Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 04:27 PM EST

PDB ID	:	3WMM
Title	:	Crystal structure of the LH1-RC complex from Thermochromatium tepidum in C2 form
Authors	:	Niwa, S.; Takeda, K.; Wang-Otomo, Z.-Y.; Miki, K.
Deposited on	:	2013-11-22
Resolution	:	3.01 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

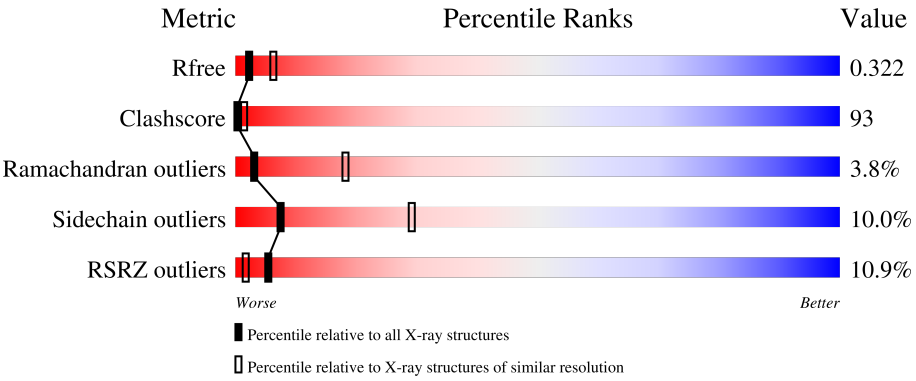
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.01 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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	C	404	4% 29% 45% 22%
2	L	281	2% 28% 66% 6%
3	M	325	2% 30% 63% 5%
4	H	259	7% 33% 59% 7%
5	1	61	18% 16% 62% 20%

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Mol	Chain	Length	Quality of chain
5	3	61	10% 11% 72% 15%
5	5	61	20% 20% 61% 18%
5	7	61	20% 18% 62% 18%
5	9	61	23% 23% 62% 13%
5	A	61	25% 15% 74% 10%
5	D	61	15% 8% 82% 8%
5	F	61	20% 18% 66% 13%
5	I	61	26% 21% 64% 13%
5	K	61	33% 26% 57% 15%
5	O	61	21% 18% 67% 13%
5	Q	61	31% 28% 64% 7%
5	S	61	23% 25% 67% 5%
5	U	61	11% 18% 66% 15%
5	W	61	10% 11% 67% 20%
5	Y	61	16% 15% 66% 18%
6	0	47	4% 11% 53% 21% 15%
6	2	47	6% 21% 55% 9% 15%
6	4	47	9% 23% 51% 11% 15%
6	6	47	6% 21% 55% 9% 15%
6	8	47	17% 15% 55% 15% 15%
6	B	47	11% 19% 53% 13% 15%
6	E	47	6% 23% 60% 15%
6	G	47	13% 6% 66% 13% 15%
6	J	47	21% 55% 9% 15%
6	N	47	9% 17% 55% 13% 15%

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Mol	Chain	Length	Quality of chain
6	P	47	13% 11% 62% 13% 15%
6	R	47	13% 19% 55% 11% 15%
6	T	47	11% 17% 51% 17% 15%
6	V	47	6% 19% 53% 13% 15%
6	X	47	11% 66% 6% 15%
6	Z	47	6% 26% 45% 13% 15%

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
11	UQ8	L	304	-	-	-	X
12	PO4	H	304	-	-	X	-
15	CRT	2	102	-	-	X	X
15	CRT	3	103	-	-	-	X
15	CRT	4	102	-	-	X	X
15	CRT	8	101	-	-	X	X
15	CRT	A	101	-	-	X	X
15	CRT	A	103	-	-	X	X
15	CRT	B	102	-	-	X	X
15	CRT	G	102	-	-	X	X
15	CRT	J	101	-	-	X	X
15	CRT	N	102	-	-	X	X
15	CRT	P	102	-	-	X	X
15	CRT	R	102	-	-	X	X
15	CRT	T	102	-	-	X	X
15	CRT	V	102	-	-	X	X
15	CRT	W	103	-	-	X	X
15	CRT	X	102	-	-	X	X
17	PEF	H	301	-	X	-	-
9	BCL	0	101	-	-	X	-
9	BCL	3	102	-	-	X	-
9	BCL	4	101	-	-	X	-
9	BCL	5	102	-	-	X	-
9	BCL	6	101	-	-	X	-
9	BCL	7	102	-	-	X	-
9	BCL	7	103	-	-	X	-
9	BCL	9	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	A	102	-	-	X	-
9	BCL	B	101	-	-	X	-
9	BCL	D	102	-	-	X	-
9	BCL	E	101	-	-	X	-
9	BCL	F	102	-	-	X	-
9	BCL	G	101	-	-	X	-
9	BCL	I	102	-	-	X	-
9	BCL	I	103	-	-	X	-
9	BCL	K	102	-	-	X	-
9	BCL	M	401	-	-	X	-
9	BCL	N	101	-	-	X	-
9	BCL	O	102	-	-	X	-
9	BCL	P	101	-	-	X	-
9	BCL	Q	102	-	-	X	-
9	BCL	R	101	-	-	X	-
9	BCL	S	102	-	-	X	-
9	BCL	T	101	-	-	X	-
9	BCL	U	102	-	-	X	-
9	BCL	W	102	-	-	X	-
9	BCL	X	101	-	-	X	-
9	BCL	Y	102	-	-	X	-
9	BCL	Z	101	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 25819 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 Photosynthetic reaction center C subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	0	0	0
			1983	1275	339	364	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	D	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	F	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	I	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	O	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	Q	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	S	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	U	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	W	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	Y	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	1	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	3	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	5	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	7	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	9	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	E	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	G	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	J	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	N	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	P	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	R	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

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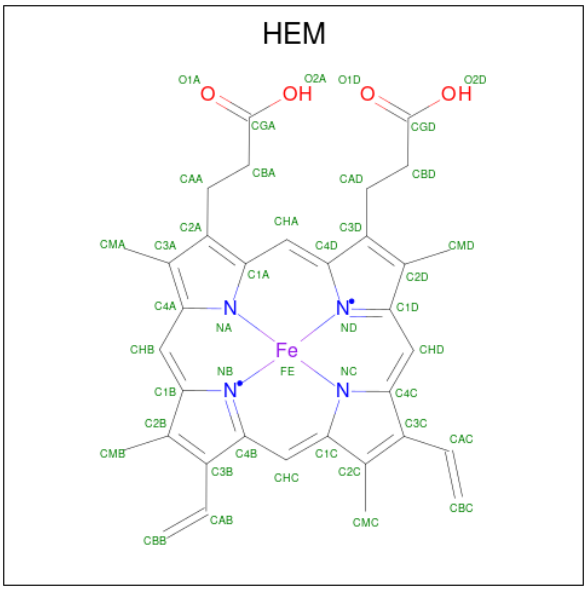
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	V	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	X	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	4	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	6	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	8	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	0	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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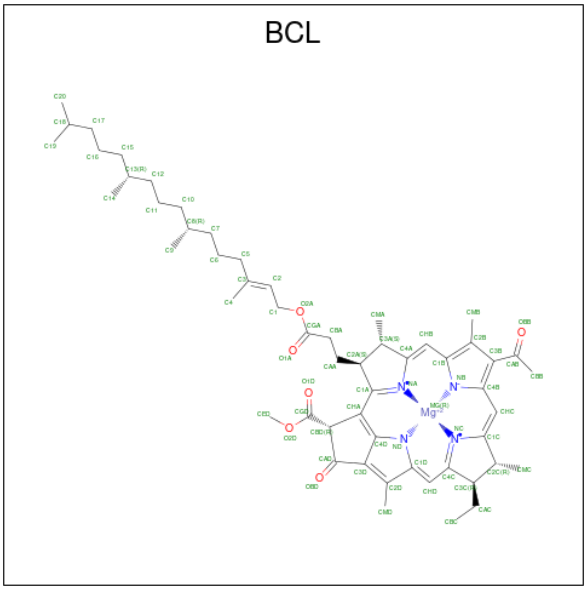
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		
8	F	1	Total	Ca	0	0
			1	1		
8	I	1	Total	Ca	0	0
			1	1		
8	K	1	Total	Ca	0	0
			1	1		
8	O	1	Total	Ca	0	0
			1	1		
8	Q	1	Total	Ca	0	0
			1	1		
8	S	1	Total	Ca	0	0
			1	1		
8	U	1	Total	Ca	0	0
			1	1		
8	W	1	Total	Ca	0	0
			1	1		
8	Y	1	Total	Ca	0	0
			1	1		
8	1	1	Total	Ca	0	0
			1	1		
8	3	1	Total	Ca	0	0
			1	1		
8	5	1	Total	Ca	0	0
			1	1		
8	7	1	Total	Ca	0	0
			1	1		
8	9	1	Total	Ca	0	0
			1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	K	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	P	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Q	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	T	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	U	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	V	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	W	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	X	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Z	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	1	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	4	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	5	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	6	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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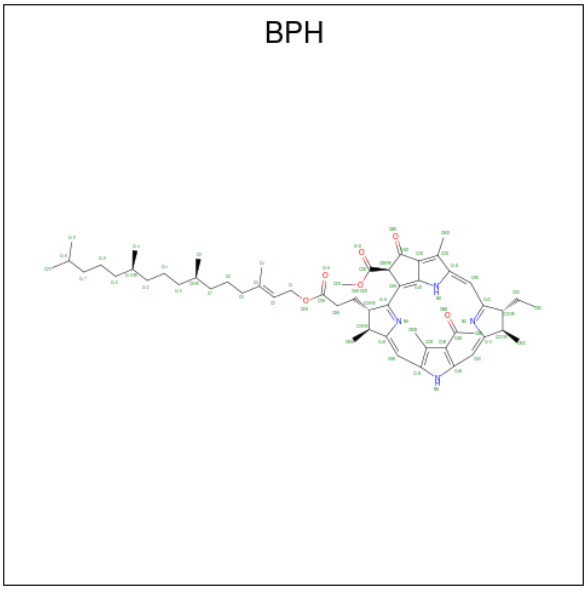
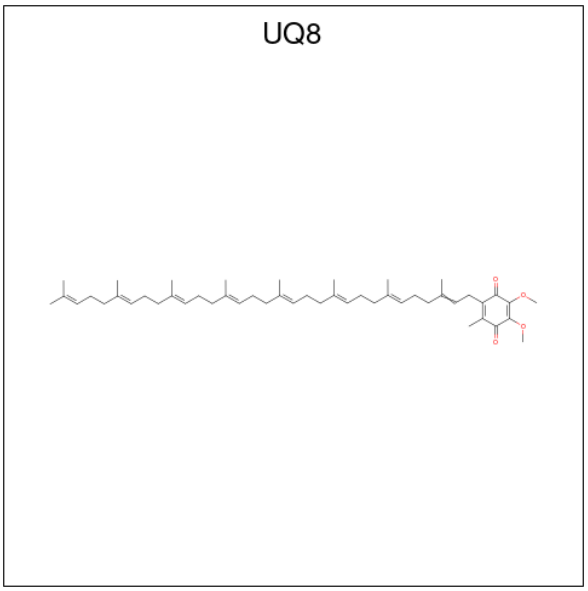
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



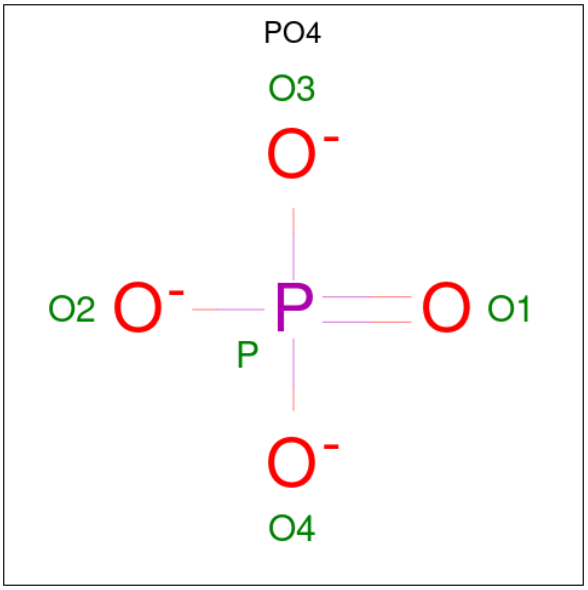
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 53 49 4	0	0

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total O P 5 4 1	0	0
12	M	1	Total O P 5 4 1	0	0
12	H	1	Total O P 5 4 1	0	0

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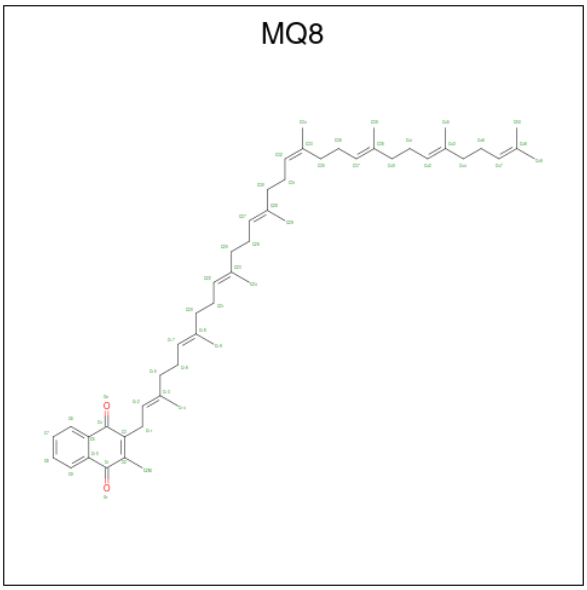
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total O P 5 4 1	0	0

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

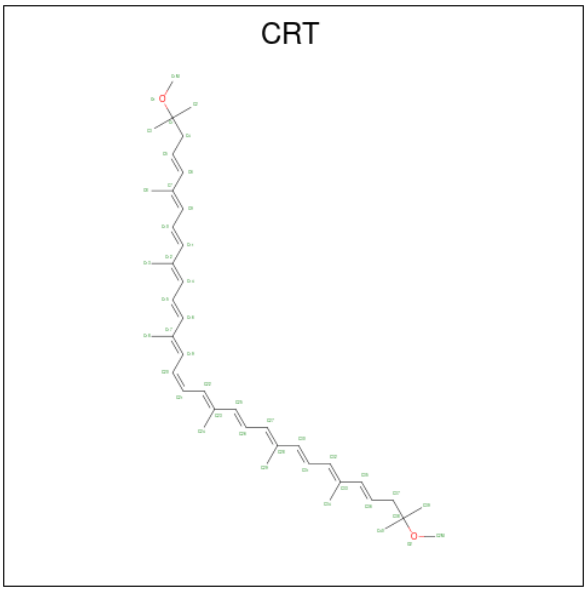
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total Fe 1 1	0	0

- Molecule 14 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	M	1	Total C O 53 51 2	0	0

- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total C O 44 42 2	0	0
15	A	1	Total C O 44 42 2	0	0
15	A	1	Total C O 44 42 2	0	0
15	B	1	Total C O 44 42 2	0	0
15	G	1	Total C O 44 42 2	0	0
15	J	1	Total C O 44 42 2	0	0
15	N	1	Total C O 44 42 2	0	0
15	P	1	Total C O 44 42 2	0	0
15	R	1	Total C O 44 42 2	0	0
15	T	1	Total C O 44 42 2	0	0
15	V	1	Total C O 44 42 2	0	0
15	W	1	Total C O 44 42 2	0	0
15	X	1	Total C O 44 42 2	0	0
15	2	1	Total C O 44 42 2	0	0

Continued on next page...

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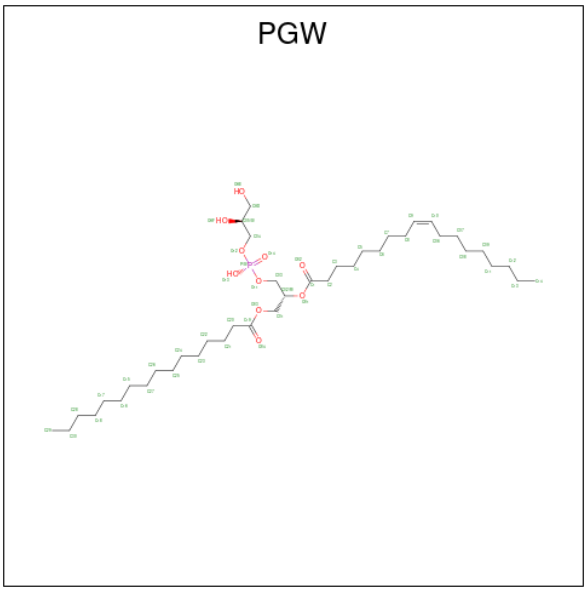
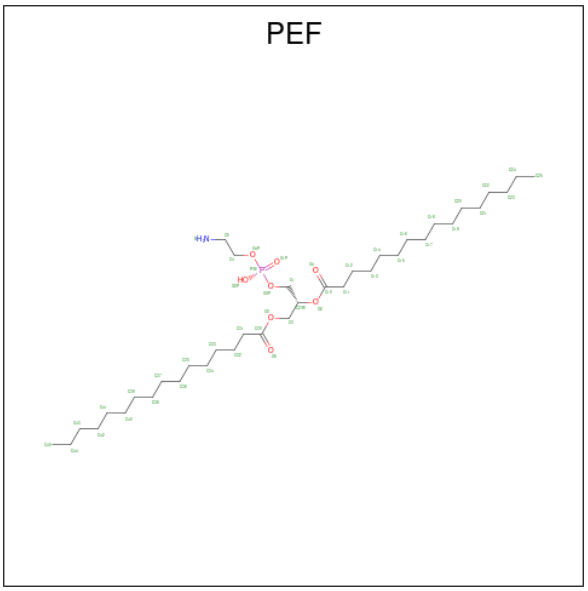
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	3	1	Total C O 44 42 2	0	0
15	4	1	Total C O 44 42 2	0	0
15	8	1	Total C O 44 42 2	0	0

- Molecule 16 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C O P 21 10 10 1	0	0
16	H	1	Total C O P 21 10 10 1	0	0

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

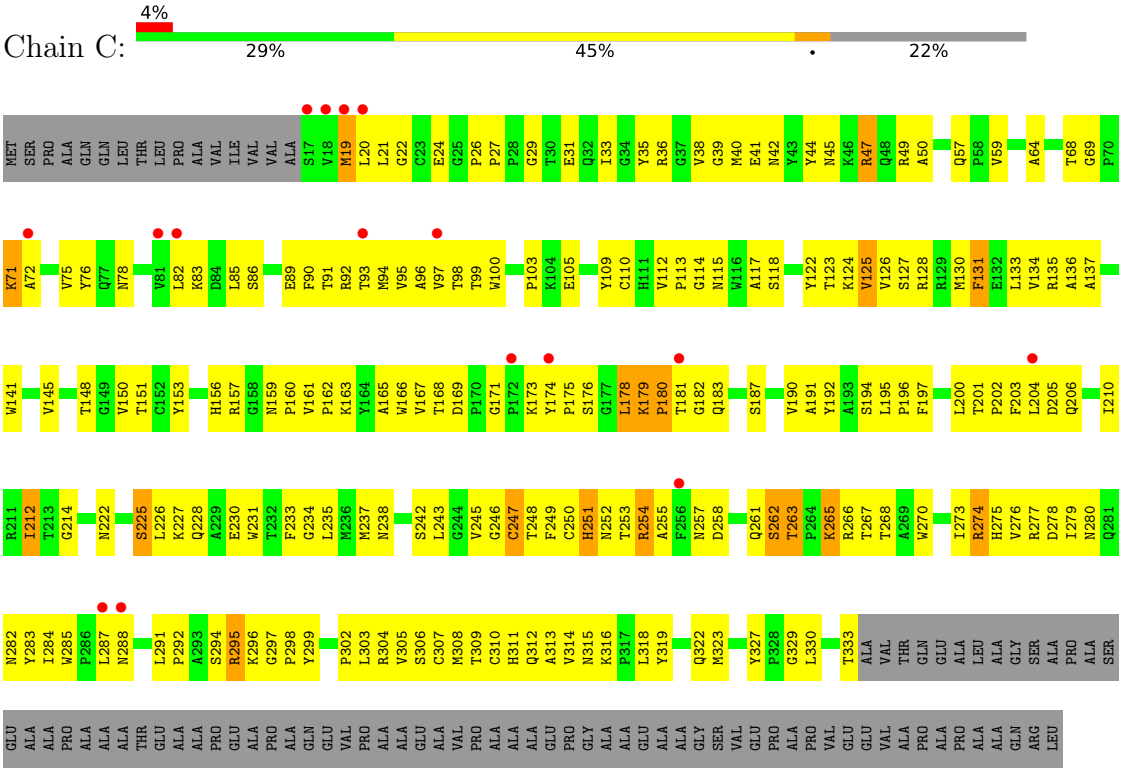
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	4	Total	O	0	0
			4	4		
18	H	1	Total	O	0	0
			1	1		

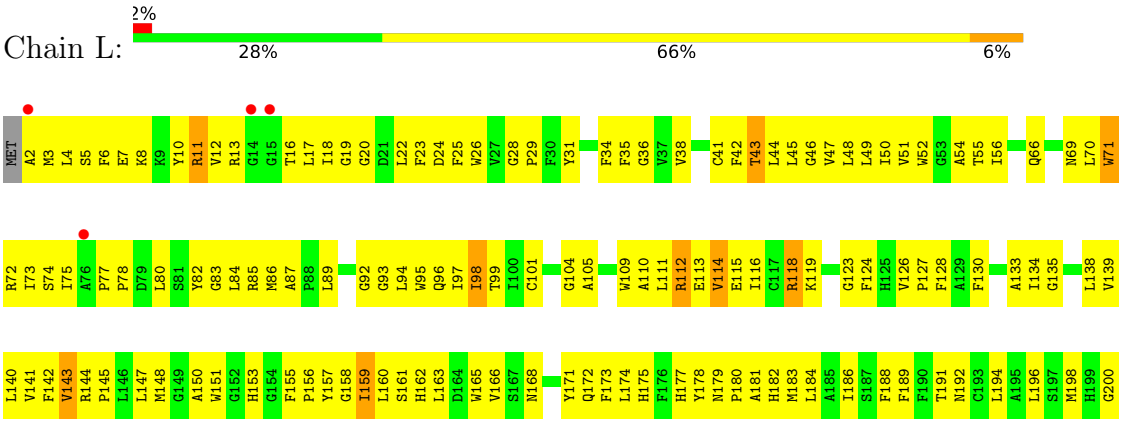
3 Residue-property plots (i)

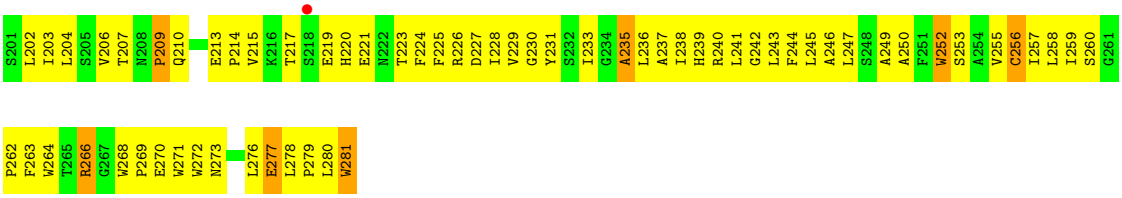
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Photosynthetic reaction center C subunit



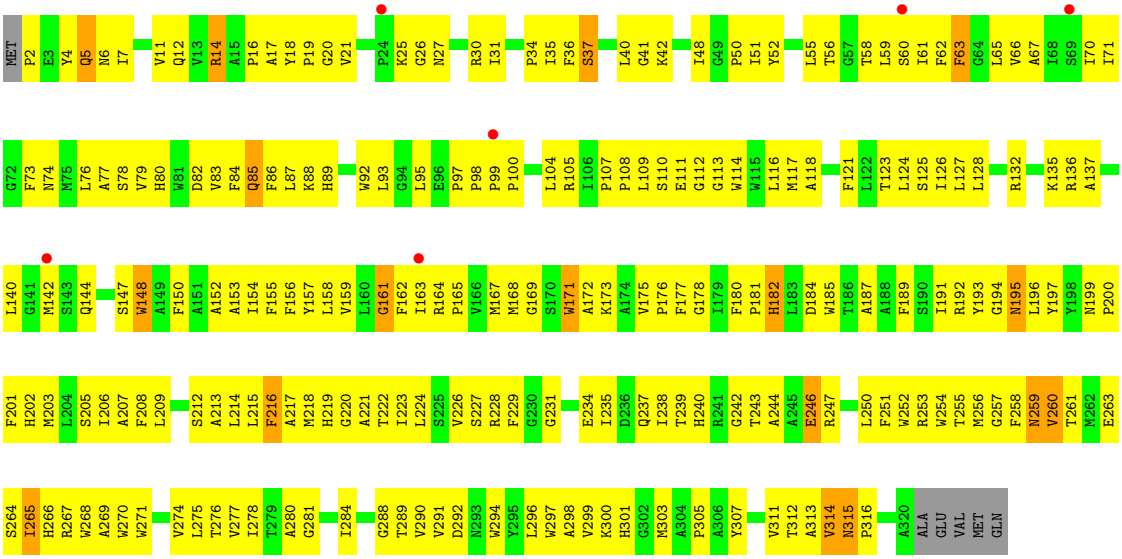
• Molecule 2: Photosynthetic reaction center L subunit





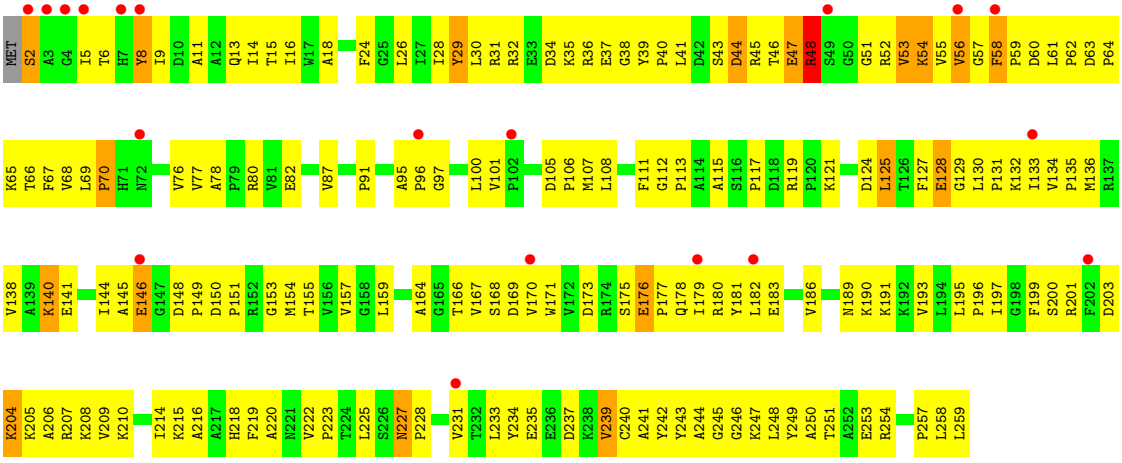
• Molecule 3: Photosynthetic reaction center M subunit

Chain M:



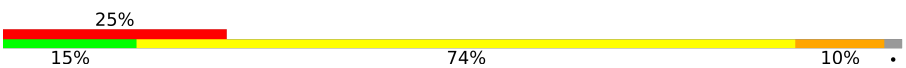
• Molecule 4: Photosynthetic reaction center H subunit

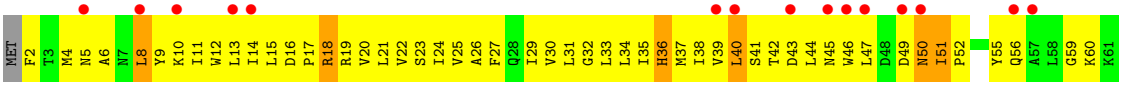
Chain H:



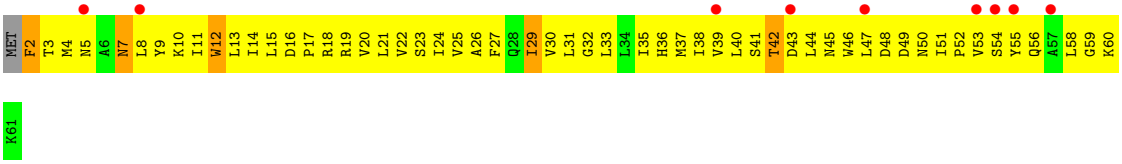
• Molecule 5: LH1 alpha polypeptide

Chain A:

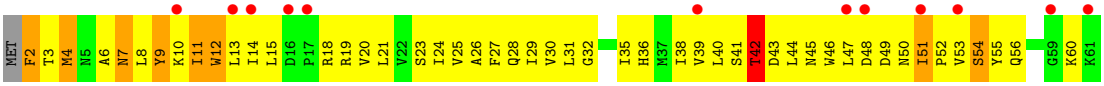




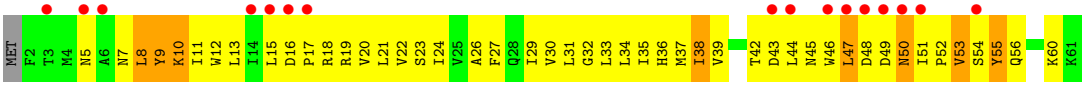
• Molecule 5: LH1 alpha polypeptide



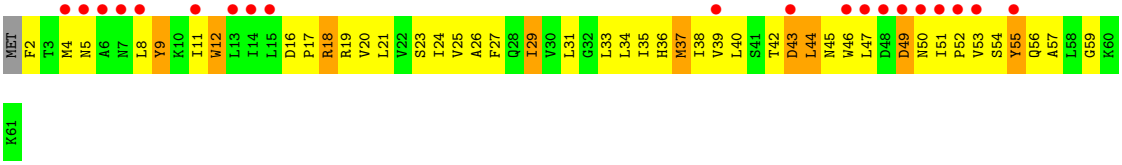
• Molecule 5: LH1 alpha polypeptide



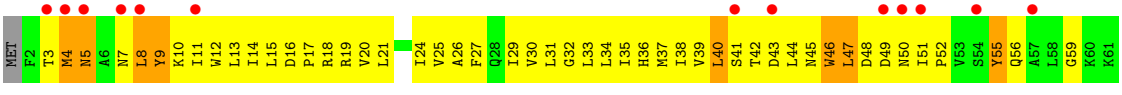
• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide

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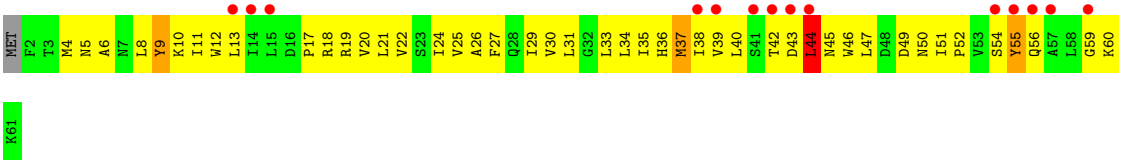
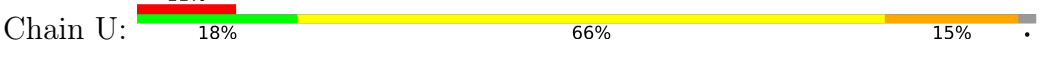
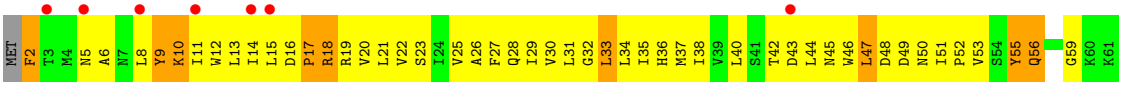
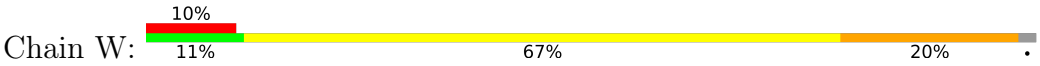


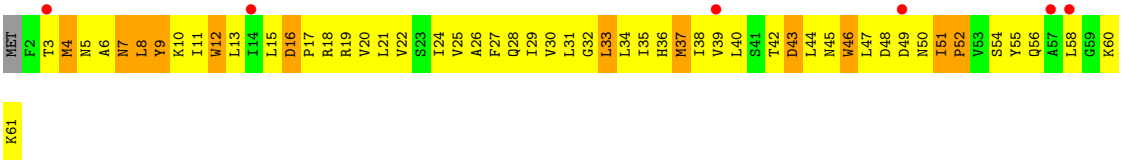
• Molecule 5: LH1 alpha polypeptide



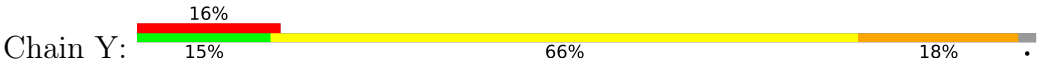


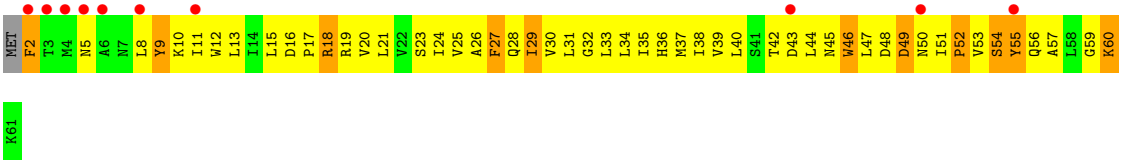
• Molecule 5: LH1 alpha polypeptide



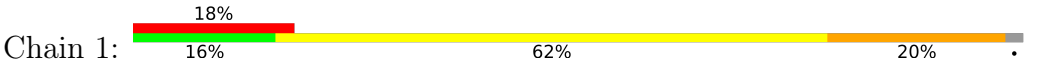


• Molecule 5: LH1 alpha polypeptide

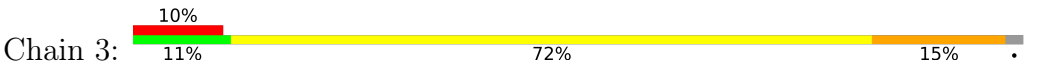


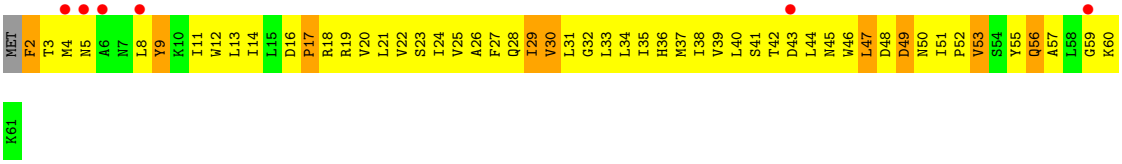


• Molecule 5: LH1 alpha polypeptide



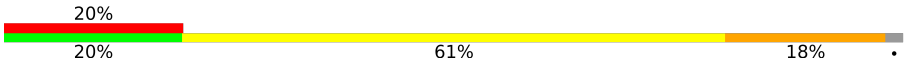
• Molecule 5: LH1 alpha polypeptide

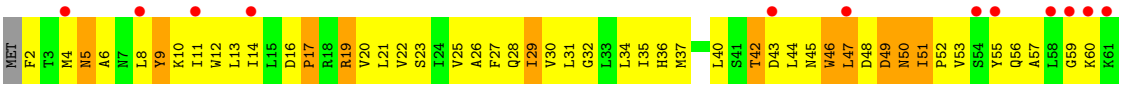




• Molecule 5: LH1 alpha polypeptide

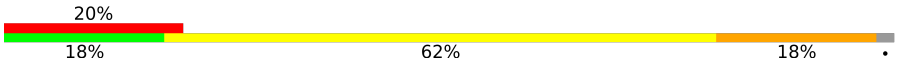
Chain 5:





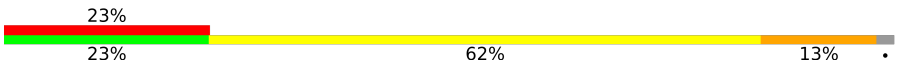
• Molecule 5: LH1 alpha polypeptide

Chain 7:



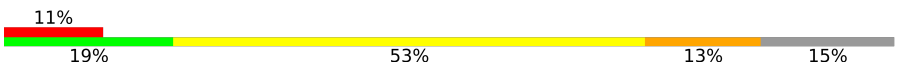
• Molecule 5: LH1 alpha polypeptide

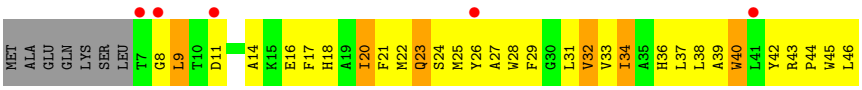
Chain 9:



• Molecule 6: LH1 beta polypeptide

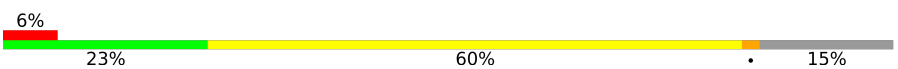
Chain B:

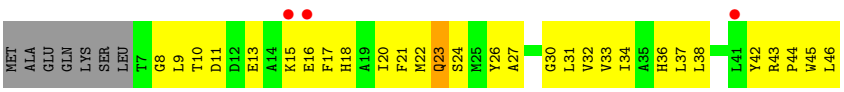




• Molecule 6: LH1 beta polypeptide

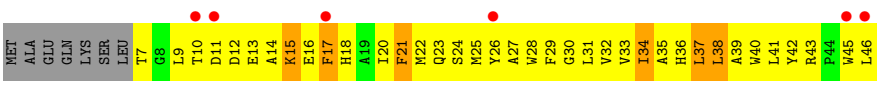
Chain E:





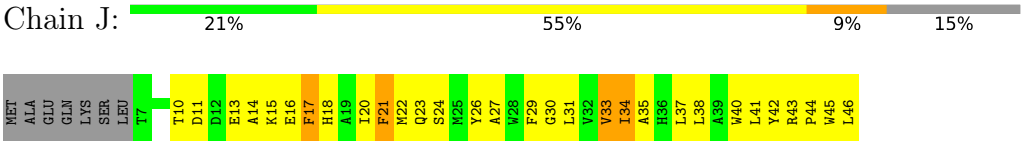
• Molecule 6: LH1 beta polypeptide

Chain G:



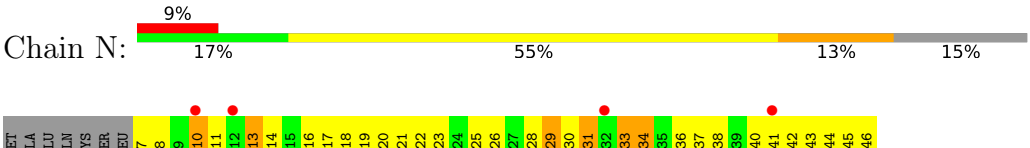
• Molecule 6: LH1 beta polypeptide

Chain J:



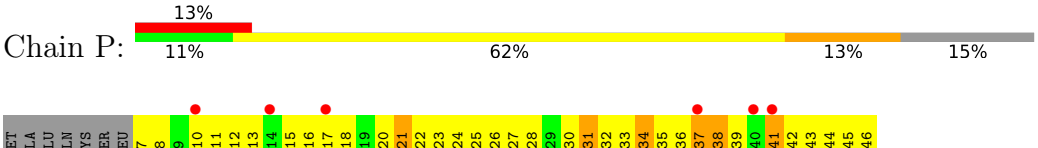
• Molecule 6: LH1 beta polypeptide

Chain N:



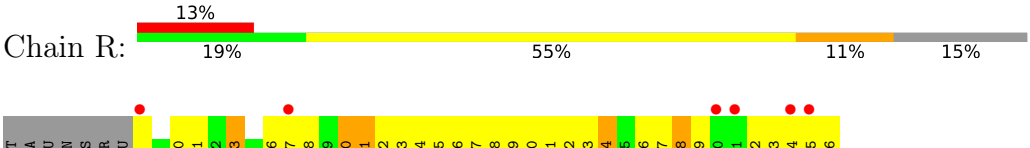
• Molecule 6: LH1 beta polypeptide

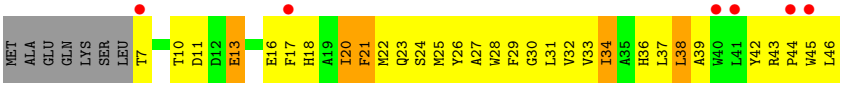
Chain P:



• Molecule 6: LH1 beta polypeptide

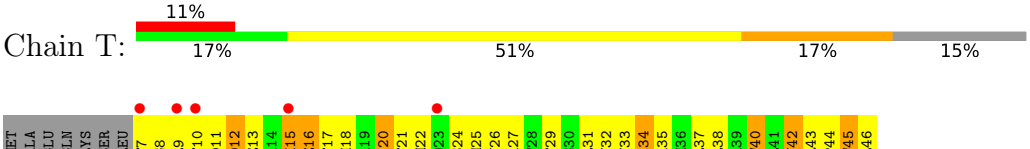
Chain R:

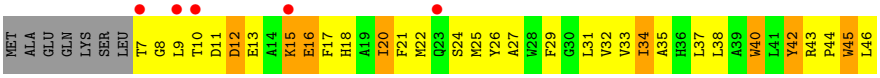




• Molecule 6: LH1 beta polypeptide

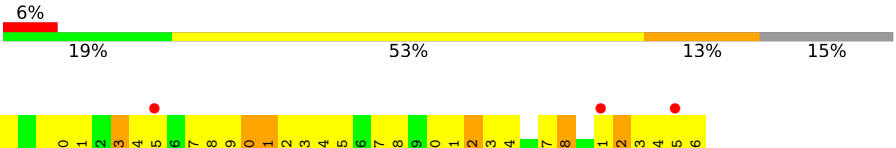
Chain T:

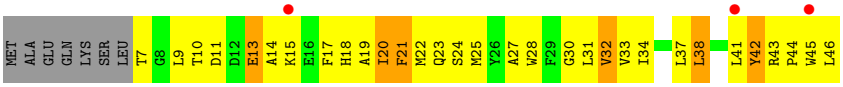




• Molecule 6: LH1 beta polypeptide

Chain V:



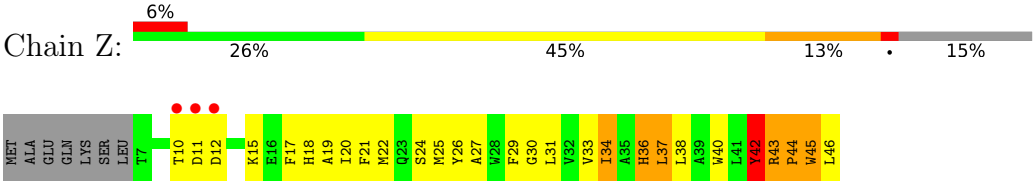


• Molecule 6: LH1 beta polypeptide

Chain X:

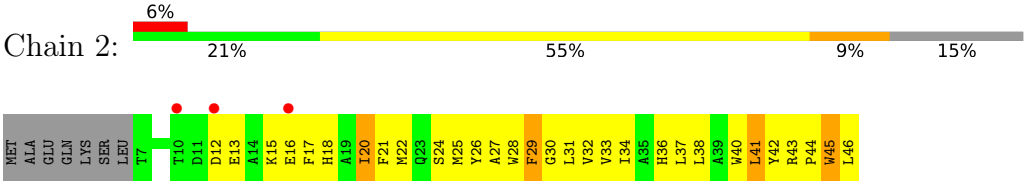
• Molecule 6: LH1 beta polypeptide

Chain Z:



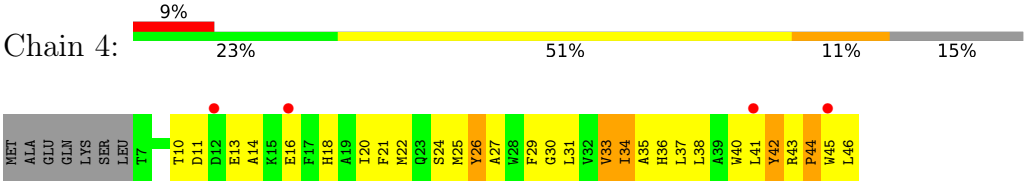
• Molecule 6: LH1 beta polypeptide

Chain 2:



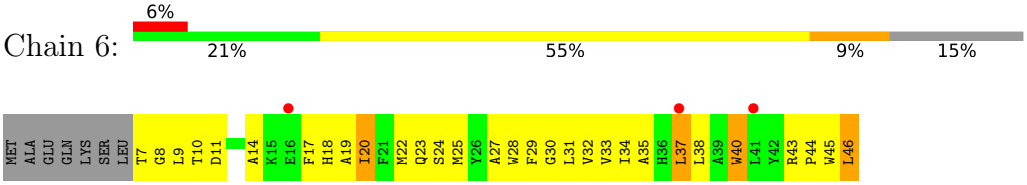
• Molecule 6: LH1 beta polypeptide

Chain 4:



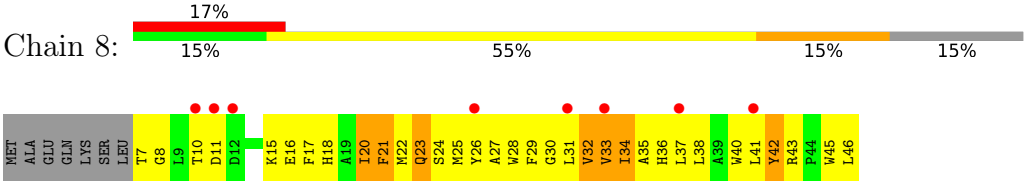
• Molecule 6: LH1 beta polypeptide

Chain 6:



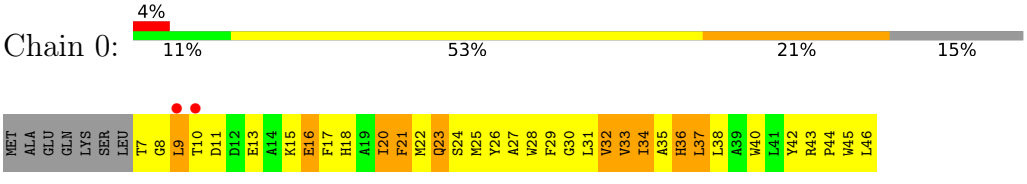
• Molecule 6: LH1 beta polypeptide

Chain 8:



• Molecule 6: LH1 beta polypeptide

Chain 0:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.34Å 148.24Å 161.79Å 90.00° 117.59° 90.00°	Depositor
Resolution (Å)	47.99 – 3.01 47.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.0 (47.99-3.01) 83.0 (47.99-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.314 , 0.337 0.315 , 0.322	Depositor DCC
R_{free} test set	3884 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	25819	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, HEM, UQ8, MQ8, PO4, BPH, CRT, BCL, CA, PGW, PEF

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	C	0.38	0/2528	0.63	0/3451
2	L	0.37	0/2318	0.57	1/3167 (0.0%)
3	M	0.30	0/2651	0.51	1/3628 (0.0%)
4	H	0.37	0/2038	0.57	1/2776 (0.0%)
5	1	0.42	0/483	0.63	0/660
5	3	0.37	0/483	0.68	0/660
5	5	0.34	0/483	0.71	0/660
5	7	0.39	0/483	0.75	0/660
5	9	0.38	0/483	0.67	0/660
5	A	0.43	0/483	0.74	0/660
5	D	0.33	0/483	0.61	0/660
5	F	0.42	0/483	0.66	0/660
5	I	0.33	0/483	0.63	0/660
5	K	0.38	0/483	0.63	0/660
5	O	0.36	0/483	0.68	0/660
5	Q	0.31	0/483	0.58	0/660
5	S	0.31	0/483	0.61	0/660
5	U	0.36	0/483	0.69	1/660 (0.2%)
5	W	0.41	1/483 (0.2%)	0.59	0/660
5	Y	0.37	0/483	0.68	0/660
6	0	0.42	0/350	0.57	0/476
6	2	0.33	0/350	0.58	0/476
6	4	0.44	0/350	0.67	0/476
6	6	0.33	0/350	0.59	1/476 (0.2%)
6	8	0.47	0/350	0.63	0/476
6	B	0.39	0/350	0.49	0/476
6	E	0.40	0/350	0.51	0/476
6	G	0.43	0/350	0.61	0/476
6	J	0.45	0/350	0.56	0/476
6	N	0.40	0/350	0.58	0/476
6	P	0.42	0/350	0.60	0/476
6	R	0.39	0/350	0.55	0/476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	T	0.35	0/350	0.52	0/476
6	V	0.40	0/350	0.64	0/476
6	X	0.40	0/350	0.56	0/476
6	Z	0.34	0/350	0.59	0/476
All	All	0.37	1/22863 (0.0%)	0.61	5/31198 (0.0%)

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
6	X	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	61	LYS	C-OXT	5.31	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	58	PHE	C-N-CD	6.24	141.50	128.40
3	M	5	GLN	N-CA-C	-5.97	94.89	111.00
5	U	10	LYS	CB-CA-C	-5.35	99.70	110.40
2	L	98	ILE	CB-CA-C	-5.10	101.39	111.60
6	6	46	LEU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	X	37	LEU	Mainchain

5.2 Too-close contacts (i)

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	C	2458	0	2377	294	0
2	L	2231	0	2192	349	0
3	M	2551	0	2526	413	0
4	H	1983	0	1981	326	0
5	1	473	0	476	149	0
5	3	473	0	476	148	0
5	5	473	0	476	150	0
5	7	473	0	476	149	0
5	9	473	0	476	137	0
5	A	473	0	476	204	0
5	D	473	0	476	152	0
5	F	473	0	476	160	0
5	I	473	0	476	150	0
5	K	473	0	476	133	0
5	O	473	0	476	133	0
5	Q	473	0	476	119	0
5	S	473	0	476	119	0
5	U	473	0	476	142	0
5	W	473	0	476	184	0
5	Y	473	0	476	165	0
6	0	337	0	323	78	0
6	2	337	0	323	88	0
6	4	337	0	323	114	0
6	6	337	0	323	55	0
6	8	337	0	323	103	0
6	B	337	0	323	77	0
6	E	337	0	323	77	0
6	G	337	0	323	92	0
6	J	337	0	323	89	0
6	N	337	0	323	75	0
6	P	337	0	323	125	0
6	R	337	0	323	80	0
6	T	337	0	323	71	0
6	V	337	0	323	106	0
6	X	337	0	323	93	0
6	Z	337	0	323	74	0
7	C	172	0	120	17	0
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	5	1	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
9	0	66	0	74	24	0
9	1	66	0	74	18	0
9	2	66	0	74	19	0
9	3	66	0	74	28	0
9	4	66	0	74	36	0
9	5	66	0	74	23	0
9	6	66	0	74	22	0
9	7	132	0	148	51	0
9	9	66	0	74	29	0
9	A	66	0	74	35	0
9	B	66	0	74	38	0
9	D	66	0	74	22	0
9	E	66	0	74	33	0
9	F	66	0	74	45	0
9	G	66	0	74	37	0
9	I	132	0	148	53	0
9	K	66	0	74	27	0
9	L	132	0	148	20	0
9	M	132	0	148	43	0
9	N	66	0	74	23	0
9	O	66	0	74	55	0
9	P	66	0	74	30	0
9	Q	66	0	74	28	0
9	R	66	0	74	31	0
9	S	66	0	74	26	0
9	T	66	0	74	24	0
9	U	66	0	74	23	0
9	V	66	0	74	14	0
9	W	66	0	74	37	0
9	X	66	0	74	39	0
9	Y	66	0	74	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Z	66	0	74	29	0
10	L	65	0	76	8	0
10	M	65	0	76	19	0
11	L	53	0	74	13	0
12	H	10	0	0	4	0
12	L	5	0	0	0	0
12	M	5	0	0	1	0
13	M	1	0	0	0	0
14	M	53	0	72	13	0
15	2	44	0	60	40	0
15	3	44	0	60	20	0
15	4	44	0	60	68	0
15	8	44	0	60	80	0
15	A	88	0	120	70	0
15	B	44	0	60	35	0
15	G	44	0	60	27	0
15	J	44	0	60	35	0
15	M	44	0	60	12	0
15	N	44	0	60	54	0
15	P	44	0	60	61	0
15	R	44	0	60	34	0
15	T	44	0	58	23	0
15	V	44	0	60	65	0
15	W	44	0	60	29	0
15	X	44	0	60	27	0
16	H	21	0	12	7	0
16	M	21	0	12	16	0
17	H	19	0	11	18	0
18	H	1	0	0	0	0
18	L	4	0	0	3	0
All	All	25819	0	25995	4814	0

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 93.

All (4814) 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)
5:W:27:PHE:CE2	5:Y:29:ILE:HD11	1.30	1.64
5:U:27:PHE:CE2	5:W:29:ILE:HD11	1.30	1.63
6:V:21:PHE:CD2	15:V:102:CRT:H14	1.37	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LYS:HD2	15:8:101:CRT:C2	1.27	1.58
6:P:17:PHE:CD1	15:P:102:CRT:H6	1.39	1.57
5:1:10:LYS:HD2	6:4:20:ILE:CD1	1.42	1.49
6:V:21:PHE:CE2	15:V:102:CRT:H16	1.43	1.49
15:V:102:CRT:C39	5:W:36:HIS:HB2	1.43	1.48
6:8:17:PHE:CE1	15:8:101:CRT:H9	1.55	1.42
3:M:31:ILE:HD11	16:M:407:PGW:C05	1.48	1.41
5:W:27:PHE:HE2	5:Y:29:ILE:CD1	1.33	1.40
3:M:70:ILE:HG21	3:M:118:ALA:CB	1.49	1.40
6:V:21:PHE:CD2	15:V:102:CRT:C14	2.06	1.37
6:V:21:PHE:CG	15:V:102:CRT:H14	1.61	1.35
6:4:25:MET:CG	15:4:102:CRT:H19	1.58	1.34
6:V:21:PHE:HD2	15:V:102:CRT:C14	1.39	1.33
5:W:27:PHE:CE2	5:Y:29:ILE:CD1	2.08	1.33
6:P:17:PHE:CE1	15:P:102:CRT:H9	1.63	1.33
5:K:54:SER:CB	5:K:56:GLN:HE22	1.41	1.31
5:3:13:LEU:HD12	15:3:103:CRT:C1M	1.59	1.31
5:1:13:LEU:HB2	15:4:102:CRT:C1M	1.61	1.31
5:Q:26:ALA:O	5:Q:29:ILE:HG22	1.15	1.29
6:T:17:PHE:CE1	15:T:102:CRT:H9	1.64	1.29
6:8:17:PHE:CZ	15:8:101:CRT:H9	1.67	1.29
5:U:26:ALA:O	5:U:29:ILE:HG22	1.33	1.28
5:3:13:LEU:CD1	15:3:103:CRT:H1M2	1.61	1.28
5:3:26:ALA:O	5:3:29:ILE:HG22	1.30	1.27
5:I:50:ASN:CB	5:K:59:GLY:HA3	1.65	1.26
6:P:17:PHE:HD1	15:P:102:CRT:C6	1.46	1.26
5:U:27:PHE:CE2	5:W:29:ILE:CD1	2.17	1.26
5:W:26:ALA:O	5:W:29:ILE:HG22	1.17	1.26
15:P:102:CRT:H2M3	5:Q:36:HIS:CB	1.65	1.26
5:3:43:ASP:HB2	5:5:47:LEU:O	1.33	1.25
6:8:27:ALA:O	6:8:31:LEU:HG	1.35	1.25
5:5:10:LYS:CD	15:8:101:CRT:H21A	1.67	1.24
5:9:16:ASP:CG	5:9:17:PRO:HD2	1.55	1.24
6:V:21:PHE:HB2	15:V:102:CRT:C11	1.68	1.24
6:V:21:PHE:CD2	15:V:102:CRT:H16	1.72	1.24
5:Q:27:PHE:CE2	5:S:29:ILE:HD11	1.73	1.23
9:3:102:BCL:C9	15:4:102:CRT:H183	1.68	1.23
6:P:38:LEU:O	6:P:41:LEU:HD23	1.31	1.22
15:P:102:CRT:H342	9:Q:102:BCL:CAA	1.68	1.22
5:U:27:PHE:CD2	5:W:29:ILE:HD11	1.75	1.21
6:P:21:PHE:CZ	15:P:102:CRT:H19	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:21:PHE:CB	15:V:102:CRT:H14	1.71	1.21
15:V:102:CRT:H391	5:W:36:HIS:CB	1.70	1.21
3:M:31:ILE:HD11	16:M:407:PGW:C04	1.67	1.20
6:R:21:PHE:HB2	15:R:102:CRT:C14	1.72	1.20
5:K:54:SER:CB	5:K:56:GLN:NE2	2.02	1.20
6:2:21:PHE:CE1	15:2:102:CRT:C16	2.25	1.20
6:J:20:ILE:HG12	15:J:101:CRT:H83	1.22	1.18
5:W:8:LEU:HD13	6:X:22:MET:CE	1.72	1.18
5:Y:49:ASP:CA	5:1:56:GLN:HE21	1.55	1.18
6:4:20:ILE:HG21	15:4:102:CRT:C6	1.74	1.17
3:M:67:ALA:O	3:M:70:ILE:HG22	1.43	1.17
5:5:10:LYS:HG3	15:8:101:CRT:H31A	1.17	1.17
6:V:27:ALA:O	6:V:31:LEU:HG	1.42	1.17
1:C:173:LYS:HG2	3:M:80:HIS:ND1	1.60	1.16
5:5:10:LYS:CD	15:8:101:CRT:C2	2.23	1.16
15:N:102:CRT:H342	9:O:102:BCL:HAA1	1.17	1.16
6:G:27:ALA:O	6:G:31:LEU:HG	1.45	1.15
5:1:26:ALA:O	5:1:29:ILE:HG22	1.46	1.15
4:H:138:VAL:O	4:H:140:LYS:HD3	1.46	1.15
5:F:36:HIS:CE1	9:G:101:BCL:HMD1	1.81	1.15
6:8:21:PHE:CD1	15:8:101:CRT:H16	1.80	1.15
5:1:10:LYS:HD2	6:4:20:ILE:HD13	1.24	1.14
6:V:21:PHE:CD2	15:V:102:CRT:C16	2.30	1.14
5:9:16:ASP:OD2	5:9:17:PRO:HD2	1.46	1.13
9:M:401:BCL:H142	10:M:403:BPH:HMA1	1.19	1.12
5:Y:49:ASP:HA	5:1:56:GLN:HE21	0.97	1.12
6:4:25:MET:CB	15:4:102:CRT:H16	1.78	1.12
15:M:406:CRT:H402	5:O:38:ILE:HG22	1.28	1.12
6:T:27:ALA:O	6:T:31:LEU:HG	1.50	1.12
15:V:102:CRT:C39	5:W:36:HIS:CB	2.25	1.12
6:2:20:ILE:HG21	15:2:102:CRT:C8	1.78	1.12
5:5:10:LYS:HB2	15:8:101:CRT:C8	1.77	1.12
3:M:31:ILE:HD11	16:M:407:PGW:H05	1.29	1.12
1:C:47:ARG:HD3	5:3:48:ASP:OD2	1.50	1.12
9:M:401:BCL:C14	10:M:403:BPH:HMA1	1.80	1.12
15:V:102:CRT:H393	5:W:33:LEU:HA	1.26	1.12
5:1:10:LYS:HD2	6:4:20:ILE:HD12	1.17	1.12
3:M:70:ILE:CG2	3:M:118:ALA:HB2	1.80	1.11
5:Q:27:PHE:HE2	5:S:29:ILE:HD11	0.97	1.11
15:X:102:CRT:H342	9:Y:102:BCL:H3A	1.13	1.11
5:5:10:LYS:HD2	15:8:101:CRT:H23	1.33	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:21:PHE:CE1	15:8:101:CRT:H19	1.86	1.11
6:G:21:PHE:HD1	6:G:22:MET:N	1.47	1.11
6:G:21:PHE:CD2	15:G:102:CRT:H14	1.86	1.11
5:5:10:LYS:CB	15:8:101:CRT:H5	1.81	1.11
4:H:45:ARG:NH1	4:H:97:GLY:H	1.48	1.10
5:W:8:LEU:CD2	5:W:11:ILE:CD1	2.29	1.10
15:W:103:CRT:H83	6:Z:20:ILE:HD13	1.26	1.10
5:1:10:LYS:HB3	15:4:102:CRT:H22A	1.29	1.10
6:0:9:LEU:HB3	6:0:13:GLU:HG3	1.14	1.10
6:2:20:ILE:CG2	15:2:102:CRT:H83	1.80	1.10
5:A:33:LEU:HG	15:A:101:CRT:H392	1.27	1.10
15:B:102:CRT:H2M3	5:D:36:HIS:HB2	1.20	1.10
6:J:20:ILE:HG12	15:J:101:CRT:C8	1.80	1.10
6:V:21:PHE:CE2	15:V:102:CRT:C16	2.34	1.10
4:H:47:GLU:HG3	5:A:19:ARG:HA	1.33	1.10
5:I:50:ASN:HB3	5:K:59:GLY:HA3	1.33	1.10
5:1:10:LYS:CD	6:4:20:ILE:CD1	2.30	1.10
5:A:60:LYS:HA	5:9:50:ASN:HB3	1.26	1.09
15:P:102:CRT:C2M	5:Q:36:HIS:HB2	1.82	1.09
5:D:5:ASN:HB2	6:E:22:MET:HG2	1.34	1.09
9:3:102:BCL:H92	15:4:102:CRT:H183	1.11	1.09
15:N:102:CRT:H403	9:O:102:BCL:HMB2	1.32	1.09
6:V:21:PHE:HB2	15:V:102:CRT:C14	1.81	1.09
6:4:25:MET:HB2	15:4:102:CRT:C16	1.83	1.09
4:H:53:VAL:HG11	5:D:22:VAL:HG21	1.29	1.09
5:3:51:ILE:HB	5:3:52:PRO:HA	1.20	1.08
5:5:10:LYS:CG	15:8:101:CRT:H31A	1.80	1.08
9:T:101:BCL:HMA1	9:U:102:BCL:HMA1	1.23	1.08
5:W:8:LEU:HD13	6:X:22:MET:HE1	1.27	1.08
6:8:21:PHE:HE1	15:8:101:CRT:H19	1.06	1.08
3:M:31:ILE:CD1	16:M:407:PGW:H05	1.83	1.07
5:A:33:LEU:CG	15:A:101:CRT:H392	1.84	1.07
6:2:17:PHE:HE1	15:2:102:CRT:C9	1.66	1.07
6:4:25:MET:HG2	15:4:102:CRT:C19	1.84	1.07
9:F:102:BCL:HBC2	9:G:101:BCL:HAC1	1.34	1.07
5:K:24:ILE:HD13	15:N:102:CRT:H21	1.09	1.07
6:8:17:PHE:CE1	15:8:101:CRT:C9	2.36	1.07
5:O:4:MET:HG3	6:R:23:GLN:HB3	1.26	1.06
5:S:26:ALA:O	5:S:29:ILE:HG22	1.53	1.06
6:4:21:PHE:HA	15:4:102:CRT:C11	1.85	1.06
5:A:36:HIS:HB3	15:A:101:CRT:H402	1.13	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:21:PHE:HB2	15:V:102:CRT:H11	1.17	1.06
5:5:10:LYS:HE3	15:8:101:CRT:H32A	1.36	1.06
15:P:102:CRT:C34	9:Q:102:BCL:HAA1	1.84	1.06
5:5:10:LYS:HB2	15:8:101:CRT:H82	1.36	1.06
6:2:21:PHE:CD1	15:2:102:CRT:C15	2.39	1.06
9:L:301:BCL:HBB3	9:M:401:BCL:HMD2	1.33	1.06
5:A:33:LEU:HG	15:A:101:CRT:C39	1.86	1.06
5:D:43:ASP:HB2	5:F:47:LEU:HD22	1.31	1.05
15:G:102:CRT:H2M3	5:I:36:HIS:HB2	1.38	1.05
9:Q:102:BCL:HBC2	9:R:101:BCL:CMD	1.86	1.05
5:Y:49:ASP:HA	5:1:56:GLN:NE2	1.69	1.05
5:1:13:LEU:HB2	15:4:102:CRT:H1M1	1.35	1.05
6:R:27:ALA:O	6:R:31:LEU:HG	1.56	1.05
5:W:26:ALA:O	5:W:29:ILE:CG2	2.04	1.05
9:M:401:BCL:H203	10:M:403:BPH:H9C3	1.32	1.05
6:4:20:ILE:CG2	15:4:102:CRT:C6	2.35	1.05
5:I:36:HIS:CE1	9:I:103:BCL:HMD1	1.92	1.05
6:2:17:PHE:CE1	15:2:102:CRT:C9	2.40	1.05
5:7:36:HIS:CE1	9:7:103:BCL:HMD1	1.92	1.05
3:M:31:ILE:CD1	16:M:407:PGW:C05	2.35	1.04
4:H:14:ILE:HD11	5:I:37:MET:HB3	1.36	1.04
4:H:54:LYS:HE2	4:H:58:PHE:HD1	1.22	1.04
9:D:102:BCL:HBA1	9:D:102:BCL:HBD	1.39	1.04
6:P:21:PHE:CE1	6:P:25:MET:HB2	1.92	1.04
5:Q:27:PHE:HE2	5:S:29:ILE:CD1	1.71	1.04
6:V:21:PHE:CB	15:V:102:CRT:C14	2.34	1.04
5:W:8:LEU:CD2	5:W:11:ILE:HD12	1.84	1.04
5:1:10:LYS:CB	15:4:102:CRT:H22A	1.87	1.04
3:M:70:ILE:CG2	3:M:118:ALA:CB	2.36	1.04
4:H:53:VAL:CG1	5:D:22:VAL:HG21	1.88	1.03
9:4:101:BCL:H43	15:4:102:CRT:C24	1.88	1.03
9:I:102:BCL:CBC	9:I:103:BCL:HHD	1.88	1.03
5:A:50:ASN:HA	5:D:60:LYS:HA	1.40	1.03
9:Q:102:BCL:CHD	9:R:101:BCL:HMD2	1.87	1.03
3:M:164:ARG:HH12	3:M:173:LYS:HB3	1.20	1.03
9:M:401:BCL:H142	10:M:403:BPH:CMA	1.88	1.03
6:G:28:TRP:NE1	6:G:32:VAL:HG21	1.74	1.03
5:O:36:HIS:CE1	9:P:101:BCL:HMD1	1.92	1.03
6:P:17:PHE:CD1	15:P:102:CRT:H9	1.94	1.03
6:N:46:LEU:HD22	6:P:42:TYR:CZ	1.93	1.03
6:B:40:TRP:HZ3	6:B:45:TRP:H	1.05	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:9:TYR:HA	6:8:18:HIS:ND1	1.74	1.02
9:I:102:BCL:HBC2	9:I:103:BCL:HHD	1.40	1.02
5:W:26:ALA:C	5:W:29:ILE:HG22	1.78	1.02
5:A:21:LEU:CD1	15:B:102:CRT:H14	1.90	1.02
15:A:103:CRT:H83	6:E:20:ILE:HD13	1.37	1.02
5:O:26:ALA:O	5:O:29:ILE:HG22	1.56	1.02
4:H:53:VAL:HG13	4:H:54:LYS:H	1.23	1.02
6:P:21:PHE:CZ	15:P:102:CRT:C19	2.43	1.02
5:S:42:THR:HG21	5:U:47:LEU:HB3	1.04	1.02
6:V:21:PHE:CD2	15:V:102:CRT:C15	2.42	1.02
5:W:8:LEU:HD23	5:W:11:ILE:CD1	1.90	1.02
3:M:242:GLY:HA2	4:H:119:ARG:HD3	1.38	1.01
4:H:225:LEU:HA	4:H:235:GLU:OE1	1.60	1.01
6:8:21:PHE:HD1	15:8:101:CRT:H16	1.10	1.01
9:Q:102:BCL:HBC2	9:R:101:BCL:HMD2	1.37	1.01
6:V:21:PHE:CB	15:V:102:CRT:H11	1.89	1.01
6:4:21:PHE:CA	15:4:102:CRT:H11	1.90	1.01
2:L:89:LEU:HA	2:L:93:GLY:HA3	1.42	1.01
6:N:45:TRP:O	6:N:46:LEU:HB2	1.61	1.00
6:8:17:PHE:HE1	15:8:101:CRT:H9	1.24	1.00
4:H:140:LYS:HD3	4:H:140:LYS:H	1.22	1.00
9:P:101:BCL:HMA1	9:Q:102:BCL:HMA1	1.43	1.00
15:T:102:CRT:H342	9:U:102:BCL:HAA1	1.39	1.00
5:1:13:LEU:HB2	15:4:102:CRT:H1M3	1.40	1.00
1:C:252:ASN:OD1	1:C:254:ARG:HD2	1.61	1.00
6:B:20:ILE:HG21	15:B:102:CRT:H83	1.38	1.00
15:3:103:CRT:H342	9:7:102:BCL:HAA1	1.41	1.00
5:7:43:ASP:HB2	5:9:47:LEU:HD12	1.44	1.00
6:8:17:PHE:HE1	15:8:101:CRT:C9	1.73	1.00
15:N:102:CRT:C34	9:O:102:BCL:HAA1	1.92	0.99
5:5:43:ASP:HB2	5:7:47:LEU:HB3	1.44	0.99
15:N:102:CRT:H403	9:O:102:BCL:CMB	1.91	0.99
9:I:102:BCL:C1D	9:I:103:BCL:HMD2	1.92	0.99
6:J:43:ARG:NH1	5:K:55:TYR:CD2	2.30	0.99
5:U:27:PHE:HE2	5:W:29:ILE:CD1	1.66	0.99
6:2:20:ILE:HG21	15:2:102:CRT:H83	0.99	0.99
6:0:29:PHE:O	6:0:32:VAL:HG12	1.63	0.99
2:L:204:LEU:HD21	3:M:267:ARG:HG3	1.41	0.99
5:S:42:THR:CG2	5:U:47:LEU:HB3	1.92	0.99
3:M:296:LEU:O	3:M:300:LYS:HG2	1.62	0.98
6:G:21:PHE:CE2	15:G:102:CRT:H16	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:10:LYS:CD	6:4:20:ILE:HD12	1.91	0.98
5:5:49:ASP:HB2	5:7:56:GLN:HB3	1.45	0.98
5:5:10:LYS:HB3	15:8:101:CRT:H5	1.42	0.98
9:F:102:BCL:CBC	9:G:101:BCL:HAC1	1.93	0.98
6:N:37:LEU:O	6:N:41:LEU:HG	1.63	0.98
5:1:13:LEU:CB	15:4:102:CRT:C1M	2.41	0.98
6:4:20:ILE:CG2	15:4:102:CRT:H6	1.92	0.98
5:Q:26:ALA:O	5:Q:29:ILE:CG2	2.12	0.98
6:V:21:PHE:HB2	15:V:102:CRT:C12	1.93	0.98
2:L:18:ILE:O	2:L:34:PHE:HB2	1.62	0.98
6:X:36:HIS:HD1	9:X:101:BCL:H151	1.25	0.98
5:3:43:ASP:CB	5:5:47:LEU:O	2.11	0.98
6:8:25:MET:HG3	15:8:101:CRT:C21	1.92	0.98
6:N:28:TRP:CE3	6:N:31:LEU:CD1	2.45	0.98
6:N:38:LEU:HA	6:N:41:LEU:HD12	1.41	0.97
6:P:17:PHE:HB2	15:P:102:CRT:H41	1.46	0.97
5:I:26:ALA:O	5:I:29:ILE:HG22	1.63	0.97
5:Q:42:THR:HG23	5:Q:43:ASP:H	1.23	0.97
6:J:43:ARG:NH1	5:K:55:TYR:CG	2.32	0.97
6:R:21:PHE:HB2	15:R:102:CRT:H14	1.42	0.97
5:1:10:LYS:CD	6:4:20:ILE:HD13	1.92	0.97
5:1:36:HIS:CE1	9:2:101:BCL:HMD1	1.99	0.97
6:2:21:PHE:HE1	15:2:102:CRT:C16	1.72	0.97
6:8:21:PHE:HE1	15:8:101:CRT:C19	1.75	0.97
2:L:44:LEU:HB2	5:9:30:VAL:HG11	1.43	0.97
5:A:60:LYS:HA	5:9:50:ASN:CB	1.95	0.97
6:P:16:GLU:OE2	15:P:102:CRT:H1M1	1.65	0.96
6:P:21:PHE:HE1	6:P:25:MET:HB2	1.27	0.96
6:V:21:PHE:HD2	15:V:102:CRT:C15	1.78	0.96
6:P:17:PHE:CE1	15:P:102:CRT:C9	2.47	0.96
5:I:50:ASN:HB2	5:K:59:GLY:HA3	1.43	0.96
6:8:17:PHE:CZ	15:8:101:CRT:H11	1.99	0.96
5:A:47:LEU:HB3	5:9:43:ASP:HB2	1.46	0.96
5:W:10:LYS:HB3	15:W:103:CRT:H23	1.47	0.96
9:M:401:BCL:C20	10:M:403:BPH:H9C3	1.95	0.96
15:A:101:CRT:H132	5:7:11:ILE:HD12	1.46	0.96
5:F:44:LEU:HB2	6:G:43:ARG:HH11	1.31	0.96
6:4:46:LEU:HB2	5:5:52:PRO:HD3	1.46	0.96
6:8:21:PHE:HD1	15:8:101:CRT:C16	1.79	0.96
5:3:29:ILE:HG23	5:3:30:VAL:N	1.81	0.96
6:4:25:MET:HG2	15:4:102:CRT:H19	1.35	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:401:BCL:H122	10:M:403:BPH:HMA1	1.48	0.95
15:B:102:CRT:C2M	5:D:36:HIS:HB2	1.95	0.95
6:4:20:ILE:HG23	15:4:102:CRT:H9	1.48	0.95
2:L:183:MET:HE1	2:L:272:TRP:HE1	1.32	0.95
3:M:31:ILE:HD11	16:M:407:PGW:H04	1.43	0.95
6:Z:10:THR:HG22	6:Z:11:ASP:H	1.30	0.95
5:U:2:PHE:HA	5:U:5:ASN:HD22	1.31	0.95
6:4:25:MET:HG3	15:4:102:CRT:H19	1.46	0.95
5:5:10:LYS:HD2	15:8:101:CRT:H21A	0.98	0.95
5:K:24:ILE:HD13	15:N:102:CRT:C21	1.95	0.95
9:3:102:BCL:H92	15:4:102:CRT:C18	1.96	0.95
3:M:314:VAL:HG12	3:M:315:ASN:H	1.31	0.95
15:A:101:CRT:H33	6:0:16:GLU:OE2	1.65	0.95
5:D:36:HIS:CE1	9:E:101:BCL:HMD1	2.02	0.95
2:L:196:LEU:HD22	3:M:269:ALA:HB1	1.48	0.95
4:H:29:TYR:CE2	16:H:302:PGW:C2	2.49	0.95
15:X:102:CRT:H342	9:Y:102:BCL:C3A	1.97	0.95
1:C:196:PRO:O	1:C:197:PHE:CD2	2.20	0.95
4:H:29:TYR:CD2	16:H:302:PGW:C2	2.50	0.95
5:A:36:HIS:HB3	15:A:101:CRT:C40	1.96	0.95
6:4:20:ILE:HG23	15:4:102:CRT:C9	1.95	0.95
6:4:25:MET:CG	15:4:102:CRT:C19	2.41	0.95
5:U:51:ILE:HB	5:U:52:PRO:HA	1.45	0.94
1:C:124:LYS:NZ	1:C:128:ARG:HH12	1.65	0.94
5:F:27:PHE:CE2	5:I:29:ILE:HD11	2.02	0.94
5:W:8:LEU:HB3	6:X:18:HIS:CE1	2.02	0.94
5:K:44:LEU:CD2	5:K:46:TRP:HB3	1.98	0.94
4:H:6:THR:O	5:F:41:SER:HA	1.66	0.94
3:M:2:PRO:HG3	3:M:42:LYS:HE2	1.50	0.94
5:A:36:HIS:NE2	9:B:101:BCL:HMD1	1.82	0.94
5:S:50:ASN:HD21	6:T:43:ARG:NH2	1.65	0.94
6:8:17:PHE:HZ	15:8:101:CRT:H11	1.33	0.94
6:G:21:PHE:CD1	6:G:22:MET:N	2.35	0.94
5:3:44:LEU:HD12	5:3:44:LEU:O	1.67	0.94
3:M:59:LEU:CD1	5:Q:29:ILE:HG21	1.98	0.94
15:M:406:CRT:C40	5:O:38:ILE:HG22	1.98	0.94
5:F:10:LYS:HD2	15:J:101:CRT:H1M1	1.50	0.94
5:S:42:THR:HG21	5:U:47:LEU:CB	1.98	0.94
5:Y:12:TRP:HE1	6:Z:18:HIS:HA	1.32	0.94
5:3:29:ILE:HG23	5:3:30:VAL:H	1.32	0.94
5:K:24:ILE:HG12	15:N:102:CRT:H243	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:50:ASN:HB3	5:O:59:GLY:HA2	1.50	0.93
6:P:17:PHE:CD1	15:P:102:CRT:C6	2.33	0.93
5:W:8:LEU:CD2	5:W:11:ILE:HD11	1.98	0.93
6:2:21:PHE:HE1	15:2:102:CRT:C17	1.81	0.93
5:9:51:ILE:HB	5:9:52:PRO:HA	1.47	0.93
3:M:70:ILE:HG21	3:M:118:ALA:HB1	1.51	0.93
9:K:102:BCL:C1D	9:N:101:BCL:HMD2	1.98	0.93
15:V:102:CRT:H401	5:W:36:HIS:HB3	1.51	0.93
5:Y:36:HIS:CE1	9:Z:101:BCL:HMD1	2.03	0.93
5:3:51:ILE:HB	5:3:52:PRO:CA	1.99	0.93
9:4:101:BCL:H43	15:4:102:CRT:H241	1.51	0.93
3:M:70:ILE:HD11	3:M:114:TRP:HE3	1.30	0.93
5:D:31:LEU:O	5:D:35:ILE:HG12	1.69	0.93
6:R:21:PHE:HD2	15:R:102:CRT:H16	1.33	0.93
5:W:8:LEU:HD22	6:X:18:HIS:HE1	1.33	0.93
5:9:2:PHE:HA	5:9:5:ASN:HD22	1.32	0.93
1:C:308:MET:HE1	1:C:312:GLN:HA	1.49	0.92
5:S:36:HIS:CE1	9:T:101:BCL:HMD1	2.04	0.92
5:9:16:ASP:CG	5:9:17:PRO:CD	2.37	0.92
4:H:11:ALA:O	4:H:14:ILE:HG22	1.69	0.92
15:B:102:CRT:H2M3	5:D:36:HIS:CB	1.98	0.92
5:Q:5:ASN:HD22	6:R:22:MET:HG2	1.32	0.92
15:V:102:CRT:H392	5:W:36:HIS:CG	2.05	0.92
4:H:48:ARG:NH2	17:H:301:PEF:O1P	2.02	0.92
5:1:44:LEU:HD13	6:2:43:ARG:HD2	1.49	0.92
6:4:25:MET:HB2	15:4:102:CRT:H16	0.92	0.92
3:M:2:PRO:HG3	3:M:42:LYS:CE	1.99	0.92
3:M:70:ILE:HG21	3:M:118:ALA:HB2	0.94	0.92
5:A:24:ILE:HG21	15:B:102:CRT:H243	1.49	0.92
5:5:13:LEU:HD12	15:8:101:CRT:H22A	1.51	0.92
4:H:45:ARG:HH11	4:H:97:GLY:H	0.92	0.92
15:W:103:CRT:C8	6:Z:20:ILE:HD13	2.00	0.92
6:4:30:GLY:O	6:4:33:VAL:HG12	1.70	0.92
5:Y:56:GLN:HG3	5:Y:57:ALA:H	1.34	0.92
1:C:308:MET:CE	1:C:312:GLN:HA	1.99	0.92
5:A:60:LYS:CA	5:9:50:ASN:HB3	2.00	0.91
1:C:250:CYS:O	1:C:263:THR:HG23	1.70	0.91
5:9:36:HIS:CE1	9:0:101:BCL:HMD1	2.05	0.91
5:A:34:LEU:O	5:A:38:ILE:HG23	1.70	0.91
15:A:103:CRT:H23	6:E:16:GLU:HG3	1.53	0.91
5:W:8:LEU:CD1	6:X:22:MET:HE1	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:32:GLY:CA	9:B:101:BCL:HED2	2.01	0.91
9:F:102:BCL:C1D	9:G:101:BCL:HMD2	2.00	0.91
6:X:46:LEU:HD22	6:Z:42:TYR:HE2	1.36	0.91
2:L:186:ILE:HD12	9:M:401:BCL:OBD	1.69	0.91
6:P:17:PHE:HE1	15:P:102:CRT:H9	1.33	0.91
5:W:7:ASN:HD22	5:W:7:ASN:H	1.14	0.90
15:P:102:CRT:H2M3	5:Q:36:HIS:HB2	0.92	0.90
4:H:138:VAL:O	4:H:140:LYS:CD	2.19	0.90
5:A:50:ASN:HA	5:D:60:LYS:CA	2.01	0.90
5:Y:45:ASN:HB3	5:Y:48:ASP:O	1.71	0.90
5:A:29:ILE:HG12	5:9:27:PHE:HE2	1.37	0.90
6:R:16:GLU:HB2	15:R:102:CRT:H31A	1.54	0.90
5:U:36:HIS:CE1	9:V:101:BCL:HMD1	2.05	0.90
6:N:46:LEU:HD22	6:P:42:TYR:OH	1.71	0.90
5:W:36:HIS:CE1	9:X:101:BCL:HMD1	2.05	0.90
6:2:17:PHE:CE1	15:2:102:CRT:H9	2.03	0.90
15:R:102:CRT:H342	9:S:102:BCL:HAA1	1.53	0.90
15:J:101:CRT:H342	9:K:102:BCL:HAA1	1.54	0.90
5:A:29:ILE:HD11	5:A:33:LEU:HD11	1.53	0.90
5:O:3:THR:HB	5:O:4:MET:SD	2.11	0.90
5:A:29:ILE:HG12	5:9:27:PHE:CE2	2.06	0.89
5:5:10:LYS:HE3	15:8:101:CRT:C3	2.01	0.89
4:H:48:ARG:HH21	4:H:48:ARG:HG2	1.37	0.89
5:Q:45:ASN:HB2	5:Q:49:ASP:HB3	1.53	0.89
6:4:21:PHE:HA	15:4:102:CRT:H11	0.94	0.89
5:5:40:LEU:HD11	5:5:47:LEU:HB2	1.53	0.89
9:7:103:BCL:HMC3	9:9:102:BCL:HBB1	1.52	0.89
9:G:101:BCL:HMB3	9:I:102:BCL:CHB	2.02	0.89
6:Z:45:TRP:CE3	9:Z:101:BCL:HBC2	2.08	0.89
5:5:10:LYS:CD	15:8:101:CRT:C3	2.50	0.89
9:B:101:BCL:C1B	9:D:102:BCL:HMB3	2.02	0.89
6:V:21:PHE:HB2	15:V:102:CRT:H14	1.37	0.89
15:X:102:CRT:C34	9:Y:102:BCL:H3A	2.03	0.89
4:H:29:TYR:CE2	16:H:302:PGW:C1	2.56	0.89
4:H:47:GLU:CG	5:A:19:ARG:HA	2.02	0.89
5:5:10:LYS:CD	15:8:101:CRT:H31A	2.02	0.89
9:W:102:BCL:CHD	9:X:101:BCL:HMD2	2.03	0.89
3:M:117:MET:HE3	5:Q:34:LEU:HD12	1.52	0.89
5:U:13:LEU:O	6:V:7:THR:HA	1.72	0.89
9:W:102:BCL:CBC	9:X:101:BCL:HHD	2.02	0.89
3:M:31:ILE:CD1	16:M:407:PGW:H04	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:101:BCL:HMB3	9:O:102:BCL:CHB	2.03	0.88
6:T:10:THR:HG22	6:T:11:ASP:H	1.38	0.88
6:Z:45:TRP:HE3	9:Z:101:BCL:HBC2	1.36	0.88
6:2:45:TRP:CE3	9:2:101:BCL:HBC2	2.08	0.88
2:L:84:LEU:HD23	2:L:151:TRP:CD1	2.07	0.88
5:7:43:ASP:HA	5:9:48:ASP:HB3	1.56	0.88
2:L:233:ILE:HG12	2:L:237:ALA:HB1	1.53	0.88
5:O:4:MET:SD	5:O:4:MET:N	2.47	0.88
5:5:10:LYS:CE	15:8:101:CRT:H32A	2.03	0.88
2:L:89:LEU:HD11	2:L:94:LEU:HD23	1.53	0.88
9:F:102:BCL:CBC	9:G:101:BCL:HHD	2.03	0.88
5:Y:18:ARG:HD2	5:Y:19:ARG:N	1.87	0.88
6:2:21:PHE:HA	15:2:102:CRT:H133	1.54	0.88
5:5:9:TYR:CE2	5:5:10:LYS:HE2	2.09	0.88
4:H:153:GLY:H	4:H:167:VAL:HG23	1.39	0.88
6:V:21:PHE:CB	15:V:102:CRT:C11	2.50	0.88
15:N:102:CRT:C40	9:O:102:BCL:HMB2	2.04	0.88
4:H:54:LYS:HE2	4:H:58:PHE:CD1	2.09	0.87
5:O:4:MET:CG	6:R:23:GLN:HB3	2.04	0.87
6:T:17:PHE:HE1	15:T:102:CRT:H9	1.09	0.87
5:U:27:PHE:HE2	5:W:29:ILE:HD11	1.10	0.87
1:C:195:LEU:HB3	1:C:196:PRO:CD	2.04	0.87
2:L:220:HIS:HB3	3:M:140:LEU:HD21	1.56	0.87
5:F:36:HIS:NE2	9:G:101:BCL:HMD1	1.88	0.87
5:Q:27:PHE:CE2	5:S:29:ILE:CD1	2.50	0.87
5:S:43:ASP:CB	5:U:56:GLN:HG3	2.04	0.87
1:C:71:LYS:H	1:C:71:LYS:HE3	1.38	0.87
5:A:36:HIS:CD2	9:B:101:BCL:HMD1	2.09	0.87
6:T:18:HIS:O	6:T:22:MET:HG2	1.73	0.87
5:U:16:ASP:HB2	5:U:19:ARG:HH21	1.39	0.87
5:7:12:TRP:CZ3	6:8:17:PHE:CD2	2.61	0.87
15:4:102:CRT:H291	9:5:102:BCL:HBA2	1.56	0.87
4:H:53:VAL:CG1	5:D:22:VAL:CG2	2.52	0.87
6:Z:45:TRP:CE3	9:Z:101:BCL:H2C	2.10	0.87
6:P:13:GLU:O	15:P:102:CRT:H32A	1.75	0.87
15:W:103:CRT:H83	6:Z:20:ILE:CD1	2.04	0.87
1:C:95:VAL:O	1:C:98:THR:HG22	1.75	0.87
3:M:37:SER:OG	3:M:40:LEU:HB3	1.74	0.87
6:2:20:ILE:CG2	15:2:102:CRT:C8	2.47	0.87
9:L:301:BCL:CBB	9:M:401:BCL:HMD2	2.04	0.86
3:M:158:LEU:HD22	3:M:162:PHE:HD2	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:9:LEU:HB3	6:0:13:GLU:CG	2.05	0.86
3:M:258:PHE:CE2	17:H:301:PEF:C31	2.59	0.86
15:G:102:CRT:H2M3	5:I:36:HIS:CB	2.05	0.86
5:K:43:ASP:OD1	5:O:47:LEU:HB3	1.75	0.86
5:7:12:TRP:CZ3	6:8:17:PHE:HD2	1.94	0.86
6:0:9:LEU:CB	6:0:13:GLU:HG3	2.04	0.86
6:G:21:PHE:CD1	6:G:21:PHE:C	2.45	0.86
9:T:101:BCL:CMA	9:U:102:BCL:HMA1	2.05	0.86
5:5:13:LEU:HD12	15:8:101:CRT:C2	2.05	0.86
5:7:12:TRP:CH2	6:8:17:PHE:CE2	2.63	0.86
5:I:10:LYS:HG3	15:N:102:CRT:H1M1	1.56	0.86
6:V:17:PHE:HD1	15:V:102:CRT:H9	1.40	0.86
15:W:103:CRT:C18	6:Z:25:MET:HA	2.06	0.86
5:7:33:LEU:HD12	5:7:33:LEU:H	1.39	0.86
1:C:175:PRO:HD2	1:C:179:LYS:HB3	1.56	0.86
6:B:23:GLN:HG3	5:9:4:MET:HE1	1.54	0.86
15:P:102:CRT:H342	9:Q:102:BCL:HAA1	0.91	0.86
5:1:50:ASN:HD22	5:1:51:ILE:HG12	1.40	0.86
6:2:17:PHE:HE1	15:2:102:CRT:H9	1.33	0.86
5:5:10:LYS:HB2	15:8:101:CRT:H83	1.57	0.86
2:L:115:GLU:HA	2:L:118:ARG:HB2	1.57	0.86
15:A:103:CRT:C2	6:E:16:GLU:HG3	2.06	0.86
5:K:36:HIS:CE1	9:N:101:BCL:HMD1	2.10	0.86
9:6:101:BCL:CHB	9:7:102:BCL:HMB3	2.06	0.86
5:7:12:TRP:HZ3	5:7:17:PRO:HB3	1.39	0.86
9:I:102:BCL:CHD	9:I:103:BCL:HMD2	2.06	0.85
2:L:11:ARG:HH12	4:H:45:ARG:CD	1.89	0.85
6:4:31:LEU:O	6:4:34:ILE:HG22	1.76	0.85
5:A:55:TYR:HA	5:A:59:GLY:H	1.40	0.85
5:W:8:LEU:HD21	5:W:11:ILE:CD1	2.05	0.85
5:Y:29:ILE:HA	9:Y:102:BCL:H11	1.56	0.85
1:C:173:LYS:O	1:C:175:PRO:HD3	1.77	0.85
2:L:219:GLU:HG3	4:H:127:PHE:HB2	1.58	0.85
5:A:36:HIS:CE1	9:A:102:BCL:NA	2.45	0.85
6:X:44:PRO:O	5:Y:52:PRO:HG2	1.77	0.85
6:6:44:PRO:HG2	5:7:52:PRO:HG2	1.58	0.85
1:C:24:GLU:CD	1:C:45:ASN:HD22	1.80	0.85
2:L:252:TRP:HE1	11:L:304:UQ8:H30B	1.40	0.85
3:M:158:LEU:HD22	3:M:162:PHE:CD2	2.12	0.85
5:D:48:ASP:HB2	5:D:56:GLN:HE22	1.42	0.85
5:S:44:LEU:HD11	9:T:101:BCL:HBC2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:46:TRP:CZ3	9:U:102:BCL:HBC3	2.11	0.85
6:2:45:TRP:O	6:2:46:LEU:HG	1.76	0.85
2:L:159:ILE:H	2:L:159:ILE:HD12	1.40	0.85
5:K:24:ILE:CD1	15:N:102:CRT:H21	2.02	0.85
15:R:102:CRT:H2M3	5:S:36:HIS:HB2	1.57	0.85
5:U:13:LEU:HG	15:X:102:CRT:H21A	1.57	0.85
3:M:25:LYS:HE3	6:P:8:GLY:HA3	1.59	0.84
4:H:5:ILE:HD12	5:D:41:SER:OG	1.77	0.84
6:J:10:THR:HB	6:J:13:GLU:OE2	1.76	0.84
6:0:10:THR:HG22	6:0:11:ASP:H	1.40	0.84
15:G:102:CRT:H342	9:I:102:BCL:HAA1	1.59	0.84
6:P:21:PHE:CZ	15:P:102:CRT:H16	2.11	0.84
5:A:14:ILE:HG13	5:A:15:LEU:HD22	1.59	0.84
5:1:43:ASP:HB2	5:3:47:LEU:CD1	2.08	0.84
2:L:4:LEU:N	3:M:253:ARG:HH12	1.74	0.84
5:F:44:LEU:HD12	5:F:44:LEU:O	1.76	0.84
5:U:10:LYS:HB3	15:X:102:CRT:H6	1.58	0.84
5:5:10:LYS:HD2	15:8:101:CRT:C1	2.08	0.84
1:C:196:PRO:O	1:C:197:PHE:CG	2.31	0.84
9:B:101:BCL:HMB3	9:D:102:BCL:CHB	2.07	0.84
6:P:17:PHE:HE1	15:P:102:CRT:C9	1.87	0.84
5:1:14:ILE:HD12	5:1:15:LEU:N	1.93	0.84
6:4:44:PRO:O	5:5:52:PRO:HG2	1.78	0.84
5:9:4:MET:O	5:9:8:LEU:HG	1.76	0.84
3:M:117:MET:HE3	5:Q:34:LEU:CD1	2.07	0.84
6:2:21:PHE:HD1	15:2:102:CRT:C15	1.86	0.84
4:H:45:ARG:NH1	4:H:97:GLY:N	2.26	0.84
4:H:48:ARG:NH1	4:H:53:VAL:O	2.10	0.84
6:2:41:LEU:HD23	6:2:42:TYR:N	1.91	0.84
2:L:252:TRP:HA	2:L:252:TRP:CE3	2.12	0.84
5:Q:42:THR:HG23	5:Q:43:ASP:N	1.91	0.84
3:M:70:ILE:CD1	3:M:114:TRP:HE3	1.88	0.84
9:M:401:BCL:H122	10:M:403:BPH:CMA	2.08	0.84
5:9:26:ALA:O	5:9:29:ILE:HG22	1.78	0.83
5:K:51:ILE:HB	5:K:52:PRO:HA	1.59	0.83
3:M:31:ILE:CD1	16:M:407:PGW:C04	2.56	0.83
15:A:101:CRT:H342	9:A:102:BCL:CGA	2.07	0.83
6:N:17:PHE:CE1	15:N:102:CRT:C9	2.61	0.83
5:1:40:LEU:HD12	5:1:45:ASN:HA	1.57	0.83
1:C:195:LEU:HB3	1:C:196:PRO:HD2	1.58	0.83
5:A:33:LEU:CB	15:A:101:CRT:H392	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:21:PHE:CE1	15:P:102:CRT:C16	2.61	0.83
5:W:26:ALA:HA	5:W:29:ILE:CG2	2.08	0.83
5:W:42:THR:HB	5:Y:48:ASP:HB2	1.60	0.83
5:1:49:ASP:CG	5:1:50:ASN:H	1.82	0.83
5:Y:27:PHE:HE2	5:1:29:ILE:CD1	1.92	0.83
3:M:31:ILE:HD11	16:M:407:PGW:CAD	2.08	0.83
15:V:102:CRT:H392	5:W:36:HIS:HB2	1.60	0.83
5:7:13:LEU:O	6:8:7:THR:N	2.11	0.83
9:B:101:BCL:CHB	9:D:102:BCL:HMB3	2.09	0.83
2:L:72:ARG:HG2	3:M:305:PRO:HA	1.60	0.83
5:F:49:ASP:HB2	5:I:56:GLN:HB3	1.59	0.83
6:N:30:GLY:O	6:N:34:ILE:HG22	1.79	0.83
6:P:38:LEU:O	6:P:41:LEU:CD2	2.22	0.83
15:J:101:CRT:H2M3	5:K:36:HIS:CB	2.08	0.83
5:3:26:ALA:O	5:3:29:ILE:CG2	2.22	0.83
5:W:9:TYR:HA	6:X:18:HIS:CG	2.12	0.82
9:9:102:BCL:C1D	9:0:101:BCL:HMD2	2.09	0.82
6:N:17:PHE:HE1	15:N:102:CRT:C9	1.90	0.82
5:Y:49:ASP:O	5:1:56:GLN:NE2	2.11	0.82
6:2:21:PHE:CE1	15:2:102:CRT:C15	2.60	0.82
5:3:29:ILE:CG2	5:3:30:VAL:H	1.91	0.82
5:A:32:GLY:O	5:A:36:HIS:HB2	1.79	0.82
5:U:12:TRP:HE1	6:V:18:HIS:HA	1.42	0.82
5:9:8:LEU:HD22	5:9:11:ILE:HD11	1.61	0.82
2:L:3:MET:HB3	2:L:7:GLU:HB3	1.61	0.82
6:P:10:THR:HG22	6:P:11:ASP:H	1.41	0.82
5:3:35:ILE:HD11	15:4:102:CRT:H372	1.61	0.82
6:6:44:PRO:CG	5:7:52:PRO:HG2	2.10	0.82
5:7:35:ILE:CD1	9:7:103:BCL:O1D	2.27	0.82
3:M:117:MET:CE	5:Q:34:LEU:CD1	2.57	0.82
15:J:101:CRT:H2M3	5:K:36:HIS:HB3	1.61	0.82
4:H:32:ARG:NH1	4:H:60:ASP:O	2.12	0.82
6:8:17:PHE:CZ	15:8:101:CRT:C9	2.57	0.82
5:Q:51:ILE:HG22	5:Q:52:PRO:HA	1.62	0.82
5:U:27:PHE:HE2	5:W:29:ILE:CG1	1.92	0.82
6:8:17:PHE:CD1	6:8:20:ILE:HG21	2.15	0.82
3:M:218:MET:HB3	3:M:252:TRP:CZ2	2.15	0.82
6:N:30:GLY:O	6:N:33:VAL:HG12	1.79	0.82
9:O:102:BCL:HAC2	9:P:101:BCL:CBC	2.10	0.82
9:E:101:BCL:C1B	9:F:102:BCL:HMB3	2.10	0.82
5:S:29:ILE:HG23	5:S:30:VAL:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:102:CRT:C40	5:W:36:HIS:HB3	2.10	0.82
6:X:45:TRP:O	6:X:46:LEU:HG	1.79	0.82
1:C:225:SER:H	1:C:228:GLN:NE2	1.78	0.81
6:N:29:PHE:O	6:N:33:VAL:HB	1.79	0.81
5:Y:51:ILE:HG22	5:1:60:LYS:N	1.95	0.81
2:L:144:ARG:HB3	2:L:145:PRO:HD3	1.62	0.81
5:A:9:TYR:HB2	6:B:18:HIS:CD2	2.14	0.81
5:A:33:LEU:HA	15:A:101:CRT:H403	1.61	0.81
5:I:43:ASP:HB2	5:K:47:LEU:HB3	1.60	0.81
15:N:102:CRT:H392	9:O:102:BCL:C1B	2.10	0.81
5:W:8:LEU:HD21	5:W:11:ILE:HD11	1.62	0.81
1:C:255:ALA:HB1	1:C:258:ASP:HB3	1.59	0.81
1:C:295:ARG:HH11	1:C:295:ARG:HG3	1.43	0.81
5:A:43:ASP:HA	5:D:48:ASP:HB3	1.60	0.81
5:I:13:LEU:HD12	15:N:102:CRT:O1	1.80	0.81
6:P:21:PHE:CE2	15:P:102:CRT:H19	2.15	0.81
5:Y:42:THR:HB	5:1:48:ASP:CG	2.01	0.81
6:2:21:PHE:CD1	15:2:102:CRT:C14	2.63	0.81
5:3:35:ILE:HA	5:3:38:ILE:HG22	1.61	0.81
5:7:16:ASP:O	5:7:20:VAL:HG22	1.80	0.81
6:E:30:GLY:O	6:E:33:VAL:HG12	1.81	0.81
5:1:10:LYS:HB3	15:4:102:CRT:H5	1.62	0.81
5:5:50:ASN:HB2	5:7:59:GLY:HA3	1.60	0.81
6:6:40:TRP:CZ3	6:6:44:PRO:HA	2.15	0.81
4:H:179:ILE:HG22	4:H:197:ILE:HD11	1.61	0.81
1:C:327:TYR:HB2	1:C:330:LEU:HD12	1.62	0.81
6:G:27:ALA:O	6:G:31:LEU:CG	2.27	0.81
6:R:46:LEU:HB3	6:T:42:TYR:OH	1.80	0.81
5:7:12:TRP:CZ3	5:7:17:PRO:HB3	2.16	0.81
15:8:101:CRT:H372	9:9:102:BCL:HMB2	1.62	0.81
1:C:24:GLU:CG	1:C:45:ASN:HD22	1.94	0.81
3:M:197:TYR:CZ	9:M:402:BCL:HMC2	2.16	0.81
6:G:40:TRP:HB2	9:G:101:BCL:H191	1.61	0.81
5:S:50:ASN:CG	5:S:51:ILE:H	1.84	0.81
6:Z:45:TRP:O	6:Z:46:LEU:HG	1.81	0.81
9:Z:101:BCL:CHB	9:1:102:BCL:HMB3	2.10	0.81
1:C:157:ARG:HH12	1:C:318:LEU:HD21	1.46	0.81
4:H:45:ARG:HH11	4:H:97:GLY:N	1.77	0.81
5:Q:55:TYR:O	5:Q:59:GLY:HA3	1.80	0.81
6:E:23:GLN:HG3	6:E:24:SER:H	1.46	0.81
6:N:28:TRP:CE3	6:N:31:LEU:HD12	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:101:CRT:H342	9:9:102:BCL:HAA1	1.63	0.81
3:M:175:VAL:HB	15:M:406:CRT:H242	1.63	0.81
4:H:6:THR:HB	5:F:41:SER:HB3	1.63	0.81
4:H:11:ALA:HA	4:H:14:ILE:HG22	1.61	0.81
5:A:29:ILE:CD1	5:A:33:LEU:HD11	2.09	0.81
9:N:101:BCL:CMA	15:N:102:CRT:H35	2.11	0.81
15:P:102:CRT:H391	5:Q:36:HIS:CB	2.11	0.81
5:Y:56:GLN:HG3	5:Y:57:ALA:N	1.95	0.81
6:0:7:THR:HG23	6:0:8:GLY:H	1.46	0.81
5:A:42:THR:HG22	5:D:48:ASP:OD2	1.80	0.80
5:W:10:LYS:HD3	15:W:103:CRT:C1M	2.10	0.80
5:Y:31:LEU:O	5:Y:35:ILE:HG12	1.80	0.80
5:7:50:ASN:CG	5:7:51:ILE:H	1.81	0.80
1:C:126:VAL:HG12	1:C:287:LEU:HD13	1.62	0.80
9:D:102:BCL:HBA1	9:D:102:BCL:CBD	2.11	0.80
5:I:9:TYR:HA	6:J:18:HIS:ND1	1.96	0.80
6:P:46:LEU:HD22	6:R:42:TYR:OH	1.81	0.80
5:1:16:ASP:HB2	5:1:19:ARG:HD3	1.64	0.80
9:M:401:BCL:HBC1	9:M:402:BCL:HAA2	1.62	0.80
15:X:102:CRT:H31	9:Y:102:BCL:HBA2	1.63	0.80
5:Y:27:PHE:CE2	5:1:29:ILE:HD11	2.16	0.80
6:4:25:MET:CB	15:4:102:CRT:H19	2.12	0.80
5:Q:50:ASN:HD22	5:Q:51:ILE:HG13	1.44	0.80
6:G:28:TRP:NE1	6:G:32:VAL:CG2	2.44	0.80
5:Y:18:ARG:HD2	5:Y:19:ARG:H	1.43	0.80
9:5:102:BCL:C1D	9:6:101:BCL:HMD2	2.12	0.80
9:V:101:BCL:HMA1	9:W:102:BCL:HMA1	1.62	0.80
5:3:16:ASP:HB2	5:3:19:ARG:HB3	1.63	0.80
2:L:10:TYR:HE1	3:M:247:ARG:HE	1.29	0.80
5:K:49:ASP:CG	5:K:50:ASN:H	1.83	0.80
6:4:24:SER:HB2	15:4:102:CRT:C12	2.12	0.80
5:5:16:ASP:HB2	5:5:19:ARG:HG2	1.64	0.80
5:A:21:LEU:HD11	15:B:102:CRT:H14	1.62	0.80
5:W:51:ILE:HB	5:W:52:PRO:HA	1.64	0.80
5:1:10:LYS:HB2	6:4:20:ILE:HD13	1.62	0.80
9:L:303:BCL:OBD	3:M:206:ILE:HD12	1.82	0.80
1:C:251:HIS:ND1	1:C:251:HIS:N	2.28	0.79
5:U:42:THR:HB	5:W:48:ASP:HB3	1.63	0.79
9:3:102:BCL:CHD	9:4:101:BCL:HMD2	2.12	0.79
6:8:17:PHE:HZ	15:8:101:CRT:H9	1.47	0.79
1:C:327:TYR:CB	1:C:330:LEU:HD12	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9:36:HIS:NE2	9:0:101:BCL:HMD1	1.97	0.79
5:A:11:ILE:HD13	15:A:103:CRT:C10	2.12	0.79
6:E:10:THR:HG22	6:E:11:ASP:H	1.47	0.79
5:A:29:ILE:HG13	5:A:33:LEU:HD13	1.63	0.79
9:E:101:BCL:HMB3	9:F:102:BCL:CHB	2.13	0.79
6:4:10:THR:HG22	6:4:11:ASP:H	1.46	0.79
5:9:44:LEU:O	5:9:44:LEU:HD22	1.82	0.79
2:L:52:TRP:HA	5:A:37:MET:HE2	1.64	0.79
9:A:102:BCL:HMD1	6:B:36:HIS:CE1	2.17	0.79
5:D:48:ASP:CB	5:D:56:GLN:HE22	1.95	0.79
15:N:102:CRT:H372	9:O:102:BCL:HMB2	1.64	0.79
15:X:102:CRT:C2M	5:Y:36:HIS:HB3	2.13	0.79
5:5:9:TYR:HE2	5:5:10:LYS:HE2	1.45	0.79
18:L:401:HOH:O	5:A:42:THR:HG23	1.81	0.79
3:M:27:ASN:ND2	5:O:19:ARG:HE	1.81	0.79
6:G:33:VAL:O	6:G:37:LEU:HB2	1.81	0.79
5:Q:16:ASP:H	5:Q:19:ARG:HH21	1.30	0.79
5:U:27:PHE:CE2	5:W:29:ILE:CG1	2.66	0.79
1:C:173:LYS:CG	3:M:80:HIS:ND1	2.44	0.79
5:I:50:ASN:HB2	5:K:59:GLY:CA	2.13	0.79
5:S:43:ASP:HB3	5:U:56:GLN:HG3	1.64	0.79
5:5:5:ASN:HB3	6:6:22:MET:HE3	1.63	0.79
5:7:36:HIS:NE2	9:7:103:BCL:HMD1	1.97	0.79
3:M:37:SER:OG	3:M:40:LEU:CB	2.30	0.79
5:I:50:ASN:CB	5:K:59:GLY:CA	2.56	0.79
5:W:27:PHE:CE2	5:Y:29:ILE:HD12	2.16	0.79
1:C:280:ASN:OD1	1:C:304:ARG:HB3	1.82	0.79
3:M:105:ARG:HA	5:O:42:THR:CG2	2.13	0.79
3:M:260:VAL:HB	4:H:34:ASP:OD1	1.83	0.79
6:J:27:ALA:O	6:J:31:LEU:HG	1.82	0.79
5:W:51:ILE:HB	5:W:52:PRO:CA	2.13	0.79
5:7:31:LEU:O	5:7:35:ILE:HG13	1.81	0.79
1:C:200:LEU:HG	1:C:204:LEU:HD12	1.65	0.78
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.48	0.78
6:P:21:PHE:CE1	15:P:102:CRT:H16	2.18	0.78
6:T:17:PHE:CE1	15:T:102:CRT:C9	2.59	0.78
5:I:30:VAL:HG13	5:I:31:LEU:H	1.48	0.78
9:A:102:BCL:CHD	9:B:101:BCL:HMD2	2.14	0.78
5:O:46:TRP:HD1	5:O:47:LEU:HD13	1.47	0.78
5:Q:29:ILE:HG23	5:Q:30:VAL:N	1.98	0.78
1:C:183:GLN:O	1:C:183:GLN:HG2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:49:ASP:CG	5:F:50:ASN:H	1.86	0.78
5:K:18:ARG:HD2	5:K:19:ARG:H	1.47	0.78
6:2:16:GLU:HB2	15:2:102:CRT:H1M1	1.64	0.78
9:5:102:BCL:CHD	9:6:101:BCL:HMD2	2.14	0.78
9:A:102:BCL:HMB3	9:0:101:BCL:CHB	2.13	0.78
9:O:102:BCL:HBC2	9:P:101:BCL:HHD	1.66	0.78
6:4:22:MET:O	6:4:26:TYR:HB2	1.84	0.78
5:A:36:HIS:HE1	9:A:102:BCL:C1A	1.97	0.78
6:J:16:GLU:OE2	15:J:101:CRT:H23	1.84	0.78
6:P:34:ILE:HD13	6:P:35:ALA:N	1.98	0.78
6:R:10:THR:HG22	6:R:11:ASP:H	1.47	0.78
6:R:18:HIS:O	6:R:22:MET:HB2	1.84	0.78
5:5:44:LEU:HD12	5:5:44:LEU:O	1.84	0.78
15:A:103:CRT:H32	5:D:31:LEU:HD21	1.65	0.78
6:E:13:GLU:N	6:E:13:GLU:OE1	2.17	0.78
9:O:102:BCL:HAC2	9:P:101:BCL:HBC1	1.66	0.78
9:T:101:BCL:HMA1	9:U:102:BCL:CMA	2.12	0.78
5:U:29:ILE:HG23	5:U:30:VAL:N	1.98	0.78
5:W:26:ALA:CA	5:W:29:ILE:HG22	2.13	0.78
15:M:406:CRT:H402	5:O:38:ILE:CG2	2.11	0.78
4:H:140:LYS:HD3	4:H:140:LYS:N	1.99	0.78
5:O:55:TYR:HD1	5:O:56:GLN:N	1.82	0.78
6:8:21:PHE:CD1	15:8:101:CRT:C16	2.61	0.78
5:1:50:ASN:HA	5:3:60:LYS:HA	1.65	0.78
1:C:285:TRP:NE1	1:C:304:ARG:HD3	1.99	0.78
15:W:103:CRT:H183	6:Z:25:MET:HA	1.66	0.78
5:Y:16:ASP:HB3	5:Y:18:ARG:HE	1.47	0.78
6:6:40:TRP:HZ3	6:6:44:PRO:HA	1.48	0.78
4:H:5:ILE:HD13	5:D:42:THR:HG23	1.65	0.77
5:A:36:HIS:CB	15:A:101:CRT:H402	2.06	0.77
5:I:17:PRO:O	5:I:21:LEU:HB2	1.83	0.77
6:P:46:LEU:N	5:Q:52:PRO:HD3	1.99	0.77
5:Q:40:LEU:HD12	5:Q:45:ASN:HA	1.65	0.77
5:9:50:ASN:HD22	5:9:51:ILE:HG12	1.49	0.77
3:M:70:ILE:HD11	3:M:114:TRP:CE3	2.16	0.77
9:F:102:BCL:HBC2	9:F:102:BCL:HHD	1.65	0.77
6:J:16:GLU:CD	15:J:101:CRT:H23	2.04	0.77
9:O:102:BCL:C1D	9:P:101:BCL:HMD2	2.14	0.77
15:P:102:CRT:H2M1	5:Q:33:LEU:O	1.84	0.77
5:1:10:LYS:HB3	15:4:102:CRT:C5	2.13	0.77
5:5:10:LYS:CE	15:8:101:CRT:C3	2.60	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:16:ASP:HB2	5:5:19:ARG:CG	2.14	0.77
2:L:179:ASN:HB3	2:L:182:HIS:HB3	1.67	0.77
5:F:11:ILE:HD12	5:F:14:ILE:HD11	1.66	0.77
5:5:5:ASN:HA	5:5:8:LEU:HD12	1.66	0.77
3:M:159:VAL:HA	3:M:163:ILE:HG22	1.66	0.77
4:H:124:ASP:HB2	4:H:233:LEU:HD21	1.65	0.77
6:G:30:GLY:O	6:G:33:VAL:HG12	1.84	0.77
5:O:43:ASP:HA	5:Q:48:ASP:HB3	1.67	0.77
5:A:36:HIS:CD2	9:B:101:BCL:CMD	2.68	0.77
6:P:27:ALA:O	6:P:31:LEU:HG	1.84	0.77
5:W:33:LEU:HD12	5:W:34:LEU:N	2.00	0.77
6:X:46:LEU:HD22	6:Z:42:TYR:CE2	2.20	0.77
5:7:4:MET:O	5:7:8:LEU:HB2	1.84	0.77
4:H:179:ILE:O	4:H:197:ILE:HG13	1.85	0.77
6:E:45:TRP:O	6:E:46:LEU:HG	1.84	0.77
6:T:45:TRP:CE3	9:T:101:BCL:H2C	2.20	0.77
9:6:101:BCL:C1B	9:7:102:BCL:HMB3	2.15	0.77
5:7:12:TRP:CH2	6:8:17:PHE:HE2	2.01	0.77
5:A:32:GLY:HA2	9:B:101:BCL:HED2	1.67	0.77
5:1:51:ILE:HB	5:1:52:PRO:HA	1.66	0.77
5:1:51:ILE:HB	5:1:52:PRO:CA	2.15	0.77
5:5:2:PHE:HB2	5:5:5:ASN:HD22	1.49	0.77
1:C:71:LYS:HE3	1:C:71:LYS:N	2.00	0.77
9:A:102:BCL:HMB3	9:0:101:BCL:C1B	2.15	0.77
9:D:102:BCL:C1D	9:E:101:BCL:HMD2	2.15	0.77
6:V:17:PHE:CD1	15:V:102:CRT:H9	2.19	0.77
6:V:20:ILE:CG2	15:V:102:CRT:C9	2.63	0.77
6:Z:38:LEU:O	6:Z:38:LEU:HD23	1.85	0.77
5:5:9:TYR:CE2	5:5:10:LYS:CE	2.68	0.77
5:5:50:ASN:ND2	5:5:51:ILE:HG13	2.00	0.77
1:C:225:SER:HB3	1:C:228:GLN:HE21	1.48	0.77
6:B:16:GLU:CD	15:B:102:CRT:H23	2.06	0.77
5:F:8:LEU:HD23	6:J:20:ILE:HD11	1.66	0.77
15:R:102:CRT:C34	9:S:102:BCL:HAA1	2.15	0.77
1:C:245:VAL:HG21	1:C:249:PHE:HD2	1.50	0.77
3:M:59:LEU:HD13	5:Q:29:ILE:HG21	1.68	0.77
5:S:44:LEU:CD1	9:T:101:BCL:HBC2	2.15	0.76
5:W:46:TRP:CH2	9:W:102:BCL:HAC1	2.20	0.76
6:Z:24:SER:O	6:Z:27:ALA:HB3	1.85	0.76
4:H:257:PRO:HG3	5:7:19:ARG:NH2	2.01	0.76
5:A:50:ASN:HA	5:D:60:LYS:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:21:PHE:HB2	15:G:102:CRT:H11	1.66	0.76
5:U:2:PHE:CA	5:U:5:ASN:HD22	1.98	0.76
9:7:103:BCL:HMA1	9:9:102:BCL:HMA1	1.67	0.76
5:A:29:ILE:HG13	5:A:33:LEU:CD1	2.15	0.76
5:O:12:TRP:HE1	6:P:18:HIS:HD1	1.30	0.76
5:S:50:ASN:HD21	6:T:43:ARG:HH22	1.30	0.76
6:T:17:PHE:CD1	15:T:102:CRT:H9	2.21	0.76
6:V:20:ILE:HD12	15:V:102:CRT:C10	2.15	0.76
5:1:13:LEU:CB	15:4:102:CRT:H1M1	2.11	0.76
2:L:36:GLY:HA2	2:L:112:ARG:HD2	1.67	0.76
2:L:182:HIS:CE1	2:L:186:ILE:HD11	2.21	0.76
15:A:103:CRT:H372	9:F:102:BCL:HMB2	1.66	0.76
6:R:30:GLY:O	6:R:33:VAL:HG12	1.86	0.76
2:L:4:LEU:HD22	4:H:38:GLY:CA	2.16	0.76
4:H:6:THR:O	5:F:41:SER:CA	2.33	0.76
5:K:18:ARG:HD2	5:K:19:ARG:N	2.00	0.76
5:W:5:ASN:OD1	5:W:8:LEU:HD12	1.84	0.76
2:L:23:PHE:HE1	5:9:22:VAL:HG21	1.50	0.76
3:M:79:VAL:HG23	3:M:85:GLN:HB3	1.67	0.76
4:H:257:PRO:HG3	5:7:19:ARG:HH22	1.51	0.76
5:O:55:TYR:HD1	5:O:56:GLN:H	1.31	0.76
15:P:102:CRT:H391	5:Q:36:HIS:HB3	1.68	0.76
5:1:7:ASN:O	5:1:10:LYS:HG3	1.85	0.76
1:C:263:THR:O	3:M:313:ALA:HB2	1.86	0.76
9:I:102:BCL:HAC2	9:I:103:BCL:HBC3	1.67	0.76
6:N:22:MET:HG3	6:N:26:TYR:HE2	1.49	0.76
15:N:102:CRT:H342	9:O:102:BCL:CAA	2.09	0.76
6:P:13:GLU:O	15:P:102:CRT:C3	2.34	0.76
6:V:21:PHE:HE2	15:V:102:CRT:H16	1.40	0.76
5:1:18:ARG:HD2	5:1:19:ARG:N	2.00	0.76
5:5:10:LYS:HD2	15:8:101:CRT:C3	2.14	0.76
1:C:31:GLU:HB2	1:C:42:ASN:HB3	1.66	0.76
2:L:11:ARG:NH1	4:H:45:ARG:NE	2.33	0.76
3:M:67:ALA:O	3:M:70:ILE:CG2	2.31	0.76
6:G:38:LEU:HA	6:G:41:LEU:HD12	1.67	0.76
6:R:46:LEU:HD21	9:R:101:BCL:H191	1.67	0.76
5:S:49:ASP:CG	5:S:50:ASN:H	1.89	0.76
5:Y:29:ILE:HA	9:Y:102:BCL:C1	2.15	0.76
2:L:3:MET:HE2	4:H:45:ARG:NE	2.01	0.75
6:J:17:PHE:O	6:J:20:ILE:HG22	1.86	0.75
5:F:50:ASN:CG	6:G:43:ARG:HH22	1.90	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:29:ILE:CG2	5:I:30:VAL:N	2.48	0.75
1:C:124:LYS:HZ1	1:C:128:ARG:HH12	1.29	0.75
2:L:19:GLY:HA2	5:7:19:ARG:HD2	1.67	0.75
4:H:47:GLU:HG3	5:A:19:ARG:CA	2.13	0.75
5:F:42:THR:HG23	5:I:48:ASP:HB3	1.68	0.75
5:I:9:TYR:HB2	6:J:15:LYS:HA	1.67	0.75
9:I:102:BCL:HAC2	9:I:103:BCL:CBC	2.16	0.75
5:K:31:LEU:O	5:K:35:ILE:HG12	1.86	0.75
6:P:17:PHE:O	6:P:20:ILE:HG22	1.86	0.75
5:Q:42:THR:CG2	5:Q:43:ASP:H	1.98	0.75
5:Y:44:LEU:HD22	6:Z:43:ARG:HD2	1.65	0.75
9:7:103:BCL:O1D	9:7:103:BCL:H2A	1.86	0.75
3:M:123:THR:HG21	3:M:162:PHE:CE2	2.20	0.75
3:M:161:GLY:HA2	3:M:165:PRO:HG2	1.67	0.75
15:A:101:CRT:H5	5:7:10:LYS:HB3	1.68	0.75
5:K:44:LEU:HD23	5:K:46:TRP:HB3	1.68	0.75
6:P:21:PHE:CG	15:P:102:CRT:H14	2.20	0.75
9:M:401:BCL:C12	10:M:403:BPH:HMA1	2.15	0.75
5:F:42:THR:HG22	5:F:43:ASP:N	2.01	0.75
5:F:42:THR:HG22	5:I:47:LEU:HD23	1.67	0.75
2:L:252:TRP:HA	2:L:252:TRP:HE3	1.48	0.75
9:B:101:BCL:HMB3	9:D:102:BCL:C1B	2.17	0.75
6:J:20:ILE:HG21	15:J:101:CRT:C6	2.16	0.75
6:N:28:TRP:CE3	6:N:31:LEU:HD13	2.22	0.75
5:O:46:TRP:NE1	9:O:102:BCL:OBB	2.19	0.75
5:Y:27:PHE:CE2	5:1:29:ILE:CD1	2.69	0.75
9:5:102:BCL:HBC1	9:6:101:BCL:HBC3	1.68	0.75
5:U:35:ILE:HA	5:U:38:ILE:HG22	1.67	0.75
15:V:102:CRT:H393	5:W:33:LEU:CA	2.12	0.75
5:K:33:LEU:HD12	5:K:34:LEU:N	2.01	0.75
5:S:36:HIS:O	5:S:40:LEU:HB2	1.87	0.75
5:9:12:TRP:HA	5:9:12:TRP:CE3	2.20	0.75
9:M:401:BCL:C20	10:M:403:BPH:C9	2.64	0.75
6:R:24:SER:O	6:R:27:ALA:HB3	1.87	0.75
6:X:32:VAL:O	6:X:36:HIS:HB2	1.87	0.75
15:X:102:CRT:H2M1	5:Y:36:HIS:HB3	1.68	0.75
6:2:46:LEU:HB2	5:3:52:PRO:HD3	1.67	0.75
3:M:178:GLY:HA3	3:M:181:PRO:HG2	1.69	0.74
4:H:48:ARG:NH2	4:H:48:ARG:HG2	2.00	0.74
5:K:9:TYR:OH	6:N:11:ASP:HB3	1.87	0.74
6:V:46:LEU:HD13	6:X:42:TYR:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:29:ILE:HG23	5:1:30:VAL:N	2.01	0.74
11:L:304:UQ8:H20A	9:M:401:BCL:H42	1.68	0.74
9:A:102:BCL:HMD1	6:B:36:HIS:ND1	2.02	0.74
5:5:56:GLN:HG3	5:5:57:ALA:N	2.02	0.74
1:C:245:VAL:HG21	1:C:249:PHE:CD2	2.22	0.74
2:L:43:THR:O	2:L:47:VAL:HG23	1.86	0.74
5:A:47:LEU:HB3	5:9:43:ASP:CB	2.17	0.74
6:G:23:GLN:O	6:G:26:TYR:HB2	1.88	0.74
6:T:21:PHE:CE2	15:T:102:CRT:H16	2.21	0.74
6:X:36:HIS:ND1	9:X:101:BCL:H151	2.00	0.74
1:C:253:THR:HG21	2:L:171:TYR:HB2	1.69	0.74
4:H:5:ILE:CD1	5:D:42:THR:HG23	2.17	0.74
6:2:46:LEU:HD22	6:4:42:TYR:HE2	1.51	0.74
1:C:195:LEU:O	1:C:197:PHE:HD2	1.70	0.74
5:A:24:ILE:CG2	15:B:102:CRT:H243	2.17	0.74
5:A:29:ILE:CD1	15:A:101:CRT:H343	2.16	0.74
5:I:43:ASP:CB	5:K:47:LEU:HB3	2.17	0.74
5:1:10:LYS:CB	6:4:20:ILE:HD13	2.17	0.74
9:3:102:BCL:HMD1	6:4:36:HIS:CE1	2.23	0.74
5:9:12:TRP:HA	5:9:12:TRP:HE3	1.51	0.74
4:H:195:LEU:HD12	4:H:196:PRO:HD2	1.69	0.74
6:G:21:PHE:HB2	15:G:102:CRT:C11	2.17	0.74
9:N:101:BCL:C1B	9:O:102:BCL:HMB3	2.18	0.74
5:A:35:ILE:O	5:A:38:ILE:HG13	1.88	0.74
5:W:39:VAL:HA	5:Y:47:LEU:HD13	1.69	0.74
3:M:301:HIS:CE1	4:H:8:TYR:HB3	2.23	0.74
5:A:47:LEU:CB	5:9:43:ASP:HB2	2.17	0.74
9:4:101:BCL:HMB3	9:5:102:BCL:CHB	2.17	0.74
5:5:43:ASP:HB2	5:7:47:LEU:CB	2.18	0.74
5:9:9:TYR:CE1	6:0:15:LYS:HG2	2.23	0.74
3:M:117:MET:CE	5:Q:34:LEU:HD12	2.17	0.73
9:E:101:BCL:CMA	9:E:101:BCL:HBA2	2.18	0.73
5:S:20:VAL:HG23	5:S:21:LEU:H	1.53	0.73
1:C:167:VAL:HG21	1:C:297:GLY:HA3	1.70	0.73
1:C:261:GLN:O	1:C:262:SER:O	2.06	0.73
5:A:21:LEU:O	5:A:25:VAL:HG23	1.87	0.73
15:A:103:CRT:H342	9:F:102:BCL:HAA1	1.71	0.73
5:F:9:TYR:CD1	6:G:15:LYS:HG3	2.23	0.73
2:L:3:MET:SD	2:L:11:ARG:HD2	2.28	0.73
14:M:405:MQ8:H401	4:H:51:GLY:CA	2.18	0.73
4:H:11:ALA:HA	4:H:14:ILE:CG2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:25:VAL:O	5:K:29:ILE:HG22	1.89	0.73
4:H:14:ILE:HD11	5:I:37:MET:CB	2.16	0.73
5:I:9:TYR:HA	6:J:18:HIS:CG	2.23	0.73
5:S:13:LEU:HD12	15:V:102:CRT:H23	1.69	0.73
6:Z:22:MET:HG3	6:Z:26:TYR:HE1	1.53	0.73
5:7:29:ILE:HG23	5:7:30:VAL:H	1.54	0.73
4:H:48:ARG:CZ	17:H:301:PEF:O1P	2.36	0.73
6:N:28:TRP:HA	6:N:31:LEU:HD12	1.70	0.73
5:S:29:ILE:HG23	5:S:30:VAL:H	1.51	0.73
5:3:13:LEU:CD1	15:3:103:CRT:C1M	2.40	0.73
5:5:16:ASP:H	5:5:19:ARG:HG3	1.54	0.73
4:H:95:ALA:HB2	5:9:16:ASP:OD2	1.89	0.73
2:L:180:PRO:HB3	2:L:271:TRP:CZ3	2.24	0.73
4:H:133:ILE:HD11	4:H:171:TRP:HB3	1.68	0.73
9:D:102:BCL:CHD	9:E:101:BCL:HMD2	2.19	0.73
9:Q:102:BCL:C1D	9:R:101:BCL:HMD2	2.19	0.73
5:Y:16:ASP:HB3	5:Y:18:ARG:NE	2.04	0.73
5:9:12:TRP:HE1	6:0:18:HIS:HA	1.52	0.73
1:C:173:LYS:HG2	3:M:80:HIS:CG	2.22	0.73
2:L:44:LEU:CB	5:9:30:VAL:HG11	2.16	0.73
2:L:112:ARG:O	2:L:116:ILE:HG13	1.88	0.73
9:R:101:BCL:CHB	9:S:102:BCL:HMB3	2.19	0.73
5:Y:29:ILE:CA	9:Y:102:BCL:H11	2.18	0.73
5:Y:50:ASN:ND2	5:Y:51:ILE:HG12	2.04	0.73
5:7:29:ILE:HG23	5:7:30:VAL:N	2.03	0.73
15:A:103:CRT:H21	5:D:24:ILE:HD13	1.69	0.73
9:E:101:BCL:HBA2	9:E:101:BCL:HMA2	1.70	0.73
5:W:8:LEU:HD22	6:X:18:HIS:CE1	2.22	0.73
9:3:102:BCL:C1D	9:4:101:BCL:HMD2	2.17	0.73
5:A:18:ARG:HG3	5:9:14:ILE:HG23	1.71	0.72
15:A:103:CRT:H83	6:E:20:ILE:CD1	2.18	0.72
5:F:10:LYS:CD	15:J:101:CRT:H1M1	2.19	0.72
5:I:16:ASP:HB2	5:I:19:ARG:CB	2.19	0.72
5:Y:43:ASP:OD1	5:Y:44:LEU:HD23	1.88	0.72
9:F:102:BCL:HBC2	9:F:102:BCL:CHD	2.18	0.72
6:J:29:PHE:O	6:J:33:VAL:HB	1.88	0.72
5:K:54:SER:CA	5:K:56:GLN:HE22	2.01	0.72
5:1:50:ASN:ND2	5:1:51:ILE:HG12	2.03	0.72
6:2:46:LEU:HB2	5:3:52:PRO:CD	2.19	0.72
5:D:12:TRP:HE1	6:E:18:HIS:HA	1.53	0.72
5:F:49:ASP:CG	5:F:50:ASN:N	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:42:THR:HB	5:Y:48:ASP:CB	2.19	0.72
15:W:103:CRT:C20	6:Z:25:MET:HG3	2.19	0.72
5:5:14:ILE:O	5:5:14:ILE:HG22	1.89	0.72
2:L:3:MET:HE2	4:H:45:ARG:HE	1.54	0.72
4:H:39:TYR:OH	17:H:301:PEF:H41	1.90	0.72
9:A:102:BCL:CHB	9:0:101:BCL:HMB3	2.19	0.72
5:I:44:LEU:HD12	5:I:44:LEU:O	1.89	0.72
9:I:102:BCL:HBC2	9:I:102:BCL:CHD	2.18	0.72
5:3:9:TYR:HA	6:4:18:HIS:HD1	1.54	0.72
3:M:171:TRP:CE3	3:M:171:TRP:HA	2.24	0.72
4:H:5:ILE:HD11	5:F:47:LEU:HD13	1.71	0.72
6:N:20:ILE:H	6:N:20:ILE:HD12	1.52	0.72
9:Q:102:BCL:HBC2	9:R:101:BCL:HMD3	1.69	0.72
5:3:2:PHE:HA	5:3:5:ASN:ND2	2.05	0.72
5:I:16:ASP:HB2	5:I:19:ARG:HB2	1.72	0.72
6:P:13:GLU:HA	6:P:16:GLU:CD	2.10	0.72
15:V:102:CRT:H391	5:W:36:HIS:HB2	0.75	0.72
6:4:40:TRP:CZ3	6:4:44:PRO:HA	2.25	0.72
1:C:72:ALA:HB3	1:C:83:LYS:HA	1.70	0.72
2:L:49:LEU:HD21	5:9:37:MET:HG2	1.72	0.72
9:2:101:BCL:CHB	9:3:102:BCL:HMB3	2.20	0.72
6:T:45:TRP:O	5:U:52:PRO:HD2	1.90	0.72
5:W:26:ALA:HA	5:W:29:ILE:HG22	1.71	0.72
5:9:40:LEU:HD13	5:9:47:LEU:HD23	1.70	0.72
3:M:61:ILE:HG23	3:M:62:PHE:HD1	1.53	0.72
6:G:16:GLU:O	6:G:20:ILE:HG22	1.89	0.72
5:I:12:TRP:HZ2	6:J:21:PHE:HD2	1.38	0.72
5:I:34:LEU:O	5:I:38:ILE:HG22	1.90	0.72
5:Y:36:HIS:NE2	9:Z:101:BCL:HMD1	2.04	0.72
5:3:53:VAL:HA	5:3:55:TYR:CZ	2.24	0.72
4:H:35:LYS:HE3	4:H:39:TYR:CD2	2.25	0.72
5:A:2:PHE:HB2	5:A:5:ASN:OD1	1.90	0.72
5:A:18:ARG:H	5:A:18:ARG:HD2	1.55	0.72
6:N:17:PHE:HE1	15:N:102:CRT:H9	1.53	0.72
5:1:43:ASP:HB2	5:3:47:LEU:HD12	1.69	0.72
6:4:13:GLU:HA	6:4:16:GLU:CD	2.10	0.72
6:6:27:ALA:O	6:6:31:LEU:HG	1.89	0.72
4:H:140:LYS:H	4:H:140:LYS:CD	1.94	0.71
5:Y:9:TYR:HA	6:Z:18:HIS:CG	2.24	0.71
9:4:101:BCL:H43	15:4:102:CRT:H242	1.72	0.71
9:4:101:BCL:C4	15:4:102:CRT:C24	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ARG:HG3	1:C:304:ARG:NH1	2.05	0.71
3:M:229:PHE:O	3:M:244:ALA:HB2	1.90	0.71
15:G:102:CRT:H342	9:I:102:BCL:CAA	2.20	0.71
5:K:12:TRP:NE1	6:N:17:PHE:HD2	1.87	0.71
5:O:29:ILE:HG23	5:O:30:VAL:N	2.05	0.71
15:R:102:CRT:H342	9:S:102:BCL:CAA	2.20	0.71
5:3:36:HIS:CE1	9:4:101:BCL:HMD1	2.25	0.71
11:L:304:UQ8:C20	9:M:401:BCL:H42	2.21	0.71
5:A:46:TRP:HB2	6:0:46:LEU:OXT	1.89	0.71
6:2:20:ILE:HD12	15:2:102:CRT:H81	1.72	0.71
5:5:10:LYS:HB3	15:8:101:CRT:C5	2.19	0.71
1:C:157:ARG:HE	1:C:312:GLN:NE2	1.89	0.71
2:L:28:GLY:HA2	4:H:46:THR:HB	1.72	0.71
2:L:238:ILE:HD11	11:L:304:UQ8:H8	1.72	0.71
3:M:70:ILE:CD1	3:M:114:TRP:CE3	2.73	0.71
5:W:10:LYS:HB3	15:W:103:CRT:H5	1.72	0.71
2:L:28:GLY:CA	4:H:46:THR:HB	2.21	0.71
2:L:29:PRO:O	3:M:254:TRP:HA	1.90	0.71
6:N:33:VAL:O	6:N:37:LEU:HD23	1.91	0.71
6:V:17:PHE:HD1	15:V:102:CRT:C9	2.03	0.71
5:W:8:LEU:HD23	5:W:11:ILE:HD11	1.64	0.71
6:X:43:ARG:HH12	5:Y:55:TYR:HB2	1.56	0.71
6:Z:27:ALA:O	6:Z:31:LEU:HG	1.91	0.71
5:1:36:HIS:NE2	9:2:101:BCL:HMD1	2.04	0.71
5:5:56:GLN:HG3	5:5:57:ALA:H	1.56	0.71
2:L:230:GLY:N	3:M:51:ILE:HD13	2.04	0.71
3:M:171:TRP:HA	3:M:171:TRP:HE3	1.56	0.71
4:H:132:LYS:HG2	4:H:173:ASP:OD1	1.91	0.71
4:H:235:GLU:O	4:H:239:VAL:HG23	1.91	0.71
6:G:31:LEU:O	6:G:34:ILE:HG23	1.90	0.71
5:O:10:LYS:HB2	15:R:102:CRT:C8	2.21	0.71
6:0:24:SER:O	6:0:27:ALA:HB3	1.90	0.71
1:C:250:CYS:C	1:C:263:THR:HG23	2.11	0.71
1:C:251:HIS:CE1	7:C:503:HEM:NC	2.59	0.71
5:A:45:ASN:O	5:A:49:ASP:HB3	1.91	0.71
5:D:39:VAL:O	5:D:43:ASP:HB3	1.91	0.71
6:G:28:TRP:CE2	6:G:32:VAL:CG2	2.74	0.71
5:1:49:ASP:CG	5:1:50:ASN:N	2.44	0.71
3:M:79:VAL:CG2	3:M:85:GLN:HB3	2.20	0.71
15:G:102:CRT:H2M1	5:I:37:MET:HG2	1.73	0.71
6:8:45:TRP:O	6:8:46:LEU:HG	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:47:LEU:HA	5:9:43:ASP:OD2	1.91	0.71
5:D:8:LEU:O	5:D:11:ILE:HG22	1.91	0.71
3:M:34:PRO:HA	3:M:48:ILE:O	1.91	0.70
5:S:29:ILE:CG2	5:S:30:VAL:H	2.04	0.70
6:V:42:TYR:CD2	6:V:43:ARG:HG3	2.26	0.70
5:9:5:ASN:HA	5:9:8:LEU:HD12	1.71	0.70
5:A:21:LEU:HD11	15:B:102:CRT:C14	2.21	0.70
5:F:49:ASP:OD2	5:I:56:GLN:HG2	1.90	0.70
5:7:13:LEU:O	6:8:7:THR:CA	2.39	0.70
5:9:17:PRO:O	5:9:21:LEU:HB2	1.91	0.70
1:C:175:PRO:CD	1:C:179:LYS:HB3	2.20	0.70
5:5:16:ASP:HB3	5:5:17:PRO:HD2	1.73	0.70
5:O:45:ASN:HB3	5:O:48:ASP:OD1	1.92	0.70
2:L:158:GLY:HA3	2:L:161:SER:HB3	1.73	0.70
3:M:243:THR:HA	3:M:246:GLU:HB3	1.72	0.70
5:D:43:ASP:CB	5:F:47:LEU:HD22	2.16	0.70
9:T:101:BCL:OBB	9:T:101:BCL:HHC	1.91	0.70
5:Y:43:ASP:HA	5:1:48:ASP:HB3	1.74	0.70
6:4:24:SER:HB2	15:4:102:CRT:C14	2.21	0.70
3:M:298:ALA:HB1	3:M:303:MET:HB2	1.73	0.70
6:J:46:LEU:HB3	6:N:42:TYR:CZ	2.27	0.70
6:N:28:TRP:CD2	6:N:31:LEU:HD12	2.27	0.70
5:3:44:LEU:HD21	9:4:101:BCL:HBC3	1.73	0.70
3:M:59:LEU:HG	3:M:128:LEU:HD21	1.72	0.70
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.74	0.70
9:W:102:BCL:HMD1	6:X:36:HIS:HD2	1.56	0.70
5:5:30:VAL:HG13	5:5:31:LEU:H	1.57	0.70
6:8:20:ILE:O	6:8:23:GLN:HG3	1.91	0.70
6:8:21:PHE:CE1	15:8:101:CRT:C19	2.61	0.70
1:C:173:LYS:HB3	3:M:80:HIS:HB2	1.73	0.70
4:H:61:LEU:HD12	4:H:62:PRO:HD2	1.73	0.70
6:B:16:GLU:OE1	15:B:102:CRT:H23	1.91	0.70
9:I:102:BCL:C1D	9:I:103:BCL:CMD	2.69	0.70
5:Q:50:ASN:HB3	5:S:56:GLN:HG3	1.74	0.70
5:Y:49:ASP:CA	5:1:56:GLN:NE2	2.39	0.70
5:5:31:LEU:HD12	5:5:34:LEU:HD23	1.74	0.70
4:H:55:VAL:HG13	4:H:56:VAL:H	1.55	0.70
5:D:11:ILE:HG23	5:D:12:TRP:CE3	2.27	0.70
5:U:16:ASP:HB3	5:U:18:ARG:NH1	2.07	0.70
5:W:10:LYS:HD3	15:W:103:CRT:H1M2	1.73	0.70
9:W:102:BCL:HBC1	9:X:101:BCL:HBC3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9:12:TRP:HZ2	6:0:21:PHE:CE2	2.09	0.70
2:L:6:PHE:CE2	3:M:250:LEU:HD11	2.26	0.70
3:M:242:GLY:HA3	4:H:119:ARG:NH2	2.07	0.70
6:E:9:LEU:HD22	6:E:13:GLU:HG3	1.72	0.70
5:I:43:ASP:OD2	5:K:47:LEU:HD12	1.92	0.70
5:Q:44:LEU:HD12	5:Q:44:LEU:O	1.92	0.70
9:Q:102:BCL:H2A	9:Q:102:BCL:O1D	1.92	0.70
6:T:33:VAL:O	6:T:37:LEU:HD23	1.92	0.70
5:3:46:TRP:CZ3	9:3:102:BCL:HBC3	2.27	0.70
9:3:102:BCL:C8	15:4:102:CRT:H183	2.21	0.70
6:G:17:PHE:CD2	15:G:102:CRT:H6	2.26	0.69
9:K:102:BCL:HMD2	9:N:101:BCL:CHD	2.22	0.69
5:S:43:ASP:CA	5:U:56:GLN:HG3	2.21	0.69
6:X:22:MET:HG3	6:X:26:TYR:HE2	1.57	0.69
5:D:49:ASP:HB2	5:F:56:GLN:CG	2.22	0.69
1:C:249:PHE:CE1	1:C:265:LYS:HG2	2.28	0.69
6:B:40:TRP:HZ3	6:B:45:TRP:N	1.86	0.69
9:Z:101:BCL:C4A	9:1:102:BCL:HMB3	2.22	0.69
5:3:32:GLY:CA	9:4:101:BCL:HED2	2.23	0.69
1:C:315:ASN:OD1	1:C:316:LYS:N	2.26	0.69
5:A:15:LEU:HD21	5:D:21:LEU:HD23	1.73	0.69
6:B:42:TYR:OH	6:0:46:LEU:HB3	1.90	0.69
5:I:24:ILE:HG21	15:J:101:CRT:H21	1.74	0.69
6:J:17:PHE:HA	6:J:20:ILE:HG22	1.73	0.69
6:P:38:LEU:C	6:P:41:LEU:HD23	2.11	0.69
5:5:26:ALA:O	5:5:29:ILE:HG22	1.91	0.69
4:H:53:VAL:HG13	4:H:54:LYS:N	2.03	0.69
5:F:42:THR:HG22	5:F:43:ASP:H	1.58	0.69
9:W:102:BCL:HHD	9:W:102:BCL:HBC2	1.75	0.69
6:4:20:ILE:HG21	15:4:102:CRT:H6	1.58	0.69
6:4:25:MET:CB	15:4:102:CRT:C16	2.56	0.69
5:5:43:ASP:CB	5:7:47:LEU:HB3	2.22	0.69
5:7:12:TRP:CH2	6:8:17:PHE:CD2	2.81	0.69
1:C:157:ARG:HE	1:C:312:GLN:CD	1.96	0.69
5:I:36:HIS:NE2	9:I:103:BCL:HMD1	2.06	0.69
15:J:101:CRT:H342	9:K:102:BCL:CAA	2.23	0.69
9:R:101:BCL:C4A	9:S:102:BCL:HMB3	2.22	0.69
5:F:44:LEU:HB2	6:G:43:ARG:NH1	2.05	0.69
5:I:44:LEU:HD12	5:I:46:TRP:HE3	1.56	0.69
3:M:199:ASN:HD22	3:M:202:HIS:HB2	1.57	0.69
5:A:51:ILE:HB	5:A:52:PRO:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:102:BCL:C1D	9:B:101:BCL:HMD2	2.23	0.69
5:I:8:LEU:HB3	6:J:18:HIS:NE2	2.07	0.69
6:P:21:PHE:C	6:P:21:PHE:CD1	2.65	0.69
6:P:21:PHE:HZ	15:P:102:CRT:C19	2.04	0.69
5:U:13:LEU:N	5:U:13:LEU:HD23	2.08	0.69
5:U:21:LEU:O	5:U:25:VAL:HG23	1.93	0.69
5:W:39:VAL:HA	5:Y:47:LEU:CD1	2.23	0.69
5:W:46:TRP:HA	5:W:49:ASP:OD1	1.91	0.69
5:7:18:ARG:N	5:7:18:ARG:HD2	2.08	0.69
1:C:225:SER:OG	1:C:228:GLN:HG3	1.91	0.69
1:C:284:ILE:HG21	1:C:304:ARG:HA	1.75	0.69
6:J:30:GLY:O	6:J:34:ILE:HG22	1.93	0.69
15:P:102:CRT:C39	5:Q:36:HIS:CG	2.74	0.69
9:1:102:BCL:C1D	9:2:101:BCL:HMD2	2.22	0.69
1:C:270:TRP:CZ2	1:C:274:ARG:NH1	2.60	0.69
3:M:228:ARG:HH12	4:H:247:LYS:HE2	1.57	0.69
6:G:45:TRP:O	6:G:46:LEU:HB2	1.92	0.69
5:K:44:LEU:O	5:K:44:LEU:HD22	1.93	0.69
6:P:21:PHE:CE2	15:P:102:CRT:H16	2.27	0.69
6:V:20:ILE:HG23	15:V:102:CRT:C9	2.23	0.69
9:V:101:BCL:HMA1	9:W:102:BCL:HHB	1.75	0.69
5:Y:49:ASP:C	5:1:56:GLN:HE21	1.95	0.69
5:1:9:TYR:HA	6:2:18:HIS:ND1	2.08	0.69
6:4:20:ILE:HG23	15:4:102:CRT:C6	2.23	0.69
3:M:70:ILE:HD13	3:M:118:ALA:HB2	1.74	0.68
3:M:82:ASP:OD1	3:M:84:PHE:HB2	1.93	0.68
4:H:24:PHE:CE1	4:H:28:ILE:HD11	2.28	0.68
5:A:13:LEU:O	6:B:9:LEU:HD13	1.93	0.68
5:A:14:ILE:HG13	5:A:15:LEU:CD2	2.23	0.68
5:F:27:PHE:CD2	5:I:29:ILE:HD11	2.27	0.68
5:K:44:LEU:O	5:K:44:LEU:HD13	1.93	0.68
6:N:28:TRP:O	6:N:31:LEU:HB2	1.93	0.68
6:N:29:PHE:HZ	9:N:101:BCL:H61	1.58	0.68
5:S:21:LEU:O	5:S:25:VAL:HG23	1.93	0.68
5:S:40:LEU:HD11	5:S:47:LEU:HD23	1.75	0.68
6:X:20:ILE:HD13	6:X:20:ILE:O	1.94	0.68
6:4:24:SER:CB	15:4:102:CRT:C12	2.71	0.68
1:C:250:CYS:HB3	1:C:251:HIS:CE1	2.28	0.68
3:M:268:TRP:CD2	4:H:30:LEU:HD13	2.27	0.68
5:A:36:HIS:HE1	9:A:102:BCL:NA	1.88	0.68
5:S:13:LEU:CD1	15:V:102:CRT:H23	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LYS:CB	15:8:101:CRT:H82	2.18	0.68
2:L:3:MET:CE	4:H:45:ARG:HE	2.05	0.68
4:H:53:VAL:O	4:H:54:LYS:HB2	1.92	0.68
5:A:46:TRP:O	6:0:46:LEU:OXT	2.11	0.68
5:Q:13:LEU:O	6:R:7:THR:HA	1.93	0.68
5:3:36:HIS:NE2	9:4:101:BCL:HMD1	2.08	0.68
4:H:39:TYR:OH	17:H:301:PEF:C4	2.42	0.68
9:A:102:BCL:HBC1	9:B:101:BCL:HBC3	1.74	0.68
5:I:29:ILE:HG23	5:I:30:VAL:N	2.08	0.68
5:7:29:ILE:HA	9:7:102:BCL:H11	1.75	0.68
6:E:45:TRP:CE3	9:E:101:BCL:HBC2	2.29	0.68
5:7:33:LEU:HD12	5:7:33:LEU:N	2.06	0.68
4:H:11:ALA:CA	4:H:14:ILE:HG22	2.23	0.68
4:H:215:LYS:HE3	4:H:250:ALA:O	1.93	0.68
5:O:9:TYR:HA	6:P:18:HIS:CE1	2.29	0.68
6:V:20:ILE:CG2	15:V:102:CRT:H9	2.24	0.68
6:4:25:MET:CA	15:4:102:CRT:C16	2.72	0.68
2:L:20:GLY:O	2:L:24:ASP:HB2	1.94	0.68
5:O:13:LEU:O	5:O:13:LEU:HD23	1.93	0.68
9:O:102:BCL:HBC2	9:O:102:BCL:CHD	2.23	0.68
6:P:38:LEU:HD23	6:P:39:ALA:N	2.09	0.68
5:W:10:LYS:HB2	15:W:103:CRT:H83	1.75	0.68
5:3:26:ALA:C	5:3:29:ILE:HG22	2.14	0.68
1:C:251:HIS:HE1	7:C:503:HEM:C4C	2.12	0.68
6:R:33:VAL:O	6:R:37:LEU:HD23	1.94	0.68
5:7:12:TRP:HH2	6:8:17:PHE:HE2	1.42	0.68
6:E:44:PRO:HD2	5:F:55:TYR:OH	1.94	0.68
5:W:7:ASN:HD22	5:W:7:ASN:N	1.86	0.68
1:C:295:ARG:HH11	1:C:295:ARG:CG	2.06	0.68
3:M:95:LEU:HB3	3:M:177:PHE:HB2	1.75	0.67
5:A:17:PRO:HB2	5:9:14:ILE:CD1	2.24	0.67
15:A:103:CRT:H23	6:E:16:GLU:CG	2.24	0.67
6:G:21:PHE:HD1	6:G:22:MET:CA	2.06	0.67
5:I:13:LEU:HD12	15:N:102:CRT:C1M	2.24	0.67
4:H:6:THR:CB	5:F:41:SER:HB3	2.24	0.67
9:I:103:BCL:HMA1	9:K:102:BCL:HMA1	1.76	0.67
6:N:17:PHE:O	6:N:21:PHE:HB3	1.94	0.67
5:S:29:ILE:CG2	5:S:30:VAL:N	2.57	0.67
6:V:33:VAL:O	6:V:37:LEU:HD23	1.94	0.67
5:Y:25:VAL:O	5:Y:29:ILE:HG22	1.94	0.67
5:Y:36:HIS:CD2	9:Z:101:BCL:HMD1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:27:PHE:O	5:1:30:VAL:HG12	1.95	0.67
5:3:32:GLY:N	9:4:101:BCL:HED2	2.10	0.67
5:7:8:LEU:HD13	5:7:8:LEU:O	1.93	0.67
5:7:26:ALA:O	5:7:29:ILE:HG22	1.94	0.67
14:M:405:MQ8:H401	4:H:51:GLY:HA2	1.76	0.67
4:H:111:PHE:HA	4:H:115:ALA:HB2	1.75	0.67
6:G:27:ALA:C	6:G:31:LEU:HG	2.14	0.67
9:G:101:BCL:C1B	9:I:102:BCL:HMB3	2.24	0.67
5:K:39:VAL:HG11	9:K:102:BCL:HBC1	1.75	0.67
5:Q:27:PHE:CD2	5:S:29:ILE:HD11	2.29	0.67
15:T:102:CRT:H391	5:U:36:HIS:HB3	1.75	0.67
5:U:35:ILE:O	5:U:38:ILE:HG22	1.94	0.67
5:U:46:TRP:CH2	9:U:102:BCL:HBC3	2.30	0.67
5:W:8:LEU:CD2	6:X:18:HIS:HE1	2.07	0.67
6:X:43:ARG:NH1	5:Y:55:TYR:HB2	2.08	0.67
5:5:10:LYS:CG	15:8:101:CRT:H5	2.23	0.67
5:5:13:LEU:HD23	6:6:14:ALA:HB2	1.75	0.67
1:C:41:GLU:O	2:L:172:GLN:NE2	2.27	0.67
4:H:31:ARG:HA	4:H:34:ASP:OD2	1.94	0.67
4:H:35:LYS:NZ	4:H:39:TYR:CE2	2.62	0.67
5:A:29:ILE:CD1	5:A:33:LEU:CD1	2.72	0.67
5:A:60:LYS:CB	5:9:49:ASP:O	2.43	0.67
5:Q:51:ILE:CG2	5:Q:52:PRO:HA	2.23	0.67
5:W:9:TYR:HA	6:X:18:HIS:ND1	2.09	0.67
5:W:43:ASP:HB2	5:Y:47:LEU:HB3	1.76	0.67
5:Y:49:ASP:HB2	5:1:56:GLN:HG2	1.76	0.67
9:5:102:BCL:CHD	9:5:102:BCL:HBC2	2.23	0.67
6:8:17:PHE:HZ	15:8:101:CRT:C11	2.06	0.67
1:C:314:VAL:HG11	1:C:319:TYR:CE1	2.30	0.67
2:L:2:ALA:HB1	4:H:41:LEU:HD13	1.77	0.67
5:A:33:LEU:HA	15:A:101:CRT:H372	1.77	0.67
9:F:102:BCL:CBC	9:G:101:BCL:CAC	2.70	0.67
9:S:102:BCL:C1D	9:T:101:BCL:HMD2	2.25	0.67
1:C:124:LYS:HZ3	1:C:128:ARG:HH12	1.41	0.67
1:C:308:MET:HE1	1:C:312:GLN:CA	2.23	0.67
2:L:253:SER:O	2:L:256:CYS:HB3	1.95	0.67
5:I:33:LEU:O	5:I:37:MET:HG2	1.94	0.67
2:L:10:TYR:HA	4:H:112:GLY:HA2	1.77	0.67
4:H:87:VAL:HG11	4:H:100:LEU:HD13	1.77	0.67
6:J:45:TRP:O	6:J:46:LEU:HB2	1.93	0.67
6:N:10:THR:HG22	6:N:11:ASP:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:20:ILE:HD12	6:N:20:ILE:N	2.09	0.67
3:M:14:ARG:HD3	3:M:36:PHE:CD1	2.30	0.67
3:M:59:LEU:HG	3:M:128:LEU:CD2	2.24	0.67
5:K:12:TRP:HB2	6:N:14:ALA:HB1	1.76	0.67
6:X:45:TRP:CZ3	9:X:101:BCL:HAC2	2.28	0.67
6:2:36:HIS:HB3	9:2:101:BCL:H151	1.77	0.67
6:6:44:PRO:HG2	5:7:52:PRO:CG	2.24	0.67
15:B:102:CRT:H82	5:9:10:LYS:HB2	1.77	0.67
6:G:29:PHE:O	6:G:33:VAL:HB	1.94	0.67
6:2:43:ARG:NH1	5:3:55:TYR:HB3	2.10	0.67
5:3:33:LEU:HD12	5:3:34:LEU:N	2.10	0.67
6:8:27:ALA:O	6:8:31:LEU:CG	2.29	0.67
5:9:31:LEU:HD23	9:0:101:BCL:HED3	1.77	0.67
1:C:141:TRP:O	1:C:145:VAL:HG22	1.94	0.67
2:L:207:THR:O	4:H:67:PHE:HE1	1.78	0.67
2:L:273:ASN:HD22	2:L:276:LEU:HB2	1.61	0.67
3:M:70:ILE:CG2	3:M:118:ALA:HB1	2.14	0.67
5:F:42:THR:CG2	5:F:43:ASP:N	2.58	0.67
6:8:25:MET:HG3	15:8:101:CRT:C22	2.24	0.67
15:8:101:CRT:C34	9:9:102:BCL:HAA1	2.25	0.67
1:C:178:LEU:HB3	3:M:110:SER:HA	1.77	0.66
1:C:182:GLY:O	1:C:197:PHE:CE2	2.48	0.66
1:C:252:ASN:OD1	1:C:254:ARG:CD	2.38	0.66
2:L:84:LEU:HD23	2:L:151:TRP:HD1	1.56	0.66
3:M:26:GLY:HA2	5:O:16:ASP:OD2	1.95	0.66
3:M:261:THR:HG22	4:H:37:GLU:HB2	1.76	0.66
4:H:5:ILE:HB	5:D:42:THR:HG23	1.77	0.66
9:O:102:BCL:HMB1	9:O:102:BCL:CBB	2.25	0.66
5:S:29:ILE:O	5:S:33:LEU:HD13	1.94	0.66
5:W:56:GLN:O	5:W:60:LYS:CB	2.44	0.66
1:C:156:HIS:CE1	1:C:162:PRO:HD3	2.30	0.66
1:C:225:SER:N	1:C:228:GLN:NE2	2.42	0.66
2:L:183:MET:HE1	2:L:272:TRP:NE1	2.09	0.66
3:M:117:MET:CE	5:Q:34:LEU:HD11	2.25	0.66
4:H:148:ASP:OD1	4:H:149:PRO:HD2	1.95	0.66
6:J:43:ARG:HH22	5:K:55:TYR:HB2	1.60	0.66
5:K:21:LEU:HD13	15:N:102:CRT:H14	1.76	0.66
15:R:102:CRT:H391	5:S:36:HIS:CG	2.31	0.66
5:U:35:ILE:HA	5:U:38:ILE:CG2	2.25	0.66
6:V:20:ILE:HG21	15:V:102:CRT:C9	2.24	0.66
5:W:35:ILE:HD11	15:X:102:CRT:H392	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9:29:ILE:O	5:9:33:LEU:HD12	1.96	0.66
2:L:226:ARG:HG2	2:L:230:GLY:O	1.95	0.66
6:B:27:ALA:O	6:B:31:LEU:HG	1.94	0.66
5:D:9:TYR:HB2	6:E:15:LYS:HA	1.77	0.66
6:J:10:THR:HG22	6:J:11:ASP:H	1.60	0.66
5:O:7:ASN:ND2	6:R:23:GLN:OE1	2.28	0.66
5:U:46:TRP:CD1	5:U:47:LEU:HD13	2.31	0.66
5:1:18:ARG:HD2	5:1:19:ARG:H	1.59	0.66
5:3:29:ILE:CG2	5:3:30:VAL:N	2.48	0.66
6:0:38:LEU:O	6:0:38:LEU:HD23	1.96	0.66
2:L:16:THR:HA	2:L:115:GLU:OE1	1.95	0.66
3:M:258:PHE:HE2	17:H:301:PEF:C31	2.07	0.66
4:H:157:VAL:HG11	4:H:208:LYS:HD3	1.77	0.66
6:G:34:ILE:HD13	6:G:35:ALA:N	2.11	0.66
5:I:12:TRP:CZ2	6:J:21:PHE:HD2	2.14	0.66
5:Q:50:ASN:HA	5:S:60:LYS:CB	2.25	0.66
6:T:9:LEU:HD22	6:T:13:GLU:HG3	1.77	0.66
5:U:10:LYS:HD2	6:X:20:ILE:HG13	1.77	0.66
6:0:31:LEU:O	6:0:34:ILE:HG23	1.95	0.66
1:C:35:TYR:HB3	1:C:38:VAL:HG21	1.77	0.66
1:C:196:PRO:HG2	1:C:231:TRP:CD1	2.30	0.66
2:L:69:ASN:O	2:L:73:ILE:HG13	1.94	0.66
3:M:275:LEU:HA	3:M:278:ILE:HD12	1.78	0.66
4:H:258:LEU:O	5:5:19:ARG:HD3	1.95	0.66
5:A:11:ILE:HD13	15:A:103:CRT:C9	2.26	0.66
5:F:44:LEU:HD22	6:G:43:ARG:HD2	1.77	0.66
6:G:46:LEU:HB3	6:J:42:TYR:OH	1.96	0.66
5:S:50:ASN:ND2	5:S:51:ILE:HG12	2.10	0.66
9:S:102:BCL:CBB	9:S:102:BCL:HMB1	2.26	0.66
9:W:102:BCL:C1D	9:X:101:BCL:HMD2	2.25	0.66
5:3:22:VAL:HA	5:3:25:VAL:HG23	1.77	0.66
5:3:38:ILE:HD12	15:4:102:CRT:H401	1.77	0.66
6:4:40:TRP:HZ3	6:4:45:TRP:N	1.94	0.66
6:4:46:LEU:HD22	6:6:43:ARG:NH2	2.11	0.66
5:7:32:GLY:HA2	5:7:35:ILE:HD12	1.76	0.66
5:7:43:ASP:OD1	5:7:44:LEU:HD12	1.95	0.66
2:L:233:ILE:HG12	2:L:237:ALA:CB	2.25	0.66
4:H:11:ALA:C	4:H:14:ILE:HG22	2.15	0.66
15:A:101:CRT:H82	5:7:11:ILE:HA	1.77	0.66
5:D:14:ILE:CG2	5:F:18:ARG:HB3	2.26	0.66
5:U:22:VAL:HG13	5:U:23:SER:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:191:THR:OG1	11:L:304:UQ8:H20B	1.95	0.66
3:M:140:LEU:HB3	3:M:142:MET:HG2	1.78	0.66
9:G:101:BCL:HMB3	9:I:102:BCL:C4A	2.25	0.66
9:O:102:BCL:CBC	9:P:101:BCL:HHD	2.25	0.66
9:U:102:BCL:C1D	9:V:101:BCL:HMD2	2.26	0.66
9:W:102:BCL:HMB1	9:W:102:BCL:CBB	2.24	0.66
9:F:102:BCL:CHD	9:G:101:BCL:HMD2	2.24	0.66
5:K:34:LEU:O	5:K:37:MET:HB2	1.95	0.66
6:T:34:ILE:O	6:T:34:ILE:HD13	1.95	0.66
15:V:102:CRT:C40	5:W:36:HIS:CB	2.73	0.66
6:Z:10:THR:HG22	6:Z:11:ASP:N	2.07	0.66
6:2:17:PHE:CD1	15:2:102:CRT:C7	2.79	0.66
6:6:20:ILE:O	6:6:20:ILE:HD13	1.96	0.66
5:7:33:LEU:H	5:7:33:LEU:CD1	2.08	0.66
2:L:105:ALA:HB1	10:L:302:BPH:H2	1.78	0.66
4:H:37:GLU:HA	4:H:37:GLU:OE2	1.95	0.66
4:H:197:ILE:HA	4:H:200:SER:OG	1.96	0.66
9:A:102:BCL:C1B	9:0:101:BCL:HMB3	2.25	0.66
5:K:50:ASN:CB	5:O:59:GLY:HA2	2.25	0.66
5:O:46:TRP:CD1	5:O:47:LEU:HD22	2.30	0.66
1:C:214:GLY:HA2	1:C:222:ASN:HD22	1.60	0.66
4:H:14:ILE:HG13	5:I:37:MET:SD	2.35	0.66
4:H:45:ARG:HA	4:H:96:PRO:HB3	1.76	0.66
4:H:113:PRO:HG2	4:H:248:LEU:HD23	1.76	0.66
5:A:17:PRO:HB2	5:9:14:ILE:HD11	1.77	0.66
15:B:102:CRT:O1	5:9:10:LYS:HB3	1.96	0.66
6:P:21:PHE:CZ	15:P:102:CRT:C16	2.78	0.66
5:S:49:ASP:CG	5:S:50:ASN:N	2.49	0.66
5:U:45:ASN:OD1	5:U:47:LEU:HB2	1.95	0.66
5:A:38:ILE:HD12	5:A:39:VAL:N	2.11	0.65
5:D:30:VAL:HG13	5:D:31:LEU:N	2.10	0.65
6:R:21:PHE:CD2	15:R:102:CRT:H16	2.24	0.65
9:9:102:BCL:CHD	9:0:101:BCL:HMD2	2.25	0.65
2:L:89:LEU:HD13	2:L:97:ILE:CD1	2.25	0.65
5:A:18:ARG:HG3	5:9:14:ILE:HG12	1.77	0.65
5:Q:43:ASP:HB2	5:S:47:LEU:HB3	1.77	0.65
1:C:292:PRO:O	1:C:296:LYS:HG3	1.97	0.65
2:L:243:LEU:O	2:L:247:LEU:HG	1.96	0.65
4:H:55:VAL:HG13	4:H:56:VAL:N	2.10	0.65
6:B:45:TRP:O	6:B:46:LEU:HG	1.97	0.65
5:O:4:MET:HG3	6:R:23:GLN:CB	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:2:PHE:HA	5:U:5:ASN:ND2	2.08	0.65
15:V:102:CRT:H392	5:W:36:HIS:ND1	2.12	0.65
5:W:3:THR:O	5:W:5:ASN:N	2.29	0.65
6:Z:33:VAL:HG22	6:Z:37:LEU:HD12	1.77	0.65
5:3:12:TRP:NE1	6:4:18:HIS:HB2	2.11	0.65
5:5:10:LYS:HB3	15:8:101:CRT:H21A	1.77	0.65
1:C:254:ARG:HH12	3:M:307:TYR:HD2	1.44	0.65
2:L:276:LEU:HD21	3:M:92:TRP:CH2	2.31	0.65
5:A:50:ASN:OD1	6:B:43:ARG:NH2	2.29	0.65
9:S:102:BCL:CHD	9:S:102:BCL:HBC2	2.26	0.65
5:U:49:ASP:CG	5:U:50:ASN:H	1.99	0.65
5:9:46:TRP:NE1	5:9:47:LEU:HD22	2.12	0.65
2:L:94:LEU:O	2:L:98:ILE:HG13	1.97	0.65
9:D:102:BCL:HMB1	9:D:102:BCL:CBB	2.25	0.65
6:E:44:PRO:CD	5:F:55:TYR:OH	2.44	0.65
9:I:103:BCL:HMB3	9:K:102:BCL:CHB	2.26	0.65
6:J:34:ILE:HD13	6:J:35:ALA:N	2.12	0.65
15:J:101:CRT:H393	5:K:36:HIS:CG	2.32	0.65
5:S:27:PHE:CZ	5:U:29:ILE:HG13	2.31	0.65
15:W:103:CRT:H183	6:Z:25:MET:CA	2.27	0.65
5:Y:12:TRP:NE1	6:Z:18:HIS:HA	2.08	0.65
4:H:215:LYS:H	4:H:218:HIS:HD2	1.42	0.65
5:D:2:PHE:N	6:E:26:TYR:HH	1.95	0.65
5:F:20:VAL:O	5:F:24:ILE:HG12	1.97	0.65
5:I:8:LEU:O	5:I:11:ILE:HG22	1.97	0.65
9:N:101:BCL:HMA1	15:N:102:CRT:H35	1.77	0.65
6:R:42:TYR:CD2	6:R:43:ARG:HG3	2.31	0.65
6:V:17:PHE:CD1	15:V:102:CRT:C9	2.78	0.65
6:X:45:TRP:CD2	9:X:101:BCL:H2C	2.32	0.65
5:1:13:LEU:CB	15:4:102:CRT:H1M3	2.21	0.65
5:7:29:ILE:CG2	5:7:30:VAL:H	2.09	0.65
9:7:103:BCL:HMB3	9:9:102:BCL:C4A	2.27	0.65
9:M:401:BCL:H8	9:M:401:BCL:H143	1.77	0.65
6:J:31:LEU:O	6:J:34:ILE:HG23	1.96	0.65
5:9:9:TYR:HA	6:0:18:HIS:CG	2.32	0.65
6:N:20:ILE:HA	6:N:23:GLN:OE1	1.97	0.65
5:Q:5:ASN:ND2	6:R:22:MET:HG2	2.10	0.65
6:R:29:PHE:O	6:R:33:VAL:HB	1.97	0.65
5:S:44:LEU:HD21	5:U:47:LEU:HD12	1.78	0.65
5:W:50:ASN:HD22	5:W:51:ILE:HG12	1.60	0.65
6:8:34:ILE:HG12	6:8:37:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:NE	1:C:312:GLN:NE2	2.44	0.65
6:E:22:MET:HG3	6:E:26:TYR:HE1	1.62	0.65
6:E:46:LEU:HD22	6:G:42:TYR:CZ	2.32	0.65
5:F:4:MET:HG2	6:J:23:GLN:HG3	1.79	0.65
9:F:102:BCL:CBC	9:F:102:BCL:CHD	2.74	0.65
6:V:46:LEU:HB3	6:X:42:TYR:OH	1.97	0.65
5:1:44:LEU:HG	5:1:44:LEU:O	1.96	0.65
5:5:10:LYS:CG	15:8:101:CRT:H21A	2.26	0.65
5:5:12:TRP:HZ3	5:5:17:PRO:HA	1.61	0.65
5:7:43:ASP:CA	5:9:48:ASP:HB3	2.25	0.65
3:M:70:ILE:HG23	3:M:71:ILE:N	2.10	0.65
3:M:144:GLN:HB3	3:M:147:SER:OG	1.97	0.65
3:M:163:ILE:O	3:M:167:MET:HB2	1.97	0.65
6:E:33:VAL:O	6:E:37:LEU:HD23	1.95	0.65
5:F:12:TRP:HB2	6:G:14:ALA:HB1	1.79	0.65
6:G:28:TRP:HE1	6:G:32:VAL:HG21	1.59	0.65
15:X:102:CRT:H343	9:Y:102:BCL:HAA1	1.78	0.65
5:Y:30:VAL:HA	5:Y:33:LEU:HG	1.78	0.65
5:1:14:ILE:CD1	5:1:15:LEU:HG	2.27	0.65
5:5:30:VAL:HG13	5:5:31:LEU:N	2.11	0.65
6:6:29:PHE:O	6:6:33:VAL:HG23	1.96	0.65
5:9:12:TRP:HZ3	5:9:15:LEU:HD12	1.61	0.65
3:M:27:ASN:HD22	5:O:19:ARG:HE	1.45	0.64
5:D:49:ASP:HB2	5:F:56:GLN:OE1	1.96	0.64
6:E:10:THR:HG22	6:E:11:ASP:N	2.11	0.64
5:W:26:ALA:HA	5:W:29:ILE:HG21	1.78	0.64
5:W:40:LEU:HD12	5:W:45:ASN:HA	1.79	0.64
6:X:37:LEU:O	6:X:37:LEU:HD23	1.96	0.64
5:3:14:ILE:CG2	5:5:17:PRO:HB2	2.28	0.64
5:5:16:ASP:HB2	5:5:19:ARG:HH21	1.61	0.64
2:L:159:ILE:H	2:L:159:ILE:CD1	2.08	0.64
3:M:228:ARG:HB3	4:H:199:PHE:CE1	2.33	0.64
5:D:4:MET:O	5:D:8:LEU:HG	1.98	0.64
15:J:101:CRT:H391	5:K:36:HIS:HB3	1.80	0.64
5:K:27:PHE:HE2	5:O:29:ILE:HD11	1.62	0.64
5:K:44:LEU:CD1	5:K:44:LEU:H	2.09	0.64
9:Q:102:BCL:HMD2	9:R:101:BCL:C1D	2.27	0.64
6:V:10:THR:HG22	6:V:11:ASP:N	2.13	0.64
15:W:103:CRT:H20	6:Z:25:MET:HG3	1.79	0.64
5:Y:36:HIS:CE1	9:Y:102:BCL:NA	2.65	0.64
6:2:17:PHE:CD1	15:2:102:CRT:C6	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:20:ILE:HG23	15:4:102:CRT:C7	2.26	0.64
3:M:164:ARG:NH1	3:M:173:LYS:HB3	2.03	0.64
5:D:30:VAL:HG13	5:D:31:LEU:H	1.61	0.64
6:G:30:GLY:O	6:G:34:ILE:HG22	1.97	0.64
5:K:20:VAL:HA	5:K:23:SER:OG	1.97	0.64
5:U:29:ILE:CG2	5:U:30:VAL:N	2.60	0.64
6:Z:12:ASP:HA	6:Z:15:LYS:HD2	1.80	0.64
5:1:10:LYS:CG	6:4:20:ILE:HD13	2.27	0.64
3:M:63:PHE:HZ	5:Q:33:LEU:HD23	1.63	0.64
4:H:130:LEU:HD12	4:H:131:PRO:HD2	1.80	0.64
5:I:18:ARG:HA	5:I:21:LEU:HB3	1.79	0.64
5:I:44:LEU:CD1	5:I:46:TRP:HE3	2.11	0.64
9:P:101:BCL:C1B	9:Q:102:BCL:HMB3	2.28	0.64
2:L:3:MET:HE1	4:H:45:ARG:HH21	1.61	0.64
3:M:175:VAL:HG22	3:M:185:TRP:CD2	2.33	0.64
4:H:13:GLN:NE2	12:H:304:PO4:P	2.70	0.64
6:G:40:TRP:CB	9:G:101:BCL:H191	2.27	0.64
15:P:102:CRT:H391	5:Q:36:HIS:CG	2.31	0.64
6:R:38:LEU:HD12	6:R:38:LEU:O	1.98	0.64
6:8:46:LEU:HB2	5:9:52:PRO:HD3	1.79	0.64
3:M:238:ILE:HG23	3:M:263:GLU:HB2	1.78	0.64
4:H:35:LYS:HE3	4:H:39:TYR:CE2	2.32	0.64
9:E:101:BCL:CHB	9:F:102:BCL:HMB3	2.27	0.64
15:X:102:CRT:C34	9:Y:102:BCL:HAA1	2.28	0.64
5:3:51:ILE:HA	5:3:53:VAL:H	1.62	0.64
6:8:17:PHE:CE1	15:8:101:CRT:H6	2.32	0.64
5:F:4:MET:CG	6:J:23:GLN:HG3	2.28	0.64
15:G:102:CRT:H391	5:I:36:HIS:CB	2.27	0.64
6:J:14:ALA:O	6:J:18:HIS:HB2	1.98	0.64
6:X:45:TRP:O	6:X:46:LEU:CG	2.46	0.64
2:L:89:LEU:HD13	2:L:97:ILE:HD12	1.79	0.64
9:M:401:BCL:C14	10:M:403:BPH:CMA	2.60	0.64
4:H:69:LEU:HB3	4:H:70:PRO:HD2	1.80	0.64
5:A:29:ILE:HD11	15:A:101:CRT:H343	1.78	0.64
5:K:24:ILE:CG1	15:N:102:CRT:H243	2.27	0.64
5:S:42:THR:HG22	5:S:43:ASP:N	2.11	0.64
5:Y:43:ASP:N	5:1:48:ASP:HB3	2.12	0.64
5:1:29:ILE:CG2	5:1:30:VAL:N	2.61	0.64
9:4:101:BCL:C4	15:4:102:CRT:H242	2.27	0.64
5:7:12:TRP:CZ3	6:8:17:PHE:CE2	2.85	0.64
6:0:11:ASP:O	6:0:15:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:34:ILE:HD13	6:0:35:ALA:N	2.13	0.64
5:I:29:ILE:CG2	5:I:30:VAL:H	2.10	0.64
5:Q:44:LEU:HD12	5:Q:46:TRP:HE3	1.63	0.64
5:U:51:ILE:HB	5:U:52:PRO:CA	2.24	0.64
6:V:10:THR:HG22	6:V:11:ASP:H	1.62	0.64
6:4:20:ILE:CG2	15:4:102:CRT:C7	2.76	0.64
5:5:53:VAL:O	5:5:57:ALA:HB3	1.98	0.64
6:8:34:ILE:HD13	6:8:34:ILE:O	1.98	0.64
1:C:85:LEU:HD11	1:C:329:GLY:HA3	1.80	0.64
4:H:5:ILE:HB	5:D:42:THR:CG2	2.28	0.64
6:G:12:ASP:O	6:G:16:GLU:HG3	1.97	0.64
9:Q:102:BCL:CBC	9:R:101:BCL:CMD	2.71	0.64
5:S:35:ILE:HD11	15:T:102:CRT:H371	1.80	0.64
5:W:10:LYS:HD2	6:Z:20:ILE:HD12	1.78	0.64
15:2:102:CRT:H393	5:3:36:HIS:CD2	2.33	0.64
5:7:47:LEU:HD22	5:7:47:LEU:H	1.62	0.64
3:M:261:THR:O	3:M:265:ILE:HG22	1.98	0.63
5:O:18:ARG:NH1	5:O:18:ARG:HB2	2.12	0.63
9:4:101:BCL:CHB	9:5:102:BCL:HMB3	2.27	0.63
5:A:16:ASP:OD1	5:A:19:ARG:HB2	1.98	0.63
5:F:9:TYR:CE1	5:F:10:LYS:HD3	2.33	0.63
9:I:103:BCL:HMC3	9:K:102:BCL:HBB1	1.80	0.63
15:J:101:CRT:H2M3	5:K:36:HIS:HB2	1.81	0.63
5:K:44:LEU:CD2	5:K:46:TRP:HE3	2.11	0.63
15:N:102:CRT:C37	9:O:102:BCL:HMB2	2.27	0.63
5:O:36:HIS:NE2	9:P:101:BCL:HMD1	2.11	0.63
6:X:42:TYR:CE2	6:X:43:ARG:HD2	2.33	0.63
5:3:46:TRP:HZ3	9:3:102:BCL:HBC3	1.63	0.63
5:5:2:PHE:CB	5:5:5:ASN:HD22	2.11	0.63
1:C:27:PRO:HD3	5:3:41:SER:OG	1.98	0.63
1:C:85:LEU:HD22	1:C:89:GLU:HG2	1.79	0.63
2:L:3:MET:HE1	4:H:45:ARG:NH2	2.13	0.63
3:M:123:THR:HG21	3:M:162:PHE:HE2	1.61	0.63
3:M:194:GLY:O	3:M:195:ASN:HB3	1.97	0.63
4:H:54:LYS:CD	4:H:58:PHE:HA	2.28	0.63
5:I:49:ASP:OD1	5:I:50:ASN:N	2.31	0.63
9:Q:102:BCL:CBC	9:R:101:BCL:HMD3	2.28	0.63
5:S:13:LEU:HD21	6:T:10:THR:O	1.98	0.63
6:6:40:TRP:HZ3	6:6:45:TRP:H	1.47	0.63
1:C:226:LEU:HD11	3:M:189:PHE:HA	1.80	0.63
3:M:31:ILE:HD12	16:M:407:PGW:H05	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:7:ASN:O	5:D:10:LYS:HD3	1.99	0.63
5:3:51:ILE:HA	5:3:53:VAL:N	2.13	0.63
5:D:14:ILE:HD12	5:D:14:ILE:N	2.13	0.63
15:G:102:CRT:H2M1	5:I:33:LEU:O	1.99	0.63
5:K:49:ASP:CG	5:K:50:ASN:N	2.52	0.63
15:N:102:CRT:H391	5:O:36:HIS:CG	2.33	0.63
5:O:46:TRP:CD1	5:O:47:LEU:HD13	2.32	0.63
6:R:44:PRO:O	5:S:52:PRO:CG	2.46	0.63
5:U:28:GLN:NE2	15:V:102:CRT:H25	2.13	0.63
9:W:102:BCL:HBC3	9:X:101:BCL:HMD2	1.80	0.63
9:M:401:BCL:H72	10:M:403:BPH:HMA3	1.79	0.63
6:B:18:HIS:HE1	6:B:22:MET:HE2	1.64	0.63
6:E:45:TRP:HA	5:F:52:PRO:CD	2.29	0.63
5:F:19:ARG:NH1	5:I:18:ARG:HH21	1.96	0.63
6:P:16:GLU:OE2	15:P:102:CRT:C1M	2.45	0.63
5:Q:29:ILE:CG2	5:Q:30:VAL:N	2.61	0.63
5:S:55:TYR:HD1	5:S:56:GLN:N	1.97	0.63
5:W:36:HIS:NE2	9:X:101:BCL:HMD1	2.13	0.63
6:4:45:TRP:O	6:4:46:LEU:HG	1.99	0.63
6:0:18:HIS:O	6:0:22:MET:HB2	1.98	0.63
2:L:175:HIS:HD1	2:L:177:HIS:HB2	1.64	0.63
2:L:207:THR:HA	2:L:215:VAL:HG13	1.80	0.63
3:M:175:VAL:CB	15:M:406:CRT:H242	2.29	0.63
4:H:125:LEU:HD23	4:H:129:GLY:O	1.99	0.63
6:B:20:ILE:HG21	15:B:102:CRT:C8	2.20	0.63
5:D:15:LEU:HB3	5:D:20:VAL:HG21	1.80	0.63
6:2:17:PHE:CD1	15:2:102:CRT:C9	2.82	0.63
6:4:41:LEU:HD23	6:4:41:LEU:O	1.99	0.63
1:C:109:TYR:OH	1:C:160:PRO:HB3	1.99	0.63
2:L:179:ASN:HB3	2:L:182:HIS:CB	2.28	0.63
3:M:136:ARG:NE	3:M:136:ARG:HA	2.14	0.63
4:H:91:PRO:HA	4:H:100:LEU:HD23	1.81	0.63
5:S:11:ILE:HA	15:V:102:CRT:C8	2.28	0.63
5:U:12:TRP:NE1	6:V:18:HIS:HA	2.14	0.63
5:Y:49:ASP:CB	5:1:56:GLN:HG2	2.29	0.63
5:5:27:PHE:CZ	5:7:29:ILE:HD11	2.34	0.63
1:C:298:PRO:HG2	1:C:299:TYR:HD1	1.64	0.63
2:L:89:LEU:CD1	2:L:97:ILE:HD12	2.29	0.63
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.81	0.63
4:H:227:ASN:HD22	4:H:228:PRO:HD2	1.64	0.63
9:A:102:BCL:H162	5:9:12:TRP:HH2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:102:CRT:H1M1	5:9:10:LYS:HG2	1.81	0.63
5:K:50:ASN:HB3	5:O:59:GLY:CA	2.27	0.63
5:Q:31:LEU:O	5:Q:35:ILE:HG12	1.98	0.63
5:Y:33:LEU:HD12	5:Y:34:LEU:N	2.14	0.63
2:L:223:THR:HG22	3:M:20:GLY:HA2	1.80	0.62
3:M:314:VAL:HG12	3:M:315:ASN:N	2.09	0.62
4:H:222:VAL:HG22	4:H:242:TYR:CE2	2.34	0.62
6:G:21:PHE:CD2	15:G:102:CRT:H16	2.34	0.62
6:T:10:THR:HG22	6:T:11:ASP:N	2.13	0.62
5:W:21:LEU:O	5:W:25:VAL:HG23	1.99	0.62
5:W:22:VAL:O	5:W:25:VAL:HB	1.97	0.62
15:W:103:CRT:H391	5:1:36:HIS:HB3	1.81	0.62
5:5:8:LEU:O	5:5:11:ILE:HG13	1.99	0.62
4:H:29:TYR:CD1	4:H:29:TYR:C	2.72	0.62
6:T:42:TYR:CD2	6:T:43:ARG:HG2	2.34	0.62
5:Y:16:ASP:CB	5:Y:18:ARG:HE	2.12	0.62
9:7:102:BCL:C1D	9:7:103:BCL:HMD2	2.29	0.62
2:L:10:TYR:CE1	3:M:247:ARG:HG2	2.34	0.62
5:F:8:LEU:HD21	6:J:24:SER:OG	1.99	0.62
9:I:102:BCL:HMD2	9:I:103:BCL:C1D	2.29	0.62
15:W:103:CRT:H9	6:Z:17:PHE:HE1	1.65	0.62
5:1:46:TRP:CZ3	9:1:102:BCL:HBC3	2.34	0.62
5:5:13:LEU:CD2	6:6:14:ALA:HB2	2.30	0.62
5:5:20:VAL:HA	5:5:23:SER:HB3	1.80	0.62
5:7:35:ILE:HD12	9:7:103:BCL:O1D	1.99	0.62
3:M:2:PRO:CG	3:M:42:LYS:CE	2.75	0.62
3:M:234:GLU:O	3:M:238:ILE:HG12	2.00	0.62
4:H:151:PRO:HA	4:H:154:MET:SD	2.40	0.62
4:H:154:MET:O	4:H:167:VAL:HG22	1.98	0.62
5:A:5:ASN:HB2	6:B:22:MET:HE1	1.80	0.62
5:A:8:LEU:HD22	6:E:20:ILE:HG23	1.82	0.62
5:D:39:VAL:HG13	5:D:43:ASP:OD2	1.99	0.62
6:J:30:GLY:O	6:J:33:VAL:HG12	2.00	0.62
5:U:42:THR:HB	5:W:48:ASP:CB	2.28	0.62
6:X:17:PHE:O	6:X:20:ILE:HG22	1.99	0.62
5:1:14:ILE:HD12	5:1:15:LEU:H	1.62	0.62
6:4:25:MET:HA	15:4:102:CRT:C16	2.29	0.62
1:C:192:TYR:HB2	2:L:270:GLU:HA	1.82	0.62
2:L:42:PHE:HD2	2:L:101:CYS:HA	1.64	0.62
4:H:193:VAL:HG11	4:H:222:VAL:HB	1.82	0.62
9:E:101:BCL:HMB3	9:F:102:BCL:C4A	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:102:BCL:CBB	9:Y:102:BCL:HMB1	2.30	0.62
1:C:314:VAL:HG11	1:C:319:TYR:CD1	2.35	0.62
4:H:121:LYS:HA	4:H:234:TYR:HB2	1.82	0.62
15:P:102:CRT:H393	5:Q:36:HIS:CG	2.35	0.62
6:R:45:TRP:CZ3	9:R:101:BCL:HAC2	2.32	0.62
9:U:102:BCL:HMB1	9:U:102:BCL:CBB	2.30	0.62
6:V:42:TYR:CE2	6:V:43:ARG:HG3	2.35	0.62
9:X:101:BCL:H43	15:X:102:CRT:H292	1.81	0.62
6:2:43:ARG:HD3	5:3:55:TYR:CG	2.34	0.62
9:5:102:BCL:CBC	9:6:101:BCL:HBC3	2.29	0.62
1:C:166:TRP:HH2	1:C:205:ASP:HB2	1.65	0.62
9:L:303:BCL:O1D	3:M:203:MET:HB3	2.00	0.62
5:A:26:ALA:O	5:A:29:ILE:HG22	2.00	0.62
6:B:24:SER:O	6:B:27:ALA:HB3	2.00	0.62
6:P:34:ILE:O	6:P:38:LEU:HB3	2.00	0.62
5:S:10:LYS:HB3	15:V:102:CRT:H21A	1.82	0.62
5:S:33:LEU:O	5:S:37:MET:HB2	1.99	0.62
6:8:45:TRP:O	6:8:46:LEU:CG	2.48	0.62
1:C:157:ARG:NE	1:C:312:GLN:HE22	1.98	0.62
4:H:222:VAL:HG22	4:H:242:TYR:HE2	1.64	0.62
6:E:23:GLN:HG3	6:E:24:SER:N	2.14	0.62
6:E:45:TRP:HA	5:F:52:PRO:HD3	1.81	0.62
5:F:40:LEU:HD11	5:F:47:LEU:HD12	1.81	0.62
9:I:103:BCL:CHB	9:K:102:BCL:HMB3	2.30	0.62
5:K:27:PHE:CE2	5:O:29:ILE:HD11	2.34	0.62
6:P:12:ASP:O	6:P:16:GLU:HG3	1.99	0.62
6:R:20:ILE:HD12	15:R:102:CRT:C10	2.29	0.62
9:B:101:BCL:HMB1	9:B:101:BCL:CBB	2.30	0.62
6:J:33:VAL:O	6:J:37:LEU:HD23	2.00	0.62
5:K:5:ASN:ND2	6:N:22:MET:HG2	2.14	0.62
5:O:5:ASN:O	5:O:8:LEU:CD2	2.47	0.62
9:9:102:BCL:HMB1	9:9:102:BCL:CBB	2.30	0.62
1:C:202:PRO:HG2	1:C:203:PHE:HD1	1.65	0.62
2:L:4:LEU:HD22	4:H:38:GLY:HA3	1.80	0.62
2:L:229:VAL:O	9:M:401:BCL:H192	1.99	0.62
3:M:61:ILE:O	3:M:65:LEU:HB2	1.99	0.62
4:H:47:GLU:HB3	5:A:19:ARG:HG3	1.81	0.62
15:A:101:CRT:H21A	5:7:10:LYS:HG2	1.82	0.62
5:I:33:LEU:HD12	5:I:34:LEU:N	2.15	0.62
5:3:12:TRP:HE1	6:4:18:HIS:HA	1.64	0.62
1:C:24:GLU:HG2	1:C:45:ASN:ND2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:303:BCL:O1A	3:M:207:ALA:HA	1.99	0.61
5:A:9:TYR:CB	6:B:18:HIS:CD2	2.83	0.61
6:E:42:TYR:CD2	6:E:43:ARG:HG3	2.35	0.61
6:P:17:PHE:CE1	15:P:102:CRT:H11	2.35	0.61
9:R:101:BCL:HBB2	9:R:101:BCL:H162	1.82	0.61
5:S:9:TYR:HA	6:T:18:HIS:CG	2.35	0.61
5:U:30:VAL:HG13	5:U:31:LEU:N	2.15	0.61
6:V:28:TRP:HA	6:V:31:LEU:HD12	1.81	0.61
15:X:102:CRT:H2M1	5:Y:36:HIS:CB	2.30	0.61
5:Y:21:LEU:O	5:Y:25:VAL:HG23	2.00	0.61
5:5:13:LEU:O	6:6:7:THR:HA	1.99	0.61
5:5:36:HIS:CE1	9:6:101:BCL:HMD1	2.35	0.61
6:8:31:LEU:O	6:8:34:ILE:HG22	2.00	0.61
6:0:10:THR:HB	6:0:13:GLU:OE2	1.98	0.61
5:D:36:HIS:NE2	9:E:101:BCL:HMD1	2.15	0.61
5:W:46:TRP:CZ3	9:W:102:BCL:HAC1	2.35	0.61
5:1:10:LYS:CG	6:4:20:ILE:CD1	2.78	0.61
15:2:102:CRT:H393	5:3:36:HIS:CG	2.34	0.61
15:8:101:CRT:H391	5:9:36:HIS:CG	2.35	0.61
2:L:89:LEU:HD12	2:L:94:LEU:N	2.15	0.61
2:L:160:LEU:HA	2:L:163:LEU:HD13	1.80	0.61
5:A:43:ASP:O	5:D:56:GLN:CD	2.39	0.61
5:A:50:ASN:CG	5:A:51:ILE:HG12	2.21	0.61
5:D:53:VAL:O	5:D:56:GLN:HB2	2.00	0.61
5:F:50:ASN:HA	5:I:60:LYS:CB	2.30	0.61
6:P:10:THR:HG22	6:P:11:ASP:N	2.14	0.61
5:U:35:ILE:CA	5:U:38:ILE:HG22	2.30	0.61
6:Z:46:LEU:HB2	5:1:52:PRO:HD3	1.81	0.61
5:1:46:TRP:CH2	9:1:102:BCL:HBC3	2.36	0.61
6:2:20:ILE:O	6:2:20:ILE:HD13	2.00	0.61
5:3:18:ARG:HA	5:3:21:LEU:HB3	1.83	0.61
6:8:22:MET:SD	6:8:26:TYR:HE2	2.23	0.61
1:C:24:GLU:CG	1:C:45:ASN:ND2	2.62	0.61
4:H:54:LYS:HD2	4:H:58:PHE:HA	1.82	0.61
5:A:45:ASN:OD1	5:A:47:LEU:HB2	2.00	0.61
6:E:38:LEU:O	6:E:38:LEU:HD23	2.00	0.61
5:F:43:ASP:CB	5:I:47:LEU:HG	2.31	0.61
5:F:51:ILE:HB	5:F:52:PRO:HA	1.82	0.61
5:I:29:ILE:HG22	5:I:30:VAL:H	1.64	0.61
5:I:50:ASN:HB3	5:K:55:TYR:O	1.99	0.61
5:K:39:VAL:HG12	5:K:46:TRP:HZ3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:12:TRP:HA	5:Q:12:TRP:CE3	2.36	0.61
5:3:49:ASP:O	5:5:60:LYS:HA	1.99	0.61
5:5:32:GLY:HA2	9:6:101:BCL:HED2	1.82	0.61
5:9:2:PHE:HA	5:9:5:ASN:ND2	2.12	0.61
5:9:29:ILE:O	5:9:33:LEU:CD1	2.47	0.61
3:M:98:PRO:HG3	3:M:112:GLY:O	2.00	0.61
3:M:246:GLU:HG3	3:M:246:GLU:O	1.99	0.61
4:H:65:LYS:HG2	4:H:66:THR:N	2.15	0.61
5:A:50:ASN:CA	5:D:60:LYS:HA	2.25	0.61
9:B:101:BCL:C1B	9:D:102:BCL:CMB	2.77	0.61
9:I:103:BCL:C1B	9:K:102:BCL:HMB3	2.31	0.61
6:N:38:LEU:HD23	6:N:38:LEU:O	2.00	0.61
9:Q:102:BCL:C1D	9:R:101:BCL:CMD	2.78	0.61
5:1:43:ASP:O	5:3:56:GLN:NE2	2.33	0.61
9:2:101:BCL:HMB3	9:3:102:BCL:C1B	2.29	0.61
2:L:186:ILE:CD1	9:M:401:BCL:OBD	2.47	0.61
5:A:35:ILE:HD11	15:B:102:CRT:H403	1.83	0.61
5:F:19:ARG:HH12	5:I:18:ARG:NH2	1.99	0.61
9:F:102:BCL:HBC2	9:G:101:BCL:HHD	1.81	0.61
5:U:27:PHE:CD2	5:W:29:ILE:CD1	2.68	0.61
9:V:101:BCL:C4A	9:W:102:BCL:HMB3	2.30	0.61
6:2:45:TRP:O	6:2:46:LEU:CG	2.48	0.61
9:I:103:BCL:CBB	9:I:103:BCL:HMB1	2.30	0.61
6:J:20:ILE:HG12	15:J:101:CRT:C7	2.30	0.61
6:N:20:ILE:H	6:N:20:ILE:CD1	2.13	0.61
6:R:16:GLU:OE1	15:R:102:CRT:H23	2.01	0.61
5:S:30:VAL:HG13	5:S:31:LEU:H	1.65	0.61
6:X:46:LEU:N	5:Y:52:PRO:HD3	2.16	0.61
6:4:29:PHE:HZ	9:4:101:BCL:H101	1.64	0.61
6:8:17:PHE:CD1	6:8:20:ILE:CG2	2.83	0.61
2:L:13:ARG:CD	4:H:101:VAL:HG22	2.31	0.61
4:H:24:PHE:O	4:H:28:ILE:HG13	2.01	0.61
5:A:36:HIS:ND1	15:A:101:CRT:H371	2.16	0.61
5:K:44:LEU:HD22	5:K:46:TRP:H	1.65	0.61
6:P:21:PHE:HB2	15:P:102:CRT:H11	1.83	0.61
5:Q:22:VAL:HA	5:Q:25:VAL:HG12	1.82	0.61
5:S:20:VAL:HG23	5:S:21:LEU:N	2.14	0.61
6:2:29:PHE:N	6:2:29:PHE:HD1	1.99	0.61
1:C:275:HIS:O	1:C:279:ILE:HG13	2.00	0.61
5:A:36:HIS:CE1	9:A:102:BCL:C1A	2.82	0.61
5:K:47:LEU:H	5:K:47:LEU:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:5:ASN:O	5:O:8:LEU:HD22	2.01	0.61
6:R:21:PHE:CB	15:R:102:CRT:C14	2.64	0.61
5:U:18:ARG:O	5:U:22:VAL:HG12	2.01	0.61
5:W:50:ASN:HA	5:Y:60:LYS:CB	2.31	0.61
5:Y:51:ILE:HG22	5:1:60:LYS:H	1.65	0.61
5:5:9:TYR:HE2	5:5:10:LYS:CE	2.10	0.61
9:7:102:BCL:HMB1	9:7:102:BCL:CBB	2.31	0.61
9:7:103:BCL:HMC3	9:9:102:BCL:CBB	2.28	0.61
1:C:38:VAL:O	1:C:38:VAL:HG12	2.01	0.61
1:C:179:LYS:HD2	1:C:180:PRO:HD3	1.81	0.61
4:H:35:LYS:CE	4:H:39:TYR:CE2	2.84	0.61
6:G:21:PHE:CD2	15:G:102:CRT:C14	2.76	0.61
15:W:103:CRT:H181	6:Z:25:MET:HA	1.81	0.61
5:1:31:LEU:O	5:1:35:ILE:HG12	2.01	0.61
5:5:10:LYS:CB	15:8:101:CRT:H21A	2.30	0.61
6:0:10:THR:HG22	6:0:11:ASP:N	2.14	0.61
6:0:40:TRP:HZ3	6:0:45:TRP:N	1.99	0.61
3:M:2:PRO:HG3	3:M:42:LYS:NZ	2.16	0.60
5:A:43:ASP:HB2	5:D:47:LEU:HD12	1.83	0.60
5:U:43:ASP:HA	5:W:47:LEU:C	2.22	0.60
5:Y:31:LEU:HD23	9:Z:101:BCL:HED3	1.82	0.60
5:1:44:LEU:HD23	5:1:44:LEU:H	1.66	0.60
5:3:51:ILE:CB	5:3:52:PRO:HA	2.13	0.60
3:M:17:ALA:HB1	3:M:34:PRO:HG2	1.83	0.60
5:A:36:HIS:CG	15:A:101:CRT:H371	2.35	0.60
5:D:5:ASN:HD22	6:E:22:MET:CB	2.13	0.60
5:F:36:HIS:O	5:F:40:LEU:N	2.34	0.60
6:T:17:PHE:HD1	15:T:102:CRT:H6	1.66	0.60
6:T:46:LEU:C	5:U:46:TRP:HB2	2.22	0.60
9:Z:101:BCL:HMB1	9:Z:101:BCL:CBB	2.31	0.60
6:2:46:LEU:HD22	6:4:42:TYR:CE2	2.35	0.60
6:4:46:LEU:HD22	6:6:43:ARG:HH22	1.66	0.60
3:M:14:ARG:CD	3:M:36:PHE:CD1	2.83	0.60
3:M:238:ILE:HD12	3:M:263:GLU:HB2	1.84	0.60
15:G:102:CRT:C39	5:I:36:HIS:CG	2.84	0.60
6:P:32:VAL:HG12	6:P:36:HIS:HD1	1.66	0.60
5:S:50:ASN:HB3	5:U:55:TYR:O	2.01	0.60
5:U:11:ILE:CG2	5:U:15:LEU:HD12	2.31	0.60
6:X:45:TRP:CE3	9:X:101:BCL:H2C	2.35	0.60
4:H:5:ILE:HD11	5:D:38:ILE:O	2.02	0.60
5:I:15:LEU:HD12	5:I:20:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:21:PHE:CD1	6:J:21:PHE:C	2.73	0.60
5:W:43:ASP:CB	5:Y:47:LEU:HD22	2.31	0.60
5:5:44:LEU:HD12	5:5:46:TRP:HE3	1.66	0.60
2:L:243:LEU:HD13	3:M:221:ALA:HB2	1.82	0.60
3:M:31:ILE:CD1	16:M:407:PGW:CAD	2.77	0.60
6:P:30:GLY:O	6:P:33:VAL:HG12	2.02	0.60
5:Q:51:ILE:HG12	5:S:59:GLY:HA3	1.82	0.60
6:R:30:GLY:O	6:R:34:ILE:HG22	2.02	0.60
5:S:51:ILE:HA	5:S:52:PRO:C	2.21	0.60
5:Y:43:ASP:CA	5:1:48:ASP:HB3	2.30	0.60
6:4:13:GLU:O	6:4:16:GLU:HG2	2.01	0.60
6:4:37:LEU:HD23	6:4:37:LEU:C	2.22	0.60
1:C:110:CYS:HA	1:C:123:THR:OG1	2.01	0.60
3:M:159:VAL:HG21	3:M:281:GLY:CA	2.32	0.60
3:M:301:HIS:HE1	4:H:8:TYR:O	1.84	0.60
5:F:36:HIS:NE2	9:G:101:BCL:CMD	2.62	0.60
9:Q:102:BCL:CBB	9:Q:102:BCL:HMB1	2.30	0.60
9:R:101:BCL:HMB1	9:R:101:BCL:CBB	2.31	0.60
9:X:101:BCL:HMA2	9:X:101:BCL:HBA2	1.81	0.60
6:2:46:LEU:HD13	6:4:42:TYR:OH	2.02	0.60
5:7:32:GLY:N	9:7:103:BCL:HED2	2.17	0.60
2:L:4:LEU:H	3:M:253:ARG:HH12	1.46	0.60
2:L:52:TRP:HA	5:A:37:MET:CE	2.31	0.60
2:L:235:ALA:HB2	4:H:176:GLU:OE2	2.02	0.60
3:M:218:MET:CE	3:M:252:TRP:CZ3	2.84	0.60
3:M:220:GLY:O	3:M:224:LEU:HG	2.02	0.60
5:D:51:ILE:CG2	5:D:52:PRO:HA	2.32	0.60
6:E:36:HIS:ND1	9:E:101:BCL:H102	2.16	0.60
5:Q:9:TYR:HA	6:R:18:HIS:CG	2.36	0.60
5:S:9:TYR:HB2	6:T:15:LYS:HA	1.84	0.60
5:3:9:TYR:HA	6:4:18:HIS:ND1	2.16	0.60
6:4:44:PRO:O	5:5:52:PRO:CG	2.48	0.60
5:5:4:MET:O	5:5:8:LEU:HG	2.01	0.60
1:C:75:VAL:HG23	1:C:76:TYR:N	2.17	0.60
1:C:200:LEU:HD11	1:C:238:ASN:ND2	2.16	0.60
2:L:128:PHE:CE2	11:L:304:UQ8:H45B	2.36	0.60
2:L:175:HIS:ND1	2:L:177:HIS:HB2	2.16	0.60
3:M:226:VAL:HG23	3:M:231:GLY:HA3	1.83	0.60
15:B:102:CRT:H2M3	5:D:36:HIS:CG	2.36	0.60
5:I:43:ASP:OD1	5:I:44:LEU:HG	2.02	0.60
9:I:102:BCL:CBC	9:I:102:BCL:CHD	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:29:ILE:CG2	5:O:30:VAL:N	2.64	0.60
5:S:30:VAL:HG13	5:S:31:LEU:N	2.16	0.60
9:T:101:BCL:HMC3	9:U:102:BCL:HBB1	1.82	0.60
9:W:102:BCL:HBC1	9:X:101:BCL:HHD	1.83	0.60
6:4:13:GLU:H	6:4:13:GLU:CD	2.06	0.60
5:7:13:LEU:O	6:8:7:THR:HA	2.01	0.60
1:C:178:LEU:N	1:C:178:LEU:HD23	2.17	0.60
5:A:29:ILE:HG23	5:A:30:VAL:N	2.17	0.60
6:G:17:PHE:C	6:G:17:PHE:CD1	2.75	0.60
6:G:21:PHE:HD1	6:G:21:PHE:C	1.87	0.60
5:K:51:ILE:HA	5:K:52:PRO:C	2.22	0.60
6:R:32:VAL:HG11	9:R:101:BCL:HAA1	1.84	0.60
5:U:17:PRO:O	5:U:21:LEU:HG	2.02	0.60
9:1:102:BCL:HMB1	9:1:102:BCL:CBB	2.31	0.60
5:3:2:PHE:HB3	5:3:5:ASN:HD22	1.66	0.60
9:5:102:BCL:HBC2	9:6:101:BCL:HMD2	1.82	0.60
1:C:254:ARG:C	1:C:254:ARG:HD3	2.22	0.60
5:K:20:VAL:O	5:K:24:ILE:HG13	2.02	0.60
6:P:16:GLU:HB2	15:P:102:CRT:C1M	2.32	0.60
6:V:25:MET:HE3	15:V:102:CRT:H19	1.83	0.60
5:Y:44:LEU:HD22	6:Z:43:ARG:CD	2.31	0.60
5:3:14:ILE:CD1	6:6:17:PHE:HE2	2.14	0.60
15:3:103:CRT:H371	5:5:35:ILE:HD11	1.82	0.60
9:7:103:BCL:HMB1	9:7:103:BCL:CBB	2.32	0.60
2:L:22:LEU:HB2	5:7:19:ARG:CB	2.32	0.59
2:L:144:ARG:O	2:L:148:MET:HG2	2.02	0.59
2:L:200:GLY:O	2:L:204:LEU:HD13	2.02	0.59
3:M:152:ALA:O	3:M:155:PHE:HB3	2.02	0.59
5:A:21:LEU:HD13	15:B:102:CRT:H14	1.80	0.59
9:D:102:BCL:C1D	9:E:101:BCL:CMD	2.80	0.59
9:E:101:BCL:NB	9:F:102:BCL:HMB3	2.17	0.59
5:F:30:VAL:HG13	5:F:31:LEU:N	2.18	0.59
5:O:44:LEU:HD12	5:O:46:TRP:N	2.16	0.59
6:P:17:PHE:CB	15:P:102:CRT:H41	2.28	0.59
5:U:10:LYS:CB	15:X:102:CRT:H6	2.29	0.59
6:6:29:PHE:CE1	9:6:101:BCL:H11	2.37	0.59
5:7:34:LEU:HD12	5:7:34:LEU:O	2.01	0.59
1:C:35:TYR:HB3	1:C:38:VAL:CG2	2.32	0.59
9:A:102:BCL:HMB1	9:A:102:BCL:CBB	2.32	0.59
5:I:52:PRO:HB2	5:I:55:TYR:CE2	2.36	0.59
9:I:102:BCL:CAC	9:I:103:BCL:HBC3	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:16:ASP:O	5:U:20:VAL:HG23	2.02	0.59
5:W:10:LYS:CB	15:W:103:CRT:H23	2.29	0.59
5:1:44:LEU:CD1	6:2:43:ARG:HD2	2.27	0.59
6:2:17:PHE:HD1	15:2:102:CRT:C7	2.16	0.59
5:7:50:ASN:CG	5:7:51:ILE:N	2.54	0.59
2:L:52:TRP:N	5:A:37:MET:HE1	2.17	0.59
5:A:33:LEU:HG	15:A:101:CRT:H393	1.80	0.59
6:B:33:VAL:O	6:B:37:LEU:HB2	2.02	0.59
5:Q:17:PRO:O	5:Q:21:LEU:HG	2.02	0.59
6:R:21:PHE:HB2	15:R:102:CRT:C12	2.31	0.59
15:R:102:CRT:H342	9:S:102:BCL:CBA	2.32	0.59
9:V:101:BCL:CHB	9:W:102:BCL:HMB3	2.31	0.59
5:W:39:VAL:HG22	5:Y:47:LEU:HD11	1.84	0.59
5:3:12:TRP:HE1	6:4:18:HIS:CA	2.16	0.59
5:7:5:ASN:O	5:7:6:ALA:O	2.20	0.59
3:M:14:ARG:HD3	3:M:36:PHE:CE1	2.38	0.59
5:Q:12:TRP:HA	5:Q:12:TRP:HE3	1.67	0.59
6:V:20:ILE:O	6:V:20:ILE:HD13	2.01	0.59
5:5:51:ILE:HG22	5:5:52:PRO:HA	1.83	0.59
3:M:123:THR:CG2	3:M:162:PHE:HE2	2.16	0.59
9:F:102:BCL:C1D	9:G:101:BCL:CMD	2.78	0.59
5:I:10:LYS:CG	15:N:102:CRT:H1M1	2.29	0.59
5:O:17:PRO:O	5:O:21:LEU:HD13	2.03	0.59
5:Q:30:VAL:HG13	5:Q:31:LEU:N	2.18	0.59
1:C:263:THR:C	3:M:313:ALA:HB2	2.23	0.59
15:A:103:CRT:H393	5:F:36:HIS:CG	2.38	0.59
6:B:20:ILE:O	6:B:20:ILE:HD13	2.02	0.59
5:I:10:LYS:HB3	15:N:102:CRT:H82	1.83	0.59
9:I:102:BCL:HBC2	9:I:102:BCL:HHD	1.83	0.59
5:K:44:LEU:HD13	5:K:44:LEU:H	1.66	0.59
6:N:28:TRP:HA	6:N:31:LEU:CD1	2.32	0.59
5:U:13:LEU:O	6:V:7:THR:CA	2.48	0.59
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.67	0.59
2:L:250:ALA:HB2	10:L:302:BPH:HBC2	1.85	0.59
3:M:155:PHE:O	3:M:159:VAL:HG23	2.01	0.59
4:H:55:VAL:HG13	4:H:56:VAL:HG22	1.85	0.59
5:F:9:TYR:CE1	6:G:15:LYS:HG3	2.37	0.59
5:F:27:PHE:CE2	5:I:29:ILE:CD1	2.83	0.59
5:K:50:ASN:ND2	5:K:51:ILE:HG12	2.17	0.59
9:K:102:BCL:C2D	9:N:101:BCL:HMD2	2.32	0.59
9:K:102:BCL:CBB	9:K:102:BCL:HMB1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:46:LEU:HB3	6:T:42:TYR:HH	1.66	0.59
5:3:46:TRP:CE3	9:3:102:BCL:H2C	2.38	0.59
6:6:28:TRP:O	6:6:31:LEU:N	2.36	0.59
6:0:32:VAL:CG1	6:0:33:VAL:N	2.64	0.59
1:C:112:VAL:HB	1:C:115:ASN:HB2	1.84	0.59
3:M:168:MET:CE	3:M:289:THR:HG22	2.33	0.59
4:H:125:LEU:HD12	4:H:125:LEU:N	2.18	0.59
6:B:16:GLU:CD	15:B:102:CRT:C2	2.70	0.59
6:B:46:LEU:HD13	6:E:42:TYR:CZ	2.38	0.59
5:D:53:VAL:HA	5:D:56:GLN:HG3	1.85	0.59
9:E:101:BCL:HMC3	9:F:102:BCL:HBB1	1.85	0.59
5:I:50:ASN:CG	5:I:51:ILE:H	2.06	0.59
6:P:17:PHE:CD1	15:P:102:CRT:C9	2.77	0.59
6:P:20:ILE:CG2	6:P:21:PHE:N	2.65	0.59
5:Q:40:LEU:HD21	5:Q:47:LEU:HD12	1.85	0.59
6:R:45:TRP:CE3	9:R:101:BCL:H2C	2.36	0.59
6:R:45:TRP:O	6:R:46:LEU:HB2	2.02	0.59
5:U:29:ILE:CG2	5:U:30:VAL:H	2.16	0.59
9:6:101:BCL:HMB1	9:6:101:BCL:CBB	2.32	0.59
3:M:108:PRO:HA	5:Q:41:SER:O	2.03	0.59
4:H:11:ALA:O	4:H:14:ILE:CG2	2.49	0.59
4:H:251:THR:HG22	4:H:253:GLU:H	1.68	0.59
5:A:40:LEU:HD12	5:A:40:LEU:O	2.02	0.59
5:F:9:TYR:CE2	6:G:15:LYS:NZ	2.68	0.59
5:F:11:ILE:O	5:F:14:ILE:HG12	2.03	0.59
9:F:102:BCL:ND	9:G:101:BCL:HMD2	2.17	0.59
6:G:46:LEU:HB3	6:J:42:TYR:CZ	2.37	0.59
15:P:102:CRT:H2M3	5:Q:36:HIS:HB3	1.74	0.59
6:R:44:PRO:O	5:S:52:PRO:HG3	2.02	0.59
5:3:36:HIS:CE1	9:3:102:BCL:NA	2.70	0.59
5:7:7:ASN:O	5:7:10:LYS:HD3	2.03	0.59
5:7:29:ILE:CG2	5:7:30:VAL:N	2.65	0.59
6:0:21:PHE:C	6:0:21:PHE:CD1	2.75	0.59
6:0:30:GLY:O	6:0:34:ILE:HG22	2.02	0.59
2:L:10:TYR:HE1	3:M:247:ARG:NE	1.99	0.59
2:L:42:PHE:CE2	2:L:104:GLY:HA3	2.37	0.59
3:M:83:VAL:HG23	3:M:84:PHE:HD1	1.67	0.59
9:M:401:BCL:C13	10:M:403:BPH:HMA1	2.33	0.59
5:A:51:ILE:CB	5:A:52:PRO:HA	2.32	0.59
15:A:103:CRT:C21	5:D:24:ILE:HD13	2.31	0.59
6:N:13:GLU:HA	6:N:16:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:38:ILE:HG13	5:O:39:VAL:N	2.17	0.59
6:P:21:PHE:CD1	6:P:21:PHE:O	2.56	0.59
6:P:21:PHE:HB2	15:P:102:CRT:C11	2.32	0.59
6:X:37:LEU:HA	9:X:101:BCL:H193	1.85	0.59
5:Y:45:ASN:O	5:Y:47:LEU:N	2.36	0.59
9:7:103:BCL:CMA	15:8:101:CRT:H35	2.32	0.59
15:8:101:CRT:H403	9:9:102:BCL:HMB2	1.84	0.59
1:C:285:TRP:HE1	1:C:304:ARG:HD3	1.68	0.58
2:L:181:ALA:HB3	2:L:256:CYS:HA	1.85	0.58
5:S:5:ASN:HD22	6:T:22:MET:HG3	1.66	0.58
6:Z:42:TYR:CD1	6:Z:43:ARG:HG3	2.38	0.58
9:4:101:BCL:HMB1	9:4:101:BCL:CBB	2.32	0.58
5:5:9:TYR:HA	6:6:18:HIS:CG	2.38	0.58
1:C:64:ALA:HA	1:C:92:ARG:NH1	2.18	0.58
9:L:301:BCL:H122	10:L:302:BPH:H3A	1.86	0.58
3:M:258:PHE:CD2	17:H:301:PEF:C31	2.86	0.58
6:B:29:PHE:CE1	9:B:101:BCL:H12	2.38	0.58
6:E:37:LEU:HD22	9:E:101:BCL:H143	1.84	0.58
5:I:30:VAL:HG13	5:I:31:LEU:N	2.16	0.58
5:K:16:ASP:CB	5:K:18:ARG:HE	2.15	0.58
5:U:12:TRP:HA	5:U:12:TRP:CE3	2.38	0.58
9:W:102:BCL:HBC3	9:X:101:BCL:CMD	2.33	0.58
1:C:20:LEU:HD22	1:C:21:LEU:H	1.68	0.58
1:C:161:VAL:HG22	7:C:502:HEM:O1D	2.03	0.58
5:A:29:ILE:CG1	5:A:33:LEU:CD1	2.82	0.58
6:E:32:VAL:HG11	9:E:101:BCL:H2	1.84	0.58
5:I:9:TYR:CD2	5:I:10:LYS:HD2	2.39	0.58
5:I:10:LYS:CB	15:N:102:CRT:H82	2.34	0.58
6:6:40:TRP:HA	6:6:40:TRP:CE3	2.39	0.58
5:7:18:ARG:HD2	5:7:18:ARG:H	1.67	0.58
5:9:46:TRP:CH2	9:9:102:BCL:HBC3	2.38	0.58
5:A:44:LEU:C	5:A:44:LEU:HD12	2.24	0.58
6:B:40:TRP:HA	6:B:40:TRP:CE3	2.37	0.58
6:P:22:MET:HG3	6:P:26:TYR:HE2	1.67	0.58
9:P:101:BCL:HMA1	9:Q:102:BCL:CMA	2.27	0.58
6:R:10:THR:HG22	6:R:11:ASP:N	2.16	0.58
5:S:27:PHE:O	5:S:31:LEU:HB3	2.03	0.58
5:U:43:ASP:HA	5:W:47:LEU:O	2.03	0.58
5:U:44:LEU:HD22	6:V:43:ARG:HD3	1.83	0.58
15:W:103:CRT:H9	6:Z:17:PHE:CE1	2.39	0.58
6:8:25:MET:HG3	15:8:101:CRT:C20	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:PRO:C	1:C:197:PHE:CD2	2.76	0.58
2:L:75:ILE:HB	2:L:157:TYR:HB2	1.84	0.58
2:L:162:HIS:O	2:L:166:VAL:HG23	2.02	0.58
3:M:137:ALA:HB3	3:M:144:GLN:HE22	1.68	0.58
4:H:5:ILE:CD1	5:D:38:ILE:O	2.52	0.58
4:H:136:MET:HG3	4:H:170:VAL:O	2.03	0.58
6:X:30:GLY:HA2	6:X:33:VAL:HG12	1.85	0.58
6:X:36:HIS:CE1	9:X:101:BCL:NB	2.70	0.58
2:L:11:ARG:HB3	2:L:26:TRP:CZ3	2.38	0.58
2:L:20:GLY:O	2:L:24:ASP:N	2.37	0.58
5:A:5:ASN:HB2	6:B:22:MET:CE	2.34	0.58
5:A:10:LYS:HD2	15:A:103:CRT:H1M1	1.85	0.58
5:O:51:ILE:HB	5:O:52:PRO:HA	1.85	0.58
5:Q:12:TRP:HE1	6:R:18:HIS:HA	1.69	0.58
5:Q:35:ILE:HA	5:Q:38:ILE:HG22	1.84	0.58
9:R:101:BCL:HMB3	9:S:102:BCL:CHB	2.33	0.58
5:S:55:TYR:HD1	5:S:56:GLN:H	1.48	0.58
6:V:20:ILE:HD13	6:V:20:ILE:C	2.23	0.58
2:L:89:LEU:HD22	5:9:37:MET:SD	2.44	0.58
2:L:279:PRO:O	2:L:280:LEU:HD23	2.04	0.58
15:A:101:CRT:C3	6:0:16:GLU:OE2	2.46	0.58
6:B:32:VAL:HG21	9:B:101:BCL:HAA1	1.86	0.58
5:I:35:ILE:HA	5:I:38:ILE:CG2	2.33	0.58
5:O:21:LEU:O	5:O:25:VAL:HG23	2.04	0.58
5:W:51:ILE:HB	5:W:52:PRO:C	2.24	0.58
5:1:10:LYS:CG	15:4:102:CRT:H22A	2.34	0.58
6:2:17:PHE:O	6:2:20:ILE:HG22	2.03	0.58
9:3:102:BCL:HBC2	9:4:101:BCL:HMD2	1.85	0.58
5:5:31:LEU:HA	5:5:34:LEU:HB3	1.85	0.58
3:M:175:VAL:HA	3:M:185:TRP:CD1	2.39	0.58
5:Q:20:VAL:O	5:Q:24:ILE:HD13	2.04	0.58
5:U:13:LEU:O	6:V:7:THR:HG22	2.04	0.58
5:U:16:ASP:HB2	5:U:19:ARG:NH2	2.15	0.58
5:Y:35:ILE:O	5:Y:38:ILE:HG13	2.03	0.58
5:Y:50:ASN:CG	5:Y:51:ILE:H	2.05	0.58
5:1:14:ILE:HD12	5:1:15:LEU:HG	1.86	0.58
6:2:33:VAL:O	6:2:37:LEU:HD23	2.03	0.58
5:9:46:TRP:CZ3	9:9:102:BCL:HBC3	2.39	0.58
6:0:10:THR:H	6:0:13:GLU:CG	2.17	0.58
3:M:31:ILE:CD1	16:M:407:PGW:HADA	2.34	0.58
6:B:16:GLU:OE2	15:B:102:CRT:C2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:29:PHE:O	6:B:32:VAL:HG12	2.03	0.58
5:I:8:LEU:HB3	6:J:18:HIS:CE1	2.39	0.58
5:O:46:TRP:CD1	5:O:47:LEU:CD2	2.87	0.58
5:U:22:VAL:HG13	5:U:23:SER:N	2.17	0.58
5:Y:27:PHE:HE2	5:1:29:ILE:HD12	1.68	0.58
9:5:102:BCL:CBB	9:5:102:BCL:HMB1	2.34	0.58
2:L:183:MET:HB3	9:M:401:BCL:O1D	2.03	0.58
15:J:101:CRT:C34	9:K:102:BCL:HAA1	2.32	0.58
6:N:22:MET:HG3	6:N:26:TYR:CE2	2.35	0.58
5:S:26:ALA:O	5:S:29:ILE:CG2	2.42	0.58
5:W:42:THR:CB	5:Y:48:ASP:HB2	2.33	0.58
6:2:29:PHE:N	6:2:29:PHE:CD1	2.69	0.58
5:3:51:ILE:CA	5:3:53:VAL:H	2.17	0.58
1:C:261:GLN:C	1:C:262:SER:O	2.42	0.57
3:M:237:GLN:HE22	4:H:119:ARG:HH22	1.50	0.57
5:O:9:TYR:HA	6:P:18:HIS:ND1	2.19	0.57
6:V:30:GLY:O	6:V:34:ILE:HG13	2.04	0.57
9:X:101:BCL:CBB	9:X:101:BCL:HMB1	2.34	0.57
5:Y:10:LYS:HB3	15:2:102:CRT:H23	1.85	0.57
6:2:46:LEU:HB3	6:4:42:TYR:OH	2.04	0.57
6:4:29:PHE:CZ	9:4:101:BCL:H101	2.39	0.57
9:4:101:BCL:C4	15:4:102:CRT:H241	2.29	0.57
5:7:44:LEU:O	5:7:44:LEU:HD22	2.03	0.57
1:C:196:PRO:HG2	1:C:231:TRP:HD1	1.68	0.57
3:M:105:ARG:HA	5:O:42:THR:HG21	1.85	0.57
3:M:274:VAL:O	3:M:278:ILE:HG13	2.04	0.57
4:H:13:GLN:NE2	12:H:304:PO4:O1	2.37	0.57
5:A:22:VAL:HA	5:A:25:VAL:CG2	2.34	0.57
9:B:101:BCL:HBA2	9:B:101:BCL:HMA2	1.85	0.57
9:T:101:BCL:C4A	9:U:102:BCL:HMB3	2.34	0.57
6:V:30:GLY:O	6:V:33:VAL:HG12	2.04	0.57
5:Y:51:ILE:HB	5:Y:52:PRO:HA	1.85	0.57
6:6:40:TRP:HA	6:6:40:TRP:HE3	1.69	0.57
2:L:56:ILE:HD12	5:9:42:THR:HG21	1.86	0.57
4:H:47:GLU:CB	5:A:19:ARG:HA	2.35	0.57
6:B:40:TRP:HA	6:B:40:TRP:HE3	1.69	0.57
5:F:45:ASN:HB3	5:F:49:ASP:HB3	1.85	0.57
5:I:49:ASP:CG	5:I:50:ASN:H	2.06	0.57
6:P:21:PHE:CD1	15:P:102:CRT:H16	2.39	0.57
6:X:29:PHE:CE1	15:X:102:CRT:H242	2.39	0.57
5:Y:17:PRO:O	5:Y:21:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:14:ILE:O	5:5:14:ILE:CG2	2.52	0.57
9:7:103:BCL:HMA3	15:8:101:CRT:H35	1.86	0.57
6:8:22:MET:O	6:8:26:TYR:HD2	1.87	0.57
6:8:23:GLN:HG3	6:8:24:SER:H	1.69	0.57
1:C:24:GLU:HG2	1:C:45:ASN:HD22	1.67	0.57
1:C:285:TRP:CD1	1:C:304:ARG:HD3	2.38	0.57
5:D:4:MET:HB3	5:D:8:LEU:CD1	2.34	0.57
5:F:7:ASN:CB	6:J:20:ILE:HD13	2.34	0.57
9:F:102:BCL:HBC3	9:G:101:BCL:HHD	1.86	0.57
5:O:52:PRO:HG2	5:O:55:TYR:CD2	2.39	0.57
5:3:16:ASP:OD2	5:3:19:ARG:HD3	2.04	0.57
5:3:20:VAL:O	5:3:24:ILE:HG12	2.04	0.57
6:6:19:ALA:O	6:6:23:GLN:HG2	2.03	0.57
9:7:102:BCL:HMD1	6:8:36:HIS:CD2	2.39	0.57
6:8:31:LEU:O	6:8:34:ILE:CG2	2.52	0.57
15:8:101:CRT:C39	5:9:36:HIS:CG	2.87	0.57
2:L:4:LEU:CD2	4:H:38:GLY:HA3	2.34	0.57
2:L:52:TRP:CA	5:A:37:MET:CE	2.83	0.57
2:L:148:MET:SD	2:L:262:PRO:HG3	2.45	0.57
2:L:196:LEU:HG	3:M:216:PHE:HD2	1.70	0.57
3:M:218:MET:CE	3:M:252:TRP:CH2	2.87	0.57
4:H:157:VAL:CG2	4:H:210:LYS:HA	2.34	0.57
5:Q:31:LEU:HD23	9:R:101:BCL:HED3	1.85	0.57
5:S:50:ASN:CG	5:S:51:ILE:N	2.56	0.57
15:3:103:CRT:H393	5:7:36:HIS:CG	2.39	0.57
9:0:101:BCL:CBB	9:0:101:BCL:HMB1	2.34	0.57
5:F:53:VAL:O	5:F:54:SER:C	2.42	0.57
5:I:29:ILE:O	5:I:33:LEU:HG	2.04	0.57
5:K:5:ASN:HD22	6:N:22:MET:HG2	1.69	0.57
5:Q:16:ASP:H	5:Q:19:ARG:NH2	2.01	0.57
5:Y:46:TRP:CZ3	9:Y:102:BCL:HBC3	2.40	0.57
5:3:51:ILE:C	5:3:53:VAL:H	2.06	0.57
5:7:35:ILE:O	5:7:36:HIS:C	2.42	0.57
2:L:47:VAL:O	2:L:51:VAL:HG23	2.05	0.57
5:D:45:ASN:HB3	5:D:49:ASP:HB3	1.85	0.57
6:N:34:ILE:HD13	6:N:34:ILE:C	2.25	0.57
5:W:16:ASP:OD2	5:W:19:ARG:HD3	2.05	0.57
6:X:13:GLU:O	6:X:16:GLU:HB3	2.05	0.57
9:Z:101:BCL:CMA	9:Z:101:BCL:HBA2	2.32	0.57
9:3:102:BCL:C1D	9:4:101:BCL:CMD	2.82	0.57
5:7:17:PRO:O	5:7:21:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:402:BCL:CBB	9:M:402:BCL:HMB1	2.35	0.57
5:F:51:ILE:HA	5:F:52:PRO:C	2.24	0.57
5:O:30:VAL:HG13	5:O:31:LEU:H	1.69	0.57
5:Q:29:ILE:CG2	5:Q:30:VAL:H	2.17	0.57
6:R:20:ILE:O	6:R:20:ILE:HD13	2.05	0.57
5:1:29:ILE:CG2	5:1:30:VAL:H	2.18	0.57
6:0:45:TRP:O	6:0:46:LEU:HB2	2.05	0.57
4:H:48:ARG:HD2	17:H:301:PEF:O1P	2.05	0.57
6:G:38:LEU:HD23	6:G:39:ALA:N	2.20	0.57
5:K:24:ILE:HD11	9:O:102:BCL:H201	1.87	0.57
5:K:44:LEU:HD21	5:K:46:TRP:HB3	1.84	0.57
5:Q:34:LEU:O	5:Q:37:MET:HB2	2.05	0.57
15:T:102:CRT:H2M3	5:U:36:HIS:CB	2.35	0.57
5:W:8:LEU:C	6:X:18:HIS:CE1	2.78	0.57
2:L:52:TRP:CH2	5:9:38:ILE:HB	2.39	0.57
2:L:173:PHE:CE2	2:L:260:SER:HB3	2.40	0.57
9:O:102:BCL:HBA1	9:O:102:BCL:CGD	2.34	0.57
5:U:9:TYR:HA	6:V:18:HIS:CG	2.39	0.57
5:W:10:LYS:HB2	15:W:103:CRT:C8	2.35	0.57
5:W:35:ILE:HA	5:W:38:ILE:CG2	2.35	0.57
5:Y:56:GLN:CG	5:Y:57:ALA:H	2.12	0.57
5:7:25:VAL:HA	9:7:102:BCL:H52	1.86	0.57
2:L:35:PHE:CE1	2:L:111:LEU:HD13	2.40	0.56
2:L:186:ILE:HD12	18:L:402:HOH:O	2.05	0.56
3:M:105:ARG:HA	5:O:42:THR:HG22	1.87	0.56
15:A:101:CRT:C8	5:7:11:ILE:HA	2.34	0.56
5:F:7:ASN:O	15:J:101:CRT:H83	2.05	0.56
15:G:102:CRT:H391	5:I:36:HIS:HB3	1.87	0.56
5:K:51:ILE:HA	5:K:52:PRO:O	2.04	0.56
6:T:24:SER:O	6:T:27:ALA:HB3	2.05	0.56
6:Z:45:TRP:O	6:Z:46:LEU:CG	2.53	0.56
6:2:43:ARG:HD3	5:3:55:TYR:CD2	2.40	0.56
6:4:34:ILE:O	6:4:34:ILE:HD13	2.05	0.56
5:7:7:ASN:HD21	6:0:23:GLN:HE22	1.51	0.56
6:8:10:THR:HG22	6:8:11:ASP:N	2.20	0.56
6:8:17:PHE:O	6:8:20:ILE:HG22	2.05	0.56
1:C:212:ILE:HD13	1:C:212:ILE:H	1.70	0.56
2:L:175:HIS:CE1	2:L:177:HIS:HB2	2.41	0.56
2:L:226:ARG:O	3:M:51:ILE:HA	2.05	0.56
3:M:150:PHE:O	3:M:154:ILE:HG13	2.04	0.56
4:H:95:ALA:CB	5:9:16:ASP:OD2	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:22:VAL:HA	5:A:25:VAL:HB	1.86	0.56
5:A:60:LYS:HA	5:9:50:ASN:CA	2.34	0.56
6:J:40:TRP:HZ3	6:J:46:LEU:HG	1.70	0.56
5:O:7:ASN:O	6:R:20:ILE:CG1	2.54	0.56
5:O:40:LEU:O	5:O:45:ASN:OD1	2.22	0.56
6:V:46:LEU:HD13	6:X:42:TYR:CE1	2.40	0.56
5:W:5:ASN:OD1	5:W:8:LEU:CD1	2.53	0.56
5:W:43:ASP:HB2	5:Y:47:LEU:HD22	1.86	0.56
5:Y:49:ASP:C	5:1:56:GLN:NE2	2.55	0.56
6:6:40:TRP:HZ3	6:6:44:PRO:CA	2.17	0.56
2:L:130:PHE:CE2	2:L:134:ILE:HD11	2.41	0.56
2:L:156:PRO:HG2	2:L:162:HIS:HA	1.85	0.56
2:L:189:PHE:CD1	2:L:249:ALA:HB1	2.40	0.56
3:M:59:LEU:HD11	5:Q:29:ILE:HD13	1.88	0.56
3:M:252:TRP:CE3	3:M:256:MET:CE	2.88	0.56
3:M:257:GLY:HA3	17:H:301:PEF:O5	2.05	0.56
9:M:401:BCL:CBB	9:M:401:BCL:HMB1	2.34	0.56
4:H:77:VAL:HG23	4:H:80:ARG:HB3	1.88	0.56
4:H:111:PHE:CA	4:H:115:ALA:HB2	2.35	0.56
5:A:18:ARG:CG	5:9:14:ILE:HG23	2.35	0.56
9:A:102:BCL:C1D	9:B:101:BCL:CMD	2.83	0.56
5:F:9:TYR:HA	6:G:18:HIS:CE1	2.40	0.56
5:K:44:LEU:HD23	6:N:43:ARG:NH2	2.19	0.56
5:K:44:LEU:HD22	5:K:46:TRP:HE3	1.70	0.56
6:N:46:LEU:HD22	6:P:42:TYR:CE2	2.39	0.56
15:N:102:CRT:H392	9:O:102:BCL:CHB	2.35	0.56
5:O:10:LYS:HB2	15:R:102:CRT:H83	1.87	0.56
5:O:10:LYS:C	15:R:102:CRT:H82	2.25	0.56
9:P:101:BCL:CBB	9:P:101:BCL:HMB1	2.34	0.56
6:R:45:TRP:CD2	9:R:101:BCL:H2C	2.40	0.56
5:U:14:ILE:O	5:U:14:ILE:HG22	2.05	0.56
5:W:20:VAL:O	5:W:24:ILE:HG12	2.04	0.56
6:X:27:ALA:O	6:X:31:LEU:HG	2.05	0.56
5:Y:40:LEU:HD13	5:Y:46:TRP:CE2	2.40	0.56
5:Y:50:ASN:ND2	5:Y:51:ILE:H	2.03	0.56
5:Y:51:ILE:HB	5:Y:52:PRO:CA	2.35	0.56
9:1:102:BCL:HMD1	6:2:36:HIS:CE1	2.40	0.56
6:2:25:MET:HA	15:2:102:CRT:H183	1.87	0.56
5:3:12:TRP:HE1	6:4:18:HIS:CB	2.18	0.56
5:5:28:GLN:O	5:5:32:GLY:N	2.35	0.56
15:8:101:CRT:C37	9:9:102:BCL:HMB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:THR:HG23	5:A:41:SER:HA	1.87	0.56
2:L:209:PRO:HG3	2:L:214:PRO:O	2.06	0.56
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.86	0.56
5:A:47:LEU:HD12	5:9:43:ASP:HB2	1.87	0.56
9:F:102:BCL:HBC1	9:G:101:BCL:CAC	2.34	0.56
5:I:52:PRO:HB2	5:I:55:TYR:CD2	2.40	0.56
15:R:102:CRT:H342	9:S:102:BCL:CGA	2.35	0.56
6:X:25:MET:HG3	15:X:102:CRT:H21	1.86	0.56
5:Y:13:LEU:HD21	6:Z:10:THR:O	2.06	0.56
9:Y:102:BCL:HMD1	6:Z:36:HIS:CD2	2.40	0.56
5:3:16:ASP:HB2	5:3:19:ARG:CB	2.33	0.56
6:8:17:PHE:CZ	15:8:101:CRT:C11	2.81	0.56
6:0:45:TRP:O	6:0:46:LEU:CB	2.53	0.56
1:C:249:PHE:CZ	1:C:265:LYS:HG2	2.41	0.56
3:M:229:PHE:CE1	4:H:244:ALA:HB2	2.40	0.56
3:M:264:SER:OG	4:H:34:ASP:OD1	2.21	0.56
4:H:52:ARG:NH1	5:D:26:ALA:HB1	2.20	0.56
4:H:154:MET:HE2	4:H:208:LYS:N	2.21	0.56
5:U:29:ILE:HG23	5:U:30:VAL:H	1.68	0.56
6:V:9:LEU:HB3	6:V:13:GLU:OE1	2.05	0.56
5:W:35:ILE:HG22	5:W:36:HIS:N	2.20	0.56
5:3:40:LEU:C	5:3:40:LEU:HD23	2.25	0.56
6:4:43:ARG:O	6:4:45:TRP:N	2.38	0.56
5:7:29:ILE:HB	9:7:102:BCL:H43	1.86	0.56
5:7:44:LEU:O	5:7:44:LEU:HD13	2.06	0.56
9:7:103:BCL:HMB3	9:9:102:BCL:CHB	2.36	0.56
1:C:192:TYR:HD2	2:L:270:GLU:HG3	1.71	0.56
3:M:84:PHE:CZ	5:W:37:MET:HG2	2.41	0.56
4:H:153:GLY:H	4:H:167:VAL:CG2	2.14	0.56
5:A:29:ILE:CD1	15:A:101:CRT:C34	2.84	0.56
6:E:36:HIS:HD1	9:E:101:BCL:H102	1.70	0.56
5:F:6:ALA:O	5:F:9:TYR:CD2	2.58	0.56
15:N:102:CRT:H392	9:O:102:BCL:C2B	2.35	0.56
5:O:14:ILE:HG23	5:O:15:LEU:HG	1.87	0.56
5:O:55:TYR:CD1	5:O:56:GLN:N	2.70	0.56
6:Z:46:LEU:HD22	6:2:42:TYR:CZ	2.40	0.56
5:3:12:TRP:CD1	6:4:18:HIS:HB2	2.41	0.56
9:4:101:BCL:C1B	9:5:102:BCL:HMB3	2.35	0.56
3:M:70:ILE:CG2	3:M:71:ILE:N	2.69	0.56
5:F:46:TRP:NE1	9:F:102:BCL:OBB	2.38	0.56
6:G:10:THR:HG22	6:G:11:ASP:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:9:TYR:OH	6:J:11:ASP:OD2	2.24	0.56
5:O:10:LYS:HB2	15:R:102:CRT:H82	1.88	0.56
5:Q:42:THR:HG23	5:S:47:LEU:HB3	1.88	0.56
9:S:102:BCL:HBD	9:T:101:BCL:OBD	2.06	0.56
5:W:13:LEU:O	6:X:7:THR:HA	2.06	0.56
5:Y:36:HIS:CG	9:Z:101:BCL:HMD1	2.41	0.56
5:1:43:ASP:HB2	5:3:47:LEU:HD13	1.84	0.56
5:5:29:ILE:HG23	5:5:30:VAL:N	2.20	0.56
9:5:102:BCL:C1D	9:6:101:BCL:CMD	2.83	0.56
1:C:125:VAL:O	1:C:128:ARG:HB2	2.06	0.56
1:C:128:ARG:O	1:C:131:PHE:HB2	2.06	0.56
2:L:204:LEU:CD2	3:M:267:ARG:HG3	2.26	0.56
3:M:2:PRO:CG	3:M:42:LYS:NZ	2.69	0.56
3:M:251:PHE:O	3:M:255:THR:HG23	2.06	0.56
5:A:35:ILE:HA	5:A:38:ILE:CG1	2.36	0.56
6:B:17:PHE:O	6:B:20:ILE:HG22	2.05	0.56
5:D:44:LEU:HD12	5:D:44:LEU:O	2.05	0.56
9:E:101:BCL:CBB	9:E:101:BCL:HMB1	2.36	0.56
5:K:36:HIS:O	5:K:40:LEU:N	2.39	0.56
5:S:36:HIS:O	5:S:40:LEU:CB	2.52	0.56
5:U:49:ASP:CG	5:U:50:ASN:N	2.58	0.56
5:Y:43:ASP:HB2	5:1:47:LEU:CD1	2.35	0.56
5:3:11:ILE:HG12	15:3:103:CRT:H81	1.87	0.56
5:3:32:GLY:HA2	9:4:101:BCL:O1D	2.06	0.56
6:0:38:LEU:HD23	6:0:38:LEU:C	2.27	0.56
2:L:10:TYR:OH	3:M:246:GLU:HG2	2.05	0.56
3:M:65:LEU:HD23	3:M:65:LEU:O	2.06	0.56
3:M:239:THR:O	4:H:76:VAL:HG11	2.06	0.56
3:M:270:TRP:CE2	3:M:274:VAL:HG21	2.41	0.56
5:A:17:PRO:HG2	5:A:18:ARG:HD2	1.86	0.56
5:A:33:LEU:CA	15:A:101:CRT:H403	2.35	0.56
5:O:9:TYR:CE1	6:P:15:LYS:HB2	2.41	0.56
5:O:21:LEU:HD11	6:P:17:PHE:HZ	1.71	0.56
6:T:22:MET:O	6:T:26:TYR:HD1	1.88	0.56
5:W:43:ASP:HB2	5:Y:47:LEU:CB	2.36	0.56
5:Y:44:LEU:HD13	6:Z:43:ARG:NE	2.21	0.56
5:Y:45:ASN:O	5:Y:48:ASP:N	2.38	0.56
5:1:4:MET:O	5:1:8:LEU:HG	2.06	0.56
9:2:101:BCL:HMB1	9:2:101:BCL:CBB	2.36	0.56
5:9:40:LEU:CD1	5:9:47:LEU:HD23	2.33	0.56
1:C:130:MET:O	1:C:133:LEU:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:ARG:HD2	4:H:101:VAL:HG22	1.88	0.56
2:L:196:LEU:HG	3:M:216:PHE:CD2	2.41	0.56
4:H:205:LYS:NZ	5:1:18:ARG:HH12	2.04	0.56
15:A:103:CRT:C21	5:D:24:ILE:HG21	2.35	0.56
6:B:20:ILE:HD11	5:9:8:LEU:HD23	1.87	0.56
5:D:45:ASN:O	5:D:49:ASP:CG	2.45	0.56
6:E:21:PHE:HZ	9:F:102:BCL:H203	1.71	0.56
5:O:16:ASP:O	5:O:20:VAL:HG23	2.06	0.56
5:S:4:MET:HB2	5:S:8:LEU:HD11	1.87	0.56
6:T:21:PHE:CD2	15:T:102:CRT:H14	2.40	0.56
5:Y:49:ASP:HB2	5:1:56:GLN:HA	1.88	0.56
5:3:5:ASN:ND2	6:4:22:MET:CG	2.69	0.56
6:4:10:THR:HG22	6:4:11:ASP:N	2.17	0.56
6:6:10:THR:HG22	6:6:11:ASP:N	2.21	0.56
6:0:32:VAL:HG13	6:0:33:VAL:N	2.21	0.56
4:H:53:VAL:HG22	4:H:54:LYS:N	2.21	0.55
5:F:11:ILE:CD1	5:F:14:ILE:HD11	2.34	0.55
5:F:31:LEU:O	5:F:35:ILE:HG12	2.06	0.55
5:I:56:GLN:C	5:I:60:LYS:CB	2.74	0.55
6:N:13:GLU:CD	6:N:13:GLU:H	2.06	0.55
5:S:26:ALA:O	5:S:30:VAL:HG12	2.06	0.55
5:1:30:VAL:HG13	5:1:31:LEU:N	2.21	0.55
5:3:5:ASN:ND2	6:4:22:MET:HG2	2.21	0.55
1:C:19:MET:HA	2:L:180:PRO:HB2	1.88	0.55
2:L:70:LEU:HA	2:L:73:ILE:CD1	2.36	0.55
4:H:6:THR:O	5:F:41:SER:CB	2.53	0.55
5:F:44:LEU:O	5:F:46:TRP:N	2.38	0.55
9:G:101:BCL:HMB1	9:G:101:BCL:CBB	2.37	0.55
6:P:44:PRO:O	5:Q:52:PRO:HG2	2.05	0.55
9:W:102:BCL:CHD	9:W:102:BCL:CBC	2.84	0.55
6:Z:34:ILE:C	6:Z:34:ILE:HD13	2.26	0.55
5:1:9:TYR:HB2	6:2:15:LYS:HA	1.86	0.55
5:1:10:LYS:HB2	6:4:20:ILE:CD1	2.35	0.55
6:2:36:HIS:CB	9:2:101:BCL:H151	2.36	0.55
5:7:25:VAL:HG13	9:7:102:BCL:H41	1.89	0.55
2:L:11:ARG:NH1	4:H:45:ARG:CD	2.61	0.55
2:L:182:HIS:O	2:L:186:ILE:HG13	2.06	0.55
5:K:20:VAL:O	5:K:24:ILE:CD1	2.54	0.55
5:O:44:LEU:HD12	5:O:46:TRP:H	1.71	0.55
5:Q:30:VAL:HG13	5:Q:31:LEU:H	1.71	0.55
15:V:102:CRT:H342	9:W:102:BCL:HAA1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:46:TRP:CH2	9:W:102:BCL:H2C	2.40	0.55
5:7:40:LEU:HD11	5:7:47:LEU:HD23	1.88	0.55
2:L:3:MET:CE	4:H:45:ARG:NE	2.66	0.55
4:H:128:GLU:OE1	4:H:128:GLU:N	2.36	0.55
4:H:244:ALA:O	4:H:247:LYS:HB2	2.06	0.55
5:A:4:MET:HE3	6:E:24:SER:HA	1.87	0.55
5:A:29:ILE:HD11	5:9:27:PHE:HZ	1.70	0.55
5:A:38:ILE:HD12	5:A:38:ILE:C	2.27	0.55
15:A:103:CRT:H342	9:F:102:BCL:CAA	2.36	0.55
6:E:9:LEU:HB3	6:E:13:GLU:OE2	2.05	0.55
9:F:102:BCL:CBB	9:F:102:BCL:HMB1	2.36	0.55
5:K:33:LEU:O	5:K:37:MET:HG3	2.06	0.55
15:N:102:CRT:H372	9:O:102:BCL:HHB	1.89	0.55
5:Q:51:ILE:HD12	6:R:43:ARG:HH22	1.71	0.55
6:V:21:PHE:HA	15:V:102:CRT:C12	2.36	0.55
5:3:53:VAL:HA	5:3:55:TYR:CE2	2.41	0.55
5:7:18:ARG:H	5:7:18:ARG:CD	2.19	0.55
6:8:20:ILE:HG23	6:8:21:PHE:N	2.20	0.55
1:C:20:LEU:HD23	2:L:271:TRP:HE1	1.71	0.55
15:B:102:CRT:H2M1	5:D:33:LEU:HA	1.89	0.55
5:F:44:LEU:HB3	5:I:55:TYR:OH	2.05	0.55
6:G:21:PHE:HD2	15:G:102:CRT:H14	1.59	0.55
5:O:46:TRP:NE1	5:O:47:LEU:HD21	2.22	0.55
6:P:10:THR:CG2	6:P:11:ASP:H	2.15	0.55
9:W:102:BCL:CHD	9:W:102:BCL:HBC2	2.35	0.55
5:3:13:LEU:HG	15:3:103:CRT:H1M1	1.89	0.55
9:4:101:BCL:HMB3	9:5:102:BCL:C1B	2.36	0.55
5:7:35:ILE:HA	5:7:38:ILE:HG22	1.89	0.55
1:C:29:GLY:N	1:C:44:TYR:O	2.34	0.55
2:L:180:PRO:HG2	2:L:181:ALA:H	1.71	0.55
3:M:56:THR:HG23	3:M:135:LYS:HZ2	1.72	0.55
3:M:159:VAL:HG21	3:M:281:GLY:HA3	1.88	0.55
4:H:53:VAL:HG11	5:D:22:VAL:CG2	2.15	0.55
5:F:42:THR:CG2	5:I:47:LEU:HB3	2.37	0.55
6:G:17:PHE:CE2	15:G:102:CRT:H9	2.41	0.55
5:O:50:ASN:CG	5:O:51:ILE:H	2.10	0.55
6:T:9:LEU:HB3	6:T:13:GLU:CG	2.36	0.55
6:2:21:PHE:CD1	15:2:102:CRT:C16	2.76	0.55
5:3:12:TRP:HE1	6:4:18:HIS:HB2	1.71	0.55
5:5:21:LEU:O	5:5:25:VAL:HG23	2.07	0.55
1:C:210:ILE:HB	7:C:503:HEM:O1D	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:ILE:HD12	2:L:159:ILE:N	2.15	0.55
9:L:303:BCL:HMB1	9:L:303:BCL:CBB	2.36	0.55
3:M:37:SER:HG	3:M:40:LEU:HB3	1.70	0.55
3:M:153:ALA:HB2	10:M:403:BPH:HAC2	1.89	0.55
9:E:101:BCL:H201	6:G:38:LEU:HD11	1.88	0.55
5:K:35:ILE:HA	5:K:38:ILE:HG22	1.89	0.55
5:K:38:ILE:O	5:K:42:THR:OG1	2.25	0.55
5:7:46:TRP:CZ3	9:7:102:BCL:HBC3	2.41	0.55
1:C:19:MET:SD	1:C:19:MET:N	2.78	0.55
1:C:118:SER:O	1:C:124:LYS:HD3	2.06	0.55
3:M:5:GLN:HB2	3:M:7:ILE:HG12	1.89	0.55
3:M:261:THR:CG2	4:H:37:GLU:HB2	2.36	0.55
6:G:21:PHE:CG	15:G:102:CRT:H14	2.40	0.55
5:K:54:SER:CB	5:K:56:GLN:HE21	2.14	0.55
6:N:10:THR:HB	6:N:13:GLU:OE2	2.07	0.55
6:N:46:LEU:CD2	6:P:42:TYR:CZ	2.81	0.55
5:O:30:VAL:HG13	5:O:31:LEU:N	2.22	0.55
5:O:50:ASN:OD1	6:P:43:ARG:NH2	2.40	0.55
5:Q:44:LEU:CD1	5:Q:46:TRP:HE3	2.20	0.55
9:3:102:BCL:CBB	9:3:102:BCL:HMB1	2.37	0.55
6:6:17:PHE:O	6:6:20:ILE:HG22	2.06	0.55
1:C:203:PHE:CD2	1:C:210:ILE:HG12	2.42	0.55
2:L:83:GLY:HA2	2:L:150:ALA:HA	1.89	0.55
3:M:196:LEU:HD12	9:M:402:BCL:CHD	2.37	0.55
5:A:35:ILE:HD13	5:A:38:ILE:HG12	1.89	0.55
15:A:101:CRT:H9	6:0:17:PHE:CE1	2.41	0.55
5:I:16:ASP:HB2	5:I:19:ARG:HB3	1.87	0.55
6:N:17:PHE:CE1	15:N:102:CRT:C11	2.89	0.55
15:N:102:CRT:C39	5:O:36:HIS:CG	2.89	0.55
5:O:43:ASP:HA	5:Q:48:ASP:CB	2.35	0.55
6:P:13:GLU:HB2	15:P:102:CRT:H33	1.87	0.55
6:P:21:PHE:CD1	15:P:102:CRT:C16	2.89	0.55
5:Q:36:HIS:CE1	9:R:101:BCL:HMD1	2.42	0.55
6:R:44:PRO:O	5:S:52:PRO:HG2	2.06	0.55
5:3:13:LEU:CG	15:3:103:CRT:C1M	2.85	0.55
5:5:49:ASP:O	5:7:56:GLN:HA	2.07	0.55
6:6:30:GLY:O	6:6:34:ILE:HG22	2.06	0.55
5:7:35:ILE:HD11	9:7:103:BCL:O1D	2.06	0.55
2:L:16:THR:CB	2:L:20:GLY:HA3	2.36	0.55
2:L:89:LEU:CD1	2:L:94:LEU:HD23	2.31	0.55
2:L:178:TYR:HD2	2:L:269:PRO:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:242:GLY:O	3:M:246:GLU:HB2	2.07	0.55
3:M:246:GLU:OE2	4:H:117:PRO:HB3	2.07	0.55
5:A:50:ASN:HB2	5:D:59:GLY:HA3	1.89	0.55
6:B:16:GLU:OE2	15:B:102:CRT:H21A	2.07	0.55
6:B:17:PHE:CE1	15:B:102:CRT:C9	2.90	0.55
15:P:102:CRT:H342	9:Q:102:BCL:HAA2	1.81	0.55
5:W:9:TYR:HB2	6:X:15:LYS:HA	1.89	0.55
6:X:34:ILE:O	6:X:34:ILE:HD13	2.07	0.55
5:5:4:MET:SD	6:8:27:ALA:HB3	2.47	0.55
1:C:75:VAL:HG23	1:C:76:TYR:H	1.71	0.54
2:L:11:ARG:HH12	4:H:45:ARG:HD3	1.67	0.54
3:M:79:VAL:O	3:M:79:VAL:HG22	2.07	0.54
5:A:11:ILE:O	5:A:11:ILE:HG13	2.07	0.54
6:E:46:LEU:HD13	6:G:42:TYR:CE1	2.42	0.54
5:Q:29:ILE:HG23	5:Q:30:VAL:H	1.69	0.54
5:S:43:ASP:OD2	5:U:48:ASP:HA	2.07	0.54
6:T:32:VAL:O	6:T:35:ALA:HB3	2.07	0.54
6:X:38:LEU:C	6:X:38:LEU:HD23	2.28	0.54
5:1:55:TYR:O	5:1:56:GLN:C	2.45	0.54
9:7:103:BCL:HMA2	15:8:101:CRT:H32	1.88	0.54
6:0:36:HIS:HE1	9:0:101:BCL:C1B	2.20	0.54
5:D:10:LYS:HB3	15:G:102:CRT:H5	1.90	0.54
15:G:102:CRT:H391	5:I:36:HIS:CG	2.42	0.54
5:O:46:TRP:CD1	5:O:47:LEU:CD1	2.90	0.54
15:R:102:CRT:H2M1	5:S:33:LEU:HA	1.88	0.54
5:1:16:ASP:HB3	5:1:18:ARG:HE	1.73	0.54
5:1:29:ILE:O	5:1:33:LEU:HG	2.07	0.54
1:C:225:SER:CB	1:C:228:GLN:HG3	2.36	0.54
3:M:218:MET:HE2	3:M:252:TRP:CZ3	2.43	0.54
3:M:234:GLU:OE2	3:M:266:HIS:CE1	2.60	0.54
4:H:151:PRO:O	4:H:167:VAL:HG21	2.07	0.54
6:N:20:ILE:HG22	15:N:102:CRT:H133	1.90	0.54
6:T:40:TRP:CZ3	6:T:44:PRO:HA	2.42	0.54
5:W:15:LEU:O	5:W:17:PRO:HD3	2.08	0.54
5:1:17:PRO:HG2	5:1:18:ARG:H	1.73	0.54
5:1:51:ILE:HB	5:1:52:PRO:C	2.28	0.54
6:4:18:HIS:C	6:4:18:HIS:CD2	2.81	0.54
6:8:34:ILE:HD13	6:8:34:ILE:C	2.27	0.54
2:L:140:LEU:CD2	2:L:257:ILE:HG21	2.37	0.54
4:H:119:ARG:NH2	4:H:237:ASP:OD2	2.39	0.54
6:B:22:MET:HG3	6:B:26:TYR:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:45:TRP:O	6:B:46:LEU:CB	2.55	0.54
9:I:102:BCL:HMD2	9:I:103:BCL:CHD	2.37	0.54
9:I:102:BCL:HMB1	9:I:102:BCL:CBB	2.37	0.54
5:O:13:LEU:O	6:P:7:THR:HA	2.06	0.54
5:U:44:LEU:HD13	6:V:43:ARG:CD	2.38	0.54
9:X:101:BCL:HBA2	9:X:101:BCL:CMA	2.38	0.54
9:Z:101:BCL:HBA2	9:Z:101:BCL:HMA2	1.88	0.54
6:8:34:ILE:O	6:8:37:LEU:HB3	2.08	0.54
15:8:101:CRT:H403	9:9:102:BCL:CMB	2.38	0.54
1:C:179:LYS:N	1:C:180:PRO:CD	2.71	0.54
2:L:11:ARG:HH11	4:H:45:ARG:NE	2.04	0.54
3:M:268:TRP:CZ3	14:M:405:MQ8:H162	2.43	0.54
6:B:34:ILE:O	6:B:34:ILE:HD13	2.08	0.54
5:D:18:ARG:O	5:D:22:VAL:HG12	2.08	0.54
6:J:17:PHE:HE1	6:J:21:PHE:HB2	1.73	0.54
6:R:34:ILE:C	6:R:34:ILE:HD13	2.27	0.54
6:X:30:GLY:O	6:X:34:ILE:HG22	2.08	0.54
5:1:11:ILE:HG23	5:1:15:LEU:HD12	1.89	0.54
1:C:250:CYS:C	1:C:251:HIS:ND1	2.61	0.54
1:C:263:THR:O	1:C:266:ARG:HB3	2.08	0.54
2:L:203:ILE:O	2:L:206:VAL:HG22	2.07	0.54
3:M:98:PRO:HA	3:M:112:GLY:HA3	1.89	0.54
4:H:240:CYS:HA	4:H:243:TYR:HD2	1.73	0.54
5:A:5:ASN:HA	5:A:8:LEU:HG	1.89	0.54
5:D:7:ASN:HD22	5:D:7:ASN:H	1.56	0.54
5:F:43:ASP:O	5:F:44:LEU:HG	2.07	0.54
5:K:16:ASP:HB3	5:K:18:ARG:NE	2.22	0.54
9:N:101:BCL:HMB3	9:O:102:BCL:C4A	2.37	0.54
5:S:20:VAL:O	5:S:24:ILE:HG12	2.07	0.54
5:U:10:LYS:HA	15:X:102:CRT:H23	1.89	0.54
15:V:102:CRT:H2M3	5:W:33:LEU:O	2.08	0.54
6:X:46:LEU:HB3	6:Z:42:TYR:OH	2.08	0.54
6:Z:30:GLY:O	6:Z:34:ILE:HG22	2.08	0.54
6:2:24:SER:O	6:2:27:ALA:HB3	2.06	0.54
5:3:14:ILE:HG21	5:5:17:PRO:HB2	1.90	0.54
2:L:233:ILE:HG21	2:L:238:ILE:CD1	2.38	0.54
3:M:31:ILE:HG13	16:M:407:PGW:HADA	1.89	0.54
4:H:5:ILE:HA	5:F:40:LEU:HD21	1.89	0.54
5:D:16:ASP:OD2	5:D:18:ARG:HG2	2.08	0.54
5:O:21:LEU:HD11	6:P:17:PHE:CZ	2.43	0.54
6:R:21:PHE:HD2	15:R:102:CRT:C16	2.12	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:33:VAL:HG13	6:V:34:ILE:N	2.23	0.54
5:W:8:LEU:HB3	6:X:18:HIS:HE1	1.70	0.54
6:2:20:ILE:CG2	15:2:102:CRT:H81	2.35	0.54
6:8:40:TRP:HH2	6:8:46:LEU:HD12	1.73	0.54
5:9:44:LEU:O	5:9:46:TRP:N	2.39	0.54
2:L:71:TRP:HB3	2:L:160:LEU:HD12	1.90	0.54
2:L:150:ALA:HB3	2:L:153:HIS:CE1	2.43	0.54
4:H:130:LEU:CD1	4:H:131:PRO:HD2	2.38	0.54
5:A:2:PHE:HB3	6:B:26:TYR:OH	2.07	0.54
5:I:10:LYS:HG3	15:N:102:CRT:C1M	2.35	0.54
5:Q:50:ASN:HB3	5:S:56:GLN:HA	1.90	0.54
5:U:35:ILE:O	5:U:38:ILE:CG2	2.55	0.54
5:Y:50:ASN:CG	5:Y:51:ILE:N	2.61	0.54
6:4:20:ILE:CG2	15:4:102:CRT:C9	2.80	0.54
3:M:67:ALA:O	3:M:71:ILE:HG13	2.07	0.54
3:M:206:ILE:HA	9:M:402:BCL:HMA1	1.89	0.54
5:D:4:MET:HB3	5:D:8:LEU:HD11	1.90	0.54
6:E:20:ILE:O	6:E:23:GLN:HG3	2.08	0.54
5:W:10:LYS:CD	15:W:103:CRT:H1M2	2.37	0.54
5:Y:50:ASN:HB2	5:1:58:LEU:O	2.08	0.54
6:2:45:TRP:CD2	9:2:101:BCL:H2C	2.43	0.54
6:4:25:MET:CB	15:4:102:CRT:C19	2.81	0.54
5:5:43:ASP:HB2	5:7:47:LEU:C	2.27	0.54
5:7:7:ASN:H	5:7:7:ASN:ND2	2.05	0.54
1:C:97:VAL:CG1	7:C:501:HEM:HBC2	2.38	0.54
1:C:307:CYS:O	1:C:311:HIS:HB2	2.08	0.54
2:L:12:VAL:HG11	4:H:113:PRO:HD3	1.88	0.54
3:M:199:ASN:HD22	3:M:202:HIS:CB	2.21	0.54
3:M:259:ASN:HD22	3:M:259:ASN:N	2.05	0.54
5:D:14:ILE:HG23	5:F:18:ARG:HB3	1.90	0.54
6:J:10:THR:HB	6:J:13:GLU:CD	2.28	0.54
6:J:20:ILE:CG1	15:J:101:CRT:C8	2.72	0.54
5:K:35:ILE:HA	5:K:38:ILE:CG2	2.37	0.54
9:K:102:BCL:HBC1	9:N:101:BCL:HBC3	1.90	0.54
5:O:31:LEU:O	5:O:35:ILE:HG12	2.07	0.54
9:P:101:BCL:NB	9:Q:102:BCL:HMB3	2.23	0.54
6:T:13:GLU:H	6:T:13:GLU:CD	2.12	0.54
5:U:26:ALA:O	5:U:29:ILE:CG2	2.29	0.54
5:W:29:ILE:HG23	5:W:30:VAL:N	2.22	0.54
5:1:4:MET:HB3	5:1:8:LEU:HD11	1.90	0.54
5:1:9:TYR:HA	6:2:18:HIS:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:19:ARG:NH2	5:3:20:VAL:HG13	2.23	0.54
6:4:25:MET:CA	15:4:102:CRT:H16	2.35	0.54
5:9:12:TRP:CD1	6:0:17:PHE:HD2	2.25	0.54
1:C:39:GLY:HA3	2:L:168:ASN:HB2	1.91	0.53
1:C:250:CYS:CB	1:C:251:HIS:CE1	2.91	0.53
2:L:140:LEU:HD23	2:L:257:ILE:HG21	1.90	0.53
2:L:192:ASN:ND2	3:M:213:ALA:HA	2.23	0.53
2:L:246:ALA:HB1	3:M:217:ALA:HB2	1.90	0.53
3:M:12:GLN:NE2	3:M:42:LYS:N	2.55	0.53
3:M:104:LEU:HD21	3:M:169:GLY:HA2	1.90	0.53
4:H:43:SER:C	4:H:44:ASP:OD1	2.46	0.53
4:H:48:ARG:CD	17:H:301:PEF:O1P	2.56	0.53
4:H:53:VAL:CG1	4:H:54:LYS:H	2.03	0.53
16:H:302:PGW:H04A	16:H:302:PGW:H03	1.90	0.53
5:A:60:LYS:N	5:9:50:ASN:HB3	2.23	0.53
5:D:2:PHE:N	5:D:2:PHE:CD1	2.75	0.53
6:N:10:THR:C	6:N:13:GLU:OE2	2.46	0.53
6:V:25:MET:HE2	15:V:102:CRT:H21	1.90	0.53
5:7:30:VAL:HG13	5:7:31:LEU:N	2.23	0.53
1:C:36:ARG:NH1	2:L:92:GLY:N	2.56	0.53
1:C:196:PRO:CG	1:C:231:TRP:CD1	2.90	0.53
3:M:242:GLY:HA2	4:H:119:ARG:CD	2.25	0.53
4:H:121:LYS:HA	4:H:234:TYR:CB	2.37	0.53
5:A:10:LYS:O	5:A:13:LEU:HD13	2.08	0.53
5:I:10:LYS:CG	15:N:102:CRT:C1M	2.86	0.53
6:V:34:ILE:HG22	6:V:38:LEU:HD21	1.89	0.53
9:W:102:BCL:C1D	9:X:101:BCL:CMD	2.86	0.53
15:X:102:CRT:C2M	5:Y:36:HIS:CB	2.84	0.53
6:Z:36:HIS:HE1	9:Z:101:BCL:C4A	2.21	0.53
5:1:10:LYS:HB3	15:4:102:CRT:C2	2.21	0.53
5:1:35:ILE:O	5:1:39:VAL:HG12	2.08	0.53
5:9:12:TRP:CE3	5:9:12:TRP:CA	2.91	0.53
1:C:251:HIS:CE1	7:C:503:HEM:C4C	2.94	0.53
1:C:266:ARG:HD2	7:C:503:HEM:HMD3	1.90	0.53
2:L:31:TYR:CE1	2:L:119:LYS:NZ	2.71	0.53
2:L:74:SER:O	2:L:75:ILE:HD13	2.08	0.53
2:L:150:ALA:HB3	2:L:153:HIS:ND1	2.22	0.53
2:L:210:GLN:HB2	2:L:213:GLU:HG3	1.89	0.53
3:M:85:GLN:HG3	3:M:89:HIS:CD2	2.44	0.53
4:H:157:VAL:CG1	4:H:208:LYS:HD3	2.38	0.53
5:A:24:ILE:HG21	15:B:102:CRT:C24	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:101:CRT:H82	5:7:11:ILE:N	2.23	0.53
6:E:27:ALA:O	6:E:31:LEU:HG	2.09	0.53
5:F:26:ALA:O	5:F:29:ILE:HG22	2.08	0.53
6:R:46:LEU:HB3	6:T:42:TYR:CZ	2.42	0.53
5:S:10:LYS:O	5:S:13:LEU:HB2	2.08	0.53
5:5:43:ASP:HB2	5:7:47:LEU:CA	2.38	0.53
5:7:11:ILE:CD1	5:7:15:LEU:HD11	2.38	0.53
5:7:42:THR:HB	5:9:48:ASP:OD2	2.07	0.53
15:8:101:CRT:H372	9:9:102:BCL:HHB	1.91	0.53
1:C:251:HIS:HE1	7:C:503:HEM:NC	2.01	0.53
4:H:11:ALA:HB2	12:H:303:PO4:O2	2.09	0.53
9:B:101:BCL:CMB	9:D:102:BCL:C1B	2.86	0.53
5:I:8:LEU:HB3	6:J:18:HIS:HE2	1.70	0.53
6:N:21:PHE:CD2	15:N:102:CRT:C16	2.92	0.53
5:O:44:LEU:HD22	6:P:43:ARG:HD3	1.90	0.53
5:Q:8:LEU:O	5:Q:11:ILE:HG12	2.08	0.53
5:3:8:LEU:O	5:3:11:ILE:HG13	2.07	0.53
5:3:50:ASN:HA	5:5:59:GLY:O	2.08	0.53
9:7:103:BCL:C1C	9:9:102:BCL:HBB3	2.38	0.53
5:9:16:ASP:O	5:9:20:VAL:HG22	2.09	0.53
6:0:28:TRP:O	6:0:31:LEU:HB2	2.07	0.53
2:L:89:LEU:HD12	2:L:93:GLY:C	2.28	0.53
2:L:217:THR:H	2:L:220:HIS:CE1	2.26	0.53
6:B:28:TRP:HA	6:B:31:LEU:HG	1.90	0.53
6:E:36:HIS:HB3	9:E:101:BCL:H122	1.91	0.53
5:F:12:TRP:HE1	6:G:17:PHE:HD1	1.56	0.53
5:Q:46:TRP:CD1	5:Q:47:LEU:N	2.77	0.53
5:W:3:THR:O	5:W:6:ALA:N	2.41	0.53
5:W:35:ILE:HA	5:W:38:ILE:HG22	1.91	0.53
5:Y:55:TYR:O	5:Y:59:GLY:HA3	2.08	0.53
6:4:10:THR:HB	6:4:13:GLU:OE2	2.08	0.53
1:C:127:SER:HB2	7:C:501:HEM:HMD1	1.90	0.53
1:C:173:LYS:CB	3:M:80:HIS:HB2	2.38	0.53
3:M:104:LEU:HD22	3:M:104:LEU:N	2.24	0.53
5:A:42:THR:HG22	5:D:48:ASP:CG	2.28	0.53
6:B:29:PHE:HE1	9:B:101:BCL:H12	1.73	0.53
6:E:13:GLU:H	6:E:13:GLU:CD	2.09	0.53
5:I:43:ASP:CA	5:K:47:LEU:HB3	2.39	0.53
5:I:50:ASN:HA	5:K:59:GLY:C	2.29	0.53
5:Q:8:LEU:HD23	6:R:22:MET:HE1	1.90	0.53
6:T:45:TRP:O	6:T:46:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:36:HIS:NE2	9:V:101:BCL:HMD1	2.24	0.53
5:Y:20:VAL:O	5:Y:24:ILE:HG12	2.08	0.53
6:2:20:ILE:HD13	6:2:20:ILE:C	2.29	0.53
5:5:16:ASP:CB	5:5:19:ARG:HH21	2.22	0.53
1:C:212:ILE:HD13	1:C:212:ILE:N	2.22	0.53
2:L:77:PRO:HB2	2:L:78:PRO:HD2	1.91	0.53
14:M:405:MQ8:H401	4:H:51:GLY:HA3	1.90	0.53
5:I:13:LEU:CD1	15:N:102:CRT:C1M	2.87	0.53
5:I:20:VAL:O	5:I:24:ILE:HG12	2.09	0.53
5:S:13:LEU:O	6:T:7:THR:HA	2.08	0.53
5:S:46:TRP:CD1	5:S:47:LEU:HD22	2.44	0.53
5:W:44:LEU:HB2	5:Y:55:TYR:OH	2.08	0.53
6:X:40:TRP:O	6:X:44:PRO:HG3	2.09	0.53
6:6:10:THR:HG22	6:6:11:ASP:H	1.74	0.53
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.44	0.53
4:H:105:ASP:OD2	4:H:107:MET:HB3	2.08	0.53
15:A:101:CRT:H82	5:7:10:LYS:C	2.29	0.53
6:G:24:SER:O	6:G:27:ALA:HB3	2.09	0.53
5:U:26:ALA:C	5:U:29:ILE:HG22	2.23	0.53
6:V:27:ALA:C	6:V:31:LEU:HG	2.24	0.53
5:W:17:PRO:HA	5:W:20:VAL:HG22	1.91	0.53
9:W:102:BCL:HMB1	9:W:102:BCL:HBB2	1.90	0.53
15:W:103:CRT:H393	5:1:36:HIS:CG	2.44	0.53
5:1:2:PHE:HB2	5:1:5:ASN:HD22	1.73	0.53
5:3:22:VAL:HA	5:3:25:VAL:CG2	2.38	0.53
2:L:221:GLU:OE1	3:M:235:ILE:HD11	2.08	0.53
2:L:237:ALA:O	2:L:240:ARG:HB2	2.09	0.53
3:M:126:ILE:HD12	3:M:157:TYR:CE2	2.43	0.53
4:H:159:LEU:HB3	4:H:215:LYS:HA	1.91	0.53
6:V:13:GLU:CD	6:V:13:GLU:H	2.11	0.53
5:Y:36:HIS:CD2	9:Z:101:BCL:CMD	2.92	0.53
6:4:18:HIS:CD2	6:4:22:MET:HB2	2.43	0.53
5:5:42:THR:OG1	5:7:47:LEU:HG	2.09	0.53
2:L:41:CYS:HA	5:9:30:VAL:CG2	2.38	0.53
2:L:255:VAL:O	2:L:259:ILE:HG12	2.08	0.53
9:L:301:BCL:HAA2	9:L:303:BCL:HBC1	1.91	0.53
3:M:67:ALA:C	3:M:70:ILE:HG22	2.24	0.53
3:M:258:PHE:CD2	17:H:301:PEF:C30	2.93	0.53
4:H:227:ASN:HD22	4:H:228:PRO:CD	2.20	0.53
5:A:33:LEU:HA	15:A:101:CRT:C40	2.36	0.53
5:F:20:VAL:HA	5:F:23:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:43:ASP:O	5:Q:48:ASP:HB3	2.09	0.53
5:W:32:GLY:HA2	9:X:101:BCL:O1D	2.07	0.53
5:Y:42:THR:O	5:Y:43:ASP:C	2.47	0.53
5:7:36:HIS:O	5:7:40:LEU:N	2.31	0.53
5:9:29:ILE:HG23	5:9:30:VAL:N	2.24	0.53
1:C:311:HIS:CE1	1:C:315:ASN:O	2.62	0.52
2:L:156:PRO:O	2:L:162:HIS:HB3	2.09	0.52
6:E:10:THR:N	6:E:13:GLU:OE2	2.41	0.52
9:S:102:BCL:HMB1	9:S:102:BCL:HBB2	1.91	0.52
5:W:8:LEU:O	6:X:18:HIS:CE1	2.63	0.52
6:X:22:MET:HG3	6:X:26:TYR:CE2	2.39	0.52
5:3:12:TRP:HA	5:3:12:TRP:HE3	1.75	0.52
6:8:45:TRP:C	5:9:52:PRO:HD2	2.29	0.52
1:C:194:SER:HB3	3:M:92:TRP:CD1	2.45	0.52
1:C:201:THR:O	1:C:205:ASP:HB3	2.09	0.52
3:M:107:PRO:HB2	3:M:111:GLU:O	2.09	0.52
3:M:135:LYS:HZ1	12:M:408:PO4:P	2.32	0.52
3:M:180:PHE:N	3:M:181:PRO:HD2	2.24	0.52
4:H:138:VAL:O	4:H:140:LYS:NZ	2.43	0.52
9:V:101:BCL:CMA	9:W:102:BCL:HMA1	2.36	0.52
5:W:8:LEU:HD13	6:X:22:MET:HE2	1.81	0.52
15:4:102:CRT:H342	9:5:102:BCL:HAA1	1.91	0.52
6:6:28:TRP:C	6:6:30:GLY:N	2.63	0.52
1:C:20:LEU:HB2	2:L:271:TRP:CZ2	2.44	0.52
1:C:91:THR:O	1:C:95:VAL:HG23	2.10	0.52
1:C:270:TRP:CD2	3:M:316:PRO:HG3	2.44	0.52
4:H:45:ARG:HH11	4:H:45:ARG:HG2	1.74	0.52
6:G:17:PHE:CD2	15:G:102:CRT:H9	2.43	0.52
9:I:103:BCL:HMB3	9:K:102:BCL:C4A	2.39	0.52
6:J:17:PHE:CE1	15:J:101:CRT:H9	2.44	0.52
5:O:11:ILE:N	15:R:102:CRT:H82	2.23	0.52
9:O:102:BCL:HED3	6:P:28:TRP:CH2	2.45	0.52
6:4:42:TYR:C	6:4:42:TYR:HD1	2.12	0.52
5:7:35:ILE:HD12	9:7:103:BCL:CGD	2.40	0.52
6:8:7:THR:HG23	6:8:8:GLY:N	2.23	0.52
1:C:33:ILE:HD13	1:C:249:PHE:HA	1.92	0.52
2:L:250:ALA:O	2:L:253:SER:OG	2.16	0.52
3:M:30:ARG:HD3	3:M:50:PRO:HG2	1.91	0.52
3:M:161:GLY:HA3	15:M:406:CRT:C29	2.38	0.52
5:A:43:ASP:CA	5:D:48:ASP:HB3	2.36	0.52
15:A:101:CRT:H132	5:7:11:ILE:CD1	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:101:CRT:H22A	5:7:10:LYS:HB3	1.91	0.52
5:S:42:THR:HG22	5:S:43:ASP:H	1.73	0.52
6:T:42:TYR:CE2	6:T:43:ARG:HG2	2.44	0.52
5:Y:18:ARG:HG2	5:Y:18:ARG:HH11	1.74	0.52
5:Y:38:ILE:HD12	5:Y:39:VAL:N	2.25	0.52
5:3:13:LEU:HD21	6:4:10:THR:O	2.10	0.52
1:C:277:ARG:HG2	1:C:277:ARG:HH11	1.74	0.52
3:M:218:MET:HE3	3:M:252:TRP:CZ3	2.44	0.52
5:A:49:ASP:O	5:A:50:ASN:HB3	2.09	0.52
6:E:42:TYR:CE2	6:E:43:ARG:HG3	2.45	0.52
6:P:13:GLU:HA	6:P:16:GLU:CG	2.39	0.52
6:R:34:ILE:HD13	6:R:34:ILE:O	2.10	0.52
6:0:20:ILE:HG23	6:0:21:PHE:N	2.25	0.52
6:0:40:TRP:HZ3	6:0:45:TRP:H	1.55	0.52
6:0:40:TRP:HA	6:0:40:TRP:CE3	2.44	0.52
2:L:54:ALA:O	2:L:66:GLN:NE2	2.42	0.52
2:L:87:ALA:H	2:L:96:GLN:HE22	1.57	0.52
3:M:27:ASN:ND2	5:O:19:ARG:HH11	2.08	0.52
4:H:189:ASN:HB3	4:H:191:LYS:HG3	1.92	0.52
5:A:33:LEU:CG	15:A:101:CRT:C39	2.63	0.52
5:D:50:ASN:CG	5:D:51:ILE:H	2.13	0.52
5:F:7:ASN:CG	6:J:20:ILE:HD13	2.30	0.52
6:J:21:PHE:C	6:J:21:PHE:HD1	2.13	0.52
5:K:18:ARG:HG2	5:K:18:ARG:HH11	1.74	0.52
5:7:56:GLN:CD	5:7:56:GLN:H	2.12	0.52
2:L:55:THR:HG23	5:A:41:SER:CA	2.40	0.52
2:L:71:TRP:HD1	3:M:303:MET:HG2	1.75	0.52
2:L:281:TRP:CG	3:M:88:LYS:HD2	2.44	0.52
3:M:124:LEU:HD23	3:M:127:LEU:HD12	1.92	0.52
4:H:55:VAL:HG11	5:D:19:ARG:HD3	1.90	0.52
15:A:101:CRT:H5	5:7:10:LYS:CB	2.38	0.52
6:B:9:LEU:N	6:B:9:LEU:HD12	2.23	0.52
6:E:9:LEU:HD13	6:E:13:GLU:HG2	1.91	0.52
6:R:29:PHE:HD1	6:R:29:PHE:H	1.58	0.52
5:7:18:ARG:O	5:7:22:VAL:HG12	2.10	0.52
6:8:38:LEU:O	6:8:38:LEU:HD23	2.10	0.52
5:9:29:ILE:CG2	5:9:30:VAL:N	2.73	0.52
1:C:194:SER:HB3	3:M:92:TRP:HD1	1.75	0.52
1:C:242:SER:O	1:C:313:ALA:HA	2.10	0.52
1:C:304:ARG:HH11	1:C:304:ARG:CG	2.19	0.52
3:M:156:PHE:HD1	3:M:281:GLY:HA2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:168:MET:HE1	3:M:289:THR:HA	1.92	0.52
3:M:242:GLY:HA3	4:H:119:ARG:HH21	1.75	0.52
5:D:16:ASP:OD1	5:D:17:PRO:HD2	2.10	0.52
5:F:10:LYS:HB2	15:J:101:CRT:H5	1.92	0.52
5:F:12:TRP:NE1	6:G:17:PHE:CD1	2.77	0.52
5:I:27:PHE:HE2	5:K:29:ILE:CD1	2.23	0.52
5:I:35:ILE:O	5:I:38:ILE:HG23	2.09	0.52
5:O:36:HIS:CE1	9:O:102:BCL:NA	2.78	0.52
15:T:102:CRT:H2M3	5:U:36:HIS:HB3	1.92	0.52
9:U:102:BCL:OBD	6:V:32:VAL:HG22	2.10	0.52
6:2:21:PHE:HD1	15:2:102:CRT:C14	2.10	0.52
5:9:16:ASP:OD1	5:9:17:PRO:HD2	2.07	0.52
1:C:200:LEU:H	1:C:200:LEU:HD12	1.75	0.52
1:C:295:ARG:CG	1:C:295:ARG:NH1	2.70	0.52
3:M:35:ILE:HG22	3:M:36:PHE:N	2.25	0.52
3:M:250:LEU:CD1	3:M:250:LEU:H	2.23	0.52
4:H:14:ILE:O	4:H:14:ILE:HG12	2.09	0.52
5:A:52:PRO:HD2	5:A:55:TYR:OH	2.09	0.52
6:B:20:ILE:HD13	6:B:20:ILE:C	2.31	0.52
5:D:7:ASN:HD22	5:D:8:LEU:N	2.06	0.52
5:F:29:ILE:HG23	5:F:30:VAL:N	2.24	0.52
5:K:51:ILE:HB	5:K:52:PRO:CA	2.35	0.52
5:W:13:LEU:HD11	6:X:11:ASP:HA	1.92	0.52
5:W:49:ASP:OD1	5:W:50:ASN:N	2.42	0.52
9:W:102:BCL:HMD2	9:X:101:BCL:C1D	2.40	0.52
6:X:28:TRP:HE3	6:X:31:LEU:HD12	1.73	0.52
5:1:2:PHE:CA	5:1:5:ASN:HD22	2.23	0.52
5:3:46:TRP:NE1	5:3:47:LEU:HD22	2.25	0.52
6:4:20:ILE:HG23	15:4:102:CRT:H6	1.84	0.52
6:8:28:TRP:HA	6:8:31:LEU:HB2	1.92	0.52
2:L:239:HIS:CD2	3:M:223:ILE:HG13	2.45	0.52
3:M:74:ASN:O	3:M:77:ALA:HB3	2.10	0.52
3:M:83:VAL:HA	3:M:86:PHE:HB3	1.92	0.52
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.44	0.52
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.75	0.52
5:A:35:ILE:O	5:A:36:HIS:C	2.48	0.52
5:D:20:VAL:O	5:D:24:ILE:HD12	2.10	0.52
5:F:44:LEU:H	5:I:56:GLN:NE2	2.08	0.52
9:N:101:BCL:CBB	9:N:101:BCL:HMB1	2.40	0.52
6:T:12:ASP:O	6:T:15:LYS:HD2	2.10	0.52
6:T:38:LEU:HD23	6:T:38:LEU:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:45:TRP:CD1	6:T:46:LEU:N	2.78	0.52
5:7:10:LYS:H	5:7:10:LYS:HD2	1.74	0.52
6:8:21:PHE:CG	6:8:22:MET:N	2.78	0.52
2:L:55:THR:HG23	5:A:41:SER:CB	2.40	0.51
2:L:78:PRO:HB3	2:L:92:GLY:HA3	1.92	0.51
2:L:241:LEU:O	2:L:244:PHE:HB3	2.10	0.51
11:L:304:UQ8:H43	11:L:304:UQ8:H40B	1.91	0.51
3:M:12:GLN:HE22	3:M:42:LYS:N	2.07	0.51
15:A:103:CRT:C22	5:D:24:ILE:HG21	2.39	0.51
9:E:101:BCL:C20	6:G:38:LEU:HD11	2.39	0.51
6:G:28:TRP:CE2	6:G:32:VAL:HG23	2.44	0.51
9:I:102:BCL:OBB	9:I:102:BCL:HHC	2.08	0.51
5:K:2:PHE:O	5:K:5:ASN:HB3	2.09	0.51
5:K:34:LEU:O	5:K:38:ILE:HG22	2.10	0.51
9:N:101:BCL:HMB3	9:O:102:BCL:C1B	2.39	0.51
5:O:44:LEU:HD12	5:O:44:LEU:C	2.31	0.51
6:P:46:LEU:HD22	6:R:42:TYR:CZ	2.44	0.51
6:V:21:PHE:CA	15:V:102:CRT:C14	2.87	0.51
9:6:101:BCL:C4B	9:7:102:BCL:HBB3	2.40	0.51
5:9:9:TYR:CD1	6:0:15:LYS:HG2	2.44	0.51
6:0:7:THR:HG23	6:0:8:GLY:N	2.20	0.51
2:L:184:LEU:HG	2:L:252:TRP:CD1	2.45	0.51
2:L:186:ILE:HD13	9:M:401:BCL:HMD1	1.91	0.51
3:M:271:TRP:CG	4:H:26:LEU:HD21	2.44	0.51
3:M:296:LEU:HA	3:M:299:VAL:HG12	1.92	0.51
4:H:132:LYS:HE2	4:H:175:SER:CB	2.41	0.51
5:A:20:VAL:HA	5:A:23:SER:HB3	1.91	0.51
6:G:36:HIS:HB3	9:G:101:BCL:H151	1.92	0.51
6:G:40:TRP:HB2	9:G:101:BCL:C19	2.35	0.51
5:K:38:ILE:O	5:K:38:ILE:HG12	2.10	0.51
15:N:102:CRT:H242	9:O:102:BCL:H18	1.91	0.51
5:U:2:PHE:HA	5:U:5:ASN:HB2	1.92	0.51
6:V:21:PHE:CG	15:V:102:CRT:C14	2.49	0.51
6:V:43:ARG:HB3	5:W:55:TYR:CZ	2.45	0.51
6:Z:10:THR:CG2	6:Z:11:ASP:H	2.13	0.51
5:3:13:LEU:CG	15:3:103:CRT:H1M1	2.41	0.51
6:4:42:TYR:C	6:4:42:TYR:CD1	2.83	0.51
9:4:101:BCL:HMB3	9:5:102:BCL:C4A	2.39	0.51
5:5:30:VAL:O	5:5:34:LEU:N	2.38	0.51
6:8:17:PHE:CE1	15:8:101:CRT:C6	2.92	0.51
1:C:202:PRO:O	1:C:206:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:PRO:HB3	2:L:95:TRP:CD2	2.45	0.51
2:L:227:ASP:O	3:M:52:TYR:HB3	2.11	0.51
3:M:218:MET:HE2	3:M:252:TRP:CH2	2.46	0.51
3:M:260:VAL:O	14:M:405:MQ8:H61	2.10	0.51
5:F:7:ASN:HB3	6:J:20:ILE:HD13	1.91	0.51
5:F:9:TYR:CD1	5:F:9:TYR:C	2.84	0.51
5:I:20:VAL:HA	5:I:23:SER:OG	2.11	0.51
5:K:8:LEU:HD22	5:K:11:ILE:HD11	1.93	0.51
5:Q:2:PHE:O	5:Q:5:ASN:HB3	2.10	0.51
9:V:101:BCL:CBB	9:V:101:BCL:HMB1	2.40	0.51
6:X:32:VAL:O	6:X:36:HIS:N	2.40	0.51
5:1:10:LYS:CA	15:4:102:CRT:H22A	2.39	0.51
9:1:102:BCL:H2A	9:1:102:BCL:O1D	2.11	0.51
5:5:19:ARG:O	5:5:23:SER:HB2	2.09	0.51
9:6:101:BCL:C1B	9:7:102:BCL:CMB	2.88	0.51
2:L:128:PHE:HE2	11:L:304:UQ8:C45	2.24	0.51
2:L:206:VAL:HG12	3:M:142:MET:HE1	1.91	0.51
2:L:224:PHE:CE1	2:L:228:ILE:HD11	2.45	0.51
4:H:36:ARG:NH1	4:H:78:ALA:O	2.43	0.51
5:A:36:HIS:CD2	9:B:101:BCL:HMD3	2.45	0.51
6:R:20:ILE:HG23	6:R:21:PHE:N	2.24	0.51
5:U:5:ASN:HA	5:U:8:LEU:HD12	1.92	0.51
6:V:20:ILE:HG23	15:V:102:CRT:H9	1.90	0.51
5:Y:5:ASN:HA	6:Z:18:HIS:CD2	2.45	0.51
6:Z:36:HIS:CE1	9:Z:101:BCL:C4A	2.93	0.51
6:8:23:GLN:HG3	6:8:24:SER:N	2.24	0.51
1:C:246:GLY:O	1:C:248:THR:N	2.43	0.51
2:L:13:ARG:HD3	4:H:101:VAL:HG22	1.92	0.51
2:L:18:ILE:HD11	4:H:259:LEU:HD12	1.92	0.51
2:L:236:LEU:HD23	2:L:237:ALA:H	1.76	0.51
3:M:60:SER:HA	3:M:128:LEU:HD23	1.91	0.51
3:M:260:VAL:CB	4:H:34:ASP:OD1	2.56	0.51
9:A:102:BCL:CMD	6:B:36:HIS:CE1	2.90	0.51
5:D:12:TRP:CE3	5:D:12:TRP:HA	2.46	0.51
5:I:15:LEU:HD22	5:I:15:LEU:N	2.26	0.51
9:K:102:BCL:CHD	9:K:102:BCL:HBC2	2.40	0.51
9:Q:102:BCL:C4C	9:R:101:BCL:HMD2	2.38	0.51
5:Y:15:LEU:HD11	9:1:102:BCL:H141	1.91	0.51
5:1:49:ASP:O	5:3:60:LYS:HA	2.11	0.51
6:0:29:PHE:N	6:0:29:PHE:HD1	2.08	0.51
1:C:203:PHE:CD2	1:C:235:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:LEU:O	5:9:18:ARG:HD2	2.10	0.51
2:L:138:LEU:O	2:L:142:PHE:HB3	2.10	0.51
2:L:194:LEU:HD12	11:L:304:UQ8:H15B	1.91	0.51
5:A:8:LEU:HB3	6:E:20:ILE:CG2	2.41	0.51
15:A:101:CRT:H82	5:7:11:ILE:CA	2.40	0.51
9:F:102:BCL:HMD2	9:G:101:BCL:CHD	2.40	0.51
5:I:18:ARG:O	5:I:22:VAL:HG12	2.11	0.51
6:N:29:PHE:CZ	9:N:101:BCL:H61	2.44	0.51
6:P:24:SER:O	6:P:27:ALA:HB3	2.11	0.51
6:R:29:PHE:HD1	6:R:29:PHE:N	2.08	0.51
15:V:102:CRT:H342	9:W:102:BCL:CAA	2.41	0.51
5:5:50:ASN:CG	5:5:51:ILE:N	2.62	0.51
5:7:11:ILE:HD13	9:9:102:BCL:H151	1.93	0.51
6:0:29:PHE:N	6:0:29:PHE:CD1	2.78	0.51
1:C:291:LEU:O	1:C:296:LYS:HE3	2.10	0.51
2:L:70:LEU:HA	2:L:73:ILE:HD12	1.91	0.51
2:L:86:MET:CE	2:L:96:GLN:HB3	2.40	0.51
2:L:189:PHE:HZ	9:L:301:BCL:O1A	1.94	0.51
6:B:43:ARG:HB3	5:D:55:TYR:OH	2.11	0.51
5:O:9:TYR:HA	6:P:18:HIS:CG	2.46	0.51
5:W:33:LEU:HD12	5:W:34:LEU:H	1.75	0.51
5:Y:34:LEU:O	5:Y:37:MET:HB2	2.11	0.51
5:Y:40:LEU:HD12	5:Y:45:ASN:HA	1.93	0.51
6:2:42:TYR:CD1	6:2:43:ARG:HG3	2.45	0.51
5:3:2:PHE:CA	5:3:5:ASN:ND2	2.74	0.51
5:5:44:LEU:C	5:5:46:TRP:H	2.13	0.51
5:7:4:MET:HG3	5:7:8:LEU:HB2	1.93	0.51
6:8:17:PHE:HE1	15:8:101:CRT:C7	2.21	0.51
6:8:20:ILE:O	6:8:23:GLN:CG	2.59	0.51
9:9:102:BCL:C1D	9:0:101:BCL:CMD	2.83	0.51
1:C:157:ARG:HG2	1:C:157:ARG:NH1	2.25	0.51
2:L:89:LEU:HD23	5:9:41:SER:HB3	1.92	0.51
3:M:11:VAL:HA	4:H:148:ASP:OD2	2.11	0.51
3:M:175:VAL:HG22	3:M:185:TRP:CE2	2.46	0.51
6:B:38:LEU:HD23	6:B:38:LEU:C	2.31	0.51
5:D:2:PHE:HD1	5:D:3:THR:H	1.56	0.51
9:D:102:BCL:HMB1	9:D:102:BCL:HBB3	1.92	0.51
5:O:3:THR:CB	5:O:4:MET:SD	2.92	0.51
6:P:20:ILE:HG23	6:P:21:PHE:N	2.24	0.51
5:S:39:VAL:O	5:S:42:THR:HB	2.10	0.51
6:X:34:ILE:HD13	6:X:34:ILE:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:27:PHE:HE2	5:3:29:ILE:HD11	1.76	0.51
6:4:40:TRP:CZ3	6:4:45:TRP:N	2.77	0.51
5:5:43:ASP:OD1	5:7:53:VAL:CB	2.59	0.51
5:7:2:PHE:O	5:7:5:ASN:HB3	2.10	0.51
1:C:191:ALA:HB3	1:C:237:MET:HE3	1.92	0.51
1:C:228:GLN:O	1:C:231:TRP:HB2	2.11	0.51
2:L:28:GLY:N	4:H:46:THR:HB	2.26	0.51
2:L:89:LEU:CA	2:L:93:GLY:HA3	2.27	0.51
3:M:291:VAL:HG12	3:M:292:ASP:N	2.26	0.51
5:F:39:VAL:HG22	5:I:47:LEU:HD21	1.92	0.51
6:R:13:GLU:H	6:R:13:GLU:CD	2.13	0.51
15:T:102:CRT:H372	9:U:102:BCL:HMB2	1.93	0.51
5:Y:52:PRO:O	5:1:60:LYS:CB	2.59	0.51
6:Z:45:TRP:CD2	9:Z:101:BCL:H2C	2.45	0.51
6:2:40:TRP:CE3	6:2:44:PRO:HA	2.46	0.51
9:4:101:BCL:HBA2	9:4:101:BCL:HMA2	1.93	0.51
6:8:43:ARG:NE	5:9:55:TYR:HB2	2.26	0.51
1:C:109:TYR:CZ	1:C:160:PRO:HB3	2.46	0.51
1:C:157:ARG:HH22	1:C:318:LEU:HG	1.76	0.51
1:C:292:PRO:HG2	1:C:295:ARG:HG2	1.93	0.51
9:A:102:BCL:C4C	9:B:101:BCL:HMD2	2.42	0.51
6:B:38:LEU:HD23	6:B:38:LEU:O	2.11	0.51
5:D:15:LEU:HB3	5:D:20:VAL:CG2	2.41	0.51
5:F:43:ASP:HB2	5:I:47:LEU:CB	2.41	0.51
5:I:12:TRP:HZ2	6:J:21:PHE:CD2	2.24	0.51
5:O:11:ILE:O	5:O:11:ILE:HG22	2.10	0.51
9:O:102:BCL:HMB1	9:O:102:BCL:HBB3	1.92	0.51
5:S:50:ASN:ND2	6:T:43:ARG:HH22	2.04	0.51
5:Y:2:PHE:CA	5:Y:5:ASN:HD22	2.24	0.51
5:Y:30:VAL:HA	5:Y:33:LEU:CG	2.40	0.51
6:4:46:LEU:CD2	6:6:43:ARG:HH22	2.23	0.51
5:5:10:LYS:CD	15:8:101:CRT:H23	2.16	0.51
5:5:44:LEU:O	5:5:46:TRP:N	2.38	0.51
5:9:43:ASP:OD1	5:9:44:LEU:HD12	2.11	0.51
1:C:20:LEU:HD13	1:C:21:LEU:N	2.26	0.50
3:M:59:LEU:HD11	5:Q:29:ILE:HG21	1.90	0.50
5:A:9:TYR:C	5:A:11:ILE:H	2.13	0.50
5:A:36:HIS:CE1	9:B:101:BCL:HMD1	2.46	0.50
6:E:23:GLN:CG	6:E:24:SER:N	2.75	0.50
5:F:10:LYS:O	5:F:13:LEU:HG	2.10	0.50
6:J:16:GLU:HG2	15:J:101:CRT:C2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:101:BCL:HBB3	9:O:102:BCL:C4B	2.41	0.50
5:O:24:ILE:HA	5:O:27:PHE:CB	2.41	0.50
6:R:10:THR:HB	6:R:13:GLU:OE2	2.11	0.50
5:S:5:ASN:ND2	6:T:22:MET:HG3	2.25	0.50
5:U:19:ARG:NH2	5:U:19:ARG:HB2	2.26	0.50
5:Y:29:ILE:CB	9:Y:102:BCL:H11	2.41	0.50
5:3:35:ILE:HA	5:3:38:ILE:CG2	2.38	0.50
5:9:16:ASP:OD1	5:9:17:PRO:CD	2.59	0.50
1:C:71:LYS:N	1:C:71:LYS:CE	2.73	0.50
3:M:277:VAL:O	3:M:280:ALA:HB3	2.12	0.50
4:H:6:THR:C	5:F:41:SER:HB3	2.31	0.50
5:A:9:TYR:CZ	5:A:10:LYS:HE2	2.45	0.50
15:G:102:CRT:H393	5:I:36:HIS:CG	2.45	0.50
6:2:28:TRP:O	6:2:32:VAL:HG23	2.10	0.50
1:C:122:TYR:O	1:C:126:VAL:HG22	2.11	0.50
1:C:166:TRP:HE1	1:C:305:VAL:C	2.14	0.50
1:C:174:TYR:O	1:C:174:TYR:HD1	1.94	0.50
1:C:195:LEU:O	1:C:197:PHE:CD2	2.58	0.50
1:C:196:PRO:CG	1:C:231:TRP:HD1	2.25	0.50
2:L:242:GLY:HA3	3:M:216:PHE:CE1	2.45	0.50
2:L:268:TRP:CE3	2:L:268:TRP:HA	2.47	0.50
3:M:218:MET:HE3	3:M:252:TRP:CH2	2.47	0.50
5:A:2:PHE:O	5:A:2:PHE:HD1	1.94	0.50
5:A:35:ILE:HA	5:A:38:ILE:HG12	1.93	0.50
5:A:36:HIS:CB	15:A:101:CRT:C40	2.77	0.50
6:B:17:PHE:HE1	15:B:102:CRT:C9	2.25	0.50
5:D:27:PHE:CE1	5:F:29:ILE:HD11	2.46	0.50
5:F:19:ARG:NH1	5:I:18:ARG:NH2	2.58	0.50
9:I:102:BCL:C2D	9:I:103:BCL:C2D	2.89	0.50
6:J:38:LEU:O	6:J:38:LEU:HD23	2.10	0.50
6:V:34:ILE:O	6:V:37:LEU:HB2	2.11	0.50
6:Z:29:PHE:N	6:Z:29:PHE:CD1	2.77	0.50
5:3:38:ILE:HD12	15:4:102:CRT:C40	2.40	0.50
1:C:59:VAL:HG21	1:C:100:TRP:HE1	1.76	0.50
2:L:236:LEU:HD12	3:M:6:ASN:OD1	2.12	0.50
5:D:12:TRP:HA	5:D:12:TRP:HE3	1.76	0.50
9:I:103:BCL:HMB3	9:K:102:BCL:C1B	2.41	0.50
5:K:44:LEU:CD1	5:K:44:LEU:N	2.73	0.50
6:N:17:PHE:CD1	15:N:102:CRT:C9	2.93	0.50
6:P:46:LEU:HD13	6:R:42:TYR:OH	2.11	0.50
6:2:40:TRP:CZ3	6:2:44:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:8:GLY:O	6:6:9:LEU:HD23	2.12	0.50
6:8:17:PHE:CE1	6:8:20:ILE:HG21	2.46	0.50
6:8:20:ILE:O	6:8:20:ILE:HD13	2.11	0.50
6:0:21:PHE:O	6:0:24:SER:N	2.45	0.50
2:L:194:LEU:O	2:L:198:MET:HG3	2.11	0.50
3:M:37:SER:OG	3:M:40:LEU:HB2	2.11	0.50
3:M:121:PHE:O	3:M:125:SER:HB2	2.12	0.50
5:A:21:LEU:HD23	5:9:14:ILE:HG21	1.93	0.50
5:K:27:PHE:CD1	5:K:27:PHE:C	2.85	0.50
5:Q:9:TYR:HA	6:R:18:HIS:ND1	2.27	0.50
5:U:40:LEU:HD11	5:U:47:LEU:HD23	1.94	0.50
6:2:38:LEU:C	6:2:38:LEU:HD23	2.32	0.50
5:3:55:TYR:O	5:3:59:GLY:HA3	2.11	0.50
5:5:31:LEU:O	5:5:35:ILE:HG12	2.11	0.50
6:6:29:PHE:CE1	9:6:101:BCL:C1	2.95	0.50
5:7:46:TRP:CD1	5:7:47:LEU:HD22	2.46	0.50
2:L:23:PHE:HA	2:L:25:PHE:CE2	2.46	0.50
3:M:178:GLY:O	3:M:182:HIS:HB3	2.11	0.50
4:H:48:ARG:NH2	17:H:301:PEF:H12	2.26	0.50
4:H:121:LYS:HG2	4:H:234:TYR:CG	2.47	0.50
9:B:101:BCL:HBA2	9:B:101:BCL:CMA	2.36	0.50
9:F:102:BCL:OBD	6:G:32:VAL:HG13	2.12	0.50
5:Q:50:ASN:CB	5:S:56:GLN:HA	2.41	0.50
6:R:29:PHE:N	6:R:29:PHE:CD1	2.79	0.50
5:U:10:LYS:CA	15:X:102:CRT:H23	2.41	0.50
5:Y:29:ILE:CA	9:Y:102:BCL:C1	2.85	0.50
5:1:20:VAL:O	5:1:24:ILE:HG12	2.11	0.50
6:2:30:GLY:O	6:2:33:VAL:HG12	2.12	0.50
5:5:43:ASP:HA	5:7:48:ASP:HB3	1.93	0.50
6:8:26:TYR:HA	6:8:29:PHE:HB3	1.93	0.50
6:0:20:ILE:HD13	6:0:20:ILE:C	2.31	0.50
1:C:20:LEU:HD13	1:C:20:LEU:C	2.31	0.50
1:C:35:TYR:O	1:C:38:VAL:HG23	2.12	0.50
1:C:250:CYS:HB3	1:C:251:HIS:ND1	2.27	0.50
1:C:252:ASN:OD1	1:C:254:ARG:HG3	2.12	0.50
9:L:301:BCL:CBB	9:L:301:BCL:HMB1	2.42	0.50
3:M:17:ALA:O	3:M:19:PRO:HD3	2.12	0.50
9:B:101:BCL:C2B	9:D:102:BCL:C2B	2.89	0.50
5:F:44:LEU:CB	6:G:43:ARG:HH11	2.14	0.50
6:G:21:PHE:CZ	15:G:102:CRT:H16	2.46	0.50
6:G:30:GLY:O	6:G:34:ILE:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:44:LEU:HD22	5:K:46:TRP:N	2.26	0.50
6:R:20:ILE:HD13	6:R:20:ILE:C	2.32	0.50
5:U:17:PRO:HB3	6:V:17:PHE:CE2	2.46	0.50
5:Y:36:HIS:HE1	9:Y:102:BCL:C1A	2.25	0.50
5:Y:54:SER:O	5:Y:55:TYR:C	2.50	0.50
5:Y:55:TYR:N	5:Y:55:TYR:CD1	2.79	0.50
6:2:20:ILE:HG23	15:2:102:CRT:C8	2.38	0.50
5:3:12:TRP:HA	5:3:12:TRP:CE3	2.46	0.50
2:L:206:VAL:HG12	3:M:142:MET:CE	2.42	0.50
3:M:228:ARG:NH1	4:H:247:LYS:HE2	2.25	0.50
5:D:50:ASN:CG	5:D:51:ILE:N	2.65	0.50
9:O:102:BCL:CAC	9:P:101:BCL:HBC3	2.42	0.50
5:Q:50:ASN:ND2	5:Q:51:ILE:HG13	2.21	0.50
6:R:25:MET:HE2	15:R:102:CRT:H242	1.94	0.50
9:T:101:BCL:HMB1	9:T:101:BCL:CBB	2.42	0.50
5:U:5:ASN:HB3	6:V:22:MET:CE	2.42	0.50
5:1:38:ILE:HG23	5:1:39:VAL:H	1.77	0.50
6:2:29:PHE:HD1	6:2:29:PHE:H	1.58	0.50
1:C:135:ARG:O	1:C:136:ALA:C	2.50	0.50
1:C:173:LYS:HG3	1:C:174:TYR:N	2.26	0.50
1:C:270:TRP:HA	1:C:273:ILE:HD12	1.94	0.50
1:C:327:TYR:HB3	1:C:330:LEU:HD12	1.93	0.50
2:L:48:LEU:HD13	5:9:34:LEU:HD22	1.94	0.50
2:L:56:ILE:O	2:L:66:GLN:HG3	2.11	0.50
3:M:234:GLU:CD	3:M:266:HIS:CE1	2.85	0.50
5:F:44:LEU:HD12	5:F:46:TRP:HE3	1.75	0.50
5:O:9:TYR:C	5:O:9:TYR:CD1	2.86	0.50
6:P:21:PHE:O	6:P:22:MET:C	2.49	0.50
6:R:13:GLU:O	15:R:102:CRT:C3	2.60	0.50
6:2:46:LEU:HB2	5:3:52:PRO:HD2	1.93	0.50
6:6:38:LEU:HD23	6:6:38:LEU:C	2.32	0.50
1:C:89:GLU:O	1:C:92:ARG:HB3	2.12	0.49
3:M:55:LEU:HD23	5:Q:22:VAL:HG23	1.93	0.49
4:H:47:GLU:O	4:H:48:ARG:C	2.49	0.49
5:O:50:ASN:HB3	5:Q:59:GLY:HA2	1.94	0.49
6:P:30:GLY:O	6:P:34:ILE:HG22	2.12	0.49
6:R:36:HIS:O	6:R:39:ALA:N	2.45	0.49
9:S:102:BCL:HBC1	9:T:101:BCL:HBC3	1.94	0.49
5:U:14:ILE:O	5:U:14:ILE:CG2	2.60	0.49
5:U:43:ASP:OD1	5:U:44:LEU:HD23	2.11	0.49
5:1:4:MET:CB	5:1:8:LEU:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:33:LEU:HD12	5:1:34:LEU:N	2.27	0.49
6:2:45:TRP:O	6:2:46:LEU:CB	2.60	0.49
5:5:5:ASN:CA	5:5:8:LEU:HD12	2.38	0.49
3:M:178:GLY:HA3	3:M:181:PRO:CG	2.40	0.49
4:H:35:LYS:HG3	4:H:39:TYR:CD2	2.47	0.49
9:F:102:BCL:ND	9:G:101:BCL:CMD	2.75	0.49
5:K:16:ASP:HB3	5:K:18:ARG:HE	1.76	0.49
9:O:102:BCL:HMB1	9:O:102:BCL:HBB2	1.94	0.49
6:X:45:TRP:CE3	9:X:101:BCL:HAC2	2.47	0.49
5:Y:36:HIS:ND1	9:Z:101:BCL:HMD1	2.24	0.49
5:9:33:LEU:HD12	5:9:33:LEU:H	1.77	0.49
6:0:34:ILE:HD13	6:0:34:ILE:C	2.32	0.49
1:C:203:PHE:HD2	1:C:210:ILE:HG12	1.78	0.49
2:L:50:ILE:HG12	2:L:98:ILE:HD13	1.94	0.49
3:M:215:LEU:HD21	14:M:405:MQ8:C19	2.42	0.49
6:N:7:THR:OG1	6:N:8:GLY:N	2.45	0.49
5:O:43:ASP:HB2	5:Q:47:LEU:HB3	1.95	0.49
5:Q:16:ASP:N	5:Q:19:ARG:HH21	2.06	0.49
5:S:34:LEU:HD23	5:U:33:LEU:HD21	1.93	0.49
5:W:54:SER:O	5:W:58:LEU:N	2.39	0.49
5:Y:29:ILE:HB	9:Y:102:BCL:H11	1.93	0.49
6:8:17:PHE:HE1	15:8:101:CRT:C6	2.24	0.49
6:8:33:VAL:CG1	6:8:34:ILE:N	2.75	0.49
6:0:21:PHE:CE1	6:0:25:MET:HB2	2.47	0.49
6:0:21:PHE:HE1	6:0:25:MET:HB2	1.77	0.49
1:C:150:VAL:HG12	7:C:504:HEM:HMD1	1.94	0.49
1:C:175:PRO:HD2	1:C:179:LYS:CB	2.37	0.49
2:L:71:TRP:N	2:L:71:TRP:CE3	2.80	0.49
2:L:189:PHE:CE1	2:L:249:ALA:HB1	2.47	0.49
3:M:105:ARG:O	3:M:107:PRO:HD3	2.13	0.49
4:H:182:LEU:HB2	4:H:195:LEU:HB3	1.95	0.49
9:A:102:BCL:CHA	9:B:101:BCL:OBD	2.60	0.49
5:D:7:ASN:H	5:D:7:ASN:ND2	2.09	0.49
5:D:49:ASP:HB2	5:F:56:GLN:CD	2.33	0.49
6:E:44:PRO:HG2	5:F:55:TYR:OH	2.13	0.49
5:I:26:ALA:O	5:I:30:VAL:HG12	2.12	0.49
6:J:33:VAL:HG22	6:J:37:LEU:HD23	1.94	0.49
5:K:44:LEU:CD2	5:K:46:TRP:CE3	2.94	0.49
5:O:17:PRO:HG2	5:O:18:ARG:H	1.77	0.49
5:S:50:ASN:CB	5:U:59:GLY:HA3	2.42	0.49
5:W:24:ILE:HG21	15:X:102:CRT:H20	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:11:ILE:CG2	5:Y:15:LEU:HD12	2.41	0.49
5:Y:43:ASP:HA	5:1:47:LEU:O	2.11	0.49
6:Z:45:TRP:O	6:Z:46:LEU:CB	2.60	0.49
15:3:103:CRT:H6	6:6:17:PHE:CE2	2.48	0.49
6:4:43:ARG:NH1	5:5:55:TYR:CD1	2.81	0.49
4:H:35:LYS:CE	4:H:39:TYR:CD2	2.96	0.49
4:H:100:LEU:HB2	4:H:111:PHE:CZ	2.47	0.49
5:A:12:TRP:HZ2	6:B:21:PHE:CE2	2.30	0.49
6:B:18:HIS:HE1	6:B:22:MET:CE	2.24	0.49
5:D:21:LEU:O	5:D:25:VAL:HG23	2.12	0.49
9:G:101:BCL:CMA	9:G:101:BCL:HBA2	2.36	0.49
5:I:53:VAL:O	5:I:54:SER:CB	2.60	0.49
6:J:17:PHE:CA	6:J:20:ILE:HG22	2.39	0.49
5:K:44:LEU:HD21	5:K:46:TRP:CE3	2.48	0.49
6:R:13:GLU:OE2	6:R:13:GLU:N	2.45	0.49
5:U:42:THR:HB	5:W:48:ASP:CG	2.33	0.49
5:1:11:ILE:CG2	5:1:15:LEU:HD12	2.42	0.49
1:C:161:VAL:HG13	7:C:502:HEM:O1D	2.12	0.49
1:C:288:ASN:HB2	1:C:302:PRO:HG3	1.93	0.49
2:L:18:ILE:HG12	4:H:259:LEU:HB2	1.95	0.49
2:L:83:GLY:O	2:L:150:ALA:HA	2.12	0.49
2:L:220:HIS:HD2	3:M:140:LEU:HD11	1.78	0.49
2:L:264:TRP:CZ3	2:L:271:TRP:HD1	2.30	0.49
3:M:268:TRP:NE1	4:H:30:LEU:HB3	2.27	0.49
4:H:9:ILE:HG21	5:F:42:THR:OG1	2.12	0.49
5:D:49:ASP:O	5:F:56:GLN:HG2	2.13	0.49
5:F:43:ASP:HB3	5:I:47:LEU:HG	1.93	0.49
5:I:46:TRP:CD1	5:I:47:LEU:HD12	2.48	0.49
6:P:46:LEU:H	5:Q:52:PRO:HD3	1.74	0.49
6:R:42:TYR:CE2	6:R:43:ARG:HG3	2.47	0.49
5:S:10:LYS:HB3	15:V:102:CRT:H31A	1.94	0.49
6:T:20:ILE:C	6:T:20:ILE:HD13	2.32	0.49
5:U:51:ILE:HA	5:U:53:VAL:N	2.27	0.49
5:W:35:ILE:O	5:W:36:HIS:C	2.49	0.49
5:1:51:ILE:CB	5:1:52:PRO:CA	2.86	0.49
6:4:46:LEU:CB	5:5:52:PRO:HD3	2.31	0.49
3:M:268:TRP:CE2	4:H:30:LEU:HB3	2.48	0.49
4:H:32:ARG:HG2	4:H:32:ARG:HH11	1.77	0.49
5:A:50:ASN:HA	5:D:59:GLY:C	2.33	0.49
6:B:20:ILE:CG2	15:B:102:CRT:H83	2.26	0.49
9:D:102:BCL:HMB1	9:D:102:BCL:HBB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:ILE:O	5:F:36:HIS:C	2.51	0.49
5:U:32:GLY:N	9:V:101:BCL:HED2	2.27	0.49
5:W:30:VAL:HG13	5:W:31:LEU:N	2.27	0.49
6:6:40:TRP:HZ3	6:6:45:TRP:N	2.09	0.49
6:0:36:HIS:CE1	9:0:101:BCL:C1B	2.95	0.49
6:B:29:PHE:HE1	9:B:101:BCL:C1	2.26	0.49
5:F:50:ASN:OD1	6:G:43:ARG:NH2	2.41	0.49
6:P:21:PHE:CG	15:P:102:CRT:C14	2.92	0.49
6:R:7:THR:HG22	5:S:18:ARG:NH2	2.27	0.49
5:W:26:ALA:CA	5:W:29:ILE:CG2	2.78	0.49
5:Y:9:TYR:CD1	5:Y:9:TYR:C	2.85	0.49
5:Y:55:TYR:N	5:Y:55:TYR:HD1	2.11	0.49
5:1:50:ASN:HB2	5:3:59:GLY:CA	2.42	0.49
5:5:22:VAL:O	5:5:25:VAL:HB	2.13	0.49
6:8:43:ARG:NH2	5:9:55:TYR:HB2	2.27	0.49
2:L:128:PHE:HE2	11:L:304:UQ8:H45B	1.76	0.49
2:L:130:PHE:HB2	10:L:302:BPH:HMD3	1.95	0.49
2:L:196:LEU:HD12	3:M:212:SER:OG	2.12	0.49
3:M:135:LYS:HE3	5:O:19:ARG:HH22	1.76	0.49
4:H:61:LEU:CD1	4:H:62:PRO:HD2	2.42	0.49
4:H:177:PRO:O	4:H:178:GLN:HB3	2.13	0.49
6:E:24:SER:O	6:E:27:ALA:HB3	2.13	0.49
5:F:2:PHE:N	5:F:2:PHE:CD1	2.81	0.49
6:G:38:LEU:HA	6:G:41:LEU:CD1	2.39	0.49
5:I:31:LEU:O	5:I:35:ILE:HG12	2.13	0.49
15:J:101:CRT:C2M	5:K:36:HIS:HB2	2.42	0.49
15:N:102:CRT:C33	9:O:102:BCL:H3A	2.42	0.49
5:O:7:ASN:O	6:R:20:ILE:HG12	2.12	0.49
5:O:24:ILE:HA	5:O:27:PHE:HB3	1.94	0.49
6:P:41:LEU:HG	6:P:42:TYR:N	2.27	0.49
6:X:37:LEU:C	6:X:37:LEU:CD2	2.81	0.49
5:5:35:ILE:O	5:5:36:HIS:C	2.49	0.49
5:7:7:ASN:HD22	5:7:7:ASN:N	2.10	0.49
5:7:42:THR:O	5:7:43:ASP:C	2.50	0.49
1:C:179:LYS:HD2	1:C:180:PRO:CD	2.43	0.49
2:L:13:ARG:HH11	2:L:13:ARG:HG3	1.78	0.49
3:M:16:PRO:HD3	4:H:141:GLU:HB2	1.93	0.49
3:M:66:VAL:HG21	5:Q:30:VAL:HG21	1.95	0.49
6:B:29:PHE:CE1	9:B:101:BCL:C1	2.96	0.49
9:G:101:BCL:HMB3	9:I:102:BCL:C1B	2.42	0.49
5:O:26:ALA:O	5:O:27:PHE:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:16:GLU:HB2	15:R:102:CRT:C3	2.37	0.49
6:V:45:TRP:O	6:V:46:LEU:CB	2.60	0.49
5:W:49:ASP:CG	5:W:50:ASN:N	2.66	0.49
9:Y:102:BCL:H2A	9:Y:102:BCL:O1D	2.12	0.49
6:0:33:VAL:O	6:0:37:LEU:HB2	2.12	0.49
1:C:47:ARG:CD	5:3:48:ASP:OD2	2.42	0.48
2:L:179:ASN:ND2	2:L:268:TRP:CE2	2.81	0.48
4:H:132:LYS:HE2	4:H:175:SER:HB2	1.96	0.48
5:A:17:PRO:CB	5:9:14:ILE:HD11	2.43	0.48
9:A:102:BCL:CMB	9:0:101:BCL:C1B	2.87	0.48
6:G:45:TRP:O	6:G:46:LEU:CB	2.61	0.48
9:I:102:BCL:HBC1	9:I:103:BCL:HHD	1.85	0.48
5:K:4:MET:SD	6:P:27:ALA:HB2	2.52	0.48
9:O:102:BCL:CHD	9:P:101:BCL:HMD2	2.43	0.48
5:S:26:ALA:C	5:S:29:ILE:HG22	2.26	0.48
6:T:29:PHE:N	6:T:29:PHE:CD1	2.80	0.48
9:W:102:BCL:HMD1	6:X:36:HIS:CD2	2.44	0.48
5:1:2:PHE:CB	5:1:5:ASN:HD22	2.26	0.48
5:1:16:ASP:CB	5:1:19:ARG:HD3	2.41	0.48
9:6:101:BCL:CHC	9:7:102:BCL:HBB3	2.43	0.48
15:8:101:CRT:C33	9:9:102:BCL:H3A	2.43	0.48
1:C:148:THR:HG23	1:C:322:GLN:HG2	1.94	0.48
2:L:126:VAL:HG11	3:M:251:PHE:CE2	2.47	0.48
2:L:159:ILE:O	9:L:303:BCL:HED1	2.13	0.48
2:L:257:ILE:HD13	9:L:301:BCL:CAD	2.43	0.48
4:H:15:THR:O	4:H:18:ALA:HB3	2.13	0.48
5:D:9:TYR:HA	6:E:18:HIS:CD2	2.47	0.48
9:S:102:BCL:CAD	9:T:101:BCL:CAD	2.91	0.48
15:W:103:CRT:C8	6:Z:20:ILE:CD1	2.76	0.48
5:Y:30:VAL:CA	5:Y:33:LEU:HG	2.43	0.48
5:1:51:ILE:HB	5:1:52:PRO:O	2.13	0.48
5:7:32:GLY:O	5:7:35:ILE:HB	2.13	0.48
5:7:56:GLN:HG2	5:7:57:ALA:H	1.78	0.48
6:0:40:TRP:HA	6:0:40:TRP:HE3	1.78	0.48
1:C:234:GLY:O	1:C:237:MET:HB2	2.13	0.48
2:L:7:GLU:OE1	3:M:254:TRP:NE1	2.32	0.48
2:L:84:LEU:HD23	2:L:151:TRP:NE1	2.29	0.48
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.49	0.48
4:H:201:ARG:O	4:H:209:VAL:HA	2.14	0.48
5:D:7:ASN:HD22	5:D:7:ASN:N	2.10	0.48
5:D:43:ASP:CG	5:D:44:LEU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:101:BCL:C2B	9:F:102:BCL:C1B	2.92	0.48
9:O:102:BCL:CAC	9:P:101:BCL:CBC	2.87	0.48
6:R:46:LEU:HD22	6:T:42:TYR:CE2	2.47	0.48
5:Y:40:LEU:O	5:Y:45:ASN:HA	2.13	0.48
6:8:28:TRP:HA	6:8:31:LEU:HD12	1.94	0.48
1:C:130:MET:HE3	1:C:284:ILE:HD11	1.95	0.48
1:C:200:LEU:HD12	1:C:200:LEU:N	2.29	0.48
2:L:10:TYR:CZ	3:M:247:ARG:HG2	2.49	0.48
2:L:191:THR:O	2:L:194:LEU:HB3	2.12	0.48
4:H:39:TYR:HA	4:H:40:PRO:C	2.34	0.48
4:H:132:LYS:HG3	4:H:175:SER:OG	2.13	0.48
4:H:134:VAL:HB	4:H:135:PRO:HD2	1.95	0.48
4:H:146:GLU:OE1	4:H:146:GLU:N	2.46	0.48
5:A:10:LYS:C	5:A:13:LEU:HD13	2.33	0.48
6:B:28:TRP:O	6:B:31:LEU:N	2.46	0.48
5:D:16:ASP:HB3	5:D:19:ARG:HB3	1.95	0.48
5:F:9:TYR:OH	5:F:10:LYS:HE2	2.13	0.48
5:U:43:ASP:HB2	5:W:47:LEU:HD22	1.96	0.48
9:X:101:BCL:C4A	9:Y:102:BCL:HMB3	2.43	0.48
5:Y:10:LYS:HB2	15:2:102:CRT:H82	1.95	0.48
5:Y:44:LEU:HD13	6:Z:43:ARG:HE	1.77	0.48
5:5:4:MET:CE	6:8:24:SER:HB3	2.43	0.48
2:L:281:TRP:HB2	3:M:88:LYS:HD2	1.95	0.48
4:H:135:PRO:HB3	4:H:171:TRP:CE2	2.48	0.48
5:A:47:LEU:CA	5:9:43:ASP:OD2	2.60	0.48
15:A:103:CRT:H401	5:D:38:ILE:HD13	1.95	0.48
15:B:102:CRT:H9	5:9:14:ILE:HD12	1.95	0.48
5:D:27:PHE:HA	5:D:30:VAL:HG12	1.95	0.48
6:E:10:THR:CG2	6:E:11:ASP:H	2.23	0.48
6:N:17:PHE:CE1	15:N:102:CRT:H11	2.48	0.48
5:O:29:ILE:CG2	5:O:30:VAL:H	2.25	0.48
6:V:19:ALA:O	6:V:23:GLN:HG3	2.13	0.48
5:1:57:ALA:O	5:1:58:LEU:O	2.32	0.48
5:5:50:ASN:HD22	5:5:51:ILE:HG13	1.75	0.48
1:C:262:SER:O	3:M:312:THR:HA	2.14	0.48
1:C:288:ASN:O	1:C:288:ASN:ND2	2.46	0.48
3:M:78:SER:C	3:M:80:HIS:H	2.16	0.48
4:H:245:GLY:O	4:H:249:TYR:N	2.46	0.48
5:F:32:GLY:N	9:G:101:BCL:HED2	2.28	0.48
9:I:102:BCL:HAC2	9:I:103:BCL:HBC1	1.95	0.48
9:I:103:BCL:HMB1	9:I:103:BCL:HBB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:BCL:C4A	9:K:102:BCL:HMB3	2.44	0.48
5:O:21:LEU:HD21	6:P:17:PHE:CZ	2.48	0.48
6:V:44:PRO:O	5:W:55:TYR:OH	2.28	0.48
5:3:30:VAL:HA	5:3:33:LEU:HD11	1.96	0.48
5:3:56:GLN:HG2	5:3:57:ALA:H	1.79	0.48
6:4:25:MET:HG2	15:4:102:CRT:C20	2.39	0.48
2:L:276:LEU:HD22	2:L:276:LEU:N	2.29	0.48
3:M:88:LYS:HE2	3:M:89:HIS:CE1	2.48	0.48
4:H:113:PRO:O	4:H:244:ALA:HB3	2.13	0.48
4:H:155:THR:HG22	4:H:166:THR:HG22	1.94	0.48
6:B:45:TRP:O	6:B:46:LEU:CG	2.61	0.48
9:E:101:BCL:HMB3	9:F:102:BCL:C1B	2.43	0.48
5:F:8:LEU:CD2	6:J:20:ILE:HD11	2.40	0.48
5:F:26:ALA:O	5:F:30:VAL:HG12	2.14	0.48
6:G:27:ALA:O	6:G:31:LEU:CD2	2.61	0.48
6:P:13:GLU:HA	6:P:16:GLU:OE1	2.14	0.48
9:P:101:BCL:HMA2	9:P:101:BCL:HBA2	1.95	0.48
9:P:101:BCL:HMB3	9:Q:102:BCL:CHB	2.43	0.48
5:U:9:TYR:HB2	6:V:15:LYS:HD3	1.95	0.48
5:Y:36:HIS:CE1	9:Y:102:BCL:C1A	2.96	0.48
5:1:29:ILE:HG23	5:1:30:VAL:H	1.72	0.48
5:3:11:ILE:N	15:3:103:CRT:H82	2.29	0.48
5:5:2:PHE:CA	5:5:5:ASN:HD22	2.26	0.48
9:5:102:BCL:CHD	9:5:102:BCL:CBC	2.91	0.48
9:7:102:BCL:CMD	6:8:36:HIS:CD2	2.97	0.48
9:7:103:BCL:H101	6:8:29:PHE:HZ	1.78	0.48
1:C:135:ARG:NH1	1:C:333:THR:HG22	2.28	0.48
1:C:180:PRO:O	1:C:182:GLY:N	2.45	0.48
2:L:22:LEU:HB2	5:7:19:ARG:HB2	1.95	0.48
3:M:268:TRP:CD1	4:H:30:LEU:HD22	2.47	0.48
5:A:45:ASN:O	5:A:49:ASP:CB	2.59	0.48
5:F:45:ASN:O	5:F:49:ASP:OD1	2.32	0.48
9:N:101:BCL:CHC	9:O:102:BCL:HBB3	2.43	0.48
5:O:47:LEU:HD22	5:O:47:LEU:H	1.78	0.48
6:P:23:GLN:O	6:P:26:TYR:N	2.46	0.48
6:T:38:LEU:HD23	6:T:38:LEU:O	2.13	0.48
5:W:9:TYR:CD1	6:X:15:LYS:HB2	2.48	0.48
6:Z:29:PHE:N	6:Z:29:PHE:HD1	2.12	0.48
5:1:50:ASN:HB2	5:3:59:GLY:C	2.33	0.48
9:3:102:BCL:HBC2	9:4:101:BCL:CMD	2.43	0.48
6:4:10:THR:O	6:4:14:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:102:BCL:HHC	9:5:102:BCL:OBB	2.14	0.48
6:8:46:LEU:HB2	5:9:52:PRO:CD	2.44	0.48
6:0:29:PHE:HD1	6:0:29:PHE:H	1.60	0.48
1:C:94:MET:HA	1:C:94:MET:CE	2.43	0.48
1:C:157:ARG:HH12	1:C:318:LEU:CD2	2.20	0.48
3:M:61:ILE:HG23	3:M:62:PHE:CD1	2.42	0.48
3:M:268:TRP:CE2	4:H:30:LEU:HD13	2.48	0.48
4:H:45:ARG:NH1	4:H:45:ARG:HG2	2.29	0.48
4:H:53:VAL:CG1	5:D:22:VAL:HG22	2.40	0.48
5:A:15:LEU:HD21	5:D:21:LEU:CD2	2.42	0.48
5:F:35:ILE:HA	5:F:38:ILE:HG22	1.94	0.48
6:N:28:TRP:O	6:N:31:LEU:N	2.47	0.48
9:O:102:BCL:HBC1	9:P:101:BCL:HBC3	1.95	0.48
6:V:21:PHE:CB	15:V:102:CRT:C12	2.71	0.48
6:X:10:THR:H	6:X:13:GLU:CD	2.16	0.48
5:1:44:LEU:HD23	5:1:44:LEU:N	2.27	0.48
5:5:13:LEU:CD1	15:8:101:CRT:C2	2.87	0.48
6:8:38:LEU:HA	6:8:41:LEU:HD12	1.96	0.48
1:C:78:ASN:HB3	1:C:117:ALA:HB1	1.96	0.48
3:M:222:THR:O	3:M:226:VAL:HG22	2.14	0.48
4:H:55:VAL:HA	5:A:19:ARG:HH12	1.77	0.48
5:D:22:VAL:HA	5:D:25:VAL:CG2	2.43	0.48
5:K:33:LEU:HD12	5:K:34:LEU:H	1.79	0.48
6:N:22:MET:O	6:N:25:MET:HB3	2.14	0.48
5:O:36:HIS:O	5:O:40:LEU:HB2	2.14	0.48
6:P:45:TRP:O	6:P:46:LEU:HD23	2.14	0.48
5:W:9:TYR:HA	6:X:18:HIS:CB	2.44	0.48
6:2:20:ILE:HG23	15:2:102:CRT:H81	1.96	0.48
5:3:26:ALA:O	5:3:30:VAL:HG12	2.14	0.48
5:3:46:TRP:CZ3	9:3:102:BCL:H2C	2.48	0.48
15:3:103:CRT:H391	5:7:36:HIS:HB3	1.95	0.48
6:4:40:TRP:CZ3	6:4:44:PRO:CA	2.96	0.48
5:7:5:ASN:O	5:7:6:ALA:C	2.52	0.48
5:7:42:THR:HB	5:9:48:ASP:CG	2.35	0.48
6:0:36:HIS:HE1	9:0:101:BCL:CHB	2.27	0.48
4:H:186:VAL:HG11	4:H:220:ALA:HA	1.96	0.47
5:D:13:LEU:C	5:D:14:ILE:HD12	2.34	0.47
5:F:8:LEU:HD23	6:J:20:ILE:CD1	2.42	0.47
5:I:46:TRP:NE1	9:I:102:BCL:OBB	2.43	0.47
5:K:54:SER:CA	5:K:56:GLN:NE2	2.70	0.47
15:N:102:CRT:C35	9:O:102:BCL:H3A	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:14:ILE:HD11	6:6:17:PHE:HE2	1.77	0.47
2:L:11:ARG:NH1	4:H:45:ARG:HE	2.12	0.47
2:L:119:LYS:O	4:H:113:PRO:HG3	2.14	0.47
3:M:161:GLY:HA3	15:M:406:CRT:H291	1.94	0.47
5:A:27:PHE:CE2	5:D:29:ILE:HD12	2.50	0.47
5:A:46:TRP:CB	6:B:43:ARG:HH12	2.26	0.47
6:J:34:ILE:HD13	6:J:34:ILE:C	2.34	0.47
5:O:26:ALA:C	5:O:29:ILE:HG22	2.29	0.47
5:S:47:LEU:HD22	5:S:47:LEU:H	1.79	0.47
6:T:29:PHE:HA	6:T:32:VAL:HG12	1.97	0.47
6:V:44:PRO:HD2	5:W:55:TYR:OH	2.14	0.47
6:4:18:HIS:CD2	6:4:18:HIS:O	2.67	0.47
6:6:28:TRP:C	6:6:30:GLY:H	2.17	0.47
5:9:17:PRO:O	5:9:21:LEU:CB	2.61	0.47
1:C:175:PRO:O	1:C:176:SER:HB3	2.13	0.47
1:C:308:MET:O	1:C:308:MET:HE3	2.14	0.47
3:M:116:LEU:HD13	3:M:171:TRP:NE1	2.29	0.47
3:M:250:LEU:N	3:M:250:LEU:HD12	2.29	0.47
4:H:24:PHE:HE1	4:H:28:ILE:HD11	1.74	0.47
4:H:76:VAL:HG12	4:H:80:ARG:HH21	1.79	0.47
4:H:169:ASP:OD1	4:H:170:VAL:N	2.47	0.47
5:A:40:LEU:HD22	5:A:46:TRP:CH2	2.50	0.47
5:D:5:ASN:HA	6:E:18:HIS:NE2	2.29	0.47
5:F:12:TRP:HA	5:F:12:TRP:CE3	2.49	0.47
5:K:16:ASP:O	5:K:19:ARG:HG2	2.14	0.47
9:O:102:BCL:HED1	6:P:32:VAL:HG22	1.95	0.47
9:T:101:BCL:NC	9:U:102:BCL:HBB3	2.29	0.47
5:W:45:ASN:O	5:W:47:LEU:N	2.47	0.47
9:W:102:BCL:HBC2	9:X:101:BCL:HHD	1.92	0.47
5:3:8:LEU:HD22	5:3:11:ILE:HD11	1.95	0.47
5:7:9:TYR:CD1	5:7:9:TYR:C	2.87	0.47
1:C:294:SER:C	1:C:295:ARG:HD3	2.34	0.47
2:L:179:ASN:O	2:L:183:MET:HG3	2.13	0.47
2:L:264:TRP:CH2	2:L:271:TRP:HA	2.50	0.47
9:B:101:BCL:HMB1	9:B:101:BCL:HBB2	1.96	0.47
9:E:101:BCL:C1B	9:F:102:BCL:CMB	2.88	0.47
5:F:35:ILE:O	5:F:38:ILE:HG22	2.14	0.47
5:I:52:PRO:O	5:I:53:VAL:O	2.33	0.47
5:K:12:TRP:CE3	5:K:12:TRP:HA	2.49	0.47
6:N:17:PHE:CE1	15:N:102:CRT:C10	2.98	0.47
5:W:8:LEU:HD23	5:W:11:ILE:HD12	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:9:TYR:HA	6:Z:18:HIS:ND1	2.29	0.47
6:Z:42:TYR:O	6:Z:44:PRO:HD3	2.13	0.47
5:1:10:LYS:HD2	6:4:20:ILE:CG1	2.32	0.47
6:6:17:PHE:CD1	6:6:17:PHE:C	2.87	0.47
1:C:20:LEU:HD22	1:C:21:LEU:N	2.29	0.47
1:C:22:GLY:HA2	2:L:263:PHE:HB3	1.97	0.47
2:L:50:ILE:HD11	10:L:302:BPH:H122	1.96	0.47
3:M:187:ALA:O	3:M:191:ILE:HG13	2.13	0.47
3:M:260:VAL:CG1	4:H:34:ASP:OD1	2.62	0.47
6:B:42:TYR:CZ	6:0:46:LEU:HD22	2.50	0.47
15:P:102:CRT:C39	5:Q:36:HIS:CB	2.86	0.47
5:S:4:MET:O	5:S:8:LEU:HG	2.14	0.47
5:W:3:THR:C	5:W:5:ASN:N	2.67	0.47
5:W:36:HIS:CE1	9:X:101:BCL:OBD	2.67	0.47
6:X:34:ILE:HG23	6:X:35:ALA:N	2.29	0.47
5:Y:34:LEU:O	5:Y:38:ILE:HG23	2.14	0.47
15:2:102:CRT:H372	9:3:102:BCL:HMB2	1.96	0.47
5:5:5:ASN:OD1	5:5:8:LEU:HD12	2.15	0.47
9:7:103:BCL:CMA	15:8:101:CRT:H32	2.44	0.47
6:8:25:MET:HB2	15:8:101:CRT:C19	2.45	0.47
6:8:43:ARG:CZ	5:9:55:TYR:HB2	2.44	0.47
1:C:59:VAL:CG2	1:C:100:TRP:HE1	2.27	0.47
2:L:143:VAL:O	2:L:147:LEU:HD13	2.14	0.47
3:M:79:VAL:HG11	3:M:86:PHE:HB2	1.97	0.47
5:A:29:ILE:CG1	5:A:33:LEU:HD11	2.42	0.47
5:I:45:ASN:OD1	5:I:48:ASP:OD1	2.33	0.47
5:K:36:HIS:NE2	9:K:102:BCL:NA	2.61	0.47
9:K:102:BCL:HBD	9:N:101:BCL:OBD	2.14	0.47
5:O:43:ASP:CA	5:Q:48:ASP:HB3	2.41	0.47
15:R:102:CRT:C2M	5:S:33:LEU:HA	2.44	0.47
6:T:10:THR:HB	6:T:13:GLU:OE2	2.14	0.47
6:V:14:ALA:O	6:V:18:HIS:HB2	2.15	0.47
6:V:43:ARG:NH1	5:W:55:TYR:HB3	2.30	0.47
5:W:9:TYR:CD1	5:W:9:TYR:C	2.87	0.47
5:1:16:ASP:OD2	5:1:19:ARG:HD3	2.15	0.47
9:7:103:BCL:HHC	9:7:103:BCL:OBB	2.14	0.47
15:8:101:CRT:H392	9:9:102:BCL:C1B	2.45	0.47
1:C:20:LEU:HD23	2:L:271:TRP:NE1	2.30	0.47
1:C:134:VAL:O	1:C:137:ALA:HB3	2.14	0.47
2:L:219:GLU:O	2:L:223:THR:HG23	2.15	0.47
9:L:301:BCL:CAA	9:L:303:BCL:HBC1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:31:ILE:CG1	16:M:407:PGW:HADA	2.45	0.47
3:M:105:ARG:NH2	5:Q:49:ASP:HA	2.29	0.47
3:M:208:PHE:CD2	3:M:276:THR:HA	2.50	0.47
4:H:164:ALA:HB2	4:H:216:ALA:HA	1.97	0.47
5:A:5:ASN:CB	6:B:22:MET:HE1	2.42	0.47
15:A:103:CRT:H11	6:E:17:PHE:HE1	1.80	0.47
6:B:23:GLN:HG3	5:9:4:MET:CE	2.34	0.47
6:B:34:ILE:HD13	6:B:34:ILE:C	2.35	0.47
6:B:45:TRP:O	6:B:46:LEU:HB2	2.13	0.47
5:D:2:PHE:N	6:E:26:TYR:CZ	2.83	0.47
5:D:33:LEU:O	5:D:37:MET:HG2	2.15	0.47
5:F:9:TYR:HA	6:G:18:HIS:ND1	2.29	0.47
6:G:34:ILE:O	6:G:38:LEU:HB3	2.13	0.47
5:I:7:ASN:HB3	6:N:20:ILE:HG13	1.96	0.47
5:I:16:ASP:OD2	5:I:19:ARG:HD2	2.15	0.47
5:I:46:TRP:HE1	5:I:47:LEU:CD1	2.28	0.47
5:K:38:ILE:O	5:K:38:ILE:CG1	2.63	0.47
15:N:102:CRT:C38	9:O:102:BCL:HMB2	2.44	0.47
5:O:8:LEU:O	5:O:11:ILE:HG13	2.13	0.47
5:O:43:ASP:OD1	5:O:44:LEU:HD23	2.14	0.47
9:O:102:BCL:HBD	9:P:101:BCL:OBD	2.14	0.47
6:P:7:THR:OG1	6:P:8:GLY:N	2.45	0.47
6:P:13:GLU:HA	6:P:16:GLU:HG3	1.97	0.47
6:P:21:PHE:CD2	15:P:102:CRT:H16	2.48	0.47
5:S:9:TYR:CD1	5:S:9:TYR:C	2.87	0.47
9:S:102:BCL:CHD	9:S:102:BCL:CBC	2.92	0.47
6:T:16:GLU:HG2	6:T:17:PHE:N	2.30	0.47
6:T:40:TRP:CE3	6:T:44:PRO:HA	2.50	0.47
6:V:33:VAL:CG1	6:V:34:ILE:N	2.77	0.47
5:W:10:LYS:NZ	15:W:103:CRT:H1M1	2.29	0.47
5:W:29:ILE:CG2	5:W:30:VAL:N	2.78	0.47
5:W:29:ILE:O	5:W:33:LEU:HG	2.14	0.47
5:Y:5:ASN:OD1	6:Z:19:ALA:HA	2.14	0.47
5:Y:38:ILE:HD12	5:Y:38:ILE:C	2.35	0.47
5:Y:51:ILE:CG2	5:1:60:LYS:N	2.73	0.47
6:Z:22:MET:HG3	6:Z:26:TYR:CE1	2.41	0.47
5:1:60:LYS:O	5:1:61:LYS:CB	2.63	0.47
5:3:13:LEU:HD12	15:3:103:CRT:H1M2	0.69	0.47
5:3:46:TRP:NE1	9:3:102:BCL:OBB	2.48	0.47
6:4:24:SER:HB2	15:4:102:CRT:C11	2.45	0.47
6:8:20:ILE:CG2	6:8:21:PHE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:102:BCL:HMB1	9:9:102:BCL:HBB3	1.97	0.47
1:C:157:ARG:NH1	1:C:318:LEU:HD21	2.22	0.47
2:L:17:LEU:HD12	2:L:35:PHE:HE2	1.80	0.47
3:M:61:ILE:HG13	10:M:403:BPH:H7C2	1.96	0.47
5:F:3:THR:O	5:F:4:MET:HB2	2.15	0.47
5:F:9:TYR:CD1	5:F:10:LYS:N	2.83	0.47
5:I:33:LEU:O	5:I:37:MET:CG	2.63	0.47
9:I:102:BCL:ND	9:I:103:BCL:HMD2	2.27	0.47
6:J:17:PHE:O	6:J:18:HIS:C	2.53	0.47
5:Q:15:LEU:HD11	5:S:21:LEU:HD13	1.96	0.47
9:R:101:BCL:HHC	9:R:101:BCL:OBB	2.15	0.47
5:S:27:PHE:CG	5:U:29:ILE:HD11	2.49	0.47
9:W:102:BCL:HMB1	9:W:102:BCL:HBB3	1.95	0.47
5:Y:2:PHE:HA	5:Y:5:ASN:HD22	1.79	0.47
6:6:38:LEU:HD23	6:6:38:LEU:O	2.15	0.47
1:C:294:SER:O	1:C:295:ARG:HD3	2.15	0.47
3:M:31:ILE:HD11	16:M:407:PGW:HADA	1.89	0.47
3:M:84:PHE:HD1	3:M:84:PHE:H	1.62	0.47
9:M:401:BCL:HHC	9:M:401:BCL:OBB	2.14	0.47
4:H:48:ARG:HH22	17:H:301:PEF:C1	2.27	0.47
4:H:52:ARG:HB3	5:D:26:ALA:HB1	1.96	0.47
16:H:302:PGW:H04A	16:H:302:PGW:C03	2.45	0.47
5:A:29:ILE:CG2	5:A:30:VAL:N	2.77	0.47
5:A:33:LEU:O	15:A:101:CRT:H403	2.15	0.47
5:A:35:ILE:HA	5:A:38:ILE:HG13	1.97	0.47
5:F:43:ASP:OD1	5:F:44:LEU:HD23	2.15	0.47
6:G:17:PHE:C	6:G:17:PHE:HD1	2.18	0.47
5:O:46:TRP:CE3	9:O:102:BCL:H2C	2.50	0.47
6:P:23:GLN:O	6:P:24:SER:C	2.51	0.47
6:P:45:TRP:O	6:P:46:LEU:HG	2.15	0.47
5:S:37:MET:O	5:S:40:LEU:HB3	2.15	0.47
5:W:8:LEU:HD22	5:W:11:ILE:HD12	1.83	0.47
6:X:24:SER:O	6:X:27:ALA:HB3	2.15	0.47
5:5:12:TRP:CZ3	5:5:17:PRO:HA	2.46	0.47
6:6:31:LEU:HA	6:6:34:ILE:HG22	1.97	0.47
6:8:45:TRP:O	6:8:46:LEU:CB	2.62	0.47
6:0:29:PHE:CE2	9:0:101:BCL:H42	2.50	0.47
5:A:47:LEU:O	5:9:43:ASP:OD2	2.33	0.47
6:G:21:PHE:CD1	6:G:22:MET:CA	2.94	0.47
9:I:102:BCL:CBC	9:I:103:BCL:HBC3	2.45	0.47
5:S:18:ARG:O	5:S:22:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:31:LEU:O	5:S:35:ILE:HG12	2.15	0.47
5:W:8:LEU:CB	6:X:18:HIS:CE1	2.87	0.47
5:W:12:TRP:HA	5:W:12:TRP:CE3	2.50	0.47
5:W:27:PHE:CZ	5:Y:29:ILE:HD11	2.24	0.47
5:W:33:LEU:O	5:W:37:MET:HB2	2.15	0.47
5:Y:9:TYR:CD1	6:Z:15:LYS:HG3	2.50	0.47
5:Y:9:TYR:CZ	5:Y:10:LYS:HE3	2.50	0.47
5:1:55:TYR:C	5:1:57:ALA:N	2.68	0.47
9:9:102:BCL:OBB	9:9:102:BCL:HHC	2.14	0.47
1:C:190:VAL:HG13	1:C:197:PHE:HA	1.97	0.46
1:C:196:PRO:C	1:C:197:PHE:CG	2.89	0.46
1:C:225:SER:O	1:C:228:GLN:HB2	2.15	0.46
3:M:208:PHE:HD2	3:M:276:THR:HA	1.81	0.46
5:A:36:HIS:CE1	9:A:102:BCL:C4A	2.98	0.46
5:A:36:HIS:CE1	9:B:101:BCL:OBD	2.69	0.46
6:G:28:TRP:C	6:G:30:GLY:N	2.66	0.46
5:I:46:TRP:NE1	5:I:47:LEU:HD12	2.30	0.46
5:K:8:LEU:O	5:K:11:ILE:HG13	2.15	0.46
6:N:28:TRP:CG	6:N:31:LEU:HD12	2.50	0.46
6:P:33:VAL:HG22	6:P:37:LEU:HD23	1.95	0.46
5:Q:13:LEU:HD21	6:R:11:ASP:HA	1.96	0.46
9:R:101:BCL:HMB3	9:S:102:BCL:C1B	2.46	0.46
6:T:17:PHE:CD1	15:T:102:CRT:H6	2.46	0.46
5:Y:51:ILE:HA	5:Y:52:PRO:C	2.36	0.46
5:1:2:PHE:CD1	5:1:2:PHE:N	2.82	0.46
5:5:20:VAL:HA	5:5:23:SER:CB	2.45	0.46
6:6:31:LEU:HA	6:6:34:ILE:CG2	2.45	0.46
6:6:32:VAL:O	6:6:35:ALA:HB3	2.16	0.46
1:C:85:LEU:HD11	1:C:329:GLY:CA	2.43	0.46
1:C:243:LEU:HG	1:C:311:HIS:ND1	2.31	0.46
7:C:502:HEM:O2D	7:C:502:HEM:HHA	2.15	0.46
2:L:3:MET:CE	4:H:45:ARG:HH21	2.26	0.46
3:M:109:LEU:HB3	3:M:114:TRP:NE1	2.29	0.46
4:H:57:GLY:HA3	17:H:301:PEF:O2P	2.15	0.46
4:H:80:ARG:HH11	4:H:80:ARG:HG2	1.79	0.46
5:D:12:TRP:CD1	6:E:17:PHE:CD2	3.03	0.46
9:D:102:BCL:CAD	9:E:101:BCL:CAD	2.93	0.46
5:I:9:TYR:CD1	5:I:9:TYR:C	2.88	0.46
6:J:33:VAL:HG22	6:J:37:LEU:CD2	2.45	0.46
6:J:45:TRP:CD1	6:J:46:LEU:N	2.83	0.46
15:J:101:CRT:H2M1	5:K:37:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:102:CRT:H10	15:N:102:CRT:H81	1.52	0.46
9:O:102:BCL:ND	9:P:101:BCL:HMD2	2.29	0.46
5:S:12:TRP:HE1	6:T:18:HIS:CB	2.28	0.46
5:S:38:ILE:HG23	5:S:39:VAL:N	2.30	0.46
6:T:9:LEU:HB3	6:T:13:GLU:HG3	1.95	0.46
5:U:27:PHE:HE2	5:W:29:ILE:HG12	1.76	0.46
6:V:45:TRP:O	6:V:46:LEU:HB2	2.14	0.46
5:W:31:LEU:HD13	15:X:102:CRT:H35	1.97	0.46
5:Y:15:LEU:HD22	5:Y:20:VAL:HG11	1.97	0.46
5:Y:20:VAL:HA	5:Y:23:SER:OG	2.14	0.46
6:Z:43:ARG:O	6:Z:45:TRP:N	2.48	0.46
5:3:36:HIS:CD2	9:4:101:BCL:HMD1	2.49	0.46
5:5:36:HIS:NE2	9:6:101:BCL:HMD1	2.30	0.46
6:8:20:ILE:HD13	6:8:20:ILE:C	2.36	0.46
1:C:201:THR:N	1:C:202:PRO:HD2	2.29	0.46
1:C:251:HIS:CE1	7:C:503:HEM:C1C	3.03	0.46
1:C:253:THR:HG21	2:L:171:TYR:CD2	2.51	0.46
1:C:312:GLN:O	1:C:313:ALA:HB3	2.16	0.46
2:L:192:ASN:HD21	3:M:213:ALA:N	2.14	0.46
2:L:273:ASN:ND2	2:L:277:GLU:HG3	2.30	0.46
3:M:214:LEU:O	3:M:217:ALA:HB3	2.14	0.46
3:M:259:ASN:N	3:M:259:ASN:ND2	2.63	0.46
4:H:5:ILE:CD1	5:F:47:LEU:HD13	2.42	0.46
5:A:11:ILE:N	15:A:103:CRT:H82	2.30	0.46
6:B:36:HIS:O	6:B:45:TRP:HH2	1.98	0.46
5:D:2:PHE:O	5:D:5:ASN:HB3	2.14	0.46
5:I:27:PHE:HE2	5:K:29:ILE:HD11	1.80	0.46
5:U:9:TYR:HB2	6:V:15:LYS:CD	2.45	0.46
9:Z:101:BCL:HMB1	9:Z:101:BCL:HBB2	1.98	0.46
5:5:30:VAL:CG1	5:5:31:LEU:H	2.28	0.46
6:8:22:MET:HG3	6:8:26:TYR:HE2	1.81	0.46
5:9:35:ILE:HA	5:9:38:ILE:HG12	1.97	0.46
1:C:295:ARG:NH1	7:C:502:HEM:O2A	2.48	0.46
2:L:133:ALA:HB2	10:L:302:BPH:HAC2	1.97	0.46
2:L:236:LEU:HD23	2:L:237:ALA:N	2.30	0.46
3:M:107:PRO:HG2	3:M:113:GLY:HA2	1.97	0.46
3:M:200:PRO:HD3	3:M:297:TRP:CZ3	2.51	0.46
4:H:149:PRO:HG3	4:H:204:LYS:HD3	1.96	0.46
5:A:50:ASN:ND2	5:A:51:ILE:HG12	2.31	0.46
5:I:32:GLY:N	9:I:103:BCL:HED2	2.31	0.46
9:N:101:BCL:HMA3	15:N:102:CRT:H35	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:47:LEU:HD22	5:O:47:LEU:N	2.31	0.46
6:T:33:VAL:HG13	6:T:34:ILE:N	2.30	0.46
15:T:102:CRT:H2M3	5:U:36:HIS:HB2	1.97	0.46
5:W:12:TRP:HZ2	6:X:21:PHE:CG	2.34	0.46
6:X:29:PHE:CZ	15:X:102:CRT:H242	2.50	0.46
5:1:55:TYR:O	5:1:57:ALA:N	2.48	0.46
5:7:15:LEU:HB3	5:7:20:VAL:HG11	1.97	0.46
5:9:44:LEU:HD22	5:9:46:TRP:HB3	1.97	0.46
5:9:50:ASN:ND2	5:9:51:ILE:HG12	2.25	0.46
2:L:228:ILE:HG21	10:M:403:BPH:HED1	1.98	0.46
2:L:258:LEU:O	2:L:262:PRO:HD2	2.16	0.46
3:M:12:GLN:NE2	3:M:42:LYS:CA	2.78	0.46
3:M:12:GLN:HE21	3:M:42:LYS:HA	1.80	0.46
15:B:102:CRT:H10	15:B:102:CRT:H81	1.59	0.46
5:D:35:ILE:HA	5:D:38:ILE:HG22	1.97	0.46
6:J:16:GLU:HG2	15:J:101:CRT:H21A	1.98	0.46
6:P:21:PHE:CD1	15:P:102:CRT:C14	2.99	0.46
5:U:9:TYR:HA	6:V:18:HIS:ND1	2.30	0.46
6:V:21:PHE:CD1	6:V:22:MET:N	2.84	0.46
6:2:25:MET:HA	15:2:102:CRT:C18	2.46	0.46
6:6:29:PHE:HA	6:6:32:VAL:HG12	1.96	0.46
5:7:44:LEU:HB2	6:8:43:ARG:NH1	2.30	0.46
1:C:115:ASN:HB3	1:C:118:SER:HB2	1.98	0.46
9:M:401:BCL:H111	9:M:401:BCL:H152	1.51	0.46
4:H:215:LYS:HB2	4:H:218:HIS:CD2	2.51	0.46
5:A:35:ILE:HG22	5:A:36:HIS:N	2.30	0.46
6:B:33:VAL:O	6:B:37:LEU:HD23	2.15	0.46
5:F:13:LEU:O	6:G:7:THR:HA	2.15	0.46
5:I:46:TRP:NE1	5:I:47:LEU:CD1	2.79	0.46
9:I:103:BCL:HAC2	6:J:45:TRP:CZ3	2.51	0.46
5:O:46:TRP:NE1	5:O:47:LEU:CD2	2.79	0.46
9:O:102:BCL:HED1	6:P:32:VAL:CG2	2.45	0.46
9:P:101:BCL:HBA2	9:P:101:BCL:CMA	2.44	0.46
9:X:101:BCL:CHB	9:Y:102:BCL:HMB3	2.45	0.46
9:Y:102:BCL:HMB1	9:Y:102:BCL:HBB3	1.95	0.46
9:4:101:BCL:HBA2	9:4:101:BCL:CMA	2.46	0.46
5:9:17:PRO:HG2	5:9:18:ARG:H	1.81	0.46
5:9:35:ILE:O	5:9:38:ILE:HG12	2.14	0.46
6:0:40:TRP:CE3	6:0:44:PRO:HA	2.50	0.46
1:C:133:LEU:HD23	1:C:134:VAL:N	2.31	0.46
2:L:46:GLY:HA3	10:L:302:BPH:H9C3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:TRP:CZ3	5:9:38:ILE:HB	2.51	0.46
2:L:71:TRP:CZ2	4:H:2:SER:OG	2.66	0.46
3:M:18:TYR:HD1	3:M:20:GLY:H	1.64	0.46
3:M:297:TRP:O	3:M:300:LYS:HB2	2.16	0.46
4:H:55:VAL:CG1	4:H:56:VAL:H	2.26	0.46
5:A:22:VAL:HA	5:A:25:VAL:CB	2.45	0.46
5:A:50:ASN:O	5:D:59:GLY:O	2.32	0.46
9:A:102:BCL:H162	5:9:12:TRP:CH2	2.48	0.46
6:B:17:PHE:HE1	15:B:102:CRT:C10	2.28	0.46
5:I:55:TYR:CE1	5:I:56:GLN:HG3	2.51	0.46
5:K:16:ASP:HB2	5:K:19:ARG:HG2	1.98	0.46
5:O:21:LEU:HD21	6:P:17:PHE:HZ	1.81	0.46
5:1:33:LEU:HD12	5:1:33:LEU:C	2.36	0.46
5:3:51:ILE:CA	5:3:53:VAL:N	2.77	0.46
6:4:38:LEU:HD23	6:4:38:LEU:O	2.15	0.46
5:5:10:LYS:HG3	15:8:101:CRT:H5	1.94	0.46
2:L:42:PHE:CD2	2:L:104:GLY:HA3	2.50	0.46
3:M:84:PHE:CE1	5:U:38:ILE:HD12	2.51	0.46
3:M:168:MET:HE1	3:M:289:THR:HG22	1.96	0.46
9:A:102:BCL:HBC2	9:B:101:BCL:HMD2	1.98	0.46
5:D:30:VAL:CG1	5:D:31:LEU:N	2.78	0.46
5:F:25:VAL:O	5:F:29:ILE:HG22	2.15	0.46
5:F:36:HIS:CD2	9:G:101:BCL:CMD	2.99	0.46
9:G:101:BCL:HBA2	9:G:101:BCL:HMA2	1.97	0.46
9:I:102:BCL:HBC2	9:I:103:BCL:CHD	2.27	0.46
5:Q:16:ASP:HB2	5:Q:19:ARG:NE	2.31	0.46
5:S:8:LEU:HD22	5:S:11:ILE:HD11	1.97	0.46
5:S:46:TRP:CE3	9:S:102:BCL:H2C	2.51	0.46
6:T:15:LYS:HG2	6:T:16:GLU:N	2.30	0.46
15:T:102:CRT:H2M1	5:U:37:MET:HG2	1.97	0.46
5:W:30:VAL:O	5:W:33:LEU:CD1	2.64	0.46
5:W:51:ILE:CB	5:W:52:PRO:CA	2.90	0.46
5:1:20:VAL:HA	5:1:23:SER:OG	2.15	0.46
5:1:46:TRP:CZ3	9:1:102:BCL:CBC	2.98	0.46
5:5:5:ASN:CB	6:6:22:MET:HE3	2.40	0.46
5:5:16:ASP:N	5:5:19:ARG:HG3	2.28	0.46
1:C:252:ASN:OD1	1:C:254:ARG:CG	2.64	0.46
2:L:194:LEU:C	2:L:194:LEU:HD13	2.37	0.46
3:M:63:PHE:CE2	3:M:124:LEU:HB2	2.51	0.46
3:M:123:THR:CG2	3:M:162:PHE:CE2	2.94	0.46
14:M:405:MQ8:H302	17:H:301:PEF:C31	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:64:PRO:HA	4:H:78:ALA:O	2.15	0.46
4:H:135:PRO:HB3	4:H:171:TRP:NE1	2.31	0.46
4:H:186:VAL:O	4:H:190:LYS:HA	2.15	0.46
15:A:101:CRT:C8	5:7:11:ILE:CA	2.93	0.46
6:B:20:ILE:HD12	15:B:102:CRT:H81	1.97	0.46
5:D:5:ASN:HD22	6:E:22:MET:HB3	1.80	0.46
5:D:45:ASN:O	5:D:49:ASP:HB3	2.16	0.46
5:F:4:MET:SD	6:J:23:GLN:HG3	2.56	0.46
5:F:6:ALA:O	5:F:9:TYR:HD2	1.99	0.46
5:F:28:GLN:O	5:F:31:LEU:N	2.49	0.46
6:J:43:ARG:NH1	5:K:55:TYR:CE2	2.83	0.46
5:K:20:VAL:O	5:K:24:ILE:CG1	2.63	0.46
5:1:12:TRP:HD1	6:2:18:HIS:HB2	1.81	0.46
5:3:14:ILE:HD13	5:5:17:PRO:HB2	1.96	0.46
2:L:124:PHE:O	2:L:127:PRO:HG2	2.16	0.46
9:L:303:BCL:CGA	3:M:207:ALA:HA	2.46	0.46
4:H:48:ARG:NH2	17:H:301:PEF:C1	2.79	0.46
4:H:203:ASP:OD2	4:H:206:ALA:HB3	2.15	0.46
5:A:35:ILE:O	5:A:39:VAL:HG23	2.16	0.46
5:F:12:TRP:HA	5:F:12:TRP:HE3	1.81	0.46
5:F:50:ASN:C	5:F:51:ILE:O	2.54	0.46
5:I:43:ASP:HA	5:K:47:LEU:HB3	1.98	0.46
5:K:20:VAL:O	5:K:24:ILE:HD12	2.15	0.46
5:Q:46:TRP:NE1	5:Q:47:LEU:HG	2.31	0.46
9:Q:102:BCL:HMB1	9:Q:102:BCL:HBB2	1.97	0.46
5:3:46:TRP:CD1	5:3:47:LEU:N	2.84	0.46
5:3:49:ASP:O	5:5:60:LYS:CA	2.64	0.46
5:5:2:PHE:HB2	5:5:5:ASN:ND2	2.25	0.46
5:7:30:VAL:HG13	5:7:31:LEU:H	1.79	0.46
3:M:62:PHE:O	3:M:66:VAL:HG23	2.16	0.45
5:A:29:ILE:HD11	5:9:27:PHE:CZ	2.50	0.45
6:B:25:MET:HG2	6:B:29:PHE:CE2	2.52	0.45
5:D:12:TRP:CD1	6:E:18:HIS:HB2	2.51	0.45
5:I:10:LYS:HB3	15:N:102:CRT:H5	1.98	0.45
5:K:43:ASP:OD2	5:K:44:LEU:HD12	2.15	0.45
15:N:102:CRT:C39	5:O:36:HIS:CD2	2.99	0.45
5:O:50:ASN:CG	6:P:43:ARG:HH22	2.19	0.45
6:P:16:GLU:CB	15:P:102:CRT:H1M1	2.46	0.45
5:U:35:ILE:O	5:U:36:HIS:C	2.55	0.45
9:U:102:BCL:HMB1	9:U:102:BCL:HBB3	1.97	0.45
5:5:49:ASP:HB2	5:7:56:GLN:CB	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:45:TRP:C	6:6:46:LEU:O	2.51	0.45
9:7:102:BCL:HMB1	9:7:102:BCL:HBB2	1.98	0.45
1:C:276:VAL:HG13	1:C:277:ARG:N	2.31	0.45
3:M:27:ASN:HD22	3:M:27:ASN:N	2.13	0.45
3:M:121:PHE:HZ	5:Q:34:LEU:HA	1.81	0.45
6:J:22:MET:O	6:J:26:TYR:HD1	1.99	0.45
5:K:45:ASN:HB3	5:K:49:ASP:HB3	1.97	0.45
5:Q:17:PRO:O	5:Q:20:VAL:HG22	2.16	0.45
5:S:43:ASP:C	5:S:45:ASN:H	2.19	0.45
5:Y:5:ASN:OD1	6:Z:18:HIS:O	2.34	0.45
5:7:7:ASN:HA	5:7:10:LYS:HZ2	1.81	0.45
5:7:11:ILE:O	5:7:15:LEU:HG	2.16	0.45
6:0:26:TYR:O	6:0:29:PHE:HB2	2.16	0.45
1:C:49:ARG:HH11	1:C:49:ARG:HG2	1.81	0.45
1:C:135:ARG:HH12	1:C:333:THR:HG22	1.81	0.45
2:L:6:PHE:HE2	3:M:250:LEU:HD11	1.79	0.45
2:L:128:PHE:CE2	11:L:304:UQ8:C45	2.98	0.45
4:H:106:PRO:HB2	4:H:249:TYR:CD1	2.52	0.45
4:H:108:LEU:C	4:H:108:LEU:HD12	2.37	0.45
5:A:27:PHE:CD1	5:A:27:PHE:C	2.88	0.45
5:A:27:PHE:HE2	5:D:29:ILE:CD1	2.29	0.45
5:D:2:PHE:HD1	5:D:3:THR:N	2.14	0.45
5:D:27:PHE:CZ	5:F:29:ILE:HD11	2.51	0.45
6:N:31:LEU:O	6:N:34:ILE:CG2	2.64	0.45
5:O:35:ILE:O	5:O:36:HIS:C	2.54	0.45
9:S:102:BCL:HMB1	9:S:102:BCL:HBB3	1.96	0.45
9:U:102:BCL:HBC1	9:V:101:BCL:HBC3	1.98	0.45
6:V:25:MET:CE	15:V:102:CRT:H19	2.45	0.45
5:W:46:TRP:CZ2	9:W:102:BCL:H2C	2.51	0.45
9:X:101:BCL:HHC	9:X:101:BCL:OBB	2.15	0.45
6:Z:40:TRP:O	6:Z:40:TRP:CD1	2.69	0.45
5:1:12:TRP:HZ2	6:2:21:PHE:CE2	2.33	0.45
6:8:22:MET:HG3	6:8:26:TYR:CE2	2.51	0.45
15:8:101:CRT:H20	15:8:101:CRT:H181	1.79	0.45
5:9:2:PHE:CD1	5:9:2:PHE:N	2.85	0.45
1:C:20:LEU:HB2	2:L:271:TRP:CE2	2.51	0.45
2:L:18:ILE:CD1	4:H:259:LEU:HD12	2.46	0.45
2:L:69:ASN:HB2	2:L:72:ARG:HH21	1.82	0.45
2:L:111:LEU:O	2:L:114:VAL:HB	2.17	0.45
2:L:266:ARG:HD2	2:L:266:ARG:HA	1.76	0.45
4:H:13:GLN:HE21	12:H:304:PO4:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:80:ARG:HG3	4:H:82:GLU:HG3	1.99	0.45
5:A:46:TRP:HA	6:B:43:ARG:HH12	1.80	0.45
5:D:49:ASP:OD2	5:F:56:GLN:HG3	2.16	0.45
9:E:101:BCL:C1C	9:F:102:BCL:HBB3	2.47	0.45
5:O:5:ASN:HA	5:O:8:LEU:HD22	1.99	0.45
6:V:21:PHE:CA	15:V:102:CRT:C11	2.93	0.45
6:Z:42:TYR:O	6:Z:44:PRO:CD	2.64	0.45
6:2:21:PHE:CE1	15:2:102:CRT:C17	2.70	0.45
1:C:273:ILE:O	1:C:277:ARG:HG3	2.17	0.45
3:M:184:ASP:HA	3:M:187:ALA:HB3	1.98	0.45
3:M:193:TYR:CE1	3:M:288:GLY:HA2	2.52	0.45
9:M:401:BCL:H3A	9:M:401:BCL:HBA1	1.68	0.45
9:G:101:BCL:H141	9:G:101:BCL:H161	1.83	0.45
6:J:20:ILE:HG23	6:J:21:PHE:N	2.32	0.45
5:K:24:ILE:HG21	15:N:102:CRT:C21	2.47	0.45
6:P:20:ILE:HG21	15:P:102:CRT:C7	2.46	0.45
6:R:24:SER:C	15:R:102:CRT:H183	2.37	0.45
5:U:16:ASP:HB2	5:U:19:ARG:HD3	1.98	0.45
9:U:102:BCL:O2D	6:V:32:VAL:HG23	2.17	0.45
5:Y:45:ASN:O	5:Y:46:TRP:C	2.55	0.45
5:1:38:ILE:HG23	5:1:39:VAL:N	2.31	0.45
9:1:102:BCL:HMB1	9:1:102:BCL:HBB2	1.99	0.45
5:7:18:ARG:HG2	5:7:18:ARG:HH11	1.80	0.45
5:9:44:LEU:CD2	5:9:46:TRP:HB3	2.47	0.45
2:L:99:THR:HG21	2:L:141:VAL:HG11	1.99	0.45
9:M:401:BCL:H142	10:M:403:BPH:HMA2	1.90	0.45
4:H:6:THR:O	5:F:41:SER:HB3	2.17	0.45
4:H:44:ASP:OD1	4:H:44:ASP:N	2.49	0.45
4:H:214:ILE:HG22	4:H:246:GLY:HA3	1.98	0.45
5:A:40:LEU:HD11	5:A:47:LEU:HD23	1.98	0.45
15:A:101:CRT:H11	6:0:17:PHE:CE1	2.51	0.45
6:E:31:LEU:HA	6:E:34:ILE:HG22	1.97	0.45
6:G:25:MET:SD	6:G:29:PHE:CZ	3.10	0.45
6:N:44:PRO:O	5:O:52:PRO:HG3	2.16	0.45
5:O:34:LEU:O	5:O:37:MET:HB2	2.16	0.45
5:Q:50:ASN:HB3	5:S:56:GLN:CG	2.45	0.45
5:W:8:LEU:HB3	6:X:18:HIS:NE2	2.28	0.45
5:W:19:ARG:NH2	5:W:20:VAL:HG12	2.31	0.45
6:X:29:PHE:HE1	15:X:102:CRT:H242	1.81	0.45
6:X:29:PHE:N	6:X:29:PHE:CD1	2.85	0.45
15:X:102:CRT:H15	15:X:102:CRT:H131	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:51:ILE:HB	5:Y:52:PRO:C	2.37	0.45
6:0:40:TRP:CZ3	6:0:44:PRO:HA	2.51	0.45
3:M:79:VAL:HG21	3:M:86:PHE:N	2.31	0.45
3:M:229:PHE:CZ	4:H:244:ALA:HB2	2.52	0.45
3:M:260:VAL:HA	4:H:34:ASP:HB3	1.99	0.45
3:M:277:VAL:HA	3:M:280:ALA:CB	2.47	0.45
6:B:16:GLU:OE2	15:B:102:CRT:H23	2.16	0.45
6:B:33:VAL:HG13	6:B:34:ILE:N	2.31	0.45
9:F:102:BCL:HBD	9:F:102:BCL:HBA1	1.98	0.45
6:N:28:TRP:HA	6:N:31:LEU:CG	2.47	0.45
5:O:4:MET:HA	5:O:7:ASN:HD21	1.82	0.45
6:P:36:HIS:CE1	9:P:101:BCL:NA	2.83	0.45
6:T:22:MET:HB3	6:T:26:TYR:HE1	1.80	0.45
9:V:101:BCL:CMA	9:W:102:BCL:HHB	2.44	0.45
5:W:27:PHE:HE2	5:Y:29:ILE:HD11	0.42	0.45
5:Y:35:ILE:O	5:Y:36:HIS:C	2.53	0.45
6:4:21:PHE:N	15:4:102:CRT:H9	2.32	0.45
5:7:29:ILE:O	5:7:33:LEU:CD1	2.65	0.45
6:8:30:GLY:O	6:8:33:VAL:N	2.50	0.45
2:L:3:MET:HG2	2:L:11:ARG:CZ	2.47	0.45
2:L:228:ILE:HG12	3:M:136:ARG:HG3	1.98	0.45
2:L:238:ILE:HD13	2:L:238:ILE:HA	1.83	0.45
3:M:27:ASN:HD21	5:O:19:ARG:HH11	1.63	0.45
3:M:243:THR:CA	3:M:246:GLU:HB3	2.45	0.45
4:H:29:TYR:HE2	16:H:302:PGW:C1	2.24	0.45
4:H:66:THR:O	4:H:66:THR:HG23	2.16	0.45
4:H:144:ILE:HG13	4:H:150:ASP:OD1	2.17	0.45
4:H:205:LYS:HZ1	5:1:18:ARG:HH12	1.64	0.45
5:F:44:LEU:O	5:F:44:LEU:CD1	2.57	0.45
9:O:102:BCL:CED	6:P:32:VAL:HG22	2.46	0.45
5:Q:45:ASN:O	5:Q:47:LEU:N	2.50	0.45
9:Q:102:BCL:OBD	6:R:32:VAL:HG13	2.17	0.45
9:R:101:BCL:C1B	9:S:102:BCL:HMB3	2.46	0.45
6:T:21:PHE:HD2	15:T:102:CRT:H14	1.82	0.45
5:W:49:ASP:HB2	5:Y:56:GLN:HB2	1.98	0.45
6:Z:44:PRO:O	6:Z:45:TRP:O	2.34	0.45
9:Z:101:BCL:OBB	9:Z:101:BCL:HHC	2.16	0.45
5:3:36:HIS:CE1	9:4:101:BCL:OBD	2.70	0.45
5:3:56:GLN:HG2	5:3:57:ALA:N	2.31	0.45
5:7:36:HIS:CD2	9:7:103:BCL:HMD1	2.51	0.45
1:C:26:PRO:HD3	2:L:263:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HB2	1:C:90:PHE:CE2	2.51	0.45
1:C:167:VAL:HG22	1:C:168:THR:N	2.32	0.45
2:L:171:TYR:O	2:L:174:LEU:N	2.50	0.45
2:L:189:PHE:HB3	3:M:209:LEU:HD11	1.98	0.45
2:L:243:LEU:HD21	11:L:304:UQ8:H46A	1.99	0.45
9:L:301:BCL:C4A	9:M:402:BCL:HBB2	2.47	0.45
3:M:55:LEU:C	3:M:55:LEU:HD13	2.37	0.45
3:M:137:ALA:CB	3:M:144:GLN:HE22	2.29	0.45
3:M:243:THR:HB	4:H:117:PRO:HD2	1.99	0.45
9:B:101:BCL:CHC	9:D:102:BCL:HBB3	2.47	0.45
5:F:51:ILE:CB	5:F:52:PRO:HA	2.46	0.45
9:I:103:BCL:C2B	9:K:102:BCL:C1B	2.95	0.45
6:P:39:ALA:O	6:P:42:TYR:N	2.49	0.45
5:U:36:HIS:CE1	9:U:102:BCL:NA	2.85	0.45
6:V:20:ILE:HD12	15:V:102:CRT:H10	1.94	0.45
6:Z:38:LEU:HD23	6:Z:38:LEU:C	2.36	0.45
6:2:21:PHE:HA	15:2:102:CRT:C13	2.37	0.45
5:3:27:PHE:CD1	5:3:27:PHE:C	2.90	0.45
5:3:30:VAL:O	5:3:34:LEU:HB2	2.16	0.45
5:3:46:TRP:NE1	5:3:47:LEU:CD2	2.80	0.45
5:5:32:GLY:CA	9:6:101:BCL:HED2	2.46	0.45
1:C:41:GLU:OE1	2:L:80:LEU:HD11	2.17	0.45
1:C:267:THR:O	1:C:270:TRP:HB3	2.16	0.45
3:M:63:PHE:CZ	5:Q:33:LEU:HD23	2.47	0.45
3:M:192:ARG:HH11	3:M:192:ARG:HG3	1.82	0.45
4:H:119:ARG:HB2	4:H:234:TYR:HA	1.99	0.45
5:A:33:LEU:O	5:A:37:MET:HB2	2.16	0.45
15:A:101:CRT:H9	6:0:17:PHE:HE1	1.82	0.45
15:A:101:CRT:C33	9:A:102:BCL:H3A	2.47	0.45
6:E:45:TRP:HA	5:F:52:PRO:CG	2.47	0.45
5:F:9:TYR:CZ	5:F:10:LYS:HE2	2.52	0.45
5:F:28:GLN:HE22	9:G:101:BCL:HBA1	1.82	0.45
5:F:29:ILE:HB	9:F:102:BCL:H43	1.99	0.45
9:F:102:BCL:HMD2	9:G:101:BCL:C1D	2.46	0.45
6:J:22:MET:HG3	6:J:26:TYR:HE1	1.81	0.45
15:J:101:CRT:C39	5:K:36:HIS:CG	2.99	0.45
5:K:12:TRP:HA	5:K:12:TRP:HE3	1.81	0.45
6:N:19:ALA:HB3	6:N:20:ILE:HD12	1.98	0.45
6:P:24:SER:O	6:P:27:ALA:CB	2.65	0.45
9:P:101:BCL:HMB1	9:P:101:BCL:HBB2	1.99	0.45
9:Q:102:BCL:HMB1	9:Q:102:BCL:HBB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:101:BCL:HBB2	9:R:101:BCL:HMB1	1.99	0.45
9:S:102:BCL:CHD	9:T:101:BCL:HMD2	2.47	0.45
9:T:101:BCL:HMA1	9:U:102:BCL:HHB	1.98	0.45
5:U:30:VAL:HG13	5:U:31:LEU:H	1.81	0.45
5:U:36:HIS:ND1	9:V:101:BCL:HMD1	2.30	0.45
6:X:28:TRP:O	6:X:31:LEU:N	2.50	0.45
5:Y:42:THR:HB	5:1:48:ASP:OD2	2.15	0.45
6:2:46:LEU:OXT	6:4:43:ARG:NH2	2.47	0.45
5:3:29:ILE:O	5:3:33:LEU:HG	2.17	0.45
5:3:56:GLN:NE2	5:3:56:GLN:H	2.14	0.45
9:3:102:BCL:H8	15:4:102:CRT:H183	1.96	0.45
5:5:27:PHE:CZ	5:7:29:ILE:CD1	3.00	0.45
5:5:30:VAL:CG1	5:5:31:LEU:N	2.80	0.45
5:5:44:LEU:C	5:5:46:TRP:N	2.70	0.45
5:7:35:ILE:O	5:7:38:ILE:HG22	2.17	0.45
2:L:223:THR:HG21	3:M:21:VAL:H	1.82	0.44
4:H:76:VAL:CG1	4:H:80:ARG:HH21	2.29	0.44
5:A:8:LEU:O	5:A:11:ILE:HG22	2.16	0.44
5:A:13:LEU:C	6:B:9:LEU:HD22	2.37	0.44
5:A:43:ASP:O	5:D:56:GLN:NE2	2.50	0.44
9:A:102:BCL:HBB3	9:0:101:BCL:CHC	2.47	0.44
9:A:102:BCL:OBB	9:A:102:BCL:HHC	2.17	0.44
5:F:11:ILE:HD12	5:F:14:ILE:CD1	2.44	0.44
6:N:21:PHE:CD2	15:N:102:CRT:H16	2.52	0.44
5:Q:31:LEU:CD2	9:R:101:BCL:HED3	2.47	0.44
5:Q:43:ASP:OD1	5:Q:44:LEU:HD23	2.16	0.44
5:U:36:HIS:NE2	9:U:102:BCL:NA	2.65	0.44
5:W:10:LYS:CE	15:W:103:CRT:H1M2	2.47	0.44
5:W:45:ASN:O	5:W:49:ASP:HB3	2.17	0.44
5:Y:29:ILE:HB	9:Y:102:BCL:H43	1.99	0.44
5:Y:43:ASP:HB2	5:1:47:LEU:HD12	1.98	0.44
5:3:2:PHE:CB	5:3:5:ASN:ND2	2.80	0.44
2:L:112:ARG:HH22	3:M:255:THR:HA	1.82	0.44
2:L:276:LEU:C	2:L:278:LEU:H	2.20	0.44
4:H:52:ARG:HD3	4:H:54:LYS:NZ	2.32	0.44
5:A:47:LEU:CG	5:9:43:ASP:HB2	2.47	0.44
5:D:26:ALA:O	5:D:29:ILE:HG22	2.17	0.44
9:E:101:BCL:HHB	9:F:102:BCL:HMA1	1.99	0.44
6:G:21:PHE:CD1	6:G:22:MET:HA	2.52	0.44
6:J:15:LYS:O	6:J:18:HIS:HB3	2.18	0.44
6:J:16:GLU:CD	15:J:101:CRT:C2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:17:PHE:CE1	15:N:102:CRT:H9	2.37	0.44
5:W:30:VAL:HG23	5:W:33:LEU:HD11	1.99	0.44
5:3:43:ASP:HB2	5:5:47:LEU:HD13	1.99	0.44
5:7:44:LEU:HD23	6:8:43:ARG:HH11	1.81	0.44
5:9:48:ASP:CG	5:9:48:ASP:O	2.56	0.44
1:C:112:VAL:O	1:C:114:GLY:N	2.51	0.44
1:C:133:LEU:HD23	1:C:133:LEU:C	2.37	0.44
3:M:218:MET:HB3	3:M:252:TRP:HZ2	1.73	0.44
3:M:271:TRP:CD2	4:H:26:LEU:HD21	2.52	0.44
4:H:138:VAL:O	4:H:140:LYS:CE	2.65	0.44
9:A:102:BCL:HMB1	9:A:102:BCL:HBB2	2.00	0.44
6:E:17:PHE:CE1	6:E:21:PHE:HB2	2.52	0.44
6:G:28:TRP:CD1	6:G:32:VAL:CG2	3.00	0.44
6:N:40:TRP:CE2	6:N:44:PRO:HB3	2.52	0.44
5:O:32:GLY:N	9:P:101:BCL:HED2	2.32	0.44
6:R:21:PHE:CD2	15:R:102:CRT:C16	2.94	0.44
6:X:37:LEU:O	6:X:37:LEU:CD2	2.65	0.44
5:1:36:HIS:CE1	9:1:102:BCL:NA	2.86	0.44
9:1:102:BCL:HMB1	9:1:102:BCL:HBB3	1.99	0.44
5:3:56:GLN:H	5:3:56:GLN:CD	2.20	0.44
15:3:103:CRT:H2M3	5:7:36:HIS:HB3	1.98	0.44
5:5:4:MET:C	5:5:6:ALA:H	2.21	0.44
2:L:80:LEU:HD22	2:L:153:HIS:ND1	2.32	0.44
3:M:109:LEU:HD13	3:M:114:TRP:CZ2	2.52	0.44
5:A:32:GLY:N	9:B:101:BCL:HED2	2.32	0.44
15:B:102:CRT:C1M	5:9:10:LYS:HB3	2.47	0.44
6:N:40:TRP:NE1	6:N:44:PRO:HB3	2.33	0.44
9:O:102:BCL:O2D	6:P:32:VAL:HG22	2.17	0.44
9:Q:102:BCL:OBB	9:Q:102:BCL:HHC	2.17	0.44
6:R:28:TRP:HA	6:R:28:TRP:CE3	2.53	0.44
6:X:7:THR:OG1	6:X:8:GLY:N	2.48	0.44
6:X:10:THR:HG22	6:X:11:ASP:N	2.32	0.44
6:X:17:PHE:HA	6:X:20:ILE:HG22	1.99	0.44
5:Y:48:ASP:O	5:Y:49:ASP:HB3	2.17	0.44
9:Y:102:BCL:HMB1	9:Y:102:BCL:HBB2	1.99	0.44
5:1:10:LYS:HB2	15:4:102:CRT:H83	2.00	0.44
6:0:32:VAL:CG1	6:0:33:VAL:H	2.28	0.44
9:0:101:BCL:HMA2	9:0:101:BCL:HBA2	1.99	0.44
1:C:40:MET:CG	1:C:252:ASN:HD22	2.31	0.44
2:L:110:ALA:O	2:L:113:GLU:HB2	2.18	0.44
2:L:178:TYR:HE1	3:M:180:PHE:CG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:186:ILE:CD1	18:L:402:HOH:O	2.65	0.44
5:D:48:ASP:HB2	5:D:56:GLN:NE2	2.22	0.44
5:I:30:VAL:CG1	5:I:31:LEU:H	2.26	0.44
9:I:102:BCL:ND	9:I:103:BCL:CMD	2.81	0.44
5:K:18:ARG:HG2	5:K:18:ARG:NH1	2.32	0.44
5:O:49:ASP:OD1	5:O:50:ASN:N	2.37	0.44
6:P:21:PHE:HB2	15:P:102:CRT:H14	1.98	0.44
6:T:40:TRP:HZ3	6:T:44:PRO:CA	2.30	0.44
6:T:46:LEU:HB3	6:V:42:TYR:OH	2.17	0.44
5:U:5:ASN:HB3	6:V:22:MET:HE3	1.98	0.44
6:V:21:PHE:CA	15:V:102:CRT:C12	2.95	0.44
6:X:21:PHE:O	6:X:22:MET:C	2.54	0.44
5:Y:43:ASP:HB2	5:1:47:LEU:HG	2.00	0.44
5:1:50:ASN:CB	5:3:59:GLY:C	2.86	0.44
6:4:41:LEU:HD23	6:4:41:LEU:C	2.38	0.44
15:8:101:CRT:H342	9:9:102:BCL:CAA	2.39	0.44
2:L:4:LEU:HD22	4:H:38:GLY:C	2.38	0.44
5:A:17:PRO:HB2	5:9:14:ILE:HD13	1.97	0.44
15:A:101:CRT:H10	15:A:101:CRT:H81	1.68	0.44
5:D:30:VAL:CG1	5:D:31:LEU:H	2.28	0.44
9:G:101:BCL:CHB	9:I:102:BCL:HMB3	2.47	0.44
6:J:34:ILE:O	6:J:38:LEU:HB2	2.18	0.44
5:O:40:LEU:O	5:O:40:LEU:HD23	2.17	0.44
5:U:30:VAL:CG1	5:U:31:LEU:N	2.79	0.44
15:W:103:CRT:H2M3	5:1:36:HIS:CB	2.47	0.44
9:X:101:BCL:HBB1	9:Y:102:BCL:HMC3	1.99	0.44
6:2:22:MET:O	6:2:26:TYR:HD1	2.01	0.44
6:2:42:TYR:CE1	6:2:43:ARG:HG3	2.52	0.44
5:3:2:PHE:HB3	5:3:5:ASN:ND2	2.31	0.44
6:4:34:ILE:CG2	6:4:35:ALA:N	2.80	0.44
7:C:503:HEM:HBB1	2:L:174:LEU:HD23	1.99	0.44
2:L:70:LEU:HD23	2:L:73:ILE:CD1	2.48	0.44
2:L:99:THR:OG1	2:L:157:TYR:OH	2.25	0.44
4:H:47:GLU:HG3	5:A:19:ARG:N	2.33	0.44
5:A:47:LEU:HB3	5:9:43:ASP:CA	2.48	0.44
15:A:103:CRT:H81	6:E:20:ILE:HG21	1.99	0.44
5:D:9:TYR:CA	6:E:18:HIS:CD2	3.01	0.44
5:D:22:VAL:HA	5:D:25:VAL:HG23	1.98	0.44
5:F:27:PHE:CE2	5:I:29:ILE:CG1	3.01	0.44
5:F:50:ASN:ND2	5:F:51:ILE:O	2.51	0.44
5:K:12:TRP:CD1	6:N:14:ALA:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:102:BCL:OBB	9:K:102:BCL:HHC	2.17	0.44
5:U:46:TRP:CE2	5:U:47:LEU:HD22	2.52	0.44
6:V:21:PHE:CD1	6:V:21:PHE:C	2.91	0.44
6:V:43:ARG:NH1	5:W:55:TYR:CG	2.86	0.44
6:Z:20:ILE:HG23	6:Z:21:PHE:N	2.32	0.44
9:Z:101:BCL:HMA1	9:1:102:BCL:HHB	2.00	0.44
5:3:19:ARG:O	5:3:23:SER:HB2	2.18	0.44
5:5:36:HIS:NE2	9:5:102:BCL:NA	2.66	0.44
5:7:40:LEU:HD12	5:7:45:ASN:HA	1.99	0.44
1:C:33:ILE:O	3:M:311:VAL:HG21	2.18	0.44
1:C:59:VAL:O	1:C:59:VAL:HG23	2.18	0.44
1:C:96:ALA:HB1	1:C:100:TRP:CH2	2.53	0.44
1:C:162:PRO:HG2	1:C:165:ALA:HB2	2.00	0.44
1:C:250:CYS:CB	1:C:251:HIS:ND1	2.81	0.44
2:L:10:TYR:O	2:L:12:VAL:N	2.49	0.44
3:M:59:LEU:O	3:M:63:PHE:HB2	2.18	0.44
3:M:84:PHE:CE2	5:W:37:MET:HA	2.52	0.44
3:M:84:PHE:N	3:M:84:PHE:CD1	2.86	0.44
3:M:289:THR:OG1	3:M:290:VAL:N	2.49	0.44
9:M:402:BCL:HHC	9:M:402:BCL:OBB	2.17	0.44
5:A:27:PHE:HA	5:A:30:VAL:HG12	1.99	0.44
5:A:33:LEU:CA	15:A:101:CRT:H392	2.48	0.44
9:A:102:BCL:C1B	9:0:101:BCL:CMB	2.96	0.44
5:F:9:TYR:HA	6:G:18:HIS:CG	2.52	0.44
5:K:12:TRP:CE3	5:K:12:TRP:CA	3.01	0.44
5:K:27:PHE:HE2	5:O:29:ILE:CD1	2.29	0.44
5:K:45:ASN:O	5:K:49:ASP:HB3	2.17	0.44
9:K:102:BCL:HMB1	9:K:102:BCL:HBB2	1.99	0.44
6:T:45:TRP:CE3	9:T:101:BCL:HAC2	2.52	0.44
6:T:45:TRP:HD1	6:T:46:LEU:H	1.66	0.44
5:W:36:HIS:HE1	9:X:101:BCL:OBD	2.01	0.44
5:W:54:SER:C	5:W:56:GLN:N	2.71	0.44
9:Y:102:BCL:HED1	6:Z:31:LEU:C	2.38	0.44
6:2:21:PHE:CZ	9:3:102:BCL:H203	2.53	0.44
5:5:26:ALA:O	5:5:29:ILE:CG2	2.63	0.44
6:8:26:TYR:O	6:8:30:GLY:N	2.50	0.44
1:C:124:LYS:O	1:C:125:VAL:C	2.55	0.44
1:C:280:ASN:O	1:C:285:TRP:HB2	2.18	0.44
2:L:178:TYR:CD2	2:L:269:PRO:HG3	2.50	0.44
11:L:304:UQ8:H22	11:L:304:UQ8:H25	1.66	0.44
3:M:27:ASN:ND2	5:O:19:ARG:NE	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:271:TRP:O	3:M:275:LEU:HB2	2.18	0.44
16:M:407:PGW:OAE	5:Q:19:ARG:NH1	2.51	0.44
5:A:30:VAL:HG13	5:A:31:LEU:N	2.33	0.44
6:B:11:ASP:HA	6:B:14:ALA:HB3	1.99	0.44
5:F:26:ALA:HA	5:F:29:ILE:HG22	2.00	0.44
5:I:36:HIS:CE1	9:I:102:BCL:NA	2.86	0.44
9:I:103:BCL:HMB1	9:I:103:BCL:HBB3	2.00	0.44
6:J:17:PHE:CE1	6:J:21:PHE:HB2	2.51	0.44
9:R:101:BCL:HBA2	9:R:101:BCL:H3A	1.32	0.44
5:U:9:TYR:CB	6:V:15:LYS:HD3	2.47	0.44
6:V:43:ARG:HB3	5:W:55:TYR:CE2	2.53	0.44
6:X:45:TRP:CE2	9:X:101:BCL:H2C	2.52	0.44
5:Y:27:PHE:C	5:Y:27:PHE:CD1	2.91	0.44
6:Z:22:MET:O	6:Z:25:MET:HB3	2.18	0.44
5:3:16:ASP:HB2	5:3:19:ARG:HD3	1.99	0.44
5:3:36:HIS:HE1	9:3:102:BCL:C1A	2.31	0.44
9:3:102:BCL:HMD1	6:4:36:HIS:ND1	2.33	0.44
5:5:46:TRP:CZ2	9:5:102:BCL:CHC	3.01	0.44
5:9:49:ASP:CG	5:9:50:ASN:OD1	2.56	0.44
1:C:253:THR:HG21	2:L:171:TYR:CB	2.43	0.43
2:L:20:GLY:O	2:L:24:ASP:CB	2.64	0.43
2:L:144:ARG:HG2	2:L:144:ARG:HH11	1.83	0.43
2:L:233:ILE:CG1	2:L:237:ALA:HB1	2.38	0.43
3:M:260:VAL:HG23	3:M:261:THR:N	2.32	0.43
4:H:257:PRO:HG3	5:7:19:ARG:CZ	2.48	0.43
9:F:102:BCL:C2D	9:G:101:BCL:C2D	2.96	0.43
6:G:22:MET:HG3	6:G:26:TYR:CZ	2.53	0.43
5:I:55:TYR:CD1	5:I:55:TYR:C	2.92	0.43
5:K:9:TYR:CD1	5:K:9:TYR:C	2.91	0.43
5:O:29:ILE:O	5:O:33:LEU:HB2	2.18	0.43
9:S:102:BCL:CBD	9:T:101:BCL:OBD	2.66	0.43
6:T:11:ASP:O	6:T:15:LYS:HD2	2.18	0.43
5:U:8:LEU:O	5:U:11:ILE:HG13	2.18	0.43
5:U:31:LEU:HA	5:U:34:LEU:HB3	2.00	0.43
6:X:22:MET:O	6:X:26:TYR:CD2	2.70	0.43
6:2:46:LEU:HD13	6:4:42:TYR:CZ	2.52	0.43
6:4:25:MET:HG2	15:4:102:CRT:C21	2.48	0.43
5:7:41:SER:OG	5:7:42:THR:N	2.51	0.43
5:7:56:GLN:HG2	5:7:57:ALA:N	2.31	0.43
1:C:90:PHE:C	1:C:90:PHE:CD1	2.92	0.43
2:L:45:LEU:N	5:9:30:VAL:HG13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:171:TYR:HA	2:L:174:LEU:O	2.18	0.43
3:M:89:HIS:O	3:M:93:LEU:HG	2.19	0.43
3:M:98:PRO:HA	3:M:99:PRO:HD3	1.90	0.43
4:H:65:LYS:HG2	4:H:66:THR:H	1.83	0.43
5:D:51:ILE:HG22	5:D:52:PRO:HA	2.00	0.43
6:E:44:PRO:CG	5:F:55:TYR:OH	2.66	0.43
6:E:45:TRP:O	6:E:46:LEU:CG	2.60	0.43
5:F:8:LEU:HA	15:J:101:CRT:H81	2.00	0.43
5:F:30:VAL:CG1	5:F:31:LEU:N	2.80	0.43
5:I:24:ILE:HG21	15:J:101:CRT:C21	2.46	0.43
5:K:19:ARG:HG3	5:K:20:VAL:N	2.33	0.43
6:P:31:LEU:O	6:P:34:ILE:HG23	2.18	0.43
5:Q:42:THR:CG2	5:Q:43:ASP:N	2.61	0.43
6:R:17:PHE:O	6:R:20:ILE:HG22	2.18	0.43
15:R:102:CRT:H1M2	15:R:102:CRT:H32A	1.77	0.43
6:V:10:THR:CG2	6:V:11:ASP:N	2.80	0.43
5:Y:13:LEU:HD23	5:Y:13:LEU:HA	1.81	0.43
6:Z:33:VAL:HG13	6:Z:34:ILE:N	2.33	0.43
5:3:9:TYR:CD1	5:3:9:TYR:C	2.92	0.43
5:3:42:THR:OG1	5:5:48:ASP:CG	2.57	0.43
5:5:16:ASP:HB2	5:5:19:ARG:CD	2.47	0.43
5:7:9:TYR:CE1	6:8:15:LYS:HB2	2.53	0.43
6:0:27:ALA:O	6:0:31:LEU:HG	2.18	0.43
1:C:200:LEU:O	1:C:204:LEU:HB2	2.18	0.43
3:M:56:THR:HG23	3:M:135:LYS:NZ	2.32	0.43
3:M:165:PRO:HB2	3:M:171:TRP:HZ3	1.83	0.43
3:M:256:MET:HE3	14:M:405:MQ8:H112	2.01	0.43
4:H:48:ARG:HH22	17:H:301:PEF:H12	1.83	0.43
5:A:11:ILE:C	5:A:13:LEU:H	2.20	0.43
5:D:43:ASP:CG	5:D:44:LEU:N	2.71	0.43
6:E:21:PHE:C	6:E:21:PHE:CD1	2.91	0.43
6:J:17:PHE:O	6:J:20:ILE:CG2	2.61	0.43
6:J:17:PHE:HA	6:J:20:ILE:CG2	2.43	0.43
6:J:45:TRP:HA	5:K:52:PRO:HD2	1.99	0.43
9:N:101:BCL:OBB	9:N:101:BCL:HHC	2.18	0.43
9:N:101:BCL:CMB	9:O:102:BCL:C1B	2.96	0.43
5:Q:51:ILE:HG22	5:Q:52:PRO:CA	2.39	0.43
6:T:45:TRP:HD1	6:T:46:LEU:N	2.15	0.43
6:V:30:GLY:O	6:V:34:ILE:CG1	2.66	0.43
15:V:102:CRT:H241	15:V:102:CRT:H26	1.49	0.43
9:Z:101:BCL:HMB1	9:Z:101:BCL:HBB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:32:GLY:HA2	9:4:101:BCL:CGD	2.48	0.43
15:3:103:CRT:H20	15:3:103:CRT:H181	1.83	0.43
9:7:103:BCL:H141	6:8:36:HIS:ND1	2.34	0.43
5:9:55:TYR:H	5:9:55:TYR:HD1	1.63	0.43
1:C:310:CYS:O	1:C:312:GLN:HG3	2.19	0.43
2:L:3:MET:CE	4:H:45:ARG:NH2	2.79	0.43
2:L:87:ALA:HB3	2:L:96:GLN:HE22	1.82	0.43
3:M:150:PHE:HB2	10:M:403:BPH:HMD3	2.00	0.43
3:M:201:PHE:HZ	4:H:15:THR:HG22	1.84	0.43
4:H:180:ARG:O	4:H:197:ILE:HG12	2.19	0.43
5:A:9:TYR:CE2	5:A:10:LYS:HE2	2.54	0.43
6:B:44:PRO:C	5:D:52:PRO:HG3	2.39	0.43
6:B:46:LEU:HB3	6:E:42:TYR:OH	2.18	0.43
5:F:14:ILE:HG13	5:F:15:LEU:N	2.33	0.43
5:F:43:ASP:HB2	5:I:47:LEU:C	2.39	0.43
6:G:16:GLU:HB2	15:G:102:CRT:H21A	2.00	0.43
6:G:28:TRP:CD1	6:G:32:VAL:HG21	2.49	0.43
5:I:24:ILE:HG23	15:J:101:CRT:H243	2.00	0.43
6:J:46:LEU:HD13	6:N:42:TYR:CD1	2.53	0.43
5:O:29:ILE:HG23	5:O:30:VAL:H	1.81	0.43
15:P:102:CRT:H36	15:P:102:CRT:H341	1.75	0.43
9:T:101:BCL:HMA2	9:T:101:BCL:HBA2	1.99	0.43
15:T:102:CRT:H10	15:T:102:CRT:H81	1.77	0.43
5:U:16:ASP:CB	5:U:18:ARG:NH1	2.80	0.43
5:W:51:ILE:HB	5:W:52:PRO:O	2.17	0.43
5:Y:27:PHE:HD1	5:Y:28:GLN:N	2.16	0.43
6:6:44:PRO:O	5:7:52:PRO:HD2	2.18	0.43
5:7:17:PRO:O	5:7:21:LEU:CG	2.66	0.43
5:9:34:LEU:O	5:9:38:ILE:HG23	2.19	0.43
5:9:35:ILE:O	5:9:36:HIS:C	2.56	0.43
6:0:36:HIS:CE1	9:0:101:BCL:NB	2.86	0.43
1:C:20:LEU:CB	2:L:180:PRO:HG3	2.48	0.43
1:C:47:ARG:O	1:C:50:ALA:HB3	2.17	0.43
1:C:134:VAL:O	1:C:135:ARG:C	2.57	0.43
1:C:273:ILE:O	1:C:273:ILE:HG22	2.17	0.43
2:L:82:TYR:HB3	2:L:85:ARG:HB3	1.99	0.43
2:L:179:ASN:ND2	2:L:268:TRP:NE1	2.65	0.43
2:L:273:ASN:ND2	2:L:276:LEU:HB2	2.31	0.43
4:H:169:ASP:O	4:H:183:GLU:N	2.51	0.43
4:H:225:LEU:HD12	4:H:235:GLU:OE1	2.18	0.43
5:A:18:ARG:O	5:A:22:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:33:LEU:HD12	5:A:33:LEU:N	2.34	0.43
5:A:43:ASP:OD1	5:A:44:LEU:HD23	2.18	0.43
15:A:101:CRT:H2M3	15:A:101:CRT:H391	1.84	0.43
9:B:101:BCL:C4B	9:D:102:BCL:HBB3	2.49	0.43
6:N:36:HIS:CE1	9:N:101:BCL:H141	2.53	0.43
5:O:34:LEU:C	5:O:37:MET:HB2	2.39	0.43
6:T:16:GLU:OE1	15:T:102:CRT:H32A	2.18	0.43
6:V:20:ILE:HG23	15:V:102:CRT:C10	2.48	0.43
5:W:31:LEU:CD1	15:X:102:CRT:H35	2.49	0.43
9:X:101:BCL:HMB1	9:X:101:BCL:HBB2	2.00	0.43
5:Y:33:LEU:O	5:Y:37:MET:HG2	2.18	0.43
5:1:10:LYS:CB	15:4:102:CRT:H5	2.42	0.43
9:1:102:BCL:HMD2	9:2:101:BCL:CHD	2.48	0.43
6:4:21:PHE:CD1	6:4:22:MET:N	2.86	0.43
9:7:103:BCL:HMB1	9:7:103:BCL:HBB2	1.99	0.43
6:0:29:PHE:O	6:0:32:VAL:CG1	2.50	0.43
1:C:282:ASN:C	1:C:283:TYR:CD1	2.92	0.43
2:L:72:ARG:HG2	3:M:305:PRO:CA	2.41	0.43
2:L:155:PHE:HB3	2:L:165:TRP:CE3	2.54	0.43
3:M:165:PRO:HG3	3:M:173:LYS:O	2.18	0.43
3:M:196:LEU:HD12	9:M:402:BCL:C1D	2.48	0.43
3:M:200:PRO:HA	3:M:203:MET:CE	2.47	0.43
3:M:218:MET:HB3	14:M:405:MQ8:H2M3	2.00	0.43
3:M:268:TRP:CE3	4:H:30:LEU:HD13	2.52	0.43
5:A:27:PHE:HE2	5:D:29:ILE:HD12	1.84	0.43
5:D:46:TRP:HE1	9:D:102:BCL:HHC	1.84	0.43
9:E:101:BCL:CHC	9:F:102:BCL:HBB3	2.48	0.43
5:F:8:LEU:HA	6:J:20:ILE:HD11	2.00	0.43
5:F:50:ASN:HA	5:I:60:LYS:CA	2.49	0.43
5:O:27:PHE:C	5:O:27:PHE:CD1	2.91	0.43
15:R:102:CRT:H2M1	5:S:33:LEU:CA	2.49	0.43
9:S:102:BCL:OBD	6:T:32:VAL:HG23	2.19	0.43
5:W:10:LYS:CD	15:W:103:CRT:C1M	2.90	0.43
9:W:102:BCL:CBC	9:X:101:BCL:HBC3	2.46	0.43
5:Y:2:PHE:N	5:Y:2:PHE:CD1	2.86	0.43
5:Y:26:ALA:O	5:Y:30:VAL:HG23	2.18	0.43
5:1:24:ILE:O	5:1:25:VAL:C	2.57	0.43
5:5:34:LEU:O	5:5:34:LEU:HG	2.18	0.43
6:8:18:HIS:CD2	6:8:18:HIS:C	2.92	0.43
6:8:28:TRP:C	6:8:30:GLY:N	2.70	0.43
15:8:101:CRT:C35	9:9:102:BCL:H3A	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:42:TYR:CE2	6:0:43:ARG:HD2	2.54	0.43
1:C:99:THR:HA	1:C:103:PRO:HB3	1.99	0.43
1:C:148:THR:HG23	1:C:322:GLN:HA	2.00	0.43
1:C:169:ASP:OD1	1:C:171:GLY:N	2.52	0.43
1:C:306:SER:O	1:C:309:THR:HB	2.19	0.43
3:M:277:VAL:HG13	10:M:403:BPH:HBC2	2.00	0.43
5:F:43:ASP:CB	5:I:47:LEU:CG	2.96	0.43
6:P:21:PHE:CZ	15:P:102:CRT:C17	3.01	0.43
6:P:31:LEU:C	6:P:34:ILE:HG23	2.38	0.43
5:Q:46:TRP:NE1	9:Q:102:BCL:OBB	2.50	0.43
6:R:45:TRP:CD1	6:R:46:LEU:N	2.87	0.43
5:W:28:GLN:NE2	15:X:102:CRT:H27	2.34	0.43
5:3:14:ILE:HG23	5:5:17:PRO:HB2	1.98	0.43
6:6:24:SER:O	6:6:27:ALA:HB3	2.18	0.43
6:0:21:PHE:CG	6:0:22:MET:N	2.84	0.43
1:C:38:VAL:O	2:L:168:ASN:ND2	2.51	0.43
1:C:187:SER:HB2	1:C:197:PHE:HB2	2.00	0.43
1:C:201:THR:HB	1:C:202:PRO:CD	2.49	0.43
1:C:274:ARG:HA	1:C:277:ARG:HG3	1.99	0.43
2:L:135:GLY:O	2:L:139:VAL:HG23	2.19	0.43
4:H:113:PRO:HB2	4:H:245:GLY:HA2	2.01	0.43
5:A:60:LYS:HA	5:9:49:ASP:O	2.19	0.43
15:A:101:CRT:C35	9:A:102:BCL:H3A	2.49	0.43
5:D:45:ASN:O	5:D:49:ASP:CB	2.67	0.43
6:E:33:VAL:HG22	6:E:37:LEU:HD23	2.00	0.43
9:F:102:BCL:OBB	9:F:102:BCL:HHC	2.18	0.43
5:O:5:ASN:HD22	5:O:8:LEU:HD21	1.83	0.43
5:O:36:HIS:NE2	9:P:101:BCL:CMD	2.82	0.43
6:P:20:ILE:HG21	15:P:102:CRT:C9	2.48	0.43
9:R:101:BCL:HMB1	9:R:101:BCL:HBB3	2.00	0.43
9:R:101:BCL:HBA2	9:R:101:BCL:CMA	2.34	0.43
5:W:18:ARG:HG2	5:W:18:ARG:HH11	1.84	0.43
9:W:102:BCL:HBC1	9:X:101:BCL:CBC	2.48	0.43
6:X:21:PHE:CD1	6:X:22:MET:N	2.87	0.43
5:3:17:PRO:HG2	5:3:18:ARG:H	1.82	0.43
9:4:101:BCL:HMB1	9:4:101:BCL:HBB3	2.00	0.43
9:7:103:BCL:H101	6:8:29:PHE:CZ	2.53	0.43
2:L:180:PRO:HB3	2:L:271:TRP:CH2	2.52	0.43
2:L:202:LEU:HD22	2:L:225:PHE:HE2	1.83	0.43
2:L:214:PRO:HA	4:H:68:VAL:O	2.19	0.43
3:M:250:LEU:CD1	3:M:250:LEU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:251:THR:HB	4:H:254:ARG:HG3	2.01	0.43
6:E:9:LEU:HD22	6:E:13:GLU:CG	2.45	0.43
5:I:8:LEU:C	6:J:18:HIS:CE1	2.92	0.43
6:R:20:ILE:CG2	6:R:21:PHE:N	2.82	0.43
5:W:54:SER:O	5:W:55:TYR:C	2.56	0.43
9:4:101:BCL:OBB	9:4:101:BCL:HHC	2.19	0.43
5:9:20:VAL:HA	5:9:23:SER:OG	2.18	0.43
9:9:102:BCL:HMB1	9:9:102:BCL:HBB2	1.99	0.43
2:L:23:PHE:HA	2:L:25:PHE:HE2	1.83	0.43
2:L:86:MET:HE1	2:L:96:GLN:HB3	2.01	0.43
2:L:139:VAL:HA	2:L:143:VAL:HB	2.01	0.43
2:L:207:THR:O	4:H:67:PHE:CE1	2.65	0.43
3:M:84:PHE:HD1	3:M:84:PHE:N	2.16	0.43
3:M:238:ILE:HD12	3:M:263:GLU:CA	2.49	0.43
4:H:5:ILE:CB	5:D:42:THR:HG23	2.47	0.43
4:H:80:ARG:HG2	4:H:80:ARG:NH1	2.34	0.43
4:H:219:PHE:O	4:H:222:VAL:HG23	2.19	0.43
9:A:102:BCL:H141	5:9:15:LEU:HD11	2.00	0.43
5:I:13:LEU:HD21	6:J:10:THR:O	2.18	0.43
15:N:102:CRT:H372	9:O:102:BCL:CMB	2.40	0.43
9:S:102:BCL:HBC2	9:T:101:BCL:HMD2	2.00	0.43
5:U:25:VAL:HG13	9:U:102:BCL:H41	2.01	0.43
5:U:43:ASP:HB2	5:W:47:LEU:HB3	1.99	0.43
6:X:13:GLU:HG2	6:X:14:ALA:N	2.34	0.43
5:Y:44:LEU:HD13	6:Z:43:ARG:HD2	2.01	0.43
5:1:10:LYS:CE	6:4:20:ILE:HD12	2.48	0.43
5:3:33:LEU:O	5:3:37:MET:HB2	2.19	0.43
1:C:126:VAL:CG1	1:C:287:LEU:HD13	2.42	0.42
2:L:105:ALA:HB1	10:L:302:BPH:C2	2.46	0.42
3:M:12:GLN:NE2	3:M:41:GLY:C	2.71	0.42
3:M:192:ARG:HG3	3:M:192:ARG:NH1	2.34	0.42
3:M:229:PHE:HE1	4:H:244:ALA:HB2	1.83	0.42
3:M:258:PHE:HD2	17:H:301:PEF:C30	2.31	0.42
15:A:101:CRT:H26	15:A:101:CRT:H241	1.59	0.42
5:D:26:ALA:O	5:D:29:ILE:CG2	2.67	0.42
5:F:56:GLN:O	5:F:60:LYS:CB	2.67	0.42
6:G:28:TRP:O	6:G:30:GLY:N	2.52	0.42
9:G:101:BCL:HMB1	9:G:101:BCL:HBB2	2.01	0.42
5:I:12:TRP:CH2	6:J:17:PHE:CZ	3.06	0.42
5:I:24:ILE:CG2	15:J:101:CRT:H243	2.49	0.42
6:J:17:PHE:O	6:J:17:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:45:TRP:CE3	9:N:101:BCL:H2C	2.54	0.42
6:P:18:HIS:O	6:P:22:MET:HB2	2.18	0.42
5:Q:50:ASN:ND2	5:Q:51:ILE:H	2.17	0.42
5:U:6:ALA:O	6:V:15:LYS:NZ	2.44	0.42
9:U:102:BCL:HMB1	9:U:102:BCL:HBB2	1.99	0.42
5:W:54:SER:O	5:W:56:GLN:N	2.52	0.42
6:X:28:TRP:HA	6:X:31:LEU:HG	2.01	0.42
5:1:43:ASP:HB3	5:1:44:LEU:HD23	2.00	0.42
15:2:102:CRT:H342	9:3:102:BCL:HAA1	2.01	0.42
5:3:5:ASN:HB3	6:4:22:MET:HG2	2.00	0.42
6:6:37:LEU:HD23	6:6:37:LEU:O	2.19	0.42
5:7:7:ASN:ND2	5:7:7:ASN:N	2.64	0.42
2:L:144:ARG:HB3	2:L:145:PRO:CD	2.41	0.42
3:M:6:ASN:ND2	3:M:227:SER:OG	2.52	0.42
3:M:238:ILE:HD12	3:M:263:GLU:CB	2.49	0.42
5:D:51:ILE:HG22	5:D:52:PRO:CA	2.50	0.42
6:G:46:LEU:HB3	6:J:42:TYR:CE2	2.54	0.42
15:G:102:CRT:C34	9:I:102:BCL:HAA1	2.38	0.42
5:I:56:GLN:HA	5:I:60:LYS:CB	2.50	0.42
6:J:40:TRP:HA	6:J:44:PRO:HA	2.00	0.42
5:O:12:TRP:NE1	6:P:18:HIS:HA	2.35	0.42
6:P:17:PHE:HA	6:P:20:ILE:HG22	2.01	0.42
6:P:46:LEU:CA	5:Q:52:PRO:HD3	2.48	0.42
5:Q:12:TRP:CE3	5:Q:12:TRP:CA	3.01	0.42
15:T:102:CRT:H32A	15:T:102:CRT:H1M2	1.37	0.42
15:T:102:CRT:H1M3	15:T:102:CRT:H23	1.48	0.42
6:V:10:THR:HB	6:V:13:GLU:OE2	2.19	0.42
5:W:21:LEU:HD11	9:W:102:BCL:H142	2.01	0.42
5:Y:44:LEU:HD13	6:Z:43:ARG:CD	2.50	0.42
9:1:102:BCL:CHD	9:2:101:BCL:HMD2	2.49	0.42
15:3:103:CRT:H81	15:3:103:CRT:H10	1.68	0.42
6:6:25:MET:SD	6:6:29:PHE:CE2	3.12	0.42
6:6:45:TRP:O	6:6:46:LEU:HB2	2.20	0.42
1:C:105:GLU:N	1:C:105:GLU:OE2	2.52	0.42
2:L:38:VAL:O	2:L:42:PHE:HD1	2.02	0.42
3:M:275:LEU:HD12	3:M:278:ILE:HB	2.02	0.42
6:N:18:HIS:O	6:N:22:MET:CB	2.68	0.42
6:N:23:GLN:HA	6:N:26:TYR:HD2	1.84	0.42
5:O:11:ILE:O	5:O:11:ILE:CG2	2.67	0.42
9:R:101:BCL:HMA1	9:S:102:BCL:HHB	2.01	0.42
6:V:10:THR:CG2	6:V:11:ASP:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:28:TRP:CE3	6:X:31:LEU:HD12	2.53	0.42
5:Y:12:TRP:HE1	6:Z:18:HIS:CA	2.17	0.42
5:Y:40:LEU:HB2	5:Y:46:TRP:CH2	2.54	0.42
5:Y:51:ILE:CA	5:Y:52:PRO:C	2.88	0.42
5:1:18:ARG:HH11	5:1:18:ARG:HG2	1.85	0.42
9:2:101:BCL:HMB3	9:3:102:BCL:CHB	2.48	0.42
9:2:101:BCL:C4A	9:3:102:BCL:HMB3	2.49	0.42
9:4:101:BCL:HMB1	9:4:101:BCL:HBB2	2.00	0.42
5:7:17:PRO:HD2	5:7:18:ARG:HE	1.83	0.42
5:9:16:ASP:CG	5:9:17:PRO:N	2.71	0.42
6:0:10:THR:H	6:0:13:GLU:CD	2.22	0.42
1:C:151:THR:OG1	1:C:323:MET:HE3	2.19	0.42
2:L:13:ARG:HG3	2:L:13:ARG:NH1	2.34	0.42
2:L:84:LEU:CD2	2:L:151:TRP:HE1	2.32	0.42
2:L:224:PHE:O	2:L:228:ILE:HG13	2.19	0.42
2:L:242:GLY:HA3	3:M:216:PHE:CD1	2.55	0.42
3:M:14:ARG:HG2	3:M:14:ARG:HH11	1.85	0.42
3:M:114:TRP:CH2	5:S:37:MET:SD	3.13	0.42
3:M:154:ILE:O	3:M:157:TYR:HB3	2.20	0.42
3:M:164:ARG:CB	3:M:165:PRO:HD3	2.47	0.42
3:M:168:MET:HE3	3:M:289:THR:HG22	2.02	0.42
5:A:35:ILE:HD11	15:B:102:CRT:H392	2.01	0.42
6:B:46:LEU:OXT	6:E:43:ARG:NH2	2.52	0.42
5:D:14:ILE:N	5:D:14:ILE:CD1	2.81	0.42
6:E:21:PHE:CZ	9:F:102:BCL:H203	2.54	0.42
5:F:13:LEU:HD22	6:G:9:LEU:O	2.19	0.42
9:I:103:BCL:C1C	9:K:102:BCL:HBB3	2.49	0.42
6:J:33:VAL:CG1	6:J:34:ILE:N	2.83	0.42
5:O:30:VAL:O	5:O:34:LEU:N	2.51	0.42
6:P:17:PHE:HA	6:P:20:ILE:CG2	2.50	0.42
5:U:13:LEU:O	6:V:7:THR:CG2	2.67	0.42
5:U:15:LEU:HD11	9:W:102:BCL:H141	2.00	0.42
5:U:15:LEU:HD23	5:U:15:LEU:HA	1.92	0.42
5:W:7:ASN:N	5:W:7:ASN:ND2	2.58	0.42
15:W:103:CRT:H391	5:1:36:HIS:CB	2.48	0.42
15:W:103:CRT:H10	15:W:103:CRT:H81	1.62	0.42
6:X:43:ARG:HB3	5:Y:55:TYR:HE2	1.83	0.42
9:Z:101:BCL:HMB3	9:1:102:BCL:C1B	2.50	0.42
6:2:40:TRP:CE3	6:2:40:TRP:HA	2.54	0.42
5:7:19:ARG:N	5:7:19:ARG:HD3	2.35	0.42
2:L:4:LEU:HD13	2:L:6:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:301:BCL:HHC	9:L:301:BCL:OBB	2.19	0.42
9:L:303:BCL:H121	9:L:303:BCL:HMA1	2.02	0.42
3:M:180:PHE:H	3:M:181:PRO:HD2	1.84	0.42
4:H:66:THR:O	4:H:66:THR:CG2	2.67	0.42
5:A:36:HIS:NE2	9:A:102:BCL:NA	2.67	0.42
5:F:18:ARG:HA	5:F:21:LEU:HB3	2.01	0.42
15:G:102:CRT:C2M	5:I:36:HIS:HB2	2.27	0.42
6:X:37:LEU:HD23	6:X:37:LEU:C	2.40	0.42
5:Y:50:ASN:HD21	5:Y:51:ILE:HG12	1.81	0.42
15:2:102:CRT:H2M3	5:3:36:HIS:HB3	2.01	0.42
6:4:45:TRP:O	6:4:46:LEU:CG	2.67	0.42
9:6:101:BCL:HMB1	9:6:101:BCL:HBB3	2.00	0.42
9:0:101:BCL:HMB1	9:0:101:BCL:HBB2	2.02	0.42
1:C:206:GLN:HA	1:C:206:GLN:HE21	1.85	0.42
2:L:123:GLY:HA2	3:M:228:ARG:NH2	2.35	0.42
3:M:25:LYS:CE	6:P:8:GLY:HA3	2.42	0.42
3:M:58:THR:HA	3:M:61:ILE:HG22	2.02	0.42
3:M:224:LEU:HA	3:M:227:SER:HB2	2.00	0.42
4:H:14:ILE:CG1	5:I:37:MET:SD	3.06	0.42
4:H:170:VAL:HG12	4:H:182:LEU:HD22	2.00	0.42
4:H:176:GLU:O	4:H:178:GLN:HG2	2.20	0.42
9:B:101:BCL:HMB1	9:B:101:BCL:HBB3	2.00	0.42
5:D:9:TYR:CE1	6:E:11:ASP:HB3	2.54	0.42
15:J:101:CRT:C39	5:K:36:HIS:CB	2.98	0.42
6:N:28:TRP:HE3	6:N:31:LEU:CD1	2.22	0.42
6:N:31:LEU:O	6:N:34:ILE:HG22	2.18	0.42
6:P:32:VAL:O	6:P:35:ALA:HB3	2.19	0.42
9:P:101:BCL:HHC	9:P:101:BCL:OBB	2.19	0.42
5:Q:12:TRP:CD1	6:R:17:PHE:HD2	2.38	0.42
5:S:34:LEU:O	5:S:38:ILE:HG22	2.20	0.42
5:S:43:ASP:O	5:U:56:GLN:HG2	2.19	0.42
6:T:22:MET:O	6:T:25:MET:N	2.50	0.42
5:U:44:LEU:C	5:U:44:LEU:HD12	2.40	0.42
9:Y:102:BCL:CHD	9:Y:102:BCL:HBC2	2.50	0.42
5:3:18:ARG:HA	5:3:21:LEU:CB	2.48	0.42
6:4:40:TRP:CE3	6:4:44:PRO:HA	2.54	0.42
5:5:44:LEU:CD1	5:5:46:TRP:HE3	2.31	0.42
6:6:33:VAL:O	6:6:37:LEU:HB2	2.20	0.42
6:0:20:ILE:HD13	6:0:20:ILE:O	2.20	0.42
2:L:31:TYR:HE1	2:L:119:LYS:HZ2	1.55	0.42
2:L:273:ASN:HA	2:L:276:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:123:THR:O	3:M:127:LEU:HG	2.20	0.42
3:M:156:PHE:HE1	3:M:284:ILE:HG13	1.85	0.42
6:B:39:ALA:C	6:B:45:TRP:HZ3	2.23	0.42
5:D:44:LEU:HD13	6:E:43:ARG:HD3	2.02	0.42
9:E:101:BCL:NB	9:F:102:BCL:CMB	2.82	0.42
5:K:36:HIS:CE1	9:K:102:BCL:NA	2.87	0.42
5:K:47:LEU:HD22	5:K:47:LEU:N	2.32	0.42
5:O:35:ILE:HA	5:O:38:ILE:HG12	2.00	0.42
9:O:102:BCL:CBC	9:P:101:BCL:HBC3	2.50	0.42
15:P:102:CRT:C39	5:Q:36:HIS:CD2	3.03	0.42
9:Y:102:BCL:C1D	9:Z:101:BCL:HMD2	2.50	0.42
5:1:19:ARG:NH2	5:3:18:ARG:NH1	2.68	0.42
5:3:2:PHE:CB	5:3:5:ASN:HD22	2.29	0.42
15:3:103:CRT:C39	5:7:36:HIS:HB3	2.49	0.42
9:6:101:BCL:OBB	9:6:101:BCL:HHC	2.20	0.42
6:8:17:PHE:HZ	15:8:101:CRT:C9	2.17	0.42
6:0:26:TYR:O	6:0:27:ALA:C	2.58	0.42
1:C:57:GLN:OE1	1:C:57:GLN:HA	2.19	0.42
3:M:193:TYR:O	3:M:294:TRP:HD1	2.03	0.42
3:M:197:TYR:CE2	9:M:402:BCL:HMC2	2.55	0.42
9:M:401:BCL:H62	9:M:401:BCL:H41	1.57	0.42
4:H:31:ARG:NH2	4:H:35:LYS:NZ	2.68	0.42
4:H:32:ARG:NH1	4:H:32:ARG:HG2	2.35	0.42
4:H:35:LYS:HB3	4:H:61:LEU:CD1	2.50	0.42
4:H:133:ILE:CD1	4:H:171:TRP:HB3	2.45	0.42
6:E:9:LEU:HB3	6:E:13:GLU:HG2	2.01	0.42
5:F:11:ILE:HG23	5:F:12:TRP:N	2.34	0.42
5:F:43:ASP:OD2	5:I:47:LEU:O	2.37	0.42
5:I:18:ARG:HA	5:I:21:LEU:CB	2.48	0.42
5:I:43:ASP:OD1	5:I:44:LEU:CG	2.67	0.42
15:T:102:CRT:H36	15:T:102:CRT:H341	1.82	0.42
9:3:102:BCL:OBB	9:3:102:BCL:HHC	2.18	0.42
5:5:45:ASN:ND2	5:5:48:ASP:OD1	2.53	0.42
9:7:103:BCL:C1B	9:9:102:BCL:HMB3	2.50	0.42
1:C:130:MET:CE	1:C:284:ILE:HD11	2.49	0.42
1:C:166:TRP:O	1:C:303:LEU:HA	2.20	0.42
1:C:183:GLN:HG2	1:C:194:SER:O	2.20	0.42
2:L:52:TRP:CD2	5:9:38:ILE:HG22	2.55	0.42
2:L:80:LEU:HD22	2:L:153:HIS:CE1	2.55	0.42
2:L:188:PHE:HE2	2:L:252:TRP:CD1	2.38	0.42
3:M:76:LEU:HD12	3:M:79:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:99:PRO:HA	3:M:100:PRO:HD3	1.97	0.42
3:M:218:MET:HB3	3:M:252:TRP:CH2	2.53	0.42
15:M:406:CRT:H341	15:M:406:CRT:H36	1.82	0.42
4:H:29:TYR:HD1	4:H:30:LEU:N	2.18	0.42
5:A:47:LEU:HD12	5:9:43:ASP:CB	2.50	0.42
9:A:102:BCL:C2B	9:0:101:BCL:C2B	2.98	0.42
5:D:19:ARG:O	5:D:23:SER:HB3	2.19	0.42
5:D:42:THR:OG1	5:F:48:ASP:CG	2.58	0.42
9:E:101:BCL:HMB1	9:E:101:BCL:HBB2	2.02	0.42
5:K:24:ILE:CD1	15:N:102:CRT:H243	2.50	0.42
5:K:44:LEU:CD2	5:K:46:TRP:CB	2.84	0.42
5:O:18:ARG:CB	5:O:18:ARG:HH11	2.32	0.42
5:O:32:GLY:H	9:P:101:BCL:HED2	1.84	0.42
9:O:102:BCL:OBB	9:O:102:BCL:HHC	2.19	0.42
5:Q:2:PHE:HA	6:R:26:TYR:OH	2.20	0.42
5:S:8:LEU:HB2	6:T:18:HIS:NE2	2.35	0.42
6:T:40:TRP:CE3	6:T:40:TRP:O	2.72	0.42
5:U:15:LEU:HG	5:W:21:LEU:HD21	2.02	0.42
5:U:35:ILE:O	5:U:38:ILE:N	2.53	0.42
5:W:3:THR:O	5:W:4:MET:C	2.59	0.42
6:X:46:LEU:HB2	5:Y:52:PRO:HD3	2.02	0.42
5:1:54:SER:O	5:1:55:TYR:C	2.59	0.42
6:2:20:ILE:HG23	6:2:21:PHE:N	2.34	0.42
5:5:9:TYR:CE2	5:5:10:LYS:CD	3.03	0.42
9:7:103:BCL:HMB1	9:7:103:BCL:HBB3	2.01	0.42
15:8:101:CRT:C39	5:9:36:HIS:CD2	3.03	0.42
5:9:13:LEU:CD2	6:0:9:LEU:O	2.67	0.42
6:0:22:MET:O	6:0:26:TYR:HD2	2.03	0.42
9:0:101:BCL:HMB1	9:0:101:BCL:HBB3	2.02	0.42
1:C:225:SER:H	1:C:228:GLN:CD	2.21	0.42
2:L:231:TYR:CZ	2:L:233:ILE:HA	2.55	0.42
4:H:54:LYS:HD3	4:H:57:GLY:O	2.19	0.42
5:A:2:PHE:O	5:A:2:PHE:CD1	2.73	0.42
5:D:51:ILE:HG23	5:D:52:PRO:HA	2.01	0.42
5:F:50:ASN:OD1	6:G:43:ARG:NH1	2.51	0.42
5:S:43:ASP:OD1	5:U:56:GLN:NE2	2.52	0.42
5:W:43:ASP:OD1	5:W:44:LEU:N	2.53	0.42
6:Z:36:HIS:CE1	9:Z:101:BCL:NA	2.87	0.42
5:1:50:ASN:HB2	5:3:59:GLY:HA3	2.02	0.42
9:1:102:BCL:OBB	9:1:102:BCL:HHC	2.19	0.42
9:6:101:BCL:C4A	9:7:102:BCL:HMB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:9:TYR:HA	6:8:18:HIS:CE1	2.50	0.42
6:8:22:MET:CG	6:8:26:TYR:HE2	2.33	0.42
5:9:15:LEU:HB3	5:9:20:VAL:HG21	2.01	0.42
1:C:278:ASP:OD1	1:C:283:TYR:HE1	2.02	0.41
1:C:316:LYS:O	1:C:319:TYR:N	2.53	0.41
2:L:191:THR:HG22	2:L:245:LEU:CD1	2.50	0.41
2:L:257:ILE:CG2	2:L:258:LEU:N	2.83	0.41
3:M:71:ILE:HG23	3:M:177:PHE:HB3	2.02	0.41
4:H:52:ARG:HG3	4:H:52:ARG:O	2.20	0.41
5:A:33:LEU:HA	15:A:101:CRT:H392	2.01	0.41
5:A:47:LEU:HD22	5:A:47:LEU:N	2.35	0.41
9:F:102:BCL:HMB1	9:F:102:BCL:HBB2	2.02	0.41
6:G:24:SER:O	6:G:27:ALA:N	2.50	0.41
9:K:102:BCL:HMB1	9:K:102:BCL:HBB3	2.01	0.41
5:O:43:ASP:HA	5:Q:48:ASP:CG	2.40	0.41
9:O:102:BCL:CAD	9:P:101:BCL:CAD	2.98	0.41
5:Q:22:VAL:O	5:Q:25:VAL:HG12	2.20	0.41
15:R:102:CRT:H26	15:R:102:CRT:H241	1.83	0.41
6:T:29:PHE:N	6:T:29:PHE:HD1	2.18	0.41
9:T:101:BCL:CMA	9:T:101:BCL:HBA2	2.50	0.41
6:V:24:SER:O	6:V:27:ALA:HB3	2.21	0.41
5:W:30:VAL:HA	5:W:33:LEU:CG	2.50	0.41
6:Z:46:LEU:HD22	6:2:42:TYR:OH	2.19	0.41
9:2:101:BCL:CGD	9:2:101:BCL:H2A	2.50	0.41
5:3:11:ILE:HG12	15:3:103:CRT:C8	2.50	0.41
5:3:20:VAL:HA	5:3:23:SER:HB3	2.02	0.41
15:3:103:CRT:H183	6:6:25:MET:HA	2.02	0.41
6:4:24:SER:CB	15:4:102:CRT:C14	2.96	0.41
5:5:50:ASN:HB3	5:7:55:TYR:O	2.20	0.41
5:7:44:LEU:CD2	5:7:46:TRP:HE3	2.33	0.41
9:7:103:BCL:H11	6:8:29:PHE:CD1	2.55	0.41
1:C:277:ARG:HH11	1:C:277:ARG:CG	2.33	0.41
3:M:34:PRO:HG3	3:M:50:PRO:HD3	2.01	0.41
3:M:136:ARG:NE	3:M:136:ARG:CA	2.83	0.41
3:M:159:VAL:HG11	3:M:281:GLY:O	2.19	0.41
3:M:268:TRP:CE3	14:M:405:MQ8:H162	2.55	0.41
10:M:403:BPH:H102	10:M:403:BPH:H6C2	1.89	0.41
4:H:31:ARG:NH2	4:H:35:LYS:HZ2	2.18	0.41
4:H:154:MET:HE3	4:H:207:ARG:HA	2.02	0.41
5:A:55:TYR:O	5:A:56:GLN:C	2.58	0.41
9:B:101:BCL:HHC	9:B:101:BCL:OBB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:102:CRT:H1M1	5:9:10:LYS:CG	2.49	0.41
5:D:2:PHE:CD1	5:D:3:THR:N	2.88	0.41
5:I:39:VAL:HG12	5:I:46:TRP:HZ3	1.84	0.41
6:P:17:PHE:CE1	15:P:102:CRT:H6	2.30	0.41
5:S:35:ILE:O	5:S:36:HIS:C	2.56	0.41
5:U:19:ARG:HH21	5:U:19:ARG:HB2	1.85	0.41
6:Z:45:TRP:NE1	9:Z:101:BCL:OBB	2.54	0.41
9:2:101:BCL:HMB1	9:2:101:BCL:HBB2	2.03	0.41
5:3:43:ASP:CG	5:5:47:LEU:O	2.59	0.41
5:5:12:TRP:O	6:6:9:LEU:HD12	2.20	0.41
6:6:28:TRP:O	6:6:30:GLY:N	2.53	0.41
9:6:101:BCL:HMB1	9:6:101:BCL:HBB2	2.01	0.41
1:C:93:THR:O	1:C:93:THR:HG22	2.19	0.41
9:L:301:BCL:H2C	9:M:402:BCL:H2C	2.02	0.41
3:M:59:LEU:CD1	5:Q:29:ILE:HD13	2.50	0.41
3:M:74:ASN:ND2	3:M:95:LEU:HD13	2.34	0.41
3:M:159:VAL:HA	3:M:163:ILE:CG2	2.44	0.41
3:M:194:GLY:O	3:M:195:ASN:CB	2.62	0.41
4:H:65:LYS:N	4:H:78:ALA:O	2.42	0.41
4:H:248:LEU:HG	4:H:248:LEU:O	2.19	0.41
15:A:103:CRT:H181	15:A:103:CRT:H20	1.78	0.41
5:D:16:ASP:HB3	5:D:19:ARG:CB	2.51	0.41
5:I:11:ILE:HG23	5:I:12:TRP:N	2.35	0.41
9:I:103:BCL:C1B	9:K:102:BCL:C2B	2.99	0.41
6:P:15:LYS:O	6:P:16:GLU:C	2.58	0.41
5:Q:2:PHE:N	5:Q:2:PHE:CD1	2.89	0.41
9:Q:102:BCL:HBC2	9:Q:102:BCL:CHD	2.50	0.41
5:S:42:THR:CG2	5:S:43:ASP:N	2.81	0.41
9:S:102:BCL:O1D	9:S:102:BCL:H2A	2.19	0.41
6:T:10:THR:C	6:T:13:GLU:OE2	2.58	0.41
5:U:14:ILE:HB	15:X:102:CRT:H83	2.03	0.41
5:W:34:LEU:O	5:W:37:MET:CB	2.69	0.41
6:X:46:LEU:CA	5:Y:52:PRO:HD3	2.51	0.41
5:Y:51:ILE:CB	5:Y:52:PRO:CA	2.98	0.41
6:2:45:TRP:CE3	9:2:101:BCL:H2C	2.55	0.41
9:2:101:BCL:OBB	9:2:101:BCL:HHC	2.19	0.41
5:3:17:PRO:O	5:3:21:LEU:HB2	2.21	0.41
5:7:8:LEU:O	5:7:11:ILE:HG22	2.20	0.41
9:7:103:BCL:HMA2	9:7:103:BCL:HBA2	2.02	0.41
15:8:101:CRT:H372	9:9:102:BCL:CMB	2.43	0.41
1:C:38:VAL:O	1:C:38:VAL:CG1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LYS:HG3	7:C:504:HEM:O1A	2.19	0.41
2:L:52:TRP:CA	5:A:37:MET:HE1	2.49	0.41
2:L:71:TRP:N	2:L:71:TRP:HE3	2.19	0.41
9:L:303:BCL:HMB1	9:L:303:BCL:HBB3	2.02	0.41
4:H:241:ALA:O	4:H:244:ALA:HB3	2.21	0.41
5:A:32:GLY:HA3	9:B:101:BCL:HED2	1.93	0.41
5:D:32:GLY:O	5:D:35:ILE:N	2.49	0.41
5:F:7:ASN:O	15:J:101:CRT:C8	2.69	0.41
5:F:36:HIS:CE1	9:G:101:BCL:CMD	2.75	0.41
5:I:51:ILE:HA	5:I:52:PRO:HA	1.84	0.41
5:S:27:PHE:CE2	5:U:29:ILE:CD1	3.03	0.41
6:V:44:PRO:CD	5:W:55:TYR:OH	2.68	0.41
6:V:45:TRP:O	6:V:46:LEU:HG	2.20	0.41
5:W:12:TRP:CE3	5:W:12:TRP:CA	3.03	0.41
5:Y:29:ILE:HA	9:Y:102:BCL:H12	1.97	0.41
5:3:18:ARG:O	5:3:22:VAL:HG12	2.19	0.41
6:4:29:PHE:CE1	9:4:101:BCL:H61	2.56	0.41
5:5:13:LEU:CD2	6:6:14:ALA:CB	2.99	0.41
6:8:42:TYR:CG	6:8:43:ARG:N	2.85	0.41
1:C:20:LEU:HD12	2:L:259:ILE:HB	2.02	0.41
1:C:173:LYS:HE3	3:M:80:HIS:CE1	2.56	0.41
1:C:227:LYS:O	1:C:230:GLU:HB2	2.20	0.41
2:L:8:LYS:CD	4:H:87:VAL:HG21	2.50	0.41
2:L:52:TRP:HD1	2:L:94:LEU:HD11	1.85	0.41
3:M:63:PHE:HE2	3:M:124:LEU:HB2	1.85	0.41
3:M:196:LEU:HD23	3:M:196:LEU:HA	1.91	0.41
3:M:253:ARG:HB2	3:M:259:ASN:OD1	2.21	0.41
3:M:277:VAL:HA	3:M:280:ALA:HB3	2.02	0.41
9:M:401:BCL:HMB1	9:M:401:BCL:HBB3	2.02	0.41
15:A:103:CRT:H391	5:F:36:HIS:HB3	2.03	0.41
5:D:7:ASN:HD22	5:D:8:LEU:H	1.69	0.41
5:D:12:TRP:CE3	5:D:12:TRP:CA	3.04	0.41
5:D:46:TRP:NE1	9:D:102:BCL:HHC	2.36	0.41
5:D:55:TYR:HA	5:D:59:GLY:H	1.85	0.41
9:F:102:BCL:HBA1	9:F:102:BCL:CGD	2.50	0.41
5:I:39:VAL:HG11	9:I:102:BCL:HBC1	2.02	0.41
5:I:49:ASP:CG	5:I:50:ASN:N	2.73	0.41
6:J:21:PHE:O	6:J:22:MET:C	2.58	0.41
6:N:20:ILE:HG22	15:N:102:CRT:C13	2.50	0.41
6:P:30:GLY:O	6:P:34:ILE:CG2	2.69	0.41
5:Q:11:ILE:HG13	5:Q:12:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:20:VAL:CG2	5:S:21:LEU:H	2.29	0.41
5:S:43:ASP:HA	5:U:56:GLN:HG3	2.00	0.41
15:V:102:CRT:C33	9:W:102:BCL:HAA1	2.50	0.41
5:1:50:ASN:HA	5:3:60:LYS:CA	2.42	0.41
6:4:42:TYR:CD1	6:4:43:ARG:HG3	2.55	0.41
5:7:7:ASN:H	5:7:7:ASN:HD22	1.65	0.41
6:8:37:LEU:O	6:8:41:LEU:HG	2.19	0.41
1:C:136:ALA:O	1:C:137:ALA:C	2.59	0.41
9:L:303:BCL:HMD2	9:M:402:BCL:HBB3	2.01	0.41
4:H:63:ASP:HA	4:H:64:PRO:HD3	1.96	0.41
4:H:113:PRO:HD2	4:H:249:TYR:OH	2.20	0.41
15:A:101:CRT:C8	5:7:11:ILE:N	2.83	0.41
9:A:102:BCL:HMB1	9:A:102:BCL:HBB3	2.00	0.41
6:B:8:GLY:O	6:B:9:LEU:HG	2.21	0.41
6:B:27:ALA:CB	5:9:4:MET:HG3	2.50	0.41
5:F:3:THR:HG22	5:F:4:MET:CE	2.51	0.41
6:G:10:THR:CG2	6:G:11:ASP:N	2.82	0.41
6:G:28:TRP:O	6:G:31:LEU:N	2.53	0.41
6:T:7:THR:OG1	6:T:8:GLY:N	2.51	0.41
9:W:102:BCL:CBC	9:X:101:BCL:HMD2	2.50	0.41
6:X:43:ARG:HB3	5:Y:55:TYR:CE2	2.55	0.41
6:2:38:LEU:HD23	6:2:38:LEU:O	2.20	0.41
6:2:45:TRP:HZ2	9:2:101:BCL:H162	1.85	0.41
6:4:27:ALA:O	6:4:31:LEU:HG	2.21	0.41
5:5:47:LEU:O	5:5:47:LEU:HD13	2.20	0.41
5:7:7:ASN:HD21	6:0:23:GLN:NE2	2.17	0.41
1:C:40:MET:HG3	1:C:252:ASN:HD22	1.85	0.41
1:C:314:VAL:CG1	1:C:319:TYR:CE1	3.03	0.41
3:M:246:GLU:O	3:M:250:LEU:HD13	2.19	0.41
14:M:405:MQ8:H411	14:M:405:MQ8:H391	1.84	0.41
4:H:35:LYS:HE3	4:H:39:TYR:CG	2.55	0.41
4:H:44:ASP:O	4:H:45:ARG:C	2.58	0.41
4:H:130:LEU:CG	4:H:131:PRO:HD2	2.50	0.41
4:H:203:ASP:O	4:H:205:LYS:N	2.54	0.41
5:A:29:ILE:CD1	5:9:27:PHE:CZ	3.03	0.41
5:F:2:PHE:N	5:F:2:PHE:HD1	2.19	0.41
5:F:50:ASN:CA	5:I:60:LYS:CB	2.99	0.41
9:I:103:BCL:OBB	9:I:103:BCL:HHC	2.20	0.41
5:S:35:ILE:CD1	15:T:102:CRT:H371	2.49	0.41
5:U:35:ILE:C	5:U:38:ILE:HG22	2.40	0.41
6:V:45:TRP:CD2	9:V:101:BCL:H2C	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:10:LYS:HD3	15:W:103:CRT:O1	2.20	0.41
6:X:17:PHE:CA	6:X:20:ILE:HG22	2.50	0.41
6:Z:36:HIS:CE1	9:Z:101:BCL:CHB	3.04	0.41
5:1:34:LEU:O	5:1:37:MET:HB3	2.20	0.41
15:2:102:CRT:H241	15:2:102:CRT:H26	1.79	0.41
5:5:51:ILE:HA	5:5:52:PRO:HA	1.69	0.41
5:7:10:LYS:H	5:7:10:LYS:CD	2.33	0.41
6:8:24:SER:O	6:8:27:ALA:N	2.54	0.41
1:C:124:LYS:O	1:C:127:SER:HB2	2.20	0.41
1:C:153:TYR:HB3	1:C:323:MET:HE3	2.03	0.41
1:C:192:TYR:CD2	2:L:270:GLU:HG3	2.54	0.41
1:C:225:SER:N	1:C:228:GLN:HE21	2.18	0.41
2:L:4:LEU:CD2	4:H:38:GLY:CA	2.91	0.41
2:L:29:PRO:HB2	3:M:257:GLY:O	2.20	0.41
2:L:89:LEU:HA	2:L:93:GLY:CA	2.31	0.41
2:L:89:LEU:CD2	5:9:37:MET:SD	3.08	0.41
2:L:126:VAL:HB	2:L:127:PRO:CD	2.51	0.41
2:L:192:ASN:ND2	3:M:213:ALA:CA	2.84	0.41
3:M:12:GLN:HB2	4:H:145:ALA:HB2	2.02	0.41
3:M:242:GLY:CA	4:H:119:ARG:NH2	2.79	0.41
5:A:46:TRP:CB	6:0:46:LEU:OXT	2.65	0.41
15:B:102:CRT:H372	9:D:102:BCL:HMB2	2.03	0.41
5:D:40:LEU:CD1	5:D:47:LEU:HD23	2.51	0.41
5:I:7:ASN:O	5:I:10:LYS:HD3	2.20	0.41
5:I:55:TYR:HD1	5:I:56:GLN:N	2.19	0.41
6:J:17:PHE:HD1	6:J:17:PHE:C	2.24	0.41
6:J:20:ILE:HG21	15:J:101:CRT:C7	2.49	0.41
5:K:50:ASN:HD22	5:K:51:ILE:HG12	1.84	0.41
6:P:21:PHE:CB	15:P:102:CRT:H14	2.49	0.41
6:P:33:VAL:HG22	6:P:37:LEU:CD2	2.51	0.41
6:V:20:ILE:HG23	6:V:21:PHE:N	2.35	0.41
5:W:3:THR:C	5:W:5:ASN:H	2.23	0.41
9:W:102:BCL:CMD	6:X:36:HIS:HD2	2.29	0.41
5:Y:8:LEU:HD21	6:2:24:SER:OG	2.20	0.41
5:Y:36:HIS:NE2	9:Z:101:BCL:CMD	2.81	0.41
15:2:102:CRT:H81	15:2:102:CRT:H10	1.74	0.41
5:3:43:ASP:OD1	5:3:43:ASP:C	2.59	0.41
6:4:25:MET:HB2	15:4:102:CRT:H19	1.91	0.41
6:4:43:ARG:HA	6:4:44:PRO:HD2	1.94	0.41
5:5:19:ARG:HA	5:5:19:ARG:NE	2.36	0.41
5:9:38:ILE:O	5:9:41:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:33:VAL:O	6:0:37:LEU:N	2.47	0.41
1:C:166:TRP:CH2	1:C:205:ASP:HB2	2.52	0.41
1:C:206:GLN:HA	1:C:206:GLN:NE2	2.35	0.41
1:C:267:THR:HG21	3:M:314:VAL:HB	2.02	0.41
2:L:18:ILE:O	2:L:34:PHE:CB	2.50	0.41
2:L:109:TRP:O	2:L:113:GLU:HG3	2.21	0.41
2:L:220:HIS:O	2:L:221:GLU:C	2.59	0.41
3:M:87:LEU:HD22	3:M:87:LEU:N	2.36	0.41
3:M:206:ILE:HG12	9:M:402:BCL:CHB	2.51	0.41
3:M:250:LEU:H	3:M:250:LEU:HD12	1.86	0.41
9:M:401:BCL:HMB1	9:M:401:BCL:HBB2	2.01	0.41
9:M:402:BCL:HMB1	9:M:402:BCL:HBB2	2.02	0.41
4:H:29:TYR:CE2	16:H:302:PGW:O01	2.74	0.41
4:H:55:VAL:CG1	4:H:56:VAL:N	2.79	0.41
9:A:102:BCL:HBB3	9:0:101:BCL:C4B	2.50	0.41
5:D:5:ASN:HD22	6:E:22:MET:HB2	1.82	0.41
5:D:9:TYR:HA	6:E:18:HIS:CG	2.55	0.41
6:E:8:GLY:O	6:E:9:LEU:HG	2.20	0.41
6:E:38:LEU:HD23	6:E:38:LEU:C	2.41	0.41
5:F:29:ILE:CG2	5:F:30:VAL:N	2.83	0.41
9:F:102:BCL:C3D	9:G:101:BCL:C3D	2.99	0.41
6:G:23:GLN:O	6:G:26:TYR:CB	2.64	0.41
9:I:102:BCL:HMB1	9:I:102:BCL:HBB2	2.03	0.41
6:J:17:PHE:C	6:J:17:PHE:CD1	2.93	0.41
6:J:38:LEU:HD23	6:J:38:LEU:C	2.41	0.41
5:K:17:PRO:HB3	6:N:17:PHE:CE2	2.55	0.41
5:K:44:LEU:HD22	5:K:44:LEU:C	2.40	0.41
5:O:9:TYR:CD1	6:P:15:LYS:HB2	2.56	0.41
5:O:44:LEU:CD1	5:O:46:TRP:N	2.83	0.41
15:P:102:CRT:H291	9:Q:102:BCL:O2A	2.21	0.41
5:Q:43:ASP:HB2	5:S:47:LEU:CB	2.47	0.41
5:S:27:PHE:CD2	5:U:29:ILE:CD1	3.04	0.41
5:U:49:ASP:O	5:W:60:LYS:HA	2.21	0.41
5:W:43:ASP:HA	5:Y:47:LEU:O	2.20	0.41
6:X:45:TRP:CZ3	9:X:101:BCL:H2C	2.56	0.41
6:2:31:LEU:O	6:2:34:ILE:HG22	2.20	0.41
6:2:41:LEU:HD23	6:2:41:LEU:C	2.39	0.41
6:2:41:LEU:HD23	6:2:42:TYR:CA	2.50	0.41
5:3:38:ILE:HG23	5:3:39:VAL:N	2.36	0.41
5:3:46:TRP:HE1	5:3:47:LEU:HD22	1.84	0.41
5:5:46:TRP:CZ2	9:5:102:BCL:HHC	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:31:LEU:O	6:6:34:ILE:HG23	2.19	0.41
5:7:40:LEU:HD11	5:7:47:LEU:CD2	2.51	0.41
9:7:102:BCL:HHC	9:7:102:BCL:OBB	2.21	0.41
6:8:32:VAL:O	6:8:35:ALA:HB3	2.20	0.41
5:9:12:TRP:NE1	6:0:17:PHE:HD2	2.19	0.41
2:L:6:PHE:CD2	3:M:246:GLU:HG3	2.56	0.41
2:L:11:ARG:HA	2:L:26:TRP:CH2	2.56	0.41
2:L:84:LEU:CD2	2:L:151:TRP:NE1	2.84	0.41
2:L:98:ILE:HD13	2:L:98:ILE:HG21	1.81	0.41
2:L:268:TRP:O	2:L:269:PRO:C	2.59	0.41
3:M:100:PRO:HG3	3:M:172:ALA:HB2	2.02	0.41
3:M:252:TRP:NE1	14:M:405:MQ8:C2	2.84	0.41
5:A:38:ILE:CD1	5:A:39:VAL:N	2.80	0.41
6:B:28:TRP:CE3	6:B:31:LEU:HD12	2.56	0.41
9:B:101:BCL:HBB3	9:D:102:BCL:C4B	2.51	0.41
5:I:50:ASN:CG	5:I:51:ILE:N	2.72	0.41
5:K:26:ALA:O	5:K:29:ILE:HG22	2.21	0.41
5:O:18:ARG:NH1	5:O:18:ARG:CB	2.82	0.41
5:O:29:ILE:HA	9:O:102:BCL:H11	2.03	0.41
6:P:21:PHE:CG	15:P:102:CRT:H16	2.56	0.41
5:S:43:ASP:HB2	5:U:47:LEU:O	2.21	0.41
5:U:45:ASN:H	5:W:56:GLN:NE2	2.19	0.41
6:V:30:GLY:C	6:V:33:VAL:HG12	2.42	0.41
5:W:30:VAL:HA	5:W:33:LEU:HD11	2.02	0.41
6:2:40:TRP:HH2	6:2:46:LEU:HG	1.85	0.41
5:5:29:ILE:HG23	5:5:30:VAL:H	1.86	0.41
5:5:52:PRO:HB2	5:5:55:TYR:OH	2.20	0.41
9:5:102:BCL:HMB1	9:5:102:BCL:HBB2	2.01	0.41
5:7:36:HIS:NE2	9:7:102:BCL:NA	2.69	0.41
9:7:102:BCL:CHD	9:7:103:BCL:HMD2	2.51	0.41
1:C:130:MET:HE2	1:C:133:LEU:HD13	2.04	0.40
1:C:159:ASN:HA	1:C:160:PRO:HD3	1.96	0.40
1:C:248:THR:HA	1:C:251:HIS:O	2.21	0.40
2:L:160:LEU:CA	2:L:163:LEU:HD13	2.48	0.40
3:M:70:ILE:O	3:M:73:PHE:HB3	2.21	0.40
3:M:201:PHE:CZ	4:H:16:ILE:HD13	2.55	0.40
4:H:6:THR:CG2	5:F:41:SER:HB3	2.50	0.40
4:H:168:SER:O	4:H:169:ASP:HB2	2.20	0.40
4:H:225:LEU:HD11	4:H:231:VAL:HA	2.03	0.40
4:H:235:GLU:O	4:H:239:VAL:N	2.54	0.40
5:A:5:ASN:OD1	5:A:6:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:14:ILE:HG22	5:F:18:ARG:HB3	1.98	0.40
9:E:101:BCL:H62	9:E:101:BCL:H41	1.90	0.40
9:E:101:BCL:HHC	9:E:101:BCL:OBB	2.19	0.40
6:G:38:LEU:HD23	6:G:38:LEU:C	2.41	0.40
5:I:42:THR:O	5:I:43:ASP:C	2.59	0.40
6:J:17:PHE:C	6:J:20:ILE:HG22	2.41	0.40
6:R:10:THR:H	6:R:13:GLU:CD	2.25	0.40
6:T:33:VAL:CG1	6:T:34:ILE:N	2.83	0.40
5:U:17:PRO:HG2	5:U:18:ARG:H	1.85	0.40
6:V:15:LYS:O	6:V:18:HIS:HB3	2.21	0.40
9:X:101:BCL:HMB1	9:X:101:BCL:HBB3	2.03	0.40
9:4:101:BCL:CMB	9:5:102:BCL:C1B	2.99	0.40
5:5:10:LYS:CE	15:8:101:CRT:H31A	2.39	0.40
5:7:4:MET:O	5:7:4:MET:HG3	2.21	0.40
1:C:274:ARG:NH2	7:C:503:HEM:O2D	2.55	0.40
2:L:98:ILE:O	2:L:101:CYS:HB2	2.21	0.40
2:L:191:THR:HG22	2:L:245:LEU:HD11	2.04	0.40
2:L:273:ASN:HD21	2:L:277:GLU:HG3	1.87	0.40
3:M:161:GLY:CA	3:M:165:PRO:HG2	2.47	0.40
3:M:175:VAL:HB	15:M:406:CRT:C24	2.41	0.40
3:M:215:LEU:HD21	14:M:405:MQ8:C18	2.51	0.40
3:M:252:TRP:HE3	3:M:256:MET:HE2	1.84	0.40
4:H:189:ASN:N	4:H:189:ASN:HD22	2.18	0.40
5:O:18:ARG:HB2	5:O:18:ARG:CZ	2.51	0.40
6:R:20:ILE:HG21	15:R:102:CRT:C6	2.51	0.40
5:U:12:TRP:HA	5:U:12:TRP:HE3	1.80	0.40
5:W:43:ASP:O	5:Y:56:GLN:NE2	2.53	0.40
1:C:305:VAL:HG12	1:C:306:SER:N	2.36	0.40
2:L:158:GLY:O	2:L:159:ILE:C	2.60	0.40
2:L:203:ILE:HD13	2:L:203:ILE:HA	1.90	0.40
3:M:17:ALA:HB1	3:M:34:PRO:CG	2.51	0.40
3:M:161:GLY:HA3	15:M:406:CRT:H292	2.03	0.40
3:M:200:PRO:HB2	4:H:16:ILE:HD11	2.02	0.40
3:M:219:HIS:O	3:M:220:GLY:C	2.57	0.40
4:H:5:ILE:HD12	5:D:38:ILE:O	2.20	0.40
5:D:7:ASN:ND2	5:D:7:ASN:N	2.68	0.40
5:D:54:SER:O	5:D:58:LEU:CB	2.69	0.40
5:I:18:ARG:HH11	5:I:18:ARG:HG3	1.85	0.40
5:K:51:ILE:CA	5:K:52:PRO:C	2.90	0.40
9:N:101:BCL:NB	9:O:102:BCL:HMB3	2.36	0.40
9:O:102:BCL:C1D	9:P:101:BCL:CMD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:24:SER:O	6:P:27:ALA:N	2.51	0.40
5:S:43:ASP:O	5:S:45:ASN:N	2.48	0.40
5:U:36:HIS:CE1	9:U:102:BCL:C1A	3.04	0.40
5:U:44:LEU:HD22	6:V:43:ARG:CD	2.49	0.40
5:W:30:VAL:HA	5:W:33:LEU:HD21	2.03	0.40
5:Y:32:GLY:HA2	9:Z:101:BCL:O1D	2.20	0.40
5:7:9:TYR:CE2	5:7:10:LYS:HE3	2.57	0.40
9:7:102:BCL:HMB1	9:7:102:BCL:HBB3	2.00	0.40
6:0:29:PHE:O	6:0:32:VAL:N	2.54	0.40
1:C:68:THR:O	1:C:86:SER:HB2	2.21	0.40
1:C:202:PRO:HG2	1:C:203:PHE:CD1	2.49	0.40
1:C:267:THR:O	1:C:270:TRP:N	2.54	0.40
2:L:23:PHE:CE1	5:9:22:VAL:HG21	2.40	0.40
2:L:55:THR:HG23	5:A:41:SER:HB2	2.03	0.40
3:M:70:ILE:CG2	3:M:71:ILE:H	2.32	0.40
15:A:101:CRT:H36	15:A:101:CRT:H341	1.30	0.40
6:G:23:GLN:HA	6:G:26:TYR:CD2	2.56	0.40
15:J:101:CRT:H26	15:J:101:CRT:H241	1.78	0.40
5:K:2:PHE:O	5:K:2:PHE:CD1	2.74	0.40
5:K:9:TYR:HA	6:N:18:HIS:CG	2.56	0.40
6:X:13:GLU:HA	6:X:16:GLU:HB3	2.03	0.40
6:X:36:HIS:CE1	9:X:101:BCL:H141	2.56	0.40
5:3:4:MET:O	5:3:8:LEU:HG	2.22	0.40
5:7:9:TYR:CD2	5:7:10:LYS:HD2	2.57	0.40
9:7:103:BCL:H2A	9:7:103:BCL:CGD	2.50	0.40
5:9:43:ASP:OD1	5:9:44:LEU:N	2.55	0.40
1:C:40:MET:SD	1:C:252:ASN:HB2	2.60	0.40
2:L:171:TYR:C	2:L:173:PHE:N	2.75	0.40
2:L:223:THR:CG2	3:M:20:GLY:HA2	2.50	0.40
2:L:276:LEU:N	2:L:276:LEU:CD2	2.85	0.40
3:M:164:ARG:NH2	3:M:189:PHE:HE1	2.19	0.40
15:M:406:CRT:H291	15:M:406:CRT:H31	1.89	0.40
15:M:406:CRT:H15	15:M:406:CRT:H131	1.96	0.40
4:H:135:PRO:HA	4:H:171:TRP:HA	2.03	0.40
6:G:46:LEU:HB3	6:J:42:TYR:HH	1.84	0.40
5:I:15:LEU:HD12	5:I:20:VAL:CG1	2.50	0.40
5:I:52:PRO:HB2	5:I:55:TYR:HE2	1.84	0.40
5:K:56:GLN:HE21	5:K:57:ALA:H	1.69	0.40
6:N:40:TRP:CD1	6:N:40:TRP:C	2.95	0.40
15:R:102:CRT:H391	5:S:36:HIS:CB	2.51	0.40
5:S:4:MET:C	5:S:6:ALA:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:17:PRO:HA	5:S:20:VAL:HG22	2.03	0.40
5:S:27:PHE:CD2	5:U:29:ILE:HD11	2.56	0.40
5:S:55:TYR:CD1	5:S:56:GLN:N	2.84	0.40
9:T:101:BCL:CMA	9:U:102:BCL:HHB	2.52	0.40
5:U:51:ILE:CB	5:U:52:PRO:CA	2.95	0.40
15:V:102:CRT:H181	15:V:102:CRT:H20	1.60	0.40
6:X:10:THR:N	6:X:13:GLU:OE1	2.53	0.40
6:Z:34:ILE:HD13	6:Z:34:ILE:O	2.21	0.40
5:3:28:GLN:O	5:3:31:LEU:HB3	2.21	0.40
5:3:43:ASP:O	5:5:56:GLN:NE2	2.55	0.40
9:4:101:BCL:HMC3	9:5:102:BCL:HBB1	2.04	0.40
5:7:49:ASP:CG	5:7:50:ASN:N	2.75	0.40
5:9:46:TRP:CE2	5:9:47:LEU:CD2	3.04	0.40
6:0:17:PHE:HA	6:0:20:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

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	C	315/404 (78%)	230 (73%)	79 (25%)	6 (2%)	8 36
2	L	278/281 (99%)	219 (79%)	51 (18%)	8 (3%)	4 24
3	M	317/325 (98%)	254 (80%)	60 (19%)	3 (1%)	17 55
4	H	256/259 (99%)	204 (80%)	43 (17%)	9 (4%)	3 20
5	1	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0 1
5	3	58/61 (95%)	38 (66%)	15 (26%)	5 (9%)	1 3
5	5	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0 1
5	7	58/61 (95%)	37 (64%)	15 (26%)	6 (10%)	0 2
5	9	58/61 (95%)	39 (67%)	13 (22%)	6 (10%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	A	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9 39
5	D	58/61 (95%)	40 (69%)	18 (31%)	0	100 100
5	F	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	I	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	K	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2 12
5	O	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9 39
5	Q	58/61 (95%)	42 (72%)	14 (24%)	2 (3%)	3 20
5	S	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	U	58/61 (95%)	34 (59%)	23 (40%)	1 (2%)	9 39
5	W	58/61 (95%)	41 (71%)	12 (21%)	5 (9%)	1 3
5	Y	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0 1
6	0	38/47 (81%)	29 (76%)	9 (24%)	0	100 100
6	2	38/47 (81%)	28 (74%)	8 (21%)	2 (5%)	2 11
6	4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	5 27
6	6	38/47 (81%)	35 (92%)	3 (8%)	0	100 100
6	8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	5 27
6	B	38/47 (81%)	33 (87%)	5 (13%)	0	100 100
6	E	38/47 (81%)	33 (87%)	5 (13%)	0	100 100
6	G	38/47 (81%)	32 (84%)	6 (16%)	0	100 100
6	J	38/47 (81%)	29 (76%)	9 (24%)	0	100 100
6	N	38/47 (81%)	33 (87%)	4 (10%)	1 (3%)	5 27
6	P	38/47 (81%)	25 (66%)	12 (32%)	1 (3%)	5 27
6	R	38/47 (81%)	31 (82%)	7 (18%)	0	100 100
6	T	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1 4
6	V	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	5 27
6	X	38/47 (81%)	32 (84%)	6 (16%)	0	100 100
6	Z	38/47 (81%)	28 (74%)	6 (16%)	4 (10%)	0 2
All	All	2702/2997 (90%)	2030 (75%)	570 (21%)	102 (4%)	3 18

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	235	ALA

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Mol	Chain	Res	Type
4	H	53	VAL
5	I	50	ASN
5	I	53	VAL
5	Q	46	TRP
5	W	4	MET
5	W	43	ASP
5	Y	27	PHE
5	Y	46	TRP
6	Z	42	TYR
6	Z	45	TRP
5	1	43	ASP
5	1	55	TYR
5	1	57	ALA
5	1	58	LEU
6	2	12	ASP
5	3	53	VAL
5	5	19	ARG
5	5	37	MET
5	7	6	ALA
5	9	17	PRO
5	9	43	ASP
5	9	53	VAL
1	C	181	THR
1	C	247	CYS
1	C	262	SER
3	M	161	GLY
4	H	204	LYS
5	A	50	ASN
5	K	49	ASP
6	N	31	LEU
5	W	46	TRP
5	W	51	ILE
5	Y	49	ASP
5	7	29	ILE
6	8	42	TYR
1	C	113	PRO
1	C	125	VAL
2	L	277	GLU
4	H	48	ARG
5	F	54	SER
5	I	5	ASN
5	Q	53	VAL

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Mol	Chain	Res	Type
5	S	37	MET
5	S	44	LEU
5	S	54	SER
6	V	42	TYR
5	Y	54	SER
5	3	49	ASP
6	4	44	PRO
5	5	5	ASN
5	5	42	THR
5	5	49	ASP
2	L	11	ARG
2	L	43	THR
2	L	114	VAL
5	K	43	ASP
5	O	46	TRP
6	T	12	ASP
6	T	42	TYR
6	T	45	TRP
5	W	52	PRO
5	Y	52	PRO
5	Y	60	LYS
5	1	5	ASN
5	1	49	ASP
5	5	50	ASN
5	7	41	SER
5	7	46	TRP
3	M	195	ASN
4	H	54	LYS
4	H	59	PRO
4	H	223	PRO
4	H	239	VAL
6	P	31	LEU
6	Z	43	ARG
6	2	45	TRP
5	3	3	THR
5	3	17	PRO
5	7	49	ASP
5	9	5	ASN
5	9	6	ALA
2	L	143	VAL
4	H	47	GLU
5	F	42	THR

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Mol	Chain	Res	Type
6	Z	44	PRO
5	1	17	PRO
5	7	47	LEU
5	K	53	VAL
5	U	17	PRO
5	Y	53	VAL
5	1	52	PRO
2	L	159	ILE
3	M	314	VAL
5	1	51	ILE
5	9	14	ILE
1	C	69	GLY
2	L	209	PRO
4	H	70	PRO
5	F	11	ILE
5	3	29	ILE
5	5	17	PRO

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	C	265/317 (84%)	245 (92%)	20 (8%)	13 43
2	L	228/229 (100%)	220 (96%)	8 (4%)	36 71
3	M	256/261 (98%)	239 (93%)	17 (7%)	16 49
4	H	210/211 (100%)	198 (94%)	12 (6%)	20 56
5	1	50/56 (89%)	47 (94%)	3 (6%)	19 53
5	3	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	5	50/56 (89%)	45 (90%)	5 (10%)	7 29
5	7	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	9	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	A	50/56 (89%)	45 (90%)	5 (10%)	7 29
5	D	50/56 (89%)	45 (90%)	5 (10%)	7 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	I	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	K	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	O	50/56 (89%)	42 (84%)	8 (16%)	2 12
5	Q	50/56 (89%)	47 (94%)	3 (6%)	19 53
5	S	50/56 (89%)	46 (92%)	4 (8%)	12 40
5	U	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	W	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	Y	50/56 (89%)	45 (90%)	5 (10%)	7 29
6	0	33/39 (85%)	23 (70%)	10 (30%)	0 1
6	2	33/39 (85%)	29 (88%)	4 (12%)	5 21
6	4	33/39 (85%)	29 (88%)	4 (12%)	5 21
6	6	33/39 (85%)	30 (91%)	3 (9%)	9 34
6	8	33/39 (85%)	26 (79%)	7 (21%)	1 5
6	B	33/39 (85%)	27 (82%)	6 (18%)	1 9
6	E	33/39 (85%)	32 (97%)	1 (3%)	41 75
6	G	33/39 (85%)	26 (79%)	7 (21%)	1 5
6	J	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	N	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	P	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	R	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	T	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	V	33/39 (85%)	27 (82%)	6 (18%)	1 9
6	X	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	Z	33/39 (85%)	29 (88%)	4 (12%)	5 21
All	All	2287/2538 (90%)	2058 (90%)	229 (10%)	7 29

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	MET
1	C	47	ARG
1	C	71	LYS

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Mol	Chain	Res	Type
1	C	131	PHE
1	C	163	LYS
1	C	178	LEU
1	C	179	LYS
1	C	180	PRO
1	C	212	ILE
1	C	225	SER
1	C	233	PHE
1	C	247	CYS
1	C	251	HIS
1	C	254	ARG
1	C	257	ASN
1	C	263	THR
1	C	265	LYS
1	C	268	THR
1	C	274	ARG
1	C	295	ARG
2	L	5	SER
2	L	71	TRP
2	L	112	ARG
2	L	118	ARG
2	L	252	TRP
2	L	256	CYS
2	L	266	ARG
2	L	281	TRP
3	M	4	TYR
3	M	14	ARG
3	M	37	SER
3	M	63	PHE
3	M	85	GLN
3	M	132	ARG
3	M	148	TRP
3	M	171	TRP
3	M	182	HIS
3	M	205	SER
3	M	216	PHE
3	M	240	HIS
3	M	246	GLU
3	M	259	ASN
3	M	260	VAL
3	M	265	ILE
3	M	315	ASN

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Mol	Chain	Res	Type
4	H	2	SER
4	H	8	TYR
4	H	29	TYR
4	H	44	ASP
4	H	48	ARG
4	H	56	VAL
4	H	125	LEU
4	H	128	GLU
4	H	140	LYS
4	H	146	GLU
4	H	176	GLU
4	H	227	ASN
5	A	8	LEU
5	A	18	ARG
5	A	36	HIS
5	A	40	LEU
5	A	51	ILE
6	B	9	LEU
6	B	20	ILE
6	B	23	GLN
6	B	32	VAL
6	B	34	ILE
6	B	40	TRP
5	D	2	PHE
5	D	7	ASN
5	D	12	TRP
5	D	29	ILE
5	D	42	THR
6	E	23	GLN
5	F	2	PHE
5	F	4	MET
5	F	7	ASN
5	F	9	TYR
5	F	12	TRP
5	F	42	THR
5	F	51	ILE
6	G	13	GLU
6	G	15	LYS
6	G	17	PHE
6	G	21	PHE
6	G	34	ILE
6	G	37	LEU

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Mol	Chain	Res	Type
6	G	38	LEU
5	I	8	LEU
5	I	9	TYR
5	I	10	LYS
5	I	38	ILE
5	I	47	LEU
5	I	55	TYR
6	J	17	PHE
6	J	21	PHE
6	J	33	VAL
6	J	34	ILE
6	J	41	LEU
5	K	9	TYR
5	K	12	TRP
5	K	18	ARG
5	K	29	ILE
5	K	37	MET
5	K	44	LEU
5	K	55	TYR
6	N	10	THR
6	N	13	GLU
6	N	29	PHE
6	N	33	VAL
6	N	34	ILE
5	O	4	MET
5	O	5	ASN
5	O	8	LEU
5	O	9	TYR
5	O	40	LEU
5	O	41	SER
5	O	47	LEU
5	O	55	TYR
6	P	21	PHE
6	P	34	ILE
6	P	37	LEU
6	P	38	LEU
6	P	41	LEU
5	Q	9	TYR
5	Q	45	ASN
5	Q	55	TYR
6	R	13	GLU
6	R	20	ILE

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Mol	Chain	Res	Type
6	R	21	PHE
6	R	34	ILE
6	R	38	LEU
5	S	9	TYR
5	S	19	ARG
5	S	44	LEU
5	S	55	TYR
6	T	15	LYS
6	T	16	GLU
6	T	20	ILE
6	T	34	ILE
6	T	40	TRP
5	U	2	PHE
5	U	9	TYR
5	U	18	ARG
5	U	33	LEU
5	U	47	LEU
5	U	55	TYR
5	U	56	GLN
6	V	13	GLU
6	V	20	ILE
6	V	21	PHE
6	V	32	VAL
6	V	38	LEU
6	V	41	LEU
5	W	7	ASN
5	W	8	LEU
5	W	9	TYR
5	W	12	TRP
5	W	16	ASP
5	W	33	LEU
5	W	37	MET
6	X	12	ASP
6	X	20	ILE
6	X	34	ILE
6	X	36	HIS
6	X	37	LEU
5	Y	2	PHE
5	Y	9	TYR
5	Y	18	ARG
5	Y	29	ILE
5	Y	55	TYR

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Mol	Chain	Res	Type
6	Z	34	ILE
6	Z	36	HIS
6	Z	37	LEU
6	Z	42	TYR
5	1	2	PHE
5	1	9	TYR
5	1	18	ARG
6	2	13	GLU
6	2	20	ILE
6	2	29	PHE
6	2	41	LEU
5	3	2	PHE
5	3	9	TYR
5	3	30	VAL
5	3	45	ASN
5	3	47	LEU
5	3	56	GLN
6	4	26	TYR
6	4	33	VAL
6	4	34	ILE
6	4	42	TYR
5	5	9	TYR
5	5	29	ILE
5	5	46	TRP
5	5	47	LEU
5	5	51	ILE
6	6	20	ILE
6	6	37	LEU
6	6	40	TRP
5	7	7	ASN
5	7	9	TYR
5	7	18	ARG
5	7	24	ILE
5	7	34	LEU
5	7	44	LEU
6	8	16	GLU
6	8	20	ILE
6	8	21	PHE
6	8	23	GLN
6	8	32	VAL
6	8	33	VAL
6	8	34	ILE

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Mol	Chain	Res	Type
5	9	2	PHE
5	9	9	TYR
5	9	12	TRP
5	9	19	ARG
5	9	44	LEU
5	9	56	GLN
6	0	9	LEU
6	0	16	GLU
6	0	20	ILE
6	0	21	PHE
6	0	23	GLN
6	0	32	VAL
6	0	33	VAL
6	0	34	ILE
6	0	36	HIS
6	0	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	ASN
1	C	80	GLN
1	C	206	GLN
1	C	228	GLN
1	C	257	ASN
1	C	261	GLN
1	C	288	ASN
2	L	96	GLN
2	L	168	ASN
2	L	172	GLN
2	L	182	HIS
2	L	192	ASN
2	L	222	ASN
2	L	273	ASN
3	M	6	ASN
3	M	27	ASN
3	M	74	ASN
3	M	89	HIS
3	M	144	GLN
3	M	195	ASN
3	M	199	ASN
3	M	237	GLN

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Mol	Chain	Res	Type
3	M	259	ASN
3	M	301	HIS
3	M	315	ASN
4	H	178	GLN
4	H	189	ASN
4	H	218	HIS
4	H	227	ASN
5	A	7	ASN
6	B	18	HIS
6	B	23	GLN
5	D	5	ASN
5	D	7	ASN
5	D	56	GLN
5	F	7	ASN
5	F	28	GLN
6	G	18	HIS
5	K	56	GLN
5	O	5	ASN
5	O	45	ASN
5	Q	5	ASN
6	T	23	GLN
5	U	5	ASN
5	U	56	GLN
5	W	7	ASN
5	W	56	GLN
6	X	18	HIS
5	Y	56	GLN
6	Z	23	GLN
5	1	56	GLN
5	3	5	ASN
5	3	56	GLN
6	4	23	GLN
5	5	5	ASN
5	5	56	GLN
5	7	7	ASN
6	8	23	GLN
5	9	5	ASN
5	9	7	ASN
5	9	45	ASN
5	9	56	GLN
6	0	23	GLN
6	0	36	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 86 ligands modelled in this entry, 18 are monoatomic - leaving 68 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	$\#\|Z\| > 2$
15	CRT	A	103	-	41,43,43	1.76	10 (24%)	50,54,54	1.63	12 (24%)
9	BCL	A	102	-	64,74,74	1.38	9 (14%)	78,115,115	2.29	20 (25%)
9	BCL	9	102	-	64,74,74	1.47	9 (14%)	78,115,115	2.29	21 (26%)
11	UQ8	L	304	-	53,53,53	1.50	4 (7%)	64,67,67	1.89	19 (29%)
9	BCL	N	101	-	64,74,74	1.48	10 (15%)	78,115,115	2.35	24 (30%)
10	BPH	L	302	-	51,70,70	0.89	3 (5%)	52,101,101	1.15	4 (7%)
15	CRT	V	102	-	41,43,43	1.79	10 (24%)	50,54,54	2.57	20 (40%)
15	CRT	2	102	-	41,43,43	1.52	10 (24%)	50,54,54	1.94	20 (40%)
10	BPH	M	403	-	51,70,70	0.99	2 (3%)	52,101,101	1.18	3 (5%)
15	CRT	4	102	-	41,43,43	1.50	9 (21%)	50,54,54	1.84	18 (36%)
9	BCL	7	103	-	64,74,74	1.48	11 (17%)	78,115,115	2.43	24 (30%)
9	BCL	D	102	-	64,74,74	1.49	11 (17%)	78,115,115	2.33	23 (29%)
9	BCL	1	102	-	64,74,74	1.49	10 (15%)	78,115,115	2.26	20 (25%)
9	BCL	4	101	-	64,74,74	1.50	12 (18%)	78,115,115	2.37	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	I	103	-	64,74,74	1.59	13 (20%)	78,115,115	2.31	25 (32%)
9	BCL	3	102	-	64,74,74	1.43	11 (17%)	78,115,115	2.34	24 (30%)
12	PO4	H	304	-	4,4,4	1.62	0	6,6,6	0.41	0
15	CRT	J	101	-	41,43,43	2.16	11 (26%)	50,54,54	2.51	20 (40%)
9	BCL	R	101	-	64,74,74	1.54	10 (15%)	78,115,115	2.37	24 (30%)
15	CRT	A	101	-	41,43,43	2.00	14 (34%)	50,54,54	3.07	21 (42%)
9	BCL	L	301	-	64,74,74	1.45	9 (14%)	78,115,115	2.39	24 (30%)
15	CRT	W	103	-	41,43,43	1.97	10 (24%)	50,54,54	2.14	17 (34%)
17	PEF	H	301	-	18,18,46	3.12	7 (38%)	21,23,51	1.96	5 (23%)
9	BCL	F	102	-	64,74,74	1.50	11 (17%)	78,115,115	2.29	21 (26%)
7	HEM	C	503	1	41,50,50	2.12	13 (31%)	45,82,82	1.54	8 (17%)
9	BCL	Z	101	-	64,74,74	1.46	12 (18%)	78,115,115	2.33	23 (29%)
9	BCL	5	102	-	64,74,74	1.51	10 (15%)	78,115,115	2.29	21 (26%)
15	CRT	M	406	-	41,43,43	1.60	7 (17%)	50,54,54	1.48	11 (22%)
12	PO4	L	305	-	4,4,4	1.67	0	6,6,6	0.43	0
15	CRT	P	102	-	41,43,43	2.56	16 (39%)	50,54,54	2.55	17 (34%)
15	CRT	8	101	-	41,43,43	1.57	7 (17%)	50,54,54	1.76	13 (26%)
9	BCL	I	102	-	64,74,74	1.50	12 (18%)	78,115,115	2.33	23 (29%)
12	PO4	M	408	-	4,4,4	1.77	1 (25%)	6,6,6	0.44	0
7	HEM	C	504	1	41,50,50	2.17	11 (26%)	45,82,82	1.59	6 (13%)
9	BCL	7	102	-	64,74,74	1.41	9 (14%)	78,115,115	2.30	21 (26%)
9	BCL	G	101	-	64,74,74	1.37	8 (12%)	78,115,115	2.37	25 (32%)
9	BCL	M	402	-	64,74,74	1.55	9 (14%)	78,115,115	2.30	22 (28%)
9	BCL	P	101	-	64,74,74	1.45	12 (18%)	78,115,115	2.32	25 (32%)
9	BCL	E	101	-	64,74,74	1.59	13 (20%)	78,115,115	2.34	26 (33%)
15	CRT	R	102	-	41,43,43	1.67	11 (26%)	50,54,54	2.64	18 (36%)
15	CRT	3	103	-	41,43,43	1.97	12 (29%)	50,54,54	1.83	13 (26%)
9	BCL	V	101	-	64,74,74	1.48	11 (17%)	78,115,115	2.31	24 (30%)
9	BCL	W	102	-	64,74,74	1.39	8 (12%)	78,115,115	2.31	21 (26%)
9	BCL	L	303	-	64,74,74	1.38	9 (14%)	78,115,115	2.33	24 (30%)
15	CRT	N	102	-	41,43,43	1.68	10 (24%)	50,54,54	2.25	14 (28%)
7	HEM	C	501	1	41,50,50	1.90	13 (31%)	45,82,82	1.68	9 (20%)
9	BCL	T	101	-	64,74,74	1.52	11 (17%)	78,115,115	2.34	24 (30%)
9	BCL	U	102	-	64,74,74	1.50	12 (18%)	78,115,115	2.30	20 (25%)
16	PGW	M	407	-	20,20,50	0.96	1 (5%)	23,26,56	1.64	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	K	102	-	64,74,74	1.46	11 (17%)	78,115,115	2.31	23 (29%)
9	BCL	B	101	-	64,74,74	1.43	10 (15%)	78,115,115	2.30	23 (29%)
9	BCL	2	101	-	64,74,74	1.52	13 (20%)	78,115,115	2.28	24 (30%)
15	CRT	T	102	-	41,43,43	1.90	9 (21%)	50,54,54	3.30	21 (42%)
9	BCL	6	101	-	64,74,74	1.46	10 (15%)	78,115,115	2.34	25 (32%)
9	BCL	O	102	-	64,74,74	1.42	10 (15%)	78,115,115	2.25	22 (28%)
16	PGW	H	302	-	20,20,50	0.95	1 (5%)	23,26,56	1.63	4 (17%)
9	BCL	S	102	-	64,74,74	1.50	14 (21%)	78,115,115	2.24	21 (26%)
15	CRT	X	102	-	41,43,43	2.93	13 (31%)	50,54,54	2.48	16 (32%)
9	BCL	0	101	-	64,74,74	1.40	12 (18%)	78,115,115	2.37	26 (33%)
9	BCL	M	401	-	64,74,74	1.57	11 (17%)	78,115,115	2.26	23 (29%)
12	PO4	H	303	-	4,4,4	1.68	0	6,6,6	0.43	0
15	CRT	G	102	-	41,43,43	1.44	8 (19%)	50,54,54	1.68	15 (30%)
9	BCL	Y	102	-	64,74,74	1.46	13 (20%)	78,115,115	2.25	21 (26%)
14	MQ8	M	405	-	54,54,54	0.91	2 (3%)	66,69,69	1.67	16 (24%)
7	HEM	C	502	1	41,50,50	2.10	12 (29%)	45,82,82	1.64	9 (20%)
9	BCL	X	101	-	64,74,74	1.54	13 (20%)	78,115,115	2.38	25 (32%)
15	CRT	B	102	-	41,43,43	1.50	6 (14%)	50,54,54	2.42	20 (40%)
9	BCL	Q	102	-	64,74,74	1.49	13 (20%)	78,115,115	2.30	20 (25%)

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
15	CRT	A	103	-	-	1/51/51/51	-
9	BCL	A	102	-	-	16/37/137/137	-
9	BCL	9	102	-	-	16/37/137/137	-
11	UQ8	L	304	-	-	6/51/75/75	0/1/1/1
9	BCL	N	101	-	-	11/37/137/137	-
10	BPH	L	302	-	-	15/37/105/105	0/5/6/6
15	CRT	V	102	-	-	7/51/51/51	-
15	CRT	2	102	-	-	2/51/51/51	-
10	BPH	M	403	-	-	12/37/105/105	0/5/6/6
15	CRT	4	102	-	-	2/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	7	103	-	-	10/37/137/137	-
9	BCL	D	102	-	-	19/37/137/137	-
9	BCL	1	102	-	-	15/37/137/137	-
9	BCL	4	101	-	-	11/37/137/137	-
9	BCL	I	103	-	-	12/37/137/137	-
9	BCL	3	102	-	-	18/37/137/137	-
15	CRT	J	101	-	-	2/51/51/51	-
17	PEF	H	301	-	-	16/20/20/50	-
9	BCL	R	101	-	-	14/37/137/137	-
15	CRT	A	101	-	-	2/51/51/51	-
9	BCL	L	301	-	-	13/37/137/137	-
15	CRT	W	103	-	-	1/51/51/51	-
9	BCL	F	102	-	-	21/37/137/137	-
7	HEM	C	503	1	-	6/12/54/54	-
9	BCL	Z	101	-	-	12/37/137/137	-
9	BCL	5	102	-	-	21/37/137/137	-
15	CRT	M	406	-	-	0/51/51/51	-
15	CRT	P	102	-	-	2/51/51/51	-
15	CRT	8	101	-	-	2/51/51/51	-
9	BCL	I	102	-	-	19/37/137/137	-
7	HEM	C	504	1	-	6/12/54/54	-
9	BCL	7	102	-	-	15/37/137/137	-
9	BCL	G	101	-	-	8/37/137/137	-
9	BCL	M	402	-	-	15/37/137/137	-
9	BCL	P	101	-	-	12/37/137/137	-
9	BCL	E	101	-	-	8/37/137/137	-
15	CRT	R	102	-	-	2/51/51/51	-
15	CRT	3	103	-	-	2/51/51/51	-
9	BCL	V	101	-	-	17/37/137/137	-
9	BCL	W	102	-	-	22/37/137/137	-
9	BCL	L	303	-	-	9/37/137/137	-
15	CRT	N	102	-	-	2/51/51/51	-
7	HEM	C	501	1	-	7/12/54/54	-
9	BCL	T	101	-	-	12/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	U	102	-	-	15/37/137/137	-
16	PGW	M	407	-	-	11/23/23/55	-
9	BCL	K	102	-	-	17/37/137/137	-
9	BCL	B	101	-	-	15/37/137/137	-
9	BCL	2	101	-	-	14/37/137/137	-
15	CRT	T	102	-	-	5/51/51/51	-
9	BCL	6	101	-	-	19/37/137/137	-
9	BCL	O	102	-	-	21/37/137/137	-
16	PGW	H	302	-	-	10/23/23/55	-
9	BCL	S	102	-	-	20/37/137/137	-
15	CRT	X	102	-	-	2/51/51/51	-
9	BCL	0	101	-	-	16/37/137/137	-
9	BCL	M	401	-	-	19/37/137/137	-
15	CRT	G	102	-	-	1/51/51/51	-
9	BCL	Y	102	-	-	14/37/137/137	-
14	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
7	HEM	C	502	1	-	7/12/54/54	-
9	BCL	X	101	-	-	13/37/137/137	-
15	CRT	B	102	-	-	4/51/51/51	-
9	BCL	Q	102	-	-	21/37/137/137	-

All (635) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	HEM	C3C-CAC	-7.90	1.31	1.47
11	L	304	UQ8	C43-C44	7.79	1.54	1.32
15	X	102	CRT	C14-C12	7.74	1.46	1.35
15	X	102	CRT	C4-C5	7.26	1.61	1.50
17	H	301	PEF	O4-C10	7.19	1.47	1.20
15	P	102	CRT	C19-C17	7.17	1.45	1.35
7	C	502	HEM	C3C-CAC	-7.06	1.33	1.47
15	J	101	CRT	C22-C23	6.92	1.45	1.35
7	C	504	HEM	C3C-CAC	-6.91	1.33	1.47
15	X	102	CRT	C22-C23	6.23	1.44	1.35
9	M	402	BCL	O2D-CGD	6.10	1.48	1.33
17	H	301	PEF	O2-C10	6.03	1.48	1.35
15	P	102	CRT	C14-C12	5.97	1.43	1.35
15	X	102	CRT	C19-C17	5.97	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	102	CRT	C14-C12	5.83	1.43	1.35
15	X	102	CRT	C9-C7	5.71	1.43	1.35
9	X	101	BCL	O2D-CGD	5.59	1.46	1.33
15	J	101	CRT	C15-C16	5.56	1.48	1.34
7	C	501	HEM	C3C-CAC	-5.54	1.36	1.47
17	H	301	PEF	P-O1P	5.43	1.70	1.50
15	T	102	CRT	C4-C5	-5.42	1.41	1.50
9	B	101	BCL	O2D-CGD	5.41	1.46	1.33
9	4	101	BCL	O2D-CGD	5.40	1.46	1.33
9	T	101	BCL	O2D-CGD	5.33	1.46	1.33
9	P	101	BCL	O2D-CGD	5.32	1.46	1.33
17	H	301	PEF	O5-C30	5.29	1.40	1.20
9	N	101	BCL	O2D-CGD	5.24	1.46	1.33
15	W	103	CRT	C19-C17	5.22	1.42	1.35
9	E	101	BCL	O2D-CGD	5.19	1.45	1.33
9	R	101	BCL	O2D-CGD	5.19	1.45	1.33
9	V	101	BCL	O2D-CGD	5.19	1.45	1.33
9	0	101	BCL	O2D-CGD	5.18	1.45	1.33
9	G	101	BCL	O2D-CGD	5.17	1.45	1.33
9	O	102	BCL	O2D-CGD	5.13	1.45	1.33
9	Z	101	BCL	O2D-CGD	5.12	1.45	1.33
9	S	102	BCL	O2D-CGD	5.10	1.45	1.33
9	9	102	BCL	O2D-CGD	5.09	1.45	1.33
9	F	102	BCL	O2D-CGD	5.06	1.45	1.33
9	I	102	BCL	O2D-CGD	5.05	1.45	1.33
11	L	304	UQ8	C41-C42	-5.04	1.36	1.53
15	X	102	CRT	C27-C28	5.03	1.42	1.35
9	L	301	BCL	O2D-CGD	4.99	1.45	1.33
7	C	502	HEM	C1B-NB	-4.98	1.31	1.40
9	6	101	BCL	O2D-CGD	4.96	1.45	1.33
9	3	102	BCL	O2D-CGD	4.93	1.45	1.33
7	C	504	HEM	C1B-NB	-4.92	1.31	1.40
9	U	102	BCL	O2D-CGD	4.90	1.45	1.33
9	I	103	BCL	O2D-CGD	4.83	1.45	1.33
15	P	102	CRT	C27-C28	4.81	1.42	1.35
9	7	103	BCL	O2D-CGD	4.80	1.44	1.33
9	F	102	BCL	C1B-NB	4.78	1.39	1.35
9	Q	102	BCL	O2D-CGD	4.77	1.44	1.33
15	W	103	CRT	C18-C17	-4.77	1.41	1.50
9	1	102	BCL	O2D-CGD	4.75	1.44	1.33
9	K	102	BCL	O2D-CGD	4.74	1.44	1.33
9	D	102	BCL	O2D-CGD	4.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	401	BCL	O2D-CGD	4.71	1.44	1.33
9	A	102	BCL	O2D-CGD	4.69	1.44	1.33
9	Y	102	BCL	O2D-CGD	4.68	1.44	1.33
9	5	102	BCL	O2D-CGD	4.66	1.44	1.33
9	7	102	BCL	O2D-CGD	4.66	1.44	1.33
9	M	402	BCL	C1B-NB	4.63	1.39	1.35
15	W	103	CRT	C16-C17	-4.62	1.36	1.45
9	2	101	BCL	O2D-CGD	4.62	1.44	1.33
15	P	102	CRT	C15-C16	4.60	1.46	1.34
9	D	102	BCL	C1B-NB	4.54	1.39	1.35
15	A	103	CRT	C27-C28	4.53	1.41	1.35
9	W	102	BCL	O2D-CGD	4.52	1.44	1.33
15	3	103	CRT	C18-C17	-4.52	1.41	1.50
7	C	501	HEM	C1B-NB	-4.50	1.32	1.40
9	S	102	BCL	C1B-NB	4.49	1.39	1.35
15	P	102	CRT	C37-C36	4.48	1.57	1.50
9	L	303	BCL	O2D-CGD	4.48	1.44	1.33
9	N	101	BCL	C1B-NB	4.46	1.39	1.35
15	3	103	CRT	C22-C23	4.43	1.41	1.35
15	A	101	CRT	C32-C33	4.41	1.41	1.35
9	E	101	BCL	O2A-CGA	4.34	1.46	1.33
9	Q	102	BCL	C1B-NB	4.32	1.39	1.35
15	3	103	CRT	C19-C17	4.29	1.41	1.35
15	3	103	CRT	C27-C28	4.29	1.41	1.35
9	M	401	BCL	C1B-NB	4.24	1.39	1.35
9	7	103	BCL	O2A-CGA	4.23	1.45	1.33
9	0	101	BCL	O2A-CGA	4.19	1.45	1.33
15	X	102	CRT	C10-C11	4.18	1.45	1.34
7	C	504	HEM	C1D-C2D	4.17	1.52	1.44
7	C	503	HEM	C1D-C2D	4.16	1.52	1.44
9	R	101	BCL	MG-NA	-4.12	1.96	2.06
15	A	103	CRT	C22-C23	4.10	1.41	1.35
9	2	101	BCL	MG-NA	-4.09	1.96	2.06
9	M	402	BCL	O2A-CGA	4.09	1.45	1.33
9	T	101	BCL	O2A-CGA	4.06	1.45	1.33
15	A	101	CRT	O2-C2M	4.06	1.56	1.43
9	K	102	BCL	O2A-CGA	4.05	1.45	1.33
9	V	101	BCL	C1B-NB	4.04	1.38	1.35
9	I	103	BCL	O2A-CGA	4.02	1.45	1.33
15	T	102	CRT	C22-C23	4.01	1.41	1.35
15	X	102	CRT	C15-C16	3.99	1.44	1.34
9	L	301	BCL	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	103	CRT	C22-C23	3.97	1.41	1.35
9	F	102	BCL	O2A-CGA	3.97	1.44	1.33
9	I	103	BCL	C1B-NB	3.95	1.38	1.35
9	T	101	BCL	C1B-NB	3.94	1.38	1.35
9	9	102	BCL	C1B-NB	3.93	1.38	1.35
9	E	101	BCL	C5-C3	3.93	1.59	1.51
9	6	101	BCL	O2A-CGA	3.92	1.44	1.33
9	2	101	BCL	O2A-CGA	3.92	1.44	1.33
9	Z	101	BCL	O2A-CGA	3.90	1.44	1.33
15	P	102	CRT	C32-C33	3.90	1.41	1.35
9	7	102	BCL	O2A-CGA	3.87	1.44	1.33
9	P	101	BCL	O2A-CGA	3.87	1.44	1.33
9	I	102	BCL	O2A-CGA	3.86	1.44	1.33
9	3	102	BCL	O2A-CGA	3.86	1.44	1.33
15	J	101	CRT	C14-C12	3.85	1.40	1.35
9	1	102	BCL	O2A-CGA	3.84	1.44	1.33
15	V	102	CRT	C30-C28	-3.84	1.37	1.45
9	1	102	BCL	C1B-NB	3.83	1.38	1.35
9	5	102	BCL	O2A-CGA	3.82	1.44	1.33
9	V	101	BCL	O2A-CGA	3.82	1.44	1.33
9	N	101	BCL	O2A-CGA	3.81	1.44	1.33
9	X	101	BCL	C1B-NB	3.80	1.38	1.35
15	3	103	CRT	C16-C17	-3.79	1.37	1.45
9	L	303	BCL	O2A-CGA	3.78	1.44	1.33
9	B	101	BCL	O2A-CGA	3.77	1.44	1.33
15	P	102	CRT	C22-C23	3.76	1.40	1.35
9	U	102	BCL	MG-NA	3.75	2.15	2.06
9	5	102	BCL	MG-NA	-3.75	1.97	2.06
15	J	101	CRT	C19-C17	3.75	1.40	1.35
9	R	101	BCL	O2A-CGA	3.75	1.44	1.33
15	A	103	CRT	C19-C17	3.74	1.40	1.35
9	S	102	BCL	O2A-CGA	3.74	1.44	1.33
9	Y	102	BCL	O2A-CGA	3.73	1.44	1.33
9	O	102	BCL	O2A-CGA	3.73	1.44	1.33
15	2	102	CRT	C22-C23	3.72	1.40	1.35
9	U	102	BCL	O2A-CGA	3.71	1.44	1.33
9	5	102	BCL	C1B-NB	3.69	1.38	1.35
9	W	102	BCL	O2A-CGA	3.69	1.44	1.33
9	Q	102	BCL	O2A-CGA	3.69	1.44	1.33
9	L	301	BCL	C1B-NB	3.69	1.38	1.35
9	I	103	BCL	MG-NA	-3.69	1.97	2.06
15	N	102	CRT	C22-C23	3.68	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	102	BCL	O2A-CGA	3.68	1.44	1.33
9	M	401	BCL	O2A-CGA	3.67	1.44	1.33
15	A	101	CRT	C37-C36	3.67	1.56	1.50
9	L	301	BCL	C4B-NB	3.65	1.38	1.35
9	4	101	BCL	O2A-CGA	3.65	1.44	1.33
15	T	102	CRT	C16-C17	-3.65	1.38	1.45
9	X	101	BCL	O2A-CGA	3.64	1.44	1.33
9	D	102	BCL	O2A-CGA	3.63	1.43	1.33
9	I	102	BCL	C1B-NB	3.62	1.38	1.35
15	T	102	CRT	C27-C28	3.62	1.40	1.35
7	C	504	HEM	C4A-CHB	-3.62	1.30	1.41
15	X	102	CRT	C32-C33	3.61	1.40	1.35
9	A	102	BCL	O2A-CGA	3.60	1.43	1.33
15	P	102	CRT	C21-C20	3.60	1.45	1.36
9	G	101	BCL	O2A-CGA	3.60	1.43	1.33
7	C	502	HEM	C1D-C2D	3.60	1.51	1.44
15	N	102	CRT	C19-C17	3.57	1.40	1.35
9	M	401	BCL	C5-C3	3.54	1.58	1.51
9	4	101	BCL	MG-NA	-3.54	1.97	2.06
16	M	407	PGW	C01-C02	3.53	1.61	1.50
16	H	302	PGW	C01-C02	3.51	1.61	1.50
15	B	102	CRT	C22-C23	3.50	1.40	1.35
9	U	102	BCL	C1B-NB	3.49	1.38	1.35
15	X	102	CRT	C6-C5	3.48	1.41	1.32
15	X	102	CRT	C26-C25	3.47	1.43	1.34
9	M	401	BCL	MG-NA	3.47	2.14	2.06
15	8	101	CRT	C22-C23	3.46	1.40	1.35
15	8	101	CRT	C27-C28	3.43	1.40	1.35
15	A	101	CRT	C14-C12	3.42	1.40	1.35
9	T	101	BCL	C2C-C3C	-3.37	1.45	1.54
9	I	103	BCL	MG-NC	3.37	2.14	2.06
15	V	102	CRT	C15-C16	3.36	1.43	1.34
9	4	101	BCL	MG-NC	3.36	2.14	2.06
9	I	102	BCL	CAA-C2A	3.34	1.60	1.54
7	C	504	HEM	CMB-C2B	-3.34	1.43	1.50
15	J	101	CRT	C27-C28	3.34	1.40	1.35
9	D	102	BCL	C4B-NB	3.33	1.38	1.35
15	8	101	CRT	O1-C1M	-3.32	1.32	1.43
7	C	502	HEM	O2A-CGA	-3.32	1.19	1.30
15	M	406	CRT	C19-C17	3.30	1.40	1.35
9	E	101	BCL	MG-NA	-3.29	1.98	2.06
9	O	102	BCL	C1B-NB	3.29	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	BPH	C3A-C2A	-3.29	1.51	1.54
9	B	101	BCL	C1B-NB	3.27	1.38	1.35
9	A	102	BCL	C1B-NB	3.27	1.38	1.35
7	C	504	HEM	O2A-CGA	-3.27	1.19	1.30
15	M	406	CRT	C22-C23	3.26	1.40	1.35
9	0	101	BCL	C2-C3	3.25	1.40	1.33
9	1	102	BCL	MG-NC	3.25	2.14	2.06
9	7	102	BCL	MG-NC	3.25	2.14	2.06
15	A	101	CRT	C19-C17	3.24	1.40	1.35
9	7	103	BCL	C5-C3	3.21	1.58	1.51
15	T	102	CRT	C19-C17	3.20	1.40	1.35
9	X	101	BCL	C4B-NB	3.20	1.38	1.35
15	V	102	CRT	C25-C23	-3.20	1.39	1.45
9	W	102	BCL	C3B-C2B	-3.20	1.33	1.39
15	A	101	CRT	C4-C5	3.19	1.55	1.50
15	R	102	CRT	C19-C17	3.16	1.40	1.35
7	C	501	HEM	C2C-C1C	3.15	1.49	1.42
9	7	102	BCL	C1B-NB	3.15	1.38	1.35
15	R	102	CRT	C9-C7	-3.15	1.31	1.35
9	O	102	BCL	C3B-C2B	-3.12	1.33	1.39
9	6	101	BCL	MG-NC	3.12	2.13	2.06
15	A	101	CRT	C22-C23	3.12	1.39	1.35
15	N	102	CRT	C11-C12	-3.12	1.39	1.45
9	E	101	BCL	MG-NC	3.07	2.13	2.06
15	M	406	CRT	C14-C12	3.06	1.39	1.35
7	C	503	HEM	C3B-C2B	3.06	1.43	1.37
9	9	102	BCL	MG-NC	3.05	2.13	2.06
9	Z	101	BCL	C3B-C2B	-3.05	1.34	1.39
17	H	301	PEF	P-O2P	3.05	1.69	1.55
15	W	103	CRT	C11-C12	-3.04	1.39	1.45
9	R	101	BCL	MG-NC	3.04	2.13	2.06
9	K	102	BCL	C1B-NB	3.03	1.37	1.35
9	6	101	BCL	C1B-NB	3.02	1.37	1.35
15	N	102	CRT	C16-C17	-2.99	1.39	1.45
9	R	101	BCL	C3B-C2B	-2.98	1.34	1.39
9	N	101	BCL	C4B-NB	2.98	1.37	1.35
9	P	101	BCL	MG-NC	2.98	2.13	2.06
7	C	504	HEM	C4D-C3D	2.97	1.50	1.45
15	T	102	CRT	C3-C1	2.97	1.59	1.52
9	T	101	BCL	MG-NC	2.97	2.13	2.06
9	X	101	BCL	MG-NC	2.97	2.13	2.06
10	M	403	BPH	C3D-C2D	-2.97	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	102	BCL	MG-NC	2.96	2.13	2.06
7	C	501	HEM	O2A-CGA	-2.96	1.20	1.30
7	C	501	HEM	C1A-NA	2.95	1.42	1.36
15	G	102	CRT	C16-C17	-2.95	1.39	1.45
9	4	101	BCL	C2C-C3C	-2.94	1.46	1.54
15	M	406	CRT	C27-C28	2.94	1.39	1.35
9	E	101	BCL	C2-C3	2.94	1.40	1.33
9	K	102	BCL	MG-NC	2.93	2.13	2.06
9	D	102	BCL	MG-NA	2.93	2.13	2.06
7	C	503	HEM	C1B-NB	-2.93	1.35	1.40
7	C	503	HEM	O2A-CGA	-2.93	1.20	1.30
9	I	103	BCL	C2-C3	2.93	1.40	1.33
15	P	102	CRT	C10-C11	2.93	1.42	1.34
15	J	101	CRT	C18-C17	-2.92	1.44	1.50
15	W	103	CRT	C27-C28	2.92	1.39	1.35
9	9	102	BCL	C2C-C3C	-2.91	1.46	1.54
15	8	101	CRT	C14-C12	2.91	1.39	1.35
7	C	502	HEM	C4D-ND	-2.90	1.35	1.40
9	7	103	BCL	C2-C3	2.90	1.39	1.33
9	K	102	BCL	CAA-C2A	2.90	1.59	1.54
9	2	101	BCL	MG-NC	2.90	2.13	2.06
15	A	103	CRT	C16-C17	-2.90	1.39	1.45
15	G	102	CRT	C4-C5	2.89	1.54	1.50
9	M	402	BCL	C4D-ND	-2.88	1.33	1.37
10	L	302	BPH	C3D-C2D	-2.88	1.34	1.39
9	S	102	BCL	C4B-NB	2.87	1.37	1.35
9	5	102	BCL	C4D-ND	-2.87	1.33	1.37
15	B	102	CRT	C30-C28	-2.87	1.39	1.45
15	2	102	CRT	C11-C12	-2.87	1.39	1.45
15	G	102	CRT	C25-C23	-2.87	1.39	1.45
9	2	101	BCL	O2D-CED	-2.85	1.38	1.45
9	M	402	BCL	C2C-C3C	-2.84	1.46	1.54
15	B	102	CRT	C25-C23	-2.84	1.39	1.45
9	K	102	BCL	C2-C3	2.84	1.39	1.33
9	M	401	BCL	C20-C18	-2.83	1.36	1.51
9	3	102	BCL	C4B-NB	2.83	1.37	1.35
9	2	101	BCL	C2-C3	2.83	1.39	1.33
9	Y	102	BCL	C4B-NB	2.83	1.37	1.35
15	A	103	CRT	C4-C5	2.82	1.54	1.50
15	P	102	CRT	C29-C28	2.81	1.56	1.50
7	C	503	HEM	CBA-CGA	2.81	1.57	1.50
15	4	102	CRT	C19-C17	2.81	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	102	CRT	C25-C23	-2.81	1.39	1.45
15	R	102	CRT	C8-C7	2.80	1.56	1.50
9	V	101	BCL	C2-C3	2.79	1.39	1.33
14	M	405	MQ8	C10-C5	2.79	1.45	1.40
9	L	301	BCL	C2C-C3C	-2.79	1.46	1.54
9	Z	101	BCL	C2C-C3C	-2.79	1.46	1.54
9	7	103	BCL	C2C-C3C	-2.78	1.46	1.54
9	U	102	BCL	C3B-C2B	-2.78	1.34	1.39
9	G	101	BCL	MG-NC	2.78	2.12	2.06
9	F	102	BCL	MG-NC	2.78	2.12	2.06
9	6	101	BCL	C2-C3	2.78	1.39	1.33
15	4	102	CRT	C4-C5	2.77	1.54	1.50
15	R	102	CRT	C11-C12	-2.77	1.40	1.45
15	3	103	CRT	C11-C12	-2.76	1.40	1.45
15	8	101	CRT	C19-C17	2.75	1.39	1.35
9	Y	102	BCL	C1B-NB	2.75	1.37	1.35
9	Z	101	BCL	C2-C3	2.74	1.39	1.33
15	2	102	CRT	C27-C28	2.74	1.39	1.35
9	P	101	BCL	C2-C3	2.74	1.39	1.33
9	P	101	BCL	C1B-NB	2.73	1.37	1.35
9	R	101	BCL	C2-C3	2.73	1.39	1.33
15	4	102	CRT	C16-C17	-2.73	1.40	1.45
7	C	501	HEM	C3B-C2B	2.73	1.42	1.37
9	7	103	BCL	MG-NA	2.73	2.12	2.06
9	G	101	BCL	C2-C3	2.73	1.39	1.33
15	J	101	CRT	C4-C5	2.72	1.54	1.50
9	R	101	BCL	C2C-C3C	-2.72	1.46	1.54
9	S	102	BCL	C3B-C2B	-2.72	1.34	1.39
9	L	303	BCL	C1B-NB	2.72	1.37	1.35
9	E	101	BCL	C4B-NB	2.72	1.37	1.35
9	I	102	BCL	C2C-C3C	-2.72	1.46	1.54
15	G	102	CRT	C30-C28	-2.71	1.40	1.45
9	L	303	BCL	C2C-C3C	-2.71	1.46	1.54
9	Z	101	BCL	MG-NC	2.71	2.12	2.06
15	2	102	CRT	C16-C17	-2.69	1.40	1.45
9	X	101	BCL	C2C-C3C	-2.69	1.46	1.54
15	A	101	CRT	C35-C33	2.68	1.51	1.45
9	Q	102	BCL	MG-NA	2.68	2.12	2.06
7	C	502	HEM	CHB-C1B	2.68	1.41	1.35
9	6	101	BCL	MG-NA	-2.68	1.99	2.06
9	L	303	BCL	C3C-C4C	-2.68	1.48	1.51
15	A	103	CRT	C11-C12	-2.67	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	HEM	CHB-C1B	2.66	1.41	1.35
15	J	101	CRT	C11-C12	-2.65	1.40	1.45
9	7	103	BCL	C3B-C2B	-2.65	1.34	1.39
9	E	101	BCL	C2C-C3C	-2.64	1.47	1.54
9	N	101	BCL	C2C-C3C	-2.64	1.47	1.54
9	G	101	BCL	C2C-C3C	-2.64	1.47	1.54
9	S	102	BCL	C2-C3	2.64	1.39	1.33
9	I	102	BCL	C2-C3	2.64	1.39	1.33
9	L	301	BCL	MG-NC	2.63	2.12	2.06
15	T	102	CRT	C39-C38	-2.62	1.46	1.52
15	P	102	CRT	C4-C5	2.62	1.54	1.50
9	T	101	BCL	C2-C3	2.62	1.39	1.33
7	C	502	HEM	C3B-C4B	-2.62	1.39	1.44
9	B	101	BCL	MG-NC	2.62	2.12	2.06
9	3	102	BCL	CAA-C2A	2.62	1.59	1.54
9	Z	101	BCL	MG-NA	-2.62	2.00	2.06
15	4	102	CRT	C25-C23	-2.61	1.40	1.45
15	N	102	CRT	C9-C7	2.61	1.39	1.35
9	7	103	BCL	C1B-NB	2.61	1.37	1.35
9	N	101	BCL	C2-C3	2.61	1.39	1.33
9	B	101	BCL	C4B-NB	2.61	1.37	1.35
9	Q	102	BCL	C3B-C2B	-2.60	1.34	1.39
9	V	101	BCL	MG-NC	2.60	2.12	2.06
9	7	102	BCL	C4B-NB	2.59	1.37	1.35
7	C	503	HEM	CAA-C2A	2.59	1.55	1.52
9	Y	102	BCL	C3B-C2B	-2.59	1.34	1.39
15	W	103	CRT	C32-C33	2.59	1.39	1.35
15	R	102	CRT	C16-C17	-2.59	1.40	1.45
15	N	102	CRT	C27-C28	2.58	1.39	1.35
7	C	501	HEM	C4D-ND	-2.58	1.35	1.40
9	F	102	BCL	C2-C3	2.58	1.39	1.33
9	U	102	BCL	MG-NC	2.58	2.12	2.06
9	1	102	BCL	C2-C3	2.57	1.39	1.33
9	W	102	BCL	C2C-C3C	-2.57	1.47	1.54
9	M	402	BCL	CMA-C3A	2.57	1.58	1.53
7	C	501	HEM	C1D-C2D	2.57	1.49	1.44
15	W	103	CRT	C37-C36	2.56	1.54	1.50
10	L	302	BPH	C3A-C2A	-2.56	1.52	1.54
9	F	102	BCL	C2C-C3C	-2.56	1.47	1.54
7	C	503	HEM	C4A-CHB	-2.56	1.33	1.41
7	C	501	HEM	C1D-ND	-2.56	1.33	1.38
9	2	101	BCL	C2C-C3C	-2.56	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	102	BCL	C2-C3	2.55	1.39	1.33
9	K	102	BCL	C3B-C2B	-2.55	1.34	1.39
9	B	101	BCL	C2-C3	2.55	1.39	1.33
9	W	102	BCL	C2-C3	2.55	1.39	1.33
9	Q	102	BCL	C2-C3	2.55	1.39	1.33
15	X	102	CRT	C21-C20	2.54	1.42	1.36
15	B	102	CRT	C4-C5	2.54	1.54	1.50
15	3	103	CRT	C26-C25	2.54	1.41	1.34
9	I	103	BCL	C3B-C2B	-2.54	1.34	1.39
15	P	102	CRT	C31-C30	2.53	1.41	1.34
15	8	101	CRT	C11-C12	-2.53	1.40	1.45
9	X	101	BCL	C2-C3	2.53	1.39	1.33
9	S	102	BCL	C2C-C3C	-2.53	1.47	1.54
17	H	301	PEF	O3-C30	2.53	1.45	1.33
9	V	101	BCL	C2C-C3C	-2.53	1.47	1.54
9	A	102	BCL	C2C-C3C	-2.53	1.47	1.54
9	1	102	BCL	C2C-C3C	-2.52	1.47	1.54
9	0	101	BCL	C4B-NB	2.52	1.37	1.35
9	L	303	BCL	C4B-NB	2.51	1.37	1.35
9	O	102	BCL	C4B-NB	2.51	1.37	1.35
9	7	102	BCL	C2-C3	2.51	1.39	1.33
9	6	101	BCL	C4B-NB	2.51	1.37	1.35
9	7	103	BCL	MG-NC	2.51	2.12	2.06
9	Q	102	BCL	C4B-NB	2.50	1.37	1.35
7	C	504	HEM	C2C-C1C	2.50	1.48	1.42
15	A	101	CRT	O1-C1M	2.50	1.51	1.43
9	4	101	BCL	C3B-C2B	-2.50	1.34	1.39
9	D	102	BCL	C3B-C2B	-2.50	1.34	1.39
9	L	301	BCL	O2D-CED	-2.50	1.39	1.45
9	5	102	BCL	C2-C3	2.50	1.39	1.33
9	I	102	BCL	MG-NC	2.50	2.12	2.06
15	T	102	CRT	C11-C12	-2.49	1.40	1.45
9	Q	102	BCL	C2C-C3C	-2.49	1.47	1.54
9	7	102	BCL	C2C-C3C	-2.49	1.47	1.54
9	N	101	BCL	O2D-CED	-2.49	1.39	1.45
15	P	102	CRT	C16-C17	2.49	1.51	1.45
15	N	102	CRT	C25-C23	-2.49	1.40	1.45
9	I	103	BCL	O2D-CED	-2.48	1.39	1.45
7	C	504	HEM	C3B-C2B	2.48	1.42	1.37
15	N	102	CRT	C30-C28	-2.48	1.40	1.45
9	3	102	BCL	MG-NC	2.47	2.12	2.06
9	R	101	BCL	O2D-CED	-2.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	102	BCL	C2C-C3C	-2.47	1.47	1.54
9	N	101	BCL	MG-NC	2.47	2.12	2.06
9	U	102	BCL	C4B-NB	2.47	1.37	1.35
9	D	102	BCL	MG-NC	2.46	2.12	2.06
9	3	102	BCL	C2-C3	2.46	1.38	1.33
15	A	101	CRT	C13-C12	2.46	1.56	1.50
9	0	101	BCL	C5-C3	2.46	1.56	1.51
15	3	103	CRT	C4-C5	2.45	1.54	1.50
9	Z	101	BCL	O2D-CED	-2.45	1.39	1.45
9	5	102	BCL	C2C-C3C	-2.45	1.47	1.54
15	V	102	CRT	C4-C5	2.44	1.54	1.50
9	K	102	BCL	C2C-C3C	-2.44	1.47	1.54
9	5	102	BCL	C3B-C2B	-2.44	1.35	1.39
9	Y	102	BCL	C4D-ND	-2.44	1.34	1.37
9	6	101	BCL	C2C-C3C	-2.44	1.47	1.54
15	4	102	CRT	O1-C1M	-2.43	1.35	1.43
15	R	102	CRT	C30-C28	-2.43	1.40	1.45
9	1	102	BCL	C3B-C2B	-2.43	1.35	1.39
9	T	101	BCL	C3B-C2B	-2.43	1.35	1.39
9	U	102	BCL	C2-C3	2.43	1.38	1.33
15	W	103	CRT	C15-C16	2.43	1.40	1.34
15	M	406	CRT	C4-C5	2.42	1.54	1.50
9	W	102	BCL	C1B-NB	2.42	1.37	1.35
7	C	502	HEM	C4A-CHB	-2.42	1.34	1.41
15	A	101	CRT	C26-C27	-2.42	1.35	1.43
9	U	102	BCL	C2C-C3C	-2.42	1.47	1.54
9	O	102	BCL	O2D-CED	-2.42	1.39	1.45
15	J	101	CRT	O1-C1M	-2.42	1.35	1.43
9	P	101	BCL	MG-NA	-2.41	2.00	2.06
9	F	102	BCL	MG-NA	2.40	2.12	2.06
15	V	102	CRT	C26-C27	-2.40	1.36	1.43
15	B	102	CRT	C16-C17	-2.39	1.40	1.45
9	A	102	BCL	C2-C3	2.39	1.38	1.33
9	S	102	BCL	MG-NA	2.39	2.12	2.06
9	4	101	BCL	C1B-NB	2.39	1.37	1.35
15	G	102	CRT	C11-C12	-2.39	1.40	1.45
15	R	102	CRT	C22-C23	2.39	1.39	1.35
9	I	103	BCL	C4D-ND	-2.39	1.34	1.37
15	N	102	CRT	C4-C5	2.38	1.54	1.50
9	2	101	BCL	C3B-C2B	-2.38	1.35	1.39
9	G	101	BCL	C4B-NB	2.37	1.37	1.35
9	I	102	BCL	MG-NA	2.37	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302	BPH	C3B-C2B	2.37	1.43	1.39
9	3	102	BCL	C1B-NB	2.37	1.37	1.35
9	F	102	BCL	O2D-CED	-2.37	1.39	1.45
9	X	101	BCL	CMB-C2B	2.37	1.56	1.51
15	A	101	CRT	C35-C36	2.36	1.38	1.32
9	O	102	BCL	C2-C3	2.36	1.38	1.33
9	Q	102	BCL	CMD-C2D	2.36	1.55	1.50
15	J	101	CRT	C26-C25	2.36	1.40	1.34
9	7	102	BCL	C3B-C2B	-2.36	1.35	1.39
9	2	101	BCL	C3C-C4C	-2.36	1.48	1.51
9	6	101	BCL	C3B-C2B	-2.35	1.35	1.39
9	V	101	BCL	O2D-CED	-2.35	1.39	1.45
15	R	102	CRT	C37-C36	2.35	1.53	1.50
9	Y	102	BCL	O2D-CED	-2.35	1.39	1.45
15	4	102	CRT	C22-C23	2.35	1.38	1.35
9	V	101	BCL	C5-C3	2.35	1.56	1.51
7	C	501	HEM	C4B-NB	2.35	1.43	1.38
9	V	101	BCL	CMB-C2B	2.34	1.56	1.51
15	P	102	CRT	C39-C38	2.34	1.57	1.52
9	4	101	BCL	C2-C3	2.34	1.38	1.33
15	V	102	CRT	C9-C7	2.34	1.38	1.35
9	9	102	BCL	C3B-C2B	-2.34	1.35	1.39
9	N	101	BCL	C5-C3	2.34	1.56	1.51
7	C	502	HEM	O1A-CGA	2.33	1.29	1.22
9	M	401	BCL	CAA-C2A	2.33	1.58	1.54
9	9	102	BCL	C2-C3	2.33	1.38	1.33
9	2	101	BCL	CMA-C3A	2.33	1.58	1.53
9	I	103	BCL	C2C-C3C	-2.32	1.48	1.54
15	A	103	CRT	C31-C30	2.32	1.40	1.34
9	0	101	BCL	MG-NC	2.32	2.11	2.06
15	A	103	CRT	C26-C25	2.32	1.40	1.34
9	F	102	BCL	C4B-NB	2.32	1.37	1.35
9	E	101	BCL	O2D-CED	-2.32	1.39	1.45
9	A	102	BCL	C3B-C2B	-2.31	1.35	1.39
9	D	102	BCL	CMA-C3A	2.31	1.58	1.53
15	X	102	CRT	C31-C30	2.31	1.40	1.34
15	W	103	CRT	C26-C25	2.31	1.40	1.34
9	M	401	BCL	C4B-NB	2.31	1.37	1.35
7	C	504	HEM	C1A-NA	2.30	1.40	1.36
9	P	101	BCL	O2D-CED	-2.30	1.39	1.45
7	C	503	HEM	C1A-NA	2.30	1.40	1.36
9	0	101	BCL	C3B-C2B	-2.30	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	102	CRT	C11-C12	-2.29	1.41	1.45
9	4	101	BCL	C4D-ND	-2.29	1.34	1.37
9	Q	102	BCL	MG-NC	2.29	2.11	2.06
9	B	101	BCL	O2D-CED	-2.29	1.39	1.45
9	I	103	BCL	C5-C3	2.29	1.56	1.51
7	C	501	HEM	C4A-CHB	-2.29	1.34	1.41
7	C	504	HEM	C1D-ND	-2.29	1.34	1.38
9	B	101	BCL	C3B-C2B	-2.28	1.35	1.39
9	B	101	BCL	C2C-C3C	-2.28	1.48	1.54
9	D	102	BCL	C2-C3	2.28	1.38	1.33
9	Q	102	BCL	CAA-C2A	2.28	1.58	1.54
9	N	101	BCL	CMB-C2B	2.27	1.56	1.51
9	I	102	BCL	O2D-CED	-2.26	1.40	1.45
15	T	102	CRT	C26-C25	2.26	1.40	1.34
9	7	102	BCL	CMA-C3A	2.26	1.58	1.53
15	J	101	CRT	C25-C23	-2.26	1.41	1.45
9	3	102	BCL	CMB-C2B	2.26	1.56	1.51
15	R	102	CRT	C4-C5	2.26	1.53	1.50
15	A	103	CRT	C14-C12	2.25	1.38	1.35
9	3	102	BCL	C2C-C3C	-2.25	1.48	1.54
9	E	101	BCL	C4-C3	2.25	1.56	1.50
7	C	503	HEM	C1D-ND	-2.25	1.34	1.38
9	T	101	BCL	C5-C3	2.24	1.56	1.51
15	A	103	CRT	C32-C33	2.24	1.38	1.35
9	Y	102	BCL	MG-NC	2.24	2.11	2.06
9	2	101	BCL	C4D-ND	-2.24	1.34	1.37
9	L	301	BCL	C2-C3	2.24	1.38	1.33
9	L	303	BCL	C4D-ND	-2.24	1.34	1.37
14	M	405	MQ8	C3-C2	2.24	1.39	1.35
9	P	101	BCL	C2C-C3C	-2.24	1.48	1.54
9	Z	101	BCL	C1B-NB	2.23	1.37	1.35
9	P	101	BCL	CMB-C2B	2.23	1.56	1.51
9	M	401	BCL	C3B-C2B	-2.23	1.35	1.39
9	B	101	BCL	CMB-C2B	2.23	1.56	1.51
9	0	101	BCL	O2D-CED	-2.22	1.40	1.45
15	G	102	CRT	O1-C1M	-2.22	1.36	1.43
9	I	102	BCL	C3B-C2B	-2.22	1.35	1.39
9	S	102	BCL	CMB-C2B	2.22	1.56	1.51
15	3	103	CRT	C32-C33	2.22	1.38	1.35
9	E	101	BCL	C3B-C2B	-2.21	1.35	1.39
15	G	102	CRT	C22-C23	2.20	1.38	1.35
9	V	101	BCL	C4B-NB	2.20	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	102	CRT	C30-C28	-2.20	1.41	1.45
9	M	401	BCL	C2C-C3C	-2.20	1.48	1.54
15	V	102	CRT	C10-C11	2.20	1.40	1.34
9	P	101	BCL	C4B-NB	2.20	1.37	1.35
15	G	102	CRT	C27-C28	2.19	1.38	1.35
9	M	402	BCL	CMB-C2B	2.19	1.56	1.51
9	1	102	BCL	C4B-NB	2.18	1.37	1.35
15	P	102	CRT	C18-C17	-2.18	1.46	1.50
9	K	102	BCL	C4B-NB	2.17	1.37	1.35
9	1	102	BCL	MG-NA	-2.17	2.01	2.06
9	I	103	BCL	CMB-C2B	2.17	1.56	1.51
9	A	102	BCL	C4D-ND	-2.17	1.34	1.37
9	P	101	BCL	C3B-C2B	-2.17	1.35	1.39
9	0	101	BCL	C2C-C3C	-2.17	1.48	1.54
9	U	102	BCL	CAA-C2A	2.16	1.58	1.54
9	K	102	BCL	C5-C3	2.16	1.55	1.51
15	3	103	CRT	O1-C1M	-2.16	1.36	1.43
9	M	402	BCL	MG-ND	-2.16	2.01	2.05
15	A	101	CRT	C29-C28	2.16	1.55	1.50
7	C	502	HEM	C1D-ND	-2.16	1.34	1.38
9	X	101	BCL	O2D-CED	-2.16	1.40	1.45
15	P	102	CRT	C26-C27	2.16	1.50	1.43
9	M	401	BCL	MG-NC	2.16	2.11	2.06
9	K	102	BCL	CMB-C2B	2.15	1.56	1.51
9	T	101	BCL	O2D-CED	-2.15	1.40	1.45
9	Y	102	BCL	CMB-C2B	2.15	1.56	1.51
9	7	103	BCL	C4-C3	2.15	1.56	1.50
7	C	503	HEM	C4D-C3D	2.15	1.48	1.45
15	2	102	CRT	C15-C14	-2.15	1.36	1.43
9	0	101	BCL	C4-C3	2.14	1.56	1.50
9	Z	101	BCL	C4-C3	2.14	1.56	1.50
9	F	102	BCL	CMB-C2B	2.14	1.56	1.51
15	B	102	CRT	C9-C7	2.14	1.38	1.35
9	9	102	BCL	C4D-ND	-2.14	1.34	1.37
9	4	101	BCL	C5-C3	2.14	1.55	1.51
9	W	102	BCL	C4B-NB	2.13	1.37	1.35
7	C	501	HEM	CHB-C1B	2.13	1.40	1.35
9	9	102	BCL	CAA-C2A	2.13	1.58	1.54
9	0	101	BCL	CMB-C2B	2.13	1.56	1.51
15	3	103	CRT	C15-C16	2.12	1.40	1.34
9	L	303	BCL	C2-C3	2.12	1.38	1.33
15	2	102	CRT	C25-C23	-2.12	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	102	CRT	C14-C12	2.12	1.38	1.35
7	C	502	HEM	C3B-C2B	2.11	1.41	1.37
15	M	406	CRT	O1-C1M	-2.11	1.36	1.43
9	D	102	BCL	C2C-C3C	-2.11	1.48	1.54
9	Y	102	BCL	C2C-C3C	-2.11	1.48	1.54
9	2	101	BCL	C1D-ND	-2.11	1.35	1.37
15	V	102	CRT	C22-C23	2.10	1.38	1.35
12	M	408	PO4	P-O2	-2.10	1.48	1.54
15	A	101	CRT	C15-C16	2.10	1.40	1.34
9	L	303	BCL	C3B-C2B	-2.10	1.35	1.39
15	2	102	CRT	C15-C16	2.10	1.40	1.34
9	F	102	BCL	CAA-C2A	2.10	1.58	1.54
15	8	101	CRT	C25-C23	-2.10	1.41	1.45
9	A	102	BCL	CMB-C2B	2.09	1.56	1.51
9	G	101	BCL	CMB-C2B	2.09	1.56	1.51
9	A	102	BCL	MG-NC	2.09	2.11	2.06
9	Z	101	BCL	C1D-ND	-2.09	1.35	1.37
9	I	102	BCL	CMB-C2B	2.09	1.56	1.51
9	4	101	BCL	O2D-CED	-2.09	1.40	1.45
9	3	102	BCL	MG-NA	2.09	2.11	2.06
15	M	406	CRT	C25-C23	-2.09	1.41	1.45
15	R	102	CRT	C14-C12	2.09	1.38	1.35
9	M	402	BCL	C3B-C2B	-2.08	1.35	1.39
9	T	101	BCL	CMB-C2B	2.08	1.56	1.51
9	I	102	BCL	C4-C3	2.08	1.56	1.50
7	C	502	HEM	CMB-C2B	-2.08	1.46	1.50
9	U	102	BCL	CMA-C3A	2.07	1.57	1.53
9	Z	101	BCL	C5-C3	2.07	1.55	1.51
9	7	103	BCL	CMC-C2C	2.07	1.57	1.53
9	S	102	BCL	O2D-CED	-2.07	1.40	1.45
9	X	101	BCL	CMA-C3A	2.07	1.57	1.53
9	Q	102	BCL	C4-C3	2.07	1.56	1.50
9	P	101	BCL	C4-C3	2.06	1.56	1.50
15	N	102	CRT	O1-C1M	-2.06	1.36	1.43
9	D	102	BCL	CMB-C2B	2.06	1.55	1.51
9	G	101	BCL	C3B-C2B	-2.06	1.35	1.39
9	R	101	BCL	CMB-C2B	2.06	1.55	1.51
9	I	103	BCL	C4-C3	2.06	1.56	1.50
9	T	101	BCL	C4-C3	2.06	1.56	1.50
9	W	102	BCL	MG-NC	2.06	2.11	2.06
9	X	101	BCL	C4-C3	2.05	1.56	1.50
9	Y	102	BCL	C4-C3	2.05	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	102	BCL	CMA-C3A	2.05	1.57	1.53
7	C	503	HEM	C4D-ND	-2.05	1.36	1.40
15	4	102	CRT	C32-C33	2.05	1.38	1.35
15	2	102	CRT	C19-C17	2.05	1.38	1.35
9	V	101	BCL	C4-C3	2.05	1.55	1.50
9	O	102	BCL	MG-NC	2.05	2.11	2.06
17	H	301	PEF	P-O4P	2.05	1.67	1.59
9	U	102	BCL	C4-C3	2.04	1.55	1.50
9	S	102	BCL	CMD-C2D	2.04	1.55	1.50
15	4	102	CRT	C6-C5	2.04	1.37	1.32
9	2	101	BCL	C4-C3	2.04	1.55	1.50
11	L	304	UQ8	C6-C1	2.03	1.38	1.35
9	L	301	BCL	C4-C3	2.03	1.55	1.50
9	E	101	BCL	CMB-C2B	2.03	1.55	1.51
9	0	101	BCL	C1B-NB	2.03	1.37	1.35
9	X	101	BCL	C1D-ND	-2.03	1.35	1.37
9	X	101	BCL	C5-C3	2.03	1.55	1.51
9	3	102	BCL	C3B-C2B	-2.02	1.35	1.39
9	1	102	BCL	CMB-C2B	2.02	1.55	1.51
11	L	304	UQ8	C45-C44	2.02	1.55	1.50
9	E	101	BCL	C4D-ND	-2.02	1.34	1.37
9	Y	102	BCL	MG-NA	-2.01	2.01	2.06
9	O	102	BCL	C4-C3	2.01	1.55	1.50
9	R	101	BCL	CMA-C3A	2.01	1.57	1.53
9	S	102	BCL	C4-C3	2.01	1.55	1.50
9	4	101	BCL	CMB-C2B	2.00	1.55	1.51
7	C	501	HEM	O1D-CGD	2.00	1.28	1.22
9	5	102	BCL	C4-C3	2.00	1.55	1.50
15	3	103	CRT	C8-C7	-2.00	1.46	1.50
9	S	102	BCL	MG-NC	2.00	2.11	2.06
9	6	101	BCL	O2D-CED	-2.00	1.40	1.45
9	Q	102	BCL	CMB-C2B	2.00	1.55	1.51
15	V	102	CRT	C6-C5	2.00	1.37	1.32

All (1198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	102	CRT	C1-C4-C5	15.40	153.86	113.06
15	A	101	CRT	C36-C35-C33	-10.28	110.36	125.89
15	T	102	CRT	C3-C1-C4	-10.11	95.33	110.86
9	7	103	BCL	C1-C2-C3	9.65	142.73	126.04
9	4	101	BCL	C1-C2-C3	9.19	141.93	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	C1-C2-C3	8.89	141.43	126.04
15	V	102	CRT	C21-C22-C23	-8.89	114.62	127.31
9	0	101	BCL	C1-C2-C3	8.77	141.21	126.04
9	L	301	BCL	C1-C2-C3	8.66	141.02	126.04
15	N	102	CRT	C10-C9-C7	-8.62	115.01	127.31
15	R	102	CRT	C8-C7-C6	8.33	131.21	118.08
9	I	102	BCL	C1-C2-C3	8.23	140.27	126.04
9	E	101	BCL	C1-C2-C3	8.23	140.27	126.04
9	R	101	BCL	C1-C2-C3	8.22	140.26	126.04
9	2	101	BCL	C1-C2-C3	8.09	140.04	126.04
9	X	101	BCL	C1-C2-C3	8.09	140.04	126.04
9	I	103	BCL	C1-C2-C3	8.09	140.03	126.04
9	D	102	BCL	C1-C2-C3	8.08	140.02	126.04
9	6	101	BCL	C1-C2-C3	8.07	140.00	126.04
9	A	102	BCL	C1-C2-C3	8.06	139.98	126.04
9	K	102	BCL	C1-C2-C3	8.05	139.97	126.04
9	3	102	BCL	C1-C2-C3	8.04	139.94	126.04
9	Q	102	BCL	C1-C2-C3	7.99	139.87	126.04
9	1	102	BCL	C1-C2-C3	7.98	139.85	126.04
15	X	102	CRT	C15-C14-C12	-7.95	115.96	127.31
9	9	102	BCL	C1-C2-C3	7.92	139.74	126.04
9	U	102	BCL	C1-C2-C3	7.91	139.73	126.04
9	5	102	BCL	C1-C2-C3	7.89	139.70	126.04
9	7	102	BCL	C1-C2-C3	7.89	139.69	126.04
9	O	102	BCL	C1-C2-C3	7.88	139.67	126.04
9	T	101	BCL	C1-C2-C3	7.87	139.65	126.04
9	Y	102	BCL	C1-C2-C3	7.87	139.65	126.04
9	Z	101	BCL	C1-C2-C3	7.85	139.62	126.04
9	S	102	BCL	C1-C2-C3	7.85	139.62	126.04
9	M	402	BCL	C1-C2-C3	7.83	139.59	126.04
9	V	101	BCL	C1-C2-C3	7.80	139.54	126.04
9	F	102	BCL	C1-C2-C3	7.73	139.41	126.04
9	G	101	BCL	C1-C2-C3	7.72	139.40	126.04
9	W	102	BCL	C1-C2-C3	7.72	139.40	126.04
9	P	101	BCL	C1-C2-C3	7.71	139.37	126.04
9	L	303	BCL	C1-C2-C3	7.68	139.32	126.04
15	J	101	CRT	C21-C22-C23	-7.64	116.41	127.31
9	B	101	BCL	C1-C2-C3	7.60	139.19	126.04
9	X	101	BCL	C4A-NA-C1A	7.24	109.96	106.71
15	R	102	CRT	C6-C7-C9	-7.17	107.93	118.94
15	B	102	CRT	C10-C9-C7	-7.15	117.11	127.31
15	P	102	CRT	C20-C21-C22	-7.10	108.94	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	401	BCL	C1-C2-C3	6.90	137.97	126.04
15	X	102	CRT	C1-C4-C5	6.88	131.29	113.06
9	T	101	BCL	C4A-NA-C1A	6.84	109.78	106.71
15	R	102	CRT	C5-C6-C7	6.81	136.18	125.89
9	U	102	BCL	C4A-NA-C1A	6.81	109.77	106.71
9	I	102	BCL	C4A-NA-C1A	6.68	109.71	106.71
9	G	101	BCL	C4-C3-C5	-6.64	104.11	115.27
9	9	102	BCL	C4A-NA-C1A	6.60	109.67	106.71
9	0	101	BCL	C4-C3-C5	-6.46	104.40	115.27
9	6	101	BCL	C4-C3-C5	-6.31	104.65	115.27
11	L	304	UQ8	C46-C44-C45	6.31	128.53	114.60
9	K	102	BCL	C4-C3-C5	-6.31	104.66	115.27
9	F	102	BCL	C4-C3-C5	-6.27	104.72	115.27
9	D	102	BCL	OBB-CAB-C3B	6.26	131.09	119.99
9	I	103	BCL	C4-C3-C5	-6.25	104.76	115.27
9	W	102	BCL	C4-C3-C5	-6.25	104.76	115.27
9	Y	102	BCL	C4-C3-C5	-6.24	104.78	115.27
15	V	102	CRT	C18-C17-C19	-6.22	114.21	122.92
9	7	102	BCL	C4-C3-C5	-6.21	104.83	115.27
9	3	102	BCL	C4-C3-C5	-6.21	104.83	115.27
9	2	101	BCL	C4-C3-C5	-6.19	104.86	115.27
9	Z	101	BCL	C4-C3-C5	-6.19	104.86	115.27
9	B	101	BCL	C4-C3-C5	-6.17	104.90	115.27
9	R	101	BCL	C4-C3-C5	-6.16	104.91	115.27
9	1	102	BCL	C4-C3-C5	-6.15	104.92	115.27
9	P	101	BCL	C4-C3-C5	-6.14	104.94	115.27
9	S	102	BCL	C4-C3-C5	-6.14	104.95	115.27
9	T	101	BCL	C4-C3-C5	-6.13	104.96	115.27
9	X	101	BCL	C4-C3-C5	-6.12	104.98	115.27
9	V	101	BCL	C4-C3-C5	-6.11	105.00	115.27
9	I	102	BCL	C4-C3-C5	-6.10	105.01	115.27
9	F	102	BCL	C4A-NA-C1A	6.09	109.45	106.71
9	N	101	BCL	C4A-NA-C1A	6.09	109.44	106.71
9	P	101	BCL	C4A-NA-C1A	6.07	109.43	106.71
9	L	303	BCL	OBB-CAB-C3B	6.07	130.76	119.99
9	N	101	BCL	C4-C3-C5	-6.06	105.08	115.27
9	W	102	BCL	OBB-CAB-C3B	6.06	130.74	119.99
9	5	102	BCL	C4-C3-C5	-6.05	105.10	115.27
9	O	102	BCL	C4A-NA-C1A	6.04	109.42	106.71
9	9	102	BCL	C4-C3-C5	-6.03	105.13	115.27
9	D	102	BCL	C4-C3-C5	-6.01	105.17	115.27
9	9	102	BCL	OBB-CAB-C3B	5.99	130.62	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	102	BCL	C4-C3-C5	-5.99	105.20	115.27
9	4	101	BCL	OBB-CAB-C3B	5.99	130.62	119.99
9	Q	102	BCL	OBB-CAB-C3B	5.98	130.60	119.99
9	F	102	BCL	OBB-CAB-C3B	5.96	130.57	119.99
9	B	101	BCL	OBB-CAB-C3B	5.96	130.57	119.99
9	U	102	BCL	C4-C3-C5	-5.96	105.25	115.27
9	3	102	BCL	OBB-CAB-C3B	5.96	130.56	119.99
9	R	101	BCL	C4A-NA-C1A	5.95	109.38	106.71
9	G	101	BCL	OBB-CAB-C3B	5.95	130.55	119.99
9	P	101	BCL	OBB-CAB-C3B	5.95	130.55	119.99
9	O	102	BCL	C4-C3-C5	-5.94	105.28	115.27
9	M	402	BCL	OBB-CAB-C3B	5.93	130.52	119.99
9	0	101	BCL	OBB-CAB-C3B	5.93	130.51	119.99
9	A	102	BCL	OBB-CAB-C3B	5.92	130.51	119.99
9	7	103	BCL	OBB-CAB-C3B	5.92	130.50	119.99
9	O	102	BCL	OBB-CAB-C3B	5.92	130.50	119.99
9	Y	102	BCL	OBB-CAB-C3B	5.92	130.49	119.99
9	L	303	BCL	C4-C3-C5	-5.92	105.32	115.27
9	I	102	BCL	OBB-CAB-C3B	5.91	130.49	119.99
9	K	102	BCL	OBB-CAB-C3B	5.91	130.49	119.99
9	A	102	BCL	C4-C3-C5	-5.91	105.33	115.27
9	6	101	BCL	OBB-CAB-C3B	5.91	130.48	119.99
9	5	102	BCL	OBB-CAB-C3B	5.91	130.48	119.99
9	S	102	BCL	OBB-CAB-C3B	5.90	130.47	119.99
9	M	402	BCL	C4-C3-C5	-5.90	105.34	115.27
9	Z	101	BCL	OBB-CAB-C3B	5.90	130.46	119.99
9	7	102	BCL	OBB-CAB-C3B	5.90	130.46	119.99
9	E	101	BCL	OBB-CAB-C3B	5.90	130.46	119.99
9	2	101	BCL	OBB-CAB-C3B	5.88	130.42	119.99
15	A	101	CRT	C31-C32-C33	-5.87	118.93	127.31
9	I	103	BCL	OBB-CAB-C3B	5.87	130.41	119.99
9	U	102	BCL	OBB-CAB-C3B	5.85	130.37	119.99
9	3	102	BCL	C4A-NA-C1A	5.85	109.33	106.71
15	W	103	CRT	C11-C12-C14	-5.84	109.98	118.94
9	Z	101	BCL	C4A-NA-C1A	5.83	109.33	106.71
9	L	301	BCL	OBB-CAB-C3B	5.82	130.33	119.99
9	1	102	BCL	OBB-CAB-C3B	5.82	130.32	119.99
9	M	401	BCL	OBB-CAB-C3B	5.81	130.30	119.99
9	B	101	BCL	CAA-C2A-C3A	-5.79	96.91	112.78
9	L	301	BCL	C4-C3-C5	-5.78	105.54	115.27
9	4	101	BCL	C4-C3-C5	-5.78	105.54	115.27
9	V	101	BCL	OBB-CAB-C3B	5.78	130.25	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	101	BCL	C4A-NA-C1A	5.78	109.30	106.71
9	X	101	BCL	OBB-CAB-C3B	5.77	130.23	119.99
9	N	101	BCL	OBB-CAB-C3B	5.76	130.21	119.99
15	A	101	CRT	C10-C9-C7	-5.75	119.10	127.31
9	R	101	BCL	OBB-CAB-C3B	5.73	130.16	119.99
15	J	101	CRT	C18-C17-C19	-5.71	114.92	122.92
15	J	101	CRT	C16-C17-C19	5.70	127.68	118.94
9	7	103	BCL	C4-C3-C5	-5.69	105.69	115.27
9	E	101	BCL	C4A-NA-C1A	5.69	109.27	106.71
9	D	102	BCL	C4A-NA-C1A	5.68	109.26	106.71
9	K	102	BCL	C4A-NA-C1A	5.66	109.25	106.71
9	E	101	BCL	CAA-C2A-C3A	-5.65	97.32	112.78
9	6	101	BCL	C4A-NA-C1A	5.64	109.24	106.71
15	X	102	CRT	C11-C12-C14	5.59	127.52	118.94
9	7	102	BCL	C4A-NA-C1A	5.55	109.20	106.71
15	N	102	CRT	C5-C6-C7	-5.55	117.51	125.89
9	I	103	BCL	C4A-NA-C1A	5.55	109.20	106.71
9	M	402	BCL	C4A-NA-C1A	5.53	109.19	106.71
9	4	101	BCL	C4A-NA-C1A	5.53	109.19	106.71
9	2	101	BCL	C4A-NA-C1A	5.53	109.19	106.71
9	B	101	BCL	C4A-NA-C1A	5.52	109.19	106.71
15	P	102	CRT	C20-C19-C17	5.51	135.17	127.31
15	T	102	CRT	C39-C38-C37	-5.50	102.41	110.86
15	J	101	CRT	C20-C21-C22	5.48	134.70	123.47
9	G	101	BCL	CAA-C2A-C3A	-5.46	97.83	112.78
9	L	301	BCL	O2A-CGA-CBA	5.42	128.92	111.91
9	4	101	BCL	CAA-C2A-C3A	-5.40	98.00	112.78
9	A	102	BCL	O2D-CGD-CBD	5.38	120.83	111.27
9	M	401	BCL	C4A-NA-C1A	5.38	109.12	106.71
9	7	102	BCL	O2D-CGD-CBD	5.35	120.77	111.27
15	P	102	CRT	C21-C22-C23	5.33	134.92	127.31
15	A	101	CRT	C26-C27-C28	-5.33	119.71	127.31
15	A	101	CRT	C38-C37-C36	5.30	127.10	113.06
9	A	102	BCL	C4A-NA-C1A	5.30	109.09	106.71
9	W	102	BCL	C4A-NA-C1A	5.30	109.09	106.71
15	A	101	CRT	C1-C4-C5	5.28	127.05	113.06
9	Q	102	BCL	C4A-NA-C1A	5.27	109.07	106.71
9	T	101	BCL	C4B-C3B-CAB	-5.25	116.98	127.13
9	M	401	BCL	C4-C3-C5	-5.25	106.44	115.27
9	5	102	BCL	O2D-CGD-CBD	5.23	120.57	111.27
15	P	102	CRT	C21-C20-C19	5.23	134.18	123.47
9	E	101	BCL	C4-C3-C5	-5.21	106.50	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	303	BCL	O2D-CGD-CBD	5.21	120.53	111.27
15	W	103	CRT	C10-C9-C7	-5.21	119.88	127.31
9	P	101	BCL	CAA-C2A-C3A	-5.20	98.55	112.78
9	7	103	BCL	C4A-NA-C1A	5.19	109.04	106.71
9	M	401	BCL	O2D-CGD-CBD	5.18	120.48	111.27
9	R	101	BCL	CAA-C2A-C3A	-5.16	98.64	112.78
9	1	102	BCL	C4A-NA-C1A	5.14	109.02	106.71
9	T	101	BCL	CAA-C2A-C3A	-5.13	98.74	112.78
9	L	301	BCL	C4A-NA-C1A	5.12	109.01	106.71
11	L	304	UQ8	C42-C41-C39	5.11	129.80	112.98
9	1	102	BCL	O2D-CGD-CBD	5.11	120.35	111.27
9	T	101	BCL	OBB-CAB-C3B	5.11	129.06	119.99
15	P	102	CRT	C18-C17-C16	5.11	126.13	118.08
9	7	103	BCL	CAA-C2A-C3A	-5.11	98.79	112.78
9	6	101	BCL	CAA-C2A-C3A	-5.11	98.80	112.78
9	K	102	BCL	O2D-CGD-CBD	5.10	120.33	111.27
9	W	102	BCL	O2D-CGD-CBD	5.10	120.33	111.27
15	A	101	CRT	C35-C33-C32	5.08	126.73	118.94
9	D	102	BCL	O2D-CGD-CBD	5.07	120.27	111.27
9	Z	101	BCL	CAA-C2A-C3A	-5.06	98.93	112.78
9	Z	101	BCL	CBA-CAA-C2A	-5.05	98.95	113.86
9	Q	102	BCL	O2D-CGD-CBD	5.05	120.24	111.27
15	A	101	CRT	C34-C33-C32	-5.01	115.91	122.92
15	R	102	CRT	C21-C22-C23	-5.00	120.17	127.31
9	R	101	BCL	CBA-CAA-C2A	-4.98	99.16	113.86
15	X	102	CRT	C3-C1-C4	-4.96	103.24	110.86
9	X	101	BCL	CAA-C2A-C3A	-4.96	99.20	112.78
9	E	101	BCL	CBA-CAA-C2A	-4.96	99.22	113.86
15	B	102	CRT	C21-C22-C23	-4.95	120.24	127.31
9	Y	102	BCL	O2D-CGD-CBD	4.94	120.05	111.27
15	4	102	CRT	C10-C9-C7	-4.94	120.26	127.31
9	3	102	BCL	O2D-CGD-CBD	4.94	120.05	111.27
9	L	303	BCL	C4A-NA-C1A	4.94	108.92	106.71
9	G	101	BCL	C4A-NA-C1A	4.93	108.92	106.71
9	0	101	BCL	C4A-NA-C1A	4.92	108.92	106.71
15	B	102	CRT	C21-C20-C19	-4.92	113.40	123.47
9	L	301	BCL	O2A-CGA-O1A	-4.91	111.19	123.59
9	7	103	BCL	O2D-CGD-CBD	4.90	119.97	111.27
9	5	102	BCL	C4A-NA-C1A	4.90	108.91	106.71
9	G	101	BCL	CBA-CAA-C2A	-4.89	99.42	113.86
9	F	102	BCL	O2A-CGA-CBA	4.88	127.22	111.91
9	U	102	BCL	O2D-CGD-CBD	4.87	119.93	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	101	BCL	CAA-C2A-C3A	-4.87	99.44	112.78
9	I	103	BCL	CAA-C2A-C3A	-4.84	99.53	112.78
16	H	302	PGW	O01-C1-C2	4.84	119.99	111.09
16	M	407	PGW	O01-C1-C2	4.82	119.97	111.09
9	L	301	BCL	CBA-CAA-C2A	-4.81	99.66	113.86
9	S	102	BCL	C4A-NA-C1A	4.80	108.86	106.71
9	W	102	BCL	O2A-CGA-CBA	4.80	126.96	111.91
7	C	504	HEM	C2C-C3C-C4C	-4.79	103.55	106.90
9	N	101	BCL	CAA-C2A-C3A	-4.79	99.66	112.78
9	0	101	BCL	CAA-C2A-C3A	-4.76	99.75	112.78
9	D	102	BCL	C1C-NC-C4C	4.74	108.84	106.71
9	U	102	BCL	O2A-CGA-CBA	4.73	126.76	111.91
9	7	102	BCL	O2A-CGA-CBA	4.70	126.64	111.91
9	W	102	BCL	O2A-CGA-O1A	-4.69	111.77	123.59
7	C	501	HEM	C2C-C3C-C4C	-4.65	103.65	106.90
9	F	102	BCL	O2A-CGA-O1A	-4.64	111.88	123.59
9	W	102	BCL	C1C-NC-C4C	4.63	108.79	106.71
15	P	102	CRT	C10-C9-C7	4.63	133.92	127.31
7	C	502	HEM	C2C-C3C-C4C	-4.63	103.66	106.90
9	O	102	BCL	O2A-CGA-CBA	4.63	126.44	111.91
15	J	101	CRT	C15-C16-C17	-4.62	113.43	126.42
9	X	101	BCL	CBA-CAA-C2A	-4.62	100.22	113.86
9	U	102	BCL	O2A-CGA-O1A	-4.60	111.98	123.59
9	7	102	BCL	O2A-CGA-O1A	-4.60	111.99	123.59
9	9	102	BCL	O2D-CGD-CBD	4.59	119.42	111.27
15	2	102	CRT	C21-C22-C23	-4.58	120.77	127.31
9	5	102	BCL	O2A-CGA-CBA	4.56	126.22	111.91
15	V	102	CRT	C15-C14-C12	-4.56	120.80	127.31
9	6	101	BCL	O2D-CGD-CBD	4.54	119.33	111.27
9	M	401	BCL	C1C-NC-C4C	4.53	108.74	106.71
9	M	402	BCL	O2A-CGA-CBA	4.53	126.12	111.91
9	L	303	BCL	CAA-C2A-C3A	-4.53	100.38	112.78
9	S	102	BCL	O2A-CGA-CBA	4.52	126.11	111.91
9	Q	102	BCL	O2A-CGA-CBA	4.51	126.08	111.91
9	P	101	BCL	CBA-CAA-C2A	-4.50	100.58	113.86
9	G	101	BCL	C5-C3-C2	4.50	130.22	121.12
9	O	102	BCL	O2A-CGA-O1A	-4.49	112.25	123.59
9	M	402	BCL	C1C-NC-C4C	4.47	108.72	106.71
9	5	102	BCL	O2A-CGA-O1A	-4.46	112.33	123.59
9	S	102	BCL	C1C-NC-C4C	4.46	108.71	106.71
9	Y	102	BCL	C1C-NC-C4C	4.46	108.71	106.71
9	9	102	BCL	O2A-CGA-CBA	4.44	125.85	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	102	BCL	O2A-CGA-O1A	-4.44	112.40	123.59
9	S	102	BCL	O2A-CGA-O1A	-4.43	112.42	123.59
9	1	102	BCL	O2A-CGA-CBA	4.43	125.80	111.91
9	9	102	BCL	O2A-CGA-O1A	-4.42	112.44	123.59
9	B	101	BCL	CBA-CAA-C2A	-4.41	100.85	113.86
15	8	101	CRT	C21-C22-C23	-4.40	121.03	127.31
15	A	101	CRT	C21-C22-C23	-4.38	121.05	127.31
9	2	101	BCL	CAA-C2A-C3A	-4.38	100.80	112.78
9	K	102	BCL	O2A-CGA-O1A	-4.37	112.55	123.59
15	B	102	CRT	C5-C6-C7	-4.35	119.31	125.89
15	R	102	CRT	C10-C11-C12	-4.34	114.21	126.42
9	3	102	BCL	C1C-NC-C4C	4.34	108.66	106.71
9	L	303	BCL	O2A-CGA-O1A	-4.34	112.65	123.59
9	1	102	BCL	O2A-CGA-O1A	-4.33	112.66	123.59
9	3	102	BCL	O2A-CGA-O1A	-4.32	112.69	123.59
9	S	102	BCL	O2D-CGD-CBD	4.31	118.93	111.27
15	3	103	CRT	C8-C7-C9	-4.31	116.88	122.92
9	M	402	BCL	O2A-CGA-O1A	-4.31	112.72	123.59
10	L	302	BPH	C1-C2-C3	4.30	133.49	126.04
9	K	102	BCL	O2A-CGA-CBA	4.30	125.41	111.91
17	H	301	PEF	C2-O2-C10	4.30	125.91	117.90
9	I	102	BCL	O2A-CGA-O1A	-4.29	112.76	123.59
9	Y	102	BCL	O2A-CGA-O1A	-4.29	112.77	123.59
9	K	102	BCL	C5-C3-C2	4.29	129.79	121.12
9	0	101	BCL	CBA-CAA-C2A	-4.28	101.23	113.86
9	Y	102	BCL	O2A-CGA-CBA	4.28	125.34	111.91
9	A	102	BCL	O2A-CGA-O1A	-4.27	112.80	123.59
9	A	102	BCL	O2A-CGA-CBA	4.26	125.28	111.91
9	3	102	BCL	O2A-CGA-CBA	4.25	125.25	111.91
9	W	102	BCL	C5-C3-C2	4.24	129.69	121.12
9	I	103	BCL	C5-C3-C2	4.23	129.68	121.12
9	4	101	BCL	CBA-CAA-C2A	-4.23	101.38	113.86
9	P	101	BCL	C5-C3-C2	4.22	129.66	121.12
9	Z	101	BCL	C5-C3-C2	4.22	129.65	121.12
15	A	101	CRT	C5-C6-C7	-4.22	119.52	125.89
9	L	303	BCL	O2A-CGA-CBA	4.21	125.11	111.91
9	F	102	BCL	C5-C3-C2	4.20	129.61	121.12
9	T	101	BCL	C5-C3-C2	4.20	129.61	121.12
9	7	102	BCL	C5-C3-C2	4.20	129.61	121.12
9	6	101	BCL	C5-C3-C2	4.20	129.61	121.12
15	A	103	CRT	C20-C19-C17	-4.19	121.33	127.31
9	V	101	BCL	C5-C3-C2	4.19	129.60	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Y	102	BCL	C5-C3-C2	4.19	129.60	121.12
9	3	102	BCL	C5-C3-C2	4.18	129.58	121.12
9	X	101	BCL	C5-C3-C2	4.18	129.57	121.12
9	I	102	BCL	O2A-CGA-CBA	4.18	125.01	111.91
15	W	103	CRT	C13-C12-C11	4.17	124.65	118.08
9	B	101	BCL	C5-C3-C2	4.17	129.56	121.12
15	T	102	CRT	C10-C9-C7	-4.16	121.37	127.31
9	V	101	BCL	CBA-CAA-C2A	-4.16	101.59	113.86
9	1	102	BCL	C5-C3-C2	4.16	129.53	121.12
9	V	101	BCL	CMB-C2B-C1B	-4.14	122.10	128.46
9	F	102	BCL	C1C-NC-C4C	4.14	108.57	106.71
9	I	102	BCL	C4B-C3B-CAB	-4.14	119.14	127.13
9	B	101	BCL	C1C-NC-C4C	4.13	108.56	106.71
9	I	102	BCL	O2D-CGD-CBD	4.13	118.61	111.27
9	0	101	BCL	C5-C3-C2	4.12	129.46	121.12
9	F	102	BCL	O2D-CGD-CBD	4.12	118.59	111.27
9	S	102	BCL	C5-C3-C2	4.12	129.45	121.12
15	B	102	CRT	C39-C38-C37	-4.11	104.55	110.86
7	C	503	HEM	C2C-C3C-C4C	-4.11	104.03	106.90
9	D	102	BCL	O2A-CGA-O1A	-4.10	113.24	123.59
15	V	102	CRT	C32-C31-C30	-4.10	110.42	123.22
9	2	101	BCL	C5-C3-C2	4.10	129.41	121.12
15	T	102	CRT	C40-C38-C37	4.09	117.14	110.86
9	5	102	BCL	C5-C3-C2	4.09	129.38	121.12
9	R	101	BCL	C5-C3-C2	4.08	129.38	121.12
15	N	102	CRT	C8-C7-C9	-4.08	117.21	122.92
9	6	101	BCL	CBA-CAA-C2A	-4.07	101.84	113.86
9	M	402	BCL	CAA-C2A-C3A	-4.07	101.64	112.78
9	G	101	BCL	O2D-CGD-CBD	4.06	118.48	111.27
9	L	301	BCL	CMB-C2B-C1B	-4.06	122.22	128.46
9	L	303	BCL	C5-C3-C2	4.06	129.33	121.12
15	T	102	CRT	C40-C38-C39	-4.06	102.74	110.37
9	U	102	BCL	C5-C3-C2	4.05	129.31	121.12
9	M	401	BCL	O2A-CGA-CBA	4.05	124.61	111.91
9	0	101	BCL	C1C-NC-C4C	4.05	108.53	106.71
9	7	103	BCL	CBA-CAA-C2A	-4.04	101.93	113.86
9	D	102	BCL	C5-C3-C2	4.04	129.29	121.12
9	I	102	BCL	C5-C3-C2	4.04	129.29	121.12
17	H	301	PEF	O2-C10-C11	4.03	118.51	111.09
9	9	102	BCL	C5-C3-C2	4.03	129.27	121.12
9	D	102	BCL	O2A-CGA-CBA	4.03	124.55	111.91
9	Q	102	BCL	C1C-NC-C4C	4.01	108.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	102	BCL	C5-C3-C2	3.99	129.19	121.12
9	7	103	BCL	C1C-NC-C4C	3.98	108.50	106.71
9	M	402	BCL	O2D-CGD-CBD	3.98	118.34	111.27
15	X	102	CRT	C13-C12-C14	-3.98	117.35	122.92
9	Q	102	BCL	C5-C3-C2	3.97	129.16	121.12
9	M	402	BCL	CMB-C2B-C1B	-3.96	122.37	128.46
9	N	101	BCL	C5-C3-C2	3.96	129.13	121.12
9	L	303	BCL	CMB-C2B-C1B	-3.94	122.41	128.46
9	M	402	BCL	C5-C3-C2	3.94	129.08	121.12
9	R	101	BCL	O2A-CGA-O1A	-3.94	113.66	123.59
14	M	405	MQ8	C45-C43-C44	3.93	121.89	115.27
17	H	301	PEF	O3-C3-C2	3.93	119.88	108.43
9	U	102	BCL	CMB-C2B-C1B	-3.93	122.42	128.46
15	P	102	CRT	C6-C7-C9	-3.93	112.91	118.94
9	M	401	BCL	C4B-C3B-CAB	-3.92	119.56	127.13
15	N	102	CRT	C11-C12-C14	-3.92	112.93	118.94
15	P	102	CRT	C15-C16-C17	3.92	137.42	126.42
15	G	102	CRT	C21-C22-C23	-3.92	121.72	127.31
9	L	303	BCL	C1C-NC-C4C	3.91	108.47	106.71
15	V	102	CRT	C20-C19-C17	-3.91	121.73	127.31
9	M	401	BCL	O2A-CGA-O1A	-3.90	113.74	123.59
15	B	102	CRT	C30-C28-C27	-3.89	112.97	118.94
15	A	101	CRT	C26-C25-C23	-3.89	115.49	126.42
15	V	102	CRT	C26-C27-C28	-3.89	121.76	127.31
15	V	102	CRT	C26-C25-C23	-3.88	115.51	126.42
9	5	102	BCL	C4B-C3B-CAB	-3.88	119.63	127.13
9	X	101	BCL	C4B-C3B-CAB	-3.87	119.65	127.13
9	Q	102	BCL	CMB-C2B-C1B	-3.87	122.52	128.46
14	M	405	MQ8	C29-C28-C30	3.86	121.77	115.27
9	F	102	BCL	C4B-C3B-CAB	-3.86	119.67	127.13
9	A	102	BCL	C5-C3-C2	3.86	128.92	121.12
15	P	102	CRT	C16-C17-C19	-3.85	113.03	118.94
10	M	403	BPH	C1A-C2A-C3A	-3.85	99.18	102.84
9	3	102	BCL	CMB-C2B-C1B	-3.85	122.55	128.46
9	M	401	BCL	C5-C3-C2	3.84	128.89	121.12
14	M	405	MQ8	C39-C38-C40	3.84	121.73	115.27
9	M	401	BCL	CAA-C2A-C3A	-3.83	102.28	112.78
7	C	504	HEM	C4A-C3A-C2A	3.83	109.66	107.00
15	W	103	CRT	C5-C6-C7	-3.83	120.11	125.89
9	2	101	BCL	CMB-C2B-C1B	-3.83	122.58	128.46
9	7	103	BCL	C1-O2A-CGA	3.83	126.48	116.44
9	G	101	BCL	CMB-C2B-C1B	-3.81	122.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	102	BCL	O2D-CGD-CBD	3.81	118.03	111.27
9	M	402	BCL	C4B-C3B-CAB	-3.80	119.78	127.13
9	7	102	BCL	CMB-C2B-C1B	-3.80	122.62	128.46
9	N	101	BCL	C4B-C3B-CAB	-3.80	119.80	127.13
9	M	401	BCL	CMB-C2B-C1B	-3.79	122.64	128.46
9	I	103	BCL	CBA-CAA-C2A	-3.79	102.67	113.86
9	T	101	BCL	CBA-CAA-C2A	-3.78	102.69	113.86
9	G	101	BCL	O2A-CGA-O1A	-3.78	114.05	123.59
9	D	102	BCL	CMB-C2B-C1B	-3.77	122.67	128.46
9	I	103	BCL	CMB-C2B-C1B	-3.77	122.68	128.46
9	T	101	BCL	O2D-CGD-CBD	3.76	117.96	111.27
9	N	101	BCL	CBA-CAA-C2A	-3.76	102.76	113.86
7	C	501	HEM	C2B-C1B-NB	3.76	114.30	109.84
9	5	102	BCL	CMB-C2B-C1B	-3.76	122.69	128.46
9	I	103	BCL	O2A-CGA-O1A	-3.75	114.12	123.59
9	I	103	BCL	O2D-CGD-CBD	3.75	117.94	111.27
9	A	102	BCL	C4B-C3B-CAB	-3.74	119.90	127.13
9	9	102	BCL	C4B-C3B-CAB	-3.74	119.91	127.13
9	E	101	BCL	O2D-CGD-CBD	3.74	117.91	111.27
9	K	102	BCL	CMB-C2B-C1B	-3.73	122.72	128.46
9	P	101	BCL	O2A-CGA-O1A	-3.73	114.18	123.59
15	8	101	CRT	C20-C19-C17	-3.73	121.99	127.31
9	0	101	BCL	CMB-C2B-C1B	-3.73	122.74	128.46
9	E	101	BCL	C5-C3-C2	3.72	128.65	121.12
9	V	101	BCL	O2A-CGA-O1A	-3.72	114.20	123.59
9	0	101	BCL	O2D-CGD-CBD	3.72	117.88	111.27
9	L	301	BCL	C4B-C3B-CAB	-3.72	119.95	127.13
9	V	101	BCL	C4B-C3B-CAB	-3.71	119.96	127.13
9	R	101	BCL	O2A-CGA-CBA	3.71	123.56	111.91
9	7	103	BCL	CMB-C2B-C1B	-3.71	122.76	128.46
9	4	101	BCL	C5-C3-C2	3.71	128.63	121.12
9	7	103	BCL	C4B-C3B-CAB	-3.71	119.97	127.13
15	X	102	CRT	C10-C9-C7	-3.70	122.03	127.31
9	6	101	BCL	CMB-C2B-C1B	-3.69	122.79	128.46
9	3	102	BCL	C4B-C3B-CAB	-3.68	120.02	127.13
9	Z	101	BCL	O2A-CGA-O1A	-3.68	114.30	123.59
9	2	101	BCL	O2A-CGA-O1A	-3.68	114.32	123.59
9	T	101	BCL	O2A-CGA-O1A	-3.67	114.33	123.59
15	J	101	CRT	C9-C10-C11	-3.67	111.77	123.22
15	V	102	CRT	C35-C33-C32	-3.67	113.31	118.94
9	F	102	BCL	CMB-C2B-C1B	-3.66	122.83	128.46
9	W	102	BCL	CMB-C2B-C1B	-3.66	122.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	102	BCL	CMB-C2B-C1B	-3.65	122.85	128.46
9	4	101	BCL	O2D-CGD-CBD	3.65	117.76	111.27
9	N	101	BCL	O2A-CGA-O1A	-3.65	114.38	123.59
9	Y	102	BCL	CMB-C2B-C1B	-3.65	122.86	128.46
9	A	102	BCL	C1C-NC-C4C	3.64	108.34	106.71
9	L	301	BCL	C5-C3-C2	3.64	128.47	121.12
15	N	102	CRT	C14-C15-C16	-3.64	111.87	123.22
9	2	101	BCL	O2D-CGD-CBD	3.63	117.73	111.27
9	O	102	BCL	C1C-NC-C4C	3.63	108.34	106.71
9	1	102	BCL	C4B-C3B-CAB	-3.63	120.11	127.13
9	2	101	BCL	C4B-C3B-CAB	-3.63	120.12	127.13
9	R	101	BCL	C4B-C3B-CAB	-3.63	120.13	127.13
9	E	101	BCL	CMB-C2B-C1B	-3.62	122.89	128.46
9	4	101	BCL	CMB-C2B-C1B	-3.62	122.91	128.46
9	X	101	BCL	O2A-CGA-O1A	-3.62	114.47	123.59
9	K	102	BCL	C4B-C3B-CAB	-3.61	120.15	127.13
9	U	102	BCL	C1C-NC-C4C	3.61	108.33	106.71
9	Z	101	BCL	C4B-C3B-CAB	-3.61	120.16	127.13
9	Q	102	BCL	C4B-C3B-CAB	-3.61	120.16	127.13
9	4	101	BCL	C4B-C3B-CAB	-3.61	120.17	127.13
9	1	102	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
9	Z	101	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
9	7	103	BCL	C5-C3-C2	3.59	128.38	121.12
15	2	102	CRT	C10-C9-C7	-3.58	122.20	127.31
15	J	101	CRT	C6-C7-C9	-3.58	113.45	118.94
9	Y	102	BCL	C4A-NA-C1A	3.58	108.31	106.71
9	N	101	BCL	CMB-C2B-C1B	-3.57	122.97	128.46
15	V	102	CRT	C21-C20-C19	-3.57	116.16	123.47
9	P	101	BCL	C4B-C3B-CAB	-3.57	120.24	127.13
15	A	101	CRT	C29-C28-C30	3.57	123.69	118.08
9	L	303	BCL	C4B-C3B-CAB	-3.57	120.24	127.13
15	R	102	CRT	C3-C1-C4	-3.56	105.39	110.86
9	6	101	BCL	C4B-C3B-CAB	-3.56	120.25	127.13
9	0	101	BCL	O2A-CGA-O1A	-3.56	114.61	123.59
15	A	101	CRT	C20-C19-C17	-3.56	122.23	127.31
9	D	102	BCL	CAA-C2A-C3A	-3.56	103.04	112.78
9	I	103	BCL	C4B-C3B-CAB	-3.55	120.27	127.13
9	E	101	BCL	O2A-CGA-O1A	-3.55	114.63	123.59
15	3	103	CRT	C11-C12-C14	-3.54	113.51	118.94
9	I	102	BCL	C1C-NC-C4C	3.54	108.30	106.71
9	B	101	BCL	C4B-C3B-CAB	-3.54	120.29	127.13
15	P	102	CRT	C15-C14-C12	3.54	132.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	CMB-C2B-C1B	-3.54	123.02	128.46
9	K	102	BCL	C1C-NC-C4C	3.53	108.29	106.71
9	4	101	BCL	O2A-CGA-O1A	-3.53	114.68	123.59
9	S	102	BCL	CMB-C2B-C1B	-3.53	123.04	128.46
9	E	101	BCL	C4B-C3B-CAB	-3.52	120.32	127.13
7	C	504	HEM	C2B-C1B-NB	3.52	114.01	109.84
9	V	101	BCL	O2D-CGD-CBD	3.52	117.53	111.27
9	G	101	BCL	C4B-C3B-CAB	-3.52	120.33	127.13
15	4	102	CRT	C8-C7-C9	-3.51	118.00	122.92
9	A	102	BCL	CMB-C2B-C1B	-3.51	123.07	128.46
15	P	102	CRT	C8-C7-C6	3.50	123.60	118.08
9	7	102	BCL	C4B-C3B-CAB	-3.50	120.37	127.13
15	N	102	CRT	C6-C7-C9	3.50	124.31	118.94
15	W	103	CRT	C8-C7-C9	-3.49	118.04	122.92
9	R	101	BCL	O2D-CGD-CBD	3.48	117.46	111.27
9	B	101	BCL	CMB-C2B-C1B	-3.48	123.12	128.46
15	B	102	CRT	C32-C31-C30	-3.47	112.38	123.22
9	9	102	BCL	CMB-C2B-C1B	-3.47	123.13	128.46
9	B	101	BCL	O2D-CGD-CBD	3.47	117.43	111.27
9	Y	102	BCL	C4B-C3B-CAB	-3.47	120.44	127.13
14	M	405	MQ8	C34-C33-C35	3.46	121.09	115.27
9	N	101	BCL	C1C-NC-C4C	3.45	108.26	106.71
9	L	301	BCL	OBB-CAB-CBB	-3.45	112.40	120.17
15	W	103	CRT	C15-C14-C12	3.45	132.23	127.31
15	3	103	CRT	C10-C9-C7	-3.45	122.39	127.31
15	B	102	CRT	C8-C7-C9	-3.45	118.10	122.92
15	J	101	CRT	C8-C7-C6	3.44	123.50	118.08
9	G	101	BCL	O2A-CGA-CBA	3.43	122.69	111.91
9	L	303	BCL	OBB-CAB-CBB	-3.42	112.47	120.17
11	L	304	UQ8	C46-C44-C43	-3.42	112.75	122.65
9	2	101	BCL	CBA-CAA-C2A	-3.42	103.76	113.86
15	3	103	CRT	C20-C19-C17	-3.42	122.43	127.31
15	2	102	CRT	C8-C7-C9	-3.42	118.14	122.92
15	2	102	CRT	C26-C27-C28	-3.41	122.44	127.31
9	3	102	BCL	OBB-CAB-CBB	-3.41	112.50	120.17
15	B	102	CRT	C18-C17-C16	3.40	123.43	118.08
9	L	301	BCL	O2D-CGD-CBD	3.40	117.30	111.27
15	N	102	CRT	C13-C12-C11	3.39	123.42	118.08
15	W	103	CRT	C14-C15-C16	-3.39	112.65	123.22
9	R	101	BCL	OBB-CAB-CBB	-3.39	112.55	120.17
15	V	102	CRT	C34-C33-C35	3.39	123.41	118.08
9	Q	102	BCL	C4D-CHA-C1A	3.39	125.37	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	OBB-CAB-CBB	-3.38	112.57	120.17
11	L	304	UQ8	C40-C39-C41	3.37	120.94	115.27
9	E	101	BCL	OBB-CAB-CBB	-3.37	112.58	120.17
9	6	101	BCL	O2A-CGA-O1A	-3.37	115.08	123.59
9	N	101	BCL	O2D-CGD-CBD	3.37	117.26	111.27
9	L	301	BCL	CAA-C2A-C3A	-3.37	103.55	112.78
9	0	101	BCL	OBB-CAB-CBB	-3.37	112.60	120.17
9	2	101	BCL	O2A-CGA-CBA	3.36	122.46	111.91
15	B	102	CRT	C29-C28-C30	3.36	123.37	118.08
9	V	101	BCL	OBB-CAB-CBB	-3.36	112.61	120.17
15	4	102	CRT	C11-C12-C14	-3.36	113.79	118.94
9	P	101	BCL	OBB-CAB-CBB	-3.36	112.62	120.17
15	M	406	CRT	C31-C32-C33	-3.35	122.52	127.31
15	R	102	CRT	C26-C27-C28	-3.35	122.53	127.31
9	F	102	BCL	OBB-CAB-CBB	-3.35	112.63	120.17
9	V	101	BCL	O2A-CGA-CBA	3.35	122.42	111.91
9	O	102	BCL	CMB-C2B-C1B	-3.35	123.32	128.46
15	R	102	CRT	C39-C38-C37	-3.35	105.72	110.86
9	G	101	BCL	OBB-CAB-CBB	-3.35	112.64	120.17
9	I	102	BCL	OBB-CAB-CBB	-3.34	112.64	120.17
9	2	101	BCL	OBB-CAB-CBB	-3.34	112.65	120.17
9	O	102	BCL	C4B-C3B-CAB	-3.34	120.68	127.13
9	R	101	BCL	CMB-C2B-C1B	-3.33	123.34	128.46
9	M	402	BCL	C4D-CHA-C1A	3.33	125.30	121.25
9	X	101	BCL	O2D-CGD-CBD	3.32	117.17	111.27
9	Z	101	BCL	O2A-CGA-CBA	3.32	122.31	111.91
15	V	102	CRT	C30-C28-C27	-3.31	113.86	118.94
9	A	102	BCL	OBB-CAB-CBB	-3.31	112.73	120.17
9	I	103	BCL	O2A-CGA-CBA	3.30	122.28	111.91
9	U	102	BCL	OBB-CAB-CBB	-3.29	112.76	120.17
9	P	101	BCL	O2D-CGD-CBD	3.29	117.12	111.27
9	7	103	BCL	OBB-CAB-CBB	-3.29	112.77	120.17
9	5	102	BCL	OBB-CAB-CBB	-3.29	112.78	120.17
9	K	102	BCL	OBB-CAB-CBB	-3.28	112.78	120.17
7	C	503	HEM	C2B-C1B-NB	3.28	113.72	109.84
9	Q	102	BCL	OBB-CAB-CBB	-3.28	112.80	120.17
9	0	101	BCL	C4B-C3B-CAB	-3.27	120.81	127.13
9	X	101	BCL	CMB-C2B-C1B	-3.27	123.43	128.46
11	L	304	UQ8	C16-C17-C18	-3.27	101.13	111.88
9	S	102	BCL	C4B-C3B-CAB	-3.27	120.81	127.13
9	T	101	BCL	O2A-CGA-CBA	3.27	122.17	111.91
15	V	102	CRT	C18-C17-C16	3.26	123.22	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	O2A-CGA-CBA	3.26	122.14	111.91
9	L	301	BCL	C2C-C3C-C4C	3.26	106.22	101.34
9	4	101	BCL	OBB-CAB-CBB	-3.26	112.84	120.17
9	7	103	BCL	C2C-C3C-C4C	3.25	106.21	101.34
9	6	101	BCL	OBB-CAB-CBB	-3.25	112.85	120.17
9	W	102	BCL	C4B-C3B-CAB	-3.25	120.85	127.13
9	7	102	BCL	OBB-CAB-CBB	-3.25	112.86	120.17
9	D	102	BCL	OBB-CAB-CBB	-3.24	112.87	120.17
7	C	501	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
9	B	101	BCL	O2A-CGA-O1A	-3.24	115.42	123.59
9	I	102	BCL	CAA-C2A-C3A	-3.23	103.92	112.78
9	X	101	BCL	OBB-CAB-CBB	-3.23	112.89	120.17
9	V	101	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
9	M	401	BCL	OBB-CAB-CBB	-3.23	112.90	120.17
15	R	102	CRT	C1-C4-C5	3.23	121.61	113.06
9	O	102	BCL	OBB-CAB-CBB	-3.23	112.90	120.17
7	C	502	HEM	C2B-C1B-NB	3.23	113.66	109.84
9	5	102	BCL	C4D-CHA-C1A	3.23	125.18	121.25
9	S	102	BCL	OBB-CAB-CBB	-3.22	112.91	120.17
15	B	102	CRT	C16-C17-C19	-3.22	113.99	118.94
9	X	101	BCL	C4B-CHC-C1C	-3.22	123.74	130.12
15	3	103	CRT	C13-C12-C11	3.21	123.14	118.08
9	0	101	BCL	O2A-CGA-CBA	3.21	121.99	111.91
9	7	103	BCL	O2A-CGA-O1A	-3.21	115.49	123.59
9	M	401	BCL	C4D-CHA-C1A	3.21	125.15	121.25
7	C	502	HEM	CMA-C3A-C4A	-3.21	123.54	128.46
9	G	101	BCL	C4B-CHC-C1C	-3.20	123.77	130.12
15	8	101	CRT	C15-C14-C12	-3.20	122.74	127.31
9	B	101	BCL	OBB-CAB-CBB	-3.20	112.97	120.17
15	J	101	CRT	C35-C33-C32	-3.20	114.03	118.94
9	2	101	BCL	C4B-CHC-C1C	-3.19	123.79	130.12
9	R	101	BCL	C2C-C3C-C4C	3.19	106.12	101.34
14	M	405	MQ8	C19-C18-C20	3.19	120.64	115.27
9	U	102	BCL	C4B-C3B-CAB	-3.18	120.98	127.13
15	8	101	CRT	C8-C7-C6	3.18	123.09	118.08
9	I	103	BCL	C4B-CHC-C1C	-3.18	123.81	130.12
15	J	101	CRT	C32-C31-C30	-3.18	113.29	123.22
9	X	101	BCL	O2A-CGA-CBA	3.18	121.88	111.91
14	M	405	MQ8	C36-C37-C38	-3.17	120.02	127.66
9	7	102	BCL	C1C-NC-C4C	3.17	108.13	106.71
11	L	304	UQ8	C7-C8-C9	-3.17	121.51	126.79
9	7	102	BCL	C2C-C3C-C4C	3.17	106.09	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	102	BCL	OBB-CAB-CBB	-3.17	113.04	120.17
9	M	402	BCL	OBB-CAB-CBB	-3.17	113.04	120.17
15	X	102	CRT	C18-C17-C19	-3.17	118.49	122.92
9	Z	101	BCL	OBB-CAB-CBB	-3.17	113.04	120.17
9	9	102	BCL	OBB-CAB-CBB	-3.17	113.05	120.17
9	Y	102	BCL	OBB-CAB-CBB	-3.16	113.05	120.17
9	V	101	BCL	C1C-NC-C4C	3.16	108.13	106.71
9	W	102	BCL	OBB-CAB-CBB	-3.16	113.06	120.17
7	C	503	HEM	C4A-C3A-C2A	3.16	109.19	107.00
9	7	102	BCL	C4D-CHA-C1A	3.16	125.09	121.25
15	W	103	CRT	C21-C22-C23	-3.15	122.81	127.31
9	9	102	BCL	C4D-CHA-C1A	3.15	125.08	121.25
9	P	101	BCL	C4B-CHC-C1C	-3.14	123.89	130.12
9	D	102	BCL	C2C-C3C-C4C	3.14	106.05	101.34
9	I	103	BCL	OBB-CAB-CBB	-3.14	113.11	120.17
9	3	102	BCL	CAA-C2A-C3A	-3.13	104.21	112.78
15	B	102	CRT	C15-C14-C12	-3.13	122.85	127.31
15	2	102	CRT	C11-C12-C14	-3.12	114.16	118.94
9	R	101	BCL	C4B-CHC-C1C	-3.12	123.95	130.12
9	T	101	BCL	C2C-C3C-C4C	3.12	106.01	101.34
7	C	504	HEM	CMA-C3A-C4A	-3.11	123.68	128.46
15	P	102	CRT	C9-C10-C11	-3.11	113.51	123.22
9	1	102	BCL	C2C-C3C-C4C	3.11	106.00	101.34
9	9	102	BCL	CAA-C2A-C3A	-3.10	104.28	112.78
9	I	102	BCL	C4D-CHA-C1A	3.10	125.02	121.25
9	Z	101	BCL	O2D-CGD-CBD	3.10	116.78	111.27
9	N	101	BCL	O2A-CGA-CBA	3.10	121.64	111.91
9	X	101	BCL	C2C-C3C-C4C	3.10	105.98	101.34
15	B	102	CRT	C36-C35-C33	-3.09	121.22	125.89
9	5	102	BCL	C2C-C3C-C4C	3.09	105.97	101.34
9	4	101	BCL	C2C-C3C-C4C	3.09	105.97	101.34
15	4	102	CRT	C29-C28-C30	3.09	122.94	118.08
9	6	101	BCL	C4B-CHC-C1C	-3.08	124.01	130.12
9	E	101	BCL	C2C-C3C-C4C	3.08	105.96	101.34
9	4	101	BCL	C4B-CHC-C1C	-3.08	124.01	130.12
9	M	402	BCL	C2C-C3C-C4C	3.08	105.95	101.34
9	E	101	BCL	C4B-CHC-C1C	-3.08	124.02	130.12
9	Y	102	BCL	C4B-CHC-C1C	-3.08	124.03	130.12
9	Z	101	BCL	C4B-CHC-C1C	-3.07	124.03	130.12
9	9	102	BCL	C2C-C3C-C4C	3.07	105.93	101.34
9	O	102	BCL	C2C-C3C-C4C	3.07	105.93	101.34
15	X	102	CRT	C3-C1-C2	-3.06	104.61	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	6	101	BCL	C2C-C3C-C4C	3.06	105.92	101.34
9	T	101	BCL	CMB-C2B-C1B	-3.06	123.76	128.46
9	K	102	BCL	C2C-C3C-C4C	3.06	105.92	101.34
9	N	101	BCL	C2C-C3C-C4C	3.06	105.92	101.34
9	7	102	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
9	A	102	BCL	C2C-C3C-C4C	3.05	105.91	101.34
15	3	103	CRT	C21-C22-C23	-3.05	122.95	127.31
9	T	101	BCL	C4B-CHC-C1C	-3.05	124.08	130.12
9	D	102	BCL	C4D-CHA-C1A	3.05	124.95	121.25
9	G	101	BCL	C2C-C3C-C4C	3.04	105.89	101.34
9	P	101	BCL	C2C-C3C-C4C	3.04	105.89	101.34
9	E	101	BCL	O2A-CGA-CBA	3.04	121.44	111.91
9	1	102	BCL	C4D-CHA-C1A	3.03	124.94	121.25
15	2	102	CRT	C13-C12-C11	3.03	122.85	118.08
15	2	102	CRT	C15-C16-C17	-3.03	117.91	126.42
15	2	102	CRT	C21-C20-C19	-3.03	117.27	123.47
15	J	101	CRT	C20-C19-C17	-3.02	123.00	127.31
15	A	101	CRT	C13-C12-C11	3.02	122.84	118.08
9	M	401	BCL	C2C-C3C-C4C	3.02	105.86	101.34
9	V	101	BCL	C2C-C3C-C4C	3.02	105.86	101.34
9	1	102	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
9	O	102	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
9	S	102	BCL	C2C-C3C-C4C	3.01	105.85	101.34
15	P	102	CRT	C25-C23-C22	-3.01	114.32	118.94
9	I	103	BCL	C2C-C3C-C4C	3.01	105.85	101.34
9	F	102	BCL	C2C-C3C-C4C	3.01	105.85	101.34
9	K	102	BCL	C4D-CHA-C1A	3.01	124.91	121.25
9	U	102	BCL	C2C-C3C-C4C	3.00	105.84	101.34
9	G	101	BCL	C1C-NC-C4C	3.00	108.05	106.71
9	L	301	BCL	CAA-CBA-CGA	3.00	122.01	113.25
9	Q	102	BCL	C2C-C3C-C4C	3.00	105.83	101.34
9	3	102	BCL	C2C-C3C-C4C	3.00	105.83	101.34
9	0	101	BCL	C4B-CHC-C1C	-3.00	124.18	130.12
9	Y	102	BCL	C2C-C3C-C4C	3.00	105.83	101.34
9	F	102	BCL	C4D-CHA-C1A	3.00	124.89	121.25
9	L	301	BCL	C1C-NC-C4C	2.99	108.05	106.71
9	N	101	BCL	C4B-CHC-C1C	-2.99	124.20	130.12
9	4	101	BCL	O2A-CGA-CBA	2.98	121.27	111.91
9	T	101	BCL	OBB-CAB-CBB	-2.98	113.45	120.17
9	I	102	BCL	C2C-C3C-C4C	2.98	105.80	101.34
10	M	403	BPH	C4C-C3C-C2C	-2.98	100.00	102.84
9	D	102	BCL	C4B-C3B-CAB	-2.97	121.38	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	103	BCL	O2D-CGD-O1D	-2.97	118.02	123.84
9	L	303	BCL	C2C-C3C-C4C	2.97	105.79	101.34
15	T	102	CRT	C3-C1-C2	2.97	115.96	110.37
14	M	405	MQ8	C31-C32-C33	-2.97	120.51	127.66
7	C	501	HEM	C4C-CHD-C1D	2.97	126.47	122.56
9	5	102	BCL	C4B-CHC-C1C	-2.96	124.25	130.12
17	H	301	PEF	O3-C30-C31	2.96	125.29	112.38
14	M	405	MQ8	C14-C13-C15	2.96	120.25	115.27
9	K	102	BCL	CAA-C2A-C3A	-2.95	104.70	112.78
15	P	102	CRT	C24-C23-C25	2.95	122.72	118.08
9	W	102	BCL	C4D-CHA-C1A	2.94	124.83	121.25
9	W	102	BCL	C4B-CHC-C1C	-2.94	124.29	130.12
9	Z	101	BCL	C2C-C3C-C4C	2.94	105.74	101.34
9	E	101	BCL	C1-O2A-CGA	2.94	124.15	116.44
9	A	102	BCL	C4B-CHC-C1C	-2.94	124.30	130.12
15	N	102	CRT	C32-C31-C30	-2.93	114.08	123.22
7	C	501	HEM	C4A-C3A-C2A	2.93	109.03	107.00
9	G	101	BCL	C2A-C3A-C4A	2.93	106.59	101.87
15	G	102	CRT	C10-C9-C7	-2.92	123.14	127.31
9	0	101	BCL	C2C-C3C-C4C	2.92	105.72	101.34
15	X	102	CRT	C20-C19-C17	-2.92	123.15	127.31
9	L	303	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
9	L	301	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
9	2	101	BCL	C2C-C3C-C4C	2.91	105.70	101.34
7	C	502	HEM	C4A-C3A-C2A	2.91	109.02	107.00
11	L	304	UQ8	C15-C14-C16	2.91	120.16	115.27
9	5	102	BCL	C1C-NC-C4C	2.90	108.01	106.71
9	R	101	BCL	C2A-C3A-C4A	2.90	106.55	101.87
15	T	102	CRT	C36-C35-C33	-2.90	121.51	125.89
9	7	103	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
7	C	503	HEM	CMA-C3A-C4A	-2.90	124.01	128.46
15	G	102	CRT	C21-C20-C19	-2.89	117.55	123.47
9	Z	101	BCL	C1C-NC-C4C	2.89	108.01	106.71
15	3	103	CRT	C14-C15-C16	-2.89	114.21	123.22
9	L	303	BCL	CAC-C3C-C4C	-2.89	106.18	112.58
9	A	102	BCL	C4D-CHA-C1A	2.88	124.76	121.25
9	S	102	BCL	C4B-CHC-C1C	-2.88	124.42	130.12
15	G	102	CRT	C32-C31-C30	-2.88	114.23	123.22
9	9	102	BCL	C4B-CHC-C1C	-2.88	124.42	130.12
9	W	102	BCL	C2C-C3C-C4C	2.87	105.64	101.34
9	U	102	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
9	3	102	BCL	C4B-CHC-C1C	-2.87	124.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	102	BCL	C1C-NC-C4C	2.86	107.99	106.71
15	R	102	CRT	C34-C33-C35	2.86	122.59	118.08
15	M	406	CRT	C36-C35-C33	-2.86	121.57	125.89
15	N	102	CRT	C30-C28-C27	-2.85	114.56	118.94
9	E	101	BCL	C2A-C3A-C4A	2.85	106.47	101.87
14	M	405	MQ8	C15-C13-C12	-2.85	115.35	121.12
9	K	102	BCL	C4B-CHC-C1C	-2.85	124.47	130.12
11	L	304	UQ8	C20-C19-C21	2.84	120.06	115.27
9	B	101	BCL	C4B-CHC-C1C	-2.84	124.49	130.12
15	T	102	CRT	C21-C22-C23	-2.84	123.26	127.31
9	Q	102	BCL	CAA-C2A-C3A	-2.84	105.01	112.78
15	X	102	CRT	C15-C16-C17	-2.83	118.47	126.42
11	L	304	UQ8	C22-C23-C24	-2.83	120.85	127.66
9	4	101	BCL	C1-O2A-CGA	2.83	123.86	116.44
15	A	103	CRT	C8-C7-C6	2.82	122.52	118.08
15	3	103	CRT	C32-C31-C30	-2.81	114.43	123.22
15	B	102	CRT	C27-C26-C25	-2.81	114.44	123.22
9	V	101	BCL	CMB-C2B-C3B	2.81	129.94	124.68
9	6	101	BCL	C1C-NC-C4C	2.81	107.97	106.71
15	T	102	CRT	C13-C12-C11	2.80	122.50	118.08
15	4	102	CRT	C20-C21-C22	-2.80	117.75	123.47
15	8	101	CRT	C32-C31-C30	-2.80	114.49	123.22
9	X	101	BCL	C2A-C3A-C4A	2.80	106.39	101.87
9	Q	102	BCL	O2D-CGD-O1D	-2.79	118.38	123.84
15	R	102	CRT	C20-C19-C17	-2.79	123.33	127.31
9	3	102	BCL	C4D-CHA-C1A	2.79	124.64	121.25
15	G	102	CRT	C29-C28-C30	2.78	122.46	118.08
9	5	102	BCL	CAA-C2A-C3A	-2.78	105.16	112.78
9	E	101	BCL	C6-C5-C3	2.78	120.75	113.45
9	T	101	BCL	C2A-C3A-C4A	2.78	106.36	101.87
9	M	402	BCL	C4B-CHC-C1C	-2.78	124.62	130.12
15	4	102	CRT	C5-C6-C7	-2.77	121.70	125.89
9	2	101	BCL	CAC-C3C-C4C	-2.77	106.43	112.58
15	2	102	CRT	C8-C7-C6	2.77	122.44	118.08
15	3	103	CRT	C16-C17-C19	2.77	123.19	118.94
9	0	101	BCL	C1-O2A-CGA	2.77	123.70	116.44
9	W	102	BCL	CAA-C2A-C3A	-2.76	105.21	112.78
15	W	103	CRT	C39-C38-C37	-2.76	106.61	110.86
15	X	102	CRT	C10-C11-C12	-2.76	118.67	126.42
15	X	102	CRT	C5-C6-C7	-2.75	121.74	125.89
9	U	102	BCL	CAA-C2A-C3A	-2.75	105.25	112.78
9	M	401	BCL	C4B-CHC-C1C	-2.75	124.67	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	C1-O2A-CGA	2.74	123.64	116.44
9	B	101	BCL	C2A-C3A-C4A	2.74	106.29	101.87
9	Q	102	BCL	C4B-CHC-C1C	-2.74	124.69	130.12
15	4	102	CRT	C24-C23-C25	2.74	122.39	118.08
9	P	101	BCL	C2A-C3A-C4A	2.73	106.28	101.87
9	A	102	BCL	CAA-C2A-C3A	-2.73	105.31	112.78
9	I	102	BCL	C4B-CHC-C1C	-2.73	124.72	130.12
9	1	102	BCL	O2D-CGD-O1D	-2.73	118.51	123.84
15	G	102	CRT	C20-C19-C17	-2.72	123.42	127.31
9	A	102	BCL	O2D-CGD-O1D	-2.72	118.52	123.84
7	C	502	HEM	C1D-C2D-C3D	-2.72	104.10	106.96
9	D	102	BCL	C4B-CHC-C1C	-2.72	124.74	130.12
15	A	101	CRT	C40-C38-C37	-2.71	106.69	110.86
15	3	103	CRT	C40-C38-C39	-2.71	105.27	110.37
15	V	102	CRT	C29-C28-C30	2.70	122.34	118.08
15	A	103	CRT	C40-C38-C39	-2.70	105.29	110.37
7	C	504	HEM	C4B-C3B-C2B	-2.70	104.97	107.11
9	Y	102	BCL	C4D-CHA-C1A	2.70	124.53	121.25
11	L	304	UQ8	C41-C42-C43	2.69	120.73	111.88
9	7	102	BCL	O2D-CGD-O1D	-2.69	118.58	123.84
9	L	303	BCL	C4D-CHA-C1A	2.69	124.52	121.25
15	A	101	CRT	C3-C1-C4	-2.69	106.73	110.86
15	2	102	CRT	C20-C19-C17	-2.69	123.48	127.31
15	A	103	CRT	C13-C12-C11	2.68	122.30	118.08
9	6	101	BCL	O2A-CGA-CBA	2.67	120.30	111.91
15	T	102	CRT	C1M-O1-C1	-2.67	100.34	117.25
9	B	101	BCL	C2C-C3C-C4C	2.67	105.34	101.34
9	7	102	BCL	CAA-C2A-C3A	-2.66	105.48	112.78
9	N	101	BCL	C2A-C3A-C4A	2.66	106.17	101.87
9	F	102	BCL	C4B-CHC-C1C	-2.66	124.86	130.12
9	S	102	BCL	CAA-C2A-C3A	-2.65	105.51	112.78
9	0	101	BCL	C2A-C3A-C4A	2.65	106.15	101.87
9	R	101	BCL	CAA-CBA-CGA	2.65	121.00	113.25
15	T	102	CRT	C14-C15-C16	-2.65	114.94	123.22
9	D	102	BCL	O2D-CGD-O1D	-2.65	118.66	123.84
15	R	102	CRT	C21-C20-C19	-2.65	118.05	123.47
15	2	102	CRT	C34-C33-C35	2.65	122.25	118.08
9	U	102	BCL	C4D-CHA-C1A	2.64	124.47	121.25
7	C	503	HEM	C3B-C2B-C1B	-2.64	104.53	106.49
15	A	103	CRT	C9-C10-C11	-2.64	114.98	123.22
15	8	101	CRT	C26-C27-C28	-2.64	123.55	127.31
15	2	102	CRT	C5-C6-C7	-2.63	121.91	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	102	CRT	C39-C38-C37	-2.63	106.82	110.86
9	5	102	BCL	O2D-CGD-O1D	-2.63	118.70	123.84
9	I	103	BCL	C4D-CHA-C1A	2.63	124.45	121.25
9	4	101	BCL	C2A-C3A-C4A	2.62	106.11	101.87
9	M	402	BCL	CMB-C2B-C3B	2.62	129.59	124.68
9	M	401	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
9	S	102	BCL	C4D-CHA-C1A	2.62	124.44	121.25
9	1	102	BCL	CAA-C2A-C3A	-2.62	105.61	112.78
15	B	102	CRT	C38-C37-C36	-2.61	106.14	113.06
14	M	405	MQ8	C11-C12-C13	-2.60	122.47	126.79
15	T	102	CRT	C21-C20-C19	-2.59	118.17	123.47
15	A	103	CRT	C11-C12-C14	-2.59	114.97	118.94
9	K	102	BCL	O2D-CGD-O1D	-2.59	118.78	123.84
15	X	102	CRT	C14-C15-C16	2.58	131.28	123.22
15	N	102	CRT	C29-C28-C30	2.58	122.15	118.08
9	Y	102	BCL	CAA-C2A-C3A	-2.58	105.71	112.78
9	X	101	BCL	C1-O2A-CGA	2.57	123.20	116.44
15	2	102	CRT	C32-C31-C30	-2.57	115.19	123.22
15	G	102	CRT	C34-C33-C35	2.57	122.13	118.08
9	B	101	BCL	C1-O2A-CGA	2.57	123.19	116.44
11	L	304	UQ8	C30-C29-C31	2.57	119.59	115.27
9	6	101	BCL	C1-O2A-CGA	2.57	123.18	116.44
15	P	102	CRT	C3-C1-C4	-2.57	106.92	110.86
15	V	102	CRT	C5-C6-C7	-2.56	122.02	125.89
9	W	102	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
9	L	303	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
9	P	101	BCL	C1C-NC-C4C	2.55	107.85	106.71
15	A	101	CRT	C30-C28-C27	-2.55	115.03	118.94
16	H	302	PGW	P-O12-C04	-2.55	106.75	121.68
9	2	101	BCL	CMB-C2B-C3B	2.55	129.44	124.68
16	H	302	PGW	P-O11-C03	-2.55	106.75	121.68
15	B	102	CRT	C14-C15-C16	-2.54	115.28	123.22
16	M	407	PGW	P-O12-C04	-2.54	106.76	121.68
7	C	502	HEM	C3B-C2B-C1B	-2.54	104.60	106.49
16	M	407	PGW	P-O11-C03	-2.54	106.78	121.68
11	L	304	UQ8	C10-C9-C11	2.53	119.53	115.27
9	3	102	BCL	O2D-CGD-O1D	-2.53	118.89	123.84
15	4	102	CRT	C26-C27-C28	-2.52	123.71	127.31
15	N	102	CRT	C21-C20-C19	-2.52	118.30	123.47
15	4	102	CRT	C18-C17-C16	2.52	122.05	118.08
15	G	102	CRT	C30-C28-C27	-2.52	115.07	118.94
15	R	102	CRT	C32-C31-C30	-2.52	115.37	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	101	CRT	C31-C32-C33	2.51	130.89	127.31
9	E	101	BCL	C1C-NC-C4C	2.51	107.83	106.71
9	L	301	BCL	CMB-C2B-C3B	2.51	129.38	124.68
9	Y	102	BCL	O2D-CGD-O1D	-2.51	118.94	123.84
9	B	101	BCL	O2A-CGA-CBA	2.50	119.77	111.91
9	5	102	BCL	CMB-C2B-C3B	2.50	129.36	124.68
14	M	405	MQ8	C24-C23-C25	2.50	119.48	115.27
15	N	102	CRT	C21-C22-C23	-2.50	123.75	127.31
9	4	101	BCL	C4D-CHA-C1A	2.50	124.29	121.25
9	I	103	BCL	C1-O2A-CGA	2.49	122.98	116.44
15	J	101	CRT	C29-C28-C30	2.49	122.00	118.08
9	7	103	BCL	C2A-C3A-C4A	2.49	105.89	101.87
7	C	504	HEM	C4C-CHD-C1D	2.49	125.84	122.56
9	G	101	BCL	CMB-C2B-C3B	2.49	129.33	124.68
9	F	102	BCL	CAA-C2A-C3A	-2.48	105.98	112.78
9	Z	101	BCL	CMB-C2B-C3B	2.48	129.31	124.68
9	0	101	BCL	CAC-C3C-C4C	-2.48	107.09	112.58
9	U	102	BCL	CHA-C1A-NA	-2.47	120.73	126.40
9	U	102	BCL	O2D-CGD-O1D	-2.47	119.00	123.84
9	L	303	BCL	CMB-C2B-C3B	2.47	129.30	124.68
15	J	101	CRT	C26-C27-C28	-2.47	123.79	127.31
7	C	501	HEM	C3B-C2B-C1B	-2.47	104.66	106.49
9	G	101	BCL	CHA-C1A-NA	-2.47	120.75	126.40
7	C	503	HEM	C4C-CHD-C1D	2.46	125.81	122.56
15	P	102	CRT	C5-C6-C7	2.45	129.59	125.89
15	A	103	CRT	C32-C31-C30	-2.44	115.59	123.22
15	G	102	CRT	C13-C12-C11	2.44	121.92	118.08
15	T	102	CRT	C5-C6-C7	-2.44	122.20	125.89
15	2	102	CRT	C29-C28-C30	2.44	121.92	118.08
14	M	405	MQ8	C44-C43-C42	-2.44	116.18	121.12
9	7	103	BCL	C6-C5-C3	2.44	119.85	113.45
9	T	101	BCL	C2A-C1A-CHA	2.43	128.12	123.86
15	8	101	CRT	C18-C17-C19	-2.43	119.52	122.92
15	M	406	CRT	C20-C19-C17	-2.43	123.84	127.31
9	X	101	BCL	CHA-C1A-NA	-2.43	120.84	126.40
15	J	101	CRT	C34-C33-C35	2.43	121.90	118.08
15	4	102	CRT	C25-C23-C22	-2.42	115.23	118.94
15	4	102	CRT	C13-C12-C11	2.41	121.87	118.08
9	6	101	BCL	C4D-CHA-C1A	2.41	124.18	121.25
9	I	103	BCL	CMB-C2B-C3B	2.41	129.18	124.68
15	A	101	CRT	C24-C23-C22	-2.41	119.55	122.92
9	3	102	BCL	CMB-C2B-C3B	2.40	129.18	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9	102	BCL	O2D-CGD-O1D	-2.40	119.15	123.84
15	3	103	CRT	C39-C38-C37	-2.40	107.18	110.86
15	T	102	CRT	C24-C23-C25	2.40	121.85	118.08
17	H	301	PEF	C3-C2-C1	-2.39	106.14	111.79
15	J	101	CRT	C10-C9-C7	2.39	130.72	127.31
9	7	103	BCL	O2A-CGA-CBA	2.39	119.40	111.91
9	T	101	BCL	CHA-C1A-NA	-2.38	120.94	126.40
9	Z	101	BCL	C2A-C3A-C4A	2.38	105.72	101.87
9	M	401	BCL	CMB-C2B-C3B	2.38	129.13	124.68
9	O	102	BCL	C4D-CHA-C1A	2.37	124.14	121.25
9	4	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
15	G	102	CRT	C8-C7-C6	2.37	121.81	118.08
9	6	101	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
15	4	102	CRT	C10-C11-C12	-2.36	119.79	126.42
7	C	502	HEM	CBA-CAA-C2A	-2.36	108.60	112.62
15	4	102	CRT	C29-C28-C27	-2.35	119.63	122.92
9	O	102	BCL	CAA-C2A-C3A	-2.35	106.34	112.78
7	C	502	HEM	C4C-CHD-C1D	2.35	125.66	122.56
9	2	101	BCL	C2A-C3A-C4A	2.35	105.67	101.87
9	7	103	BCL	CHA-C1A-NA	-2.35	121.02	126.40
15	2	102	CRT	C9-C10-C11	-2.35	115.89	123.22
9	Z	101	BCL	C3C-C2C-C1C	2.35	105.66	101.87
9	F	102	BCL	CMB-C2B-C3B	2.34	129.06	124.68
15	3	103	CRT	C8-C7-C6	2.34	121.77	118.08
15	8	101	CRT	C9-C10-C11	-2.34	115.91	123.22
15	R	102	CRT	C14-C15-C16	-2.34	115.91	123.22
15	G	102	CRT	C8-C7-C9	-2.34	119.64	122.92
15	M	406	CRT	C10-C9-C7	-2.34	123.97	127.31
15	A	103	CRT	C20-C21-C22	-2.33	118.69	123.47
9	I	102	BCL	CMB-C2B-C3B	2.33	129.05	124.68
9	K	102	BCL	CMB-C2B-C3B	2.33	129.04	124.68
9	9	102	BCL	C1C-NC-C4C	2.33	107.75	106.71
15	W	103	CRT	C16-C17-C19	2.33	122.52	118.94
9	T	101	BCL	CMB-C2B-C3B	2.33	129.04	124.68
9	Z	101	BCL	C1-O2A-CGA	2.33	122.55	116.44
9	Y	102	BCL	CMB-C2B-C3B	2.32	129.03	124.68
9	L	303	BCL	C2A-C3A-C4A	2.32	105.62	101.87
9	6	101	BCL	CMB-C2B-C3B	2.32	129.02	124.68
7	C	501	HEM	CHB-C1B-NB	-2.32	121.52	124.38
11	L	304	UQ8	C16-C14-C13	-2.32	116.42	121.12
15	T	102	CRT	C32-C31-C30	-2.32	115.98	123.22
9	L	301	BCL	C3A-C2A-C1A	2.32	104.81	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	X	102	CRT	C29-C28-C30	2.32	121.73	118.08
9	0	101	BCL	CMB-C2B-C3B	2.31	129.01	124.68
9	X	101	BCL	C4D-CHA-C1A	2.31	124.06	121.25
9	2	101	BCL	C1C-NC-C4C	2.31	107.75	106.71
9	Q	102	BCL	CMB-C2B-C3B	2.31	129.00	124.68
10	L	302	BPH	C1A-C2A-C3A	-2.31	100.64	102.84
9	N	101	BCL	CMA-C3A-C2A	-2.31	104.50	113.83
9	6	101	BCL	C2A-C3A-C4A	2.30	105.59	101.87
9	L	303	BCL	CMA-C3A-C2A	-2.30	104.55	113.83
15	W	103	CRT	C9-C10-C11	-2.30	116.04	123.22
15	M	406	CRT	C15-C14-C12	-2.30	124.03	127.31
15	X	102	CRT	C8-C7-C9	-2.30	119.71	122.92
15	A	103	CRT	C2-C1-C4	-2.30	107.33	110.86
9	0	101	BCL	C6-C5-C3	2.29	119.47	113.45
14	M	405	MQ8	C30-C28-C27	-2.29	116.48	121.12
15	T	102	CRT	C27-C26-C25	-2.29	116.07	123.22
9	M	402	BCL	C1B-CHB-C4A	-2.29	125.58	130.12
15	V	102	CRT	C16-C17-C19	2.29	122.45	118.94
15	8	101	CRT	C29-C28-C30	2.29	121.68	118.08
9	5	102	BCL	C1B-CHB-C4A	-2.29	125.59	130.12
9	B	101	BCL	CHA-C1A-NA	-2.28	121.17	126.40
9	R	101	BCL	CHA-C1A-NA	-2.28	121.18	126.40
15	V	102	CRT	C24-C23-C22	-2.28	119.73	122.92
9	P	101	BCL	CMB-C2B-C3B	2.28	128.94	124.68
15	B	102	CRT	C34-C33-C35	2.28	121.66	118.08
9	T	101	BCL	C3C-C2C-C1C	2.27	105.54	101.87
15	W	103	CRT	C18-C17-C16	-2.27	114.50	118.08
9	7	103	BCL	CMB-C2B-C3B	2.27	128.93	124.68
15	W	103	CRT	C20-C19-C17	-2.27	124.07	127.31
9	7	102	BCL	CMB-C2B-C3B	2.26	128.91	124.68
9	A	102	BCL	CMB-C2B-C3B	2.26	128.91	124.68
9	B	101	BCL	C4D-CHA-C1A	2.26	124.00	121.25
9	W	102	BCL	C3C-C2C-C1C	2.26	105.52	101.87
9	M	401	BCL	CMA-C3A-C2A	-2.25	104.74	113.83
9	3	102	BCL	CHA-C1A-NA	-2.25	121.24	126.40
9	E	101	BCL	CMB-C2B-C3B	2.25	128.89	124.68
15	R	102	CRT	C35-C33-C32	-2.25	115.49	118.94
9	2	101	BCL	CMA-C3A-C2A	-2.25	104.75	113.83
15	A	101	CRT	C8-C7-C9	-2.25	119.78	122.92
15	W	103	CRT	C29-C28-C30	2.24	121.61	118.08
15	2	102	CRT	C15-C14-C12	-2.24	124.11	127.31
15	3	103	CRT	C29-C28-C30	2.24	121.60	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	CMB-C2B-C3B	2.24	128.86	124.68
15	8	101	CRT	C35-C33-C32	-2.24	115.51	118.94
9	I	102	BCL	CHA-C1A-NA	-2.24	121.28	126.40
9	Z	101	BCL	CHA-C1A-NA	-2.24	121.28	126.40
15	T	102	CRT	C11-C12-C14	-2.24	115.51	118.94
11	L	304	UQ8	C25-C24-C26	2.23	119.03	115.27
15	R	102	CRT	C29-C28-C30	2.23	121.59	118.08
9	E	101	BCL	CAA-C2A-C1A	2.23	119.29	111.97
15	A	103	CRT	C39-C38-C37	-2.23	107.43	110.86
9	G	101	BCL	CAA-CBA-CGA	2.23	119.77	113.25
15	4	102	CRT	C40-C38-C37	-2.23	107.44	110.86
15	2	102	CRT	C3-C1-C4	-2.22	107.44	110.86
15	A	103	CRT	C24-C23-C25	2.22	121.58	118.08
11	L	304	UQ8	C37-C38-C39	-2.22	122.31	127.66
9	1	102	BCL	C3C-C2C-C1C	2.22	105.46	101.87
9	X	101	BCL	C2A-C1A-CHA	2.22	127.74	123.86
9	I	103	BCL	C1C-NC-C4C	2.22	107.70	106.71
9	N	101	BCL	C6-C5-C3	2.22	119.28	113.45
15	8	101	CRT	C34-C33-C35	2.22	121.57	118.08
9	7	102	BCL	CMA-C3A-C2A	-2.22	104.88	113.83
9	1	102	BCL	CMB-C2B-C3B	2.22	128.83	124.68
9	S	102	BCL	O2D-CGD-O1D	-2.21	119.51	123.84
9	T	101	BCL	C1-O2A-CGA	2.21	122.25	116.44
9	P	101	BCL	CHA-C1A-NA	-2.21	121.33	126.40
9	L	301	BCL	C4D-CHA-C1A	2.21	123.94	121.25
9	T	101	BCL	C4D-CHA-C1A	2.21	123.94	121.25
9	V	101	BCL	C4D-CHA-C1A	2.21	123.94	121.25
9	F	102	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
15	M	406	CRT	C26-C27-C28	-2.21	124.16	127.31
9	G	101	BCL	C3C-C2C-C1C	2.21	105.43	101.87
15	B	102	CRT	C13-C12-C11	2.20	121.55	118.08
9	P	101	BCL	C1-O2A-CGA	2.20	122.22	116.44
9	F	102	BCL	C3C-C2C-C1C	2.20	105.43	101.87
15	N	102	CRT	C27-C26-C25	-2.20	116.35	123.22
9	6	101	BCL	C3C-C2C-C1C	2.20	105.42	101.87
16	H	302	PGW	O01-C02-C03	2.20	116.37	108.40
9	X	101	BCL	CAA-C2A-C1A	2.20	119.18	111.97
9	O	102	BCL	C2A-C1A-CHA	2.20	127.70	123.86
9	G	101	BCL	O2D-CGD-O1D	-2.20	119.54	123.84
9	N	101	BCL	C4D-CHA-C1A	2.20	123.92	121.25
9	S	102	BCL	CHD-C1D-ND	-2.20	122.43	124.45
9	A	102	BCL	CMA-C3A-C2A	-2.20	104.96	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	101	BCL	C3C-C2C-C1C	2.20	105.42	101.87
16	M	407	PGW	O01-C02-C03	2.20	116.35	108.40
10	L	302	BPH	CAC-C3C-C4C	-2.19	108.83	113.73
9	0	101	BCL	C3C-C2C-C1C	2.19	105.41	101.87
9	U	102	BCL	C2A-C1A-CHA	2.19	127.69	123.86
9	W	102	BCL	CHA-C1A-NA	-2.19	121.38	126.40
15	T	102	CRT	C8-C7-C6	2.19	121.53	118.08
10	L	302	BPH	OBB-CAB-CBB	-2.19	115.25	120.17
9	O	102	BCL	C3C-C2C-C1C	2.19	105.40	101.87
9	B	101	BCL	C3C-C2C-C1C	2.19	105.40	101.87
15	G	102	CRT	C14-C15-C16	-2.19	116.39	123.22
15	W	103	CRT	C40-C38-C39	-2.19	106.26	110.37
9	K	102	BCL	C6-C5-C3	2.19	119.19	113.45
9	3	102	BCL	CMA-C3A-C2A	-2.19	105.01	113.83
9	E	101	BCL	CHA-C1A-NA	-2.18	121.40	126.40
9	V	101	BCL	CHA-C1A-NA	-2.18	121.40	126.40
9	5	102	BCL	C3C-C2C-C1C	2.18	105.39	101.87
9	R	101	BCL	C1C-NC-C4C	2.18	107.69	106.71
9	I	102	BCL	C2A-C3A-C4A	2.18	105.39	101.87
9	D	102	BCL	CHD-C1D-ND	-2.18	122.45	124.45
9	S	102	BCL	C3C-C2C-C1C	2.18	105.38	101.87
9	P	101	BCL	C4D-CHA-C1A	2.18	123.90	121.25
9	I	103	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
9	O	102	BCL	CHA-C1A-NA	-2.17	121.42	126.40
15	V	102	CRT	C15-C16-C17	-2.17	120.31	126.42
15	M	406	CRT	C21-C22-C23	-2.17	124.21	127.31
15	2	102	CRT	C35-C33-C32	-2.17	115.61	118.94
9	X	101	BCL	C3C-C2C-C1C	2.17	105.37	101.87
9	0	101	BCL	CMA-C3A-C2A	-2.17	105.08	113.83
9	R	101	BCL	CMB-C2B-C3B	2.17	128.73	124.68
9	2	101	BCL	C1-O2A-CGA	2.17	122.13	116.44
15	G	102	CRT	C24-C23-C25	2.16	121.49	118.08
9	4	101	BCL	C3C-C2C-C1C	2.16	105.36	101.87
9	I	103	BCL	C2A-C3A-C4A	2.16	105.36	101.87
9	Y	102	BCL	CHD-C1D-ND	-2.16	122.47	124.45
15	J	101	CRT	C39-C38-C37	-2.16	107.54	110.86
14	M	405	MQ8	C16-C17-C18	-2.16	122.46	127.66
15	T	102	CRT	C8-C7-C9	-2.16	119.90	122.92
9	M	402	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
9	9	102	BCL	CMB-C2B-C3B	2.16	128.72	124.68
7	C	503	HEM	CHB-C1B-NB	-2.15	121.72	124.38
15	M	406	CRT	C24-C23-C25	2.15	121.47	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	405	MQ8	C50-C48-C49	2.15	119.35	114.60
9	7	103	BCL	CMA-C3A-C2A	-2.15	105.15	113.83
9	5	102	BCL	CHD-C1D-ND	-2.15	122.48	124.45
9	G	101	BCL	CMA-C3A-C2A	-2.15	105.16	113.83
9	9	102	BCL	CMA-C3A-C2A	-2.15	105.16	113.83
9	D	102	BCL	C3C-C2C-C1C	2.15	105.33	101.87
10	M	403	BPH	CMA-C3A-C4A	-2.14	109.68	114.38
7	C	503	HEM	C1D-C2D-C3D	-2.14	104.70	106.96
15	M	406	CRT	C13-C12-C11	2.14	121.45	118.08
9	V	101	BCL	C1-O2A-CGA	2.14	122.06	116.44
9	E	101	BCL	C3C-C2C-C1C	2.14	105.33	101.87
9	9	102	BCL	C3C-C2C-C1C	2.14	105.33	101.87
9	4	101	BCL	CHA-C1A-NA	-2.14	121.49	126.40
15	N	102	CRT	C34-C33-C35	2.14	121.45	118.08
9	V	101	BCL	C2A-C3A-C4A	2.14	105.33	101.87
9	W	102	BCL	CMB-C2B-C3B	2.14	128.68	124.68
15	2	102	CRT	C26-C25-C23	-2.14	120.41	126.42
9	N	101	BCL	C3C-C2C-C1C	2.14	105.32	101.87
9	D	102	BCL	CMA-C3A-C2A	-2.14	105.21	113.83
9	D	102	BCL	CHA-C1A-NA	-2.14	121.50	126.40
9	I	103	BCL	C3C-C2C-C1C	2.14	105.32	101.87
9	U	102	BCL	CMB-C2B-C3B	2.13	128.67	124.68
9	M	402	BCL	CHD-C1D-ND	-2.13	122.50	124.45
9	I	102	BCL	C3C-C2C-C1C	2.13	105.31	101.87
9	3	102	BCL	C3C-C2C-C1C	2.13	105.31	101.87
9	L	303	BCL	C6-C5-C3	2.13	119.04	113.45
9	7	103	BCL	C4D-CHA-C1A	2.13	123.84	121.25
15	X	102	CRT	C32-C31-C30	-2.13	116.58	123.22
15	G	102	CRT	C35-C33-C32	-2.13	115.68	118.94
9	E	101	BCL	C2A-C1A-CHA	2.13	127.58	123.86
9	I	102	BCL	O2D-CGD-O1D	-2.13	119.68	123.84
9	L	303	BCL	C3C-C2C-C1C	2.13	105.30	101.87
9	R	101	BCL	C2A-C1A-CHA	2.13	127.58	123.86
9	4	101	BCL	CMA-C3A-C2A	-2.12	105.26	113.83
15	T	102	CRT	C29-C28-C30	2.12	121.42	118.08
9	X	101	BCL	C6-C5-C3	2.12	119.02	113.45
15	8	101	CRT	C21-C20-C19	-2.12	119.13	123.47
9	Q	102	BCL	C1B-CHB-C4A	-2.12	125.91	130.12
9	I	102	BCL	C2A-C1A-CHA	2.12	127.57	123.86
9	K	102	BCL	C3C-C2C-C1C	2.12	105.30	101.87
9	2	101	BCL	C3C-C2C-C1C	2.12	105.30	101.87
9	B	101	BCL	CMA-C3A-C2A	-2.12	105.27	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	102	BCL	CMA-C3A-C2A	-2.12	105.27	113.83
9	X	101	BCL	CMB-C2B-C3B	2.12	128.64	124.68
9	0	101	BCL	O2D-CGD-O1D	-2.12	119.70	123.84
9	Q	102	BCL	C3C-C2C-C1C	2.11	105.27	101.87
9	R	101	BCL	CHD-C1D-ND	-2.11	122.52	124.45
9	D	102	BCL	C2A-C1A-CHA	2.11	127.54	123.86
9	P	101	BCL	CAC-C3C-C4C	-2.11	107.91	112.58
9	3	102	BCL	CHD-C1D-ND	-2.11	122.52	124.45
15	A	101	CRT	C10-C11-C12	-2.10	120.50	126.42
9	6	101	BCL	CAC-C3C-C4C	-2.10	107.91	112.58
9	B	101	BCL	CMB-C2B-C3B	2.10	128.61	124.68
9	4	101	BCL	C6-C5-C3	2.10	118.97	113.45
9	2	101	BCL	CHA-C1A-NA	-2.10	121.59	126.40
15	W	103	CRT	C34-C33-C35	2.10	121.39	118.08
9	Z	101	BCL	C4D-CHA-C1A	2.10	123.80	121.25
9	K	102	BCL	CHA-C1A-NA	-2.10	121.59	126.40
9	O	102	BCL	CBA-CAA-C2A	-2.10	107.67	113.86
15	4	102	CRT	C32-C31-C30	-2.10	116.67	123.22
15	J	101	CRT	C11-C12-C14	-2.10	115.72	118.94
9	T	101	BCL	C6-C5-C3	2.10	118.95	113.45
9	R	101	BCL	C3C-C2C-C1C	2.09	105.25	101.87
9	M	402	BCL	C3C-C2C-C1C	2.09	105.25	101.87
15	B	102	CRT	C2-C1-C4	-2.09	107.64	110.86
9	F	102	BCL	CHA-C1A-NA	-2.09	121.61	126.40
9	D	102	BCL	CMB-C2B-C3B	2.09	128.59	124.68
15	A	101	CRT	C9-C10-C11	-2.09	116.69	123.22
9	0	101	BCL	CHA-C1A-NA	-2.09	121.61	126.40
9	Z	101	BCL	C6-C5-C3	2.09	118.94	113.45
9	Y	102	BCL	CMA-C3A-C2A	-2.09	105.40	113.83
9	Y	102	BCL	C3C-C2C-C1C	2.09	105.24	101.87
9	7	102	BCL	C3C-C2C-C1C	2.09	105.24	101.87
11	L	304	UQ8	C42-C43-C44	-2.09	120.61	127.75
9	V	101	BCL	C2A-C1A-CHA	2.08	127.50	123.86
9	M	401	BCL	CHA-C1A-NA	-2.08	121.63	126.40
11	L	304	UQ8	C3M-O3-C3	-2.08	109.10	116.47
15	B	102	CRT	C10-C11-C12	-2.08	120.58	126.42
9	1	102	BCL	CMA-C3A-C2A	-2.07	105.46	113.83
9	N	101	BCL	CHA-C1A-NA	-2.07	121.65	126.40
7	C	501	HEM	C1D-C2D-C3D	-2.07	104.78	106.96
9	I	103	BCL	CHD-C1D-ND	-2.07	122.55	124.45
9	I	103	BCL	C6-C5-C3	2.07	118.87	113.45
9	A	102	BCL	C3C-C2C-C1C	2.07	105.20	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	CMA-C3A-C2A	-2.06	105.50	113.83
15	J	101	CRT	C21-C20-C19	-2.06	119.25	123.47
15	J	101	CRT	C30-C28-C27	-2.06	115.78	118.94
7	C	501	HEM	C4B-C3B-C2B	-2.06	105.48	107.11
9	T	101	BCL	O2D-CGD-O1D	-2.05	119.82	123.84
9	W	102	BCL	CHD-C1D-ND	-2.05	122.57	124.45
9	O	102	BCL	CHD-C1D-ND	-2.05	122.57	124.45
15	4	102	CRT	C27-C26-C25	-2.05	116.82	123.22
9	V	101	BCL	C6-C5-C3	2.05	118.83	113.45
9	F	102	BCL	CMA-C3A-C2A	-2.05	105.56	113.83
9	K	102	BCL	C2A-C3A-C4A	2.05	105.18	101.87
9	R	101	BCL	CMA-C3A-C2A	-2.05	105.56	113.83
15	2	102	CRT	C40-C38-C37	-2.05	107.71	110.86
9	L	301	BCL	C2A-C1A-CHA	2.05	127.44	123.86
9	E	101	BCL	O2D-CGD-O1D	-2.05	119.83	123.84
9	M	401	BCL	C2A-C3A-C4A	2.05	105.18	101.87
9	M	402	BCL	C2A-C3A-C4A	2.05	105.18	101.87
9	L	301	BCL	CMA-C3A-C2A	-2.05	105.57	113.83
11	L	304	UQ8	C31-C29-C28	-2.05	116.98	121.12
9	2	101	BCL	O2D-CGD-O1D	-2.04	119.84	123.84
9	G	101	BCL	CAA-C2A-C1A	2.04	118.67	111.97
15	M	406	CRT	C5-C6-C7	-2.04	122.81	125.89
9	S	102	BCL	CMB-C2B-C3B	2.04	128.50	124.68
9	L	301	BCL	CHA-C1A-NA	-2.04	121.72	126.40
9	I	102	BCL	CHD-C1D-ND	-2.04	122.58	124.45
15	P	102	CRT	C29-C28-C27	-2.04	120.06	122.92
15	G	102	CRT	C27-C26-C25	-2.04	116.86	123.22
9	0	101	BCL	CAA-CBA-CGA	2.03	119.19	113.25
15	A	103	CRT	C14-C15-C16	-2.03	116.87	123.22
9	I	103	BCL	C1B-CHB-C4A	-2.03	126.10	130.12
9	E	101	BCL	C4D-CHA-C1A	2.03	123.72	121.25
9	L	303	BCL	C1B-CHB-C4A	-2.03	126.10	130.12
15	R	102	CRT	C26-C25-C23	-2.03	120.73	126.42
15	R	102	CRT	C18-C17-C16	2.03	121.27	118.08
14	M	405	MQ8	C21-C22-C23	-2.03	122.78	127.66
9	3	102	BCL	C2A-C3A-C4A	2.02	105.14	101.87
11	L	304	UQ8	C4M-O4-C4	-2.02	109.30	116.47
9	K	102	BCL	CMA-C3A-C2A	-2.02	105.67	113.83
15	8	101	CRT	C10-C9-C7	-2.02	124.42	127.31
15	4	102	CRT	C16-C17-C19	-2.02	115.84	118.94
9	9	102	BCL	CHA-C1A-NA	-2.02	121.77	126.40
15	W	103	CRT	C8-C7-C6	2.02	121.26	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	102	BCL	C6-C5-C3	2.02	118.75	113.45
9	O	102	BCL	O2D-CGD-O1D	-2.02	119.89	123.84
9	M	401	BCL	C3C-C2C-C1C	2.02	105.13	101.87
15	4	102	CRT	C14-C15-C16	-2.02	116.92	123.22
9	6	101	BCL	CMA-C3A-C2A	-2.02	105.70	113.83
9	L	301	BCL	C3C-C2C-C1C	2.01	105.12	101.87
9	G	101	BCL	C2A-C1A-CHA	2.01	127.37	123.86
7	C	502	HEM	C4D-ND-C1D	2.01	107.15	105.07
9	P	101	BCL	C3C-C2C-C1C	2.01	105.11	101.87
9	M	401	BCL	C6-C5-C3	2.01	118.72	113.45
9	X	101	BCL	CAC-C3C-C4C	-2.01	108.13	112.58
15	V	102	CRT	C25-C23-C22	2.01	122.02	118.94
15	M	406	CRT	C18-C17-C16	2.00	121.23	118.08
9	P	101	BCL	C6-C5-C3	2.00	118.71	113.45
9	3	102	BCL	C6-C5-C3	2.00	118.71	113.45
15	V	102	CRT	C8-C7-C6	2.00	121.23	118.08
9	6	101	BCL	C6-C5-C3	2.00	118.70	113.45

There are no chirality outliers.

All (695) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C4B-C3B-CAB-CBB
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	C	504	HEM	C2B-C3B-CAB-CBB
7	C	504	HEM	C4B-C3B-CAB-CBB
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	303	BCL	C1A-C2A-CAA-CBA
9	M	401	BCL	C2-C3-C5-C6
9	M	401	BCL	C4-C3-C5-C6
9	M	402	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C3A-C2A-CAA-CBA
9	B	101	BCL	C2C-C3C-CAC-CBC
9	B	101	BCL	C4C-C3C-CAC-CBC
9	F	102	BCL	C1A-C2A-CAA-CBA
9	F	102	BCL	C4C-C3C-CAC-CBC
9	I	102	BCL	C1A-C2A-CAA-CBA
9	I	102	BCL	C2C-C3C-CAC-CBC
9	I	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	I	103	BCL	C2C-C3C-CAC-CBC
9	I	103	BCL	C4C-C3C-CAC-CBC
9	K	102	BCL	C2C-C3C-CAC-CBC
9	K	102	BCL	C4C-C3C-CAC-CBC
9	N	101	BCL	C2C-C3C-CAC-CBC
9	N	101	BCL	C4C-C3C-CAC-CBC
9	O	102	BCL	C1A-C2A-CAA-CBA
9	O	102	BCL	C2C-C3C-CAC-CBC
9	O	102	BCL	C4C-C3C-CAC-CBC
9	P	101	BCL	C2C-C3C-CAC-CBC
9	P	101	BCL	C4C-C3C-CAC-CBC
9	Q	102	BCL	C3A-C2A-CAA-CBA
9	Q	102	BCL	C4C-C3C-CAC-CBC
9	R	101	BCL	C4C-C3C-CAC-CBC
9	S	102	BCL	C1A-C2A-CAA-CBA
9	S	102	BCL	C2C-C3C-CAC-CBC
9	S	102	BCL	C4C-C3C-CAC-CBC
9	T	101	BCL	C4C-C3C-CAC-CBC
9	U	102	BCL	C1A-C2A-CAA-CBA
9	V	101	BCL	C4C-C3C-CAC-CBC
9	W	102	BCL	C4C-C3C-CAC-CBC
9	X	101	BCL	C2C-C3C-CAC-CBC
9	X	101	BCL	C4C-C3C-CAC-CBC
9	Y	102	BCL	C4C-C3C-CAC-CBC
9	1	102	BCL	C4C-C3C-CAC-CBC
9	3	102	BCL	C4C-C3C-CAC-CBC
9	5	102	BCL	C2C-C3C-CAC-CBC
9	5	102	BCL	C4C-C3C-CAC-CBC
9	6	101	BCL	C4C-C3C-CAC-CBC
9	6	101	BCL	CHA-CBD-CGD-O1D
9	6	101	BCL	CHA-CBD-CGD-O2D
9	7	102	BCL	C1A-C2A-CAA-CBA
9	7	102	BCL	C3A-C2A-CAA-CBA
9	0	101	BCL	C2C-C3C-CAC-CBC
9	0	101	BCL	C4C-C3C-CAC-CBC
10	L	302	BPH	O2A-C1-C2-C3
14	M	405	MQ8	C28-C30-C31-C32
15	A	101	CRT	C35-C36-C37-C38
15	A	103	CRT	C35-C36-C37-C38
15	B	102	CRT	C1-C4-C5-C6
15	B	102	CRT	C35-C36-C37-C38
15	B	102	CRT	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	B	102	CRT	C36-C37-C38-C40
15	G	102	CRT	C35-C36-C37-C38
15	J	101	CRT	C1-C4-C5-C6
15	N	102	CRT	C1-C4-C5-C6
15	N	102	CRT	C35-C36-C37-C38
15	P	102	CRT	C35-C36-C37-C38
15	R	102	CRT	C1-C4-C5-C6
15	T	102	CRT	C1-C4-C5-C6
15	T	102	CRT	C35-C36-C37-C38
15	V	102	CRT	C35-C36-C37-C38
15	V	102	CRT	C36-C37-C38-C39
15	V	102	CRT	C36-C37-C38-C40
15	V	102	CRT	C36-C37-C38-O2
15	W	103	CRT	C35-C36-C37-C38
15	X	102	CRT	C1-C4-C5-C6
15	2	102	CRT	C35-C36-C37-C38
15	3	103	CRT	C1-C4-C5-C6
15	3	103	CRT	C35-C36-C37-C38
15	4	102	CRT	C1-C4-C5-C6
15	4	102	CRT	C35-C36-C37-C38
15	8	101	CRT	C35-C36-C37-C38
16	M	407	PGW	C03-O11-P-O12
16	M	407	PGW	C03-O11-P-O13
16	M	407	PGW	C03-O11-P-O14
16	M	407	PGW	C2-C1-O01-C02
16	M	407	PGW	O12-C04-C05-OAF
17	H	301	PEF	O4P-C4-C5-N
17	H	301	PEF	C11-C10-O2-C2
17	H	301	PEF	O4-C10-O2-C2
17	H	301	PEF	C1-O3P-P-O1P
17	H	301	PEF	C1-O3P-P-O2P
17	H	301	PEF	C1-O3P-P-O4P
17	H	301	PEF	C4-O4P-P-O1P
17	H	301	PEF	C4-O4P-P-O2P
17	H	301	PEF	C4-O4P-P-O3P
16	H	302	PGW	C2-C1-O01-C02
9	L	301	BCL	C3-C5-C6-C7
9	M	401	BCL	C3-C5-C6-C7
9	B	101	BCL	C3-C5-C6-C7
9	D	102	BCL	C3-C5-C6-C7
9	I	103	BCL	C3-C5-C6-C7
9	R	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	X	101	BCL	C3-C5-C6-C7
9	2	101	BCL	C3-C5-C6-C7
9	6	101	BCL	C3-C5-C6-C7
9	0	101	BCL	C3-C5-C6-C7
16	M	407	PGW	O02-C1-O01-C02
17	H	301	PEF	C31-C30-O3-C3
14	M	405	MQ8	C29-C28-C30-C31
14	M	405	MQ8	C27-C28-C30-C31
9	Z	101	BCL	C3-C5-C6-C7
9	P	101	BCL	C3-C5-C6-C7
9	T	101	BCL	C3-C5-C6-C7
9	V	101	BCL	C3-C5-C6-C7
9	3	102	BCL	C3-C5-C6-C7
9	4	101	BCL	C3-C5-C6-C7
9	7	103	BCL	C3-C5-C6-C7
14	M	405	MQ8	C34-C33-C35-C36
14	M	405	MQ8	C39-C38-C40-C41
14	M	405	MQ8	C45-C43-C44-C46
14	M	405	MQ8	C32-C33-C35-C36
14	M	405	MQ8	C37-C38-C40-C41
14	M	405	MQ8	C42-C43-C44-C46
11	L	304	UQ8	C24-C26-C27-C28
16	H	302	PGW	O02-C1-O01-C02
16	M	407	PGW	O12-C04-C05-CAD
9	M	402	BCL	C13-C15-C16-C17
9	M	401	BCL	C6-C7-C8-C9
10	M	403	BPH	C14-C13-C15-C16
9	L	303	BCL	C5-C6-C7-C8
10	L	302	BPH	C5-C6-C7-C8
9	M	402	BCL	C3-C5-C6-C7
17	H	301	PEF	O5-C30-O3-C3
7	C	501	HEM	C2A-CAA-CBA-CGA
9	M	402	BCL	C8-C10-C11-C12
9	F	102	BCL	C5-C6-C7-C8
9	I	102	BCL	C5-C6-C7-C8
9	K	102	BCL	C5-C6-C7-C8
9	3	102	BCL	C15-C16-C17-C18
9	1	102	BCL	C15-C16-C17-C18
9	L	301	BCL	C11-C10-C8-C7
9	M	401	BCL	C11-C12-C13-C15
9	P	101	BCL	C6-C7-C8-C10
9	T	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	Y	102	BCL	C11-C10-C8-C7
9	5	102	BCL	C11-C10-C8-C7
9	6	101	BCL	C6-C7-C8-C10
10	M	403	BPH	C6-C7-C8-C10
9	L	303	BCL	C3-C5-C6-C7
9	D	102	BCL	C15-C16-C17-C18
9	F	102	BCL	C15-C16-C17-C18
9	U	102	BCL	C15-C16-C17-C18
9	6	101	BCL	C5-C6-C7-C8
9	A	102	BCL	C3-C5-C6-C7
9	Q	102	BCL	C3-C5-C6-C7
9	5	102	BCL	C5-C6-C7-C8
9	A	102	BCL	C5-C6-C7-C8
9	A	102	BCL	C13-C15-C16-C17
9	D	102	BCL	C8-C10-C11-C12
9	G	101	BCL	C10-C11-C12-C13
9	Q	102	BCL	C5-C6-C7-C8
9	1	102	BCL	C5-C6-C7-C8
9	7	102	BCL	C5-C6-C7-C8
9	9	102	BCL	C5-C6-C7-C8
10	M	403	BPH	C10-C11-C12-C13
9	M	401	BCL	C10-C11-C12-C13
9	A	102	BCL	C8-C10-C11-C12
9	G	101	BCL	C13-C15-C16-C17
9	O	102	BCL	C5-C6-C7-C8
9	O	102	BCL	C15-C16-C17-C18
9	S	102	BCL	C5-C6-C7-C8
9	U	102	BCL	C5-C6-C7-C8
9	3	102	BCL	C5-C6-C7-C8
9	5	102	BCL	C8-C10-C11-C12
9	D	102	BCL	C5-C6-C7-C8
9	R	101	BCL	C15-C16-C17-C18
9	X	101	BCL	C15-C16-C17-C18
9	A	102	BCL	C4-C3-C5-C6
9	F	102	BCL	C8-C10-C11-C12
9	Y	102	BCL	C3-C5-C6-C7
16	M	407	PGW	O04-C19-O03-C01
9	L	301	BCL	C15-C16-C17-C18
9	Q	102	BCL	C8-C10-C11-C12
9	1	102	BCL	C8-C10-C11-C12
9	O	102	BCL	C3-C5-C6-C7
9	B	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	P	101	BCL	C16-C17-C18-C20
9	6	101	BCL	C16-C17-C18-C20
16	M	407	PGW	C20-C19-O03-C01
9	E	101	BCL	C15-C16-C17-C18
9	M	401	BCL	C8-C10-C11-C12
9	I	103	BCL	C16-C17-C18-C20
9	T	101	BCL	C16-C17-C18-C20
9	7	103	BCL	C16-C17-C18-C20
10	L	302	BPH	C16-C17-C18-C20
9	S	102	BCL	C4-C3-C5-C6
9	A	102	BCL	C2-C3-C5-C6
9	Q	102	BCL	C2-C3-C5-C6
9	A	102	BCL	C11-C10-C8-C9
9	I	102	BCL	C11-C10-C8-C9
9	K	102	BCL	C11-C10-C8-C9
9	O	102	BCL	C11-C10-C8-C9
9	R	101	BCL	C14-C13-C15-C16
9	S	102	BCL	C11-C10-C8-C9
9	U	102	BCL	C11-C10-C8-C9
9	V	101	BCL	C6-C7-C8-C9
9	Z	101	BCL	C6-C7-C8-C9
9	2	101	BCL	C6-C7-C8-C9
9	7	102	BCL	C11-C10-C8-C9
10	L	302	BPH	C11-C10-C8-C9
9	M	401	BCL	C5-C6-C7-C8
9	B	101	BCL	C16-C17-C18-C19
9	P	101	BCL	C16-C17-C18-C19
9	T	101	BCL	C16-C17-C18-C19
9	V	101	BCL	C16-C17-C18-C20
9	X	101	BCL	C16-C17-C18-C20
9	4	101	BCL	C16-C17-C18-C20
9	7	103	BCL	C16-C17-C18-C19
9	0	101	BCL	C16-C17-C18-C19
9	0	101	BCL	C16-C17-C18-C20
10	L	302	BPH	C16-C17-C18-C19
9	S	102	BCL	C8-C10-C11-C12
10	M	403	BPH	C15-C16-C17-C18
9	I	102	BCL	C8-C10-C11-C12
9	F	102	BCL	C3A-C2A-CAA-CBA
9	I	102	BCL	C3A-C2A-CAA-CBA
9	K	102	BCL	C3A-C2A-CAA-CBA
9	O	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	S	102	BCL	C3A-C2A-CAA-CBA
9	U	102	BCL	C3A-C2A-CAA-CBA
9	W	102	BCL	C3A-C2A-CAA-CBA
9	3	102	BCL	C3A-C2A-CAA-CBA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	I	102	BCL	C15-C16-C17-C18
9	M	402	BCL	C16-C17-C18-C20
9	I	103	BCL	C16-C17-C18-C19
9	V	101	BCL	C16-C17-C18-C19
9	X	101	BCL	C16-C17-C18-C19
9	4	101	BCL	C16-C17-C18-C19
9	6	101	BCL	C16-C17-C18-C19
9	L	301	BCL	O2A-C1-C2-C3
9	G	101	BCL	C3-C5-C6-C7
9	N	101	BCL	C3-C5-C6-C7
9	Y	102	BCL	C5-C6-C7-C8
9	D	102	BCL	C4-C3-C5-C6
9	F	102	BCL	C4-C3-C5-C6
9	2	101	BCL	C4-C3-C5-C6
9	F	102	BCL	C2-C3-C5-C6
9	S	102	BCL	C2-C3-C5-C6
9	2	101	BCL	C2-C3-C5-C6
9	Y	102	BCL	C15-C16-C17-C18
9	1	102	BCL	C3-C5-C6-C7
9	W	102	BCL	C5-C6-C7-C8
9	Z	101	BCL	C5-C6-C7-C8
9	K	102	BCL	C15-C16-C17-C18
9	S	102	BCL	C15-C16-C17-C18
9	7	102	BCL	C15-C16-C17-C18
9	W	102	BCL	C15-C16-C17-C18
9	Q	102	BCL	C4-C3-C5-C6
9	V	101	BCL	C4-C3-C5-C6
9	3	102	BCL	C4-C3-C5-C6
9	5	102	BCL	C4-C3-C5-C6
9	A	102	BCL	C11-C10-C8-C7
9	A	102	BCL	C11-C12-C13-C15
9	B	101	BCL	C11-C12-C13-C15
9	D	102	BCL	C2-C3-C5-C6
9	D	102	BCL	C11-C10-C8-C7
9	I	102	BCL	C11-C10-C8-C7
9	K	102	BCL	C11-C10-C8-C7
9	O	102	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	Q	102	BCL	C11-C10-C8-C7
9	R	101	BCL	C6-C7-C8-C10
9	S	102	BCL	C11-C10-C8-C7
9	V	101	BCL	C2-C3-C5-C6
9	W	102	BCL	C11-C10-C8-C7
9	X	101	BCL	C2-C3-C5-C6
9	Y	102	BCL	C11-C12-C13-C15
9	1	102	BCL	C11-C10-C8-C7
9	3	102	BCL	C2-C3-C5-C6
9	5	102	BCL	C2-C3-C5-C6
9	6	101	BCL	C2-C3-C5-C6
9	7	102	BCL	C11-C10-C8-C7
9	7	102	BCL	C11-C12-C13-C15
9	9	102	BCL	C11-C10-C8-C7
10	L	302	BPH	C11-C10-C8-C7
10	M	403	BPH	C12-C13-C15-C16
9	5	102	BCL	C15-C16-C17-C18
9	5	102	BCL	C16-C17-C18-C20
9	O	102	BCL	C8-C10-C11-C12
9	9	102	BCL	C13-C15-C16-C17
10	M	403	BPH	C13-C15-C16-C17
17	H	301	PEF	O3P-C1-C2-O2
7	C	501	HEM	C4B-C3B-CAB-CBB
9	L	301	BCL	C5-C6-C7-C8
9	2	101	BCL	C5-C6-C7-C8
9	R	101	BCL	C4-C3-C5-C6
9	X	101	BCL	C4-C3-C5-C6
9	6	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C20-C19-C21-C22
11	L	304	UQ8	C18-C19-C21-C22
9	L	301	BCL	C11-C10-C8-C9
9	B	101	BCL	C11-C12-C13-C14
9	D	102	BCL	C11-C10-C8-C9
9	P	101	BCL	C6-C7-C8-C9
9	Q	102	BCL	C11-C10-C8-C9
9	R	101	BCL	C6-C7-C8-C9
9	T	101	BCL	C6-C7-C8-C9
9	W	102	BCL	C11-C10-C8-C9
9	W	102	BCL	C11-C12-C13-C14
9	Y	102	BCL	C11-C10-C8-C9
9	1	102	BCL	C11-C10-C8-C9
9	5	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	6	101	BCL	C6-C7-C8-C9
9	7	102	BCL	C6-C7-C8-C9
9	9	102	BCL	C11-C10-C8-C9
9	0	101	BCL	C6-C7-C8-C9
10	L	302	BPH	C6-C7-C8-C9
9	D	102	BCL	C1A-C2A-CAA-CBA
9	K	102	BCL	C1A-C2A-CAA-CBA
9	Q	102	BCL	C1A-C2A-CAA-CBA
9	W	102	BCL	C1A-C2A-CAA-CBA
9	3	102	BCL	C1A-C2A-CAA-CBA
9	9	102	BCL	C1A-C2A-CAA-CBA
9	Y	102	BCL	C13-C15-C16-C17
16	H	302	PGW	C01-C02-C03-O11
7	C	502	HEM	C3D-CAD-CBD-CGD
9	5	102	BCL	C16-C17-C18-C19
16	H	302	PGW	C20-C19-O03-C01
15	J	101	CRT	C35-C36-C37-C38
15	P	102	CRT	C1-C4-C5-C6
15	R	102	CRT	C35-C36-C37-C38
15	2	102	CRT	C1-C4-C5-C6
15	8	101	CRT	C1-C4-C5-C6
9	F	102	BCL	C2C-C3C-CAC-CBC
9	T	101	BCL	C2C-C3C-CAC-CBC
9	V	101	BCL	C2C-C3C-CAC-CBC
9	W	102	BCL	C2C-C3C-CAC-CBC
9	6	101	BCL	C2C-C3C-CAC-CBC
9	9	102	BCL	C15-C16-C17-C18
9	M	402	BCL	C16-C17-C18-C19
10	M	403	BPH	C16-C17-C18-C20
9	9	102	BCL	C3-C5-C6-C7
9	M	402	BCL	C10-C11-C12-C13
9	0	101	BCL	C4-C3-C5-C6
9	K	102	BCL	C8-C10-C11-C12
9	Y	102	BCL	C8-C10-C11-C12
9	9	102	BCL	C8-C10-C11-C12
16	M	407	PGW	C03-C02-O01-C1
9	1	102	BCL	C13-C15-C16-C17
9	2	101	BCL	C13-C15-C16-C17
9	6	101	BCL	C8-C10-C11-C12
9	M	401	BCL	C16-C17-C18-C20
10	M	403	BPH	C16-C17-C18-C19
9	L	301	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
9	B	101	BCL	C6-C7-C8-C10
9	D	102	BCL	C6-C7-C8-C10
9	D	102	BCL	C11-C12-C13-C15
9	D	102	BCL	C12-C13-C15-C16
9	F	102	BCL	C6-C7-C8-C10
9	F	102	BCL	C11-C12-C13-C15
9	F	102	BCL	C12-C13-C15-C16
9	G	101	BCL	C6-C7-C8-C10
9	K	102	BCL	C6-C7-C8-C10
9	K	102	BCL	C11-C12-C13-C15
9	O	102	BCL	C12-C13-C15-C16
9	R	101	BCL	C2-C3-C5-C6
9	S	102	BCL	C11-C12-C13-C15
9	U	102	BCL	C11-C10-C8-C7
9	U	102	BCL	C11-C12-C13-C15
9	V	101	BCL	C6-C7-C8-C10
9	W	102	BCL	C6-C7-C8-C10
9	W	102	BCL	C11-C12-C13-C15
9	W	102	BCL	C12-C13-C15-C16
9	X	101	BCL	C11-C12-C13-C15
9	Y	102	BCL	C6-C7-C8-C10
9	3	102	BCL	C6-C7-C8-C10
9	3	102	BCL	C11-C12-C13-C15
9	5	102	BCL	C11-C12-C13-C15
9	6	101	BCL	C11-C12-C13-C15
9	7	102	BCL	C6-C7-C8-C10
9	9	102	BCL	C6-C7-C8-C10
9	9	102	BCL	C11-C12-C13-C15
9	0	101	BCL	C2-C3-C5-C6
9	0	101	BCL	C6-C7-C8-C10
10	L	302	BPH	C6-C7-C8-C10
9	L	301	BCL	C14-C13-C15-C16
9	L	303	BCL	C11-C10-C8-C9
9	M	401	BCL	C11-C12-C13-C14
9	M	401	BCL	C14-C13-C15-C16
9	M	402	BCL	C11-C12-C13-C14
9	A	102	BCL	C11-C12-C13-C14
9	A	102	BCL	C14-C13-C15-C16
9	D	102	BCL	C6-C7-C8-C9
9	D	102	BCL	C11-C12-C13-C14
9	E	101	BCL	C11-C10-C8-C9
9	F	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	F	102	BCL	C11-C12-C13-C14
9	G	101	BCL	C6-C7-C8-C9
9	I	103	BCL	C6-C7-C8-C9
9	K	102	BCL	C6-C7-C8-C9
9	K	102	BCL	C11-C12-C13-C14
9	O	102	BCL	C6-C7-C8-C9
9	O	102	BCL	C11-C12-C13-C14
9	Q	102	BCL	C11-C12-C13-C14
9	S	102	BCL	C11-C12-C13-C14
9	U	102	BCL	C6-C7-C8-C9
9	U	102	BCL	C11-C12-C13-C14
9	V	101	BCL	C11-C12-C13-C14
9	V	101	BCL	C14-C13-C15-C16
9	W	102	BCL	C6-C7-C8-C9
9	W	102	BCL	C14-C13-C15-C16
9	Y	102	BCL	C6-C7-C8-C9
9	Y	102	BCL	C11-C12-C13-C14
9	1	102	BCL	C6-C7-C8-C9
9	1	102	BCL	C11-C12-C13-C14
9	3	102	BCL	C6-C7-C8-C9
9	3	102	BCL	C11-C12-C13-C14
9	6	101	BCL	C11-C12-C13-C14
9	7	102	BCL	C11-C12-C13-C14
9	7	102	BCL	C14-C13-C15-C16
9	7	103	BCL	C14-C13-C15-C16
9	9	102	BCL	C6-C7-C8-C9
9	9	102	BCL	C11-C12-C13-C14
9	K	102	BCL	C13-C15-C16-C17
9	7	103	BCL	C10-C11-C12-C13
15	V	102	CRT	O1-C1-C4-C5
9	K	102	BCL	C3-C5-C6-C7
9	5	102	BCL	C3-C5-C6-C7
9	S	102	BCL	C13-C15-C16-C17
9	V	101	BCL	C8-C10-C11-C12
9	W	102	BCL	C8-C10-C11-C12
17	H	301	PEF	O3P-C1-C2-C3
9	W	102	BCL	C3-C5-C6-C7
9	U	102	BCL	C8-C10-C11-C12
9	B	101	BCL	C4-C3-C5-C6
9	I	102	BCL	C4-C3-C5-C6
9	L	301	BCL	C16-C17-C18-C20
9	D	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C16-C17-C18-C19
9	7	102	BCL	C13-C15-C16-C17
9	I	103	BCL	C5-C6-C7-C8
9	B	101	BCL	C6-C7-C8-C9
9	F	102	BCL	C14-C13-C15-C16
9	I	102	BCL	C6-C7-C8-C9
9	I	102	BCL	C11-C12-C13-C14
9	Q	102	BCL	C14-C13-C15-C16
9	S	102	BCL	C6-C7-C8-C9
9	S	102	BCL	C14-C13-C15-C16
9	X	101	BCL	C11-C12-C13-C14
9	5	102	BCL	C11-C12-C13-C14
9	V	101	BCL	C5-C6-C7-C8
9	L	303	BCL	C11-C12-C13-C15
9	M	401	BCL	C11-C10-C8-C7
9	M	401	BCL	C12-C13-C15-C16
9	M	402	BCL	C11-C10-C8-C7
9	M	402	BCL	C11-C12-C13-C15
9	A	102	BCL	C12-C13-C15-C16
9	B	101	BCL	C2-C3-C5-C6
9	E	101	BCL	C11-C10-C8-C7
9	I	102	BCL	C6-C7-C8-C10
9	I	102	BCL	C11-C12-C13-C15
9	I	102	BCL	C12-C13-C15-C16
9	I	103	BCL	C11-C12-C13-C15
9	N	101	BCL	C6-C7-C8-C10
9	N	101	BCL	C12-C13-C15-C16
9	O	102	BCL	C6-C7-C8-C10
9	O	102	BCL	C11-C12-C13-C15
9	P	101	BCL	C11-C12-C13-C15
9	Q	102	BCL	C11-C12-C13-C15
9	Q	102	BCL	C12-C13-C15-C16
9	S	102	BCL	C6-C7-C8-C10
9	S	102	BCL	C12-C13-C15-C16
9	T	101	BCL	C11-C12-C13-C15
9	U	102	BCL	C6-C7-C8-C10
9	U	102	BCL	C12-C13-C15-C16
9	V	101	BCL	C12-C13-C15-C16
9	Y	102	BCL	C12-C13-C15-C16
9	Z	101	BCL	C11-C12-C13-C15
9	1	102	BCL	C6-C7-C8-C10
9	1	102	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	3	102	BCL	C12-C13-C15-C16
9	4	101	BCL	C6-C7-C8-C10
9	4	101	BCL	C11-C12-C13-C15
9	5	102	BCL	C6-C7-C8-C10
9	7	102	BCL	C12-C13-C15-C16
9	7	103	BCL	C6-C7-C8-C10
9	7	103	BCL	C12-C13-C15-C16
9	9	102	BCL	C12-C13-C15-C16
9	5	102	BCL	CAD-CBD-CGD-O2D
9	7	103	BCL	CAD-CBD-CGD-O2D
9	9	102	BCL	CAD-CBD-CGD-O2D
9	B	101	BCL	C8-C10-C11-C12
16	H	302	PGW	O01-C02-C03-O11
9	M	401	BCL	CHA-CBD-CGD-O1D
9	M	401	BCL	CHA-CBD-CGD-O2D
9	E	101	BCL	C13-C15-C16-C17
16	H	302	PGW	O03-C01-C02-O01
9	I	103	BCL	C11-C12-C13-C14
9	N	101	BCL	C6-C7-C8-C9
9	P	101	BCL	C11-C12-C13-C14
9	Q	102	BCL	C6-C7-C8-C9
9	3	102	BCL	C14-C13-C15-C16
9	7	103	BCL	C6-C7-C8-C9
9	W	102	BCL	C13-C15-C16-C17
9	I	102	BCL	C3-C5-C6-C7
9	4	101	BCL	C2-C1-O2A-CGA
10	L	302	BPH	C4-C3-C5-C6
11	L	304	UQ8	C30-C29-C31-C32
15	T	102	CRT	C4-C5-C6-C7
16	H	302	PGW	C04-O12-P-O14
9	M	401	BCL	C16-C17-C18-C19
9	Q	102	BCL	C15-C16-C17-C18
9	Z	101	BCL	C16-C17-C18-C20
9	M	402	BCL	CAD-CBD-CGD-O1D
9	Q	102	BCL	CAD-CBD-CGD-O1D
9	U	102	BCL	C3-C5-C6-C7
9	N	101	BCL	C4-C3-C5-C6
9	L	303	BCL	C11-C10-C8-C7
9	M	401	BCL	C6-C7-C8-C10
9	A	102	BCL	C6-C7-C8-C10
9	I	102	BCL	C2-C3-C5-C6
9	K	102	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
9	P	101	BCL	C12-C13-C15-C16
9	Q	102	BCL	C6-C7-C8-C10
9	Z	101	BCL	C12-C13-C15-C16
9	1	102	BCL	C12-C13-C15-C16
9	2	101	BCL	C11-C12-C13-C15
9	2	101	BCL	C12-C13-C15-C16
9	4	101	BCL	C12-C13-C15-C16
9	0	101	BCL	C11-C12-C13-C15
9	0	101	BCL	C12-C13-C15-C16
9	7	102	BCL	C8-C10-C11-C12
9	F	102	BCL	C3-C5-C6-C7
16	H	302	PGW	O04-C19-O03-C01
9	Z	101	BCL	C16-C17-C18-C19
16	H	302	PGW	O03-C01-C02-C03
9	X	101	BCL	C8-C10-C11-C12
9	L	303	BCL	C11-C12-C13-C14
9	D	102	BCL	C14-C13-C15-C16
9	I	102	BCL	C14-C13-C15-C16
9	K	102	BCL	C14-C13-C15-C16
9	T	101	BCL	C11-C12-C13-C14
9	U	102	BCL	C14-C13-C15-C16
9	Y	102	BCL	C14-C13-C15-C16
9	Z	101	BCL	C11-C12-C13-C14
9	1	102	BCL	C14-C13-C15-C16
9	3	102	BCL	C11-C10-C8-C9
9	4	101	BCL	C6-C7-C8-C9
9	4	101	BCL	C11-C12-C13-C14
9	5	102	BCL	C6-C7-C8-C9
9	9	102	BCL	C14-C13-C15-C16
9	0	101	BCL	C11-C12-C13-C14
10	M	403	BPH	C6-C7-C8-C9
9	E	101	BCL	C16-C17-C18-C19
10	L	302	BPH	C2-C3-C5-C6
9	O	102	BCL	C13-C15-C16-C17
9	A	102	BCL	C2-C1-O2A-CGA
9	O	102	BCL	C2-C1-O2A-CGA
9	P	101	BCL	C2-C1-O2A-CGA
9	5	102	BCL	C2-C1-O2A-CGA
16	M	407	PGW	C04-O12-P-O11
16	H	302	PGW	C04-O12-P-O11
15	T	102	CRT	C2-C1-C4-C5
9	G	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	2	101	BCL	C6-C7-C8-C10
9	6	101	BCL	C12-C13-C15-C16
9	M	401	BCL	C11-C10-C8-C9
9	M	402	BCL	C11-C10-C8-C9
9	F	102	BCL	C6-C7-C8-C9
9	N	101	BCL	C14-C13-C15-C16
9	O	102	BCL	C14-C13-C15-C16
9	4	101	BCL	C14-C13-C15-C16
9	2	101	BCL	C8-C10-C11-C12
9	E	101	BCL	C16-C17-C18-C20
7	C	504	HEM	C3D-CAD-CBD-CGD
14	M	405	MQ8	C38-C40-C41-C42
9	U	102	BCL	C13-C15-C16-C17
9	W	102	BCL	C2-C3-C5-C6
9	B	101	BCL	C2-C1-O2A-CGA
9	N	101	BCL	C2-C1-O2A-CGA
9	3	102	BCL	C2-C1-O2A-CGA
7	C	503	HEM	CAD-CBD-CGD-O2D
9	G	101	BCL	C14-C13-C15-C16
9	F	102	BCL	C13-C15-C16-C17
9	G	101	BCL	C15-C16-C17-C18
7	C	503	HEM	CAD-CBD-CGD-O1D
17	H	301	PEF	C3-C2-O2-C10
9	W	102	BCL	C4-C3-C5-C6
9	L	301	BCL	C1A-C2A-CAA-CBA
9	F	102	BCL	C11-C10-C8-C7
9	I	103	BCL	C12-C13-C15-C16
9	R	101	BCL	C12-C13-C15-C16
9	T	101	BCL	C12-C13-C15-C16
9	Z	101	BCL	C6-C7-C8-C10
9	E	101	BCL	C8-C10-C11-C12
9	0	101	BCL	C5-C6-C7-C8
7	C	502	HEM	CAD-CBD-CGD-O2D
9	I	102	BCL	C13-C15-C16-C17
11	L	304	UQ8	C26-C27-C28-C29
15	A	101	CRT	C1-C4-C5-C6
15	V	102	CRT	C1-C4-C5-C6
15	X	102	CRT	C35-C36-C37-C38
9	L	303	BCL	C4-C3-C5-C6
9	M	401	BCL	C2-C1-O2A-CGA
9	Q	102	BCL	C2-C1-O2A-CGA
9	W	102	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	R	101	BCL	C2C-C3C-CAC-CBC
9	T	101	BCL	C5-C6-C7-C8
7	C	502	HEM	CAD-CBD-CGD-O1D
7	C	503	HEM	CAA-CBA-CGA-O2A
9	5	102	BCL	C13-C15-C16-C17
9	4	101	BCL	C4-C3-C5-C6
9	N	101	BCL	C2-C3-C5-C6
7	C	503	HEM	CAA-CBA-CGA-O1A
7	C	504	HEM	CAD-CBD-CGD-O1D
9	I	103	BCL	C6-C7-C8-C10
9	V	101	BCL	C11-C12-C13-C15
9	3	102	BCL	C11-C10-C8-C7
11	L	304	UQ8	C28-C29-C31-C32
9	V	101	BCL	C10-C11-C12-C13
9	R	101	BCL	CAA-CBA-CGA-O2A
9	A	102	BCL	C6-C7-C8-C9
9	I	103	BCL	C14-C13-C15-C16
9	P	101	BCL	C14-C13-C15-C16
9	2	101	BCL	C11-C12-C13-C14
9	2	101	BCL	C14-C13-C15-C16
9	6	101	BCL	C14-C13-C15-C16
9	0	101	BCL	C14-C13-C15-C16
9	A	102	BCL	CAD-CBD-CGD-O2D
9	D	102	BCL	CAD-CBD-CGD-O2D
9	F	102	BCL	CAD-CBD-CGD-O2D
9	O	102	BCL	CAD-CBD-CGD-O2D
9	S	102	BCL	CAD-CBD-CGD-O2D
9	W	102	BCL	CAD-CBD-CGD-O2D
10	L	302	BPH	CAD-CBD-CGD-O2D
10	M	403	BPH	CAD-CBD-CGD-O2D
17	H	301	PEF	C1-C2-O2-C10
7	C	502	HEM	CAA-CBA-CGA-O1A
7	C	501	HEM	CAA-CBA-CGA-O2A
9	M	402	BCL	O2A-C1-C2-C3
9	V	101	BCL	O2A-C1-C2-C3
10	M	403	BPH	O2A-C1-C2-C3
7	C	502	HEM	CAA-CBA-CGA-O2A
7	C	501	HEM	CAD-CBD-CGD-O2D
7	C	501	HEM	CAA-CBA-CGA-O1A
7	C	501	HEM	CAD-CBD-CGD-O1D
9	O	102	BCL	CAA-CBA-CGA-O2A
9	Z	101	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	0	101	BCL	CAA-CBA-CGA-O2A
10	L	302	BPH	CHA-CBD-CGD-O1D
10	M	403	BPH	CHA-CBD-CGD-O1D
15	T	102	CRT	C3-C1-C4-C5
15	V	102	CRT	C2-C1-C4-C5
9	B	101	BCL	C12-C13-C15-C16
9	R	101	BCL	C11-C12-C13-C15
9	D	102	BCL	CAA-CBA-CGA-O2A
9	2	101	BCL	CAA-CBA-CGA-O2A
9	B	101	BCL	C14-C13-C15-C16
9	T	101	BCL	C14-C13-C15-C16
9	Z	101	BCL	C14-C13-C15-C16
9	6	101	BCL	CAA-CBA-CGA-O2A
9	L	303	BCL	C2-C3-C5-C6
9	1	102	BCL	C1A-C2A-CAA-CBA
9	5	102	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	CAA-CBA-CGA-O1A
7	C	504	HEM	CAD-CBD-CGD-O2D
9	S	102	BCL	C2-C1-O2A-CGA
9	Q	102	BCL	C13-C15-C16-C17
9	O	102	BCL	CAA-CBA-CGA-O1A
9	R	101	BCL	CAA-CBA-CGA-O1A
10	L	302	BPH	C10-C11-C12-C13
9	X	101	BCL	CAA-CBA-CGA-O2A
9	M	402	BCL	C4-C3-C5-C6
9	X	101	BCL	CAD-CBD-CGD-O1D
17	H	301	PEF	C5-C4-O4P-P
9	R	101	BCL	C11-C12-C13-C14
10	L	302	BPH	C14-C13-C15-C16
9	Q	102	BCL	CAA-CBA-CGA-O2A
9	7	103	BCL	CAA-CBA-CGA-O2A
9	3	102	BCL	C8-C10-C11-C12
9	N	101	BCL	C10-C11-C12-C13
9	L	301	BCL	C2C-C3C-CAC-CBC
9	E	101	BCL	C11-C12-C13-C15
9	5	102	BCL	C3A-C2A-CAA-CBA
10	L	302	BPH	C12-C13-C15-C16
9	D	102	BCL	CAA-CBA-CGA-O1A
9	Z	101	BCL	CAA-CBA-CGA-O1A
9	2	101	BCL	CAA-CBA-CGA-O1A
9	7	102	BCL	C3-C5-C6-C7
9	F	102	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	W	102	BCL	CAA-CBA-CGA-O2A
7	C	504	HEM	CAA-CBA-CGA-O2A
9	0	101	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

67 monomers are involved in 1470 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	103	CRT	23	0
9	A	102	BCL	35	0
9	9	102	BCL	29	0
11	L	304	UQ8	13	0
9	N	101	BCL	23	0
10	L	302	BPH	8	0
15	V	102	CRT	65	0
15	2	102	CRT	40	0
10	M	403	BPH	19	0
15	4	102	CRT	68	0
9	7	103	BCL	32	0
9	D	102	BCL	22	0
9	1	102	BCL	18	0
9	4	101	BCL	36	0
9	I	103	BCL	36	0
9	3	102	BCL	28	0
12	H	304	PO4	3	0
15	J	101	CRT	35	0
9	R	101	BCL	31	0
15	A	101	CRT	47	0
9	L	301	BCL	11	0
15	W	103	CRT	29	0
17	H	301	PEF	18	0
9	F	102	BCL	45	0
7	C	503	HEM	9	0
9	Z	101	BCL	29	0
9	5	102	BCL	23	0
15	M	406	CRT	12	0
15	P	102	CRT	61	0
15	8	101	CRT	80	0
9	I	102	BCL	34	0
12	M	408	PO4	1	0
7	C	504	HEM	2	0
9	7	102	BCL	21	0

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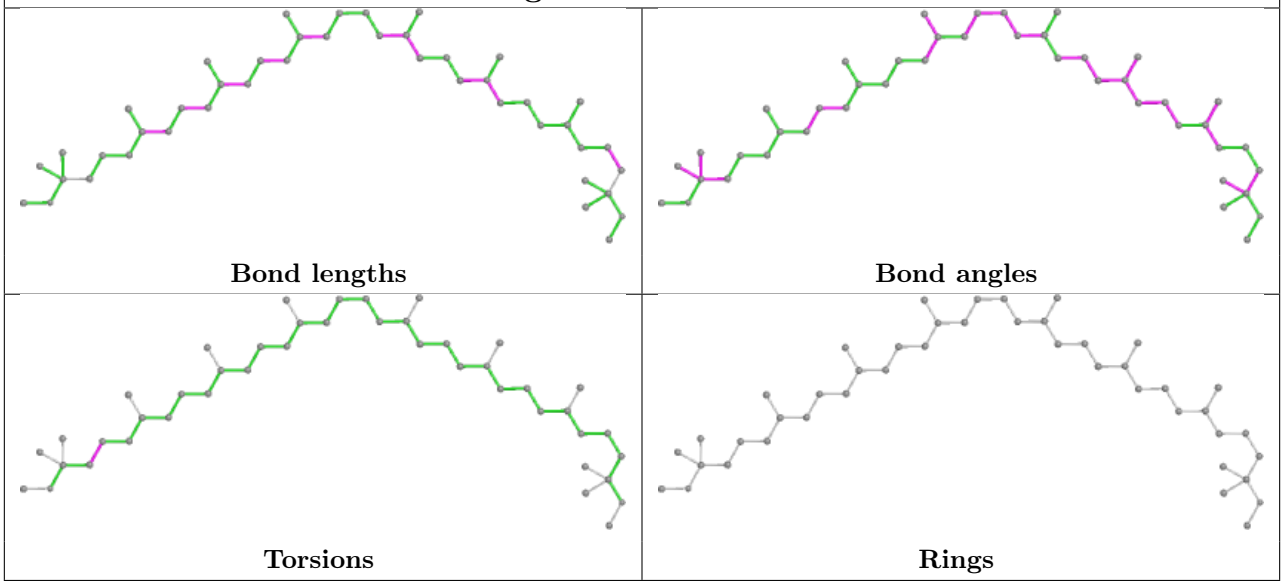
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	101	BCL	37	0
9	M	402	BCL	13	0
9	P	101	BCL	30	0
9	E	101	BCL	33	0
15	R	102	CRT	34	0
15	3	103	CRT	20	0
9	V	101	BCL	14	0
9	W	102	BCL	37	0
9	L	303	BCL	11	0
15	N	102	CRT	54	0
7	C	501	HEM	2	0
9	T	101	BCL	24	0
9	U	102	BCL	23	0
16	M	407	PGW	16	0
9	K	102	BCL	27	0
9	B	101	BCL	38	0
9	2	101	BCL	19	0
15	T	102	CRT	23	0
9	6	101	BCL	22	0
9	O	102	BCL	55	0
16	H	302	PGW	7	0
9	S	102	BCL	26	0
15	X	102	CRT	27	0
9	0	101	BCL	24	0
9	M	401	BCL	31	0
12	H	303	PO4	1	0
15	G	102	CRT	27	0
9	Y	102	BCL	29	0
14	M	405	MQ8	13	0
7	C	502	HEM	4	0
9	X	101	BCL	39	0
15	B	102	CRT	35	0
9	Q	102	BCL	28	0

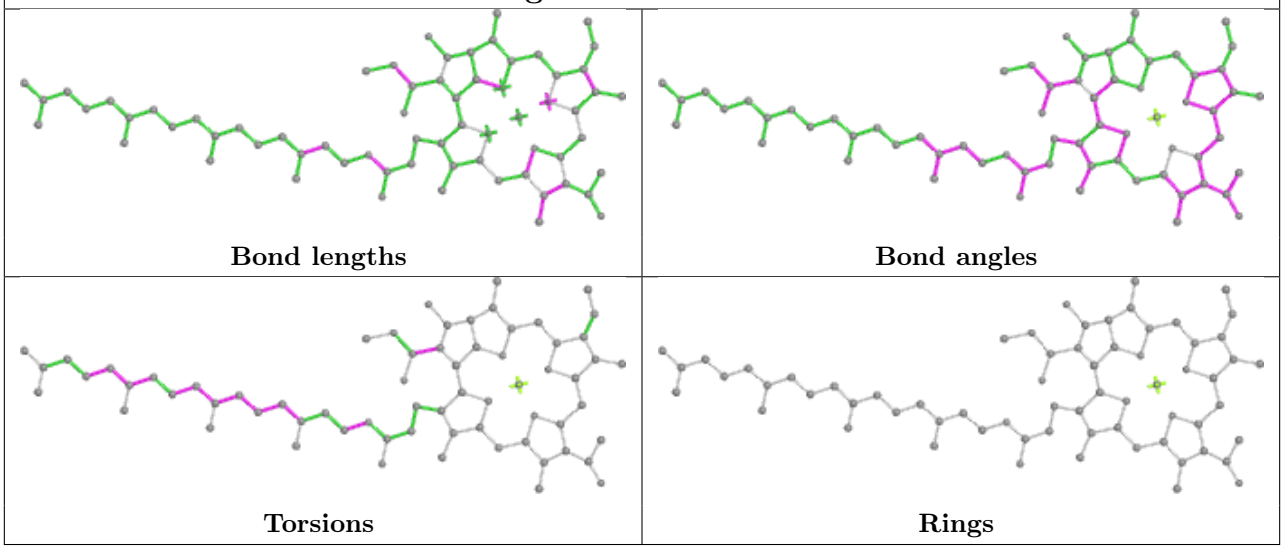
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

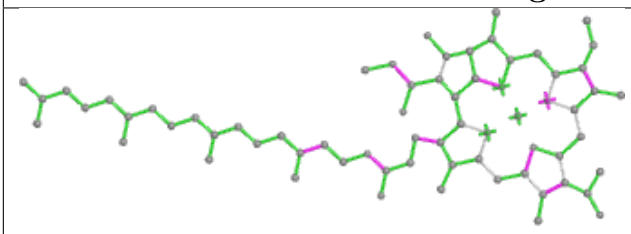
Ligand CRT A 103



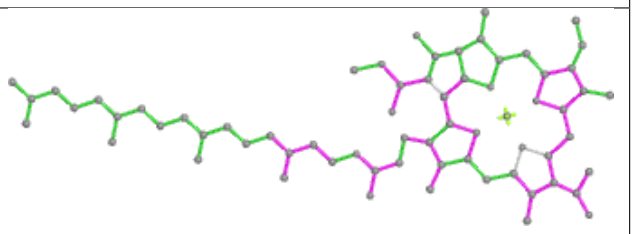
Ligand BCL A 102



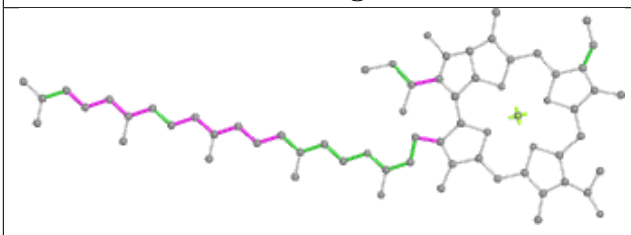
Ligand BCL 9 102



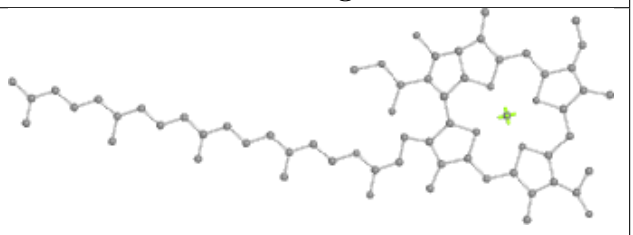
Bond lengths



Bond angles

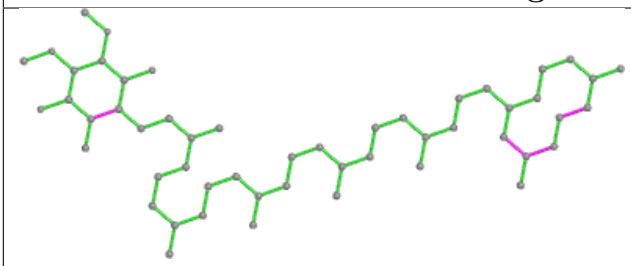


Torsions

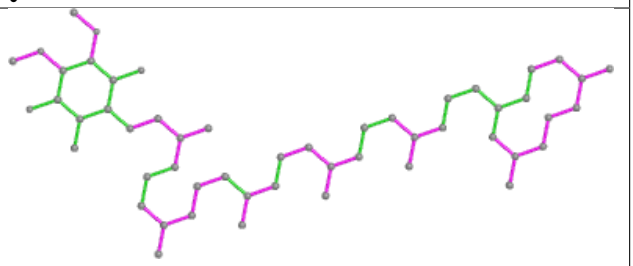


Rings

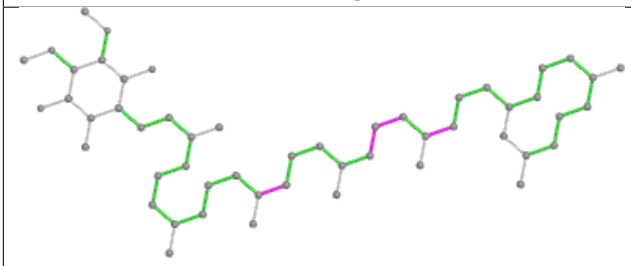
Ligand UQ8 L 304



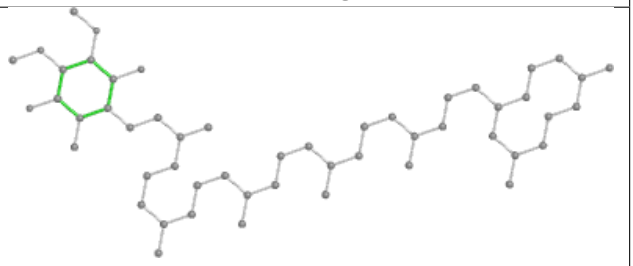
Bond lengths



Bond angles

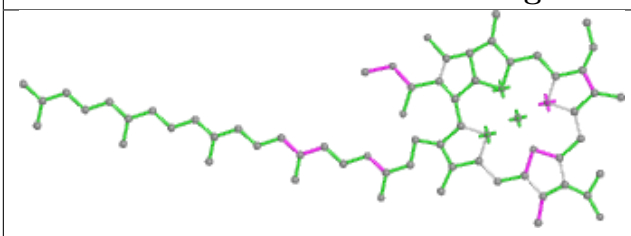


Torsions

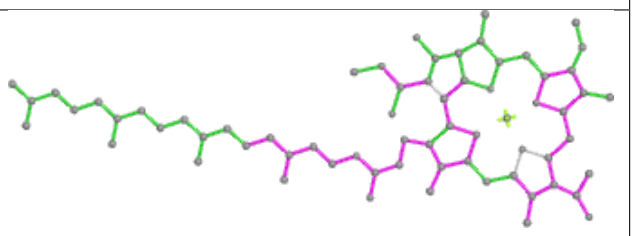


Rings

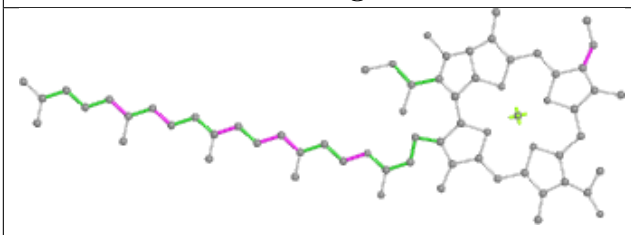
Ligand BCL N 101



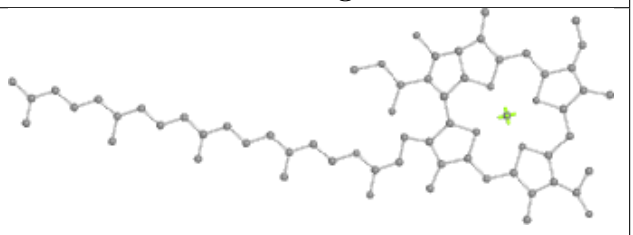
Bond lengths



Bond angles

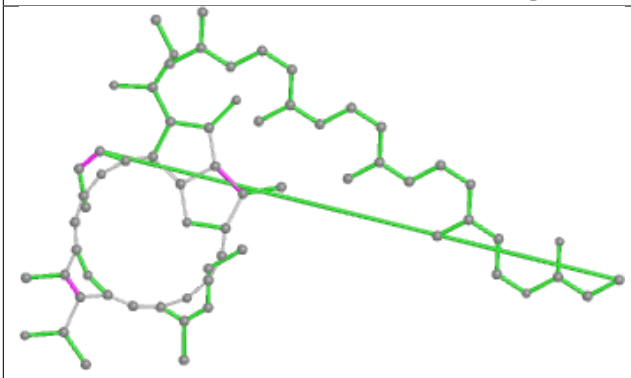


Torsions

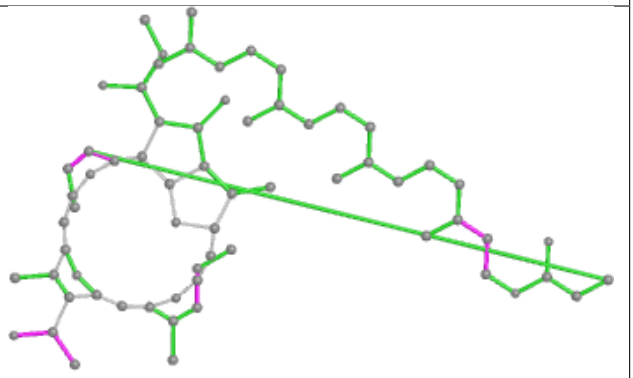


Rings

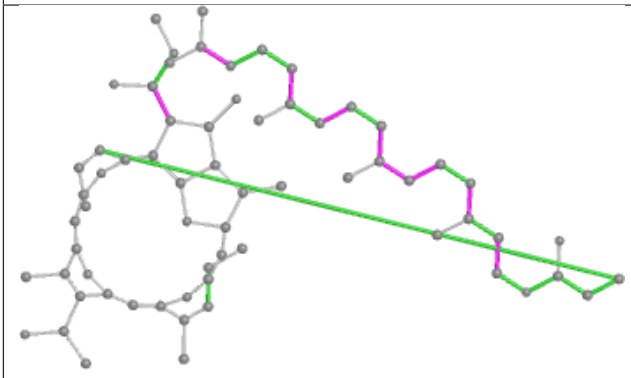
Ligand BPH L 302



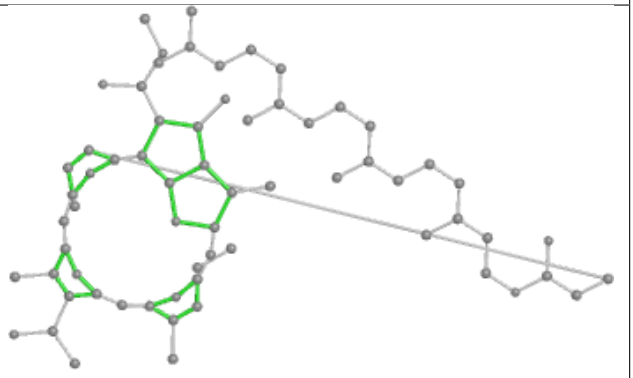
Bond lengths



Bond angles

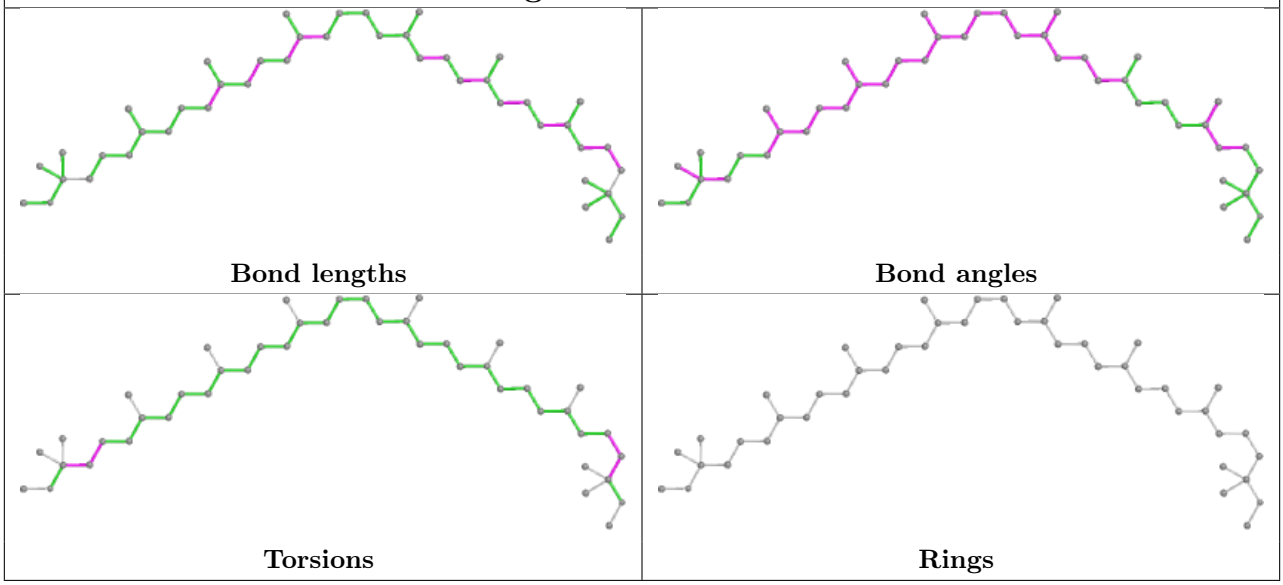


Torsions

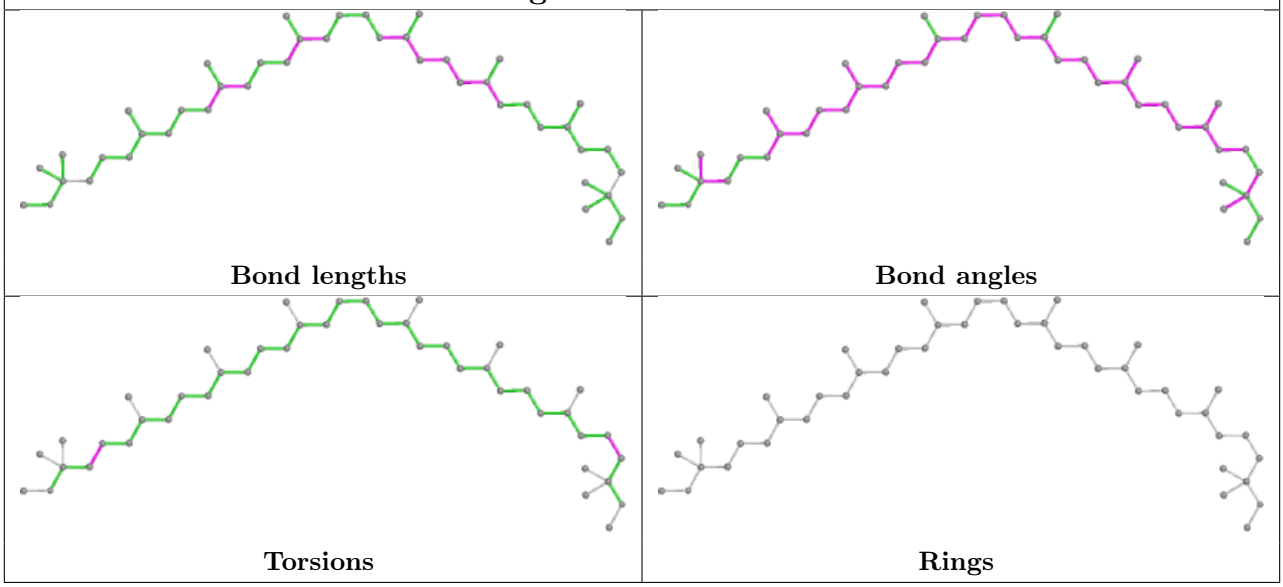


Rings

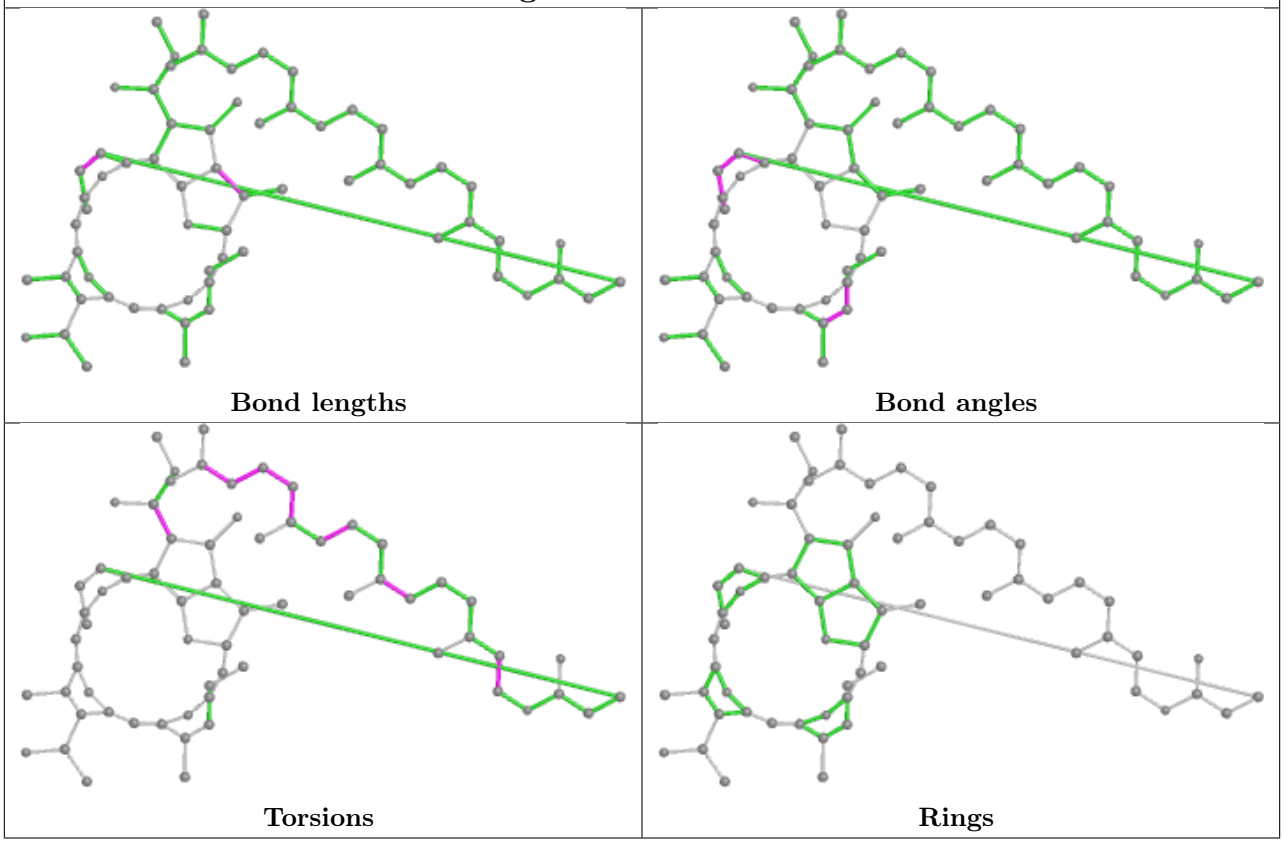
Ligand CRT V 102



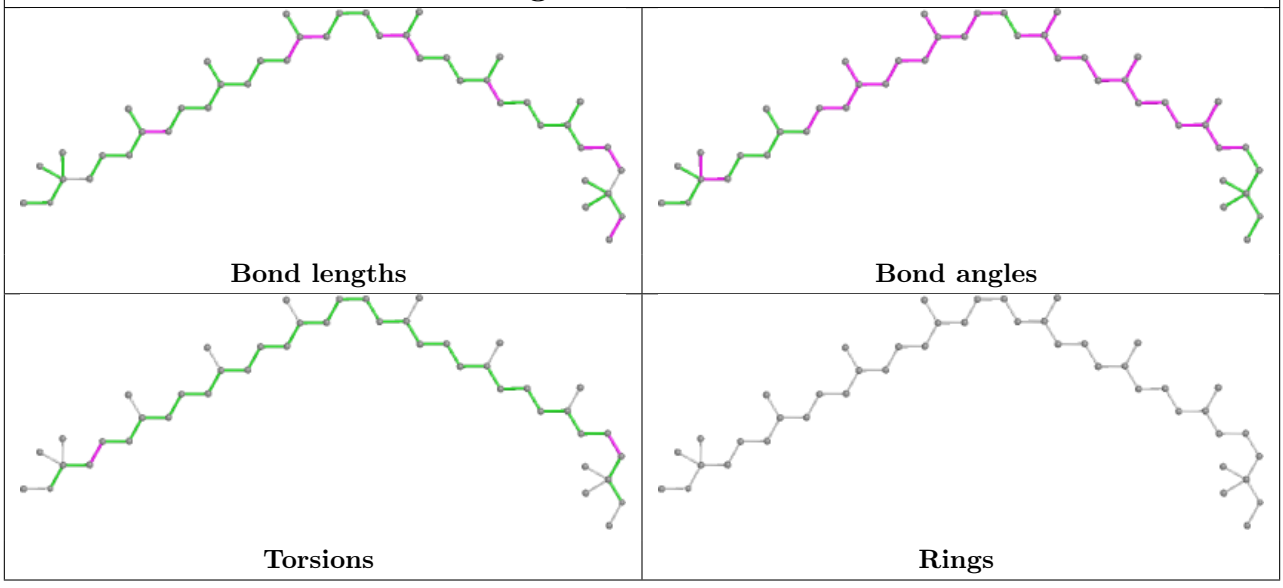
Ligand CRT 2 102



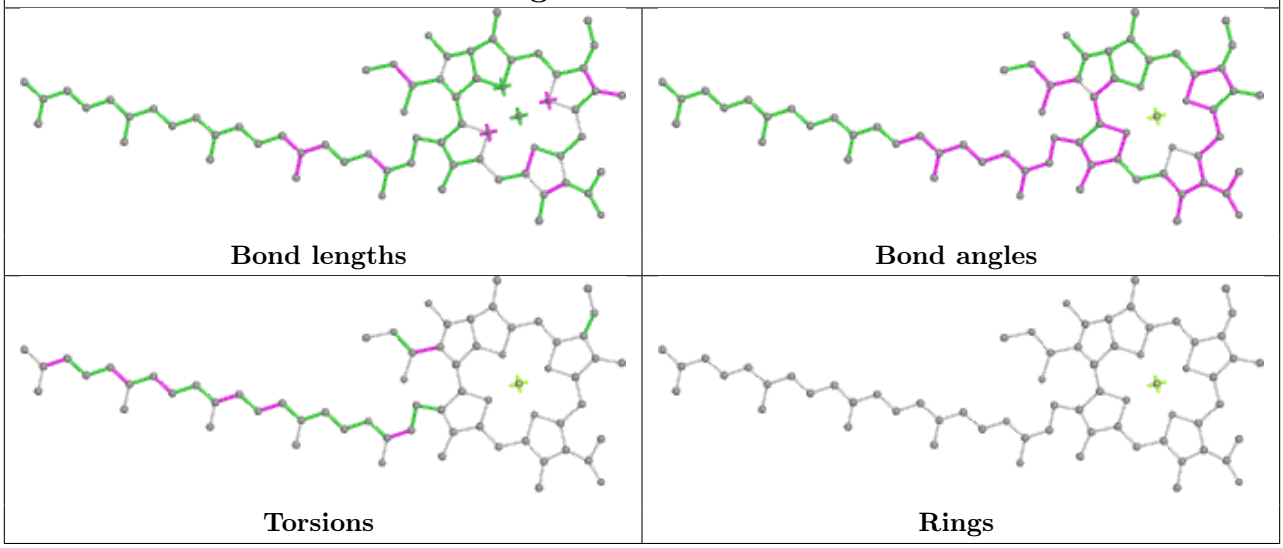
Ligand BPH M 403



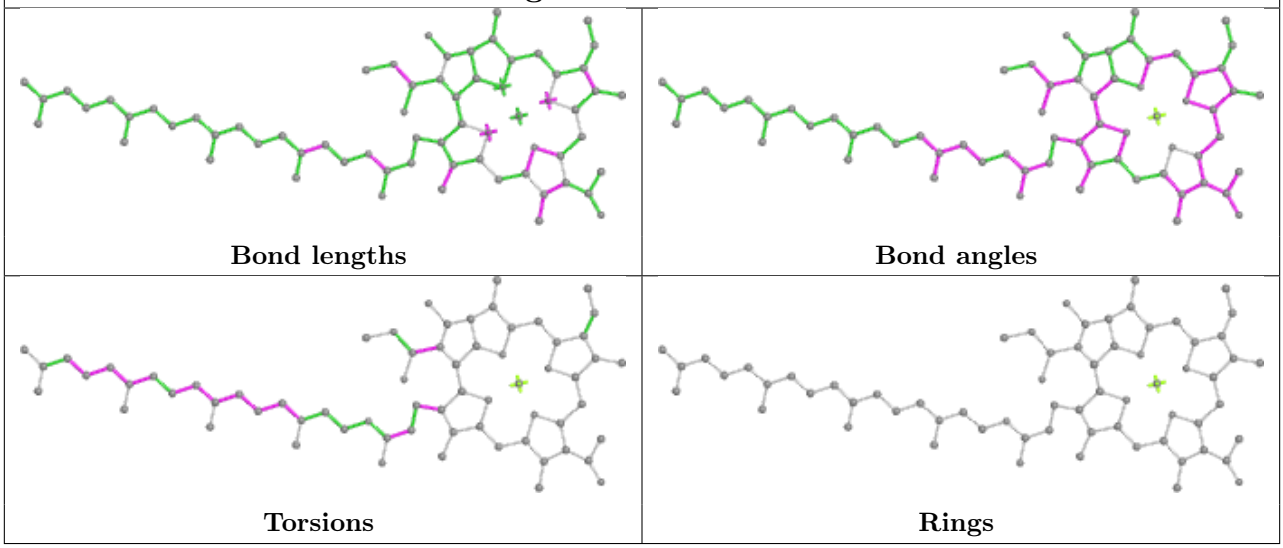
Ligand CRT 4 102



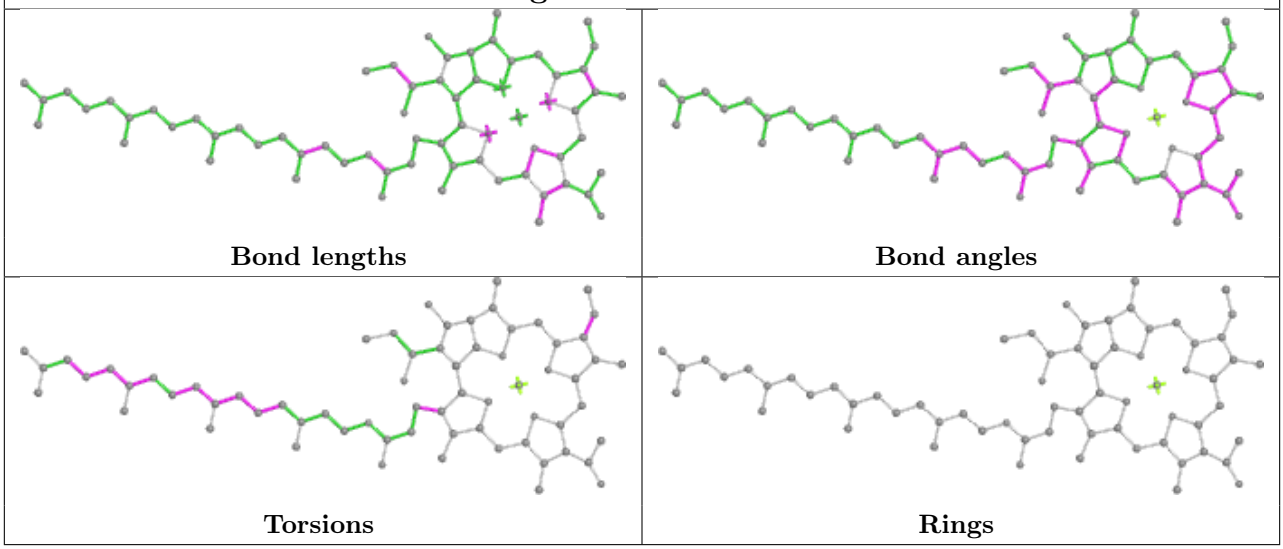
Ligand BCL 7 103



Ligand BCL D 102



Ligand BCL 1 102



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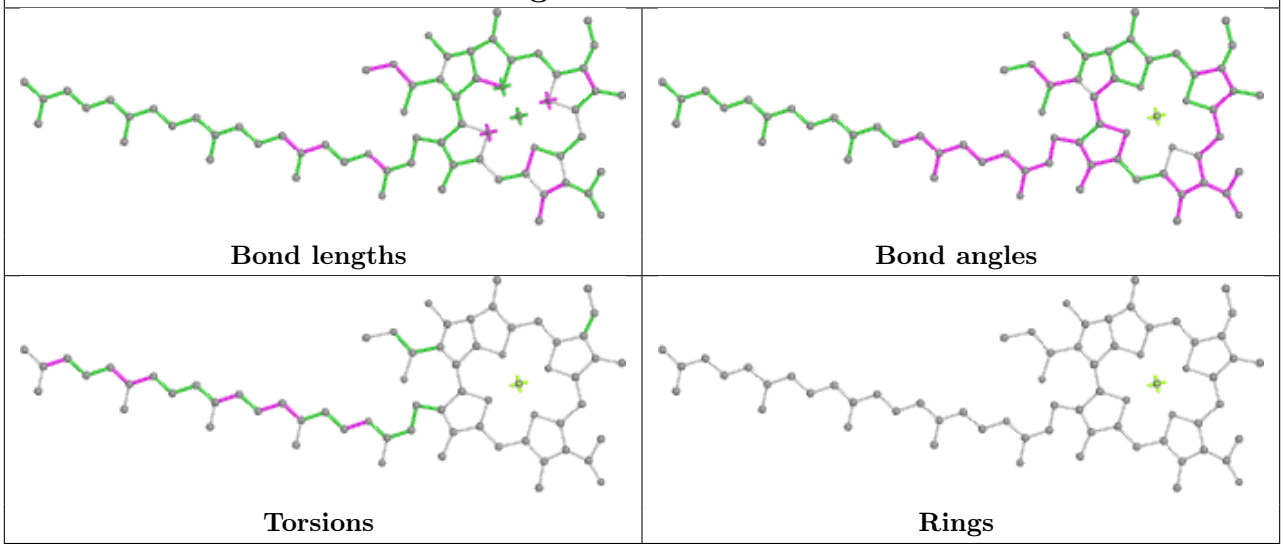
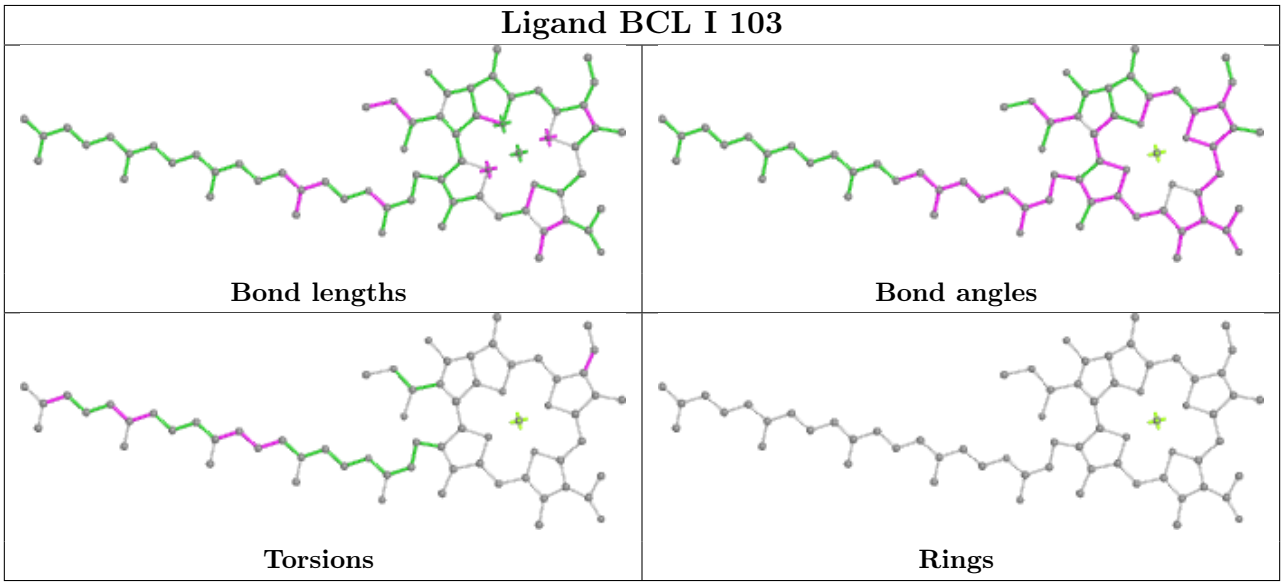
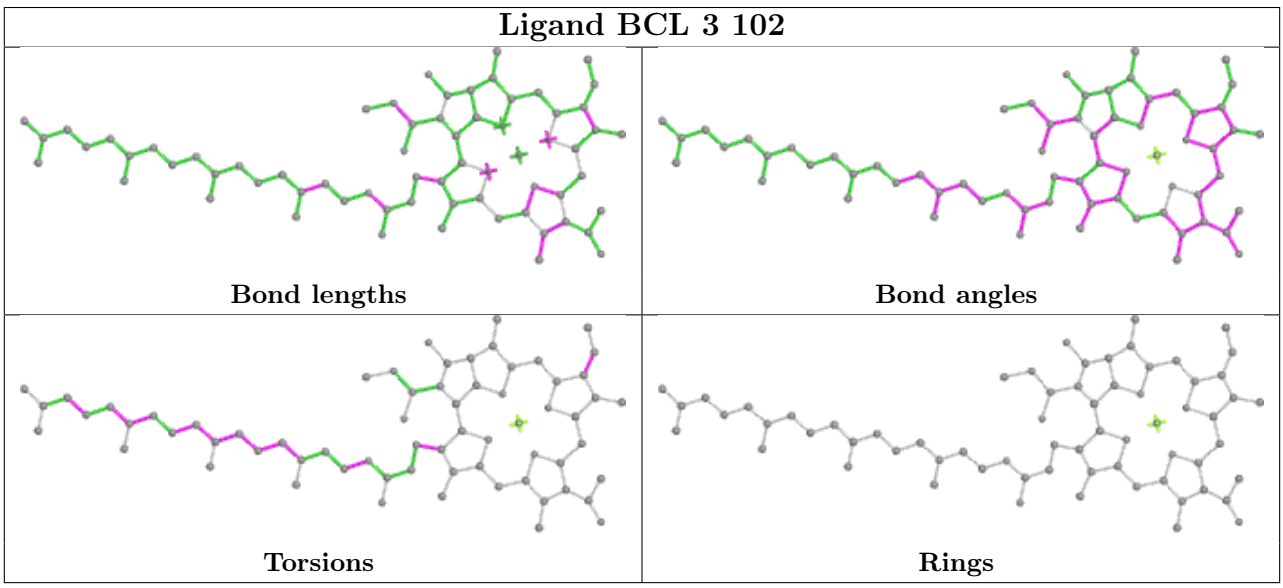


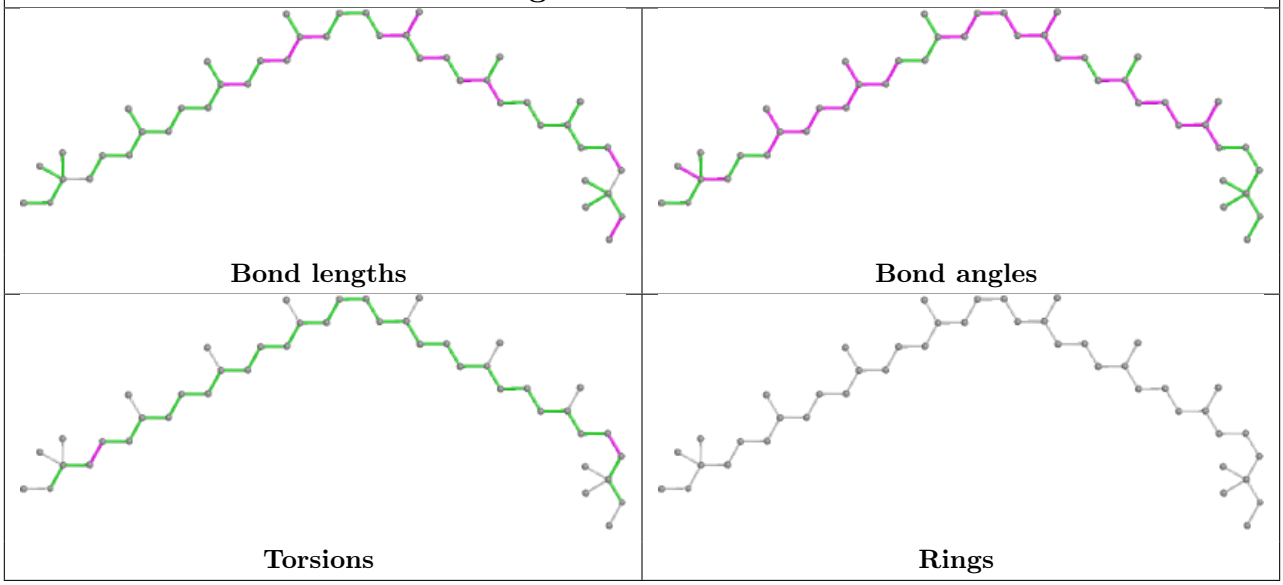
Ligand BCL I 103



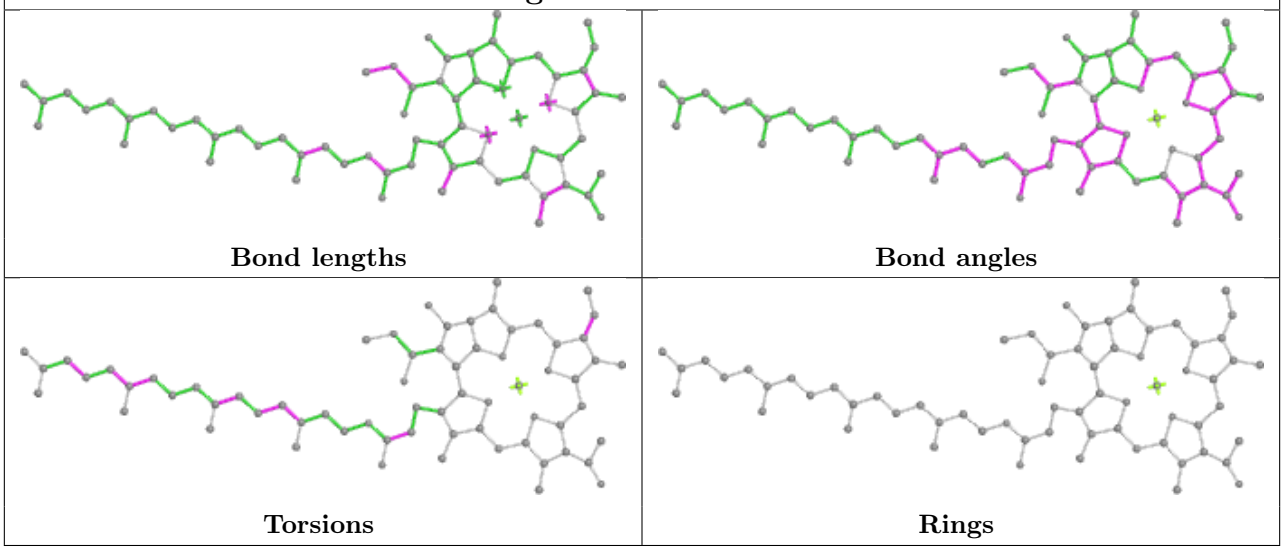
Ligand BCL 3 102



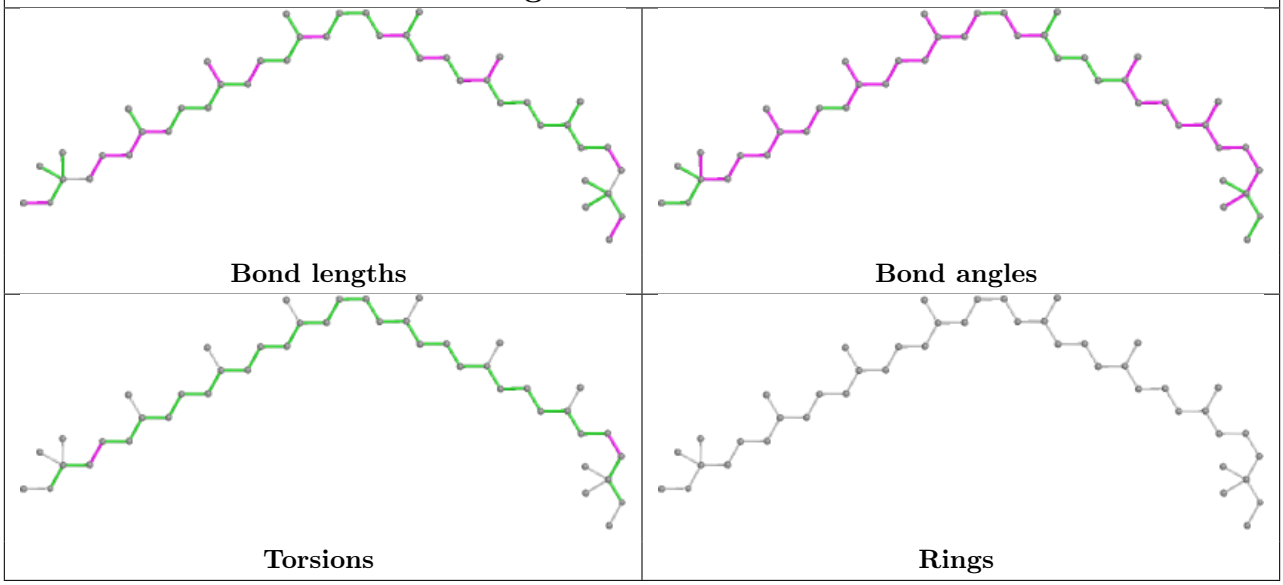
Ligand CRT J 101



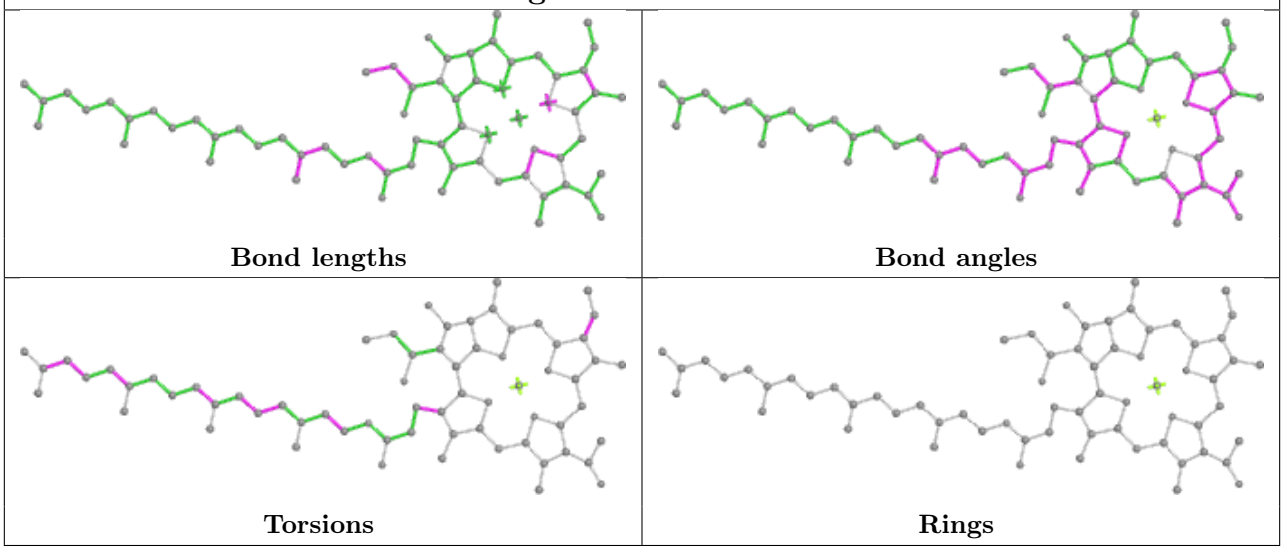
Ligand BCL R 101



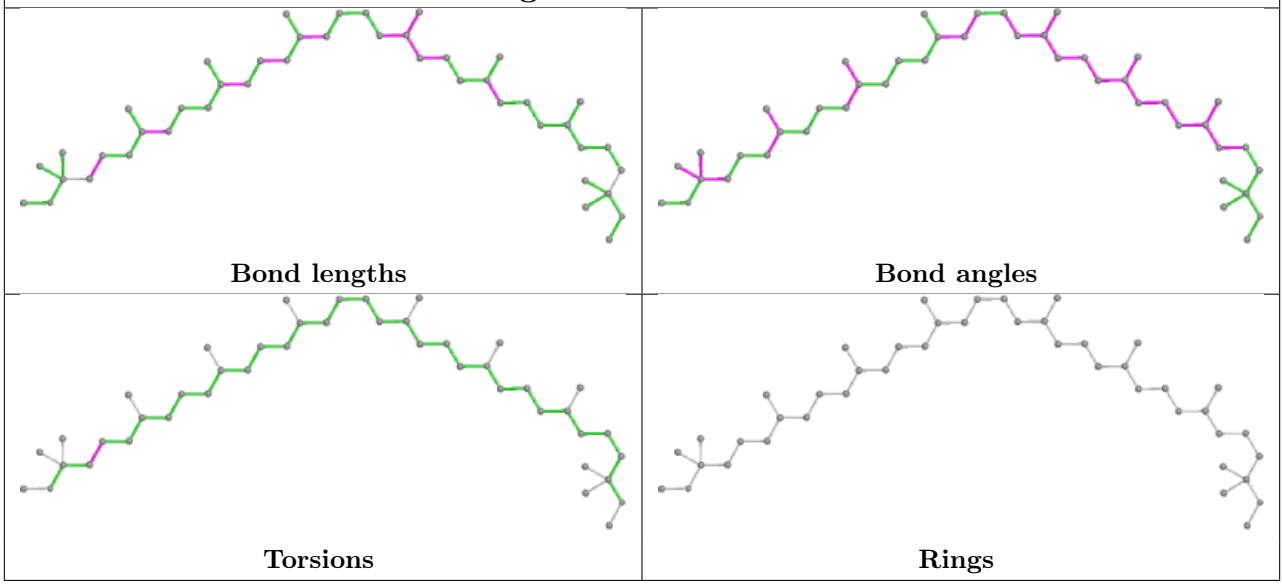
Ligand CRT A 101



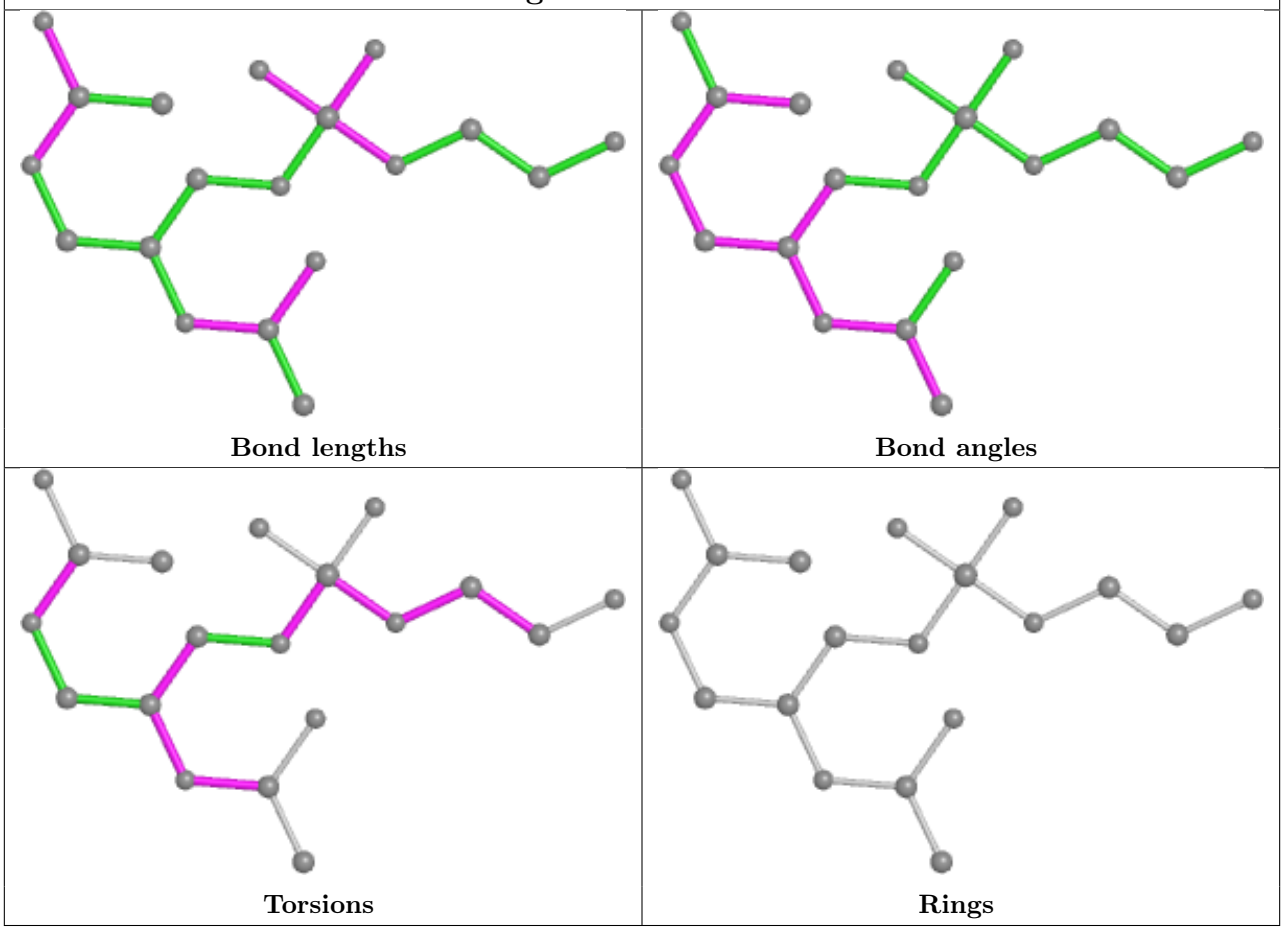
Ligand BCL L 301



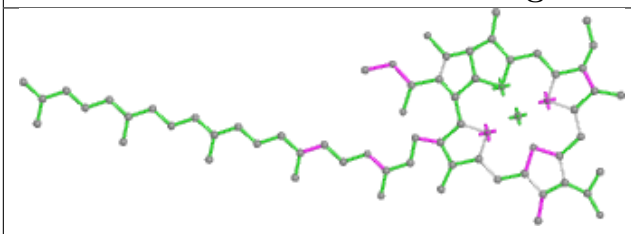
Ligand CRT W 103



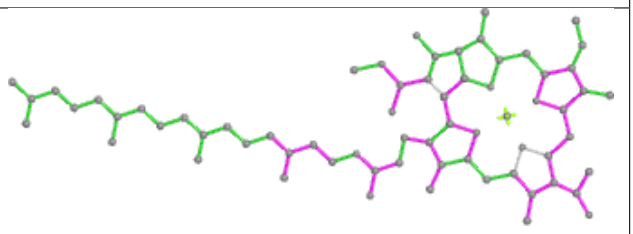
Ligand PEF H 301



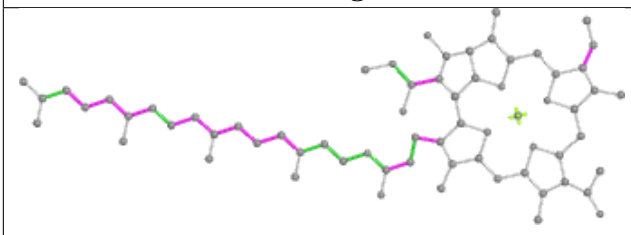
Ligand BCL F 102



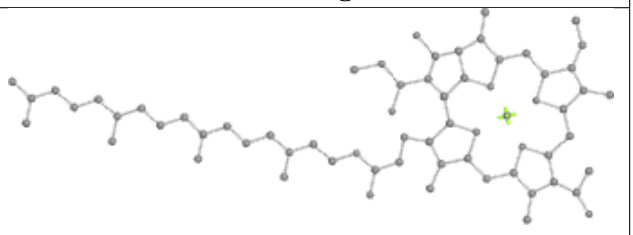
Bond lengths



Bond angles

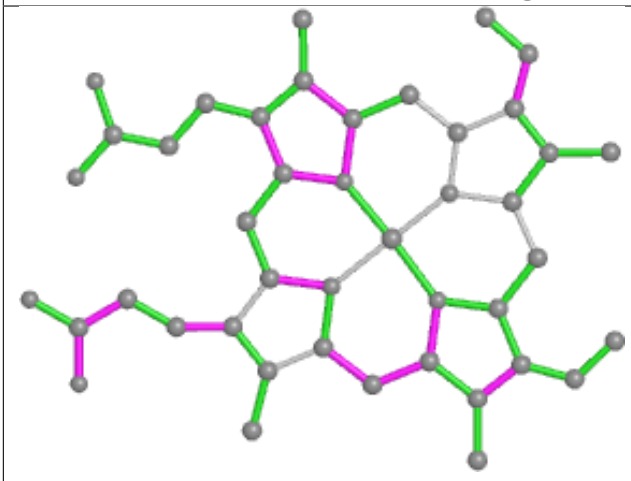


Torsions

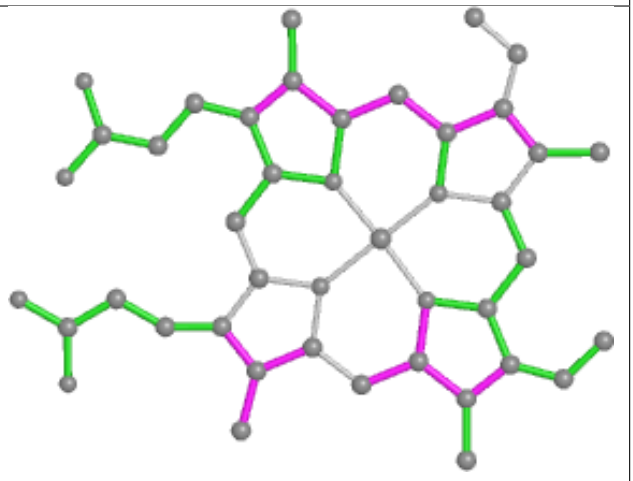


Rings

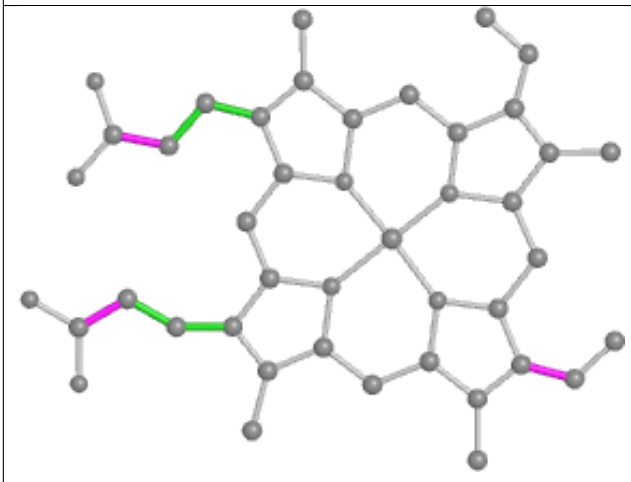
Ligand HEM C 503



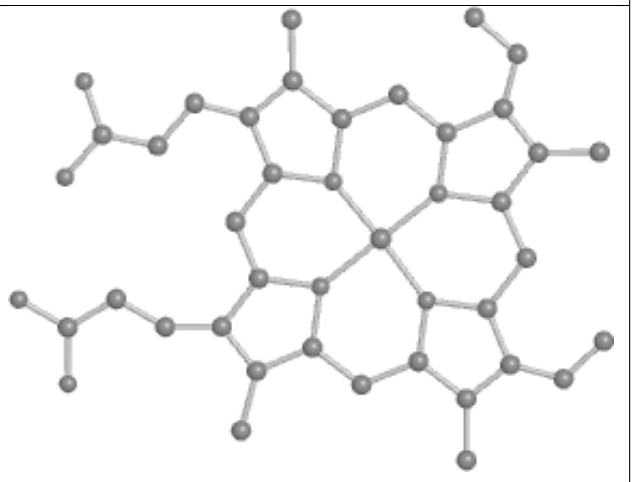
Bond lengths



Bond angles

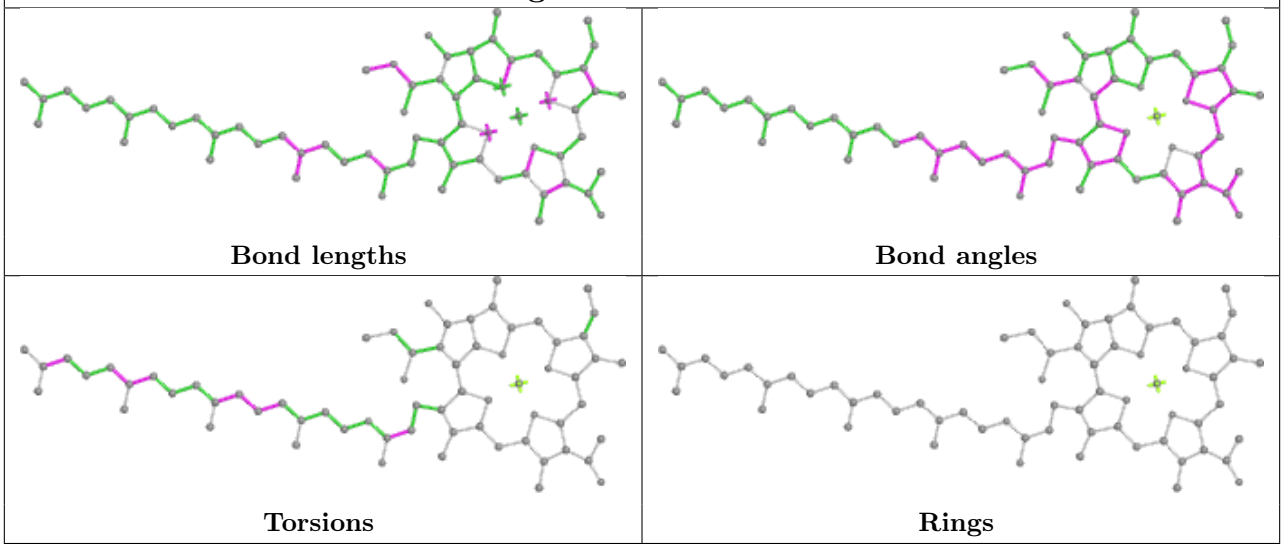


Torsions

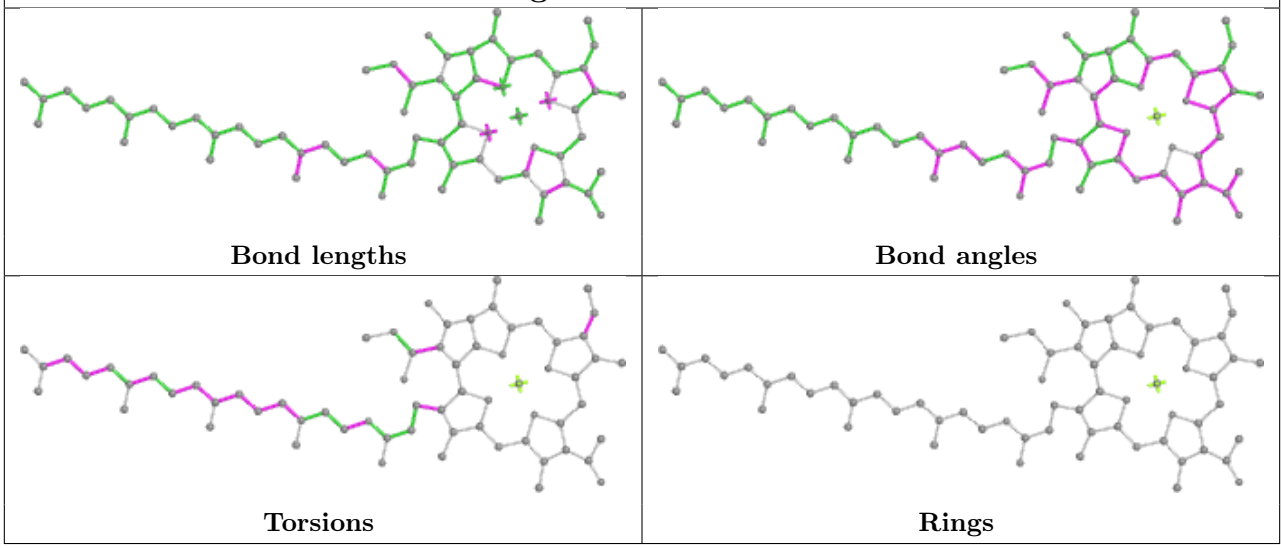


Rings

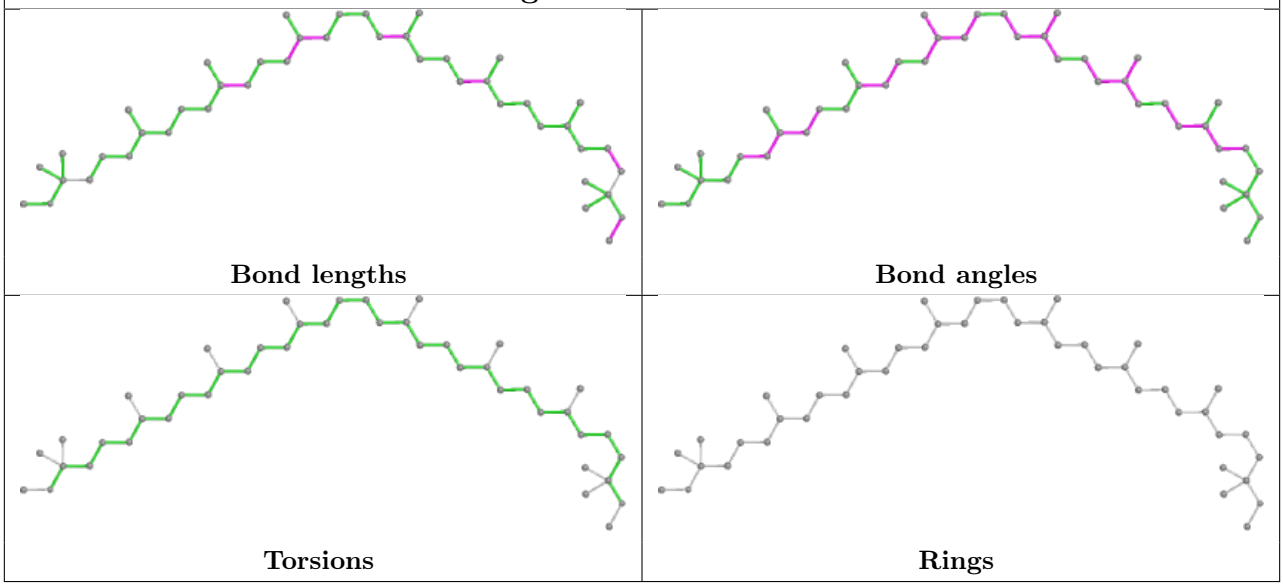
Ligand BCL Z 101



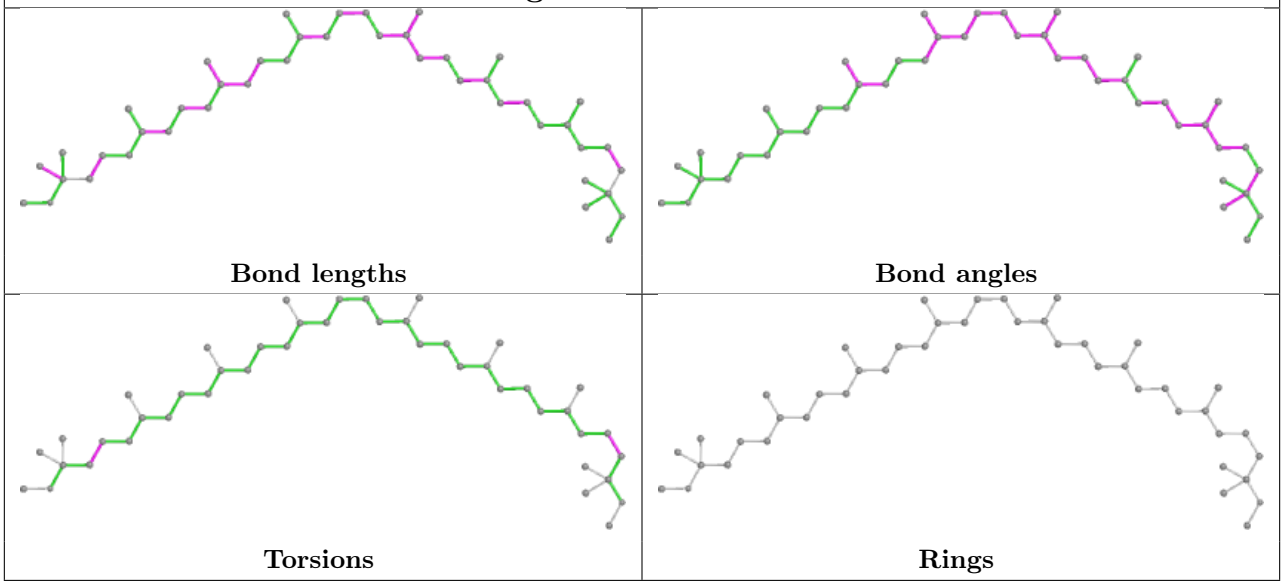
Ligand BCL 5 102



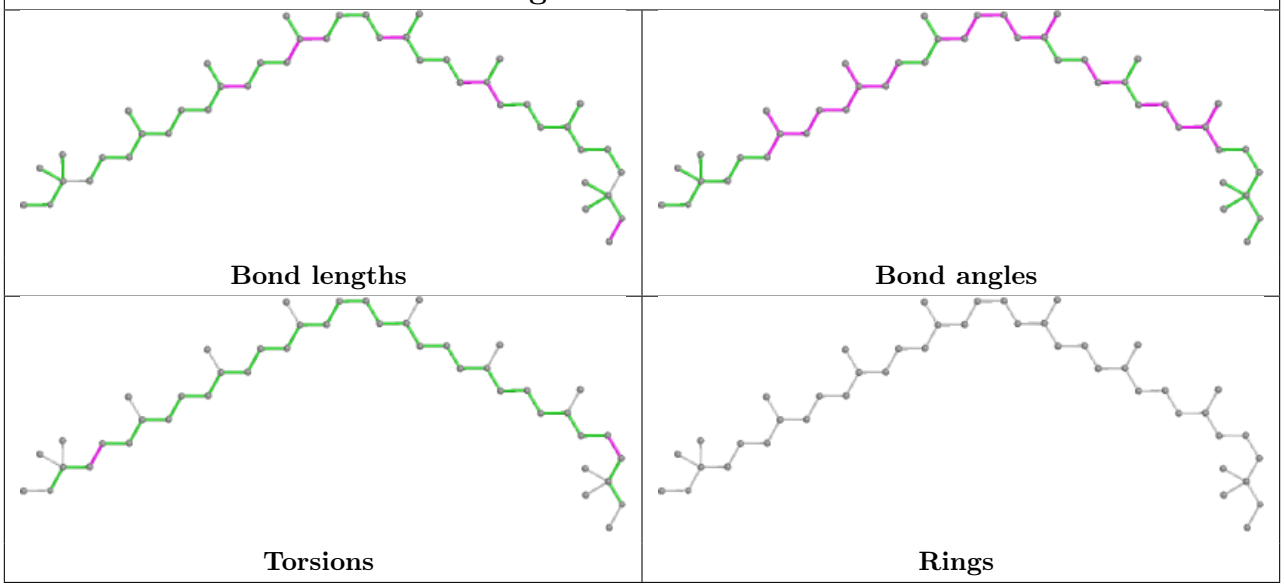
Ligand CRT M 406



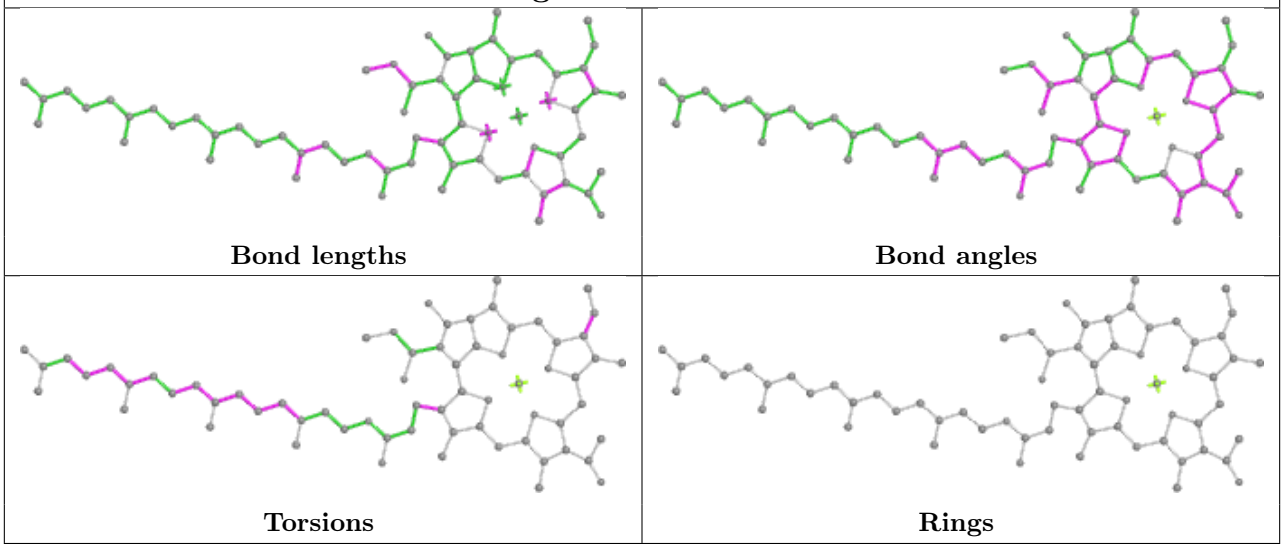
Ligand CRT P 102



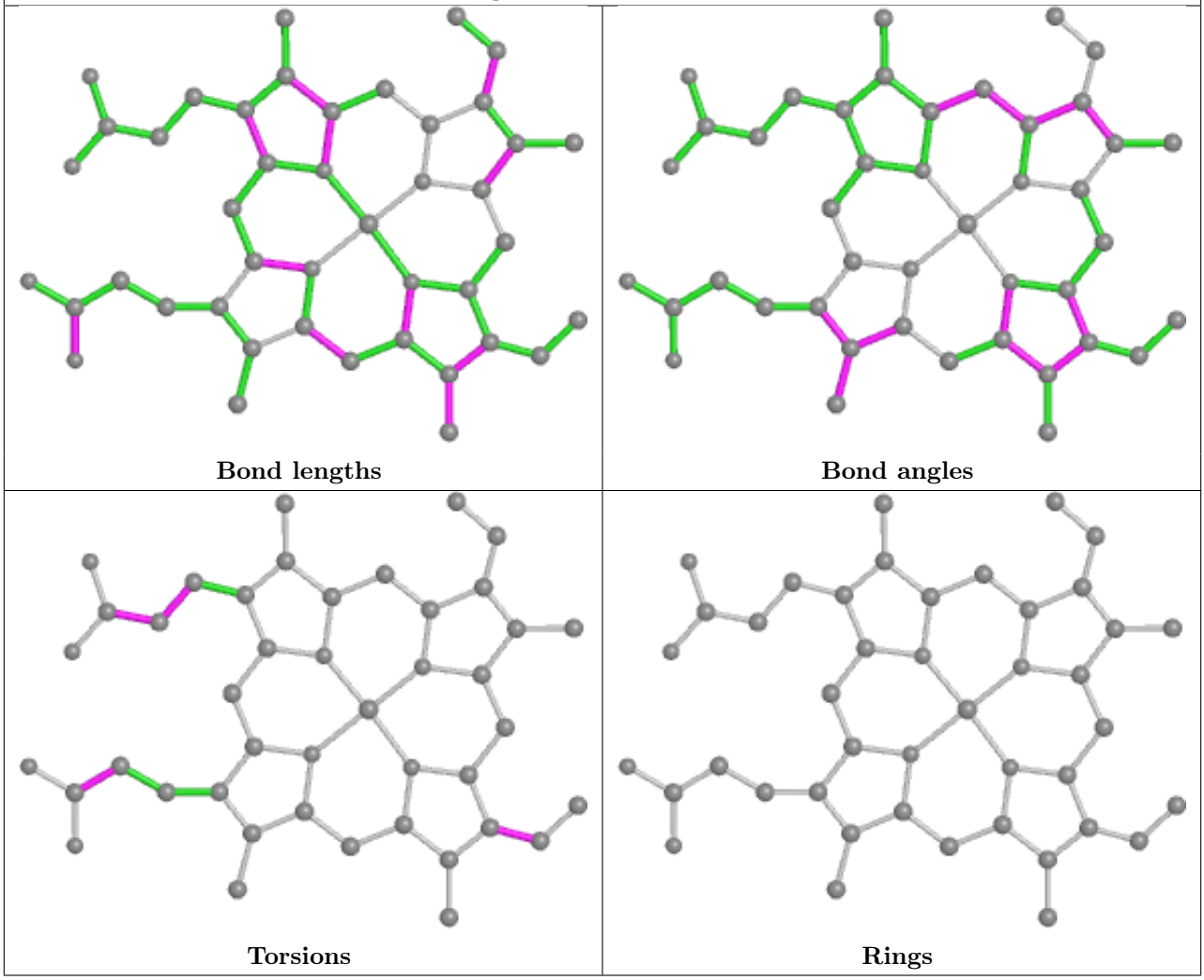
Ligand CRT 8 101



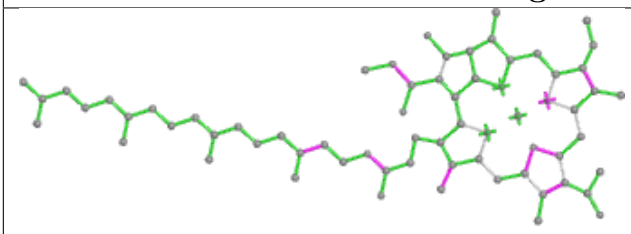
Ligand BCL I 102



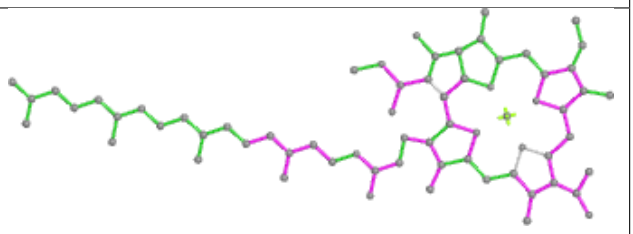
Ligand HEM C 504



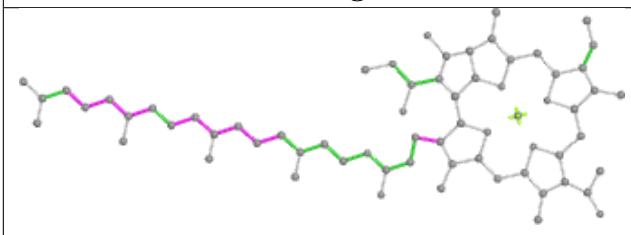
Ligand BCL 7 102



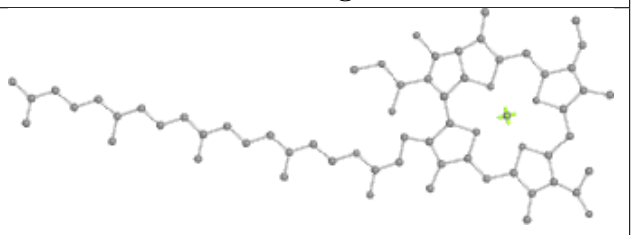
Bond lengths



Bond angles

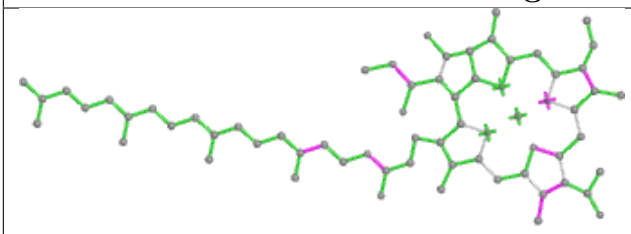


Torsions

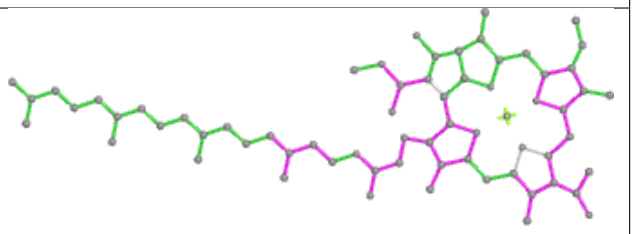


Rings

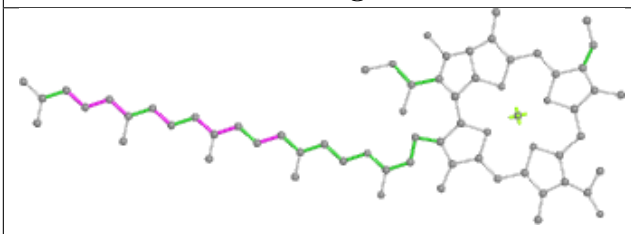
Ligand BCL G 101



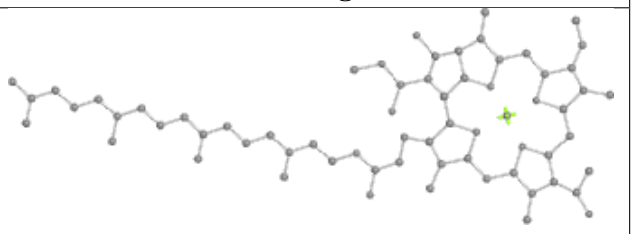
Bond lengths



Bond angles

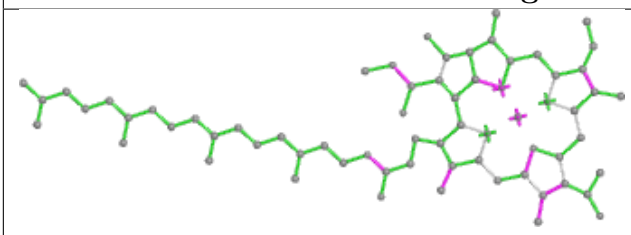


Torsions

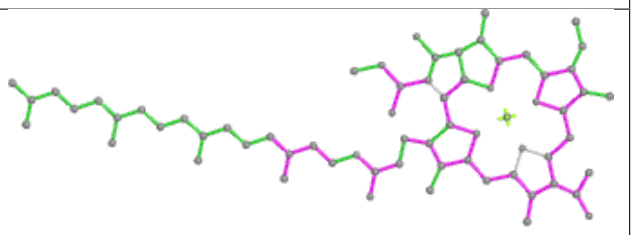


Rings

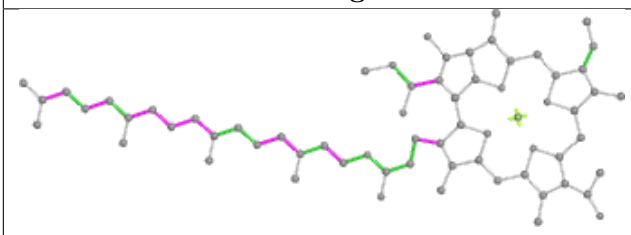
Ligand BCL M 402



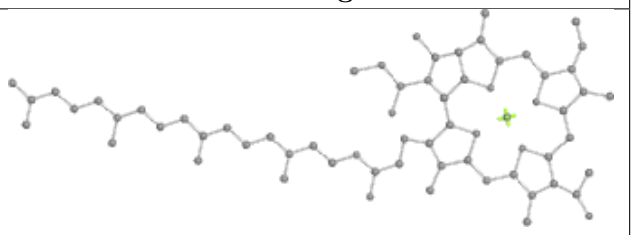
Bond lengths



Bond angles

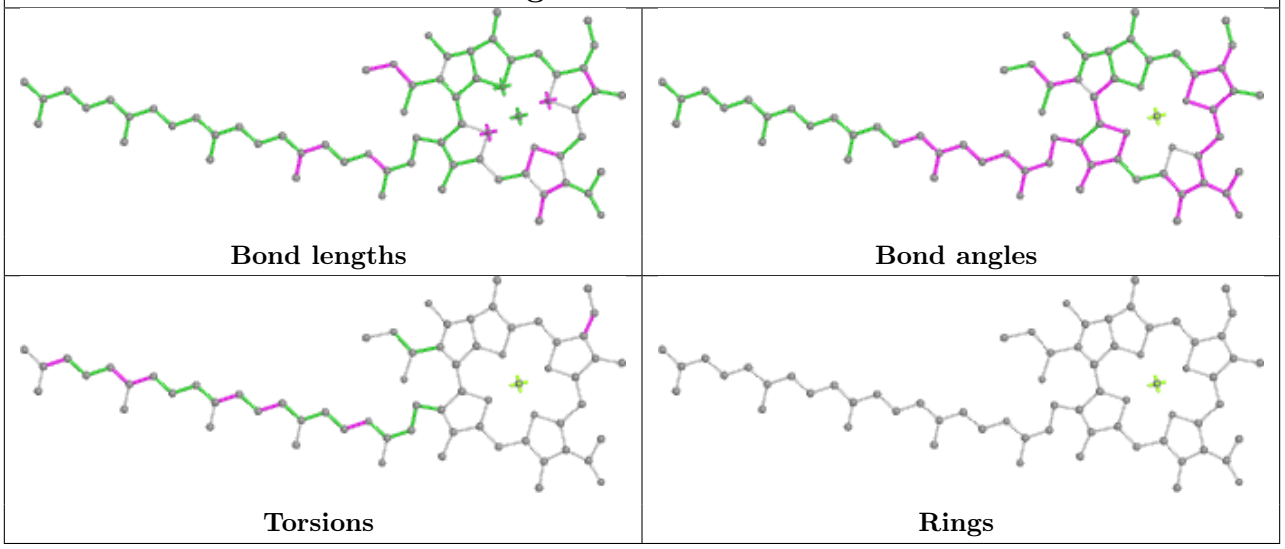


Torsions

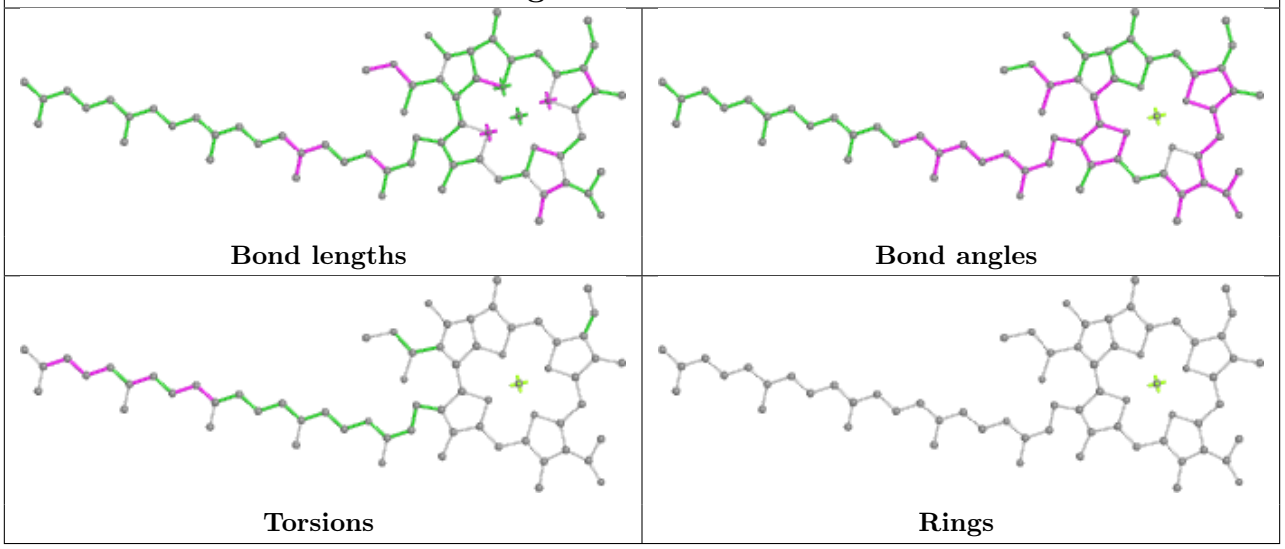


Rings

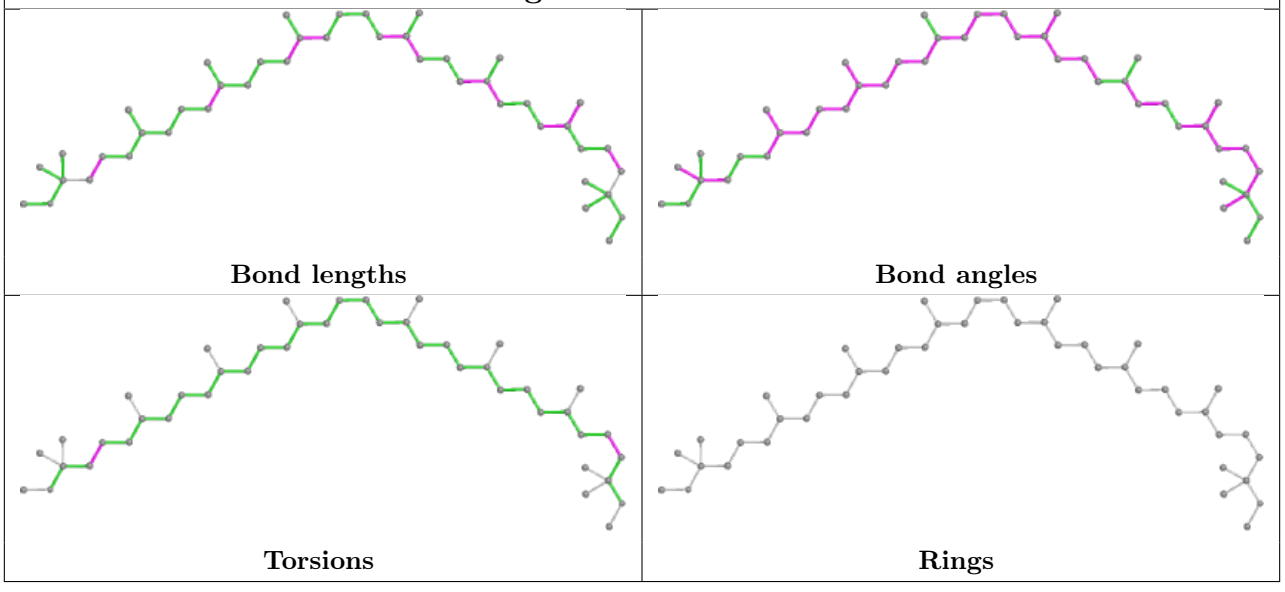
Ligand BCL P 101



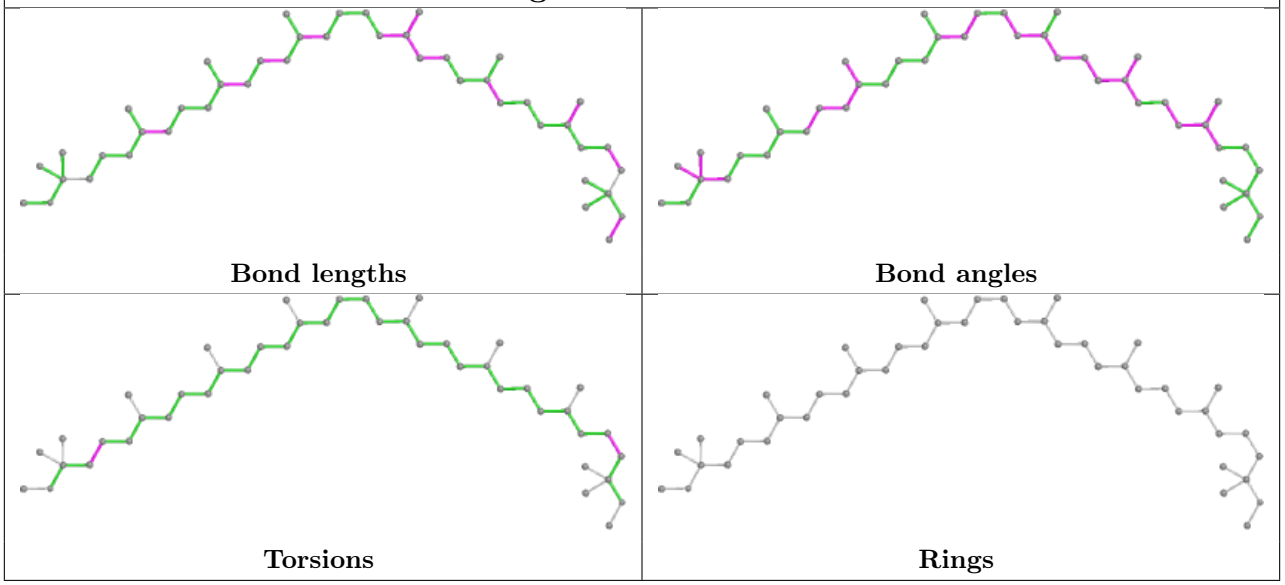
Ligand BCL E 101



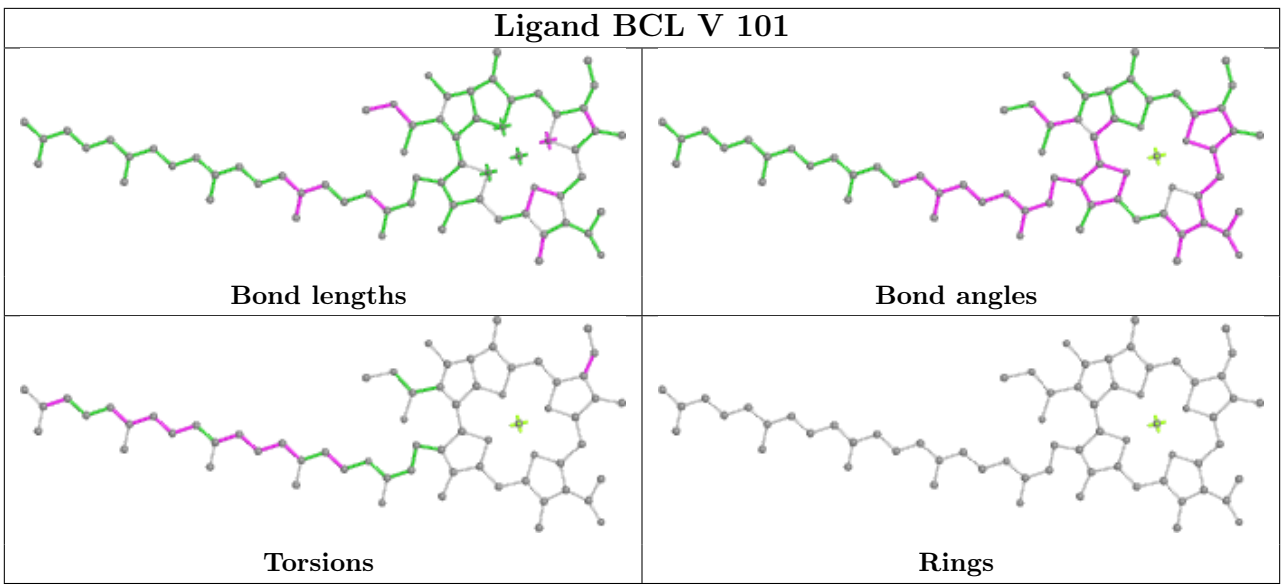
Ligand CRT R 102



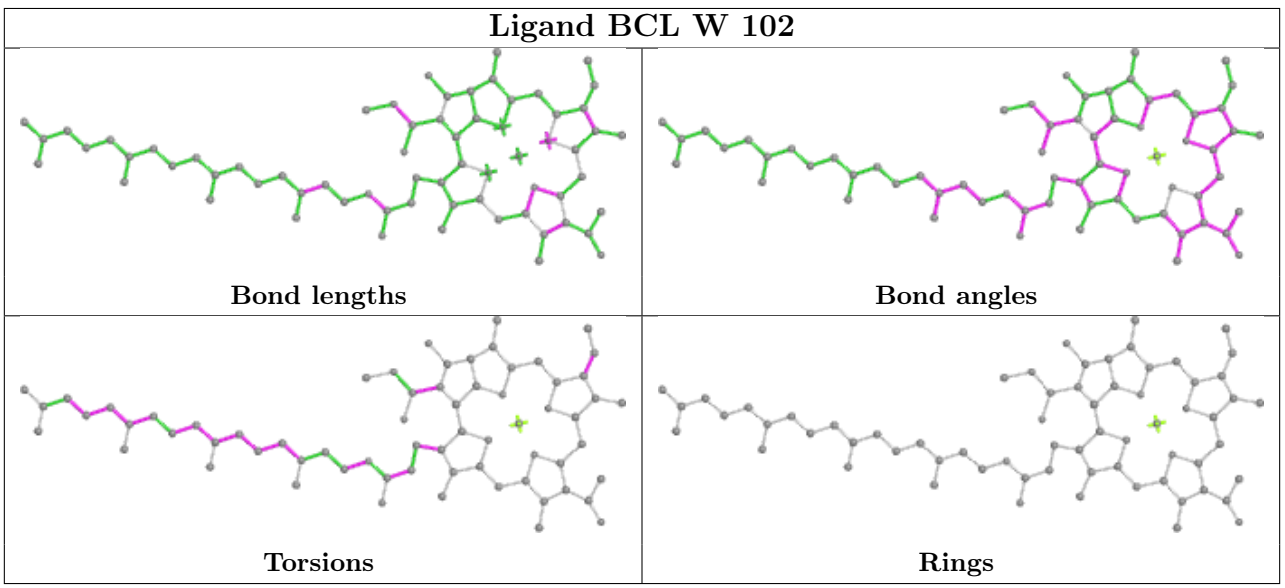
Ligand CRT 3 103



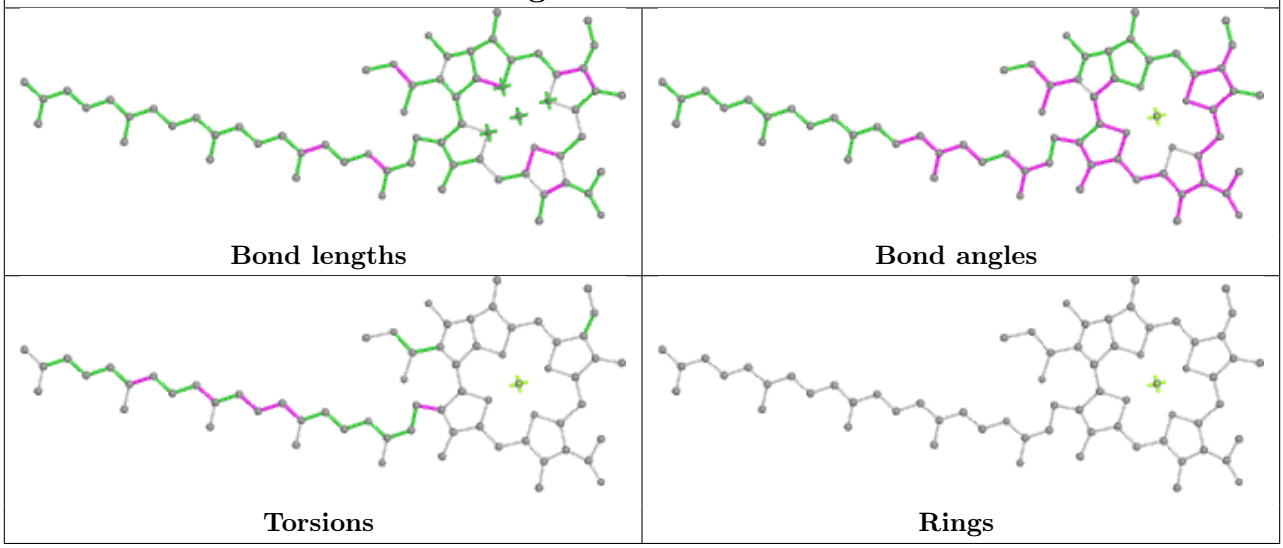
Ligand BCL V 101



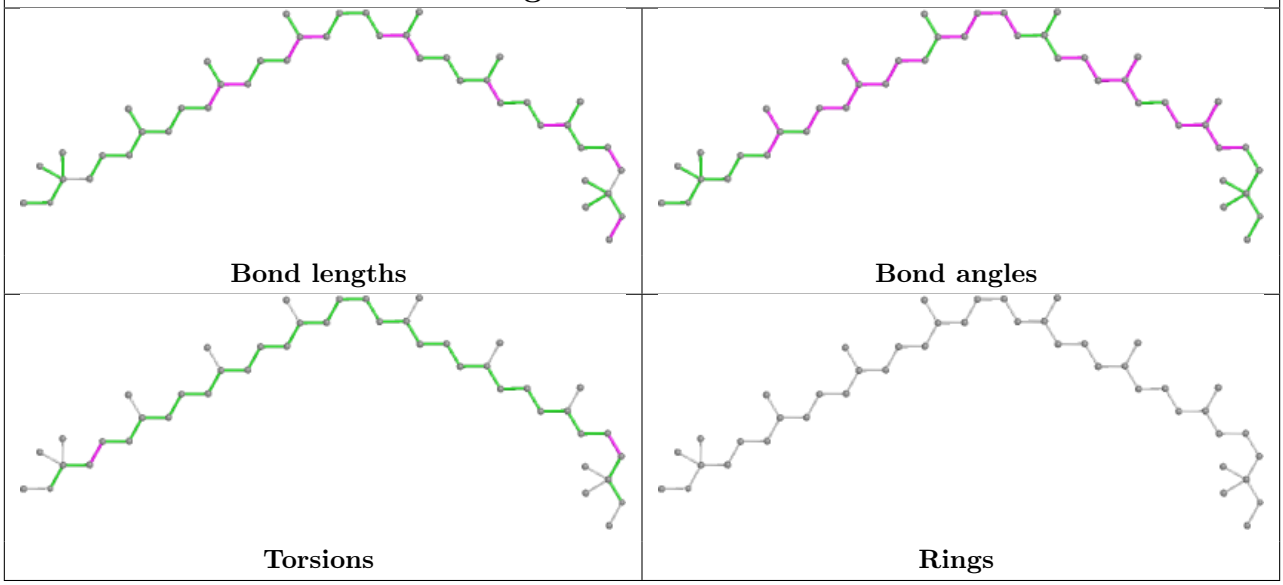
Ligand BCL W 102



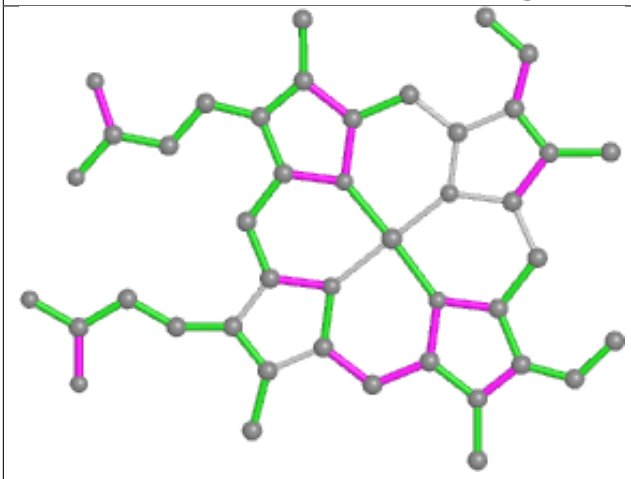
Ligand BCL L 303



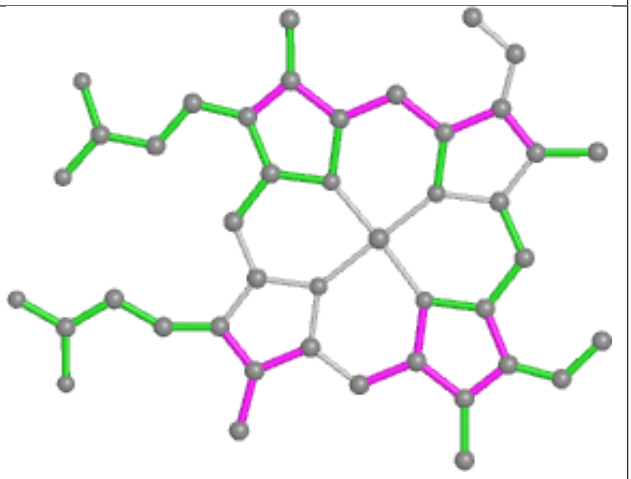
Ligand CRT N 102



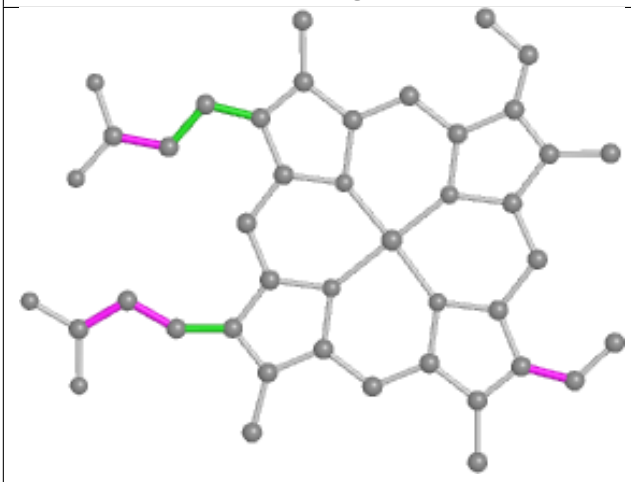
Ligand HEM C 501



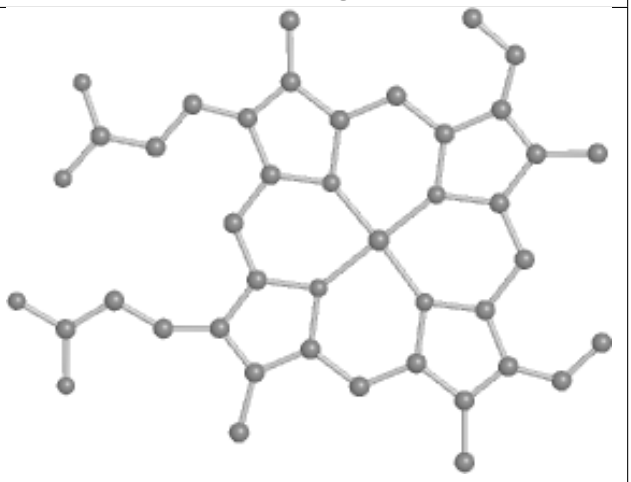
Bond lengths



Bond angles

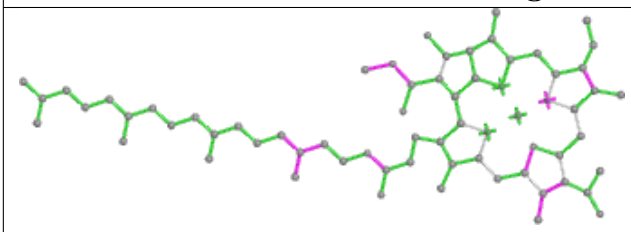


Torsions

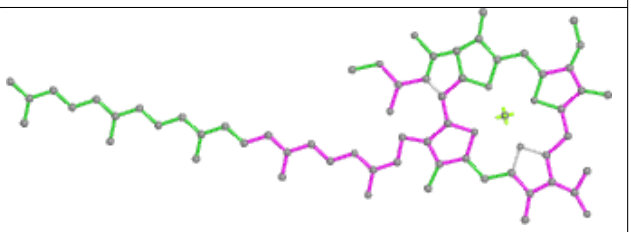


Rings

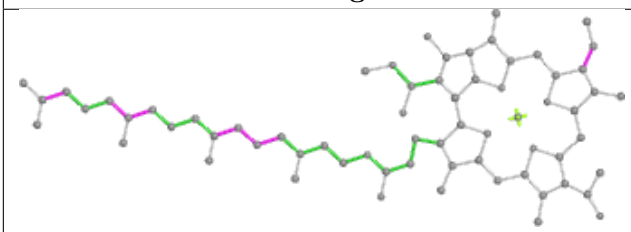
Ligand BCL T 101



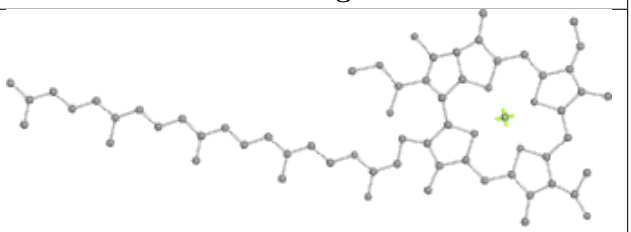
Bond lengths



Bond angles

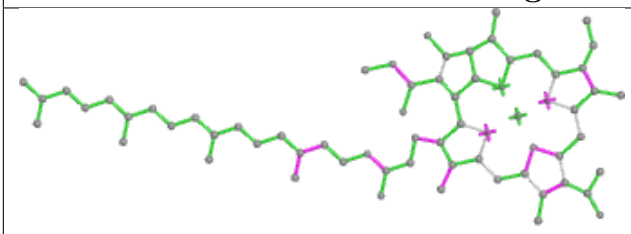


Torsions

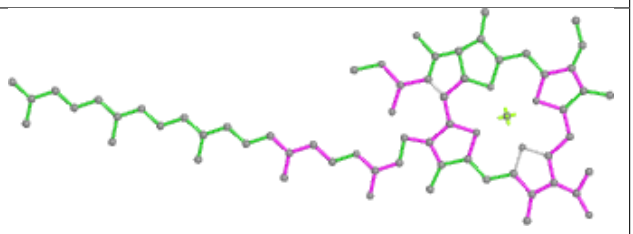


Rings

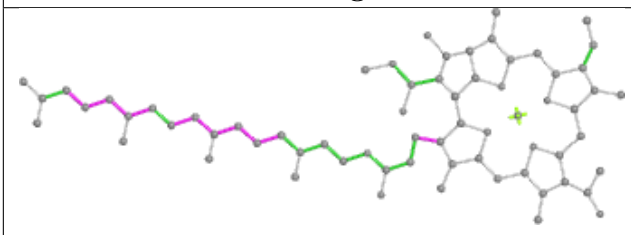
Ligand BCL U 102



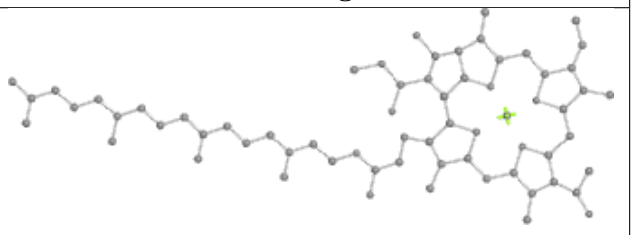
Bond lengths



Bond angles

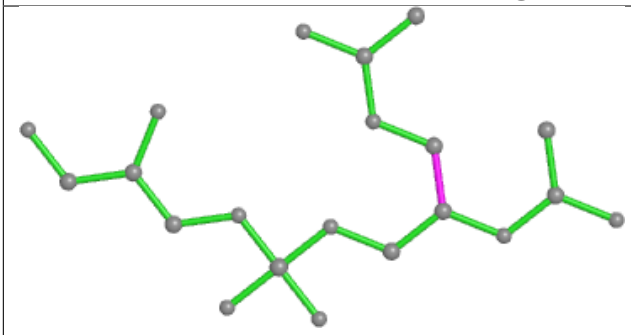


Torsions

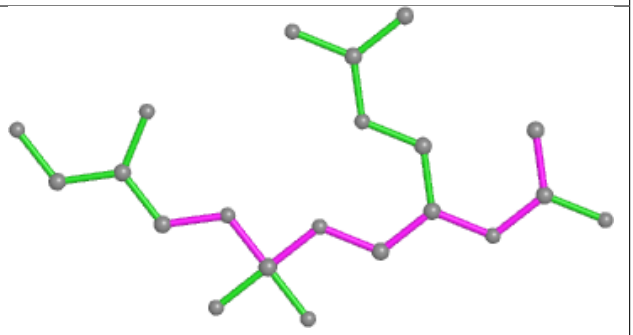


Rings

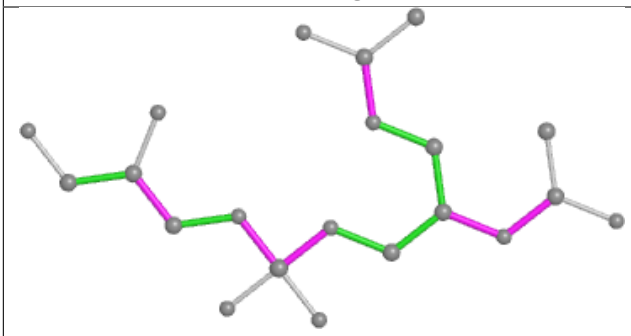
Ligand PGW M 407



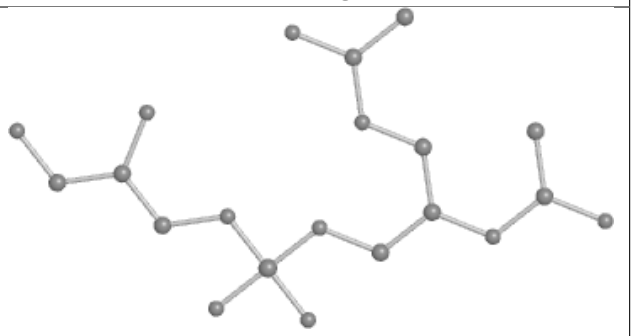
Bond lengths



Bond angles

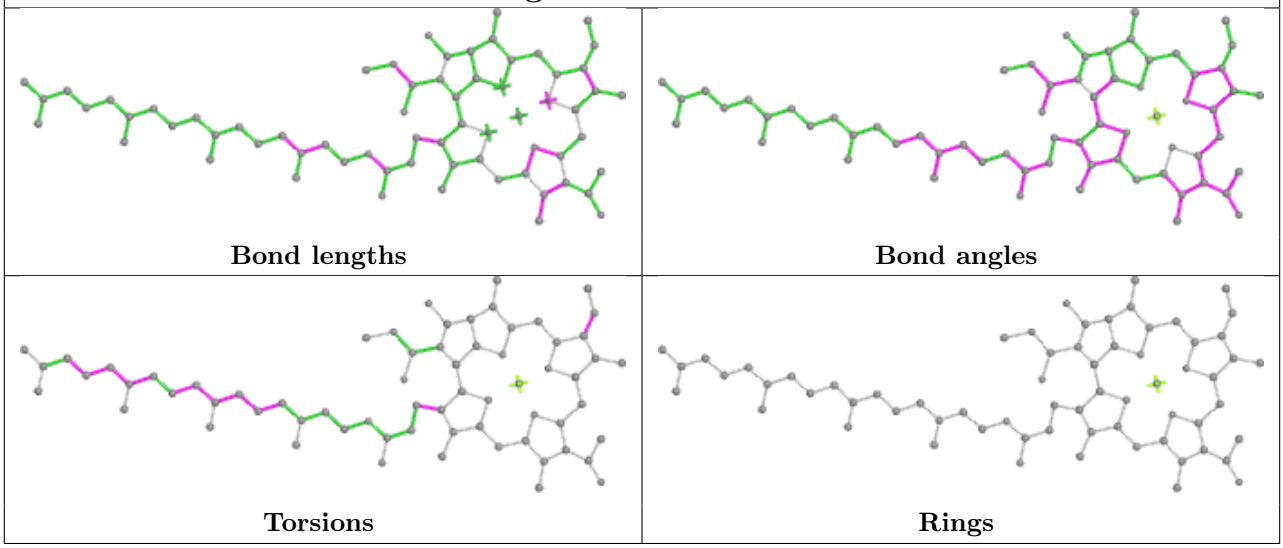


Torsions

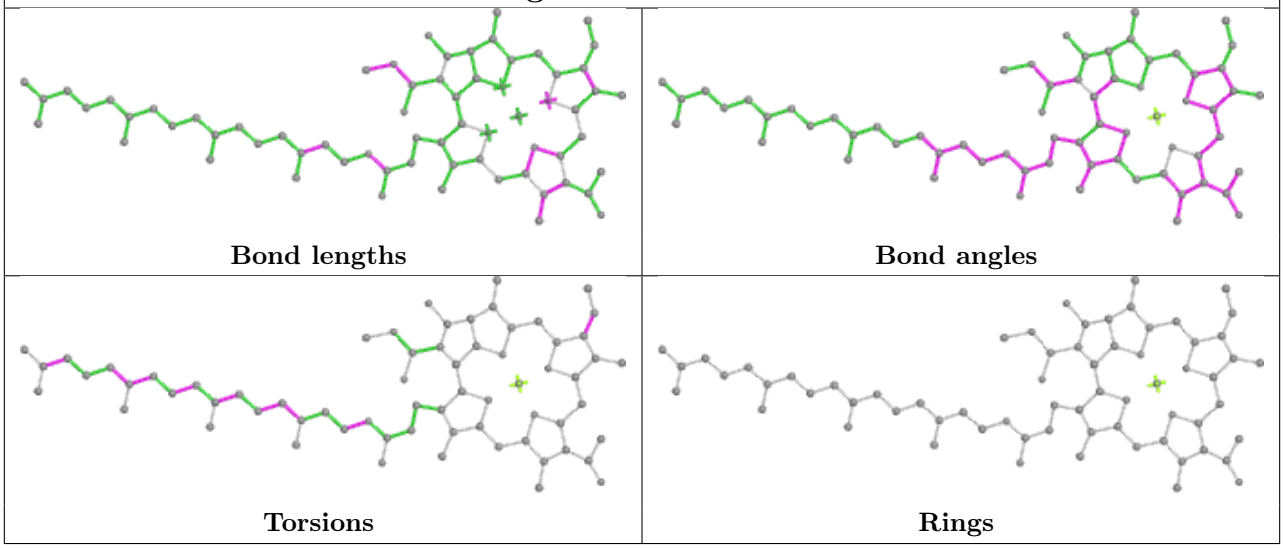


Rings

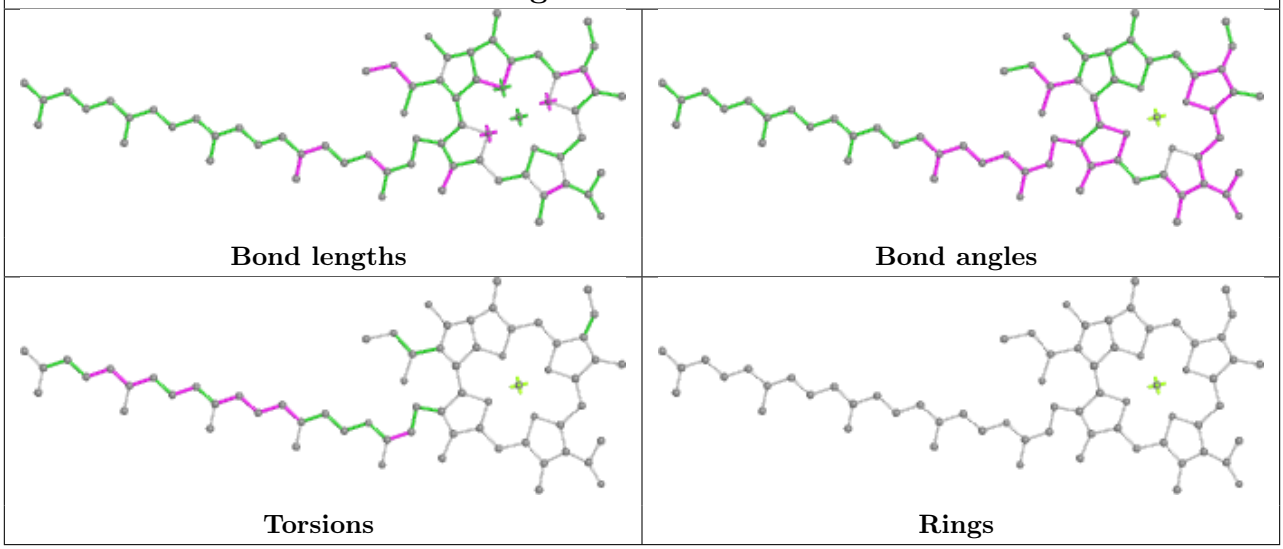
Ligand BCL K 102



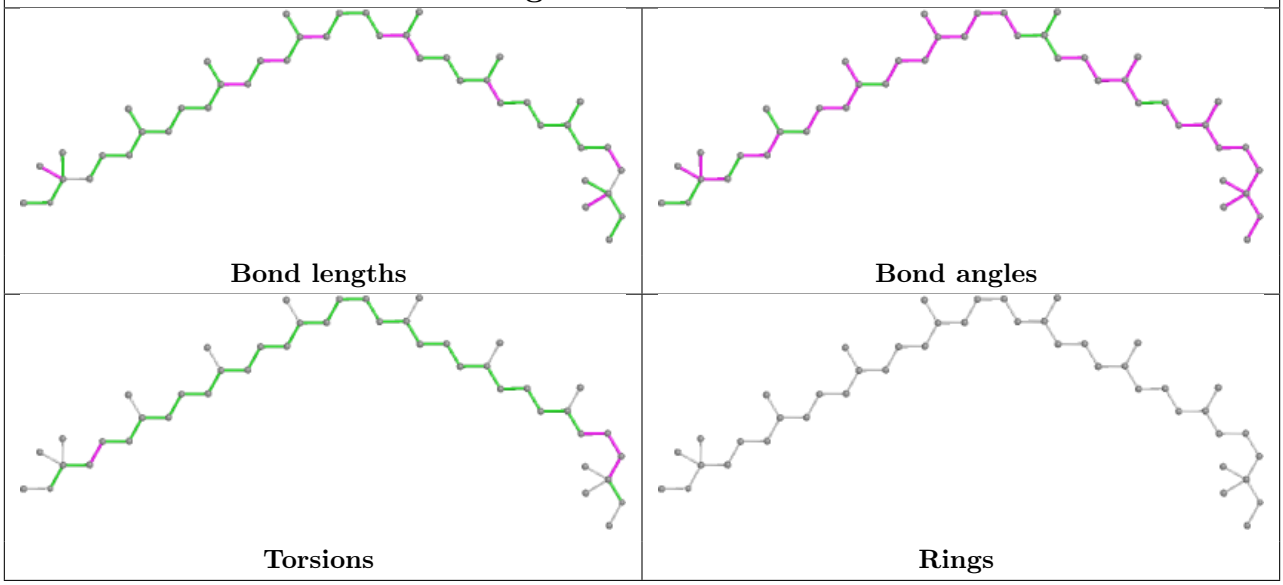
Ligand BCL B 101



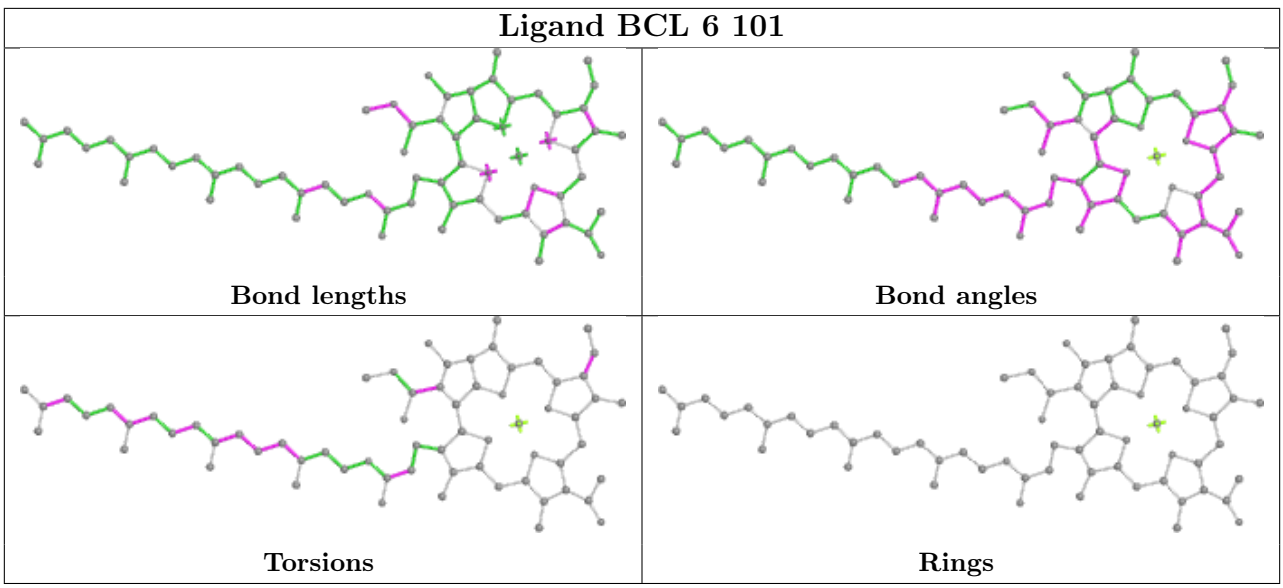
Ligand BCL 2 101



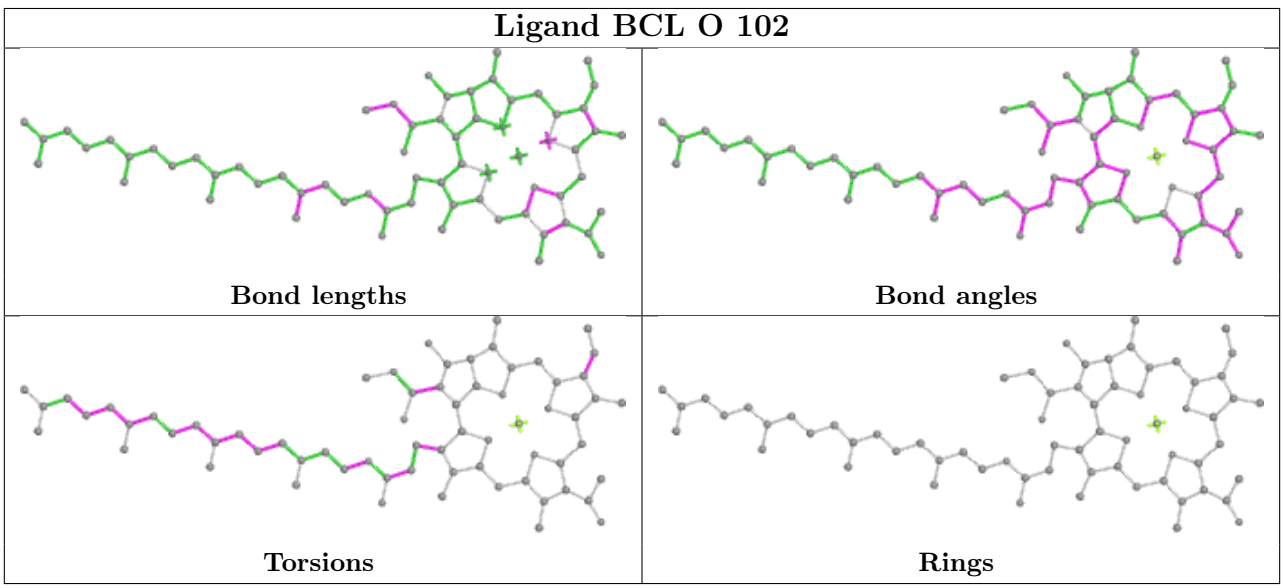
Ligand CRT T 102



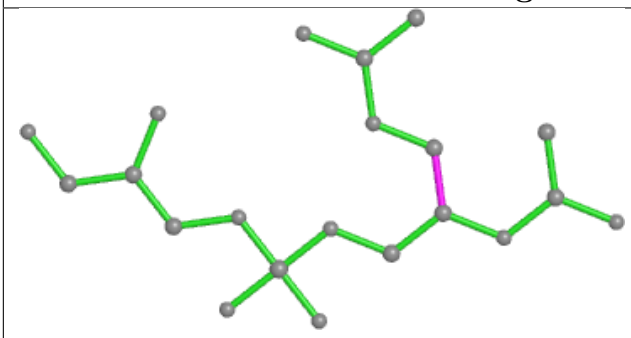
Ligand BCL 6 101



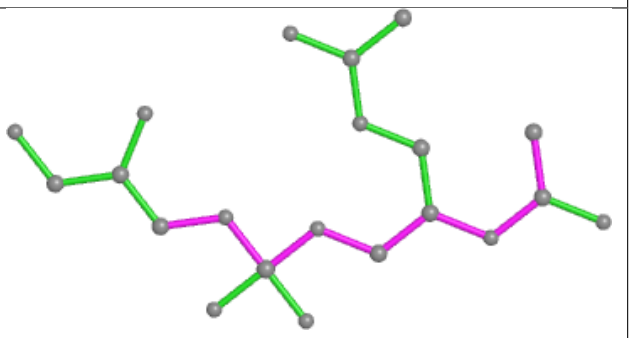
Ligand BCL O 102



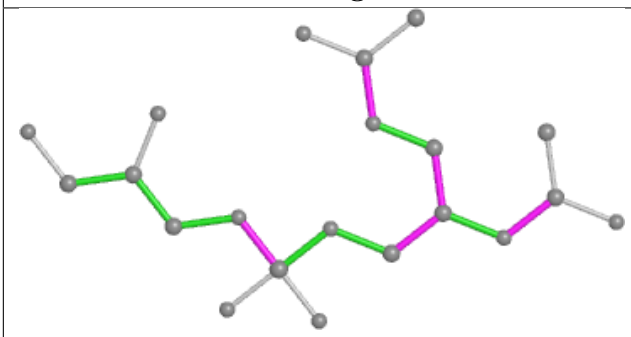
Ligand PGW H 302



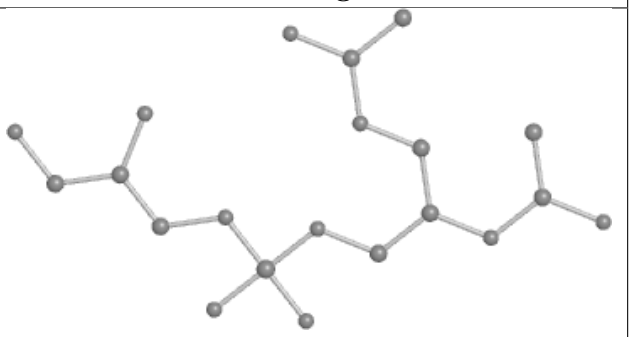
Bond lengths



Bond angles

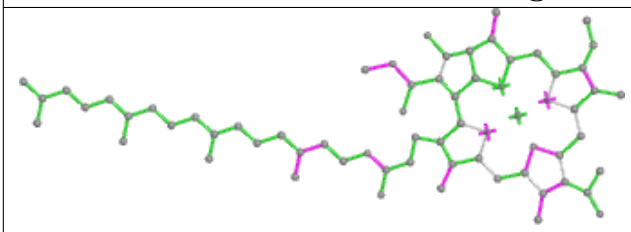


Torsions

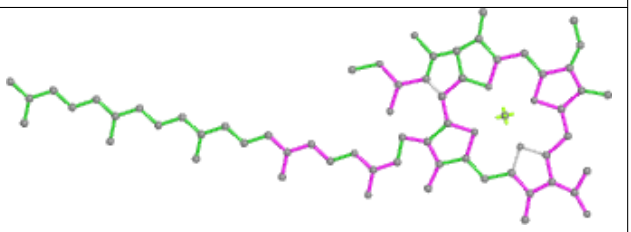


Rings

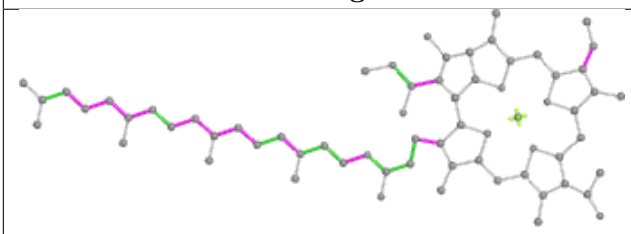
Ligand BCL S 102



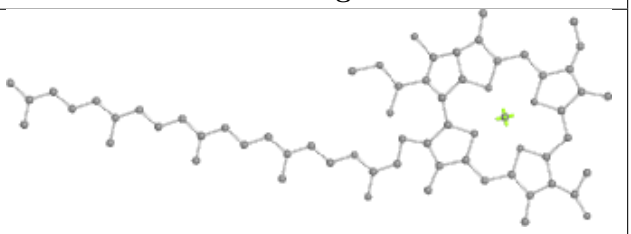
Bond lengths



Bond angles

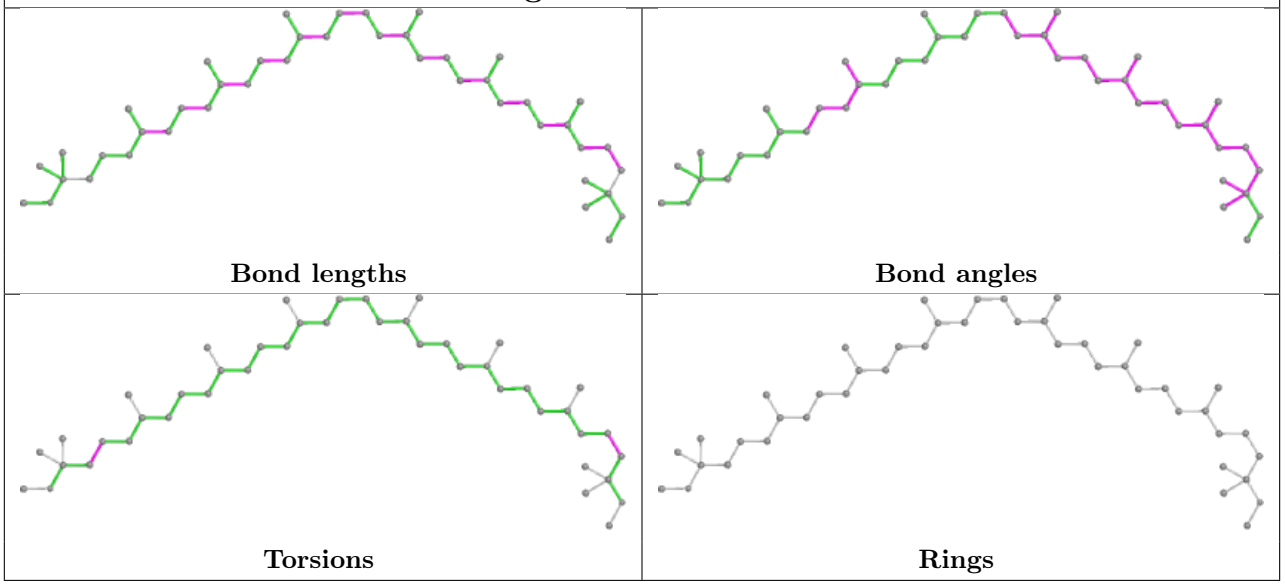


Torsions

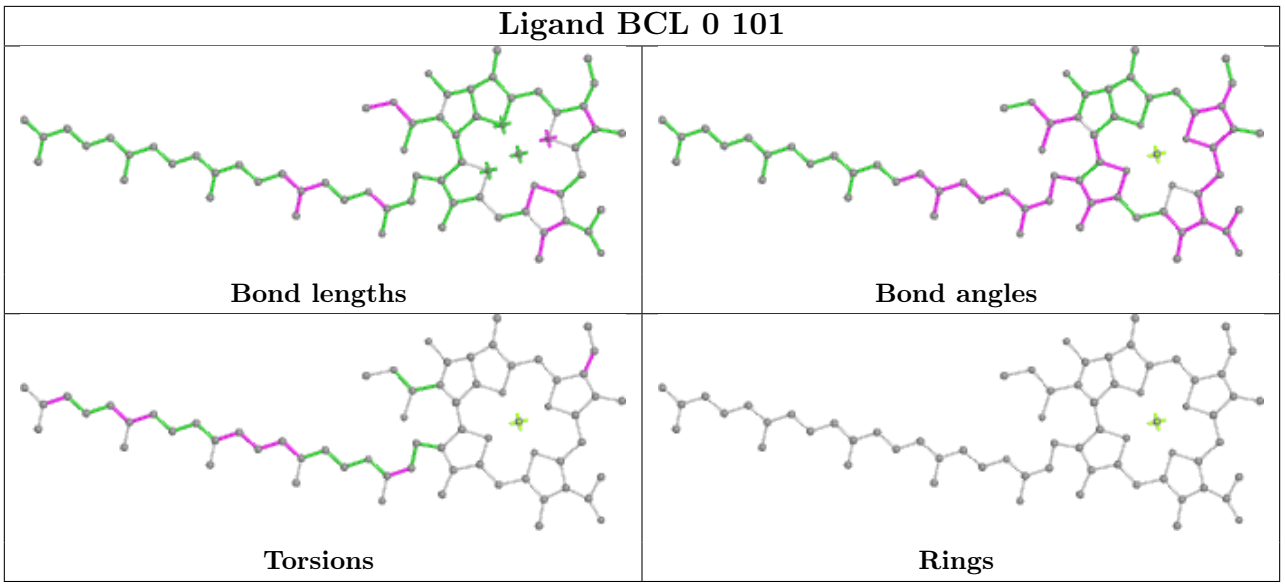


Rings

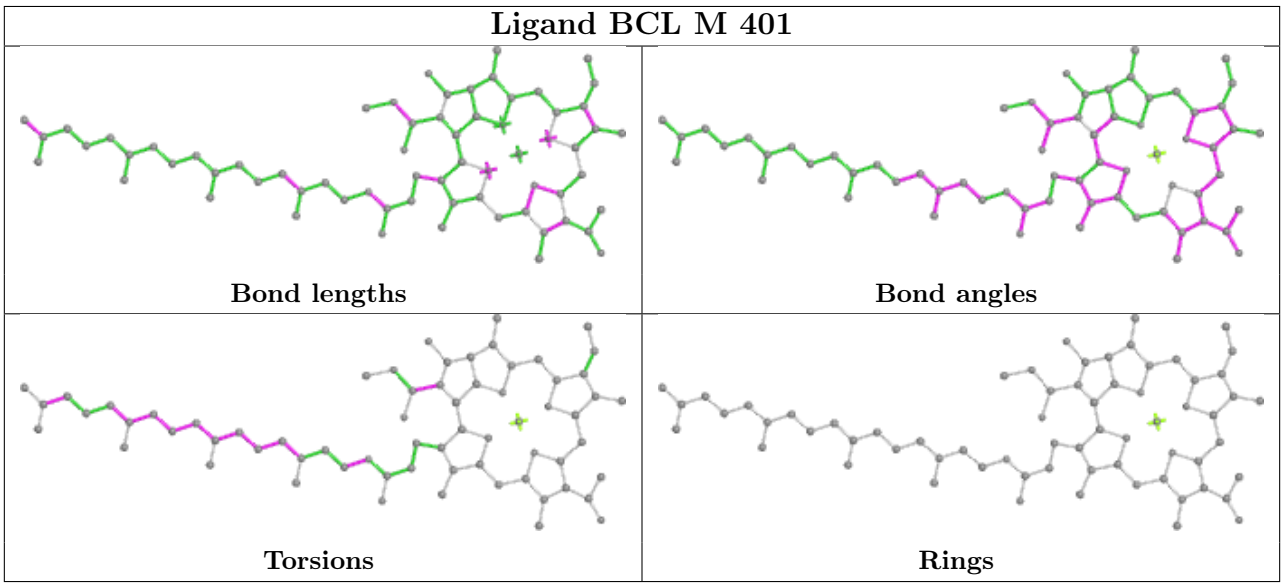
Ligand CRT X 102



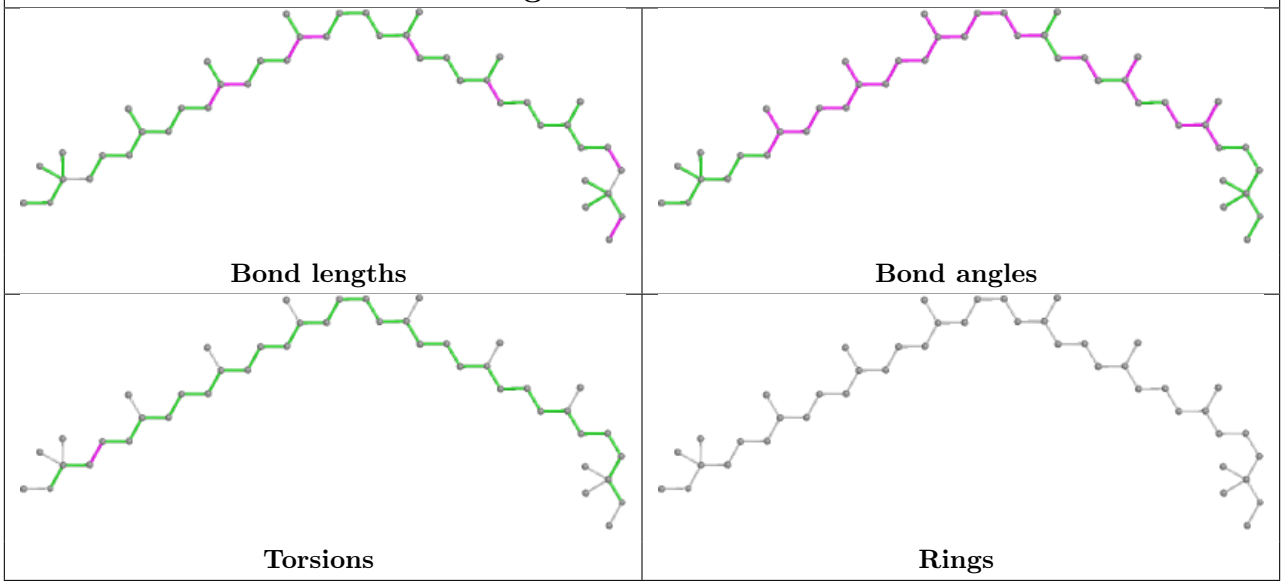
Ligand BCL 0 101



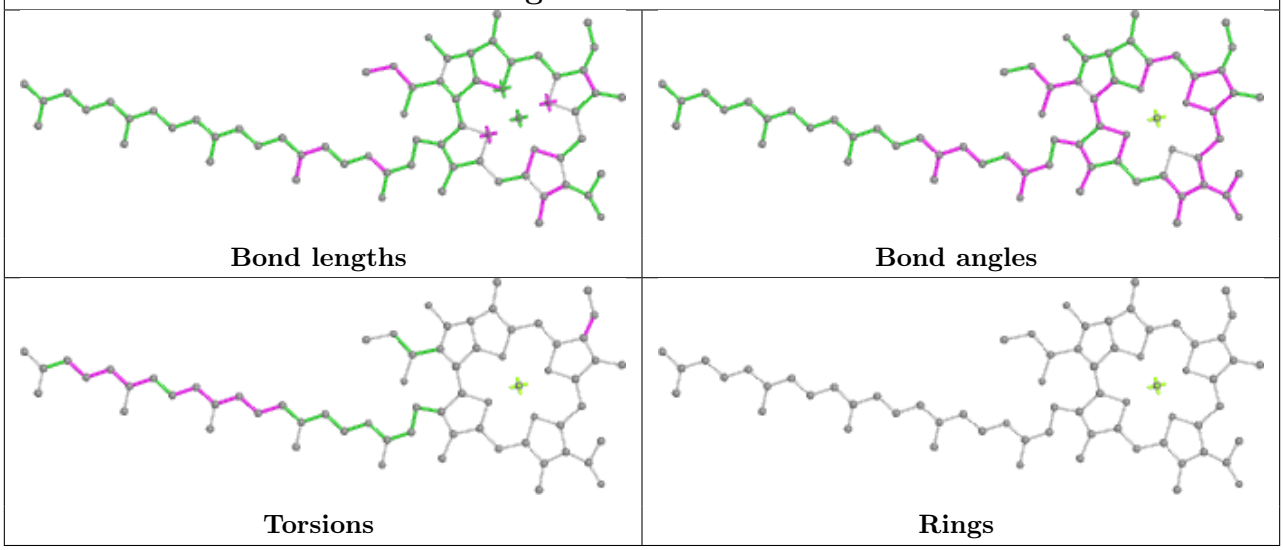
Ligand BCL M 401



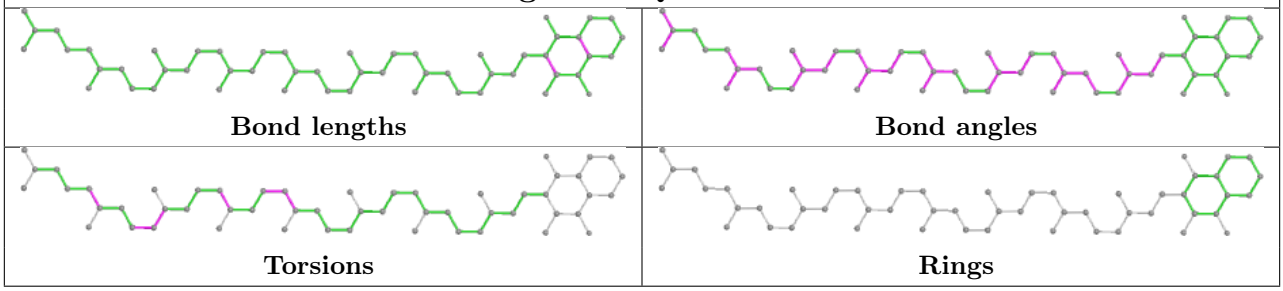
Ligand CRT G 102



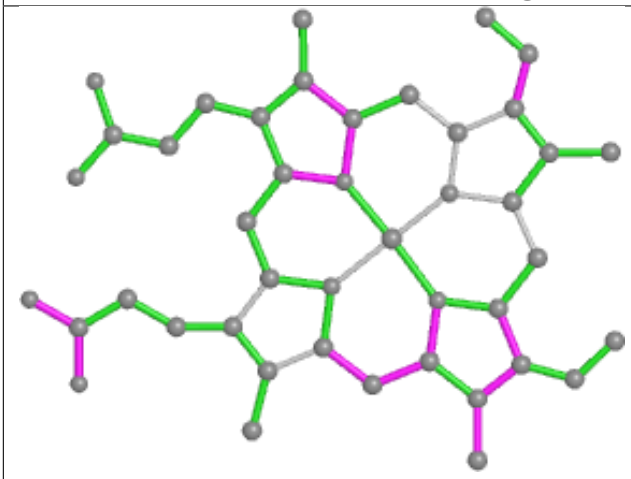
Ligand BCL Y 102



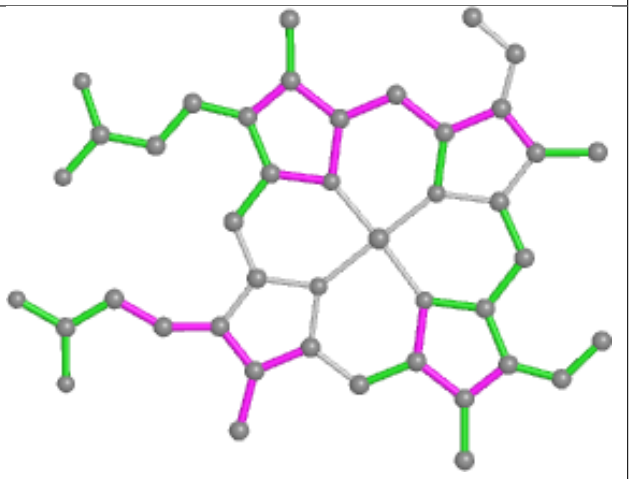
Ligand MQ8 M 405



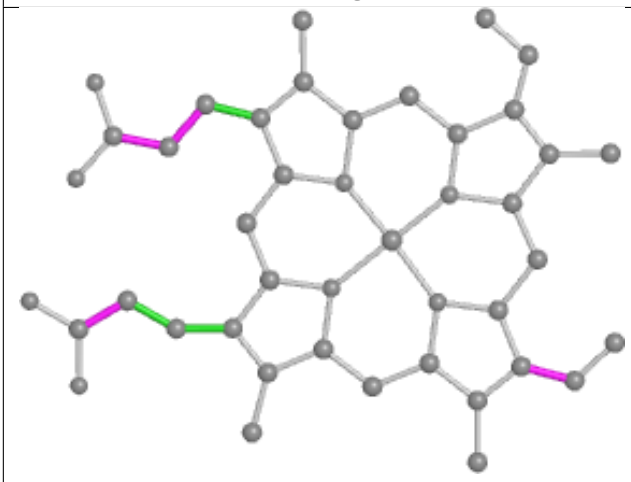
Ligand HEM C 502



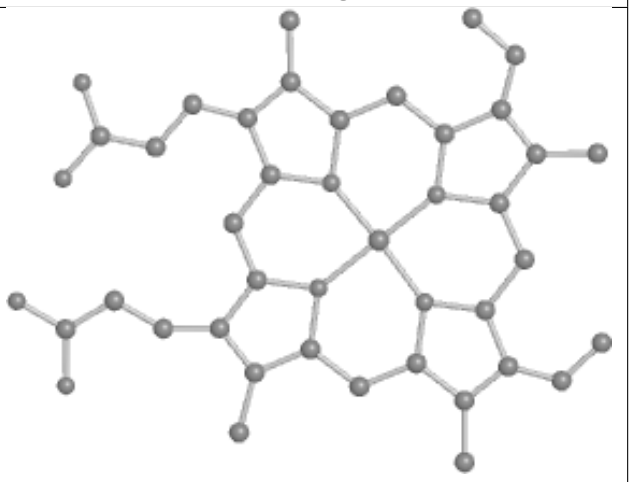
Bond lengths



Bond angles

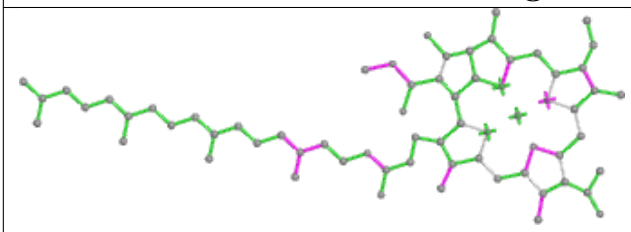


Torsions

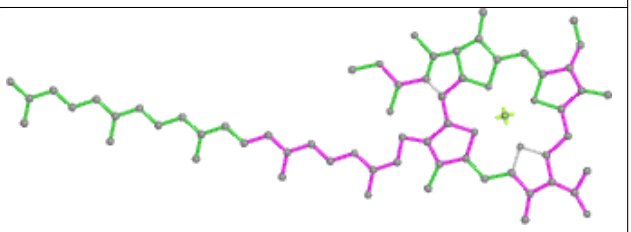


Rings

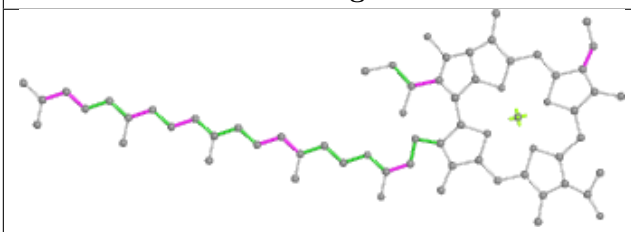
Ligand BCL X 101



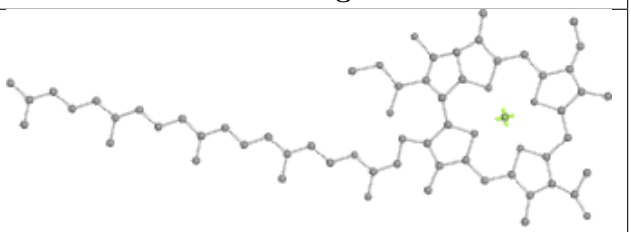
Bond lengths



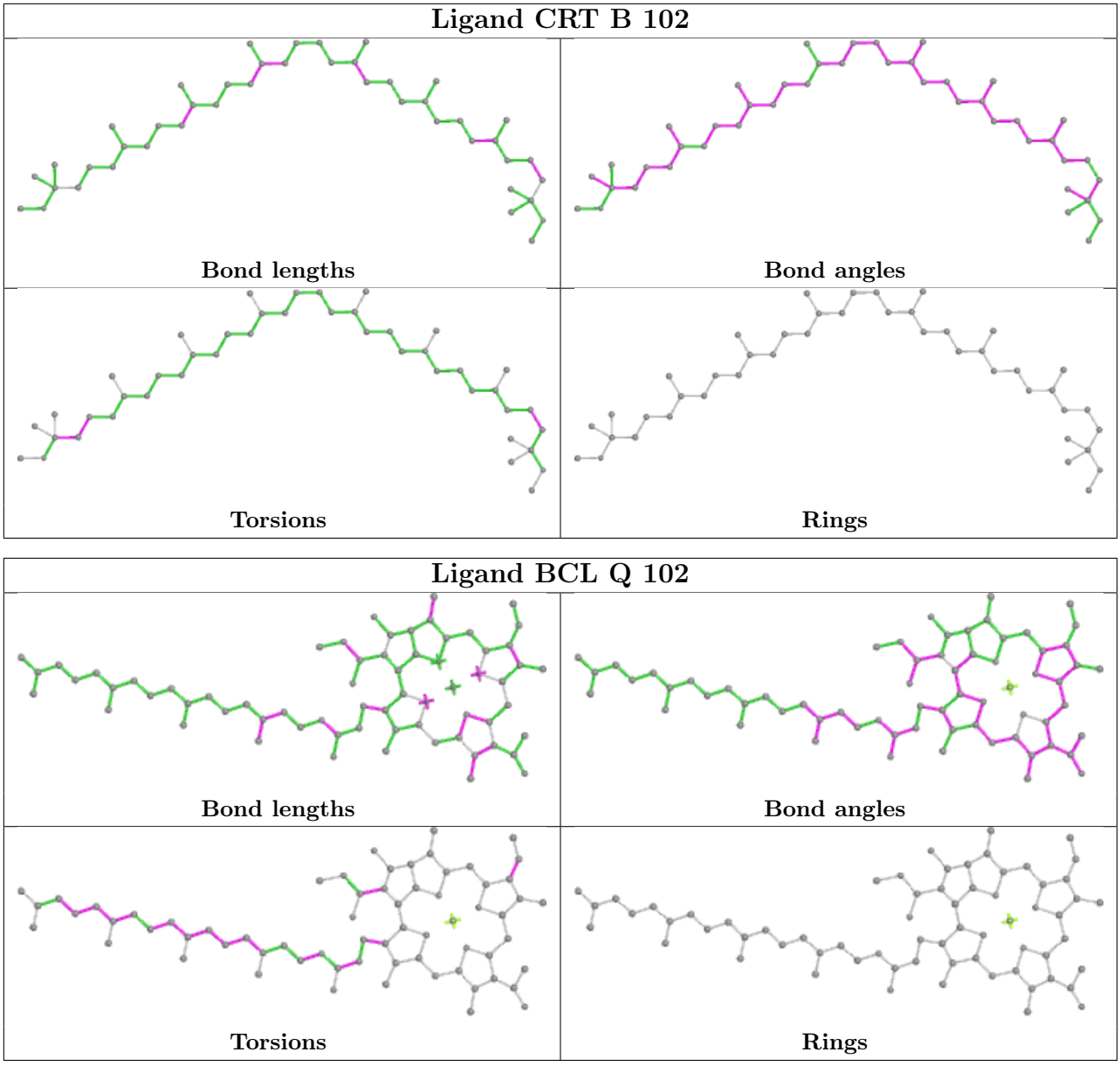
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	C	317/404 (78%)	0.03	16 (5%) 28 10	25, 67, 117, 142	1 (0%)
2	L	280/281 (99%)	-0.21	5 (1%) 68 40	15, 66, 102, 123	0
3	M	319/325 (98%)	-0.07	6 (1%) 66 37	32, 76, 115, 142	0
4	H	258/259 (99%)	0.21	19 (7%) 14 4	45, 89, 152, 198	0
5	1	60/61 (98%)	0.65	11 (18%) 1 0	62, 109, 257, 261	0
5	3	60/61 (98%)	0.45	6 (10%) 7 2	66, 137, 225, 231	0
5	5	60/61 (98%)	0.95	12 (20%) 1 0	82, 165, 250, 269	0
5	7	60/61 (98%)	0.87	12 (20%) 1 0	80, 149, 247, 254	0
5	9	60/61 (98%)	1.74	14 (23%) 0 0	74, 142, 282, 286	0
5	A	60/61 (98%)	1.18	15 (25%) 0 0	87, 147, 249, 250	0
5	D	60/61 (98%)	0.77	9 (15%) 2 1	86, 137, 260, 279	0
5	F	60/61 (98%)	1.17	12 (20%) 1 0	83, 178, 247, 256	0
5	I	60/61 (98%)	1.16	16 (26%) 0 0	81, 150, 244, 252	0
5	K	60/61 (98%)	1.32	20 (33%) 0 0	95, 155, 258, 259	0
5	O	60/61 (98%)	1.08	13 (21%) 0 0	84, 170, 249, 252	0
5	Q	60/61 (98%)	1.85	19 (31%) 0 0	105, 169, 257, 260	0
5	S	60/61 (98%)	1.20	14 (23%) 0 0	106, 167, 274, 278	0
5	U	60/61 (98%)	0.64	7 (11%) 4 1	80, 151, 265, 290	0
5	W	60/61 (98%)	0.47	6 (10%) 7 2	48, 114, 256, 264	0
5	Y	60/61 (98%)	1.07	10 (16%) 1 0	43, 105, 239, 258	0
6	0	40/47 (85%)	0.12	2 (5%) 28 10	112, 144, 199, 204	0
6	2	40/47 (85%)	0.19	3 (7%) 14 4	94, 117, 178, 181	0
6	4	40/47 (85%)	0.37	4 (10%) 7 2	100, 133, 177, 183	0
6	6	40/47 (85%)	-0.10	3 (7%) 14 4	104, 144, 171, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
6	8	40/47 (85%)	0.92	8 (20%) 1 0	107, 140, 180, 182	0
6	B	40/47 (85%)	0.34	5 (12%) 3 1	106, 141, 220, 242	0
6	E	40/47 (85%)	0.19	3 (7%) 14 4	108, 131, 156, 162	0
6	G	40/47 (85%)	0.38	6 (15%) 2 1	125, 155, 169, 179	0
6	J	40/47 (85%)	-0.19	0 100 100	124, 152, 204, 205	0
6	N	40/47 (85%)	0.37	4 (10%) 7 2	143, 160, 187, 195	0
6	P	40/47 (85%)	0.23	6 (15%) 2 1	136, 158, 179, 183	0
6	R	40/47 (85%)	0.47	6 (15%) 2 1	137, 176, 194, 197	0
6	T	40/47 (85%)	0.36	5 (12%) 3 1	141, 164, 209, 210	0
6	V	40/47 (85%)	0.04	3 (7%) 14 4	107, 141, 157, 160	0
6	X	40/47 (85%)	-0.18	0 100 100	80, 109, 154, 166	0
6	Z	40/47 (85%)	0.29	3 (7%) 14 4	60, 100, 182, 189	0
All	All	2774/2997 (92%)	0.41	303 (10%) 5 2	15, 109, 237, 290	1 (0%)

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	9	57	ALA	13.4
5	Y	5	ASN	11.9
5	Y	4	MET	11.6
5	Y	2	PHE	11.3
5	9	61	LYS	10.5
5	9	55	TYR	10.4
5	Q	61	LYS	10.3
5	9	56	GLN	9.8
5	Q	14	ILE	9.6
5	Y	3	THR	9.6
5	Q	57	ALA	9.5
5	O	50	ASN	9.1
5	F	13	LEU	8.9
5	5	55	TYR	8.7
5	9	60	LYS	8.4
5	9	58	LEU	8.3
6	0	10	THR	8.1
5	S	14	ILE	8.0
6	T	10	THR	7.9
5	Q	13	LEU	7.9
5	S	13	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
5	1	5	ASN	7.5
4	H	4	GLY	7.4
6	Z	10	THR	7.3
6	N	41	LEU	7.2
5	Q	60	LYS	7.2
5	9	54	SER	7.0
1	C	93	THR	7.0
5	K	50	ASN	7.0
5	5	54	SER	6.9
6	Z	11	ASP	6.8
6	4	12	ASP	6.8
1	C	19	MET	6.8
5	Q	56	GLN	6.8
6	2	12	ASP	6.7
5	O	49	ASP	6.6
5	1	3	THR	6.6
5	K	8	LEU	6.6
6	R	41	LEU	6.5
2	L	15	GLY	6.4
6	4	16	GLU	6.4
5	Q	8	LEU	6.3
5	U	8	LEU	6.3
5	F	10	LYS	6.3
5	3	6	ALA	6.2
5	K	53	VAL	6.2
5	I	17	PRO	6.2
5	I	48	ASP	6.0
5	O	54	SER	5.9
5	9	5	ASN	5.9
5	K	55	TYR	5.7
5	3	5	ASN	5.7
5	K	47	LEU	5.6
6	2	16	GLU	5.6
1	C	17	SER	5.5
5	S	42	THR	5.5
5	9	59	GLY	5.4
5	F	51	ILE	5.4
5	Q	11	ILE	5.3
5	O	8	LEU	5.3
5	Q	58	LEU	5.2
5	3	8	LEU	5.2
5	S	44	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
6	B	7	THR	5.2
4	H	2	SER	5.1
5	I	14	ILE	5.1
5	I	3	THR	5.1
2	L	14	GLY	5.1
4	H	3	ALA	5.1
6	8	41	LEU	5.0
4	H	133	ILE	4.9
5	A	13	LEU	4.9
5	O	43	ASP	4.9
5	U	15	LEU	4.8
5	5	8	LEU	4.8
6	8	11	ASP	4.8
6	G	46	LEU	4.7
6	2	10	THR	4.7
5	7	11	ILE	4.7
5	A	46	TRP	4.7
5	7	10	LYS	4.7
5	D	39	VAL	4.7
5	A	45	ASN	4.6
5	D	57	ALA	4.6
5	5	58	LEU	4.6
5	O	7	ASN	4.6
5	D	55	TYR	4.6
6	R	40	TRP	4.5
4	H	72	ASN	4.5
6	T	9	LEU	4.5
5	Q	55	TYR	4.5
5	O	3	THR	4.5
5	U	14	ILE	4.5
5	7	8	LEU	4.5
5	U	5	ASN	4.4
5	K	49	ASP	4.4
3	M	24	PRO	4.4
5	S	55	TYR	4.3
5	1	7	ASN	4.3
5	Q	43	ASP	4.3
6	R	45	TRP	4.3
5	I	43	ASP	4.3
6	8	10	THR	4.2
5	A	43	ASP	4.2
5	F	47	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
5	A	10	LYS	4.1
1	C	174	TYR	4.1
5	D	54	SER	4.1
5	K	48	ASP	4.1
6	N	12	ASP	4.0
4	H	7	HIS	4.0
6	V	41	LEU	4.0
5	A	56	GLN	3.9
6	Z	12	ASP	3.9
5	I	54	SER	3.9
5	Y	8	LEU	3.9
5	5	61	LYS	3.9
5	F	48	ASP	3.9
5	S	43	ASP	3.8
5	F	59	GLY	3.8
5	Q	59	GLY	3.8
5	7	43	ASP	3.8
6	6	41	LEU	3.8
5	A	57	ALA	3.7
5	7	4	MET	3.7
6	T	15	LYS	3.7
1	C	18	VAL	3.6
5	O	11	ILE	3.6
6	N	10	THR	3.6
6	4	41	LEU	3.5
5	D	43	ASP	3.5
5	Y	55	TYR	3.5
5	A	39	VAL	3.5
1	C	97	VAL	3.4
6	B	8	GLY	3.4
5	I	5	ASN	3.4
5	A	50	ASN	3.4
5	3	59	GLY	3.4
6	G	10	THR	3.4
5	S	57	ALA	3.4
6	8	26	TYR	3.4
5	I	51	ILE	3.4
5	K	51	ILE	3.4
5	K	4	MET	3.4
5	5	43	ASP	3.4
4	H	5	ILE	3.3
5	Y	6	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
6	G	26	TYR	3.3
5	1	6	ALA	3.3
5	O	41	SER	3.3
5	1	43	ASP	3.3
6	6	16	GLU	3.3
5	7	57	ALA	3.3
4	H	8	TYR	3.3
5	A	8	LEU	3.2
1	C	82	LEU	3.2
5	5	11	ILE	3.2
5	A	5	ASN	3.1
5	9	14	ILE	3.1
5	I	16	ASP	3.1
5	1	12	TRP	3.1
5	F	14	ILE	3.1
5	K	43	ASP	3.0
5	U	11	ILE	3.0
5	5	14	ILE	3.0
5	7	5	ASN	3.0
6	P	41	LEU	3.0
5	K	13	LEU	3.0
5	O	4	MET	3.0
5	O	57	ALA	3.0
5	K	7	ASN	2.9
5	I	47	LEU	2.9
6	T	7	THR	2.9
6	G	45	TRP	2.9
6	R	17	PHE	2.9
5	1	42	THR	2.9
1	C	288	ASN	2.8
5	F	53	VAL	2.8
5	1	44	LEU	2.8
5	W	3	THR	2.8
5	S	59	GLY	2.8
5	5	59	GLY	2.8
3	M	142	MET	2.8
5	K	5	ASN	2.8
4	H	182	LEU	2.8
5	W	14	ILE	2.8
2	L	218	SER	2.8
5	A	14	ILE	2.8
1	C	287	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	172	PRO	2.8
5	I	49	ASP	2.8
5	D	47	LEU	2.8
5	Y	50	ASN	2.8
5	I	6	ALA	2.8
5	A	40	LEU	2.7
5	I	44	LEU	2.7
5	S	39	VAL	2.7
5	O	5	ASN	2.7
5	5	47	LEU	2.7
5	1	47	LEU	2.6
5	K	6	ALA	2.6
5	9	8	LEU	2.6
6	B	41	LEU	2.6
5	Q	44	LEU	2.6
6	E	16	GLU	2.6
6	T	23	GLN	2.6
5	W	58	LEU	2.6
5	K	52	PRO	2.6
6	G	11	ASP	2.6
6	8	12	ASP	2.6
5	F	61	LYS	2.6
5	K	11	ILE	2.6
5	D	5	ASN	2.6
6	R	44	PRO	2.6
4	H	58	PHE	2.6
6	N	32	VAL	2.6
5	Y	11	ILE	2.6
6	6	37	LEU	2.6
6	P	17	PHE	2.6
1	C	72	ALA	2.5
5	1	61	LYS	2.5
4	H	170	VAL	2.5
5	S	54	SER	2.5
5	F	17	PRO	2.5
2	L	76	ALA	2.5
4	H	49	SER	2.5
5	W	49	ASP	2.5
5	K	39	VAL	2.5
5	K	15	LEU	2.5
5	O	51	ILE	2.5
6	V	45	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
6	R	7	THR	2.5
5	7	54	SER	2.5
5	I	15	LEU	2.5
6	8	33	VAL	2.4
2	L	2	ALA	2.4
5	7	9	TYR	2.4
5	S	56	GLN	2.4
5	D	53	VAL	2.4
5	9	53	VAL	2.4
5	A	49	ASP	2.4
5	F	39	VAL	2.4
6	E	41	LEU	2.4
6	E	15	LYS	2.4
1	C	181	THR	2.4
5	I	46	TRP	2.4
5	A	47	LEU	2.4
1	C	256	PHE	2.4
5	Q	48	ASP	2.4
5	F	16	ASP	2.4
6	P	40	TRP	2.3
4	H	146	GLU	2.3
5	Q	47	LEU	2.3
5	3	43	ASP	2.3
5	W	57	ALA	2.3
5	Q	39	VAL	2.3
5	9	4	MET	2.3
1	C	81	VAL	2.3
6	8	37	LEU	2.3
5	Q	36	HIS	2.3
5	K	14	ILE	2.2
6	B	11	ASP	2.2
5	U	43	ASP	2.2
5	5	60	LYS	2.2
6	P	14	ALA	2.2
5	9	39	VAL	2.2
5	I	50	ASN	2.2
5	Q	12	TRP	2.2
6	P	10	THR	2.2
6	B	26	TYR	2.2
4	H	96	PRO	2.2
6	8	31	LEU	2.2
6	0	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	H	202	PHE	2.2
5	1	55	TYR	2.2
5	5	4	MET	2.2
3	M	163	ILE	2.2
4	H	231	VAL	2.2
5	7	56	GLN	2.1
5	7	47	LEU	2.1
6	P	37	LEU	2.1
6	V	15	LYS	2.1
5	Q	23	SER	2.1
6	G	17	PHE	2.1
4	H	56	VAL	2.1
3	M	99	PRO	2.1
4	H	102	PRO	2.1
5	D	8	LEU	2.1
3	M	69	SER	2.1
5	S	41	SER	2.1
5	3	4	MET	2.1
5	S	15	LEU	2.1
5	K	46	TRP	2.0
1	C	204	LEU	2.0
5	S	38	ILE	2.0
3	M	60	SER	2.0
6	4	45	TRP	2.0
5	Y	43	ASP	2.0
1	C	20	LEU	2.0
5	U	3	THR	2.0
4	H	179	ILE	2.0
5	7	61	LYS	2.0
5	W	39	VAL	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)

There are no monosaccharides in this entry.

6.4 Ligands (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
8	CA	O	101	1/1	0.13	0.40	167,167,167,167	0
15	CRT	A	101	44/44	0.28	0.91	100,120,180,182	0
8	CA	Q	101	1/1	0.33	0.16	159,159,159,159	0
8	CA	7	101	1/1	0.37	0.07	161,161,161,161	0
15	CRT	B	102	44/44	0.39	0.98	125,143,171,171	0
15	CRT	J	101	44/44	0.40	0.89	133,168,197,198	0
8	CA	U	101	1/1	0.41	0.08	125,125,125,125	0
15	CRT	8	101	44/44	0.41	0.84	138,179,215,216	0
15	CRT	2	102	44/44	0.43	1.11	110,160,199,221	0
8	CA	F	101	1/1	0.46	0.24	157,157,157,157	0
15	CRT	A	103	44/44	0.46	0.89	169,184,188,189	0
15	CRT	P	102	44/44	0.51	0.80	187,222,226,227	0
15	CRT	3	103	44/44	0.56	0.71	116,145,185,187	0
15	CRT	G	102	44/44	0.58	0.82	138,158,216,217	0
15	CRT	T	102	44/44	0.62	1.14	136,158,177,178	0
15	CRT	R	102	44/44	0.63	0.48	89,127,136,137	0
15	CRT	N	102	44/44	0.63	0.66	151,161,169,169	0
15	CRT	X	102	44/44	0.63	1.18	131,163,207,207	0
15	CRT	4	102	44/44	0.66	0.76	107,121,188,189	0
15	CRT	V	102	44/44	0.67	0.52	76,133,176,179	0
8	CA	W	101	1/1	0.67	0.09	118,118,118,118	0
8	CA	I	101	1/1	0.68	0.33	158,158,158,158	0
15	CRT	W	103	44/44	0.69	0.64	77,126,154,155	0
8	CA	K	101	1/1	0.73	0.18	152,152,152,152	0
11	UQ8	L	304	53/53	0.74	0.59	84,134,142,144	0
16	PGW	M	407	21/51	0.74	0.30	65,132,182,186	0
13	FE	M	404	1/1	0.75	0.15	127,127,127,127	0
8	CA	3	101	1/1	0.75	0.21	113,113,113,113	0
8	CA	5	101	1/1	0.77	0.34	141,141,141,141	0
9	BCL	6	101	66/66	0.80	0.39	105,119,198,199	0
14	MQ8	M	405	53/53	0.81	0.40	27,87,158,160	0
15	CRT	M	406	44/44	0.82	0.38	71,78,104,107	0
8	CA	D	101	1/1	0.82	0.12	142,142,142,142	0
16	PGW	H	302	21/51	0.83	0.32	64,102,145,160	0
9	BCL	R	101	66/66	0.84	0.36	115,128,228,230	0
9	BCL	D	102	66/66	0.85	0.33	120,130,197,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	7	102	66/66	0.85	0.34	86,93,190,193	0
9	BCL	B	101	66/66	0.85	0.37	104,120,212,217	0
12	PO4	H	303	5/5	0.86	0.19	112,113,126,128	0
9	BCL	9	102	66/66	0.87	0.27	122,129,145,154	0
9	BCL	G	101	66/66	0.87	0.29	110,123,217,218	0
9	BCL	A	102	66/66	0.87	0.35	123,129,202,205	0
9	BCL	E	101	66/66	0.88	0.31	95,109,168,172	0
9	BCL	K	102	66/66	0.89	0.32	120,127,226,229	0
9	BCL	7	103	66/66	0.89	0.32	76,89,176,183	0
9	BCL	O	102	66/66	0.89	0.33	81,93,159,165	0
10	BPH	L	302	65/65	0.89	0.26	55,64,75,82	0
9	BCL	F	102	66/66	0.89	0.32	102,112,154,155	0
9	BCL	X	101	66/66	0.89	0.33	68,86,200,202	0
9	BCL	2	101	66/66	0.89	0.32	81,102,191,196	0
9	BCL	3	102	66/66	0.89	0.27	71,81,147,153	0
9	BCL	I	102	66/66	0.89	0.26	79,89,147,149	0
17	PEF	H	301	19/47	0.89	0.31	75,105,128,134	0
9	BCL	P	101	66/66	0.90	0.27	69,83,204,210	0
9	BCL	I	103	66/66	0.90	0.32	96,117,201,205	0
9	BCL	V	101	66/66	0.90	0.28	80,97,189,205	0
8	CA	9	101	1/1	0.90	0.03	124,124,124,124	0
9	BCL	Y	102	66/66	0.90	0.32	48,61,172,173	0
9	BCL	Z	101	66/66	0.90	0.29	59,71,165,167	0
12	PO4	M	408	5/5	0.90	0.18	106,119,123,135	0
9	BCL	N	101	66/66	0.90	0.24	101,123,189,191	0
8	CA	A	104	1/1	0.90	0.34	185,185,185,185	0
9	BCL	4	101	66/66	0.90	0.27	72,101,222,225	0
9	BCL	Q	102	66/66	0.91	0.32	108,115,183,188	0
9	BCL	0	101	66/66	0.91	0.29	76,101,202,207	0
9	BCL	W	102	66/66	0.91	0.29	47,69,182,185	0
9	BCL	5	102	66/66	0.91	0.34	124,134,210,214	0
9	BCL	L	303	66/66	0.92	0.22	20,53,66,82	0
12	PO4	H	304	5/5	0.92	0.33	130,131,142,148	0
9	BCL	S	102	66/66	0.92	0.27	98,112,174,177	0
9	BCL	U	102	66/66	0.92	0.39	64,119,243,246	0
9	BCL	M	401	66/66	0.92	0.23	40,55,106,109	0
8	CA	S	101	1/1	0.92	0.15	154,154,154,154	0
10	BPH	M	403	65/65	0.93	0.20	43,59,137,144	0
9	BCL	T	101	66/66	0.93	0.25	53,88,229,234	0
9	BCL	1	102	66/66	0.93	0.32	62,74,153,162	0
7	HEM	C	503	43/43	0.94	0.28	56,67,85,91	0
7	HEM	C	504	43/43	0.94	0.22	43,52,64,74	0

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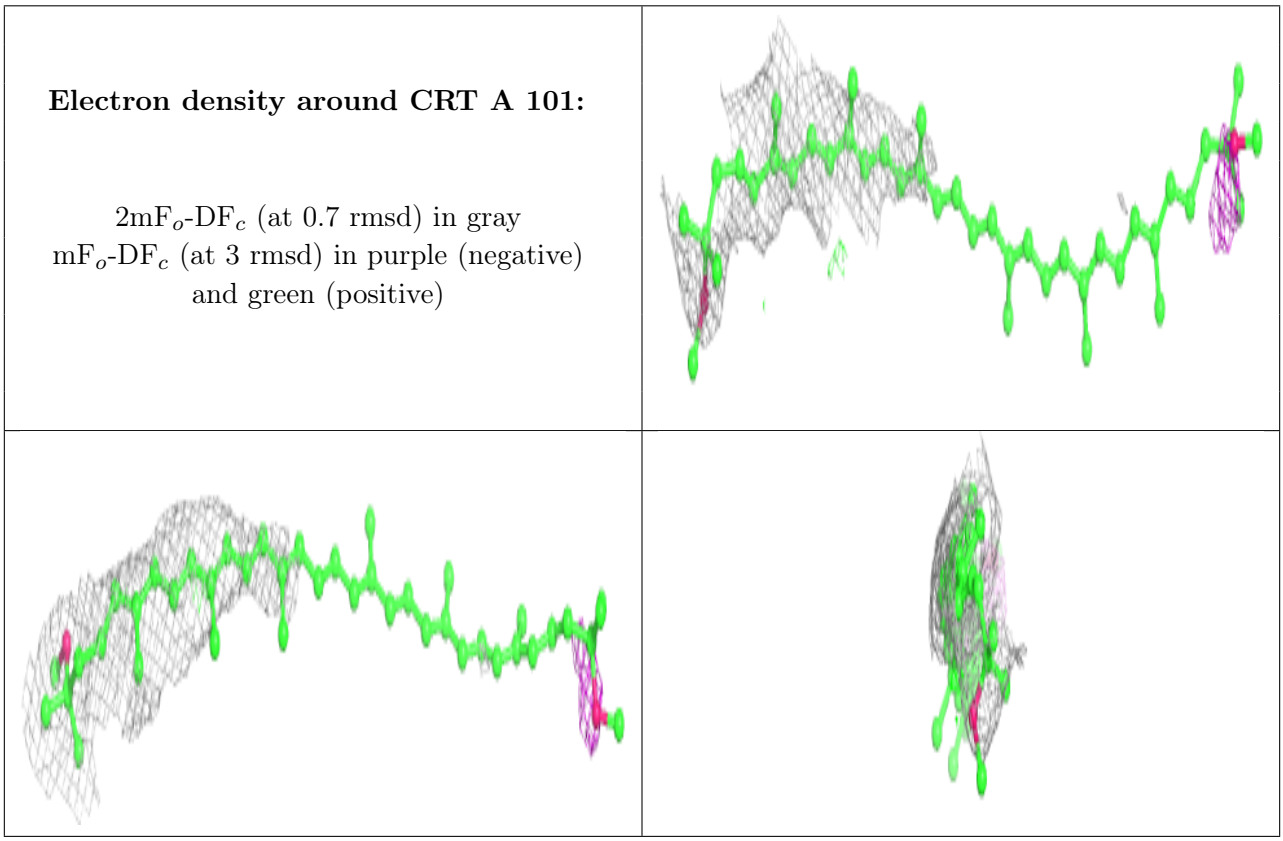
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	PO4	L	305	5/5	0.94	0.14	84,104,111,116	0
9	BCL	M	402	66/66	0.94	0.22	28,43,60,64	0
7	HEM	C	501	43/43	0.94	0.19	54,64,73,75	0
8	CA	Y	101	1/1	0.94	0.10	79,79,79,79	0
9	BCL	L	301	66/66	0.94	0.18	10,45,66,69	0
7	HEM	C	502	43/43	0.95	0.20	41,49,59,64	0
8	CA	C	505	1/1	0.95	0.23	93,93,93,93	0
8	CA	1	101	1/1	0.96	0.12	92,92,92,92	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.

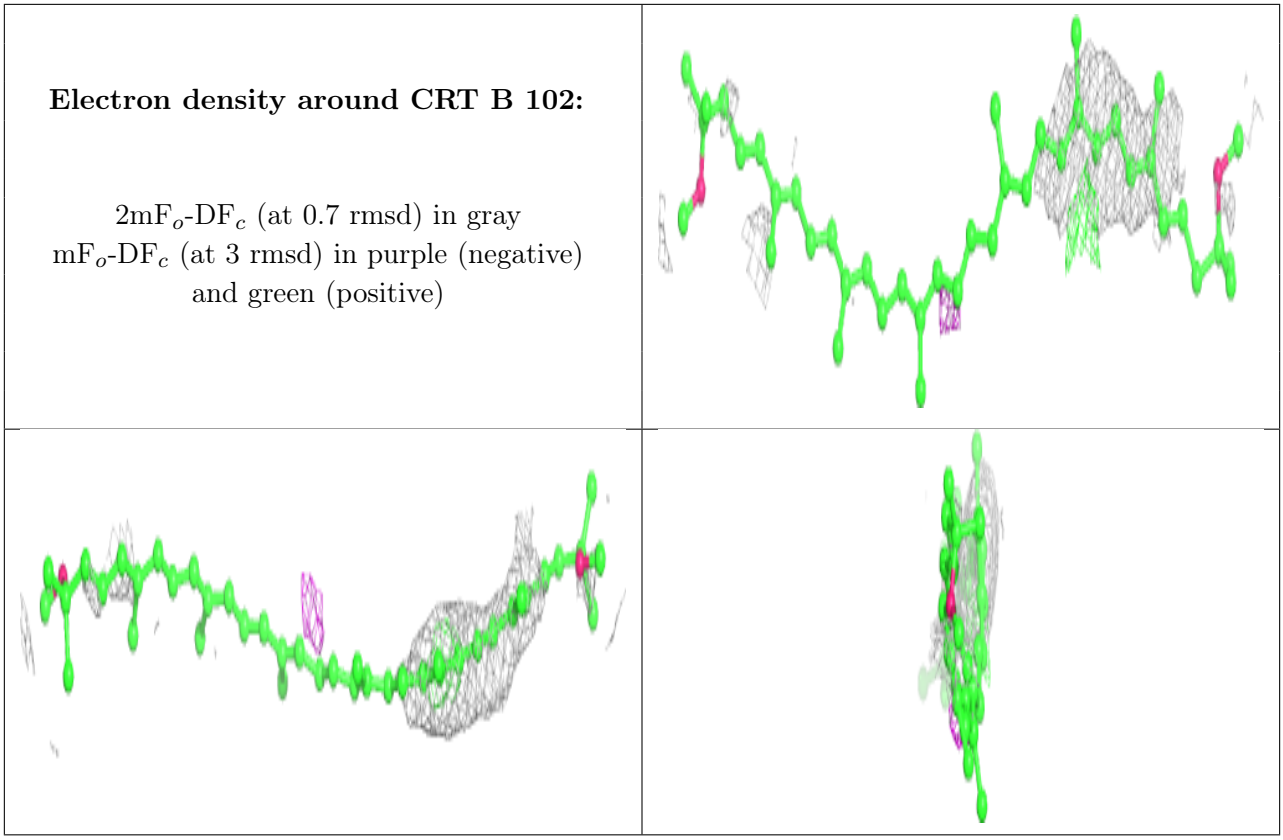
Electron density around CRT A 101:

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



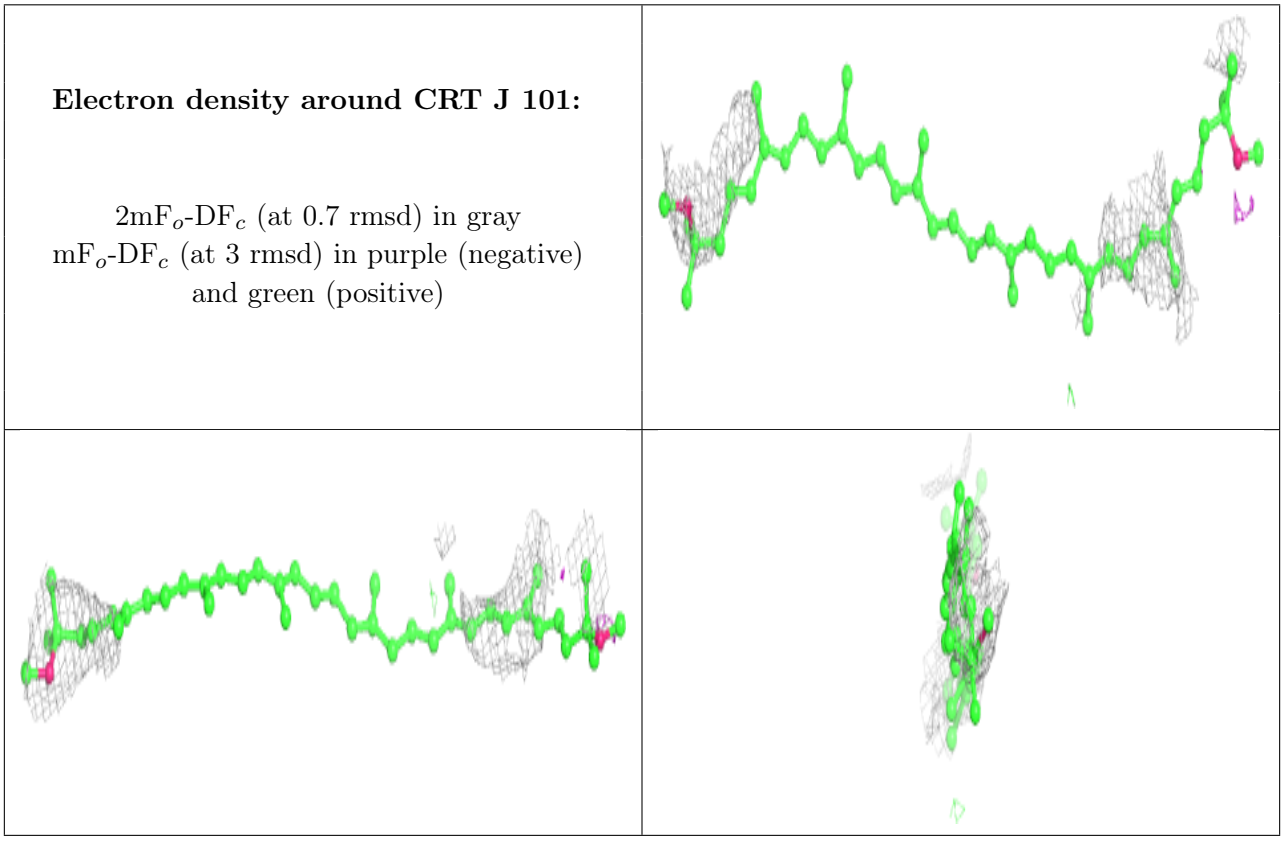
Electron density around CRT B 102:

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



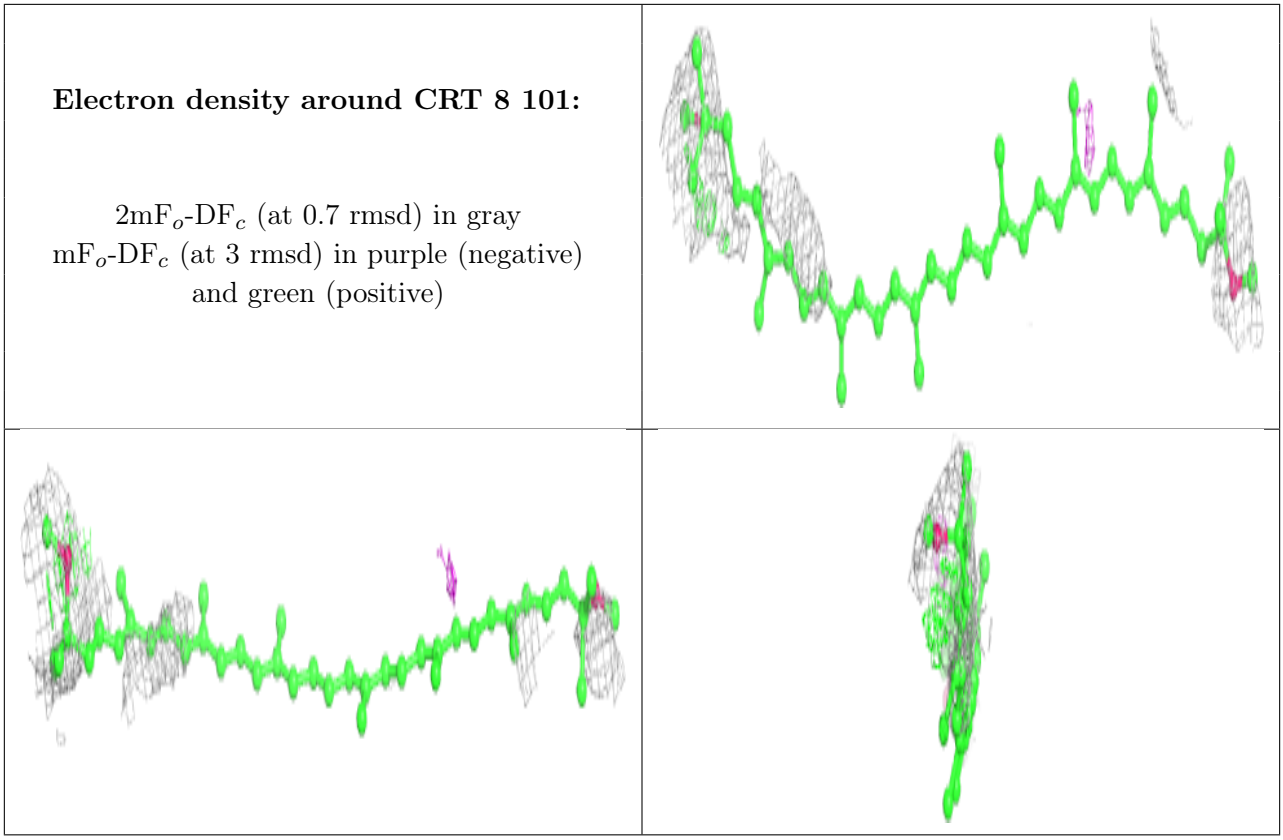
Electron density around CRT J 101:

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



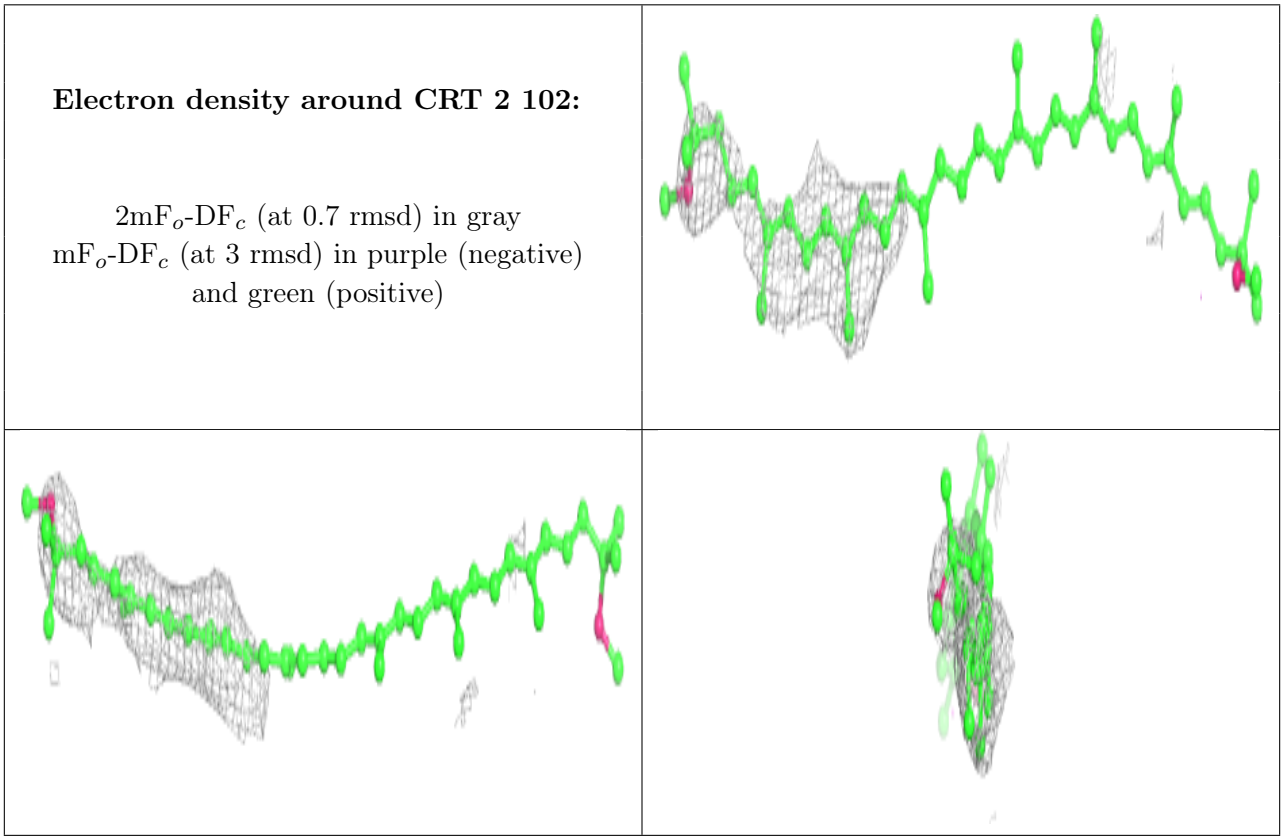
Electron density around CRT 8 101:

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



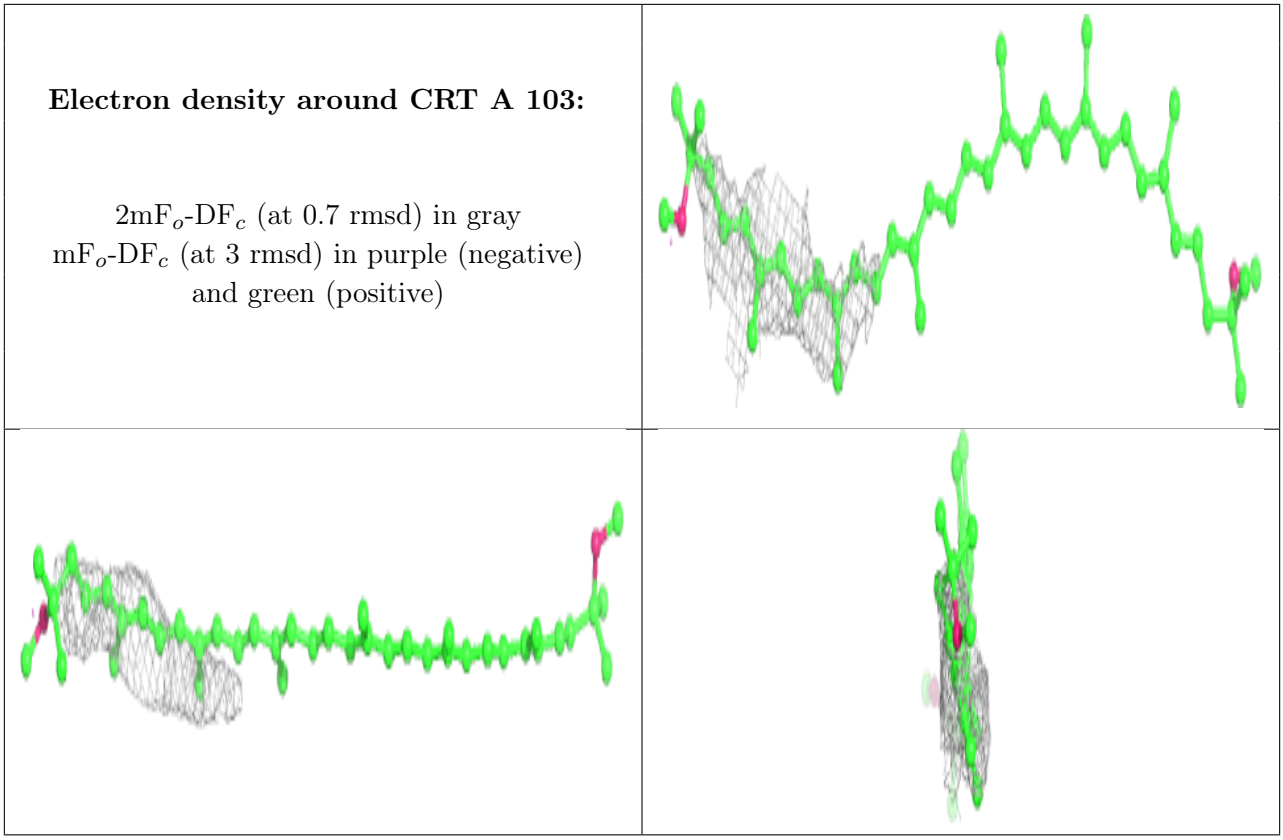
Electron density around CRT 2 102:

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



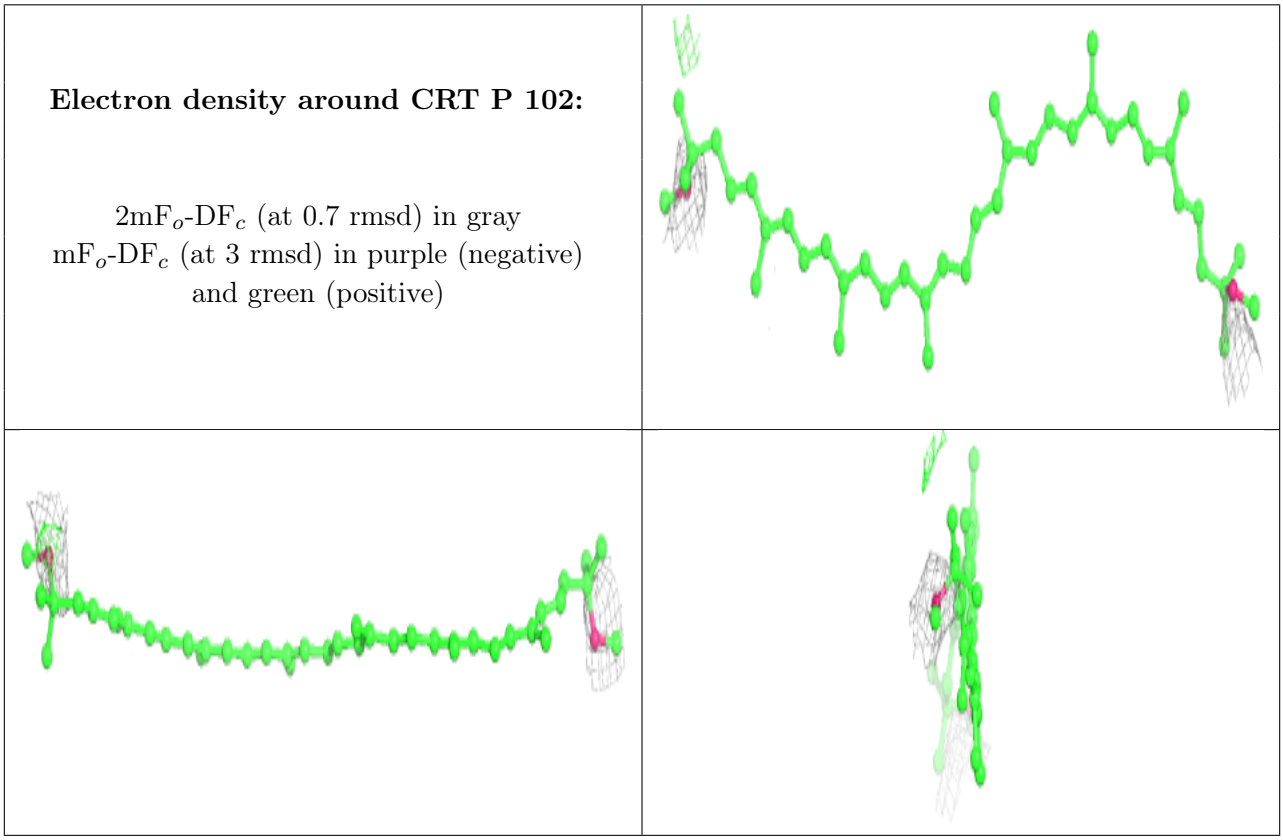
Electron density around CRT A 103:

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



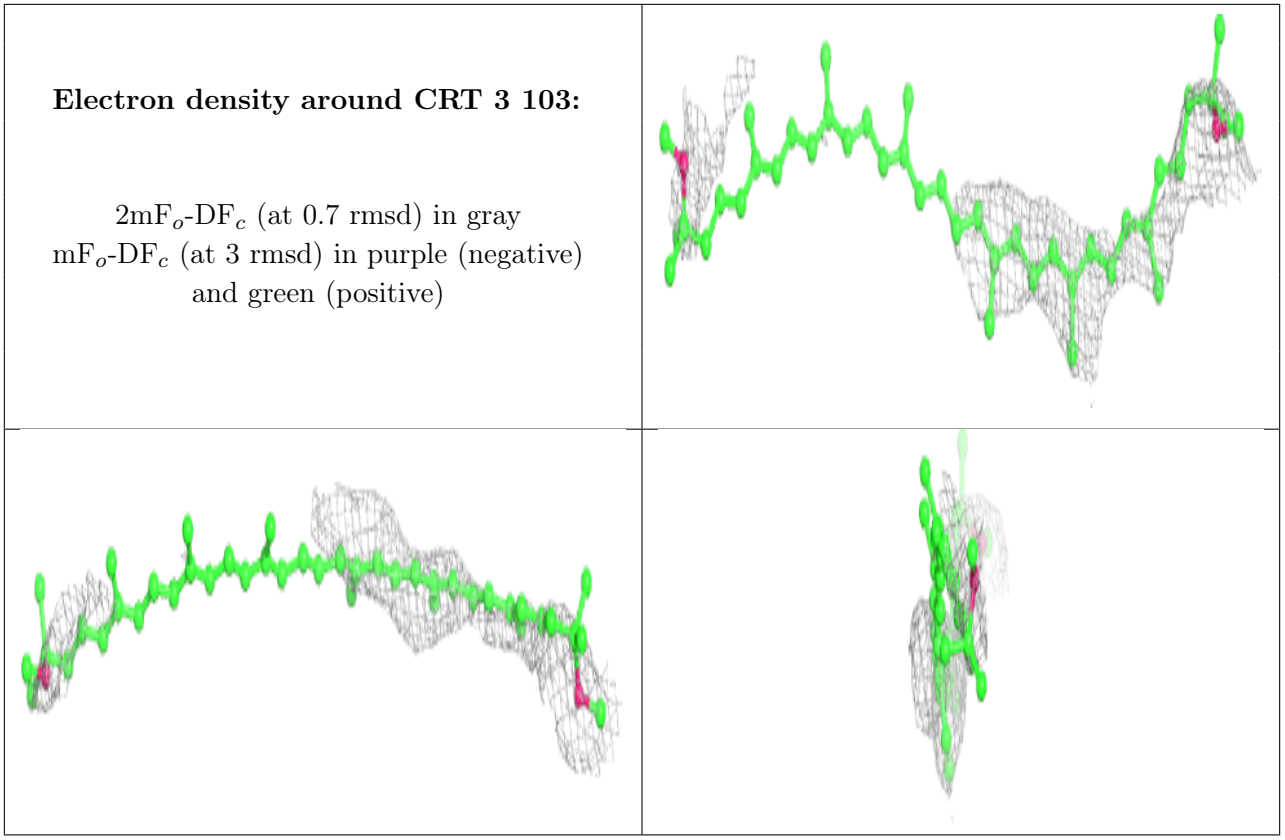
Electron density around CRT P 102:

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



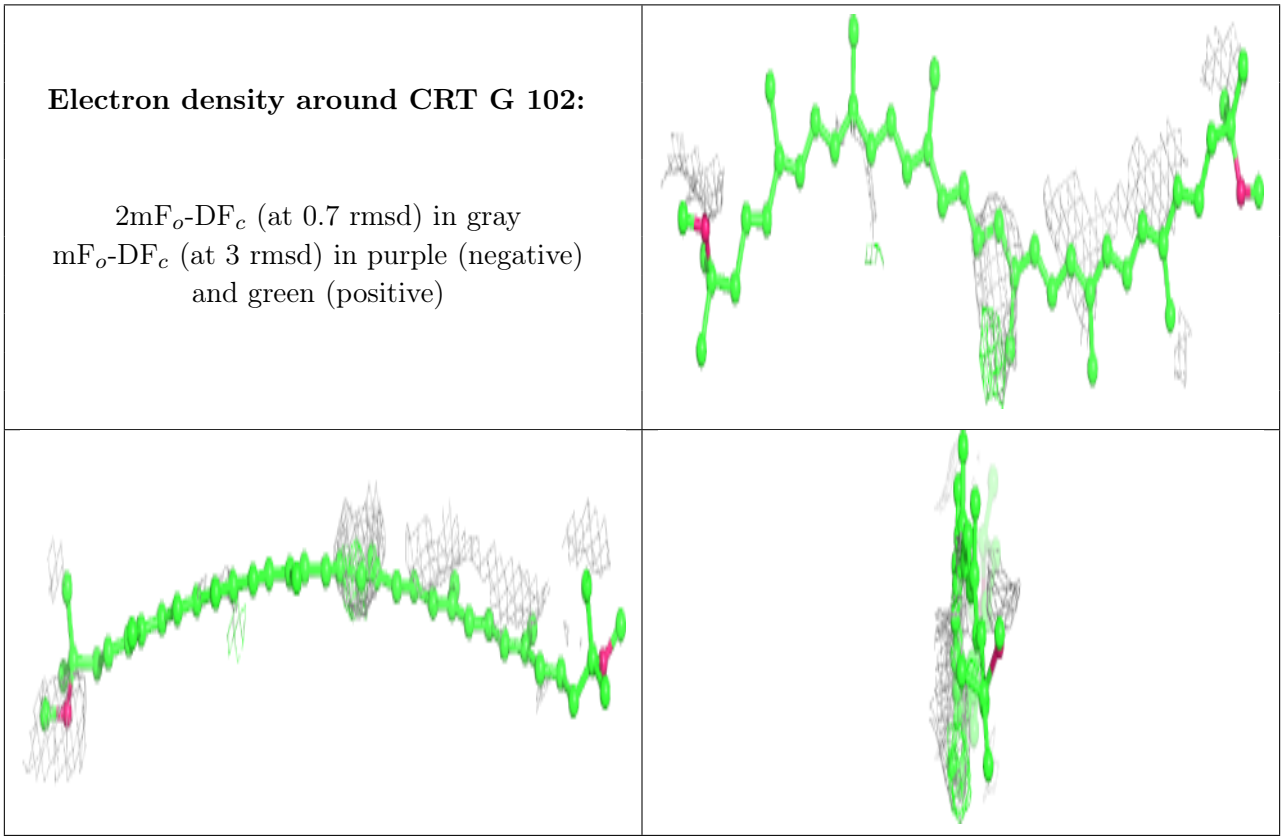
Electron density around CRT 3 103:

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



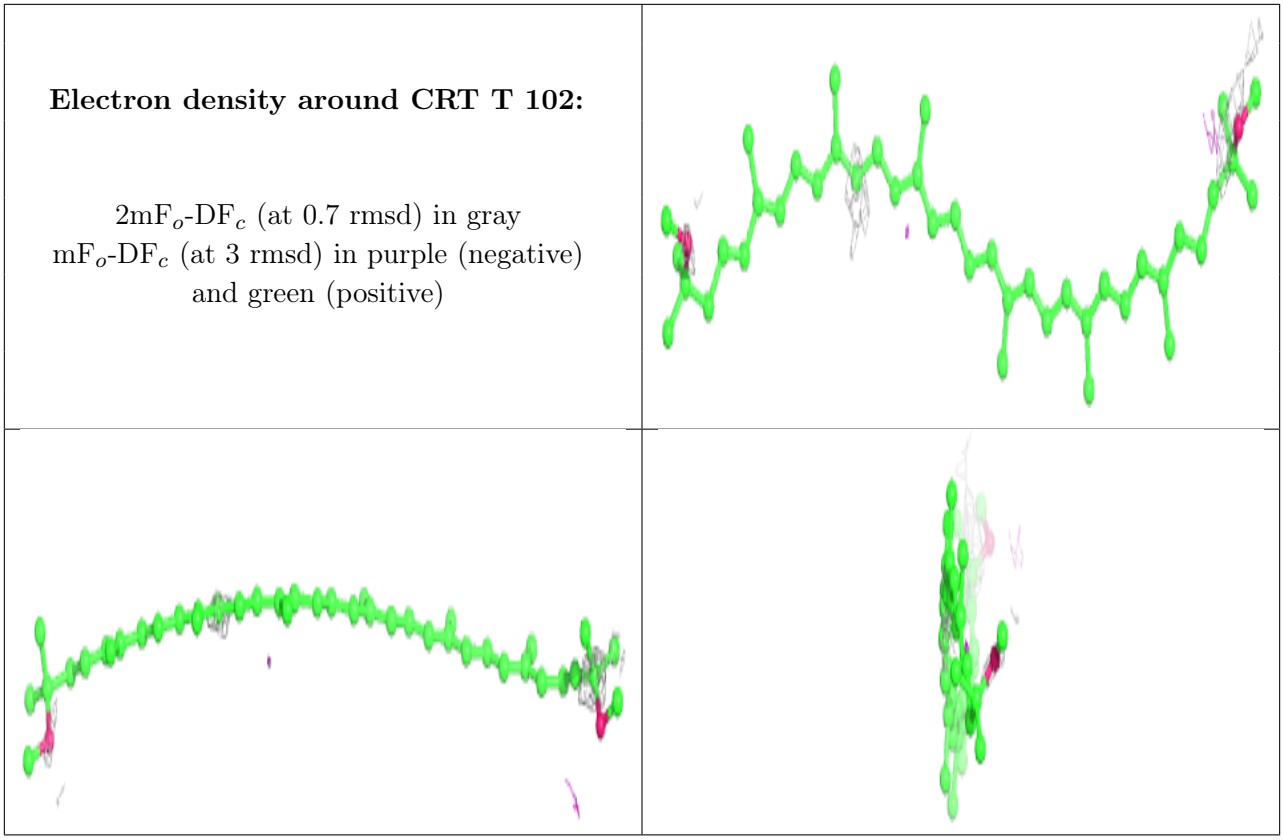
Electron density around CRT G 102:

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



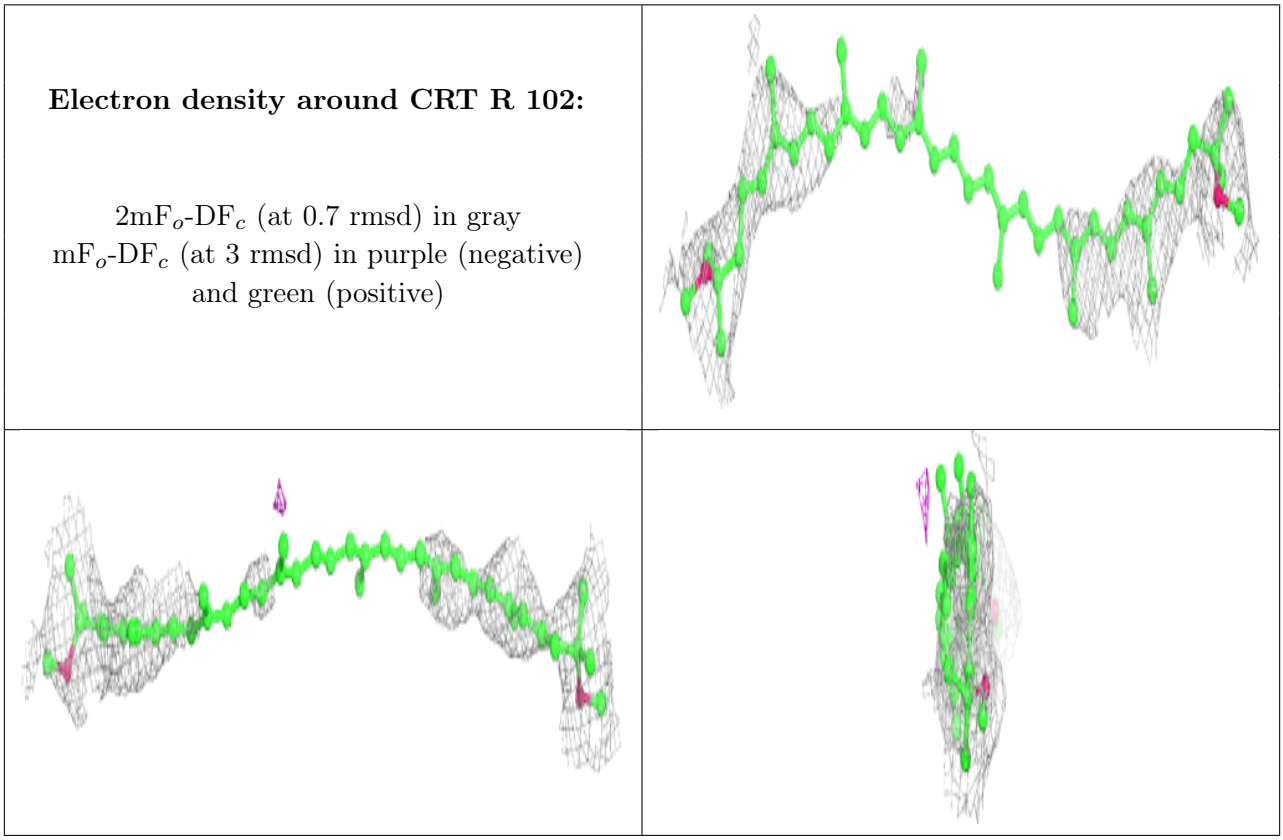
Electron density around CRT T 102:

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



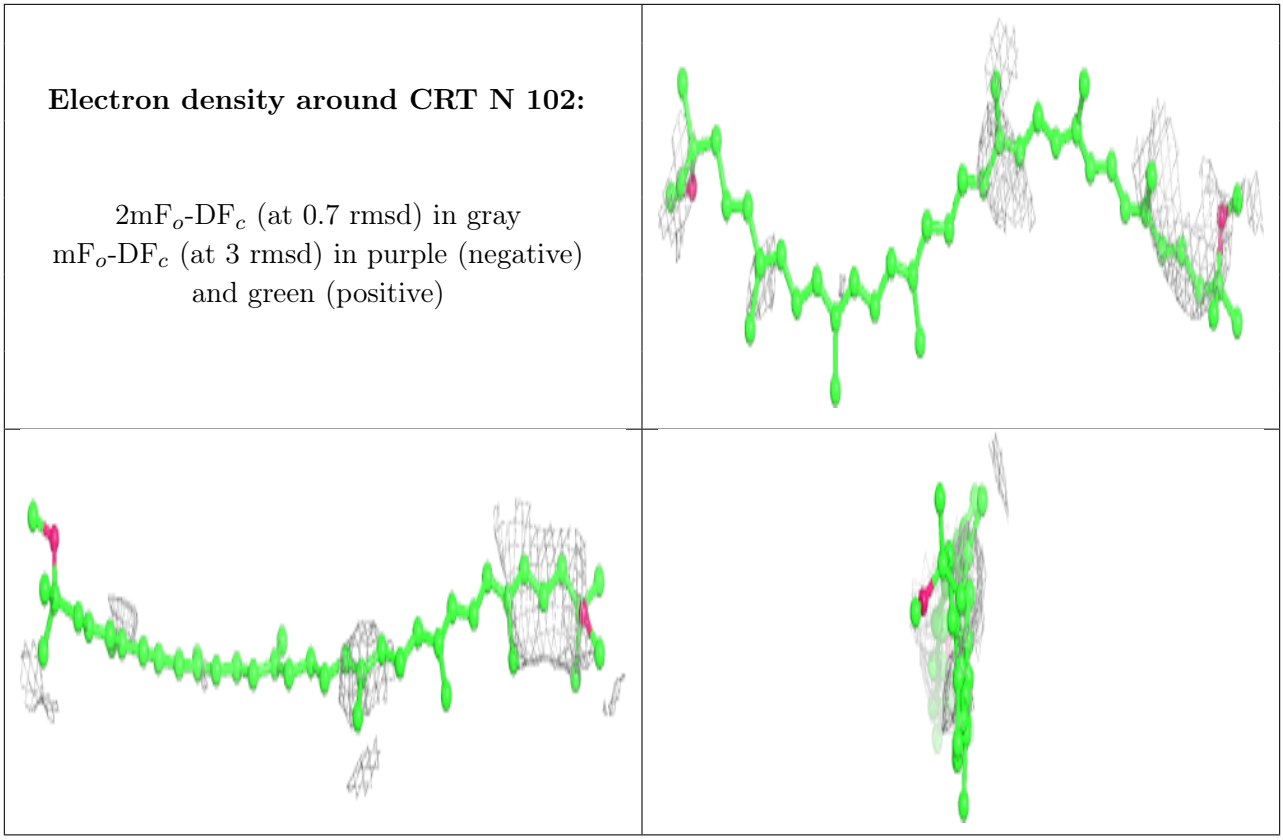
Electron density around CRT R 102:

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



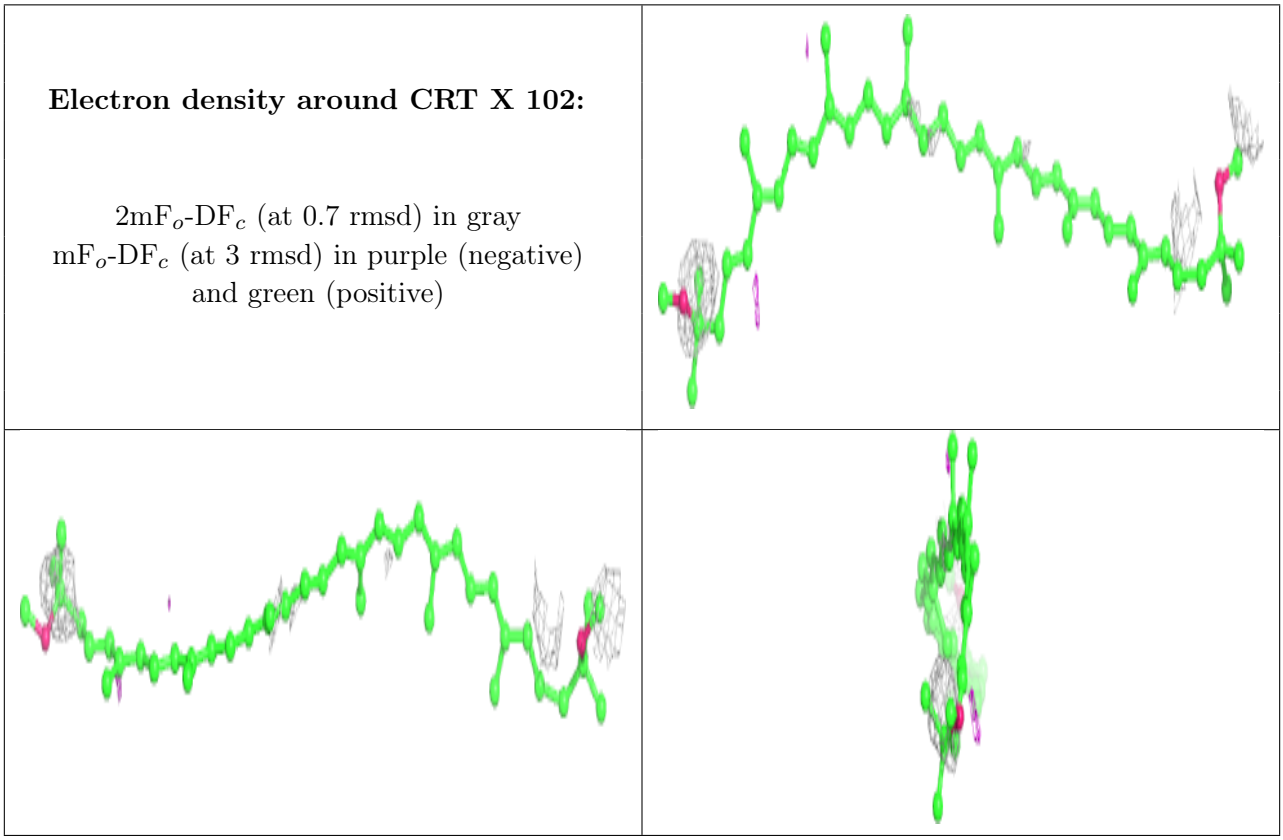
Electron density around CRT N 102:

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



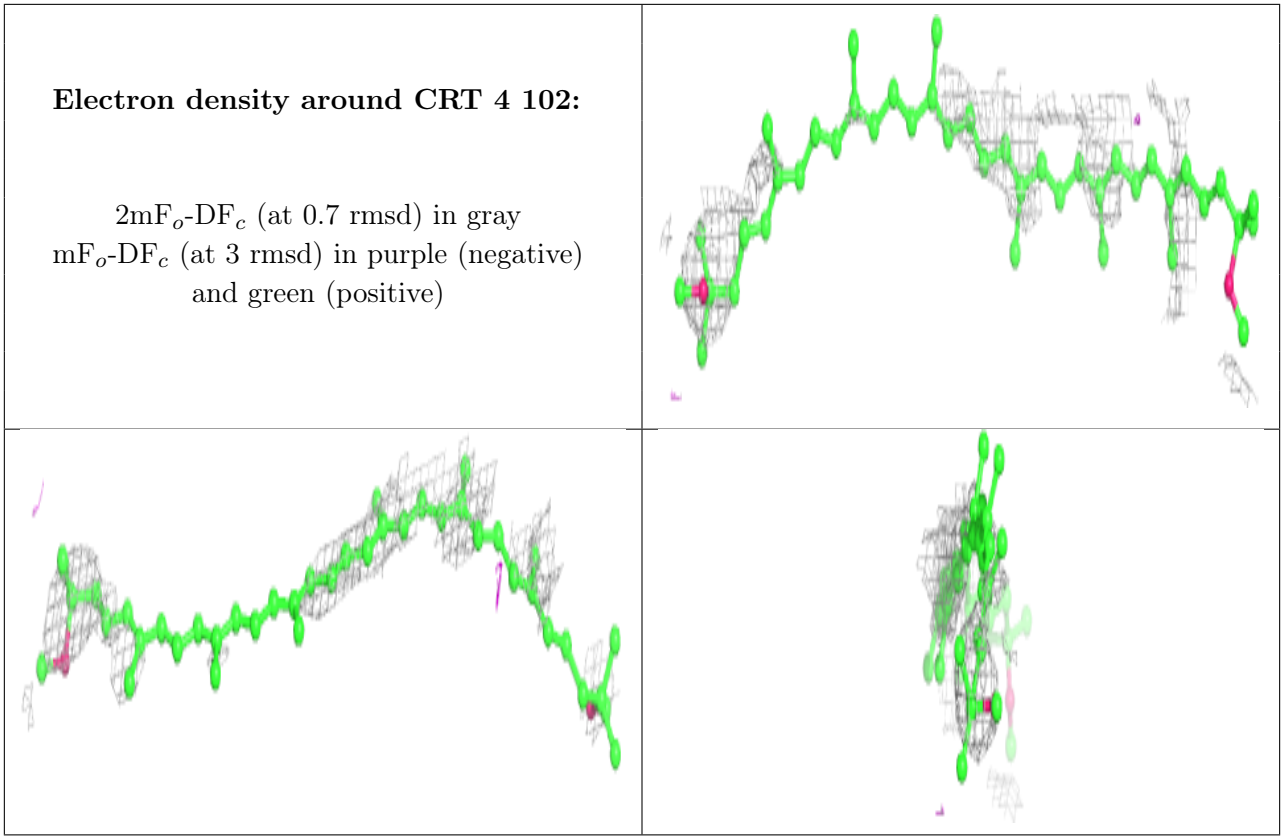
Electron density around CRT X 102:

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



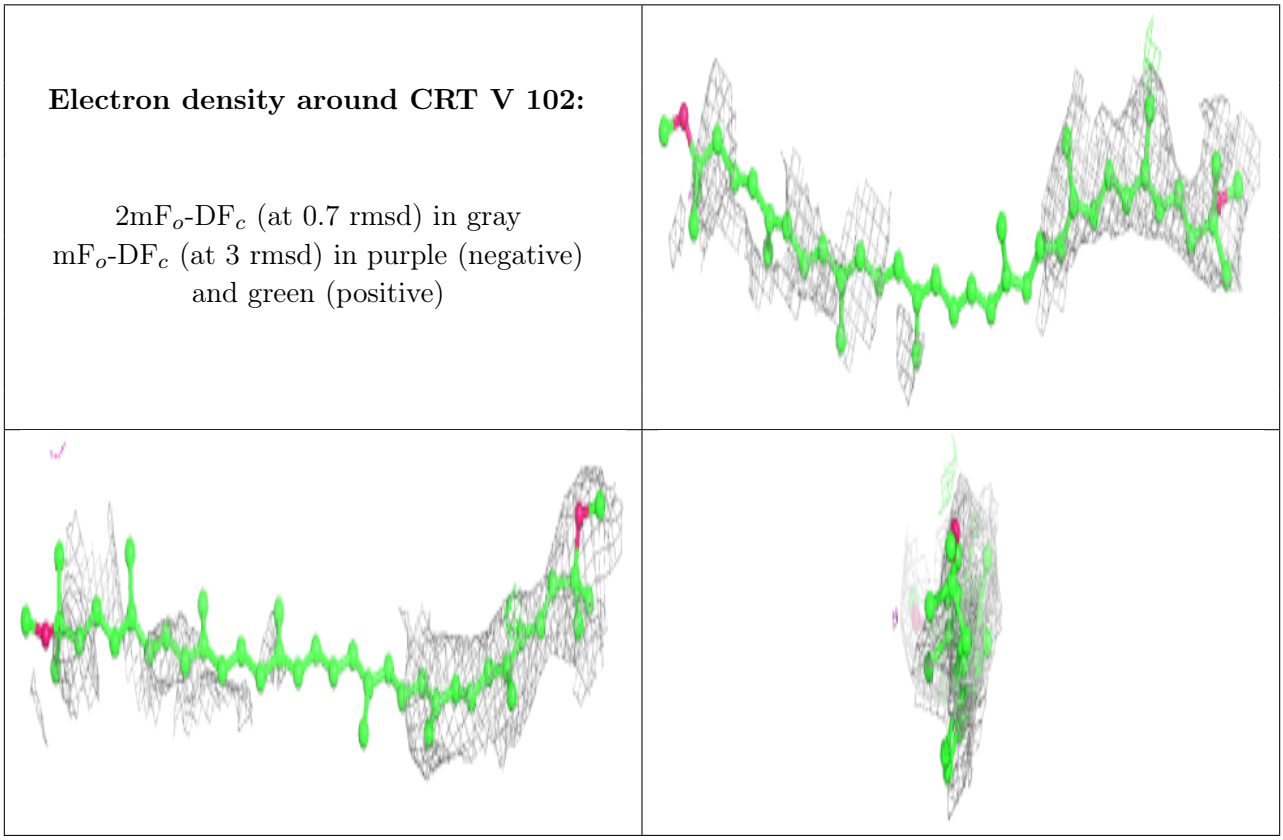
Electron density around CRT 4 102:

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



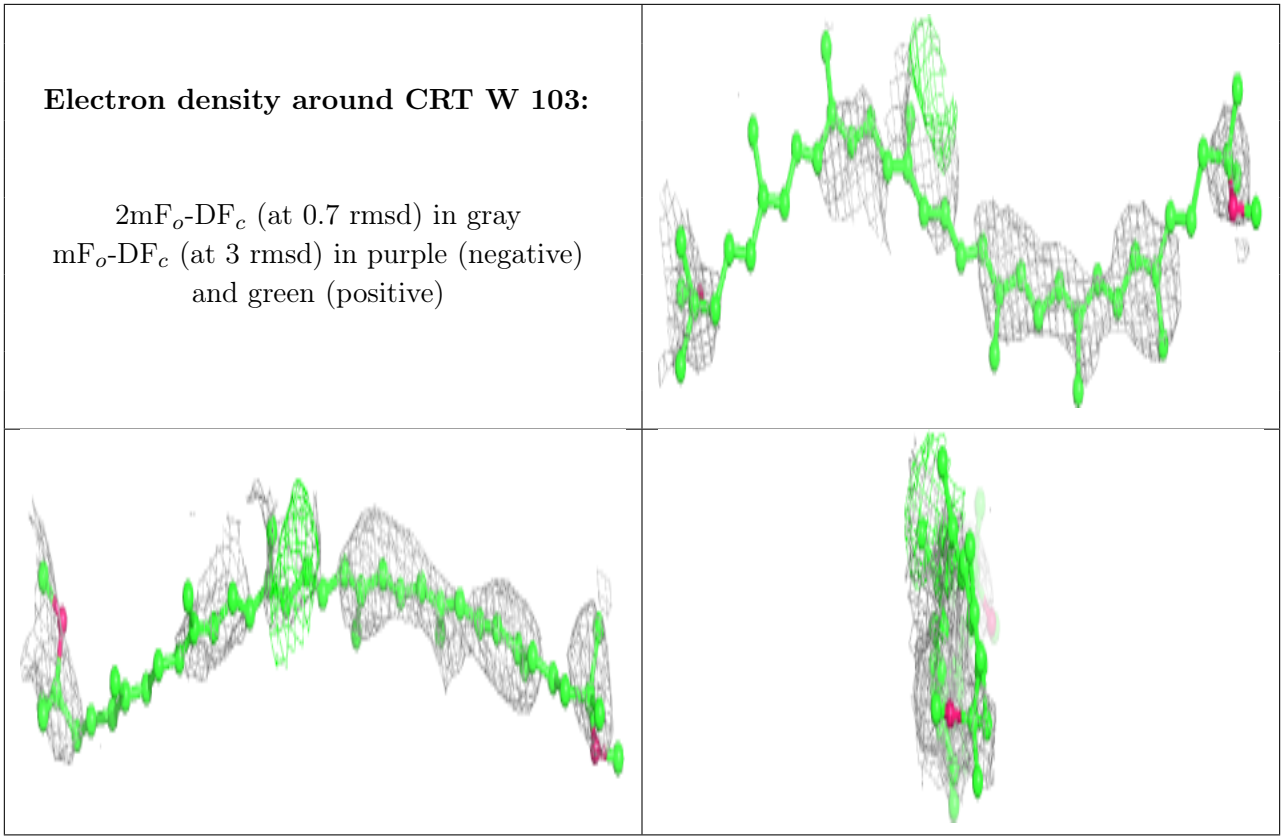
Electron density around CRT V 102:

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



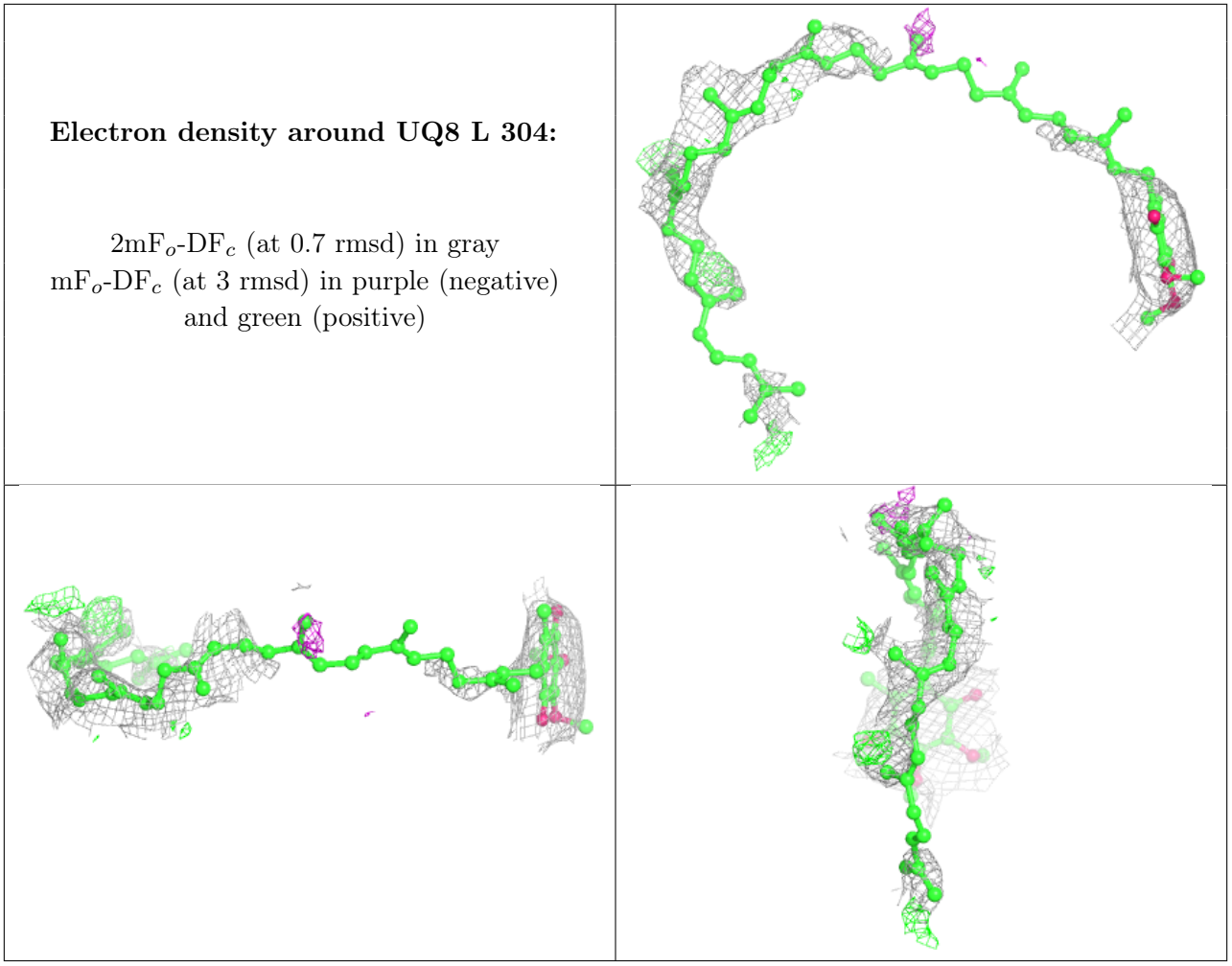
Electron density around CRT W 103:

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



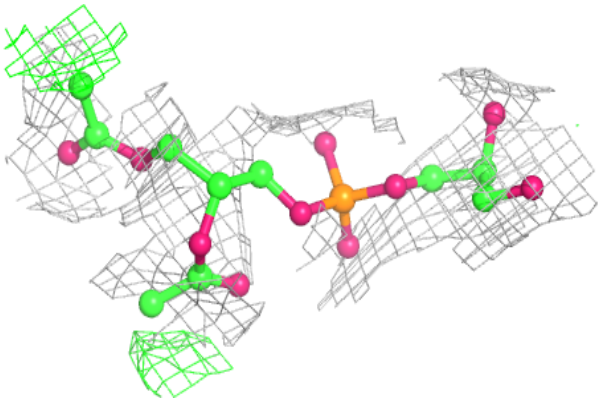
Electron density around UQ8 L 304:

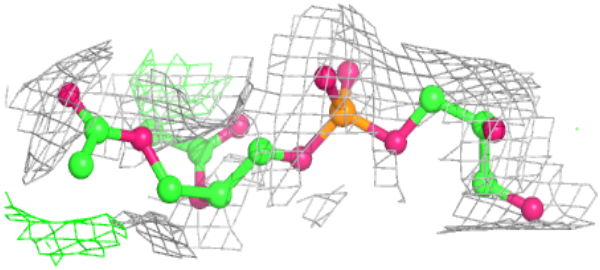
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

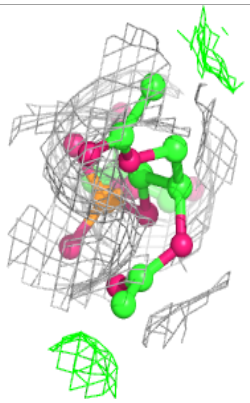


Electron density around PGW M 407:

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

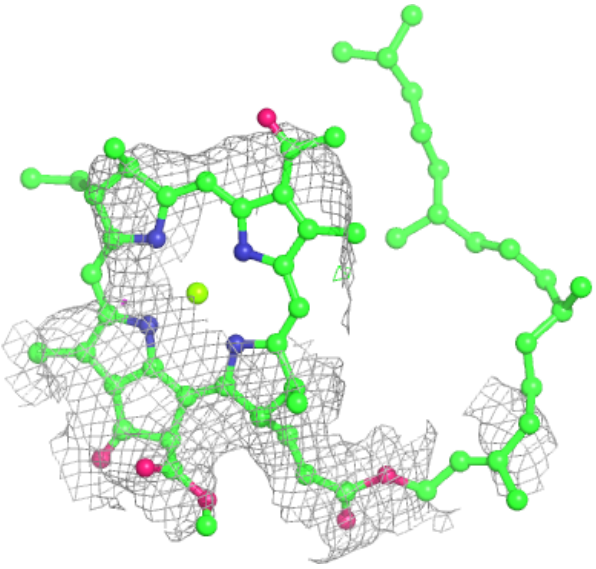


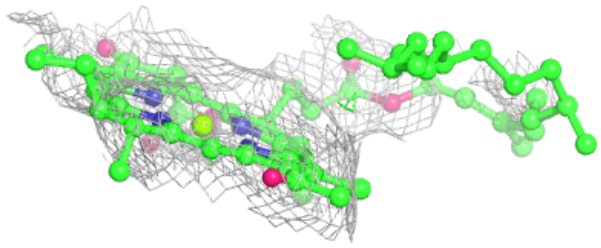


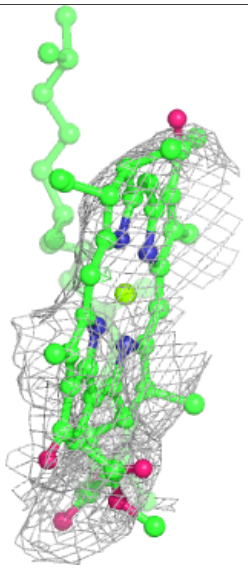


Electron density around BCL 6 101:

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

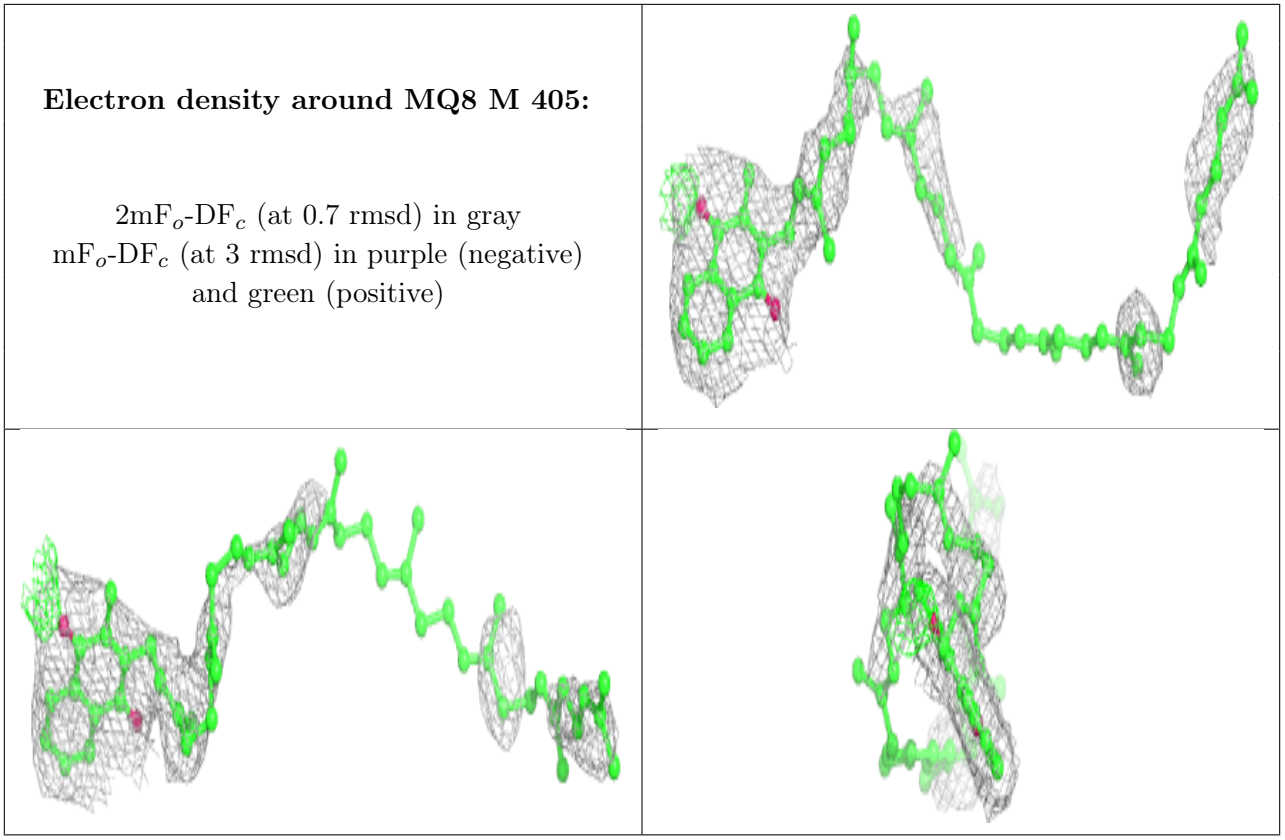






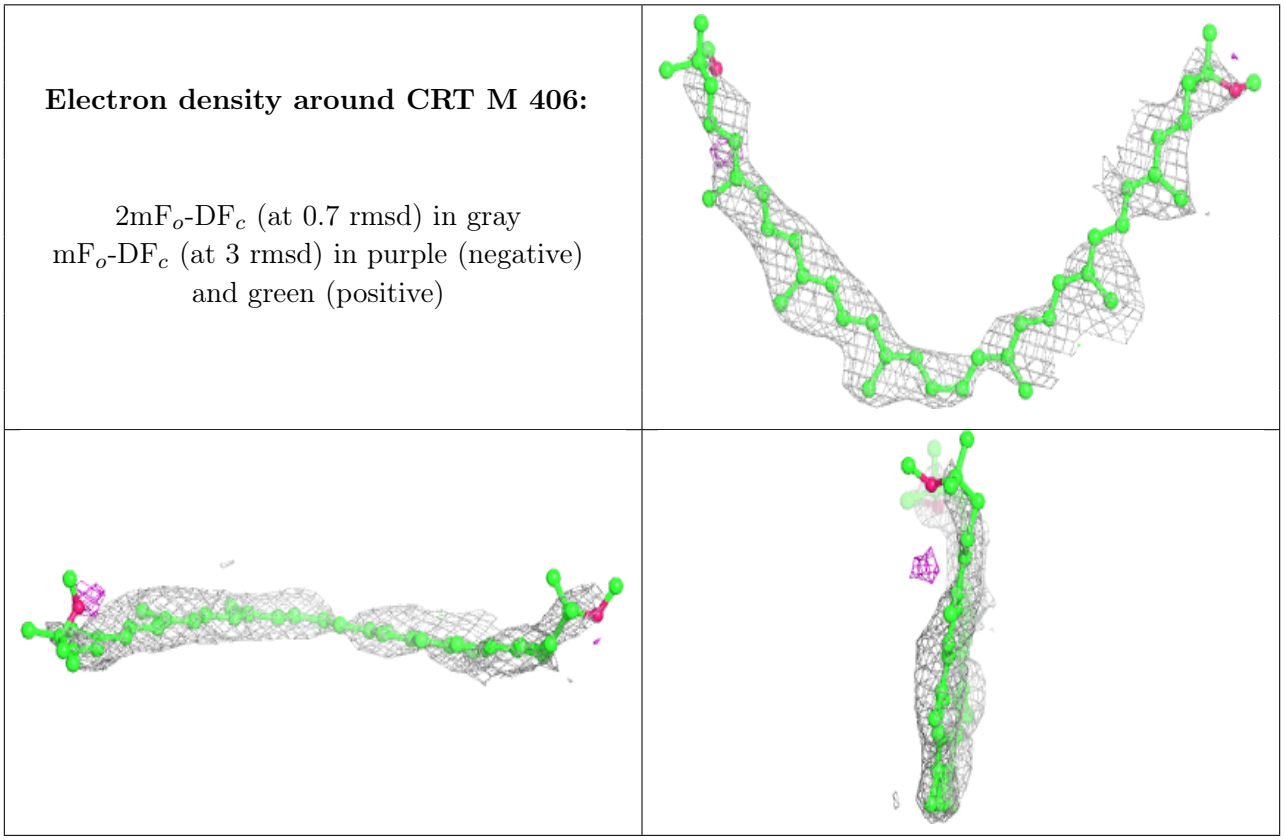
Electron density around MQ8 M 405:

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



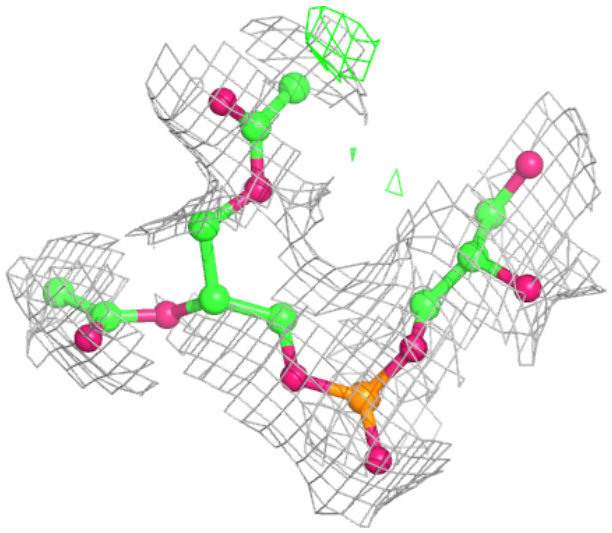
Electron density around CRT M 406:

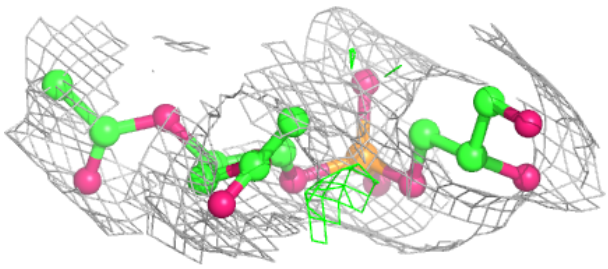
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

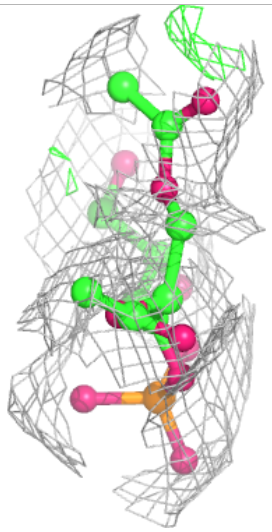


Electron density around PGW H 302:

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

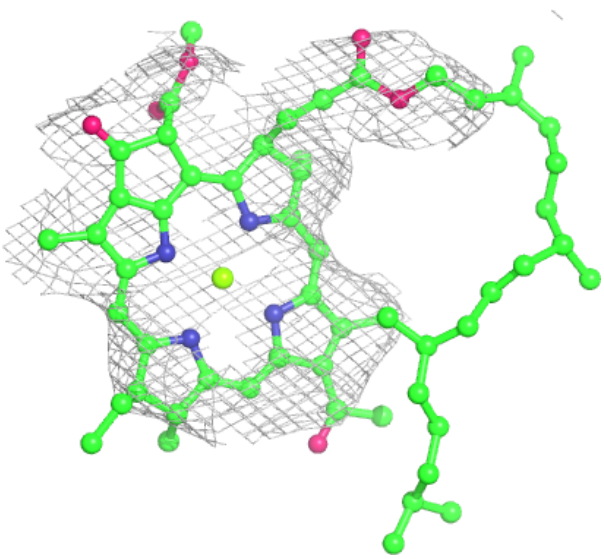


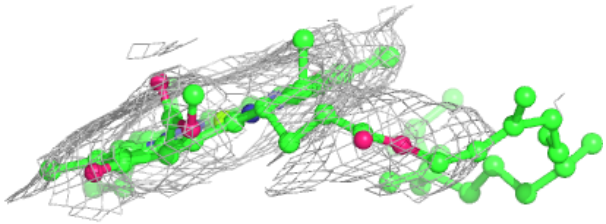


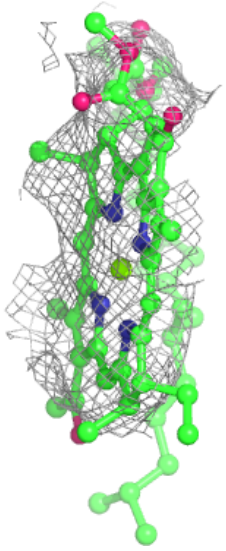


Electron density around BCL R 101:

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

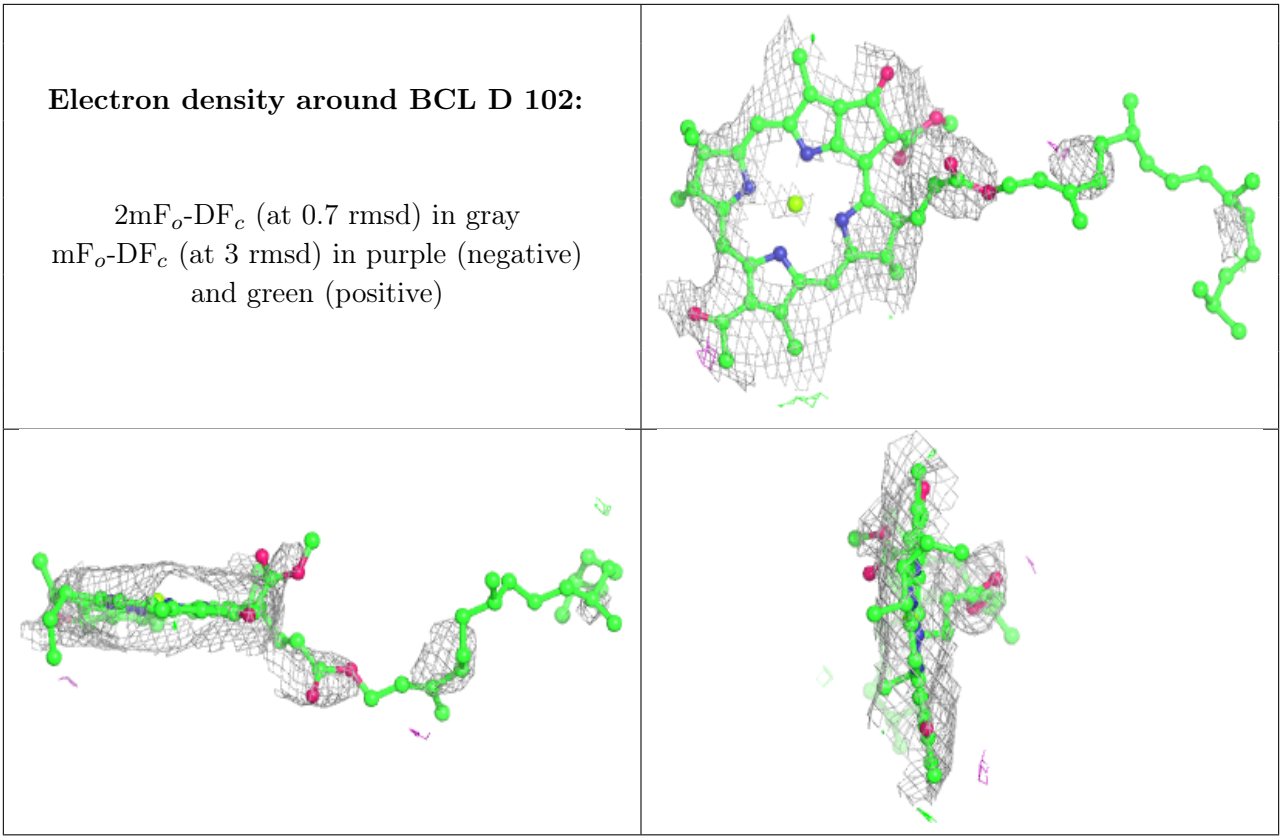






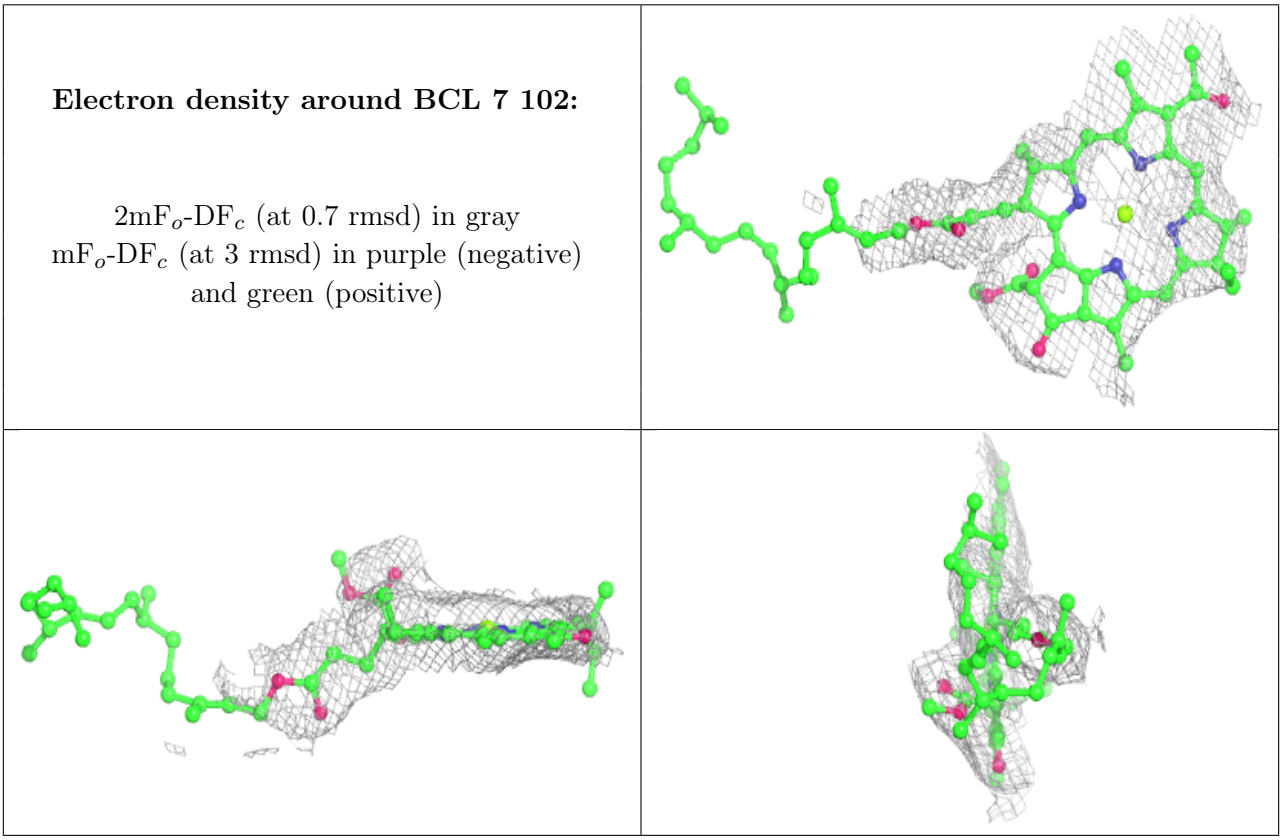
Electron density around BCL D 102:

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



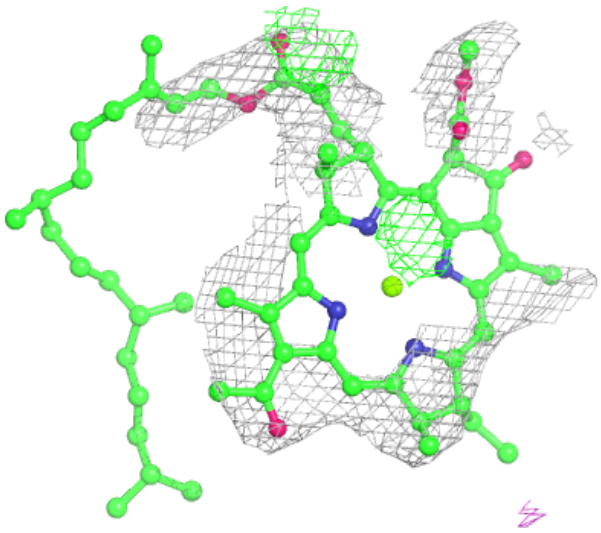
Electron density around BCL 7 102:

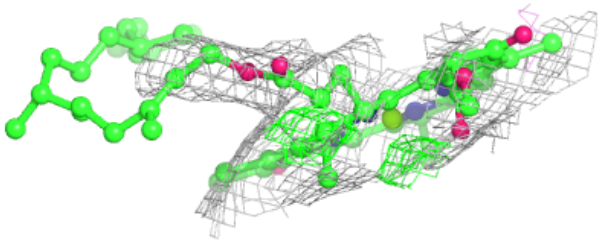
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

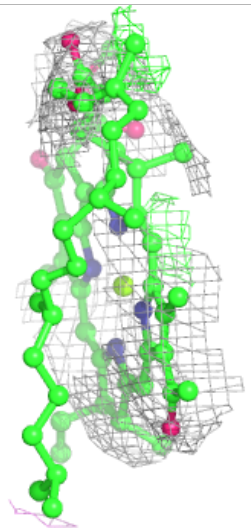


Electron density around BCL B 101:

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

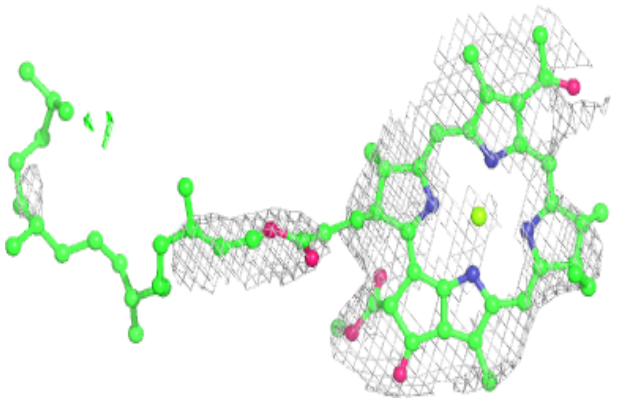


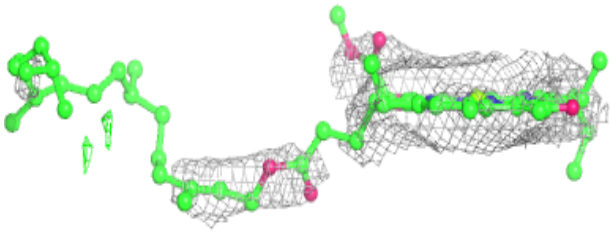


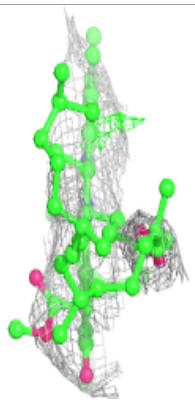


Electron density around BCL 9 102:

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

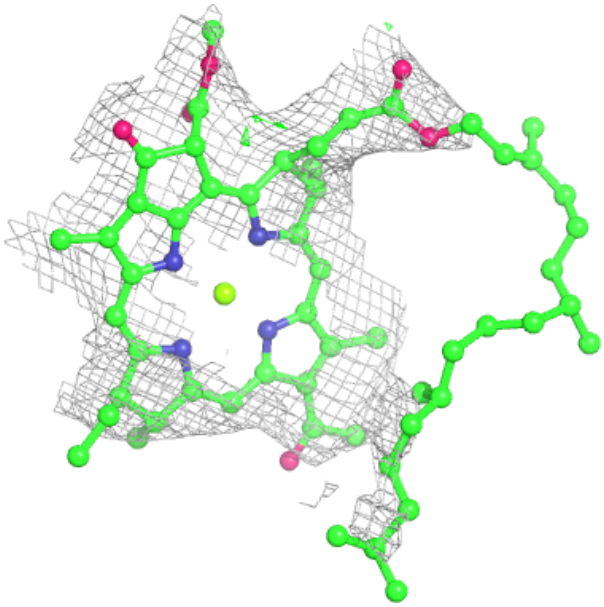


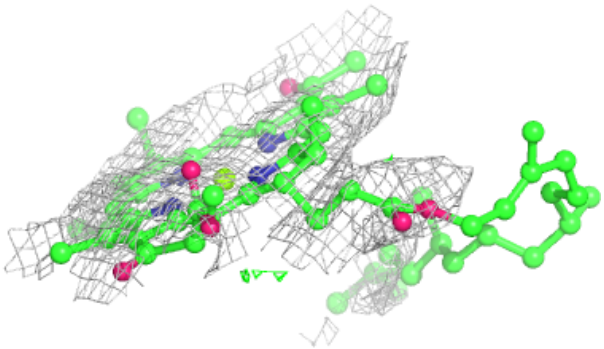


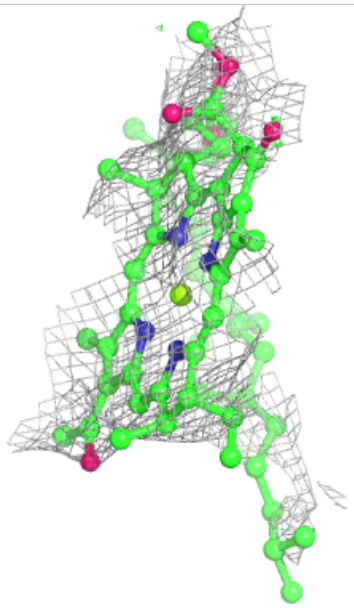


Electron density around BCL G 101:

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

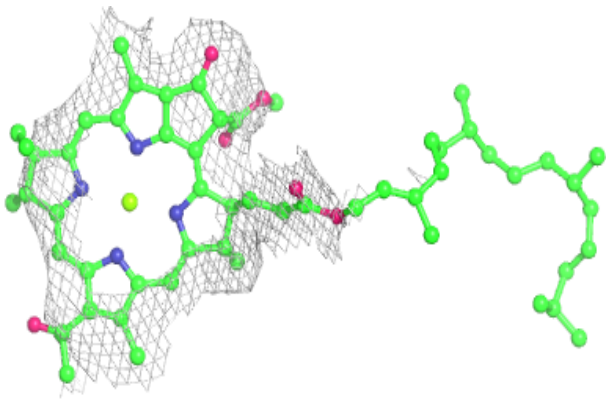


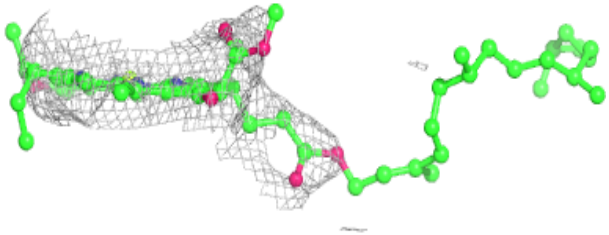


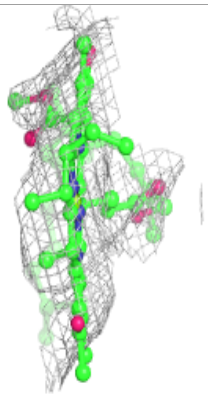


Electron density around BCL A 102:

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

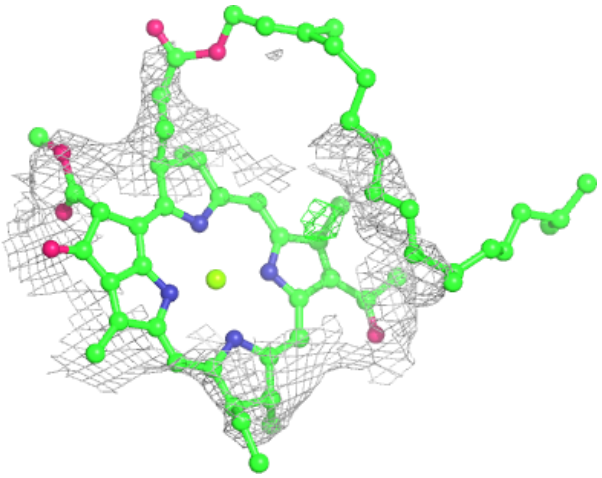


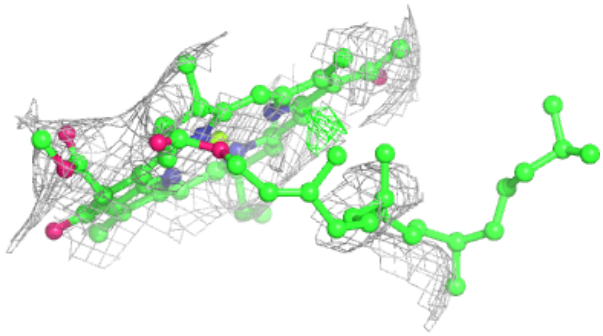


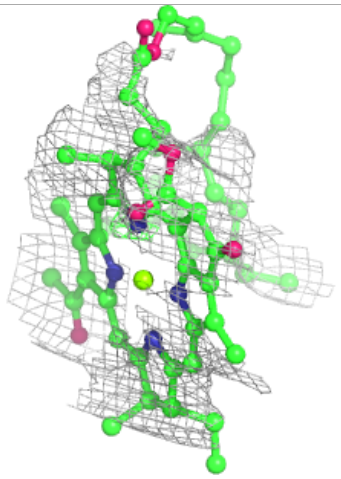


Electron density around BCL E 101:

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

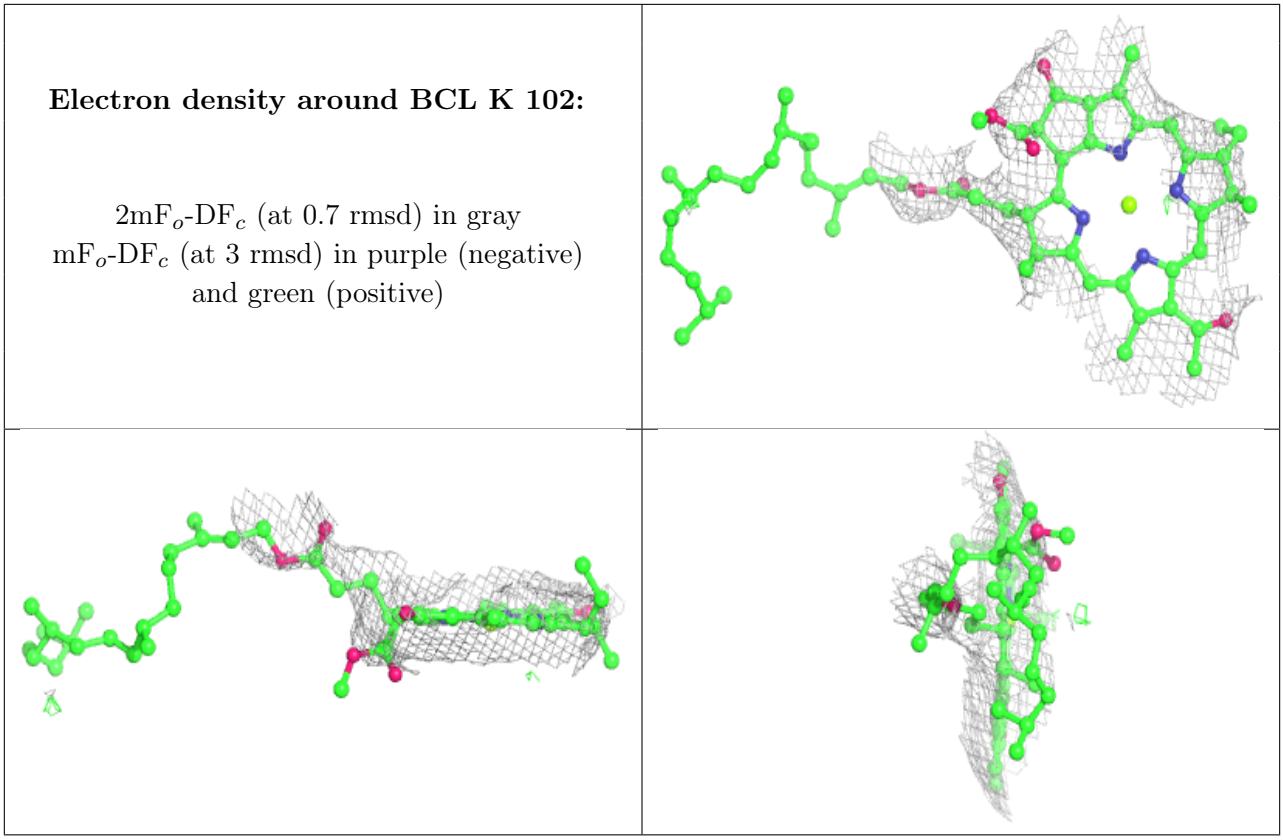






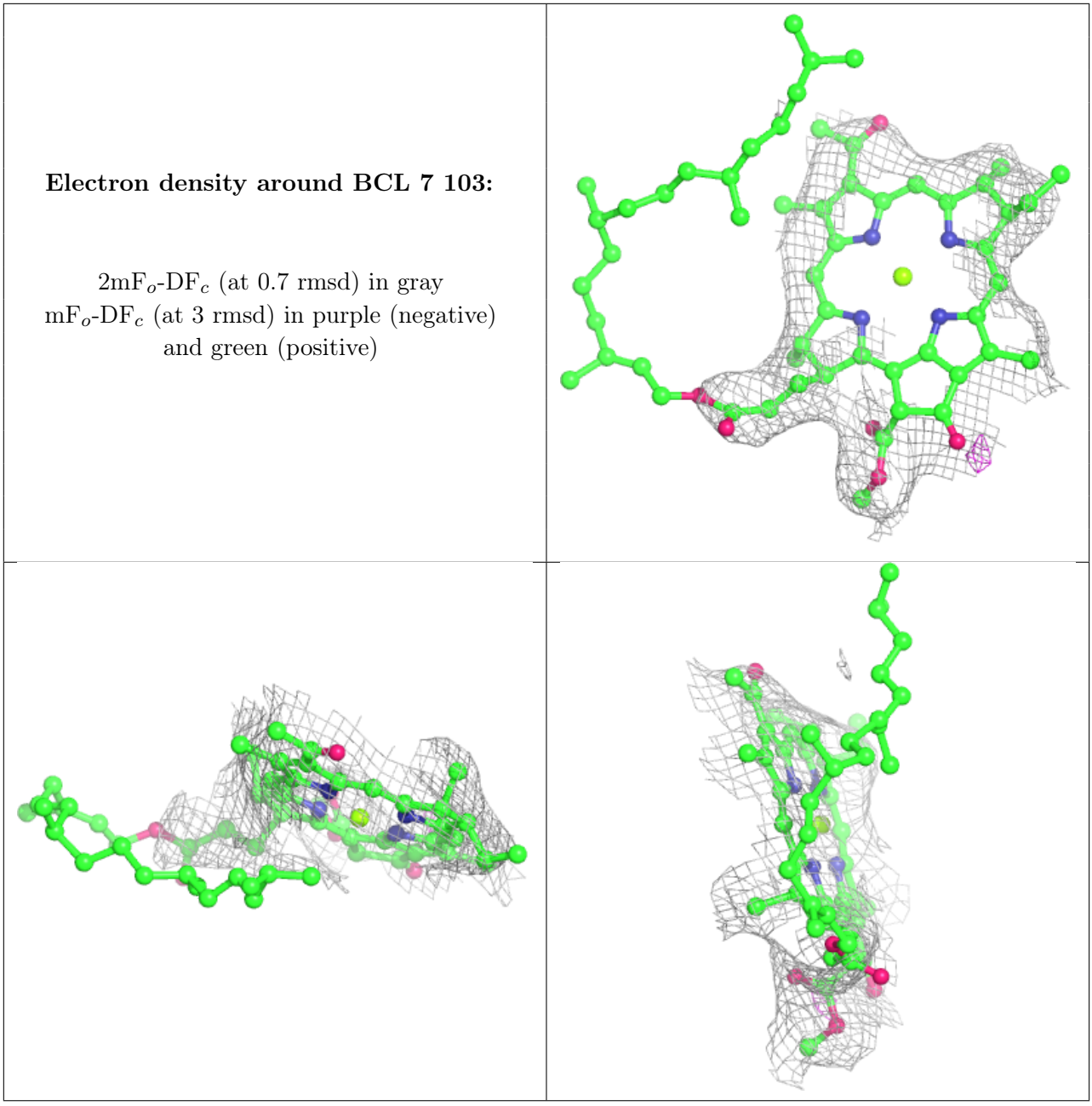
Electron density around BCL K 102:

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



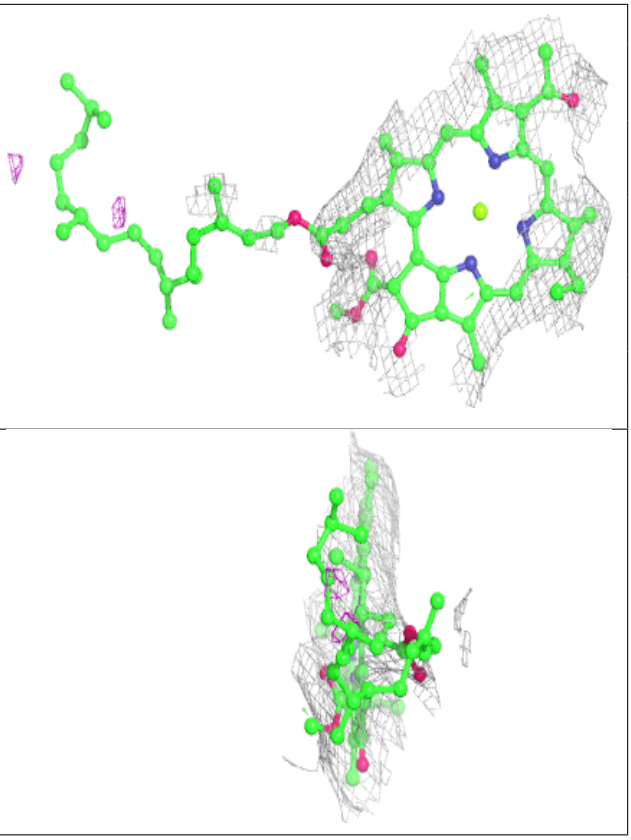
Electron density around BCL 7 103:

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



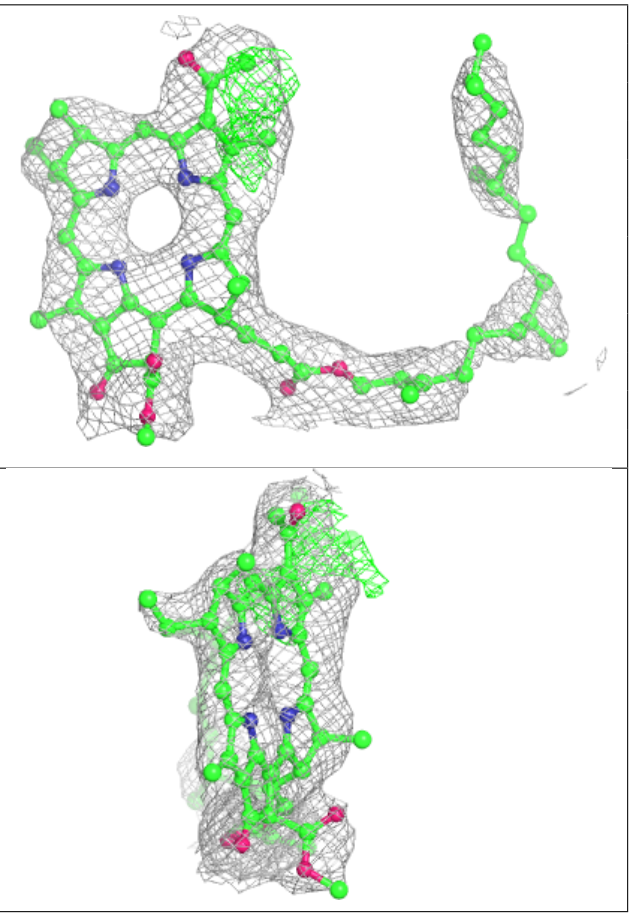
Electron density around BCL O 102:

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



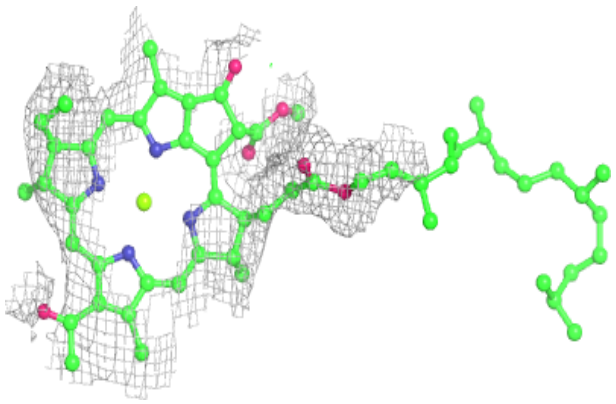
Electron density around BPH L 302:

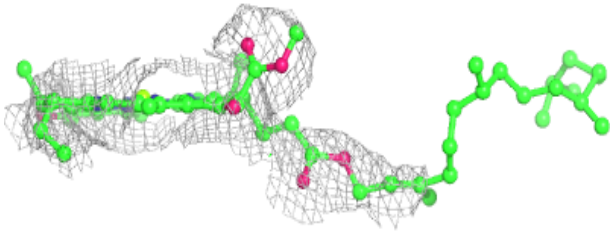
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

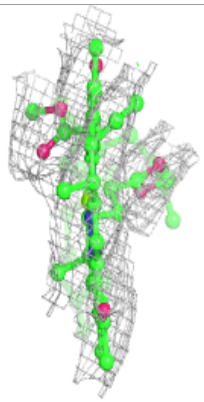


Electron density around BCL F 102:

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

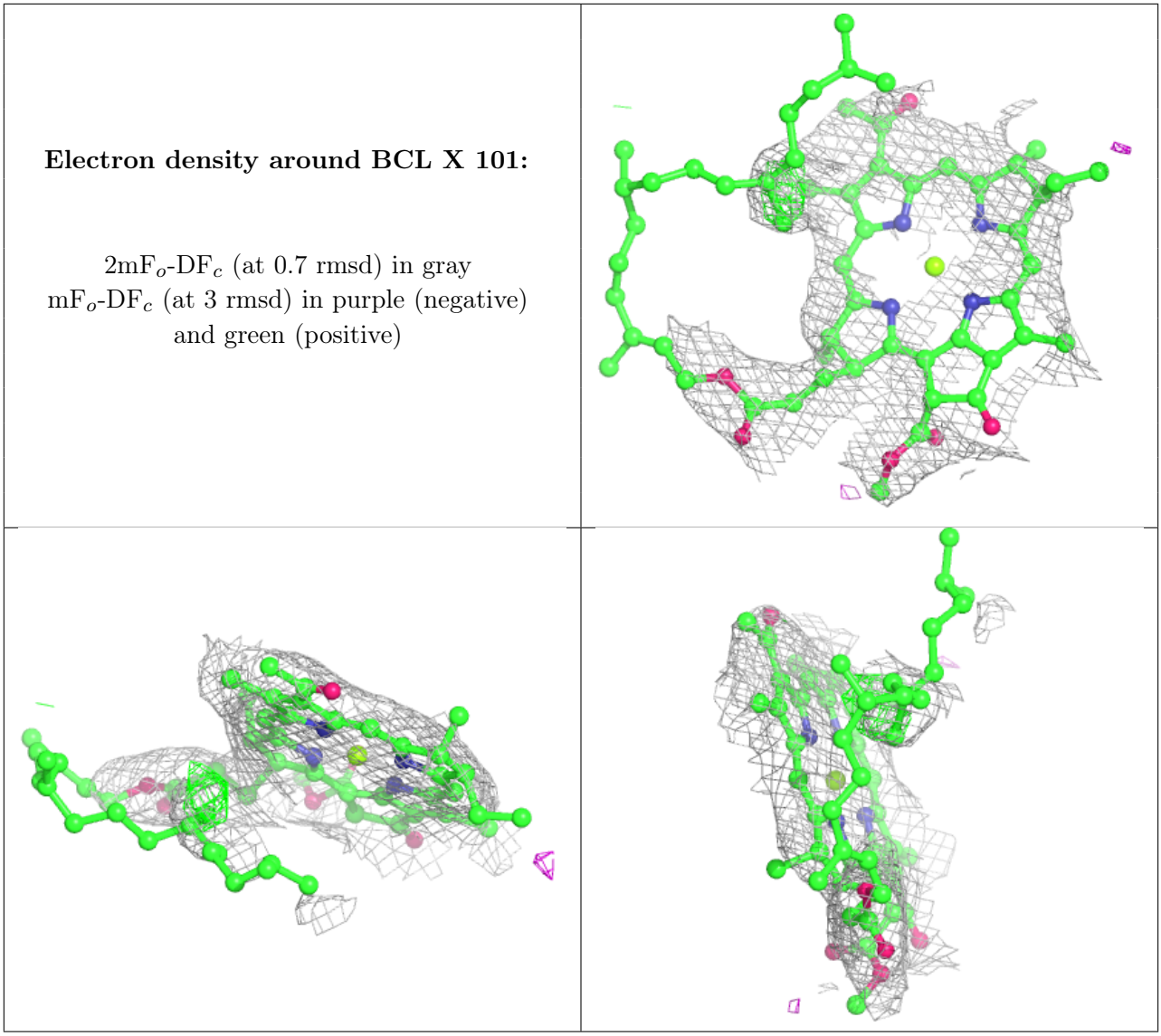






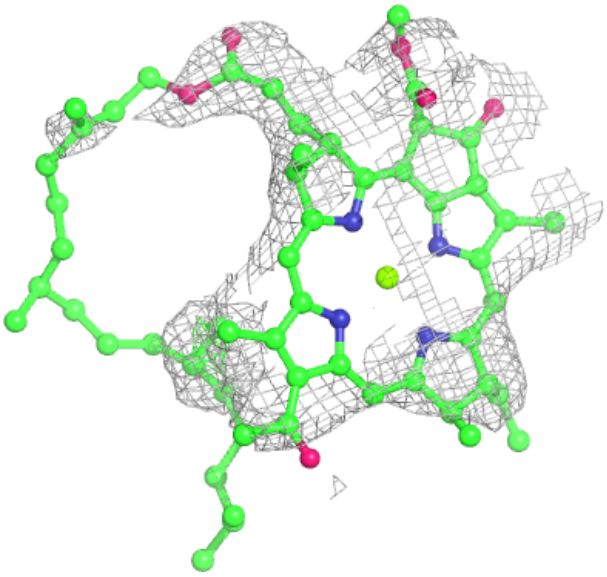
Electron density around BCL X 101:

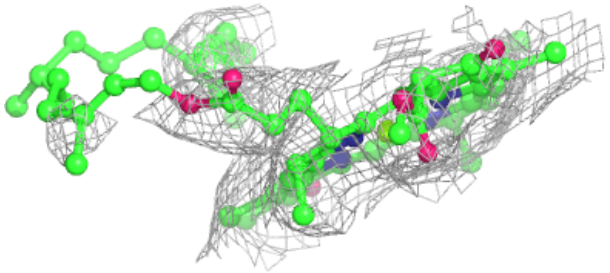
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

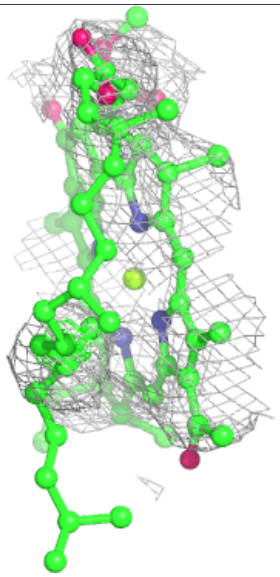


Electron density around BCL 2 101:

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

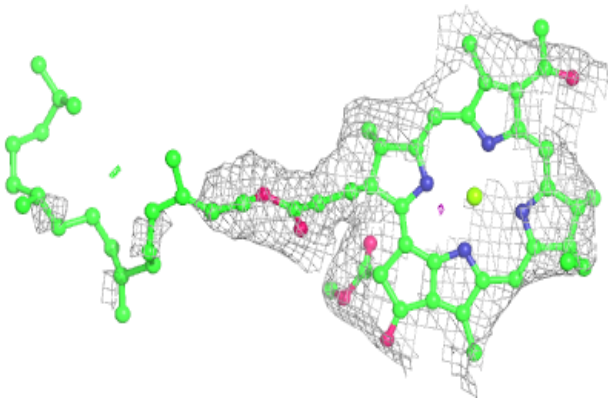


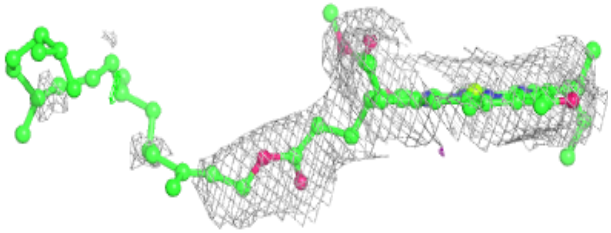


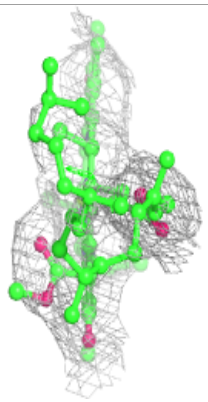


Electron density around BCL 3 102:

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

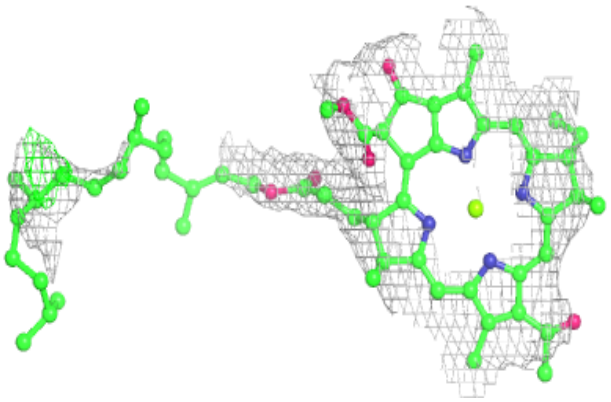


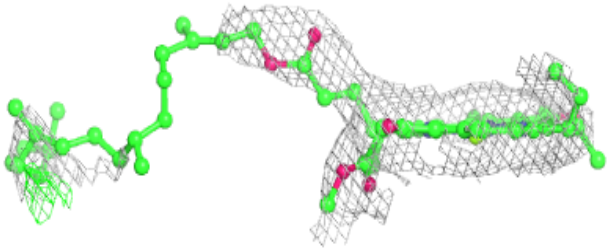


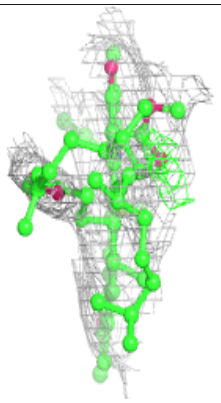


Electron density around BCL I 102:

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

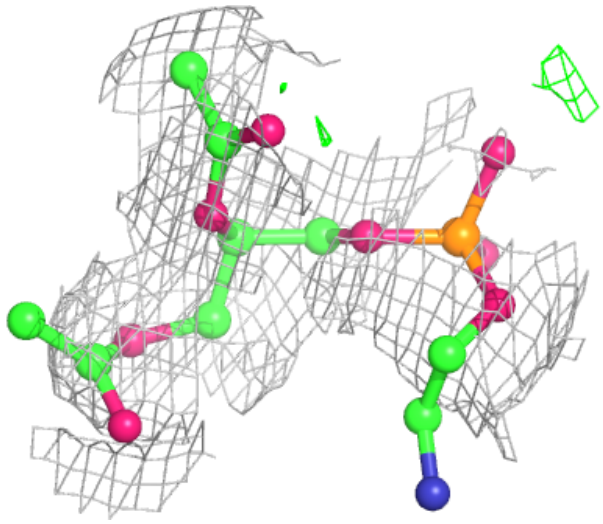


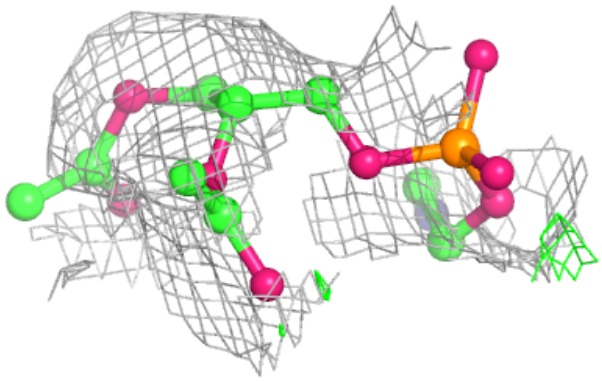


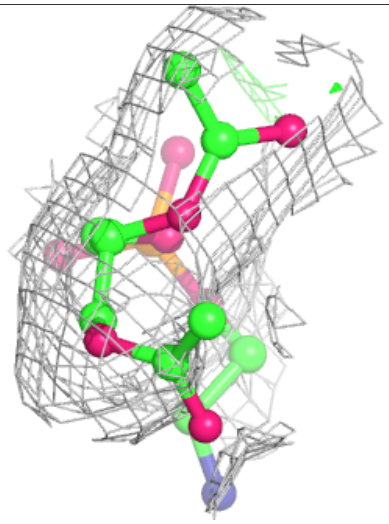


Electron density around PEF H 301:

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

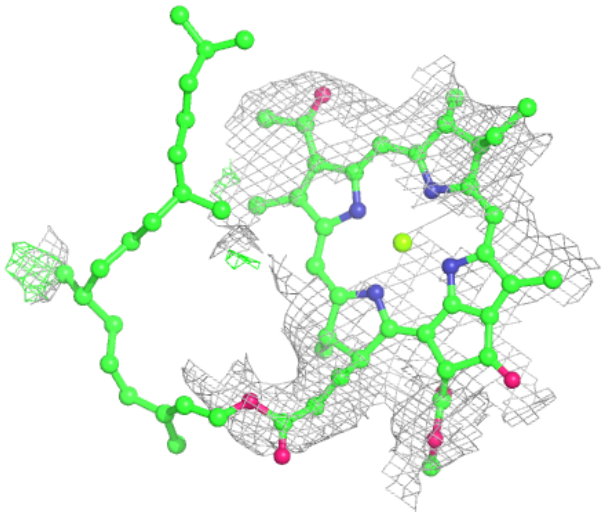


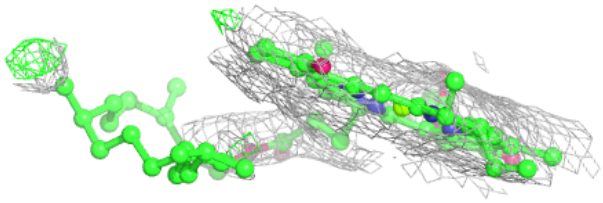


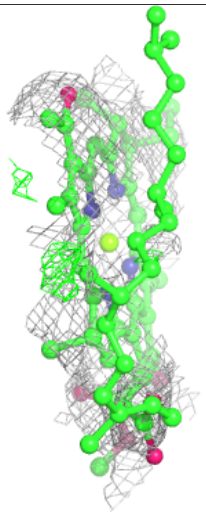


Electron density around BCL P 101:

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

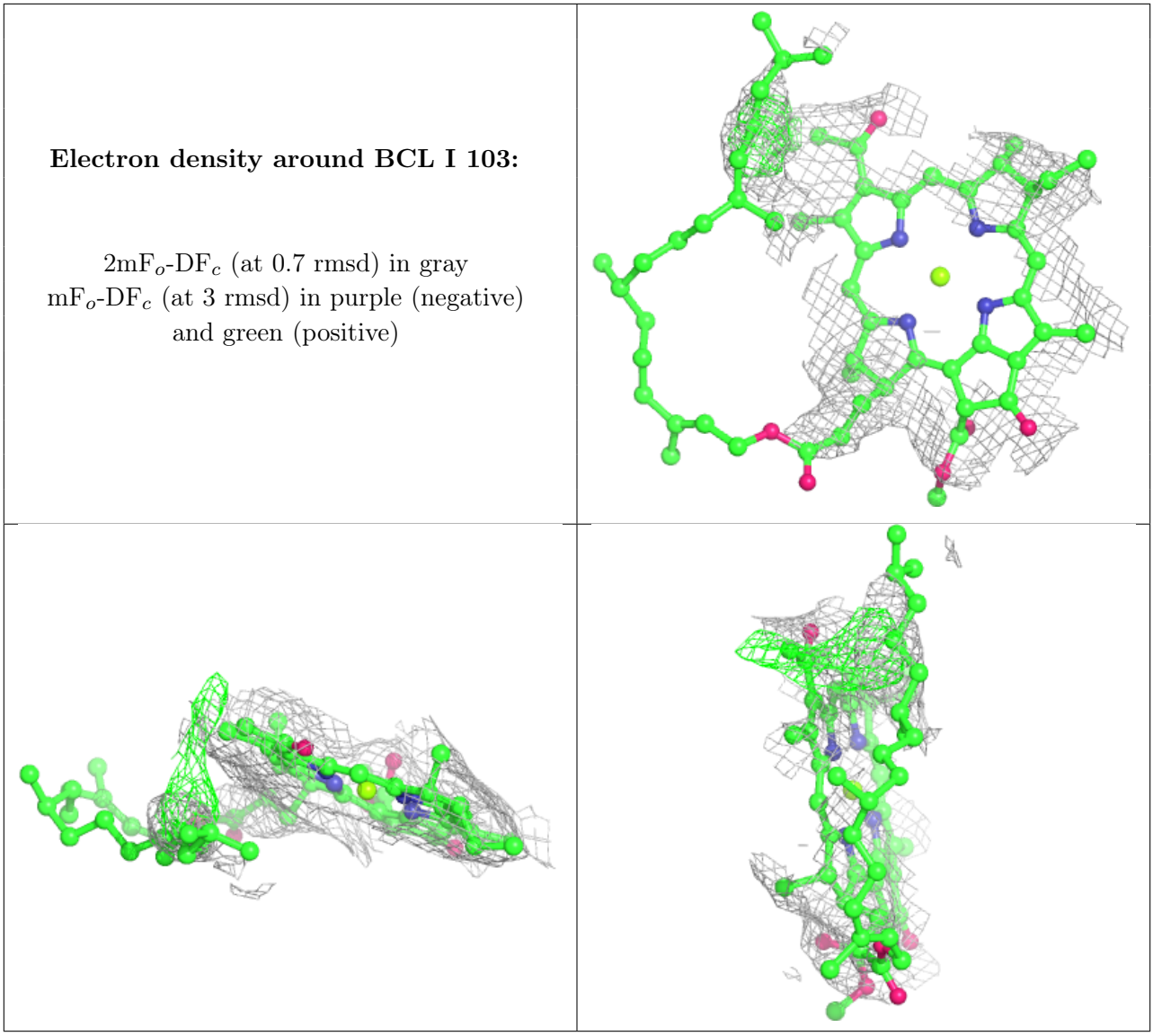






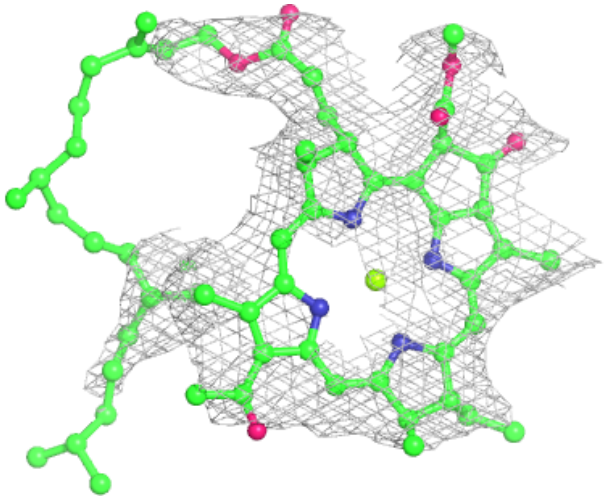
Electron density around BCL I 103:

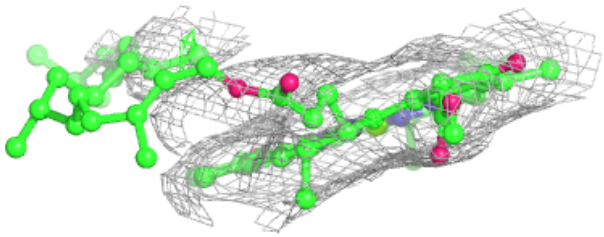
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

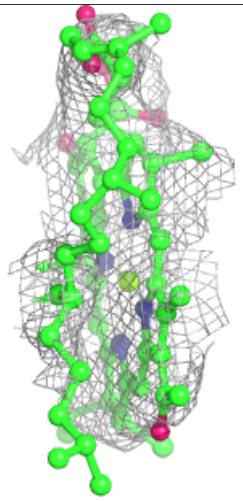


Electron density around BCL V 101:

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

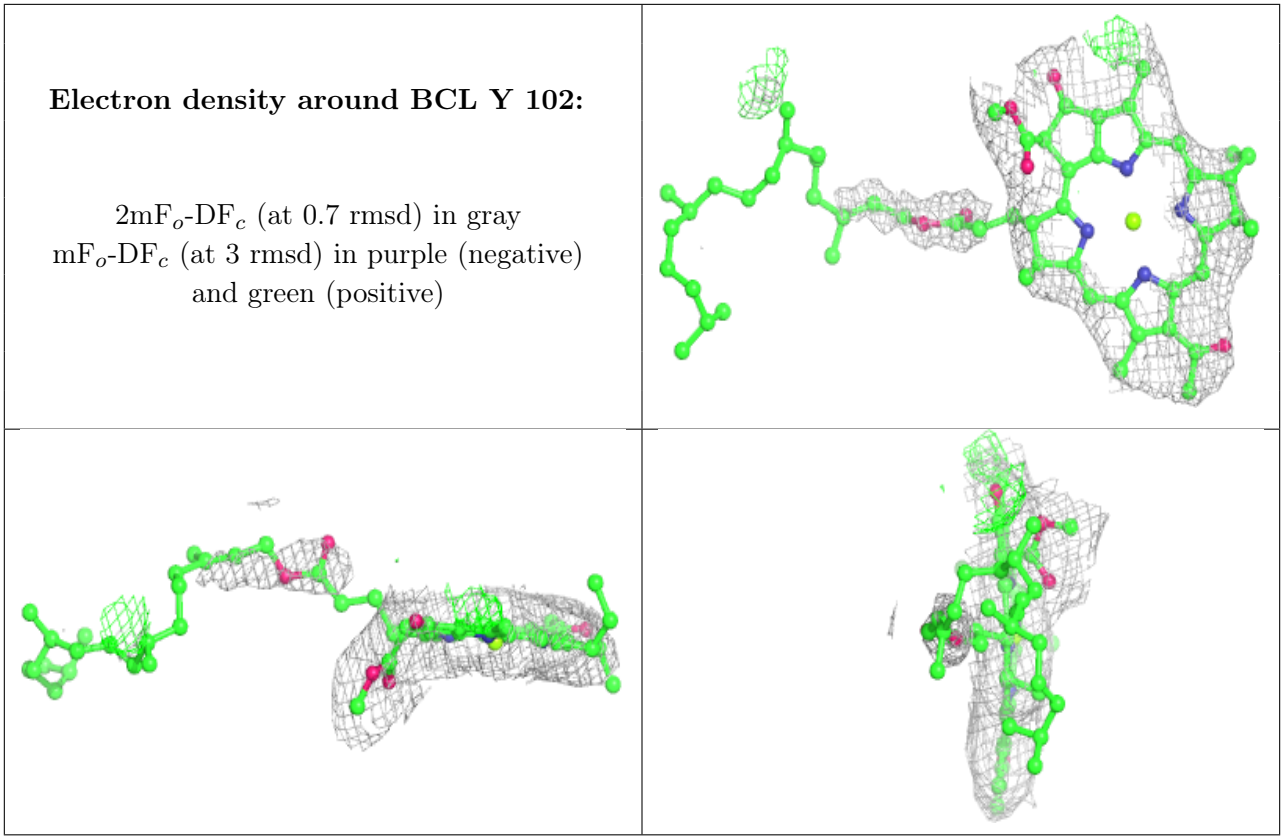






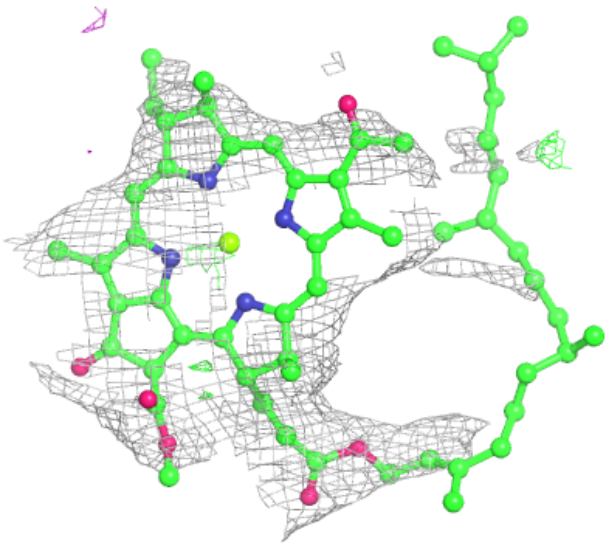
Electron density around BCL Y 102:

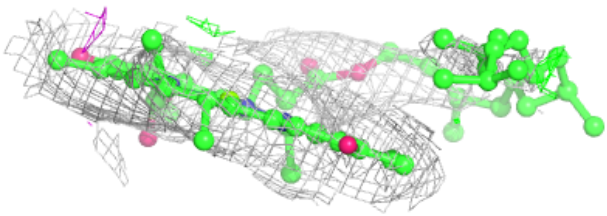
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

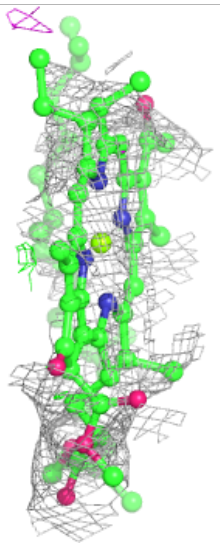


Electron density around BCL Z 101:

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

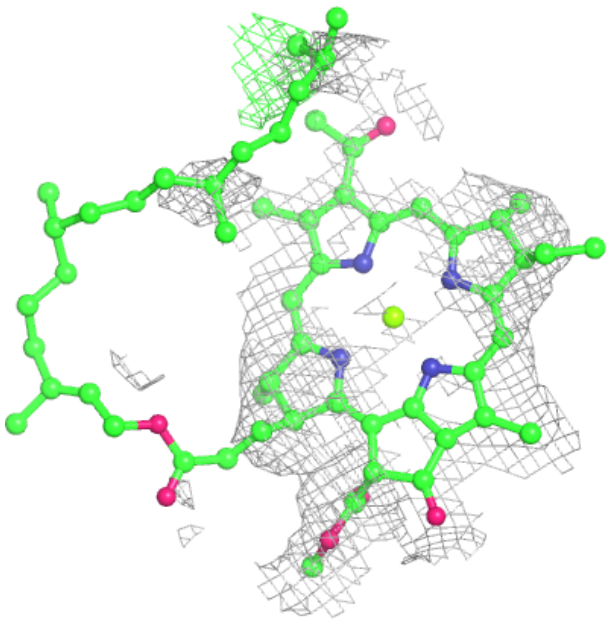


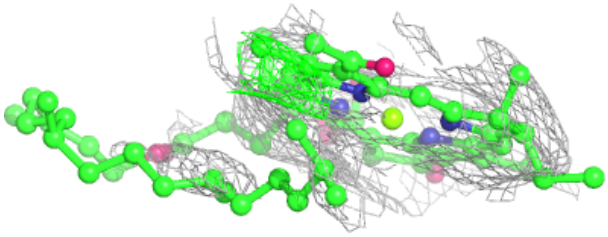


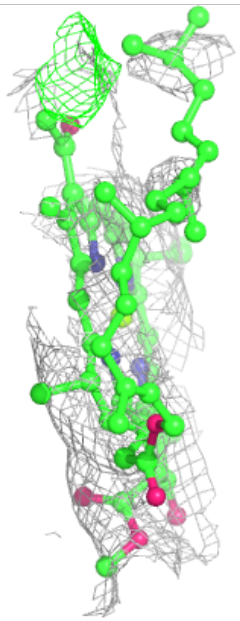


Electron density around BCL N 101:

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

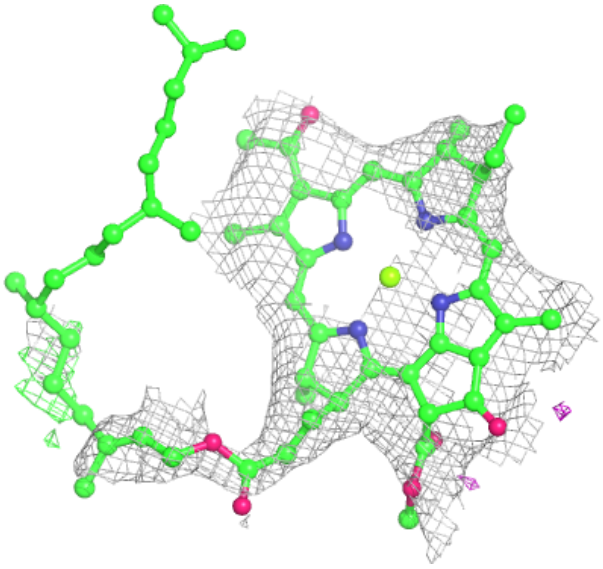


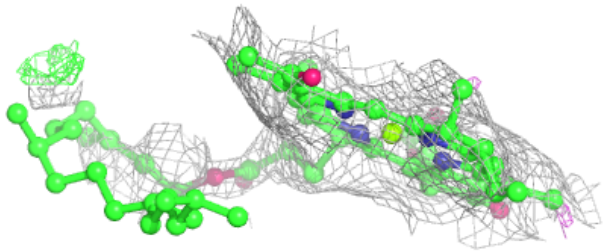


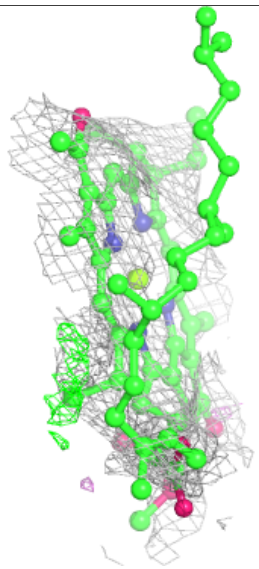


Electron density around BCL 4 101:

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

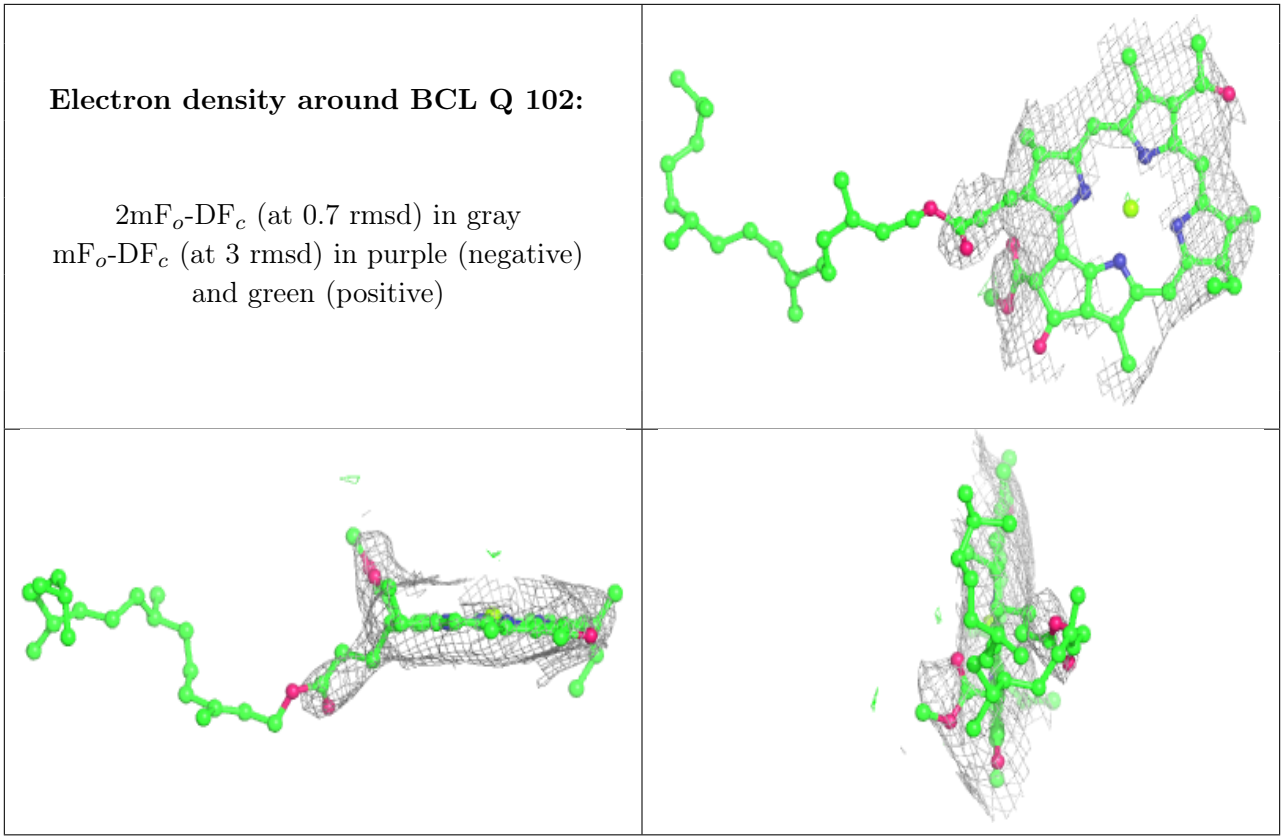






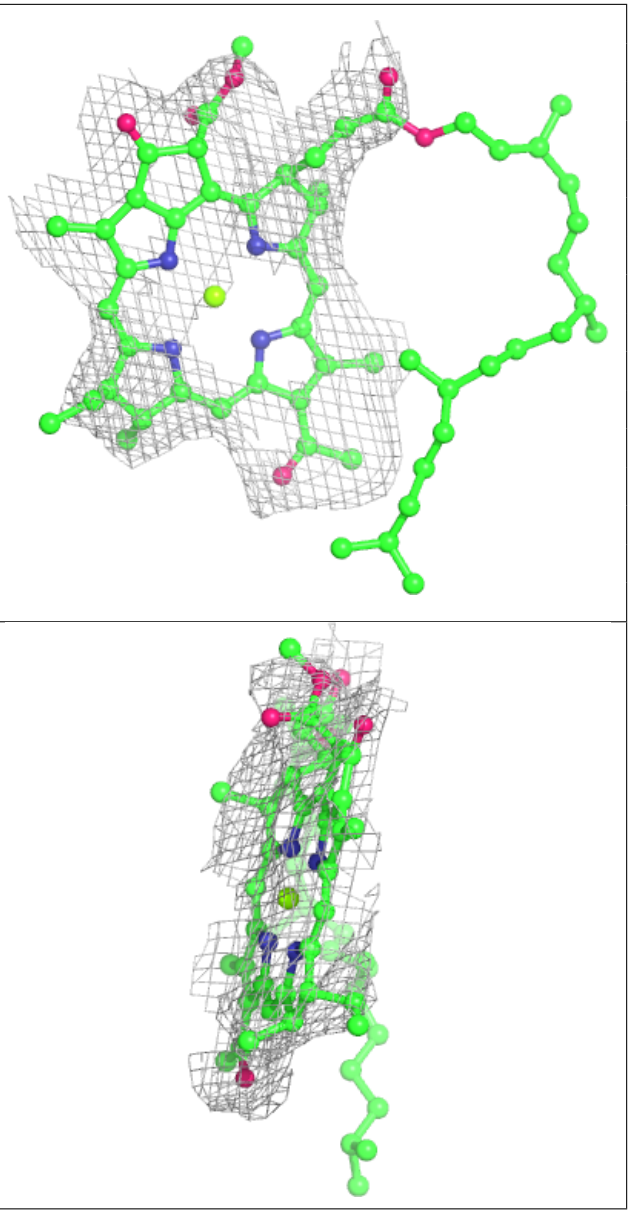
Electron density around BCL Q 102:

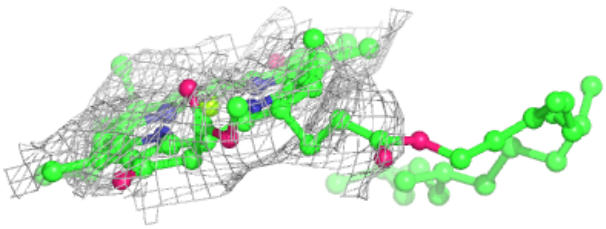
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCL 0 101:

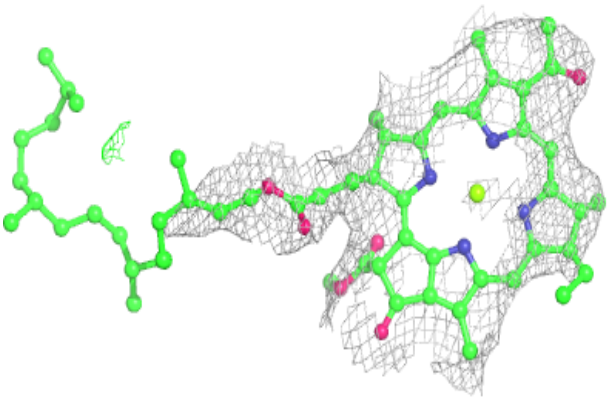
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

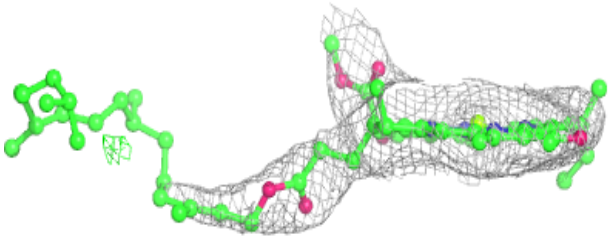


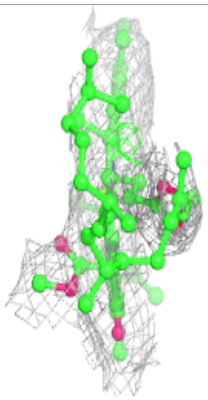


Electron density around BCL W 102:

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

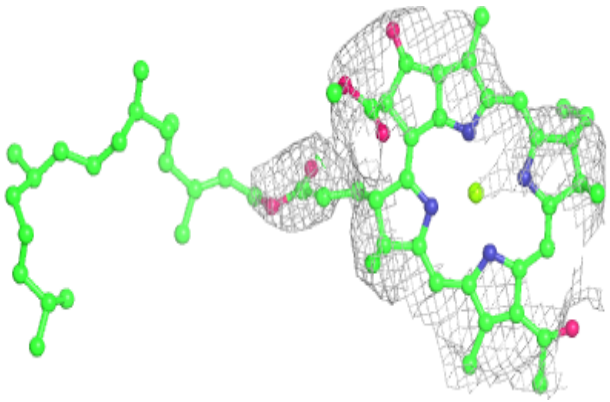


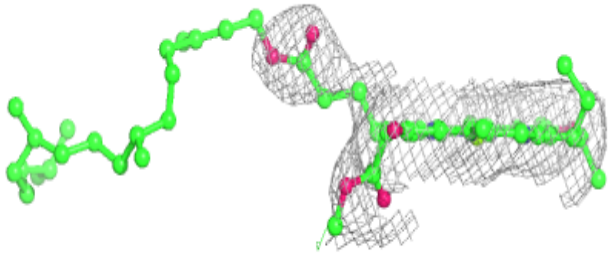


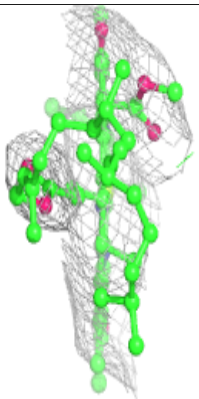


Electron density around BCL 5 102:

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

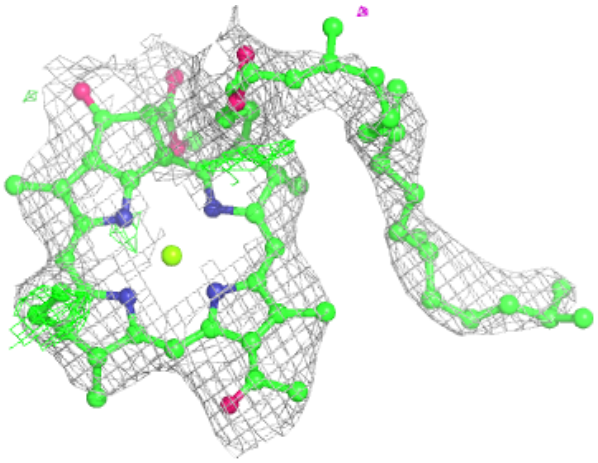


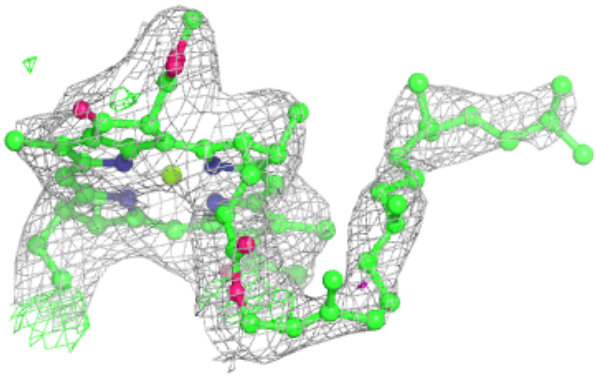


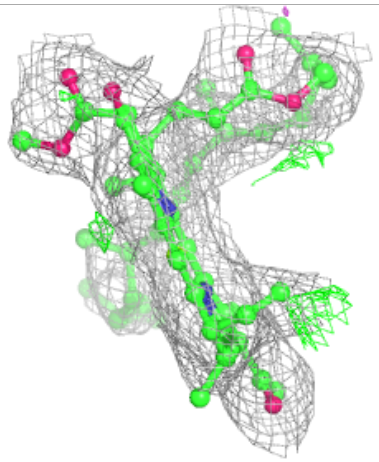


Electron density around BCL L 303:

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

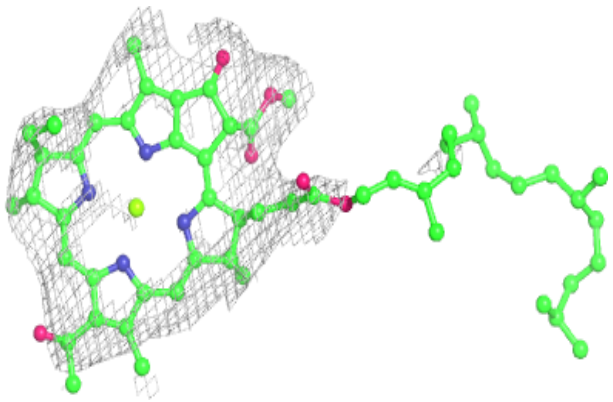


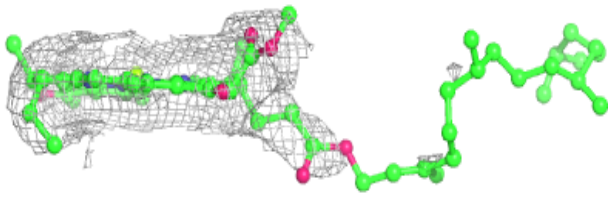


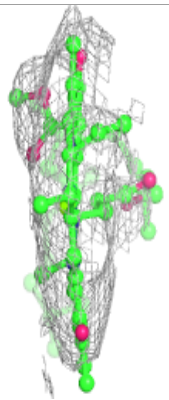


Electron density around BCL S 102:

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

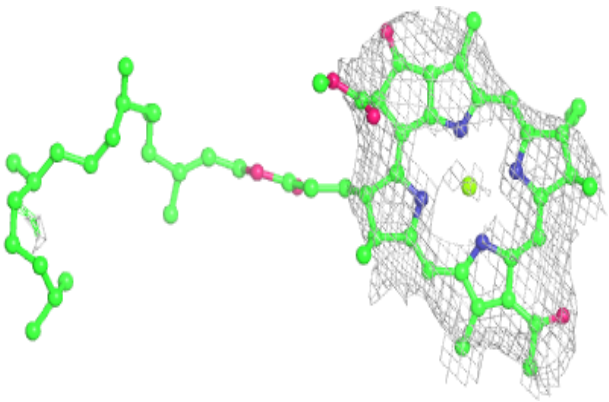


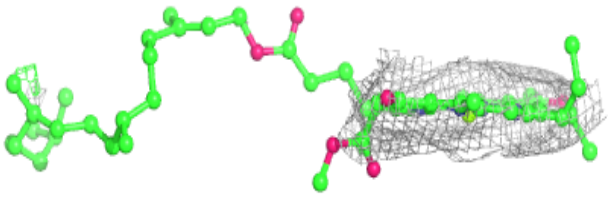


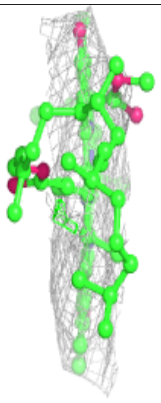


Electron density around BCL U 102:

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

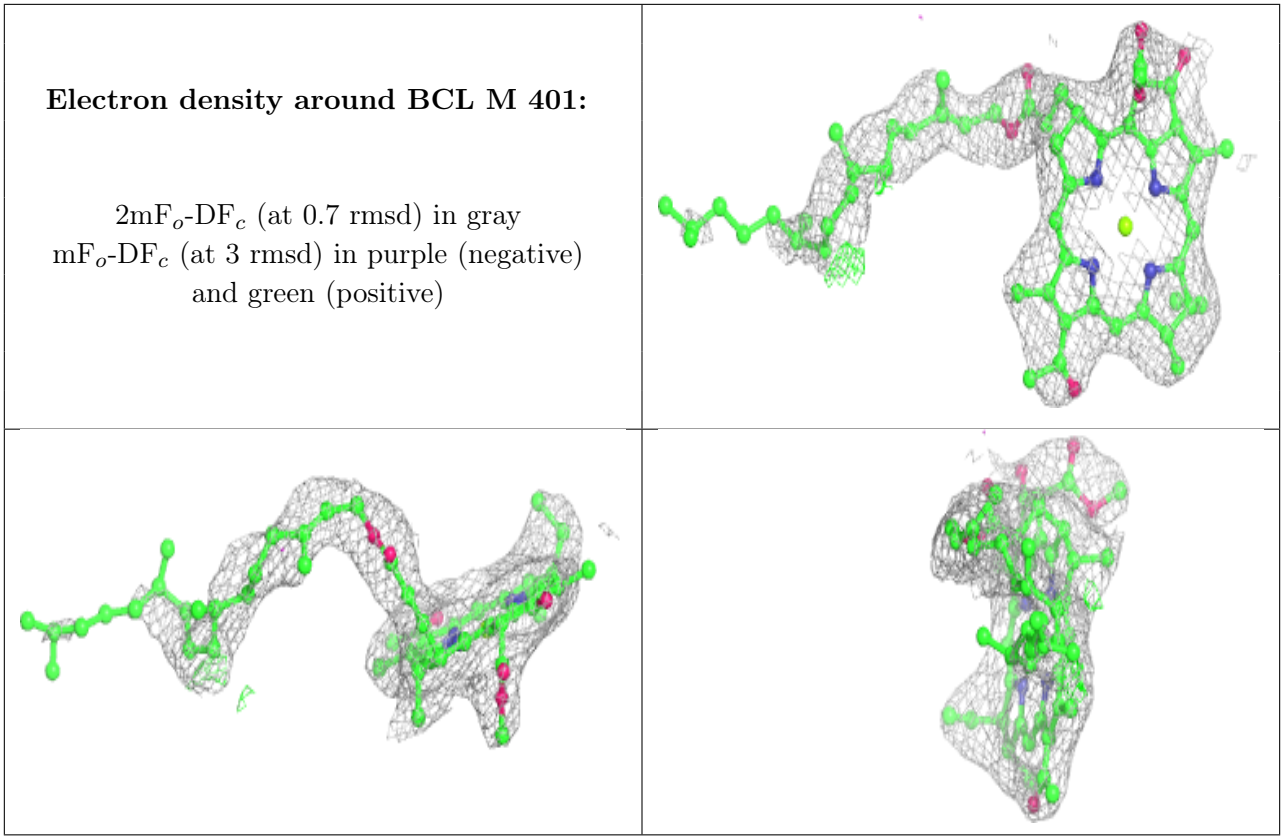






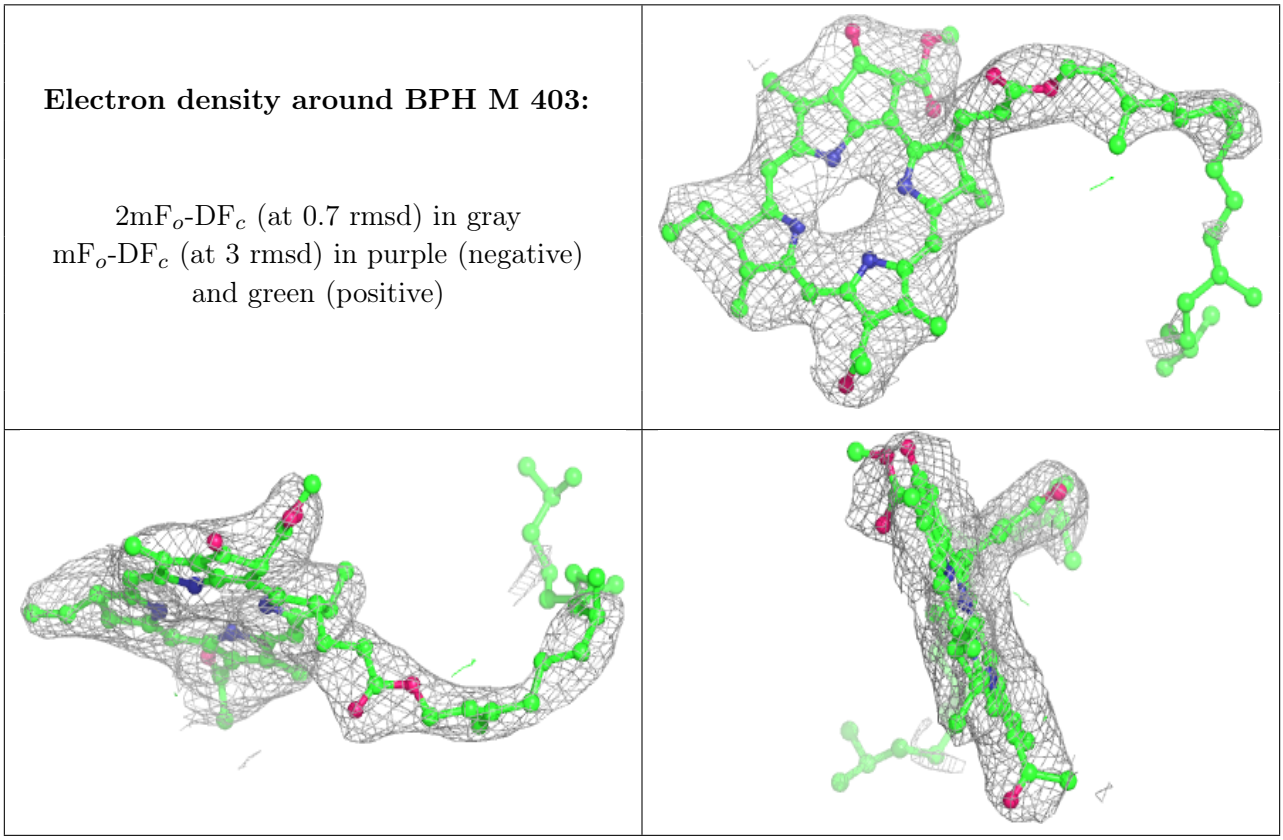
Electron density around BCL M 401:

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



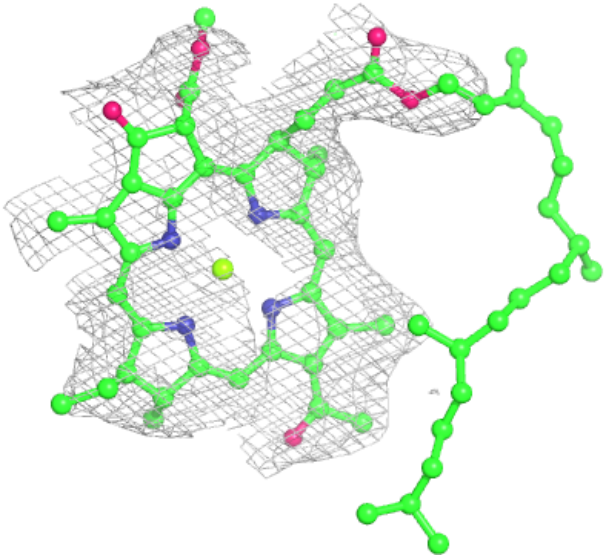
Electron density around BPH M 403:

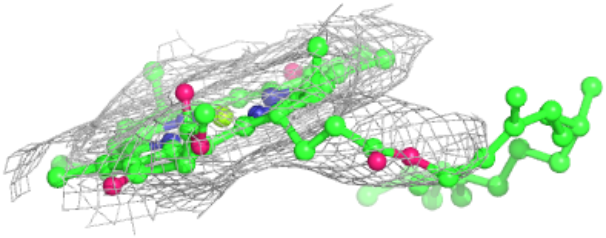
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

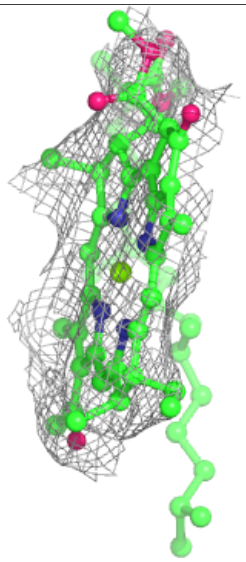


Electron density around BCL T 101:

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

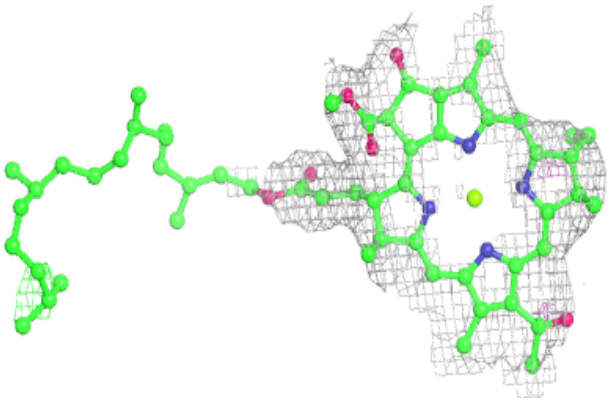


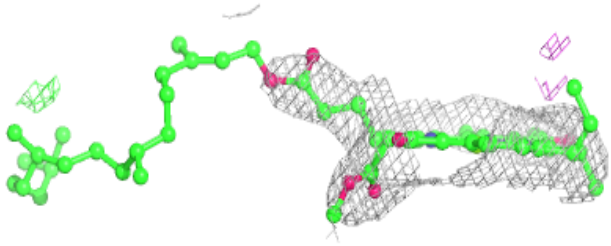


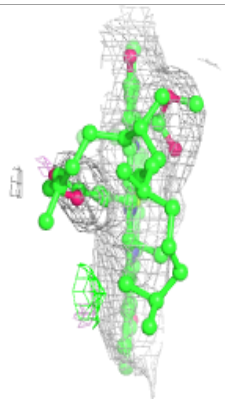


Electron density around BCL 1 102:

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

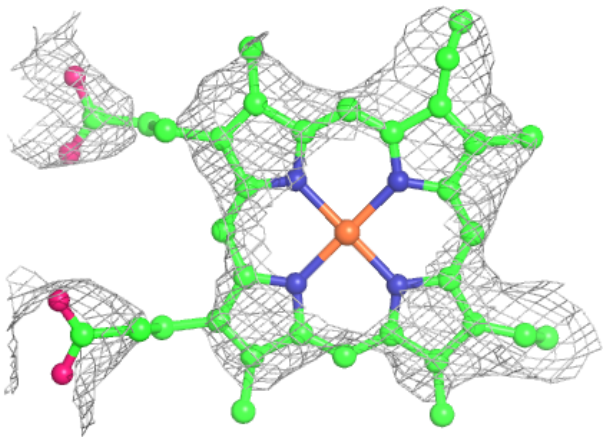


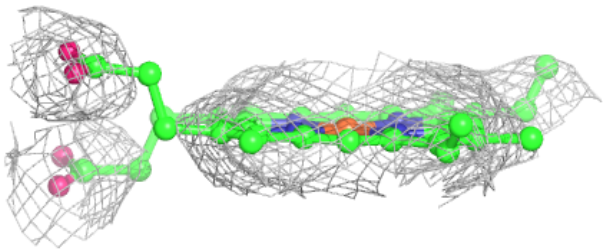


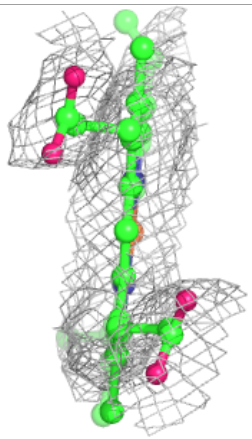


Electron density around HEM C 503:

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

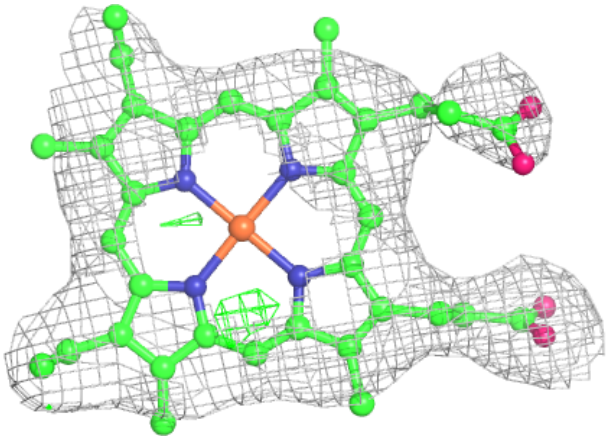


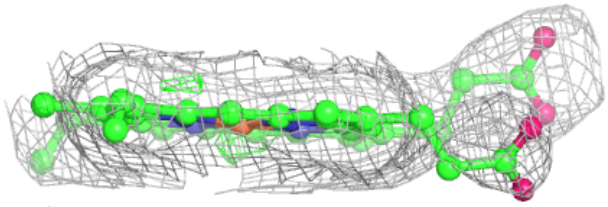


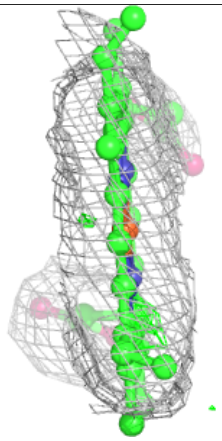


Electron density around HEM C 504:

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

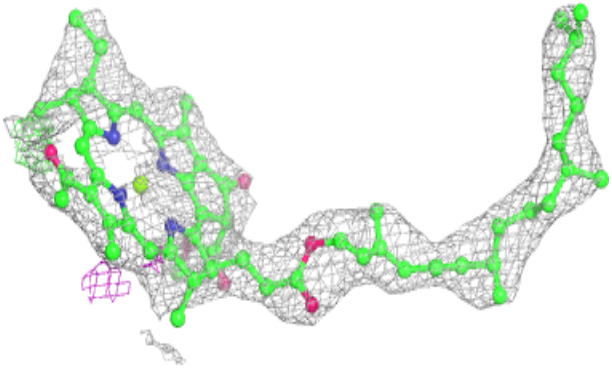


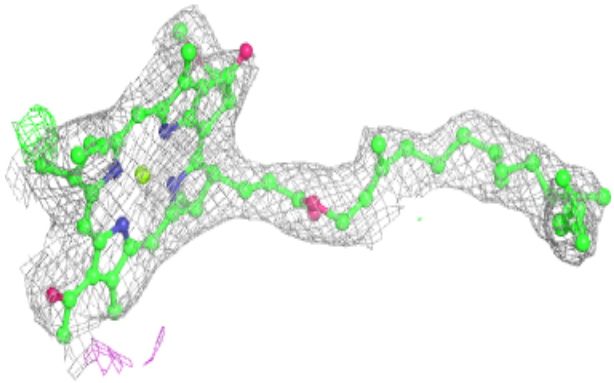


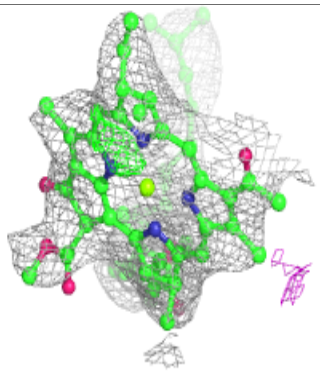


Electron density around BCL M 402:

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

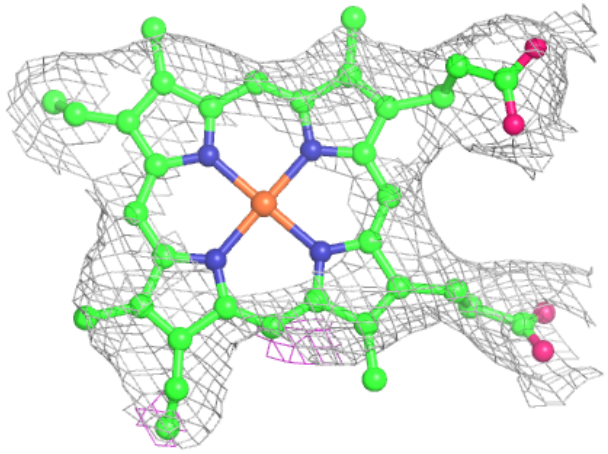


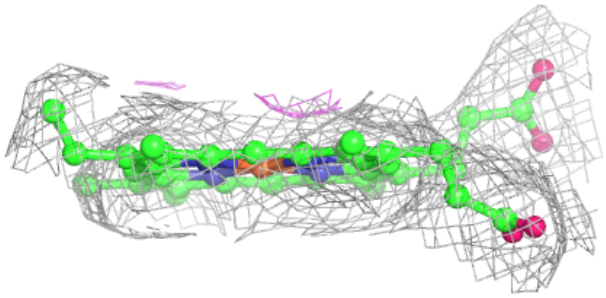


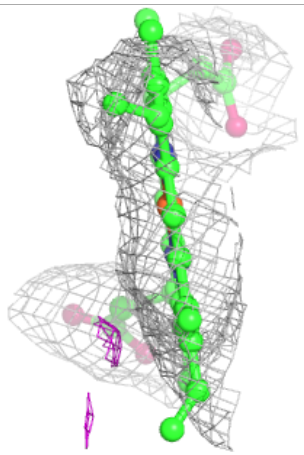


Electron density around HEM C 501:

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

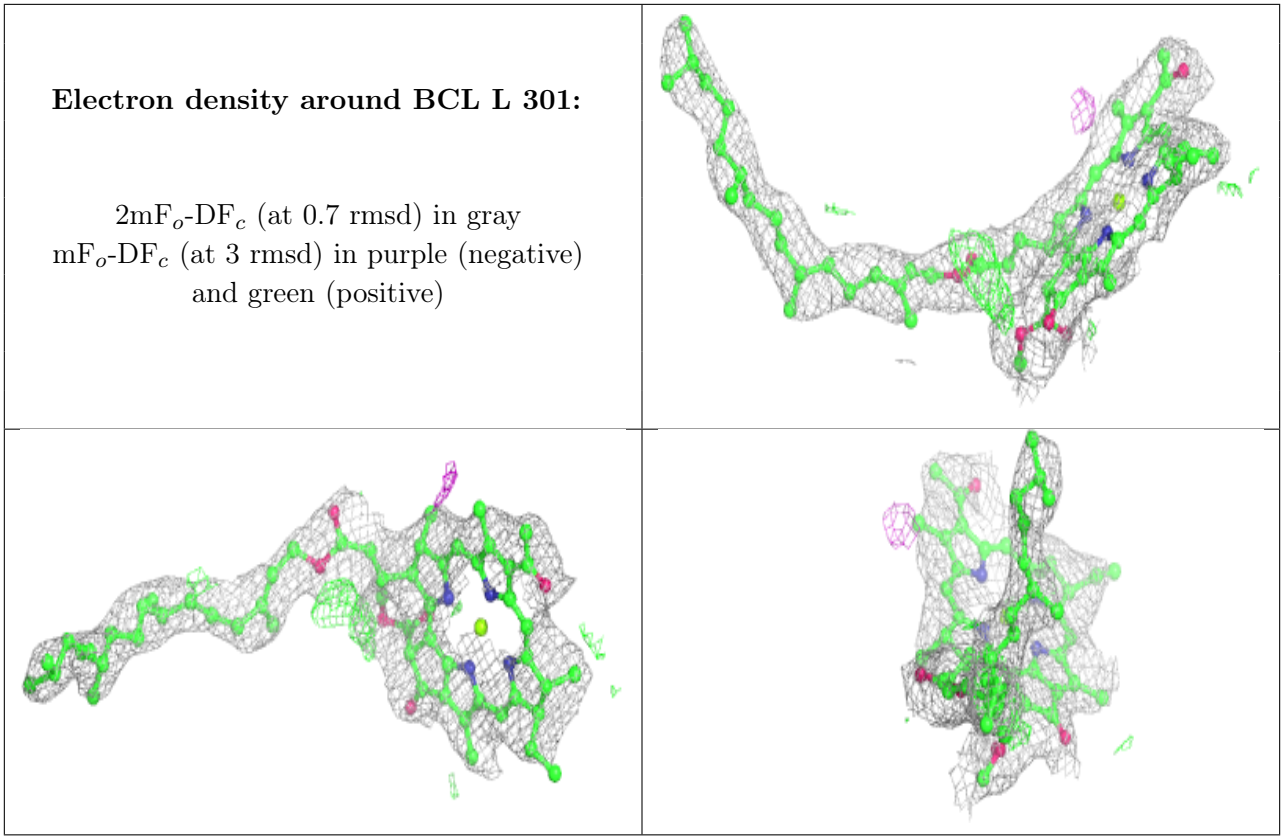






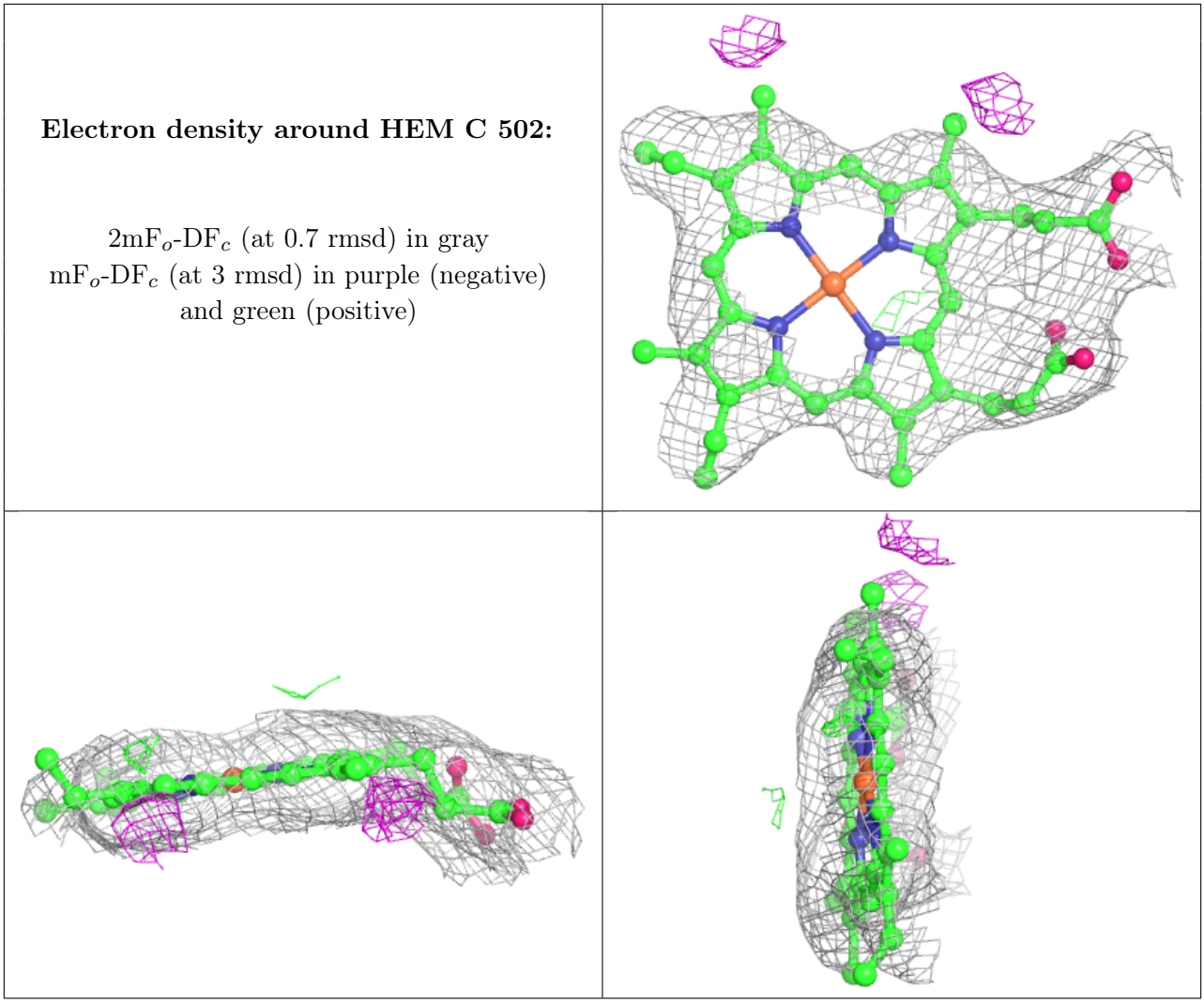
Electron density around BCL L 301:

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



Electron density around HEM C 502:

$2mF_o$-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

There are no such residues in this entry.