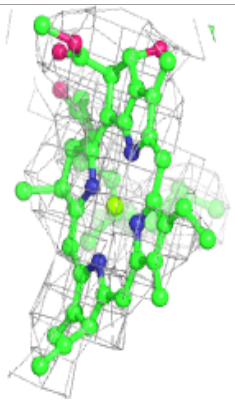


Electron density around CLA B 811:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

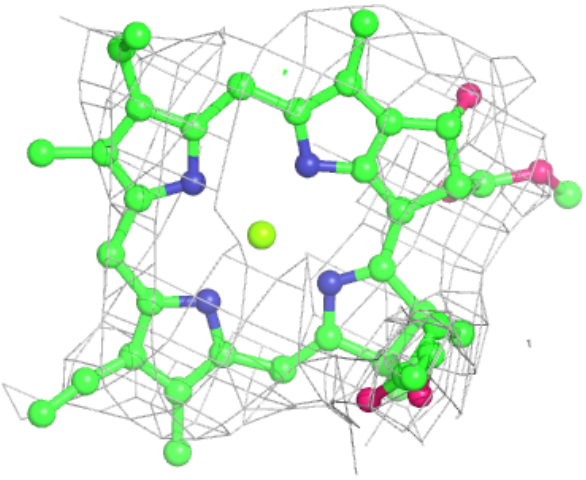


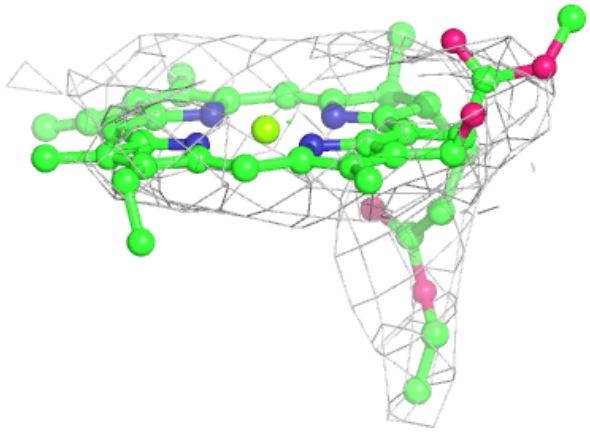


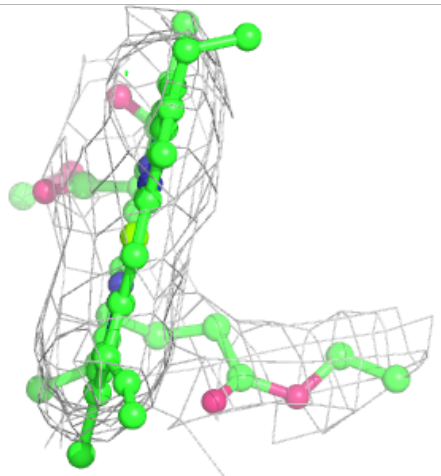


Electron density around CLA B 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

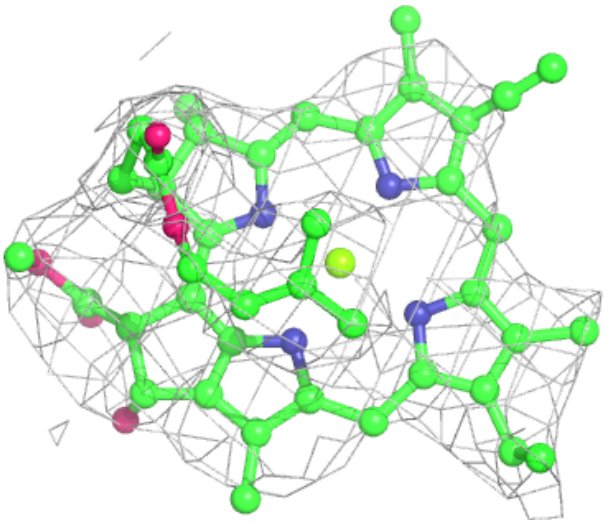


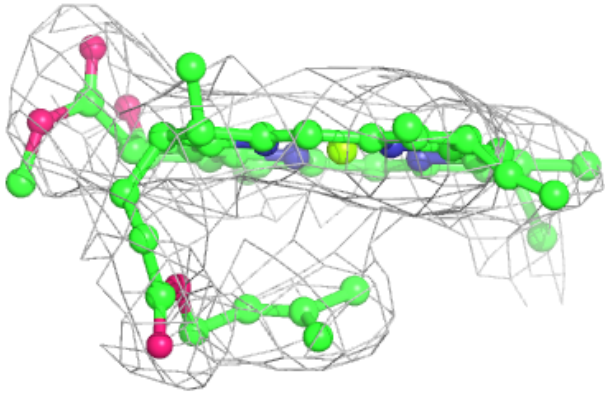


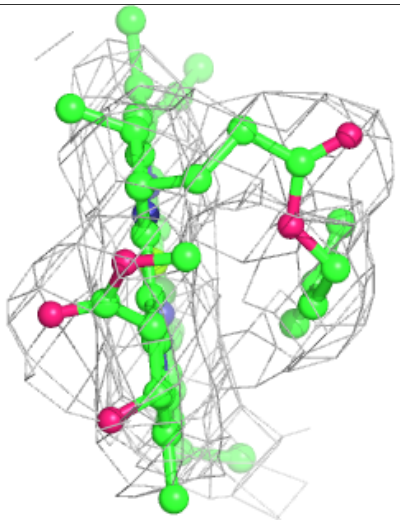


Electron density around CLA B 828:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

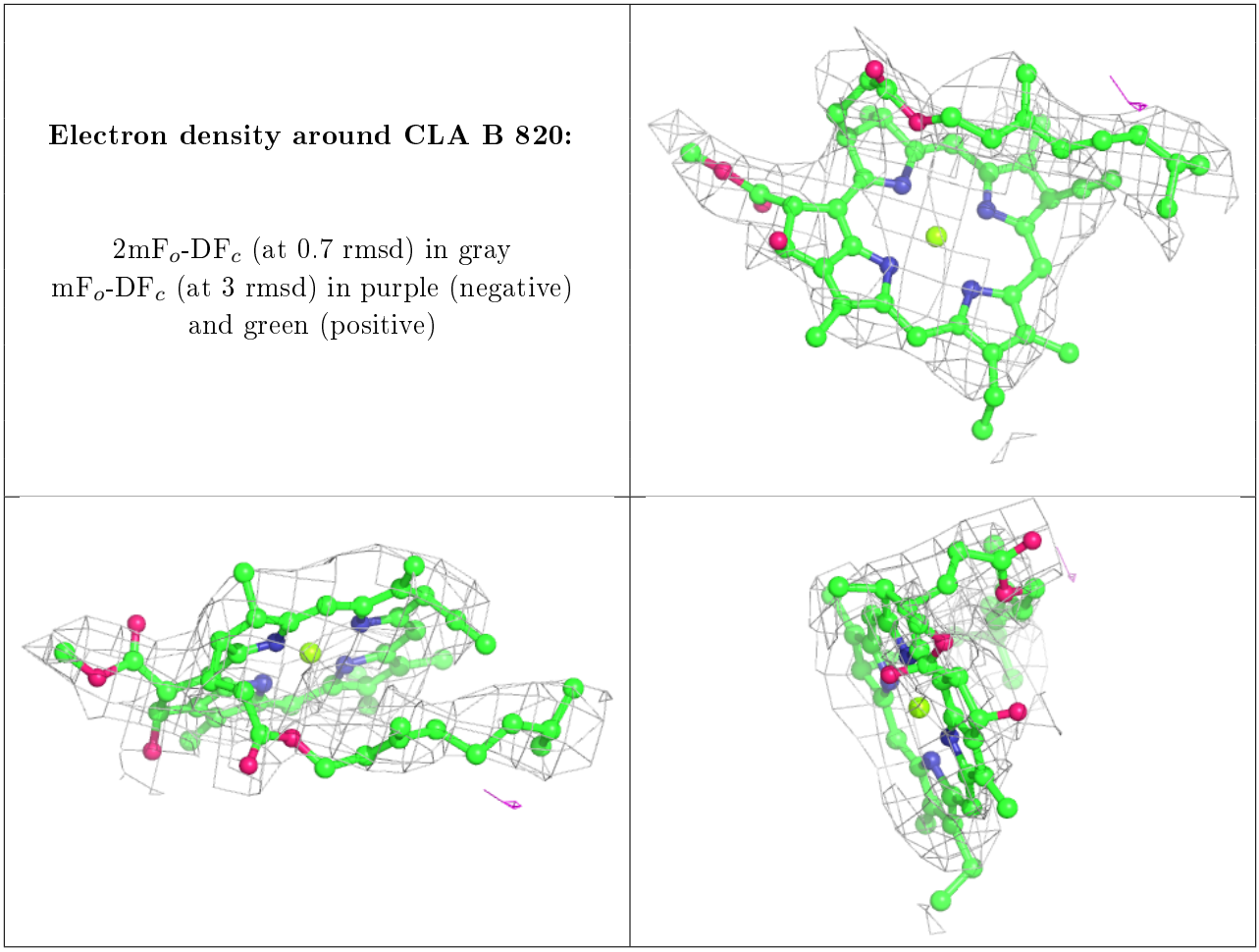






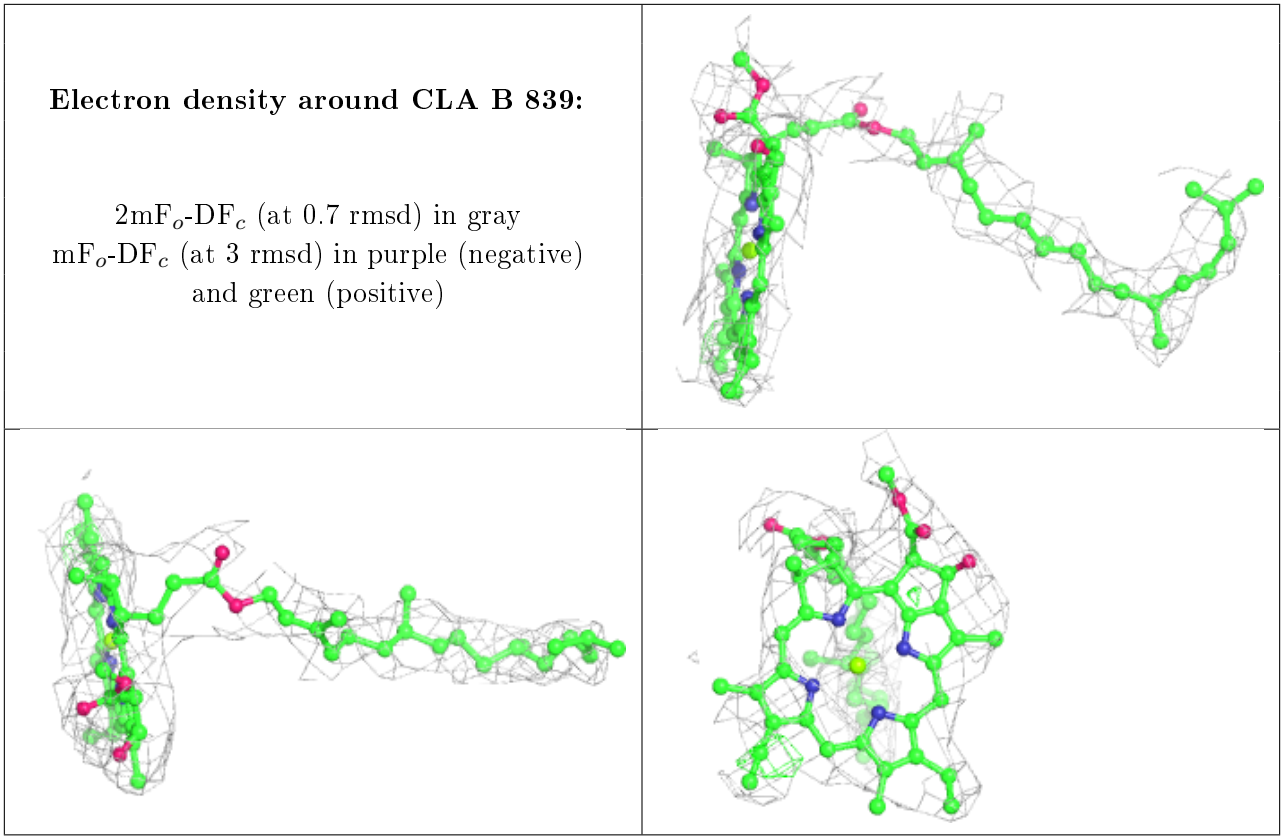
Electron density around CLA B 820:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



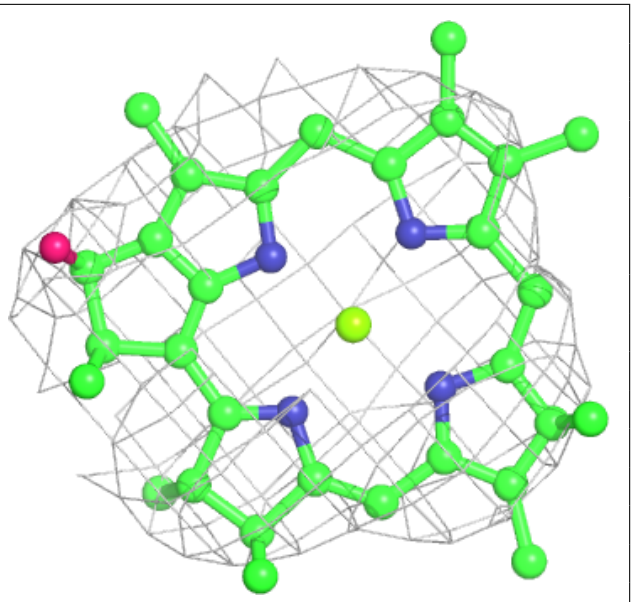
Electron density around CLA B 839:

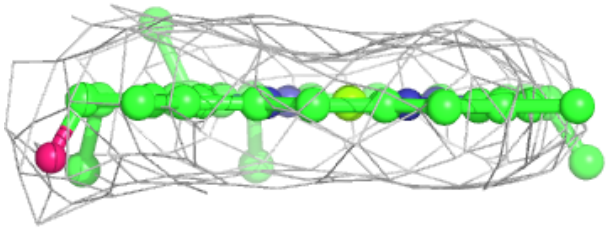
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

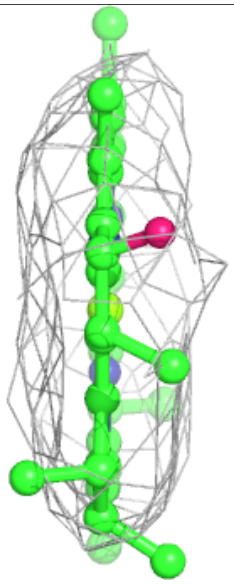


Electron density around CLA 4 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

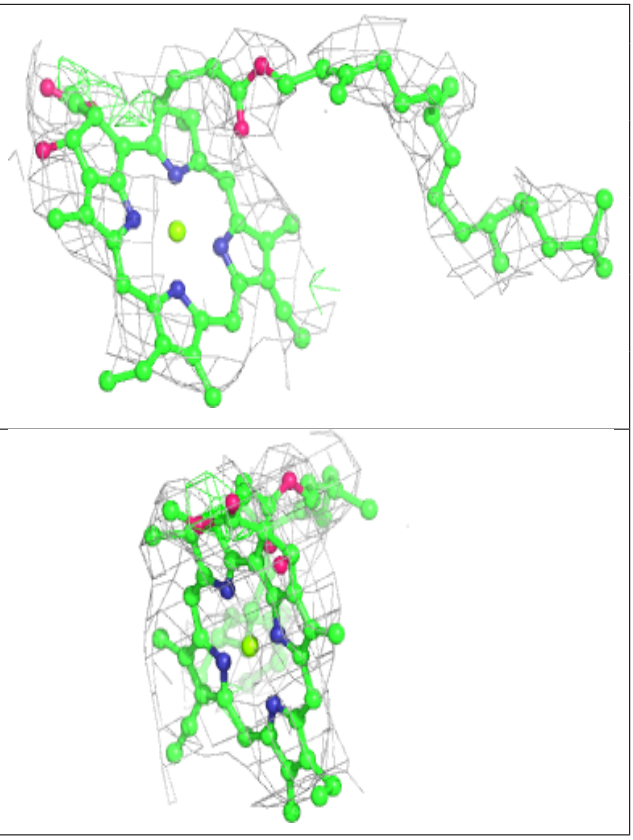


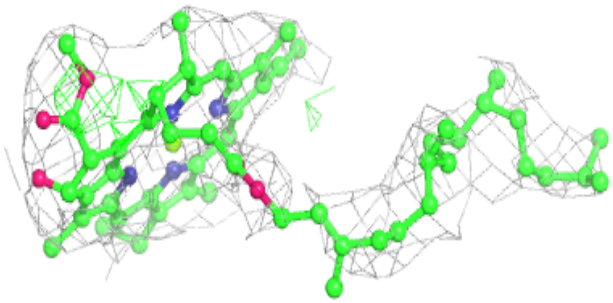




Electron density around CLA A 808:

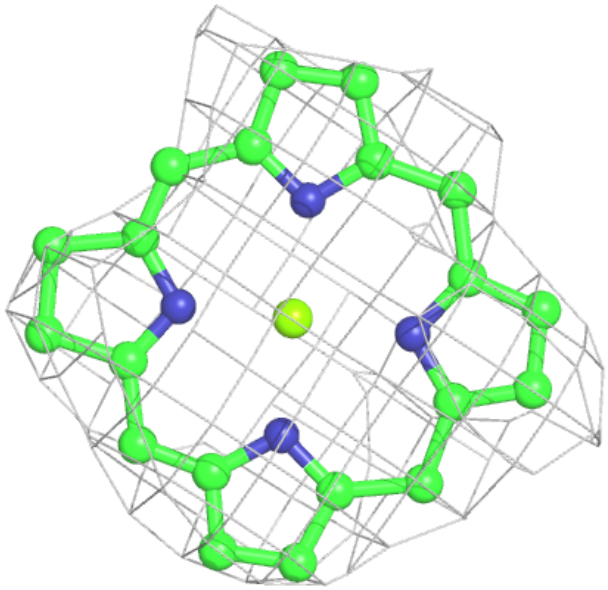
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

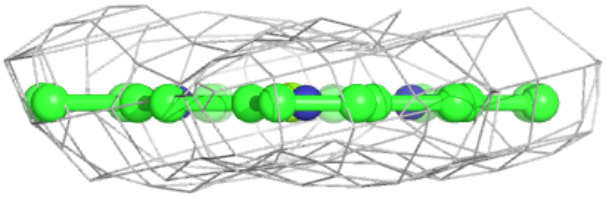


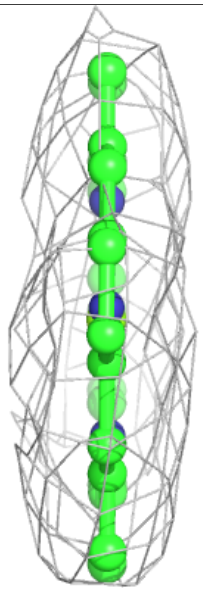


Electron density around CLA 4 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

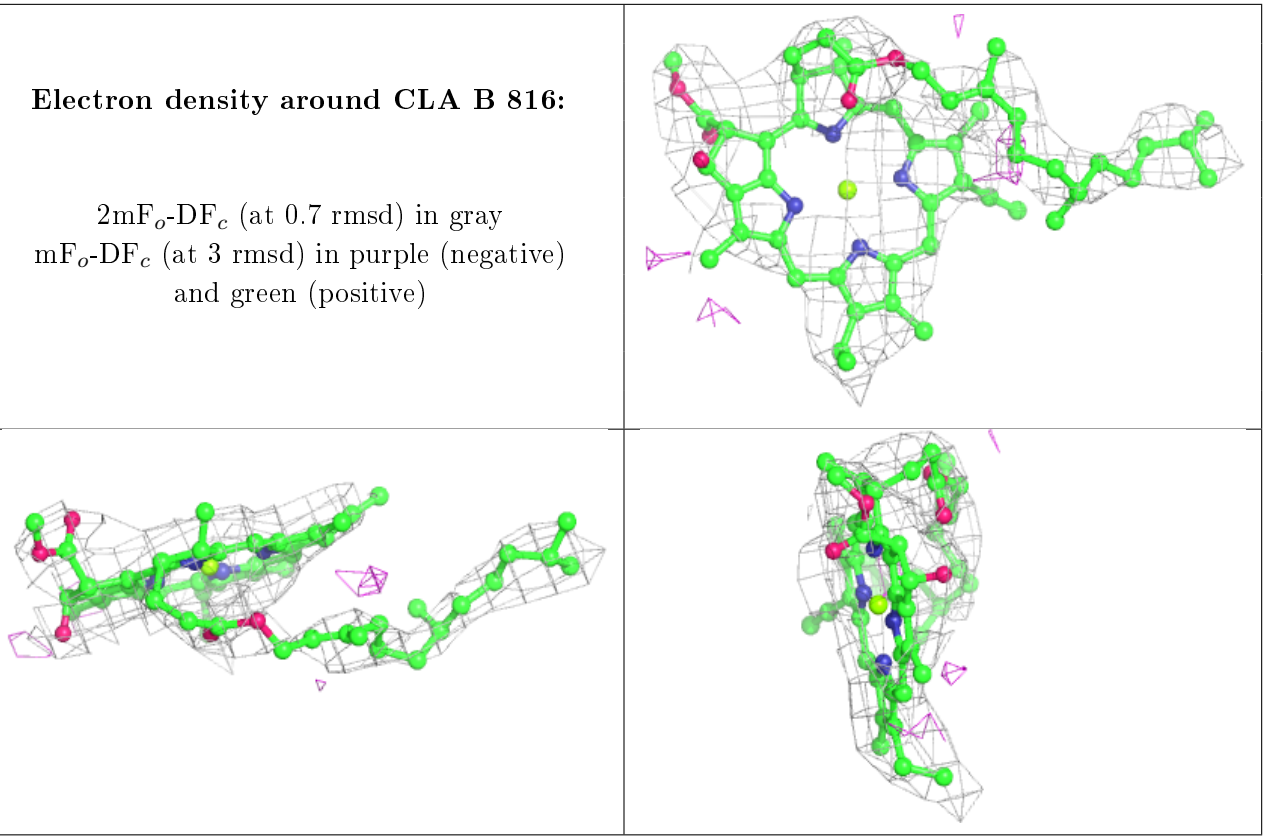






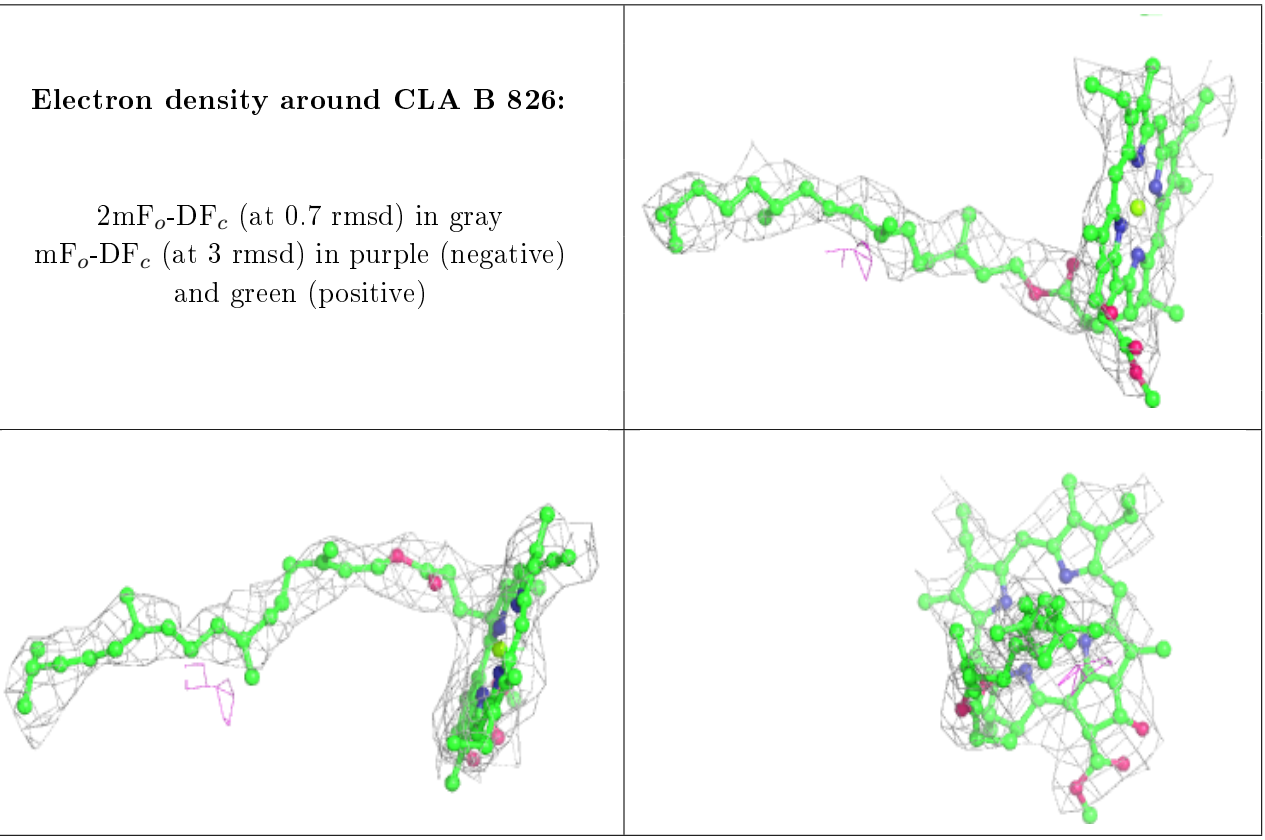
Electron density around CLA B 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



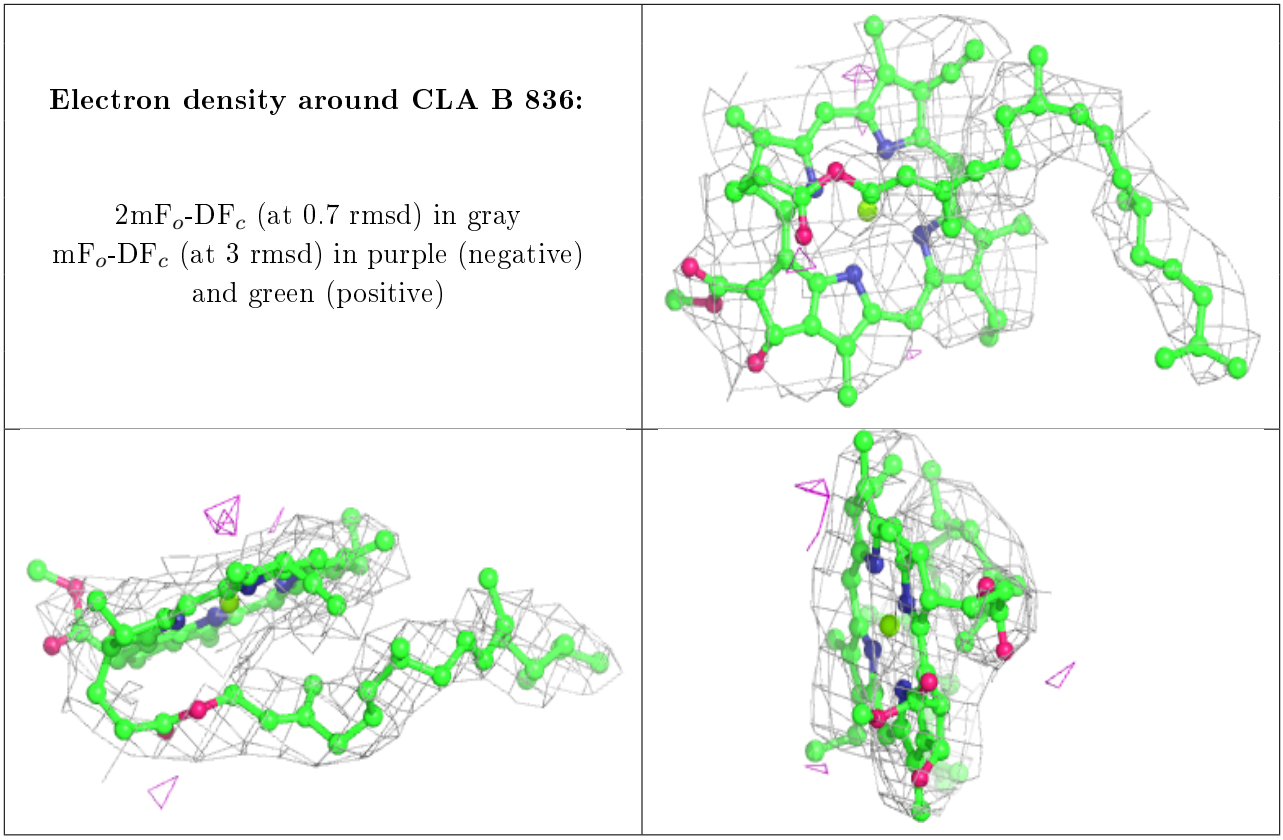
Electron density around CLA B 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



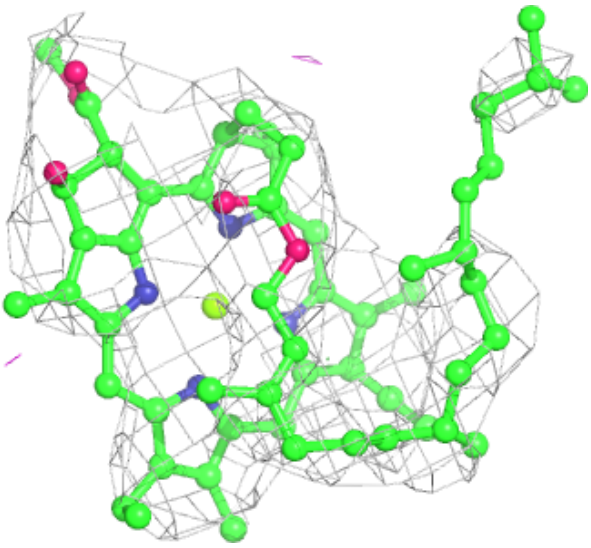
Electron density around CLA B 836:

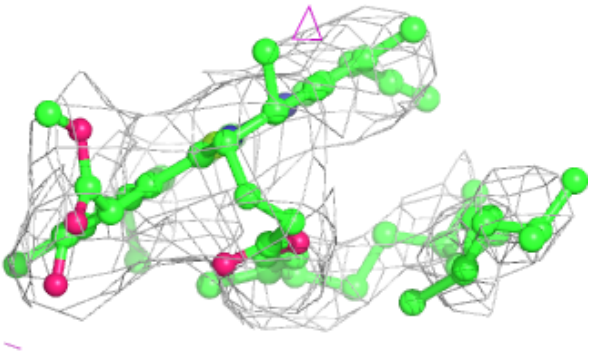
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

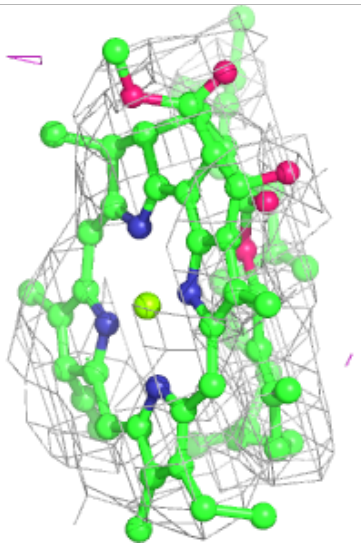


Electron density around CLA B 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

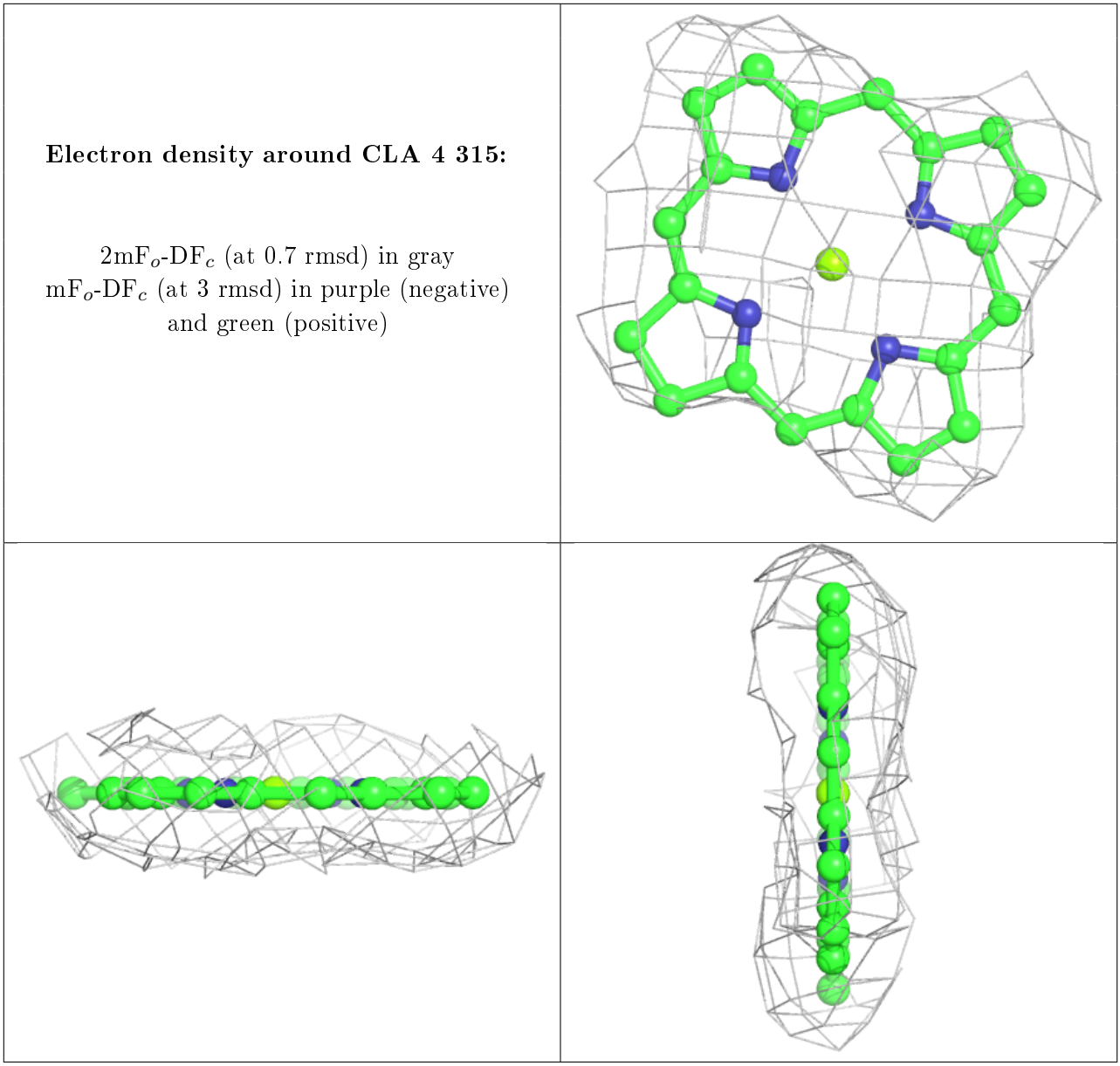






Electron density around CLA 4 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.