Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 11:29 PM JST

PDB ID	:	7Y44
Title	:	Re-refinement of damage free X-ray structure of bovine cytochrome c oxidase at 1.9 angstrom resolution
Authors	:	Tsukihara, T.; Hirata, K.; Ago, H.
Deposited on	:	2022-06-14
Resolution	:	1.90 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:

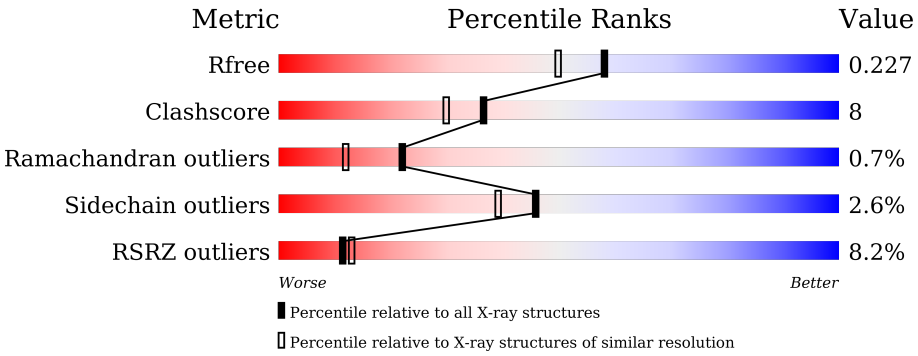
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	A	514	88% 12%
1	N	514	89% 11%
2	B	227	85% 15%
2	O	227	9% 75% 23%
3	C	261	85% 14%
3	P	261	87% 12%

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Mol	Chain	Length	Quality of chain
4	D	147	4% 90% 7%
4	Q	147	20% 88% 7%
5	E	109	12% 90% 6%
5	R	109	19% 88% 6%
6	F	98	10% 81% 16%
6	S	98	12% 80% 16%
7	G	85	22% 72% 22% 5%
7	T	85	24% 74% 18% 6%
8	H	85	14% 72% 16% 7%
8	U	85	22% 80% 12% 7%
9	I	73	18% 93% 5%
9	V	73	25% 93% 7%
10	J	59	12% 93% 5%
10	W	59	12% 81% 17%
11	K	56	5% 70% 18% 12%
11	X	56	16% 73% 14% 12%
12	L	47	4% 77% 17%
12	Y	47	9% 79% 17%
13	M	46	15% 74% 17% 7%
13	Z	46	20% 78% 15% 7%

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
20	EDO	A	612	-	-	X	-
20	EDO	N	613	-	-	X	-
20	EDO	S	107	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	DMU	A	616	-	-	-	X
21	DMU	B	306	-	-	-	X
21	DMU	D	202	-	-	-	X
21	DMU	K	102	-	-	-	X
21	DMU	K	103	-	-	-	X
21	DMU	K	105	-	-	-	X
21	DMU	X	101	-	-	-	X
26	CDL	C	304	-	-	X	-
26	CDL	G	101	-	-	X	-
27	CHD	W	101	-	-	-	X
27	CHD	X	105	-	-	-	X
7	TPO	G	11	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 34120 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	10	0
			4051	2710	623	681	37			
1	N	514	Total	C	N	O	S	0	7	0
			4046	2708	623	678	37			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	3	0
			1834	1190	281	344	19			
2	O	227	Total	C	N	O	S	0	4	0
			1844	1200	283	342	19			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	3	0
			2117	1416	336	350	15			
3	P	259	Total	C	N	O	S	0	2	0
			2115	1415	336	350	14			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1201	783	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			860	549	147	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			750	465	134	146	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

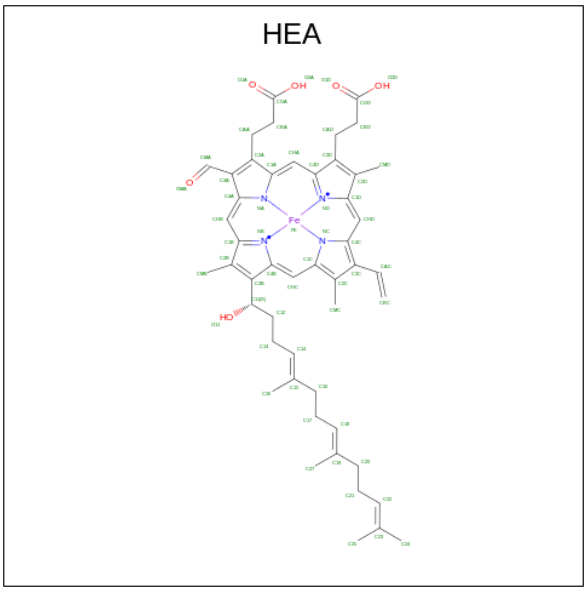
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

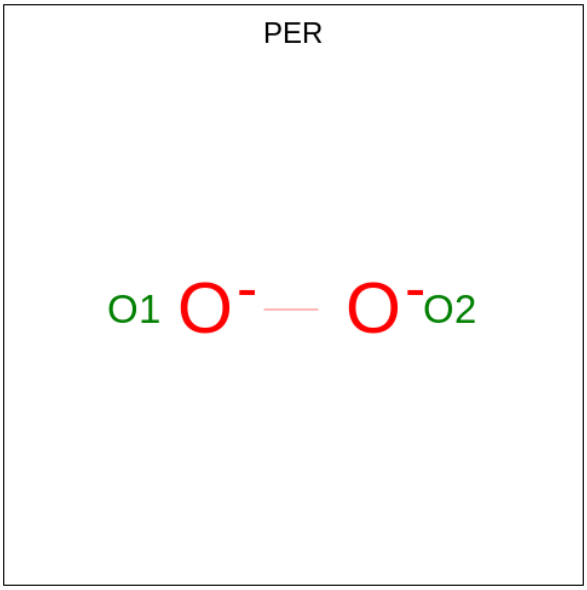
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

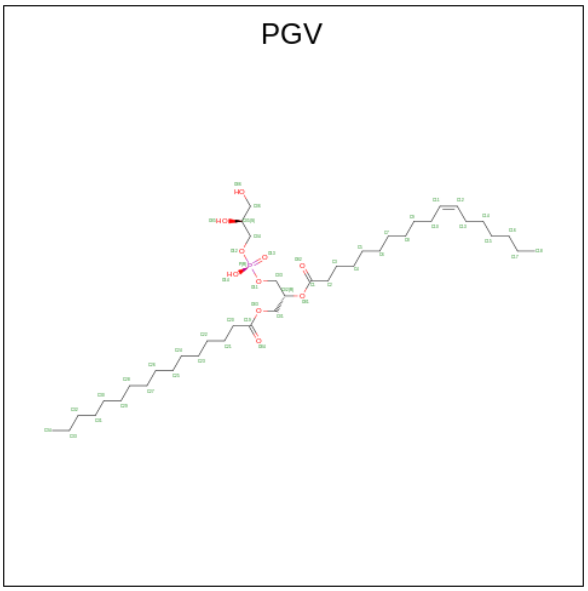
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



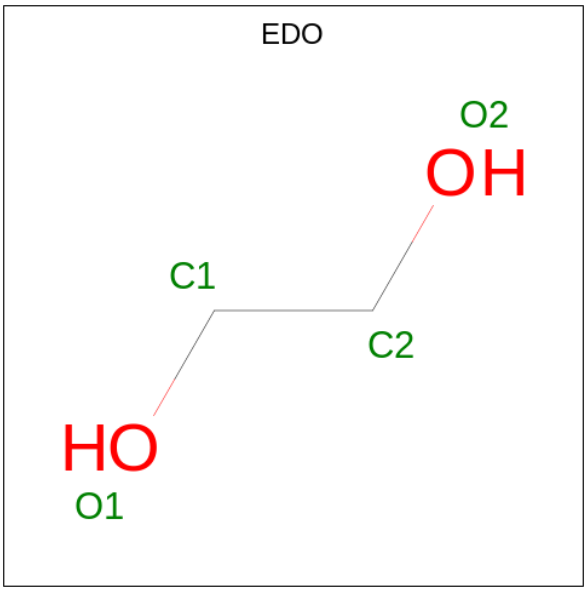
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	B	1	Total C O 4 2 2	0	0
20	B	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	F	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0
20	L	1	Total C O 4 2 2	0	0
20	L	1	Total C O 4 2 2	0	0
20	M	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0

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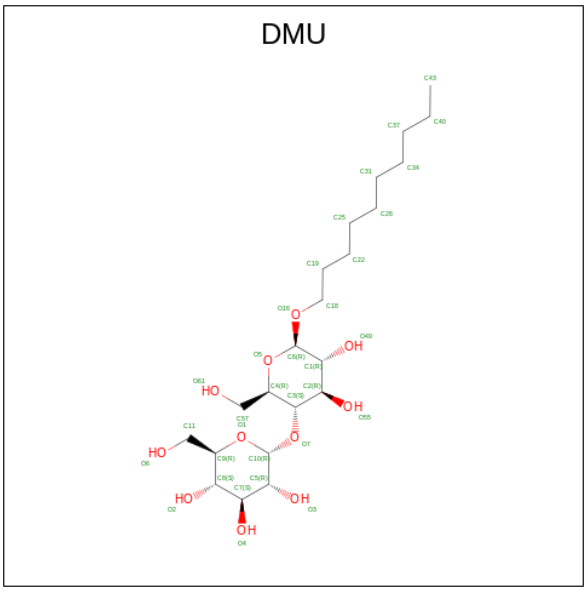
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 33 22 11	0	0
21	B	1	Total C O 33 22 11	0	0
21	C	1	Total C O 33 22 11	0	0
21	D	1	Total C O 33 22 11	0	0
21	G	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	K	1	Total C O 33 22 11	0	0
21	L	1	Total C O 33 22 11	0	0
21	M	1	Total C O 33 22 11	0	0
21	O	1	Total C O 33 22 11	0	0

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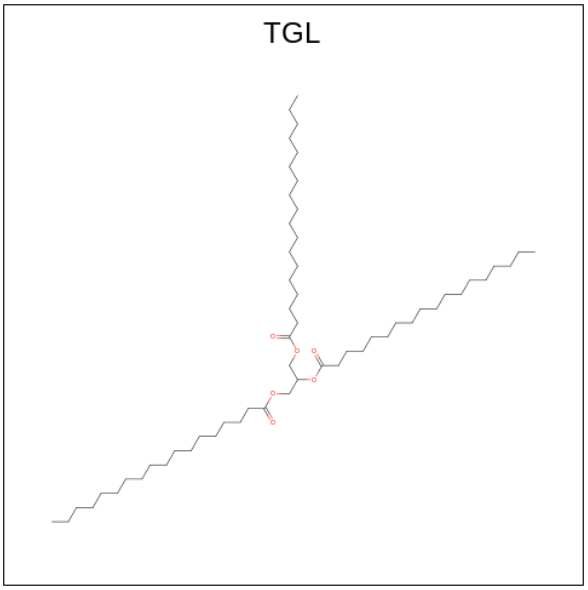
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C O 33 22 11	0	0
21	Q	1	Total C O 33 22 11	0	0
21	T	1	Total C O 33 22 11	0	0
21	X	1	Total C O 33 22 11	0	0
21	X	1	Total C O 22 16 6	0	0
21	X	1	Total C O 22 16 6	0	0
21	X	1	Total C O 22 16 6	0	0
21	Z	1	Total C O 33 22 11	0	0

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 63 57 6	0	0
22	D	1	Total C O 63 57 6	0	0

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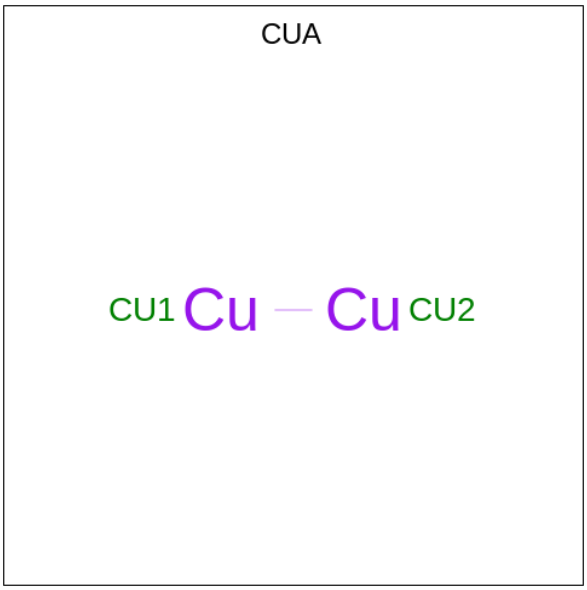
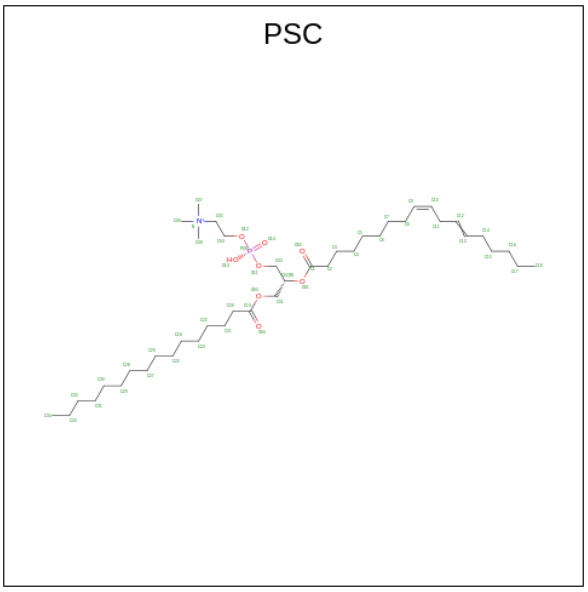
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	L	1	Total C O 63 57 6	0	0
22	O	1	Total C O 63 57 6	0	0
22	Q	1	Total C O 63 57 6	0	0
22	Y	1	Total C O 63 57 6	0	0

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



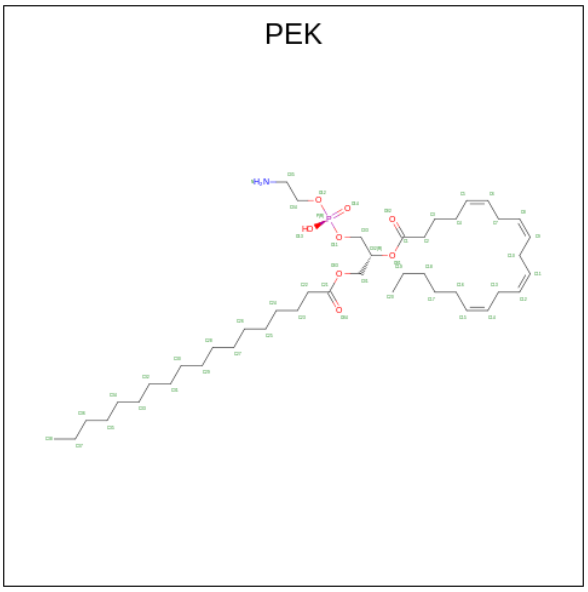
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0
23	O	1	Total Cu 2 2	0	0

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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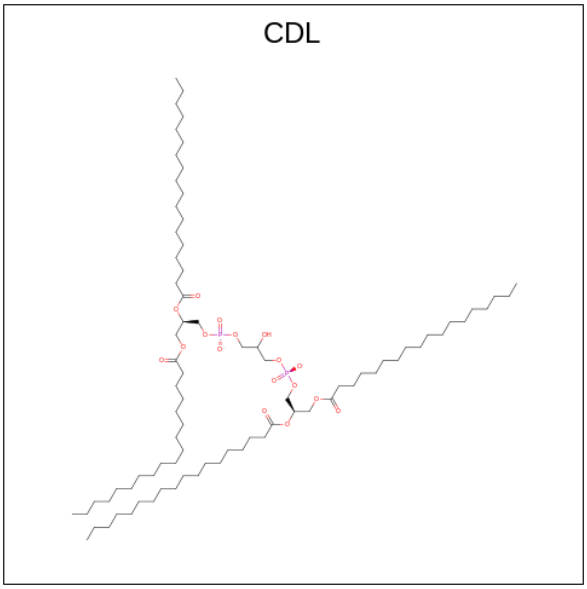
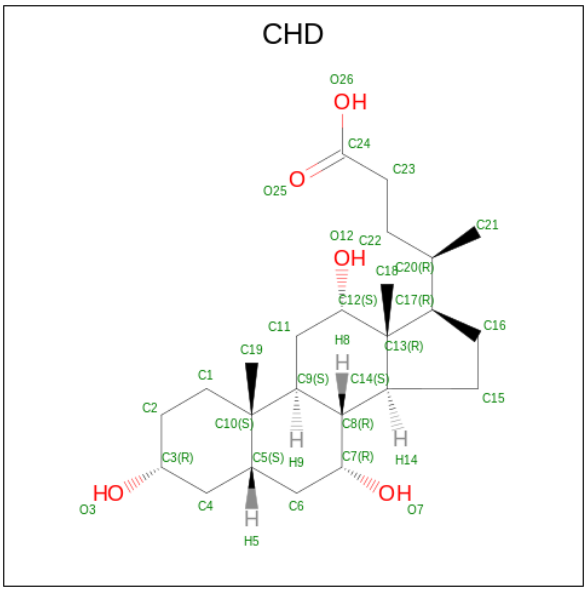
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 29 24 5	0	0
27	C	1	Total C O 29 24 5	0	0
27	G	1	Total C O 29 24 5	0	0
27	J	1	Total C O 29 24 5	0	0
27	L	1	Total C O 29 24 5	0	0
27	P	1	Total C O 29 24 5	0	0
27	P	1	Total C O 29 24 5	0	0
27	T	1	Total C O 29 24 5	0	0
27	W	1	Total C O 29 24 5	0	0
27	X	1	Total C O 29 24 5	0	0
27	Y	1	Total C O 29 24 5	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	F	1	Total Zn 1 1	0	0

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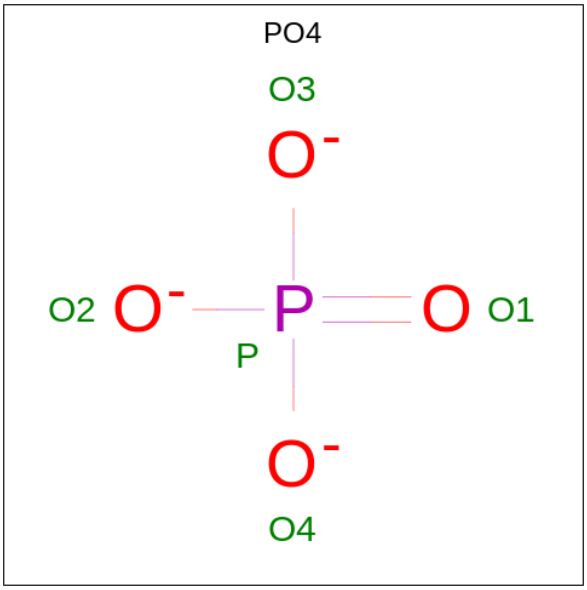
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	S	1	Total Zn 1 1	0	0

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	263	Total O 263 263	0	0
30	B	176	Total O 176 176	0	2
30	C	128	Total O 128 128	0	0
30	D	154	Total O 154 154	0	0
30	E	124	Total O 124 124	0	0
30	F	114	Total O 114 114	0	0

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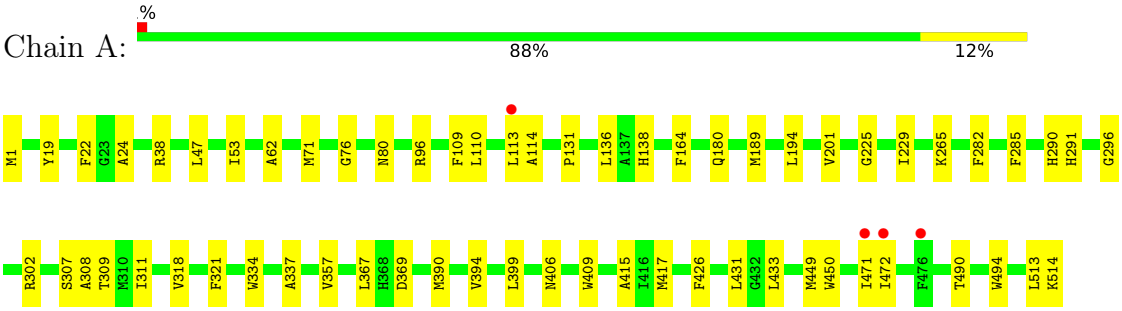
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	G	69	Total O 69 69	0	0
30	H	69	Total O 69 69	0	0
30	I	60	Total O 60 60	0	0
30	J	33	Total O 33 33	0	0
30	K	32	Total O 32 32	0	0
30	L	31	Total O 31 31	0	0
30	M	29	Total O 29 29	0	0
30	N	239	Total O 239 239	0	0
30	O	154	Total O 154 154	0	0
30	P	131	Total O 131 131	0	0
30	Q	91	Total O 91 91	0	0
30	R	93	Total O 93 93	0	0
30	S	108	Total O 108 108	0	0
30	T	61	Total O 61 61	0	0
30	U	50	Total O 50 50	0	0
30	V	41	Total O 41 41	0	0
30	W	39	Total O 39 39	0	0
30	X	31	Total O 31 31	0	0
30	Y	31	Total O 31 31	0	0
30	Z	24	Total O 24 24	0	0

3 Residue-property plots

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.

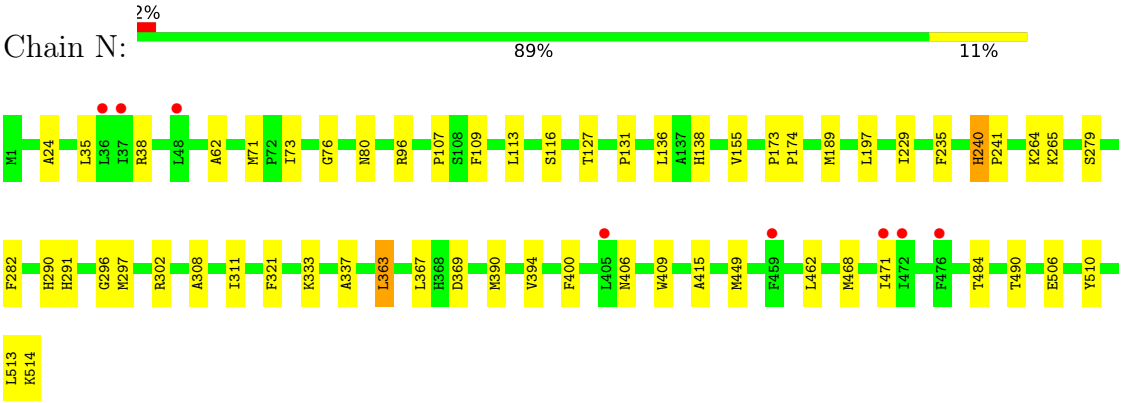
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



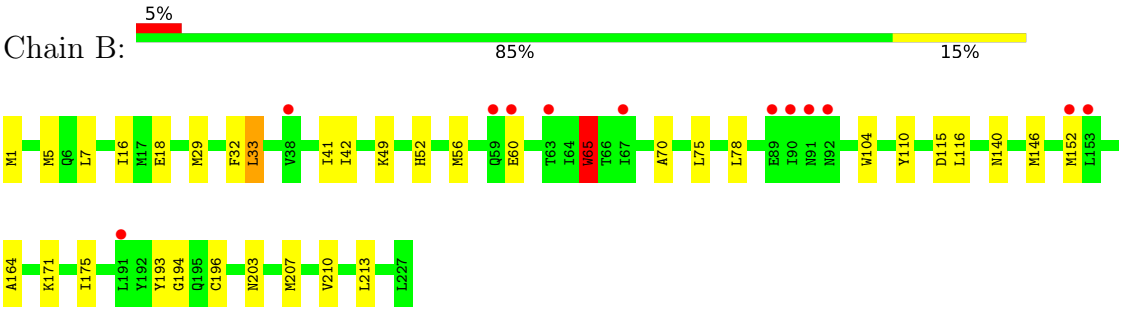
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



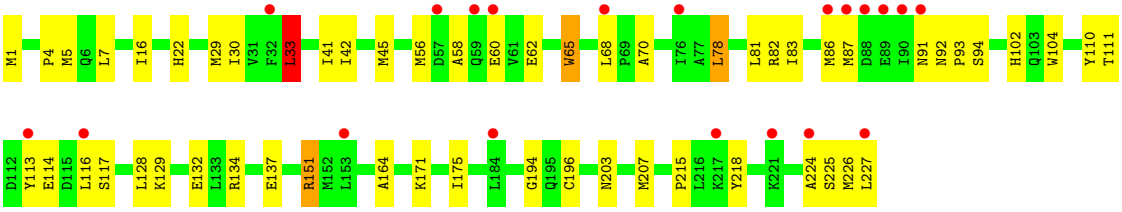
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

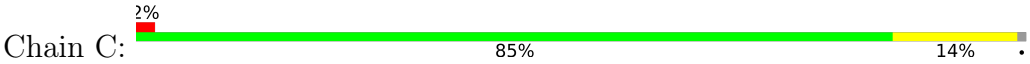


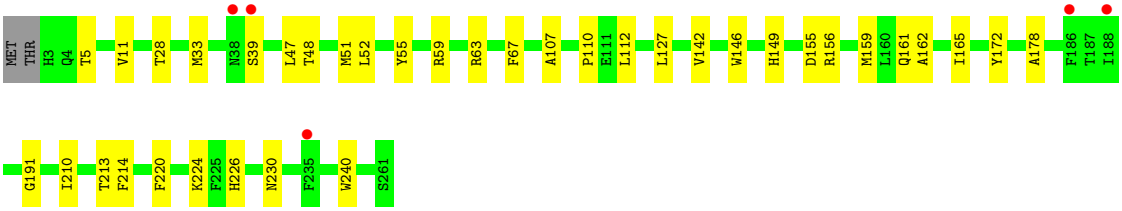
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

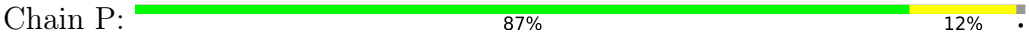


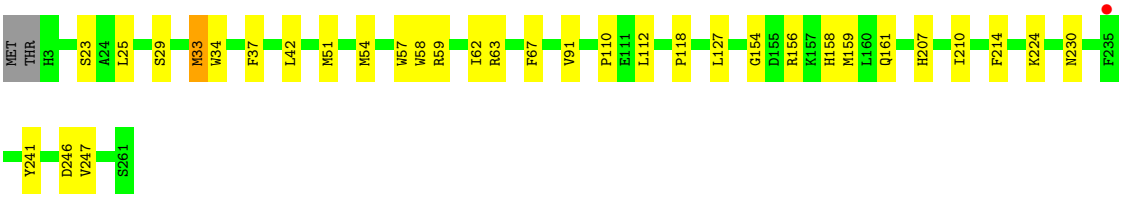
• Molecule 3: Cytochrome c oxidase subunit 3



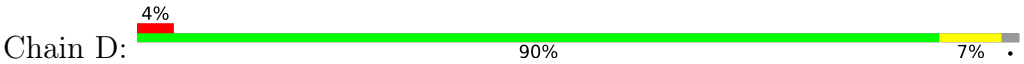


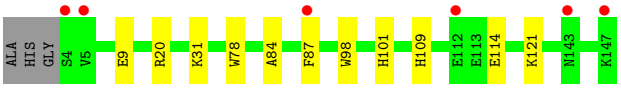
• Molecule 3: Cytochrome c oxidase subunit 3



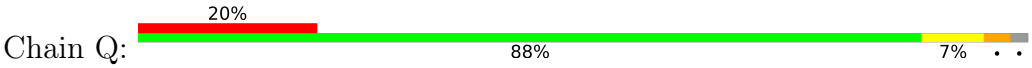


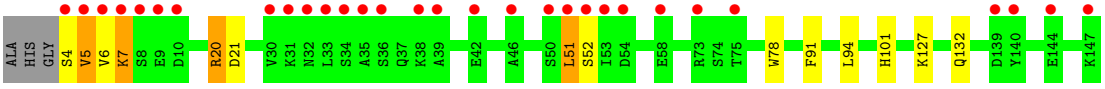
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



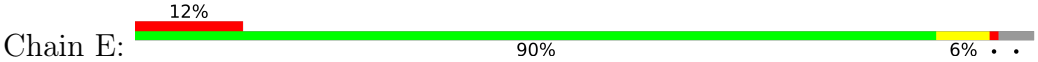


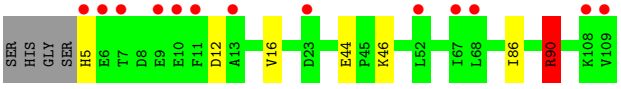
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1





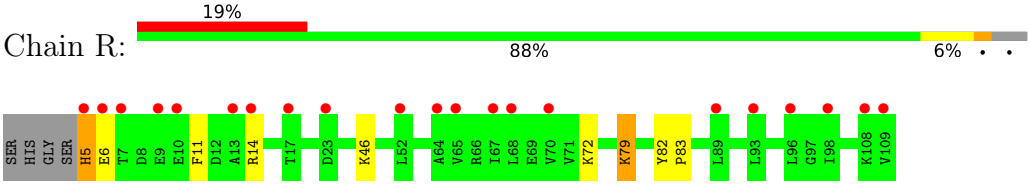
• Molecule 5: Cytochrome c oxidase subunit 5A





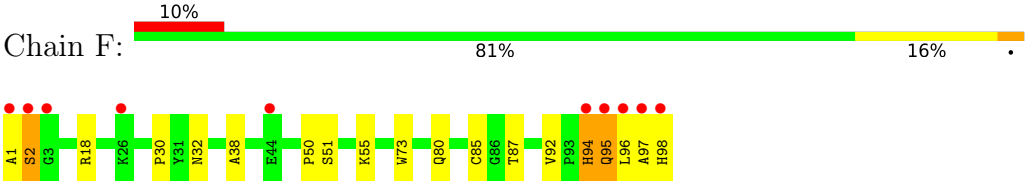
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



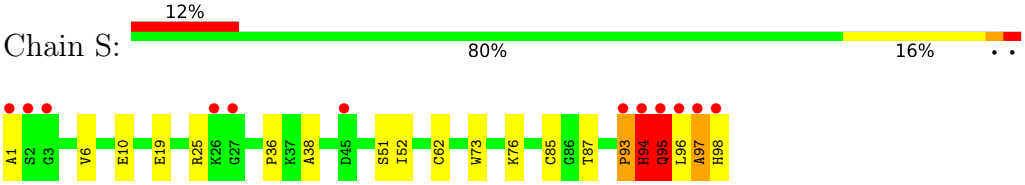
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



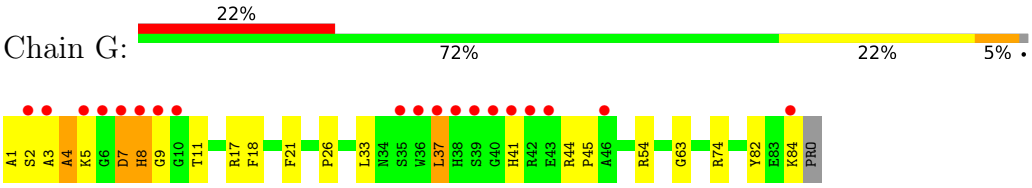
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



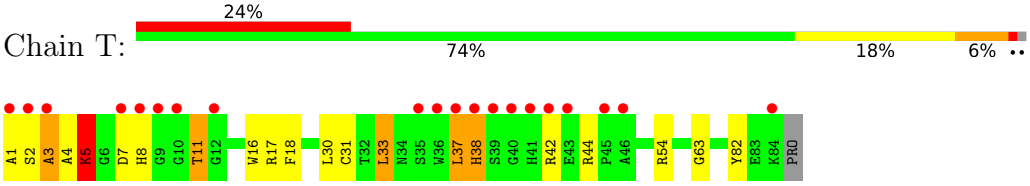
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G:



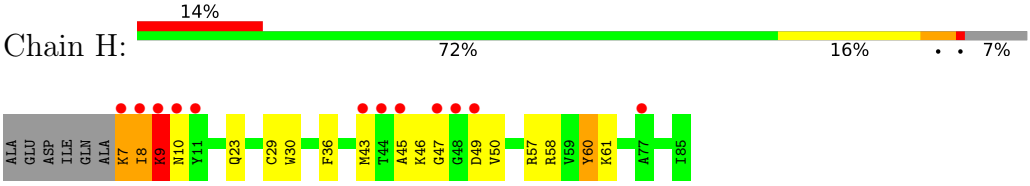
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T:



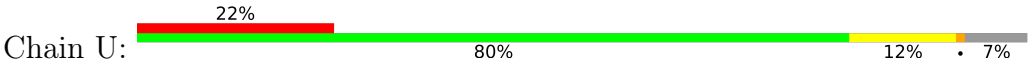
• Molecule 8: Cytochrome c oxidase subunit 6B1

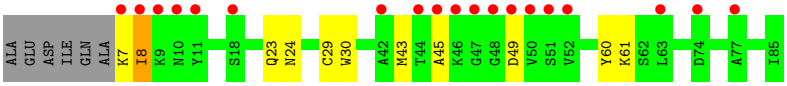
Chain H:



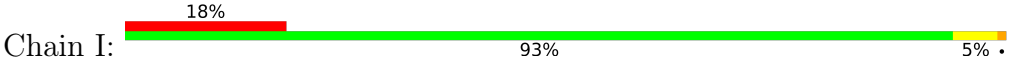
• Molecule 8: Cytochrome c oxidase subunit 6B1

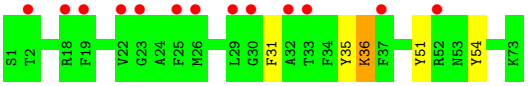
Chain U:



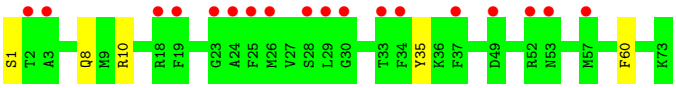


• Molecule 9: Cytochrome c oxidase subunit 6C

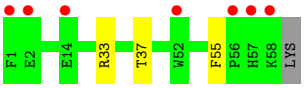




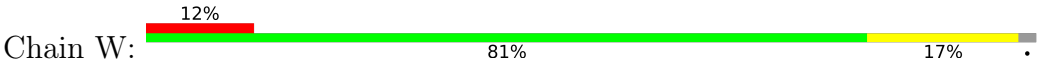
• Molecule 9: Cytochrome c oxidase subunit 6C

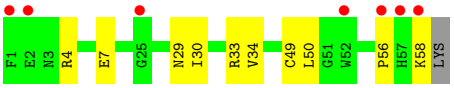


• Molecule 10: Cytochrome c oxidase subunit 7A1

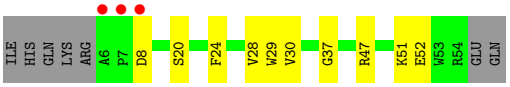


• Molecule 10: Cytochrome c oxidase subunit 7A1

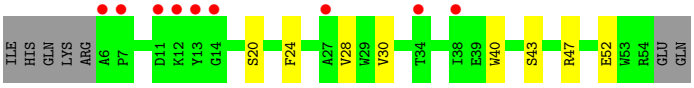




• Molecule 11: Cytochrome c oxidase subunit 7B

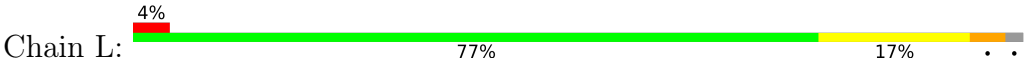


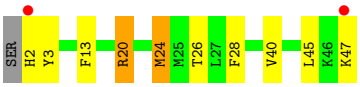
• Molecule 11: Cytochrome c oxidase subunit 7B



• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

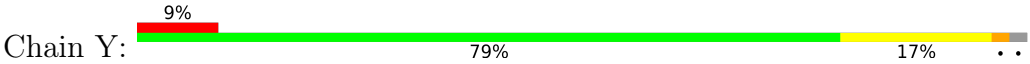
Chain L:

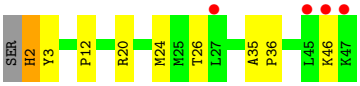




• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

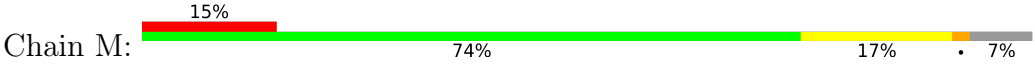
Chain Y:

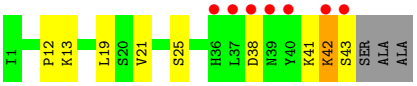




• Molecule 13: Cytochrome c oxidase subunit 8B

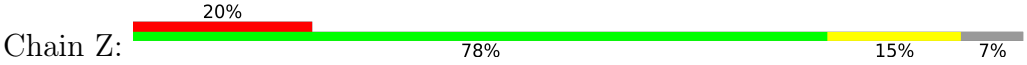
Chain M:

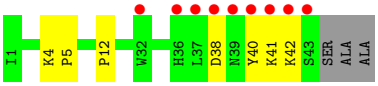




• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.31 – 1.90 27.31 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.0 (27.31-1.90) 95.3 (27.31-1.89)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.227 0.185 , 0.227	Depositor DCC
R_{free} test set	25229 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34120	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSC, CU, PGV, CHD, PER, DMU, CDL, EDO, CUA, MG, FME, NA, PEK, HEA, TGL, PO4, TPO, SAC, ZN

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	A	0.99	2/4233 (0.0%)	0.81	3/5782 (0.1%)
1	N	0.93	1/4211 (0.0%)	0.81	3/5752 (0.1%)
2	B	0.85	0/1885	0.86	3/2567 (0.1%)
2	O	0.75	0/1900	0.81	4/2587 (0.2%)
3	C	0.91	3/2221 (0.1%)	0.71	0/3035
3	P	0.86	0/2213	0.72	0/3025
4	D	0.83	0/1241	0.73	1/1674 (0.1%)
4	Q	0.60	0/1229	0.64	1/1658 (0.1%)
5	E	0.83	0/871	0.74	1/1182 (0.1%)
5	R	0.70	0/882	0.75	0/1196
6	F	0.76	0/772	0.84	1/1048 (0.1%)
6	S	0.74	0/765	0.84	1/1038 (0.1%)
7	G	0.76	0/690	0.76	0/937
7	T	0.64	0/690	0.74	0/937
8	H	0.78	0/682	0.73	1/921 (0.1%)
8	U	0.64	0/682	0.69	0/921
9	I	0.67	0/605	0.74	0/802
9	V	0.54	0/605	0.65	0/802
10	J	0.57	0/471	0.69	0/636
10	W	0.63	0/471	0.68	0/636
11	K	0.68	0/398	0.65	1/546 (0.2%)
11	X	0.51	0/398	0.58	0/546
12	L	0.81	0/401	0.80	1/536 (0.2%)
12	Y	0.71	0/393	0.61	0/526
13	M	0.74	0/345	0.70	0/470
13	Z	0.58	0/345	0.58	0/470
All	All	0.82	6/29599 (0.0%)	0.76	21/40230 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
6	F	0	1
6	S	0	2
8	H	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	VAL	CB-CG1	6.74	1.67	1.52
3	C	142	VAL	CB-CG2	6.33	1.66	1.52
3	C	11	VAL	CB-CG2	5.73	1.64	1.52
1	A	357	VAL	CB-CG1	5.29	1.64	1.52
3	C	172	TYR	CD2-CE2	5.16	1.47	1.39
1	N	264	LYS	CD-CE	5.01	1.63	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	N	71	MET	CG-SD-CE	-6.93	89.11	100.20
8	H	58	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	N	38	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	O	151	ARG	NE-CZ-NH1	6.80	123.70	120.30
6	F	18	ARG	NE-CZ-NH2	-6.64	116.98	120.30
12	L	20	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	O	65	TRP	CA-CB-CG	6.17	125.42	113.70
2	O	151	ARG	NE-CZ-NH2	-6.08	117.26	120.30
4	Q	51	LEU	CA-CB-CG	6.01	129.13	115.30
5	E	90	ARG	NE-CZ-NH1	5.87	123.23	120.30
11	K	47	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	71	MET	CG-SD-CE	-5.83	90.87	100.20
4	D	20	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	B	152[A]	MET	CG-SD-CE	5.59	109.14	100.20
2	B	152[B]	MET	CG-SD-CE	5.59	109.14	100.20
1	A	96	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	B	65	TRP	CA-CB-CG	5.36	123.88	113.70
2	O	33	LEU	CB-CG-CD2	-5.13	102.28	111.00
6	S	95	GLN	CB-CA-C	5.11	120.63	110.40
1	N	96	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	94	HIS	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide

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	A	4051	0	4040	50	0
1	N	4046	0	4040	45	0
2	B	1834	0	1840	28	0
2	O	1844	0	1852	41	0
3	C	2117	0	2034	38	0
3	P	2115	0	2033	42	0
4	D	1201	0	1188	13	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	4	0
5	R	860	0	858	6	0
6	F	750	0	731	20	0
6	S	748	0	728	21	0
7	G	675	0	643	17	0
7	T	675	0	643	21	0
8	H	662	0	623	11	0
8	U	662	0	623	9	0
9	I	601	0	613	4	0
9	V	601	0	613	4	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	383	0	389	15	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	Z	335	0	352	6	0
14	A	129	0	88	4	0
14	N	129	0	88	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	102	0	152	9	0
19	C	102	0	152	5	0
19	N	51	0	76	6	0
19	P	153	0	228	8	0
20	A	28	0	42	5	0
20	B	8	0	12	0	0
20	C	8	0	12	1	0
20	F	16	0	24	0	0
20	G	4	0	6	0	0
20	L	8	0	12	0	0
20	M	4	0	6	1	0
20	N	48	0	72	9	0
20	O	8	0	12	0	0
20	P	20	0	30	1	0
20	Q	4	0	6	1	0
20	R	4	0	6	0	0
20	S	24	0	36	5	0
20	W	8	0	12	5	0
20	Y	4	0	6	1	0
21	A	33	0	42	1	0
21	B	33	0	41	0	0
21	C	33	0	42	0	0
21	D	33	0	42	1	0
21	G	33	0	42	1	0
21	K	198	0	252	12	0
21	L	33	0	42	3	0
21	M	33	0	42	1	0
21	O	33	0	42	2	0
21	P	66	0	84	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	33	0	41	1	0
21	T	33	0	42	2	0
21	X	99	0	135	4	0
21	Z	33	0	42	0	0
22	B	63	0	110	6	0
22	D	63	0	110	10	0
22	L	63	0	108	12	0
22	O	63	0	110	1	0
22	Q	63	0	110	6	0
22	Y	63	0	110	7	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	9	0
24	N	52	0	80	12	0
25	C	159	0	231	20	0
25	G	53	0	77	4	0
25	P	106	0	154	8	0
26	C	100	0	156	23	0
26	G	100	0	156	21	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	C	58	0	78	1	0
27	G	29	0	39	0	0
27	J	29	0	39	4	0
27	L	29	0	39	1	0
27	P	58	0	78	3	0
27	T	29	0	39	0	0
27	W	29	0	38	1	0
27	X	29	0	39	5	0
27	Y	29	0	39	3	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	263	0	0	2	0
30	B	176	0	0	2	0
30	C	128	0	0	2	0
30	D	154	0	0	2	0
30	E	124	0	0	1	0
30	F	114	0	0	1	0
30	G	69	0	0	4	0
30	H	69	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	60	0	0	0	0
30	J	33	0	0	1	0
30	K	32	0	0	1	0
30	L	31	0	0	1	0
30	M	29	0	0	0	0
30	N	239	0	0	5	0
30	O	154	0	0	3	0
30	P	131	0	0	3	0
30	Q	91	0	0	4	0
30	R	93	0	0	0	0
30	S	108	0	0	2	0
30	T	61	0	0	0	0
30	U	50	0	0	0	0
30	V	41	0	0	2	0
30	W	39	0	0	1	0
30	X	31	0	0	3	0
30	Y	31	0	0	1	0
30	Z	24	0	0	0	0
All	All	34120	0	32594	510	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 8.

All (510) 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)
18:A:606:PER:O2	18:A:606:PER:O1	1.55	1.23
18:N:606:PER:O2	18:N:606:PER:O1	1.55	1.20
20:N:613:EDO:H21	6:S:36:PRO:HD3	1.38	1.03
25:C:307:PEK:H041	7:G:17:ARG:HH22	1.23	1.03
3:C:67:PHE:HE1	26:C:304:CDL:H1	1.26	0.96
26:G:101:CDL:H771	26:G:101:CDL:H582	1.54	0.88
20:W:103:EDO:H12	12:Y:46:LYS:HZ2	1.37	0.88
3:P:33:MET:HE1	3:P:42:LEU:H	1.40	0.87
4:Q:5:VAL:H	13:Z:5:PRO:HD2	1.40	0.86
3:P:210:ILE:HG12	19:P:305:PGV:H12	1.57	0.84
19:N:607:PGV:H31	19:N:607:PGV:H202	1.59	0.84
20:W:103:EDO:H12	12:Y:46:LYS:NZ	1.93	0.83
21:P:316:DMU:H10	10:W:49:CYS:HB3	1.61	0.83
26:T:102:CDL:H511	26:T:102:CDL:H202	1.60	0.83
25:P:309:PEK:H041	7:T:17:ARG:HH22	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33:MET:HB2	21:P:316:DMU:H11	1.60	0.82
2:B:70:ALA:HB1	26:T:102:CDL:H461	1.63	0.80
20:N:617:EDO:H12	30:N:777:HOH:O	1.82	0.80
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.64	0.79
3:C:67:PHE:CE1	26:C:304:CDL:H1	2.15	0.78
24:N:608:PSC:H321	24:N:608:PSC:H12	1.64	0.77
6:S:51:SER:O	6:S:94:HIS:HA	1.85	0.77
3:P:67:PHE:HE1	26:P:306:CDL:H1	1.50	0.76
6:F:94:HIS:NE2	6:F:98:HIS:HA	2.01	0.75
26:G:101:CDL:H1	26:G:101:CDL:H111	1.69	0.74
1:N:155:VAL:HG21	19:P:301:PGV:H142	1.70	0.73
7:G:37:LEU:HD21	26:G:101:CDL:H361	1.70	0.73
19:C:308:PGV:H321	7:T:1:ALA:HA	1.69	0.72
19:P:302:PGV:H11	27:P:308:CHD:H152	1.69	0.72
4:Q:7:LYS:NZ	4:Q:7:LYS:HB3	2.04	0.72
3:P:33:MET:HB2	21:P:316:DMU:C22	2.19	0.72
2:O:7:LEU:HD11	22:O:301:TGL:H152	1.73	0.71
26:G:101:CDL:H352	2:O:78:LEU:HD12	1.73	0.70
7:T:2:SER:HA	7:T:3:ALA:O	1.92	0.70
1:A:76:GLY:HA2	20:A:612:EDO:H12	1.74	0.69
1:A:110:LEU:HD12	1:A:113[B]:LEU:HD23	1.75	0.69
12:L:2:HIS:CG	12:L:3:TYR:H	2.11	0.69
3:P:63:ARG:HE	26:P:306:CDL:CA2	2.06	0.68
21:K:101:DMU:H5	21:K:105:DMU:H23	1.75	0.68
22:Q:201:TGL:HA91	22:Q:201:TGL:H231	1.76	0.67
3:C:224:LYS:CD	26:C:304:CDL:HB31	2.24	0.67
26:T:102:CDL:H732	26:T:102:CDL:H251	1.76	0.67
2:B:56:MET:HG2	24:B:303:PSC:H201	1.76	0.67
4:D:78:TRP:CA	22:D:201:TGL:HB22	2.25	0.67
25:C:307:PEK:H041	7:G:17:ARG:NH2	2.05	0.67
3:P:59:ARG:HB2	26:P:306:CDL:H521	1.76	0.67
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.76	0.66
3:C:210:ILE:HG12	19:C:303:PGV:H132	1.78	0.66
3:P:63:ARG:HE	26:P:306:CDL:HA22	1.60	0.66
1:A:19:TYR:CZ	20:A:612:EDO:H11	2.30	0.66
10:J:55:PHE:HE1	21:L:102:DMU:H29	1.61	0.66
6:F:30:PRO:HA	6:F:98:HIS:HB2	1.77	0.66
6:S:19:GLU:HG2	30:S:295:HOH:O	1.96	0.66
1:A:307:SER:HB2	26:T:102:CDL:H192	1.79	0.65
26:G:101:CDL:H511	26:G:101:CDL:H181	1.77	0.65
3:C:224:LYS:HD3	26:C:304:CDL:HB31	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:HE	26:C:304:CDL:CA2	2.09	0.64
1:A:131:PRO:HB3	20:A:611:EDO:H12	1.78	0.64
26:T:102:CDL:OA7	26:T:102:CDL:H311	1.96	0.64
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.77	0.64
24:N:608:PSC:H211	2:O:56:MET:HG2	1.79	0.64
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.62	0.64
12:L:20:ARG:NH2	22:L:101:TGL:HC32	2.13	0.64
7:T:31:CYS:SG	26:T:102:CDL:H551	2.38	0.63
1:A:47:LEU:HD12	20:M:102:EDO:H12	1.81	0.63
22:B:301:TGL:HA42	22:B:301:TGL:HA91	1.80	0.63
12:L:20:ARG:HH22	22:L:101:TGL:HC32	1.60	0.63
4:Q:78:TRP:HA	22:Q:201:TGL:HB22	1.79	0.63
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.39	0.63
3:P:33:MET:SD	21:P:316:DMU:H11	2.39	0.62
26:T:102:CDL:H561	26:T:102:CDL:H751	1.80	0.62
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.81	0.62
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.81	0.62
26:G:101:CDL:HA31	30:G:249:HOH:O	2.00	0.62
7:T:30:LEU:HD21	26:T:102:CDL:H471	1.82	0.62
20:S:105:EDO:H12	30:S:270:HOH:O	1.99	0.62
2:B:49:LYS:HE3	22:D:201:TGL:HC72	1.81	0.62
1:N:406:ASN:HD21	19:N:607:PGV:H22	1.65	0.62
3:C:5:THR:HB	6:F:98:HIS:HD2	1.65	0.62
1:N:506:GLU:OE2	20:N:618:EDO:H11	2.00	0.61
3:C:51[A]:MET:SD	26:C:304:CDL:H622	2.40	0.61
1:A:164:PHE:HE1	20:A:612:EDO:H22	1.66	0.61
3:C:127:LEU:HD13	26:G:101:CDL:OB3	2.01	0.61
3:C:52:LEU:HD23	26:C:304:CDL:H362	1.81	0.61
5:R:6:GLU:OE1	5:R:14[A]:ARG:NH2	2.29	0.60
3:P:33:MET:HG2	30:P:423:HOH:O	2.02	0.60
26:T:102:CDL:H122	26:T:102:CDL:H1	1.84	0.60
8:U:43:MET:HE3	8:U:49:ASP:H	1.65	0.60
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.84	0.60
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.32	0.59
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.83	0.59
12:Y:24:MET:SD	22:Y:101:TGL:H152	2.41	0.59
25:P:309:PEK:H6	25:P:309:PEK:H221	1.85	0.59
1:N:308:ALA:O	1:N:311[B]:ILE:HG22	2.03	0.59
20:N:613:EDO:H21	6:S:36:PRO:CD	2.24	0.59
20:N:617:EDO:H21	8:U:24:ASN:HD21	1.66	0.59
3:P:33:MET:CE	3:P:42:LEU:H	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:20:ARG:HG2	30:Q:361:HOH:O	2.02	0.58
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.42	0.58
3:P:37:PHE:O	21:P:316:DMU:O49	2.21	0.58
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.85	0.58
19:N:607:PGV:H231	13:Z:12:PRO:HG3	1.84	0.58
26:P:306:CDL:HA61	26:P:306:CDL:H131	1.86	0.58
24:N:608:PSC:H071	9:V:10:ARG:HH21	1.67	0.58
26:C:304:CDL:H862	26:C:304:CDL:H822	1.84	0.58
12:Y:12:PRO:HB2	22:Y:101:TGL:HG11	1.86	0.58
24:N:608:PSC:H241	24:N:608:PSC:H42	1.85	0.58
4:Q:78:TRP:CA	22:Q:201:TGL:HB22	2.33	0.58
11:K:29:TRP:CD2	21:K:106:DMU:H23	2.38	0.57
3:C:63:ARG:HE	26:C:304:CDL:HA22	1.67	0.57
2:B:49:LYS:HE3	22:D:201:TGL:CC7	2.34	0.57
24:N:608:PSC:H342	2:O:41:ILE:HD13	1.87	0.57
26:G:101:CDL:H712	26:G:101:CDL:H541	1.87	0.57
3:P:57:TRP:CZ2	19:P:301:PGV:H21	2.39	0.57
4:D:101:HIS:ND1	21:K:101:DMU:H30	2.19	0.57
12:L:26:THR:HG23	13:M:25:SER:CB	2.34	0.57
25:C:307:PEK:H222	7:G:21:PHE:CD2	2.40	0.57
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.86	0.57
3:P:34:TRP:HE1	21:T:103:DMU:H29	1.69	0.57
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.40	0.57
25:C:309:PEK:H371	7:T:5:LYS:HG3	1.87	0.56
24:B:303:PSC:H42	24:B:303:PSC:H241	1.86	0.56
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.87	0.56
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.87	0.56
7:G:7:ASP:O	7:G:9:GLY:N	2.38	0.56
8:U:43:MET:HE3	8:U:49:ASP:N	2.21	0.56
22:L:101:TGL:OC1	22:L:101:TGL:HC41	2.04	0.56
26:G:101:CDL:H462	2:O:70:ALA:HB1	1.87	0.56
3:P:67:PHE:CE1	26:P:306:CDL:H1	2.37	0.56
7:G:2:SER:HB2	1:N:197:LEU:HD11	1.89	0.55
3:P:127:LEU:HD13	26:T:102:CDL:OB3	2.06	0.55
3:P:246:ASP:HB2	30:P:488:HOH:O	2.06	0.55
2:B:41:ILE:HG21	24:B:303:PSC:H331	1.89	0.55
4:Q:4:SER:HA	13:Z:5:PRO:CD	2.37	0.55
2:O:128:LEU:HD22	2:O:132:GLU:HB2	1.88	0.55
1:A:415:ALA:HB1	22:D:201:TGL:H132	1.89	0.54
1:A:311[B]:ILE:HD11	25:P:309:PEK:H342	1.88	0.54
8:H:43:MET:HE3	8:H:49:ASP:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:ND1	6:S:95:GLN:O	2.31	0.54
3:P:33:MET:HB2	21:P:316:DMU:C25	2.37	0.54
1:A:19:TYR:OH	20:A:612:EDO:H11	2.07	0.54
6:S:94:HIS:HD1	6:S:95:GLN:C	2.10	0.53
1:N:297[B]:MET:HG2	30:N:741:HOH:O	2.07	0.53
2:B:7:LEU:HD12	22:B:301:TGL:HC52	1.90	0.53
4:D:78:TRP:HB3	22:D:201:TGL:HB22	1.90	0.53
25:G:102:PEK:H12	3:P:91:VAL:HG22	1.91	0.52
19:P:301:PGV:H262	19:P:305:PGV:H292	1.92	0.52
7:T:2:SER:O	7:T:2:SER:OG	2.28	0.52
7:T:63:GLY:HA2	21:T:103:DMU:H35	1.91	0.52
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.10	0.52
4:Q:127:LYS:HD2	30:V:130:HOH:O	2.08	0.52
3:C:63:ARG:HE	26:C:304:CDL:HA21	1.73	0.52
19:C:308:PGV:H312	7:T:1:ALA:O	2.10	0.52
21:A:616:DMU:H5	21:K:103:DMU:H17	1.92	0.52
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.90	0.52
25:C:307:PEK:H383	26:G:101:CDL:C27	2.40	0.52
10:J:33:ARG:HG2	27:J:101:CHD:H152	1.91	0.52
11:X:47:ARG:HD3	30:X:226:HOH:O	2.10	0.52
2:B:140:ASN:HB3	30:B:487:HOH:O	2.09	0.51
12:L:20:ARG:NH2	12:L:24[B]:MET:HE2	2.25	0.51
4:Q:5:VAL:HA	13:Z:4:LYS:HD3	1.92	0.51
6:S:52:ILE:O	6:S:94:HIS:NE2	2.43	0.51
27:L:103:CHD:H232	13:M:21:VAL:HG21	1.92	0.51
1:N:321:PHE:CD2	24:N:608:PSC:H341	2.45	0.51
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.93	0.51
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.91	0.51
3:C:149:HIS:HD2	30:C:404:HOH:O	1.93	0.51
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.36	0.51
25:G:102:PEK:H132	3:P:247:VAL:HG12	1.93	0.51
6:S:95:GLN:HB2	6:S:96:LEU:HA	1.93	0.51
20:S:107:EDO:C2	20:W:102:EDO:H11	2.40	0.51
3:C:178:ALA:HB2	25:C:302:PEK:H201	1.93	0.51
3:C:155:ASP:OD2	6:F:2:SER:HA	2.11	0.50
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.46	0.50
4:D:78:TRP:CB	22:D:201:TGL:HB22	2.41	0.50
8:H:43:MET:HE3	8:H:49:ASP:N	2.26	0.50
1:N:449:MET:SD	2:O:5:MET:HG2	2.51	0.50
3:P:63:ARG:HE	26:P:306:CDL:HA21	1.76	0.50
1:N:131:PRO:HB3	20:N:616:EDO:H21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:HA	22:D:201:TGL:HB22	1.90	0.50
12:L:26:THR:HG23	13:M:25:SER:HB2	1.92	0.50
3:C:165:ILE:HD11	25:C:307:PEK:H6	1.94	0.50
7:G:5:LYS:HG3	25:G:102:PEK:H383	1.94	0.50
1:A:311[A]:ILE:HD13	26:T:102:CDL:H221	1.93	0.50
12:L:24[A]:MET:SD	22:L:101:TGL:H152	2.51	0.50
12:L:28:PHE:HA	22:L:101:TGL:H192	1.94	0.50
19:A:608:PGV:H142	4:D:87[A]:PHE:CE2	2.47	0.50
2:O:30:ILE:HG12	21:O:305:DMU:H13	1.94	0.50
1:A:390:MET:O	1:A:394[A]:VAL:HG22	2.12	0.49
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.12	0.49
26:G:101:CDL:H542	26:G:101:CDL:C24	2.42	0.49
1:N:113:LEU:HD12	22:Y:101:TGL:H141	1.93	0.49
6:S:52:ILE:O	6:S:94:HIS:CD2	2.65	0.49
3:C:240:TRP:CD2	25:C:309:PEK:H31	2.46	0.49
26:G:101:CDL:H381	2:O:81:LEU:HD12	1.95	0.49
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.99	0.49
2:B:18[B]:GLU:HG2	30:B:537:HOH:O	2.12	0.49
25:C:307:PEK:H342	1:N:311[B]:ILE:HD11	1.95	0.49
19:A:608:PGV:H11	4:D:84:ALA:HB2	1.94	0.49
6:F:30:PRO:HA	6:F:98:HIS:CB	2.43	0.49
1:N:321:PHE:CZ	24:N:608:PSC:H162	2.47	0.49
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.48	0.49
21:X:102:DMU:O5	30:X:201:HOH:O	2.19	0.49
1:A:194:LEU:CD1	7:T:4:ALA:HB1	2.42	0.49
1:A:321:PHE:CZ	24:B:303:PSC:H162	2.47	0.49
8:H:9:LYS:O	8:H:10:ASN:HB2	2.13	0.49
8:U:7:LYS:O	8:U:8:ILE:HG22	2.12	0.49
3:C:213:THR:HG21	26:C:304:CDL:H642	1.95	0.49
2:O:227:LEU:HD21	30:O:538:HOH:O	2.13	0.49
6:S:85:CYS:SG	6:S:87:THR:HG23	2.52	0.49
10:J:37:THR:OG1	27:J:101:CHD:H5	2.13	0.49
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.49
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.93	0.49
4:Q:21:ASP:HB2	30:Q:353:HOH:O	2.11	0.49
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.48	0.48
7:G:5:LYS:HB2	25:G:102:PEK:H362	1.95	0.48
4:Q:7:LYS:HB3	4:Q:7:LYS:HZ3	1.76	0.48
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.95	0.48
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.46	0.48
19:C:303:PGV:H12	26:C:304:CDL:H621	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:608:PGV:H142	4:D:87[A]:PHE:CD2	2.49	0.48
24:N:608:PSC:C34	2:O:41:ILE:HD13	2.42	0.48
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.43	0.48
10:W:56:PRO:HD3	12:Y:46:LYS:HD2	1.95	0.48
21:K:105:DMU:H8	21:K:105:DMU:H15	1.68	0.48
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.96	0.48
6:F:30:PRO:O	6:F:98:HIS:HB2	2.14	0.48
26:G:101:CDL:H552	26:G:101:CDL:H581	1.54	0.48
8:U:8:ILE:HG23	8:U:8:ILE:O	2.14	0.48
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.94	0.48
22:B:301:TGL:HA92	22:B:301:TGL:H222	1.64	0.48
6:F:94:HIS:CD2	6:F:95:GLN:H	2.32	0.48
24:N:608:PSC:H22	24:N:608:PSC:H222	1.96	0.48
11:X:30:VAL:HG11	21:X:103:DMU:H2	1.95	0.48
22:Y:101:TGL:H172	30:Y:224:HOH:O	2.14	0.48
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.49	0.48
1:N:510:TYR:HA	20:N:613:EDO:C1	2.44	0.48
3:C:161:GLN:NE2	25:C:307:PEK:H22	2.29	0.47
2:O:4:PRO:HB2	11:X:43:SER:HA	1.95	0.47
2:O:102:HIS:O	2:O:104:TRP:HA	2.14	0.47
2:O:129:LYS:O	2:O:132:GLU:HG3	2.14	0.47
3:C:191:GLY:HA3	30:G:207:HOH:O	2.14	0.47
6:F:32:ASN:HD21	6:F:98:HIS:CD2	2.33	0.47
6:S:97:ALA:O	6:S:98:HIS:HB2	2.15	0.47
4:Q:52:SER:HB2	30:Q:354:HOH:O	2.13	0.47
2:B:52:HIS:CE1	24:B:303:PSC:H211	2.50	0.47
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.15	0.47
3:C:48:THR:HG23	26:C:304:CDL:H412	1.97	0.47
3:C:226:HIS:CE1	26:C:304:CDL:HB32	2.50	0.47
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.67	0.47
26:T:102:CDL:H782	26:T:102:CDL:C56	2.43	0.47
12:Y:2:HIS:HD1	12:Y:3:TYR:H	1.62	0.47
5:E:90:ARG:HD2	30:E:261:HOH:O	2.15	0.47
4:Q:101:HIS:ND1	21:Q:203:DMU:H29	2.30	0.47
1:A:449:MET:SD	2:B:5:MET:HG2	2.55	0.47
6:F:95:GLN:HG2	6:F:96:LEU:HG	1.96	0.47
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.14	0.47
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.96	0.47
26:T:102:CDL:H182	26:T:102:CDL:H151	1.76	0.47
6:F:92:VAL:HG23	6:F:92:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:202:EDO:H12	6:S:73:TRP:HD1	1.80	0.47
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.49	0.46
25:C:309:PEK:C37	7:T:5:LYS:HG3	2.45	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.15	0.46
13:M:42:LYS:HB3	13:M:42:LYS:HE2	1.73	0.46
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.51	0.46
19:N:607:PGV:H41	19:N:607:PGV:H221	1.97	0.46
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.49	0.46
12:L:2:HIS:CG	12:L:3:TYR:N	2.81	0.46
1:A:22:PHE:HA	22:L:101:TGL:HB72	1.97	0.46
26:C:304:CDL:H251	26:C:304:CDL:H221	1.67	0.46
25:P:304:PEK:H41	25:P:304:PEK:H71	1.46	0.46
26:P:306:CDL:H332	26:P:306:CDL:H171	1.97	0.46
11:X:20:SER:HA	27:X:105:CHD:H152	1.96	0.46
7:T:37:LEU:HD23	26:T:102:CDL:H361	1.96	0.46
2:O:33:LEU:HB3	21:O:305:DMU:H20	1.98	0.46
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.46
26:C:304:CDL:HA61	26:C:304:CDL:H312	1.72	0.46
3:P:224:LYS:CD	26:P:306:CDL:HB32	2.46	0.46
10:W:29:ASN:O	10:W:33:ARG:HG3	2.15	0.46
12:L:20:ARG:HH22	22:L:101:TGL:HC52	1.80	0.46
24:N:608:PSC:H063	24:N:608:PSC:H042	1.59	0.46
25:P:304:PEK:H132	25:P:304:PEK:H161	1.69	0.46
3:P:62:ILE:HD12	26:P:306:CDL:H511	1.98	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.45
7:G:84:LYS:N	7:G:84:LYS:HD2	2.31	0.45
1:N:116:SER:HB2	20:Y:103:EDO:H22	1.97	0.45
1:A:318:VAL:HG22	2:B:65:TRP:CD1	2.51	0.45
26:G:101:CDL:H351	2:O:81:LEU:HD12	1.99	0.45
30:O:441:HOH:O	8:U:61:LYS:HE3	2.15	0.45
25:P:304:PEK:C20	25:P:304:PEK:H15	2.46	0.45
20:P:315:EDO:O1	6:S:1:ALA:HB1	2.16	0.45
11:X:20:SER:OG	27:X:105:CHD:H182	2.17	0.45
1:A:472:ILE:HG21	22:L:101:TGL:HA82	1.98	0.45
3:C:127:LEU:HD22	26:G:101:CDL:HB62	1.99	0.45
4:D:98:TRP:CE2	21:M:101:DMU:H11	2.50	0.45
2:O:218:TYR:HB3	30:V:109:HOH:O	2.15	0.45
27:Y:102:CHD:H212	27:Y:102:CHD:H12	1.98	0.45
27:J:101:CHD:H222	27:J:101:CHD:H12	1.97	0.45
7:G:8:HIS:HB2	30:G:233:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:8:ASP:HB2	30:K:207:HOH:O	2.17	0.45
1:N:510:TYR:HA	20:N:613:EDO:H12	1.98	0.45
2:O:116:LEU:HD12	2:O:117:SER:N	2.31	0.45
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.98	0.45
2:B:56:MET:HG2	24:B:303:PSC:C20	2.45	0.45
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.45	0.45
7:G:45:PRO:HD2	30:G:206:HOH:O	2.17	0.45
1:A:113[B]:LEU:HG	1:A:114:ALA:N	2.32	0.45
6:F:51:SER:HA	6:F:98:HIS:HE1	1.82	0.45
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.00	0.45
21:P:316:DMU:O6	21:P:316:DMU:O2	2.28	0.45
5:R:5:HIS:HB3	5:R:6:GLU:H	1.54	0.45
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.52	0.45
25:C:302:PEK:H203	25:C:302:PEK:H171	1.46	0.45
19:N:607:PGV:H21	19:N:607:PGV:H52	1.61	0.45
3:P:37:PHE:CD2	21:P:316:DMU:H13	2.52	0.45
26:C:304:CDL:H182	26:C:304:CDL:H352	1.99	0.44
26:G:101:CDL:HA62	26:G:101:CDL:H311	1.74	0.44
9:I:36:LYS:HB2	9:I:36:LYS:HE3	1.53	0.44
11:K:24:PHE:CE1	11:K:28:VAL:HG21	2.52	0.44
3:C:156:ARG:HE	27:C:305:CHD:C24	2.31	0.44
25:C:302:PEK:H132	25:C:302:PEK:H161	1.50	0.44
7:G:1:ALA:HB2	19:P:302:PGV:H321	1.99	0.44
22:L:101:TGL:H261	22:L:101:TGL:H232	1.68	0.44
24:N:608:PSC:C07	9:V:10:ARG:HH21	2.29	0.44
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.99	0.44
2:B:7:LEU:HD11	22:B:301:TGL:H152	1.99	0.44
11:K:20:SER:OG	21:K:104:DMU:H6	2.17	0.44
26:C:304:CDL:H522	26:C:304:CDL:OB9	2.17	0.44
7:G:63:GLY:HA2	21:G:104:DMU:H33	1.98	0.44
3:C:5:THR:HB	6:F:98:HIS:CD2	2.49	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
3:P:67:PHE:HE1	26:P:306:CDL:C1	2.27	0.44
1:A:136[B]:LEU:HD11	30:A:948:HOH:O	2.17	0.44
8:H:50:VAL:HG23	30:H:253:HOH:O	2.16	0.44
1:N:76:GLY:O	1:N:80:ASN:HB2	2.17	0.44
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.17	0.44
3:C:55:TYR:CE1	26:C:304:CDL:H161	2.53	0.44
8:H:60:TYR:CD1	8:H:60:TYR:C	2.90	0.44
1:N:400:PHE:O	22:Y:101:TGL:H281	2.18	0.44
25:P:309:PEK:H011	25:P:309:PEK:H42	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:107:EDO:H12	30:W:216:HOH:O	2.16	0.44
8:U:43:MET:CE	8:U:49:ASP:H	2.31	0.44
2:B:32:PHE:CE2	22:B:301:TGL:HA52	2.53	0.44
3:C:220:PHE:HB2	26:C:304:CDL:H712	2.00	0.44
26:T:102:CDL:H561	26:T:102:CDL:H782	2.00	0.44
27:Y:102:CHD:H232	27:Y:102:CHD:H211	1.62	0.44
2:B:41:ILE:HD13	24:B:303:PSC:H341	2.00	0.44
3:C:59:ARG:HG3	26:C:304:CDL:H512	2.00	0.44
5:R:79:LYS:HD2	5:R:79:LYS:N	2.33	0.44
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.00	0.44
2:B:42:ILE:HG21	22:D:201:TGL:H232	1.99	0.43
3:C:107:ALA:HB2	19:C:308:PGV:H031	2.00	0.43
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.86	0.43
6:S:94:HIS:HB3	6:S:95:GLN:H	1.64	0.43
2:B:56:MET:HA	24:B:303:PSC:H201	1.99	0.43
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.53	0.43
21:D:202:DMU:H4	21:D:202:DMU:H36	1.62	0.43
11:X:40:TRP:HD1	21:X:102:DMU:H5	1.84	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.43
4:D:109:HIS:HD2	30:D:371:HOH:O	2.01	0.43
26:P:306:CDL:H401	26:P:306:CDL:H432	1.77	0.43
27:W:101:CHD:H232	27:W:101:CHD:H211	1.69	0.43
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.43
21:K:101:DMU:H13	21:K:105:DMU:H21	2.00	0.43
1:N:468:MET:HG3	30:N:928:HOH:O	2.17	0.43
3:P:51[B]:MET:CE	26:P:306:CDL:H381	2.49	0.43
26:P:306:CDL:H561	26:P:306:CDL:H531	1.69	0.43
26:C:304:CDL:H871	30:C:527:HOH:O	2.18	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.43
12:Y:20:ARG:NH2	22:Y:101:TGL:HC51	2.33	0.43
19:A:608:PGV:O06	30:A:701:HOH:O	2.14	0.43
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.54	0.43
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.43
25:C:307:PEK:H292	30:O:547:HOH:O	2.17	0.43
6:F:96:LEU:HD12	6:F:96:LEU:O	2.19	0.43
2:O:111:THR:HA	2:O:114:GLU:O	2.18	0.43
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.54	0.43
26:C:304:CDL:H561	26:C:304:CDL:H532	1.81	0.43
2:O:29:MET:HB2	9:V:35:TYR:CE2	2.54	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.84	0.43
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.18	0.43
5:E:16:VAL:HG21	5:E:46:LYS:HG3	2.00	0.43
13:M:41:LYS:C	13:M:43:SER:H	2.23	0.43
3:P:161:GLN:HE22	25:P:309:PEK:H41	1.84	0.43
4:Q:5:VAL:N	13:Z:5:PRO:HD2	2.20	0.43
20:S:107:EDO:H22	20:W:102:EDO:H11	2.01	0.43
12:Y:20:ARG:HH22	22:Y:101:TGL:HC51	1.83	0.43
19:A:608:PGV:H11	4:D:84:ALA:CB	2.49	0.43
27:Y:102:CHD:H112	27:Y:102:CHD:H12A	1.63	0.43
19:A:608:PGV:C31	13:M:19:LEU:HD23	2.49	0.42
5:E:86:ILE:O	5:E:90:ARG:HG2	2.19	0.42
11:K:30:VAL:HG11	21:K:102:DMU:H2	2.01	0.42
12:L:13:PHE:HA	22:L:101:TGL:HC31	2.01	0.42
11:X:20:SER:OG	27:X:105:CHD:H191	2.19	0.42
1:A:309:THR:HG22	14:A:602:HEA:HMB2	2.01	0.42
3:C:33[A]:MET:HG2	3:C:39:SER:HB3	2.01	0.42
20:N:612:EDO:H11	30:N:711:HOH:O	2.18	0.42
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.99	0.42
3:P:158:HIS:HE1	6:S:1:ALA:O	2.01	0.42
19:N:607:PGV:H301	19:N:607:PGV:H152	2.01	0.42
19:A:608:PGV:H251	13:M:12:PRO:HG3	2.01	0.42
25:C:307:PEK:H372	1:N:279:SER:OG	2.20	0.42
1:N:136[B]:LEU:HD21	30:N:927:HOH:O	2.19	0.42
3:P:54:MET:HE3	26:P:306:CDL:H612	2.00	0.42
3:C:47:LEU:O	3:C:51[B]:MET:HG3	2.19	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.42
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.42
3:P:156:ARG:HE	27:P:307:CHD:C23	2.32	0.42
3:P:210:ILE:HG21	19:P:305:PGV:H282	2.01	0.42
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.01	0.42
2:O:116:LEU:HD12	2:O:117:SER:H	1.84	0.42
7:T:33:LEU:HD22	7:T:37:LEU:HD22	2.02	0.42
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.91	0.42
21:X:101:DMU:H3	21:X:101:DMU:H35	2.00	0.42
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.02	0.42
3:P:58:TRP:CG	19:P:305:PGV:H41	2.55	0.42
2:B:49:LYS:HE2	30:D:417:HOH:O	2.19	0.42
26:P:306:CDL:H121	30:P:517:HOH:O	2.20	0.42
7:T:38:HIS:CE1	26:T:102:CDL:H121	2.55	0.42
1:A:406:ASN:HD21	19:A:608:PGV:H31	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:311:EDO:O2	6:F:1:ALA:HA	2.20	0.42
12:L:20:ARG:HH22	22:L:101:TGL:CC3	2.28	0.42
12:L:45:LEU:HD13	21:L:102:DMU:H32	2.02	0.42
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.01	0.42
2:O:42:ILE:HG21	22:Q:201:TGL:H232	2.02	0.42
3:P:59:ARG:HA	26:P:306:CDL:H512	2.01	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
2:B:52:HIS:HE1	24:B:303:PSC:H211	1.85	0.41
8:H:7:LYS:O	8:H:8:ILE:HB	2.20	0.41
2:O:224:ALA:O	2:O:227:LEU:HG	2.20	0.41
3:P:37:PHE:HB3	21:P:316:DMU:O49	2.20	0.41
19:A:607:PGV:H182	3:C:28:THR:HG22	2.02	0.41
3:P:29:SER:HB2	21:P:316:DMU:H23	2.02	0.41
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.54	0.41
26:G:101:CDL:H511	26:G:101:CDL:H202	2.01	0.41
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.01	0.41
24:N:608:PSC:H073	5:R:11:PHE:CG	2.55	0.41
1:A:282:PHE:HA	7:T:4:ALA:HB3	2.03	0.41
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.01	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.50	0.41
25:C:309:PEK:H372	26:T:102:CDL:H861	2.02	0.41
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.55	0.41
26:G:101:CDL:H771	26:G:101:CDL:C58	2.38	0.41
1:N:363:LEU:HD13	1:N:367:LEU:HD11	2.02	0.41
22:Q:201:TGL:HA32	22:Q:201:TGL:HB51	2.02	0.41
1:A:426:PHE:HZ	22:B:301:TGL:HA31	1.85	0.41
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.03	0.41
1:N:415:ALA:HB1	22:Q:201:TGL:H132	2.02	0.41
2:O:82:ARG:O	2:O:86:MET:HG3	2.21	0.41
26:T:102:CDL:OA7	26:T:102:CDL:H342	2.20	0.41
14:A:601[B]:HEA:H271	14:A:601[B]:HEA:H212	1.69	0.41
10:J:37:THR:OG1	27:J:101:CHD:H191	2.20	0.41
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.56	0.41
1:A:513:LEU:O	1:A:514:LYS:HB2	2.20	0.41
6:F:50:PRO:HG2	30:F:250:HOH:O	2.20	0.41
26:G:101:CDL:H381	2:O:81:LEU:CD1	2.51	0.41
1:N:73:ILE:HD11	14:N:601[B]:HEA:H22	2.02	0.41
14:N:602:HEA:HMC1	14:N:602:HEA:CBC	2.45	0.41
4:Q:132:GLN:HG2	30:Q:350:HOH:O	2.21	0.41
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.41
1:A:302:ARG:HH11	1:A:302:ARG:HD2	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:GLN:HE21	25:C:307:PEK:C5	2.33	0.41
3:C:161:GLN:HE21	25:C:307:PEK:H5	1.86	0.41
6:F:94:HIS:CE1	6:F:98:HIS:HA	2.55	0.41
10:J:55:PHE:HB2	30:J:224:HOH:O	2.21	0.41
21:K:105:DMU:H26	21:K:105:DMU:H19	1.80	0.41
21:K:105:DMU:H4	21:K:105:DMU:H35	2.03	0.41
1:N:173:PRO:HA	1:N:174:PRO:HD3	1.97	0.41
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.97	0.41
3:P:51[B]:MET:HE2	26:P:306:CDL:H381	2.02	0.41
6:S:76:LYS:HE3	6:S:93:PRO:HG2	2.03	0.41
13:Z:40:TYR:O	13:Z:42:LYS:N	2.54	0.41
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.21	0.41
6:F:94:HIS:CD2	6:F:95:GLN:N	2.89	0.41
25:C:307:PEK:H282	7:G:26:PRO:HA	2.03	0.40
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.20	0.40
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.20	0.40
1:A:194:LEU:HD12	7:T:4:ALA:HB1	2.01	0.40
1:A:282:PHE:HZ	26:T:102:CDL:H761	1.85	0.40
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.74	0.40
26:G:101:CDL:H762	26:G:101:CDL:H242	2.03	0.40
8:H:43:MET:CE	8:H:49:ASP:H	2.32	0.40
12:L:20:ARG:HH22	22:L:101:TGL:CC5	2.34	0.40
10:W:58:LYS:HD3	10:W:58:LYS:HA	1.88	0.40
11:X:52:GLU:HG2	30:X:212:HOH:O	2.19	0.40
1:A:334:TRP:CZ3	22:D:201:TGL:HA52	2.57	0.40
25:C:307:PEK:C34	1:N:311[B]:ILE:HD11	2.52	0.40
21:L:102:DMU:H6	30:L:203:HOH:O	2.20	0.40
20:S:107:EDO:O2	20:W:102:EDO:H11	2.21	0.40
27:X:105:CHD:H183	27:X:105:CHD:H20	1.72	0.40
1:A:334:TRP:CD1	22:D:201:TGL:HC41	2.57	0.40
11:K:37:GLY:HA2	21:K:103:DMU:H35	2.03	0.40
21:K:103:DMU:H36	21:K:103:DMU:H40	1.93	0.40
1:N:240:HIS:O	1:N:241:PRO:C	2.58	0.40
27:P:307:CHD:H191	27:P:307:CHD:H8	1.88	0.40
27:X:105:CHD:H162	27:X:105:CHD:H222	1.50	0.40
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.40
26:G:101:CDL:H181	26:G:101:CDL:C51	2.48	0.40
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	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	A	522/514 (102%)	508 (97%)	14 (3%)	0	100	100
1	N	519/514 (101%)	505 (97%)	14 (3%)	0	100	100
2	B	228/227 (100%)	220 (96%)	8 (4%)	0	100	100
2	O	229/227 (101%)	219 (96%)	9 (4%)	1 (0%)	34	24
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	22	12
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	97/98 (99%)	93 (96%)	2 (2%)	2 (2%)	7	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	71 (88%)	5 (6%)	5 (6%)	1	0
7	T	81/85 (95%)	70 (86%)	7 (9%)	4 (5%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	5	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6 1
All	All	3537/3614 (98%)	3411 (96%)	103 (3%)	23 (1%)	22 12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
6	S	94	HIS
7	T	5	LYS
8	U	8	ILE
6	F	97	ALA
7	G	37	LEU
4	Q	5	VAL
6	S	95	GLN
7	T	3	ALA
7	T	7	ASP
7	T	8	HIS
7	G	7	ASP
6	S	97	ALA
8	U	45	ALA
8	H	9	LYS
8	H	46	LYS
2	O	92	ASN
6	F	2	SER
7	G	3	ALA
13	M	42	LYS
13	Z	41	LYS

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	A	436/426 (102%)	430 (99%)	6 (1%)	67 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	433/426 (102%)	426 (98%)	7 (2%)	62 60
2	B	213/210 (101%)	203 (95%)	10 (5%)	26 16
2	O	214/210 (102%)	203 (95%)	11 (5%)	24 14
3	C	227/226 (100%)	224 (99%)	3 (1%)	69 68
3	P	226/226 (100%)	221 (98%)	5 (2%)	52 47
4	D	129/129 (100%)	127 (98%)	2 (2%)	62 60
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50 45
5	E	92/95 (97%)	90 (98%)	2 (2%)	52 47
5	R	93/95 (98%)	90 (97%)	3 (3%)	39 30
6	F	82/81 (101%)	80 (98%)	2 (2%)	49 43
6	S	81/81 (100%)	81 (100%)	0	100 100
7	G	67/68 (98%)	64 (96%)	3 (4%)	27 18
7	T	67/68 (98%)	60 (90%)	7 (10%)	7 2
8	H	71/75 (95%)	66 (93%)	5 (7%)	15 7
8	U	71/75 (95%)	69 (97%)	2 (3%)	43 36
9	I	57/57 (100%)	56 (98%)	1 (2%)	59 55
9	V	57/57 (100%)	56 (98%)	1 (2%)	59 55
10	J	49/50 (98%)	49 (100%)	0	100 100
10	W	49/50 (98%)	48 (98%)	1 (2%)	55 51
11	K	39/46 (85%)	39 (100%)	0	100 100
11	X	39/46 (85%)	39 (100%)	0	100 100
12	L	40/40 (100%)	37 (92%)	3 (8%)	13 5
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24 14
13	M	37/38 (97%)	35 (95%)	2 (5%)	22 13
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44 38
All	All	3073/3082 (100%)	2991 (97%)	82 (3%)	46 38

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	189	MET
1	A	369	ASP
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	110	TYR
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	116	LEU
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	9	GLU
4	D	31	LYS
5	E	5	HIS
5	E	90	ARG
6	F	80	GLN
6	F	95	GLN
7	G	18	PHE
7	G	33	LEU
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
12	L	24[A]	MET
12	L	24[B]	MET
12	L	47	LYS
13	M	13	LYS
13	M	38	ASP
1	N	109	PHE
1	N	138	HIS
1	N	189	MET
1	N	333	LYS
1	N	363	LEU
1	N	369	ASP

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Mol	Chain	Res	Type
1	N	484	THR
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	113	TYR
2	O	171	LYS
2	O	225	SER
2	O	226	MET
3	P	23	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
5	R	5	HIS
5	R	46	LYS
5	R	79	LYS
7	T	5	LYS
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	54	ARG
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
12	Y	2	HIS
12	Y	26	THR
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	3	HIS

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Mol	Chain	Res	Type
4	D	109	HIS
6	F	94	HIS
6	F	98	HIS
13	M	36	HIS
13	M	39	ASN
6	S	28	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	0.89	0	7,9,11	2.18	4 (57%)
1	FME	A	1	1	8,9,10	0.39	0	7,9,11	1.45	1 (14%)
1	FME	N	1	1	8,9,10	0.44	0	7,9,11	1.08	0
9	SAC	V	1	9	7,8,9	0.57	0	8,9,11	0.86	1 (12%)
7	TPO	G	11	7	8,10,11	1.24	1 (12%)	10,14,16	1.08	0
9	SAC	I	1	9	7,8,9	0.57	0	8,9,11	0.80	0
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.84	1 (14%)
7	TPO	T	11	7	8,10,11	1.56	1 (12%)	10,14,16	1.39	1 (10%)

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
2	FME	B	1	2	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	1/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.35	1.61	1.50
7	G	11	TPO	P-O1P	2.46	1.58	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	11	TPO	CG2-CB-CA	3.95	120.96	113.16
2	O	1	FME	CG-CB-CA	-3.84	102.27	112.95
1	A	1	FME	C-CA-N	2.91	114.99	109.73
2	B	1	FME	C-CA-N	-2.84	104.60	109.73
2	B	1	FME	O-C-CA	-2.80	117.45	124.78
2	B	1	FME	CG-CB-CA	-2.56	105.83	112.95
2	B	1	FME	CA-N-CN	2.44	126.57	122.82
9	V	1	SAC	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	CG2-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O3P
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	T	11	TPO	CB-OG1-P-O1P
7	T	11	TPO	CB-OG1-P-O2P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-CB-OG
2	B	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
1	A	1	FME	CB-CG-SD-CE
2	B	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 131 ligands modelled in this entry, 10 are monoatomic - leaving 121 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	$\#\|Z\| > 2$
25	PEK	C	307	-	52,52,52	0.99	2 (3%)	55,57,57	1.52	9 (16%)
19	PGV	P	305	-	50,50,50	0.82	2 (4%)	53,56,56	1.12	4 (7%)
20	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.11	0
25	PEK	C	302	-	52,52,52	0.97	2 (3%)	55,57,57	1.14	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	P	301	-	50,50,50	0.98	2 (4%)	53,56,56	1.28	4 (7%)
20	EDO	N	617	-	3,3,3	0.35	0	2,2,2	1.13	0
23	CUA	B	302	2	0,1,1	-	-	-		
20	EDO	N	620	-	3,3,3	0.41	0	2,2,2	0.33	0
21	DMU	P	316	-	34,34,34	0.79	1 (2%)	45,45,45	2.37	16 (35%)
20	EDO	N	611	-	3,3,3	0.49	0	2,2,2	0.32	0
27	CHD	X	105	-	32,32,32	0.75	0	51,51,51	1.69	14 (27%)
21	DMU	Z	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.97	3 (6%)
21	DMU	X	102	-	22,22,34	0.70	1 (4%)	27,27,45	1.59	6 (22%)
21	DMU	O	305	-	34,34,34	0.56	0	45,45,45	1.70	12 (26%)
20	EDO	Q	202	-	3,3,3	0.40	0	2,2,2	0.59	0
20	EDO	L	105	-	3,3,3	0.50	0	2,2,2	0.20	0
21	DMU	K	101	-	34,34,34	0.54	1 (2%)	45,45,45	1.54	10 (22%)
20	EDO	S	104	-	3,3,3	0.54	0	2,2,2	0.53	0
27	CHD	C	305	-	32,32,32	0.81	1 (3%)	51,51,51	1.40	9 (17%)
20	EDO	M	102	-	3,3,3	0.37	0	2,2,2	0.38	0
20	EDO	W	102	-	3,3,3	0.44	0	2,2,2	0.30	0
27	CHD	Y	102	-	32,32,32	0.72	0	51,51,51	2.16	15 (29%)
20	EDO	P	310	-	3,3,3	0.64	0	2,2,2	0.17	0
20	EDO	F	104	-	3,3,3	0.34	0	2,2,2	0.60	0
22	TGL	Q	201	-	62,62,62	1.07	3 (4%)	65,65,65	0.99	5 (7%)
26	CDL	G	101	-	99,99,99	1.34	12 (12%)	105,111,111	1.46	12 (11%)
20	EDO	A	611	-	3,3,3	0.40	0	2,2,2	0.08	0
22	TGL	L	101	12	62,62,62	1.17	4 (6%)	65,65,65	1.56	7 (10%)
27	CHD	J	101	-	32,32,32	0.62	0	51,51,51	2.38	21 (41%)
19	PGV	N	607	-	50,50,50	0.97	2 (4%)	53,56,56	1.30	7 (13%)
26	CDL	T	102	-	99,99,99	1.30	12 (12%)	105,111,111	1.31	7 (6%)
27	CHD	G	103	-	32,32,32	0.96	2 (6%)	51,51,51	1.52	10 (19%)
20	EDO	B	304	-	3,3,3	0.64	0	2,2,2	0.20	0
20	EDO	W	103	-	3,3,3	0.56	0	2,2,2	0.60	0
21	DMU	K	106	-	34,34,34	0.55	1 (2%)	45,45,45	1.45	6 (13%)
20	EDO	S	106	-	3,3,3	0.68	0	2,2,2	0.67	0
23	CUA	O	302	2	0,1,1	-	-	-		
27	CHD	C	306	-	32,32,32	0.92	0	51,51,51	1.38	7 (13%)
20	EDO	B	305	-	3,3,3	0.47	0	2,2,2	0.43	0
19	PGV	A	608	-	50,50,50	1.06	2 (4%)	53,56,56	1.13	4 (7%)
24	PSC	N	608	-	51,51,51	1.14	3 (5%)	57,59,59	1.54	7 (12%)
20	EDO	P	311	-	3,3,3	0.64	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	DMU	K	103	-	34,34,34	0.53	0	45,45,45	1.34	6 (13%)
20	EDO	N	615	-	3,3,3	0.36	0	2,2,2	0.78	0
20	EDO	Y	103	-	3,3,3	0.43	0	2,2,2	0.13	0
19	PGV	A	607	-	50,50,50	1.02	3 (6%)	53,56,56	1.26	4 (7%)
14	HEA	A	602	1,18	57,67,67	1.40	6 (10%)	61,103,103	1.84	20 (32%)
22	TGL	O	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.14	5 (7%)
26	CDL	C	304	-	99,99,99	1.36	12 (12%)	105,111,111	1.43	12 (11%)
20	EDO	G	105	-	3,3,3	0.54	0	2,2,2	0.13	0
21	DMU	X	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.78	10 (22%)
14	HEA	N	601[B]	-	57,67,67	1.34	8 (14%)	61,103,103	1.83	17 (27%)
25	PEK	P	309	-	52,52,52	1.05	2 (3%)	55,57,57	1.49	4 (7%)
20	EDO	P	315	-	3,3,3	0.37	0	2,2,2	1.05	0
20	EDO	P	312	-	3,3,3	0.49	0	2,2,2	1.13	0
27	CHD	W	101	-	32,32,32	0.76	0	51,51,51	2.35	17 (33%)
20	EDO	N	609	-	3,3,3	0.80	0	2,2,2	0.67	0
20	EDO	N	610	-	3,3,3	0.80	0	2,2,2	0.34	0
25	PEK	P	304	-	52,52,52	0.85	2 (3%)	55,57,57	1.23	4 (7%)
20	EDO	A	614	-	3,3,3	0.57	0	2,2,2	0.09	0
27	CHD	P	308	-	32,32,32	0.70	0	51,51,51	1.35	6 (11%)
21	DMU	X	103	-	22,22,34	0.54	0	27,27,45	0.68	0
20	EDO	C	310	-	3,3,3	0.75	0	2,2,2	0.53	0
29	PO4	H	101	-	4,4,4	0.82	0	6,6,6	0.42	0
20	EDO	P	313	-	3,3,3	0.51	0	2,2,2	0.47	0
20	EDO	S	107	-	3,3,3	0.42	0	2,2,2	0.41	0
21	DMU	D	202	-	34,34,34	0.53	0	45,45,45	1.09	3 (6%)
22	TGL	D	201	-	62,62,62	1.16	4 (6%)	65,65,65	1.04	4 (6%)
20	EDO	O	304	-	3,3,3	0.62	0	2,2,2	0.25	0
27	CHD	L	103	-	32,32,32	0.68	0	51,51,51	2.70	20 (39%)
21	DMU	B	306	-	34,34,34	0.84	1 (2%)	45,45,45	2.60	16 (35%)
21	DMU	K	105	-	34,34,34	0.49	0	45,45,45	1.33	6 (13%)
19	PGV	P	302	-	50,50,50	1.02	2 (4%)	53,56,56	1.26	6 (11%)
14	HEA	N	601[A]	-	57,67,67	1.36	8 (14%)	61,103,103	1.83	16 (26%)
20	EDO	A	612	-	3,3,3	0.37	0	2,2,2	0.30	0
21	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.17	4 (8%)
20	EDO	N	613	-	3,3,3	0.39	0	2,2,2	0.51	0
21	DMU	Q	203	-	34,34,34	0.78	1 (2%)	45,45,45	2.65	18 (40%)
18	PER	A	606	15,14	0,1,1	-	-	-		
21	DMU	P	314	-	34,34,34	0.56	0	45,45,45	1.34	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	C	311	-	3,3,3	0.35	0	2,2,2	0.77	0
29	PO4	U	101	-	4,4,4	1.02	0	6,6,6	0.58	0
22	TGL	B	301	-	62,62,62	1.09	3 (4%)	65,65,65	1.25	4 (6%)
20	EDO	A	610	-	3,3,3	0.62	0	2,2,2	0.56	0
19	PGV	C	303	-	50,50,50	0.83	2 (4%)	53,56,56	1.06	4 (7%)
20	EDO	N	614	-	3,3,3	0.60	0	2,2,2	0.15	0
20	EDO	R	201	-	3,3,3	0.38	0	2,2,2	0.40	0
14	HEA	A	601[B]	-	57,67,67	1.62	14 (24%)	61,103,103	1.95	22 (36%)
20	EDO	L	104	-	3,3,3	0.51	0	2,2,2	0.41	0
20	EDO	F	102	-	3,3,3	0.50	0	2,2,2	0.82	0
21	DMU	L	102	-	34,34,34	0.54	0	45,45,45	1.05	2 (4%)
27	CHD	P	307	-	32,32,32	0.73	0	51,51,51	1.43	9 (17%)
14	HEA	N	602	1,18	57,67,67	1.61	9 (15%)	61,103,103	1.89	17 (27%)
18	PER	N	606	15,14	0,1,1	-	-	-		
21	DMU	K	104	-	34,34,34	0.52	0	45,45,45	1.19	6 (13%)
22	TGL	Y	101	-	62,62,62	1.11	3 (4%)	65,65,65	1.41	7 (10%)
24	PSC	B	303	-	51,51,51	1.09	3 (5%)	57,59,59	1.41	5 (8%)
20	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.43	0
21	DMU	G	104	-	34,34,34	0.57	0	45,45,45	1.45	8 (17%)
27	CHD	T	101	-	32,32,32	0.85	1 (3%)	51,51,51	1.55	10 (19%)
20	EDO	O	303	-	3,3,3	0.76	0	2,2,2	0.60	0
21	DMU	K	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.40	7 (15%)
20	EDO	S	105	-	3,3,3	0.52	0	2,2,2	0.16	0
19	PGV	C	308	-	50,50,50	1.08	2 (4%)	53,56,56	1.64	8 (15%)
20	EDO	A	615	-	3,3,3	0.88	0	2,2,2	0.59	0
21	DMU	T	103	-	34,34,34	0.56	0	45,45,45	1.23	7 (15%)
25	PEK	C	309	-	52,52,52	1.00	2 (3%)	55,57,57	1.40	6 (10%)
20	EDO	F	105	-	3,3,3	0.50	0	2,2,2	0.70	0
20	EDO	A	613	-	3,3,3	0.78	0	2,2,2	0.18	0
14	HEA	A	601[A]	-	57,67,67	1.62	14 (24%)	61,103,103	1.95	21 (34%)
20	EDO	N	619	-	3,3,3	0.51	0	2,2,2	0.16	0
20	EDO	F	103	-	3,3,3	0.68	0	2,2,2	0.59	0
21	DMU	X	104	-	22,22,34	0.51	0	27,27,45	0.60	0
25	PEK	G	102	-	52,52,52	1.02	2 (3%)	55,57,57	1.07	4 (7%)
26	CDL	P	306	-	99,99,99	1.37	12 (12%)	105,111,111	1.52	17 (16%)
21	DMU	A	616	-	34,34,34	0.47	0	45,45,45	1.07	2 (4%)
21	DMU	C	312	-	34,34,34	0.48	0	45,45,45	1.45	8 (17%)
20	EDO	S	102	-	3,3,3	0.82	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.81	0
20	EDO	N	618	-	3,3,3	0.35	0	2,2,2	0.48	0
20	EDO	N	612	-	3,3,3	0.53	0	2,2,2	0.12	0

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
25	PEK	C	307	-	-	28/56/56/56	-
19	PGV	P	305	-	-	5/55/55/55	-
20	EDO	S	103	-	-	0/1/1/1	-
25	PEK	C	302	-	-	15/56/56/56	-
19	PGV	P	301	-	-	8/55/55/55	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
21	DMU	P	316	-	-	14/19/59/59	0/2/2/2
20	EDO	N	611	-	-	0/1/1/1	-
27	CHD	X	105	-	-	7/9/74/74	0/4/4/4
21	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
21	DMU	X	102	-	-	8/13/33/59	0/1/1/2
21	DMU	O	305	-	-	10/19/59/59	0/2/2/2
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	L	105	-	-	0/1/1/1	-
21	DMU	K	101	-	-	7/19/59/59	0/2/2/2
20	EDO	S	104	-	-	1/1/1/1	-
27	CHD	C	305	-	-	5/9/74/74	0/4/4/4
20	EDO	M	102	-	-	1/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
27	CHD	Y	102	-	-	0/9/74/74	0/4/4/4
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	F	104	-	-	1/1/1/1	-
22	TGL	Q	201	-	-	31/65/65/65	-
26	CDL	G	101	-	-	38/110/110/110	-
20	EDO	A	611	-	-	0/1/1/1	-
22	TGL	L	101	12	-	34/65/65/65	-
27	CHD	J	101	-	-	7/9/74/74	0/4/4/4
19	PGV	N	607	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	T	102	-	-	42/110/110/110	-
27	CHD	G	103	-	-	2/9/74/74	0/4/4/4
20	EDO	B	304	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
21	DMU	K	106	-	-	10/19/59/59	0/2/2/2
20	EDO	S	106	-	-	0/1/1/1	-
27	CHD	C	306	-	-	2/9/74/74	0/4/4/4
20	EDO	B	305	-	-	0/1/1/1	-
19	PGV	A	608	-	-	23/55/55/55	-
24	PSC	N	608	-	-	28/55/55/55	-
20	EDO	P	311	-	-	1/1/1/1	-
21	DMU	K	103	-	-	10/19/59/59	0/2/2/2
20	EDO	N	615	-	-	1/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
19	PGV	A	607	-	-	6/55/55/55	-
14	HEA	A	602	1,18	-	6/32/76/76	-
22	TGL	O	301	-	-	30/65/65/65	-
26	CDL	C	304	-	-	47/110/110/110	-
20	EDO	G	105	-	-	0/1/1/1	-
21	DMU	X	101	-	-	11/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	7/32/76/76	-
25	PEK	P	309	-	-	30/56/56/56	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
27	CHD	W	101	-	-	6/9/74/74	0/4/4/4
20	EDO	N	609	-	-	0/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
25	PEK	P	304	-	-	8/56/56/56	-
20	EDO	A	614	-	-	1/1/1/1	-
27	CHD	P	308	-	-	2/9/74/74	0/4/4/4
21	DMU	X	103	-	-	6/13/33/59	0/1/1/2
20	EDO	C	310	-	-	0/1/1/1	-
20	EDO	P	313	-	-	0/1/1/1	-
20	EDO	S	107	-	-	1/1/1/1	-
21	DMU	D	202	-	-	8/19/59/59	0/2/2/2
22	TGL	D	201	-	-	26/65/65/65	-
20	EDO	O	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHD	L	103	-	-	5/9/74/74	0/4/4/4
21	DMU	B	306	-	-	14/19/59/59	0/2/2/2
21	DMU	K	105	-	-	10/19/59/59	0/2/2/2
19	PGV	P	302	-	-	18/55/55/55	-
14	HEA	N	601[A]	-	-	4/32/76/76	-
20	EDO	A	612	-	-	0/1/1/1	-
21	DMU	M	101	-	-	4/19/59/59	0/2/2/2
20	EDO	N	613	-	-	1/1/1/1	-
21	DMU	Q	203	-	-	17/19/59/59	0/2/2/2
21	DMU	P	314	-	-	7/19/59/59	0/2/2/2
20	EDO	C	311	-	-	1/1/1/1	-
22	TGL	B	301	-	-	27/65/65/65	-
20	EDO	A	610	-	-	0/1/1/1	-
19	PGV	C	303	-	-	14/55/55/55	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	6/32/76/76	-
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
21	DMU	L	102	-	-	9/19/59/59	0/2/2/2
27	CHD	P	307	-	-	5/9/74/74	0/4/4/4
14	HEA	N	602	1,18	-	4/32/76/76	-
21	DMU	K	104	-	-	12/19/59/59	0/2/2/2
22	TGL	Y	101	-	-	29/65/65/65	-
24	PSC	B	303	-	-	26/55/55/55	-
20	EDO	N	616	-	-	1/1/1/1	-
21	DMU	G	104	-	-	9/19/59/59	0/2/2/2
27	CHD	T	101	-	-	2/9/74/74	0/4/4/4
20	EDO	O	303	-	-	0/1/1/1	-
21	DMU	K	102	-	-	11/19/59/59	0/2/2/2
20	EDO	S	105	-	-	0/1/1/1	-
19	PGV	C	308	-	-	20/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
21	DMU	T	103	-	-	8/19/59/59	0/2/2/2
25	PEK	C	309	-	-	22/56/56/56	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601[A]	-	-	4/32/76/76	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
21	DMU	X	104	-	-	7/13/33/59	0/1/1/2
25	PEK	G	102	-	-	15/56/56/56	-
26	CDL	P	306	-	-	46/110/110/110	-
21	DMU	A	616	-	-	8/19/59/59	0/2/2/2
21	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	101	TGL	OG2-CB1	5.27	1.49	1.34
19	C	308	PGV	O03-C19	5.25	1.48	1.33
22	Y	101	TGL	OG2-CB1	5.15	1.48	1.34
22	O	301	TGL	OG3-CC1	5.04	1.48	1.33
19	A	608	PGV	O03-C19	5.03	1.48	1.33
22	Y	101	TGL	OG3-CC1	5.02	1.48	1.33
25	C	307	PEK	O03-C21	4.93	1.47	1.33
22	B	301	TGL	OG1-CA1	4.81	1.47	1.33
22	L	101	TGL	OG3-CC1	4.78	1.47	1.33
25	C	309	PEK	O03-C21	4.78	1.47	1.33
25	G	102	PEK	O03-C21	4.76	1.47	1.33
25	P	309	PEK	O03-C21	4.76	1.47	1.33
19	P	302	PGV	O03-C19	4.74	1.47	1.33
26	G	101	CDL	OB8-CB7	4.74	1.47	1.33
26	P	306	CDL	OA8-CA7	4.73	1.47	1.33
26	G	101	CDL	OA6-CA5	4.71	1.47	1.34
22	D	201	TGL	OG1-CA1	4.69	1.47	1.33
26	C	304	CDL	OB8-CB7	4.67	1.47	1.33
14	N	602	HEA	CHD-C1D	4.66	1.46	1.35
22	O	301	TGL	OG2-CB1	4.66	1.47	1.34
19	N	607	PGV	O03-C19	4.65	1.46	1.33
24	N	608	PSC	O01-C1	4.64	1.47	1.34
25	G	102	PEK	O01-C1	4.63	1.47	1.34
26	C	304	CDL	OA8-CA7	4.62	1.46	1.33
22	Q	201	TGL	OG1-CA1	4.57	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	301	TGL	OG1-CA1	4.56	1.46	1.33
22	B	301	TGL	OG3-CC1	4.56	1.46	1.33
26	P	306	CDL	OB8-CB7	4.53	1.46	1.33
26	T	102	CDL	OA8-CA7	4.51	1.46	1.33
25	P	309	PEK	O01-C1	4.49	1.47	1.34
26	P	306	CDL	OA6-CA5	4.49	1.47	1.34
22	L	101	TGL	OG1-CA1	4.44	1.46	1.33
24	B	303	PSC	O01-C1	4.43	1.46	1.34
22	Q	201	TGL	OG3-CC1	4.42	1.46	1.33
14	A	601[A]	HEA	CBD-CGD	4.41	1.60	1.50
14	A	601[B]	HEA	CBD-CGD	4.41	1.60	1.50
22	B	301	TGL	OG2-CB1	4.32	1.46	1.34
19	N	607	PGV	O01-C1	4.30	1.46	1.34
22	D	201	TGL	OG2-CB1	4.25	1.46	1.34
26	G	101	CDL	OA8-CA7	4.25	1.45	1.33
25	C	309	PEK	O01-C1	4.24	1.46	1.34
26	T	102	CDL	OB6-CB5	4.23	1.46	1.34
26	G	101	CDL	OB6-CB5	4.17	1.46	1.34
19	P	301	PGV	O03-C19	4.16	1.45	1.33
25	C	302	PEK	O03-C21	4.15	1.45	1.33
26	T	102	CDL	OA6-CA5	4.11	1.45	1.34
22	Q	201	TGL	OG2-CB1	4.10	1.45	1.34
26	T	102	CDL	OB8-CB7	4.10	1.45	1.33
25	C	307	PEK	O01-C1	4.10	1.45	1.34
26	C	304	CDL	OA6-CA5	4.08	1.45	1.34
19	P	302	PGV	O01-C1	4.06	1.45	1.34
25	P	304	PEK	O03-C21	4.06	1.45	1.33
14	N	602	HEA	C4B-C3B	-4.05	1.37	1.44
22	D	201	TGL	OG3-CC1	4.04	1.45	1.33
24	N	608	PSC	C13-C12	4.03	1.55	1.31
19	A	607	PGV	O03-C19	3.99	1.45	1.33
19	A	608	PGV	O01-C1	3.92	1.45	1.34
19	C	308	PGV	O01-C1	3.85	1.45	1.34
22	Y	101	TGL	OG1-CA1	3.84	1.44	1.33
24	B	303	PSC	C13-C12	3.81	1.53	1.31
22	D	201	TGL	OB1-CB1	3.72	1.33	1.22
14	A	602	HEA	C3C-C2C	-3.71	1.35	1.40
14	N	601[A]	HEA	CHC-C4B	3.66	1.44	1.35
14	N	601[B]	HEA	CHC-C4B	3.66	1.44	1.35
26	P	306	CDL	OB6-CB5	3.57	1.44	1.34
14	A	602	HEA	CHD-C1D	3.52	1.44	1.35
25	C	302	PEK	O01-C1	3.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	608	PSC	O03-C19	3.50	1.43	1.33
26	G	101	CDL	C59-C58	-3.48	1.32	1.51
26	G	101	CDL	C62-C61	-3.46	1.32	1.51
26	C	304	CDL	OB6-CB5	3.45	1.44	1.34
26	P	306	CDL	C19-C18	-3.44	1.32	1.51
14	N	601[A]	HEA	CHD-C1D	3.43	1.43	1.35
14	N	601[B]	HEA	CHD-C1D	3.43	1.43	1.35
26	C	304	CDL	C59-C58	-3.41	1.32	1.51
24	B	303	PSC	O03-C19	3.40	1.43	1.33
26	T	102	CDL	C42-C41	-3.36	1.32	1.51
26	C	304	CDL	C79-C78	-3.35	1.32	1.51
26	P	306	CDL	C59-C58	-3.34	1.32	1.51
26	C	304	CDL	C82-C81	-3.32	1.33	1.51
26	C	304	CDL	C19-C18	-3.31	1.33	1.51
26	C	304	CDL	C62-C61	-3.30	1.33	1.51
26	P	306	CDL	C79-C78	-3.28	1.33	1.51
26	P	306	CDL	C62-C61	-3.28	1.33	1.51
26	P	306	CDL	C22-C21	-3.28	1.33	1.51
14	N	602	HEA	C1D-ND	-3.28	1.34	1.40
21	B	306	DMU	O16-C6	3.23	1.45	1.40
19	C	303	PGV	O01-C1	3.23	1.43	1.34
26	G	101	CDL	C82-C81	-3.23	1.33	1.51
26	P	306	CDL	C39-C38	-3.21	1.33	1.51
14	A	602	HEA	CHC-C4B	3.21	1.43	1.35
26	T	102	CDL	C62-C61	-3.20	1.33	1.51
26	T	102	CDL	C19-C18	-3.20	1.33	1.51
26	T	102	CDL	C82-C81	-3.19	1.33	1.51
26	C	304	CDL	C22-C21	-3.19	1.33	1.51
26	P	306	CDL	C82-C81	-3.18	1.33	1.51
26	T	102	CDL	C22-C21	-3.17	1.33	1.51
14	N	602	HEA	CHC-C4B	3.17	1.43	1.35
26	T	102	CDL	C59-C58	-3.16	1.33	1.51
26	P	306	CDL	C42-C41	-3.13	1.34	1.51
26	G	101	CDL	C79-C78	-3.13	1.34	1.51
26	C	304	CDL	C39-C38	-3.13	1.34	1.51
26	T	102	CDL	C39-C38	-3.13	1.34	1.51
26	C	304	CDL	C42-C41	-3.11	1.34	1.51
26	T	102	CDL	C79-C78	-3.09	1.34	1.51
26	G	101	CDL	C42-C41	-3.09	1.34	1.51
19	A	607	PGV	O01-C1	3.07	1.43	1.34
19	P	305	PGV	O03-C19	3.06	1.42	1.33
26	G	101	CDL	C22-C21	-3.04	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	O11-C11	3.03	1.49	1.42
14	A	601[B]	HEA	O11-C11	3.03	1.49	1.42
19	P	305	PGV	O01-C1	3.01	1.42	1.34
26	G	101	CDL	C19-C18	-2.99	1.34	1.51
27	G	103	CHD	C10-C5	-2.95	1.50	1.55
26	G	101	CDL	C39-C38	-2.93	1.35	1.51
14	N	601[A]	HEA	C1D-ND	-2.87	1.35	1.40
14	N	601[B]	HEA	C1D-ND	-2.87	1.35	1.40
14	A	601[A]	HEA	CHC-C4B	2.83	1.42	1.35
14	A	601[B]	HEA	CHC-C4B	2.83	1.42	1.35
14	A	601[A]	HEA	C3B-C2B	2.80	1.41	1.34
14	A	601[B]	HEA	C3B-C2B	2.80	1.41	1.34
19	P	301	PGV	O01-C1	2.79	1.42	1.34
14	A	601[A]	HEA	C4D-C3D	-2.75	1.40	1.45
14	A	601[B]	HEA	C4D-C3D	-2.75	1.40	1.45
19	C	303	PGV	O03-C19	2.74	1.41	1.33
14	A	601[A]	HEA	C1D-C2D	-2.67	1.39	1.44
14	A	601[B]	HEA	C1D-C2D	-2.67	1.39	1.44
14	N	602	HEA	C1D-C2D	-2.45	1.39	1.44
14	A	602	HEA	C18-C19	2.43	1.38	1.33
14	A	601[A]	HEA	CAA-C2A	2.38	1.56	1.52
14	A	601[B]	HEA	CAA-C2A	2.38	1.56	1.52
21	Q	203	DMU	O16-C6	2.36	1.44	1.40
21	X	102	DMU	O16-C6	2.33	1.44	1.40
14	A	601[A]	HEA	C1D-ND	-2.33	1.36	1.40
14	A	601[B]	HEA	C1D-ND	-2.33	1.36	1.40
14	A	601[A]	HEA	CHD-C1D	2.30	1.40	1.35
14	A	601[B]	HEA	CHD-C1D	2.30	1.40	1.35
14	N	601[A]	HEA	C4D-C3D	-2.29	1.41	1.45
14	N	601[B]	HEA	C4D-C3D	-2.29	1.41	1.45
14	A	602	HEA	CMD-C2D	2.27	1.55	1.50
14	N	602	HEA	C1B-C2B	-2.26	1.40	1.44
14	N	601[A]	HEA	O1A-CGA	2.26	1.29	1.22
14	N	601[B]	HEA	O1A-CGA	2.26	1.29	1.22
21	P	316	DMU	O16-C6	2.26	1.44	1.40
25	P	304	PEK	O01-C1	2.22	1.40	1.34
14	N	601[A]	HEA	CBD-CGD	2.22	1.55	1.50
14	N	601[B]	HEA	CBD-CGD	2.22	1.55	1.50
14	N	601[A]	HEA	CBD-CAD	2.20	1.59	1.52
14	N	601[B]	HEA	CBD-CAD	2.20	1.59	1.52
21	Z	101	DMU	O16-C6	2.20	1.43	1.40
14	A	602	HEA	C4D-ND	-2.18	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C18-C19	2.17	1.38	1.33
27	C	305	CHD	C13-C14	-2.16	1.51	1.55
14	A	601[A]	HEA	C4C-NC	-2.15	1.31	1.36
14	A	601[B]	HEA	C4C-NC	-2.15	1.31	1.36
14	N	602	HEA	CBD-CGD	2.15	1.55	1.50
14	A	601[A]	HEA	O2D-CGD	-2.09	1.23	1.30
14	A	601[B]	HEA	O2D-CGD	-2.09	1.23	1.30
21	K	101	DMU	O16-C6	2.09	1.43	1.40
21	K	106	DMU	O16-C6	2.08	1.43	1.40
14	N	602	HEA	C3B-C2B	2.08	1.39	1.34
14	A	601[A]	HEA	C4B-NB	-2.07	1.36	1.40
14	A	601[B]	HEA	C4B-NB	-2.07	1.36	1.40
27	T	101	CHD	O25-C24	2.07	1.29	1.22
21	K	102	DMU	O16-C6	2.05	1.43	1.40
14	A	601[A]	HEA	C1B-C2B	-2.04	1.40	1.44
14	A	601[B]	HEA	C1B-C2B	-2.04	1.40	1.44
22	L	101	TGL	CC2-CC1	2.03	1.56	1.50
19	A	607	PGV	C03-C02	2.02	1.56	1.50
27	G	103	CHD	O7-C7	2.02	1.47	1.43
21	X	101	DMU	O16-C6	2.02	1.43	1.40
14	N	601[A]	HEA	C1B-NB	-2.01	1.34	1.38
14	N	601[B]	HEA	C1B-NB	-2.01	1.34	1.38
14	A	601[A]	HEA	C3C-C2C	-2.01	1.37	1.40
14	A	601[B]	HEA	C3C-C2C	-2.01	1.37	1.40

All (576) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	306	DMU	O4-C7-C5	-7.29	93.49	110.35
27	J	101	CHD	C10-C9-C8	7.13	119.48	111.82
26	G	101	CDL	OA6-CA5-C11	7.03	126.66	111.50
21	B	306	DMU	C10-O1-C9	6.69	126.82	113.69
27	W	101	CHD	C13-C17-C20	6.59	127.36	119.50
21	P	316	DMU	C7-C8-C9	-6.43	98.76	110.24
27	Y	102	CHD	C6-C5-C4	-6.28	103.96	111.19
19	C	308	PGV	O03-C19-C20	6.27	131.58	111.91
22	Y	101	TGL	OG2-CB1-CB2	6.25	124.98	111.50
26	T	102	CDL	OA6-CA5-C11	6.24	124.94	111.50
21	Q	203	DMU	O4-C7-C5	-6.22	95.97	110.35
26	P	306	CDL	CB4-OB6-CB5	-6.16	102.63	117.79
21	B	306	DMU	O2-C8-C9	-6.15	94.02	109.30
24	N	608	PSC	C03-C02-C01	-5.90	97.84	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	103	CHD	C11-C12-C13	5.70	117.10	111.24
25	P	309	PEK	O03-C21-C22	5.64	129.60	111.91
27	L	103	CHD	C14-C13-C12	5.61	112.63	107.40
22	L	101	TGL	OG3-CC1-OC1	-5.44	109.87	123.59
27	L	103	CHD	C21-C20-C17	5.38	121.16	112.92
27	W	101	CHD	C11-C12-C13	5.38	116.77	111.24
27	L	103	CHD	C4-C5-C10	5.35	118.34	112.66
26	G	101	CDL	OB6-CB5-C51	5.35	123.03	111.50
21	P	316	DMU	O49-C1-C2	-5.34	98.00	110.35
27	W	101	CHD	C17-C13-C14	-5.31	94.74	100.09
27	Y	102	CHD	C14-C13-C12	5.30	112.33	107.40
25	C	309	PEK	O01-C1-C2	5.29	122.91	111.50
27	W	101	CHD	C14-C13-C12	5.20	112.24	107.40
21	Q	203	DMU	C7-C8-C9	5.18	119.48	110.24
27	L	103	CHD	C6-C5-C4	-5.18	105.22	111.19
21	Q	203	DMU	C10-O1-C9	5.14	123.78	113.69
24	N	608	PSC	O01-C1-C2	5.13	122.56	111.50
22	O	301	TGL	OG2-CB1-CB2	5.04	122.35	111.50
26	P	306	CDL	OB6-CB5-C51	5.04	122.35	111.50
24	B	303	PSC	O01-C1-C2	4.94	122.14	111.50
21	K	101	DMU	C6-O5-C4	4.94	123.38	113.69
21	Q	203	DMU	O2-C8-C9	-4.92	97.07	109.30
14	N	602	HEA	CHD-C1D-ND	4.90	130.44	124.38
21	Q	203	DMU	O7-C10-C5	4.90	120.80	108.10
21	Q	203	DMU	O1-C9-C8	4.80	118.41	109.69
27	L	103	CHD	C1-C10-C5	4.80	114.86	107.77
22	L	101	TGL	OG2-CB1-CB2	4.78	121.80	111.50
22	B	301	TGL	OG2-CB1-CB2	4.77	121.78	111.50
27	Y	102	CHD	C1-C10-C5	4.75	114.79	107.77
24	B	303	PSC	O03-C01-C02	-4.75	94.61	108.43
19	P	301	PGV	O03-C19-O04	-4.74	111.63	123.59
27	L	103	CHD	C17-C13-C12	-4.72	113.35	117.67
21	Q	203	DMU	C10-C5-C7	4.64	119.65	110.00
26	T	102	CDL	OB6-CB5-C51	4.64	121.50	111.50
27	J	101	CHD	C14-C13-C12	4.63	111.71	107.40
27	J	101	CHD	C14-C8-C9	-4.62	103.37	109.71
21	P	316	DMU	O7-C10-C5	4.61	120.05	108.10
25	C	307	PEK	O03-C21-C22	4.57	126.25	111.91
21	Q	203	DMU	C6-O5-C4	4.57	122.65	113.69
21	P	314	DMU	C10-O1-C9	4.55	122.62	113.69
27	L	103	CHD	C11-C9-C10	-4.54	109.04	113.73
21	B	306	DMU	C8-C7-C5	4.54	118.76	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	Q	203	DMU	O3-C5-C10	4.52	121.04	110.05
19	A	607	PGV	O03-C19-C20	4.52	126.10	111.91
14	N	602	HEA	CHA-C4D-ND	4.52	129.34	124.43
14	A	602	HEA	C27-C19-C20	4.47	122.80	115.27
27	J	101	CHD	C6-C5-C4	-4.46	106.05	111.19
22	L	101	TGL	OG3-CC1-CC2	4.46	125.92	111.91
19	C	308	PGV	C01-O03-C19	4.45	133.58	117.12
21	X	101	DMU	C8-C7-C5	4.41	118.52	110.82
27	W	101	CHD	C17-C13-C12	4.39	121.67	117.67
21	X	101	DMU	C7-C8-C9	4.37	118.03	110.24
21	O	305	DMU	C10-O1-C9	4.35	122.23	113.69
25	C	307	PEK	O01-C1-C2	4.34	120.85	111.50
21	B	306	DMU	C1-C2-C3	4.33	119.58	109.68
27	Y	102	CHD	C9-C11-C12	-4.30	108.62	114.30
27	J	101	CHD	C9-C8-C7	4.29	117.00	111.88
21	K	103	DMU	O5-C4-C3	4.24	118.70	109.75
21	P	316	DMU	C2-C3-C4	-4.23	101.23	110.93
26	C	304	CDL	CB4-OB6-CB5	-4.21	107.44	117.79
14	N	601[A]	HEA	C26-C15-C16	4.20	122.33	115.27
14	N	601[B]	HEA	C26-C15-C16	4.20	122.33	115.27
21	X	101	DMU	C10-C5-C7	4.18	118.70	110.00
14	N	601[A]	HEA	C3D-C4D-ND	4.18	114.40	110.36
14	N	601[B]	HEA	C3D-C4D-ND	4.18	114.40	110.36
21	X	101	DMU	O1-C9-C8	4.18	117.28	109.69
14	N	601[A]	HEA	C3C-C4C-NC	4.17	114.60	109.21
14	N	601[B]	HEA	C3C-C4C-NC	4.17	114.60	109.21
19	P	302	PGV	O03-C19-C20	4.16	124.97	111.91
21	L	102	DMU	O7-C3-C2	4.16	118.34	107.28
26	C	304	CDL	OB8-CB7-C71	4.14	124.90	111.91
25	P	309	PEK	O03-C21-O04	-4.14	113.16	123.59
14	A	601[A]	HEA	CMC-C2C-C3C	4.11	132.37	124.68
14	A	601[B]	HEA	CMC-C2C-C3C	4.11	132.37	124.68
21	K	105	DMU	O1-C9-C8	4.11	117.16	109.69
21	X	102	DMU	O16-C6-C1	4.11	114.72	108.30
27	W	101	CHD	C22-C20-C17	4.09	118.73	110.28
19	C	308	PGV	O01-C1-C2	4.07	120.28	111.50
21	B	306	DMU	C11-C9-C8	4.07	122.53	113.00
26	C	304	CDL	OB6-CB5-C51	4.07	120.27	111.50
19	P	301	PGV	O03-C19-C20	4.07	124.67	111.91
21	X	101	DMU	C10-O1-C9	4.05	121.65	113.69
27	W	101	CHD	C18-C13-C12	-4.05	104.95	109.07
27	Y	102	CHD	C14-C8-C7	4.04	117.16	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	102	DMU	O5-C4-C3	4.01	118.20	109.75
14	N	602	HEA	CHB-C1B-NB	3.99	128.77	124.43
19	P	302	PGV	O01-C1-C2	3.98	120.08	111.50
25	P	309	PEK	O01-C1-C2	3.97	120.05	111.50
25	C	309	PEK	O03-C21-C22	3.95	124.31	111.91
25	C	307	PEK	C01-O03-C21	3.94	131.72	117.12
27	L	103	CHD	C13-C14-C8	-3.94	109.70	114.74
21	B	306	DMU	O1-C9-C8	3.94	116.84	109.69
27	P	307	CHD	C19-C10-C9	-3.92	105.78	111.18
21	P	316	DMU	O3-C5-C10	3.91	119.54	110.05
25	P	309	PEK	C01-O03-C21	3.88	131.50	117.12
27	L	103	CHD	C13-C17-C20	3.88	124.12	119.50
19	A	607	PGV	O03-C19-O04	-3.86	113.84	123.59
21	K	102	DMU	C10-O1-C9	3.85	121.24	113.69
22	D	201	TGL	OG2-CB1-CB2	-3.83	103.25	111.50
21	G	104	DMU	O1-C10-C5	3.82	118.44	110.35
14	A	601[A]	HEA	C13-C12-C11	-3.82	108.61	114.35
14	A	601[B]	HEA	C13-C12-C11	-3.82	108.61	114.35
21	P	316	DMU	O7-C3-C4	3.77	119.78	109.45
26	C	304	CDL	C52-C51-CB5	-3.77	99.92	113.62
21	K	103	DMU	C6-O5-C4	3.76	121.07	113.69
25	P	304	PEK	O01-C1-O02	-3.75	114.63	123.70
27	W	101	CHD	C23-C22-C20	-3.74	107.68	114.52
22	D	201	TGL	CG2-OG2-CB1	-3.74	108.58	117.79
14	N	602	HEA	CHB-C1B-C2B	-3.73	119.15	124.98
22	Q	201	TGL	CG2-OG2-CB1	-3.73	108.60	117.79
21	K	106	DMU	C8-C7-C5	3.73	117.34	110.82
27	T	101	CHD	C17-C13-C12	3.72	121.06	117.67
21	P	316	DMU	O1-C10-C5	3.72	118.22	110.35
14	N	602	HEA	CAD-CBD-CGD	-3.71	105.62	113.60
27	J	101	CHD	C18-C13-C14	-3.70	105.42	111.21
27	L	103	CHD	C5-C4-C3	3.69	118.17	112.76
25	G	102	PEK	O01-C1-C2	3.68	119.44	111.50
14	A	602	HEA	C3D-C4D-ND	3.68	113.92	110.36
27	L	103	CHD	C18-C13-C14	-3.68	105.46	111.21
27	C	306	CHD	C18-C13-C12	3.68	112.81	109.07
24	N	608	PSC	O03-C01-C02	-3.68	97.73	108.43
21	C	312	DMU	C6-O5-C4	3.67	120.88	113.69
27	X	105	CHD	C17-C13-C14	3.65	103.78	100.09
14	A	601[A]	HEA	CMC-C2C-C1C	-3.64	122.86	128.46
14	A	601[B]	HEA	CMC-C2C-C1C	-3.64	122.86	128.46
14	A	601[A]	HEA	C2D-C1D-ND	3.64	114.16	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[B]	HEA	C2D-C1D-ND	3.64	114.16	109.84
27	X	105	CHD	C18-C13-C17	-3.63	105.53	111.21
26	C	304	CDL	OA6-CA5-C11	3.63	119.33	111.50
14	A	602	HEA	C2B-C1B-NB	3.63	114.23	109.88
21	G	104	DMU	C10-O7-C3	-3.61	109.03	117.96
21	Q	203	DMU	O5-C4-C3	3.59	117.33	109.75
21	Q	203	DMU	C8-C7-C5	3.58	117.08	110.82
27	Y	102	CHD	C19-C10-C1	-3.58	102.49	108.26
21	O	305	DMU	C10-C5-C7	3.57	117.44	110.00
24	N	608	PSC	C21-C20-C19	-3.57	100.65	113.62
27	L	103	CHD	C9-C11-C12	3.56	119.01	114.30
21	O	305	DMU	C1-C2-C3	3.54	117.77	109.68
27	X	105	CHD	C13-C17-C20	-3.54	115.27	119.50
21	X	102	DMU	O5-C6-C1	3.54	117.84	110.35
22	Y	101	TGL	OG3-CC1-CC2	3.54	123.01	111.91
21	P	316	DMU	C6-C1-C2	3.51	117.31	110.00
27	J	101	CHD	C22-C20-C17	3.50	117.53	110.28
27	W	101	CHD	C9-C11-C12	3.50	118.92	114.30
22	B	301	TGL	OG1-CA1-CA2	3.49	122.85	111.91
22	Y	101	TGL	CG3-CG2-CG1	-3.48	103.56	111.79
26	P	306	CDL	OB8-CB7-C71	3.48	122.82	111.91
21	P	316	DMU	O55-C2-C1	-3.45	102.38	110.35
19	A	608	PGV	C4-C3-C2	-3.44	100.82	113.19
26	G	101	CDL	OA6-CA5-OA7	-3.44	115.39	123.70
21	K	103	DMU	C7-C8-C9	3.43	116.36	110.24
14	A	602	HEA	CHA-C4D-C3D	-3.43	119.80	124.84
27	J	101	CHD	C4-C5-C10	3.43	116.30	112.66
21	K	106	DMU	C1-C2-C3	3.43	117.50	109.68
21	K	101	DMU	O5-C4-C3	3.42	116.96	109.75
21	P	316	DMU	O55-C2-C3	3.42	119.00	109.94
19	N	607	PGV	C03-C02-C01	3.41	119.86	111.79
21	G	104	DMU	C8-C7-C5	3.41	116.77	110.82
21	O	305	DMU	O1-C10-C5	3.41	117.56	110.35
14	A	602	HEA	C21-C22-C23	-3.40	116.11	127.75
27	L	103	CHD	C11-C9-C8	3.40	115.85	110.88
21	T	103	DMU	C10-O1-C9	3.40	120.36	113.69
19	N	607	PGV	O03-C01-C02	-3.39	98.58	108.43
21	K	101	DMU	O5-C6-C1	3.37	117.49	110.35
21	D	202	DMU	C1-C2-C3	3.36	117.36	109.68
21	P	316	DMU	C10-O7-C3	-3.36	109.64	117.96
27	X	105	CHD	C18-C13-C12	-3.36	105.65	109.07
26	P	306	CDL	OA8-CA6-CA4	3.35	118.19	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	303	PGV	O03-C19-O04	-3.35	115.14	123.59
27	J	101	CHD	C1-C10-C5	3.34	112.71	107.77
26	G	101	CDL	CB4-OB6-CB5	-3.34	109.57	117.79
21	C	312	DMU	O5-C4-C3	3.31	116.73	109.75
21	T	103	DMU	O1-C10-C5	3.31	117.35	110.35
27	L	103	CHD	C1-C2-C3	-3.30	106.23	110.47
21	K	106	DMU	C10-C5-C7	3.30	116.87	110.00
27	G	103	CHD	C6-C5-C10	-3.30	109.15	112.66
27	C	305	CHD	C6-C5-C4	-3.30	107.39	111.19
14	A	601[A]	HEA	C1D-C2D-C3D	-3.29	103.49	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-3.29	103.49	106.96
19	C	308	PGV	O03-C19-O04	-3.28	115.31	123.59
21	B	306	DMU	C10-C5-C7	3.28	116.83	110.00
14	N	602	HEA	CAD-C3D-C4D	3.27	130.37	124.66
21	K	106	DMU	C7-C8-C9	3.26	116.06	110.24
27	P	308	CHD	O25-C24-C23	-3.26	112.61	123.08
21	Q	203	DMU	O1-C10-C5	3.26	117.25	110.35
14	N	602	HEA	CHA-C4D-C3D	-3.26	120.05	124.84
21	O	305	DMU	C18-O16-C6	-3.25	108.45	113.84
26	C	304	CDL	OA8-CA6-CA4	3.25	117.90	108.43
26	P	306	CDL	OA8-CA7-C31	3.24	122.06	111.91
19	C	308	PGV	C03-C02-C01	3.23	119.44	111.79
21	P	314	DMU	O1-C9-C8	3.23	115.55	109.69
14	A	601[A]	HEA	C27-C19-C20	3.22	120.69	115.27
27	Y	102	CHD	C5-C6-C7	3.21	118.01	114.46
26	P	306	CDL	C52-C51-CB5	-3.21	101.94	113.62
19	N	607	PGV	O03-C19-C20	3.21	121.97	111.91
21	M	101	DMU	C18-O16-C6	-3.20	108.54	113.84
14	A	601[B]	HEA	C16-C17-C18	3.20	122.39	111.88
21	Q	203	DMU	C11-C9-C8	3.19	120.48	113.00
27	G	103	CHD	C13-C14-C8	-3.18	110.67	114.74
27	J	101	CHD	C13-C17-C20	3.18	123.29	119.50
25	P	304	PEK	C03-C02-C01	-3.18	104.27	111.79
14	A	602	HEA	CMB-C2B-C1B	3.18	129.88	125.04
27	P	307	CHD	C16-C17-C13	3.17	106.67	103.55
21	K	105	DMU	C7-C8-C9	3.17	115.90	110.24
21	D	202	DMU	C6-C1-C2	3.17	116.60	110.00
27	T	101	CHD	C18-C13-C12	-3.16	105.85	109.07
21	B	306	DMU	O1-C10-C5	3.15	117.03	110.35
14	N	601[A]	HEA	CMD-C2D-C1D	3.15	129.83	125.04
14	N	601[B]	HEA	CMD-C2D-C1D	3.15	129.83	125.04
14	N	602	HEA	C13-C12-C11	-3.14	109.63	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	306	DMU	C7-C8-C9	3.14	115.84	110.24
26	G	101	CDL	CA4-OA6-CA5	-3.12	110.11	117.79
26	P	306	CDL	OA6-CA5-C11	3.11	118.20	111.50
25	C	309	PEK	C2-C3-C4	-3.11	107.69	113.23
27	G	103	CHD	C5-C4-C3	-3.09	108.22	112.76
22	O	301	TGL	CG3-CG2-CG1	-3.08	104.51	111.79
22	L	101	TGL	OG1-CA1-CA2	3.08	121.56	111.91
27	P	308	CHD	C4-C5-C10	-3.07	109.39	112.66
27	G	103	CHD	C11-C9-C10	-3.07	110.56	113.73
26	P	306	CDL	O1-C1-CB2	3.06	120.29	109.56
22	B	301	TGL	CB3-CB2-CB1	-3.06	102.50	113.62
22	O	301	TGL	OG1-CA1-CA2	3.05	121.47	111.91
21	B	306	DMU	O7-C3-C2	3.04	115.38	107.28
22	B	301	TGL	OG3-CC1-CC2	3.03	121.42	111.91
27	X	105	CHD	C5-C4-C3	-3.02	108.32	112.76
21	G	104	DMU	C7-C8-C9	3.00	115.59	110.24
27	C	305	CHD	C14-C8-C7	-3.00	107.83	111.81
21	A	616	DMU	C10-O7-C3	-2.99	110.56	117.96
22	D	201	TGL	CB3-CB2-CB1	2.99	124.50	113.62
21	Q	203	DMU	O6-C11-C9	2.99	121.54	111.29
27	G	103	CHD	C4-C5-C10	-2.97	109.51	112.66
26	T	102	CDL	OA6-CA5-OA7	-2.97	116.53	123.70
21	B	306	DMU	O3-C5-C10	2.96	117.23	110.05
19	C	303	PGV	O01-C1-C2	2.95	117.86	111.50
14	N	602	HEA	C4D-CHA-C1A	-2.94	118.68	122.56
22	Y	101	TGL	OG1-CA1-CA2	2.94	121.12	111.91
21	K	103	DMU	C8-C7-C5	2.93	115.94	110.82
21	C	312	DMU	C10-O1-C9	2.93	119.44	113.69
21	C	312	DMU	O1-C10-C5	2.93	116.55	110.35
27	P	307	CHD	C18-C13-C12	-2.92	106.09	109.07
27	C	305	CHD	C1-C10-C5	2.92	112.09	107.77
14	A	602	HEA	C1D-C2D-C3D	-2.92	103.89	106.96
21	K	105	DMU	C6-O5-C4	2.92	119.42	113.69
21	P	316	DMU	C57-C4-C3	2.91	121.80	113.33
27	T	101	CHD	C4-C3-C2	2.90	114.01	110.55
27	W	101	CHD	C14-C8-C9	-2.90	105.74	109.71
14	N	601[A]	HEA	CMB-C2B-C1B	-2.89	120.64	125.04
14	N	601[B]	HEA	CMB-C2B-C1B	-2.89	120.64	125.04
27	C	306	CHD	C14-C13-C12	-2.88	104.72	107.40
14	N	601[A]	HEA	CMC-C2C-C3C	2.87	130.06	124.68
14	N	601[B]	HEA	CMC-C2C-C3C	2.87	130.06	124.68
25	C	307	PEK	O03-C21-O04	-2.86	116.37	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	101	CHD	C19-C10-C1	-2.86	103.65	108.26
27	P	308	CHD	C21-C20-C22	-2.85	105.89	110.36
21	X	101	DMU	O5-C4-C3	2.85	115.77	109.75
14	A	601[A]	HEA	CAA-CBA-CGA	-2.84	105.79	113.76
14	A	601[B]	HEA	CAA-CBA-CGA	-2.84	105.79	113.76
14	N	601[A]	HEA	C4D-CHA-C1A	2.84	126.31	122.56
14	N	601[B]	HEA	C4D-CHA-C1A	2.84	126.31	122.56
19	A	608	PGV	O01-C1-C2	2.84	117.62	111.50
27	L	103	CHD	C14-C8-C7	2.83	115.57	111.81
26	C	304	CDL	OB6-CB5-OB7	-2.83	116.86	123.70
14	A	602	HEA	CAD-CBD-CGD	-2.83	107.52	113.60
27	G	103	CHD	C1-C2-C3	-2.83	106.84	110.47
14	A	601[A]	HEA	C26-C15-C16	2.82	120.01	115.27
14	A	601[B]	HEA	C26-C15-C16	2.82	120.01	115.27
27	G	103	CHD	C19-C10-C5	-2.80	105.61	110.36
14	A	601[A]	HEA	O2A-CGA-CBA	2.80	123.02	114.03
14	A	601[B]	HEA	O2A-CGA-CBA	2.80	123.02	114.03
27	P	307	CHD	C15-C14-C13	2.80	106.30	103.55
14	A	602	HEA	CMB-C2B-C3B	-2.78	125.04	130.34
25	C	302	PEK	O03-C21-C22	2.78	120.64	111.91
27	W	101	CHD	C18-C13-C14	-2.78	106.86	111.21
14	A	601[A]	HEA	CHA-C4D-C3D	-2.78	120.75	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-2.78	120.75	124.84
22	L	101	TGL	CG3-CG2-CG1	-2.77	105.23	111.79
14	N	601[A]	HEA	CHB-C1B-C2B	-2.77	120.65	124.98
14	N	601[B]	HEA	CHB-C1B-C2B	-2.77	120.65	124.98
21	K	101	DMU	O1-C10-C5	2.76	116.20	110.35
25	P	304	PEK	O03-C21-C22	2.76	120.57	111.91
14	A	601[B]	HEA	C25-C23-C24	2.76	120.70	114.60
14	N	601[A]	HEA	CBA-CAA-C2A	2.76	117.25	112.60
14	N	601[B]	HEA	CBA-CAA-C2A	2.76	117.25	112.60
14	A	601[A]	HEA	OMA-CMA-C3A	-2.76	118.90	124.91
14	A	601[B]	HEA	OMA-CMA-C3A	-2.76	118.90	124.91
27	T	101	CHD	C19-C10-C1	-2.76	103.82	108.26
27	P	308	CHD	C18-C13-C17	-2.75	106.90	111.21
21	K	104	DMU	O1-C9-C8	2.75	114.69	109.69
21	P	316	DMU	O1-C9-C11	2.75	113.27	106.44
21	G	104	DMU	C10-C5-C7	2.75	115.71	110.00
25	C	309	PEK	O01-C1-O02	-2.74	117.08	123.70
19	P	305	PGV	C27-C26-C25	-2.74	100.51	114.42
19	C	308	PGV	O04-C19-C20	-2.73	113.08	123.73
26	G	101	CDL	CB6-OB8-CB7	2.73	127.23	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Y	102	CHD	C21-C20-C17	2.72	117.09	112.92
21	X	101	DMU	C2-C3-C4	2.71	117.13	110.93
14	N	601[A]	HEA	O2A-CGA-CBA	2.70	122.71	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	2.70	122.71	114.03
14	A	601[A]	HEA	C3C-C4C-NC	2.70	112.69	109.21
14	A	601[B]	HEA	C3C-C4C-NC	2.70	112.69	109.21
27	W	101	CHD	C18-C13-C17	2.70	115.43	111.21
14	A	602	HEA	C27-C19-C18	-2.69	116.77	123.68
14	A	601[A]	HEA	CHC-C4B-NB	-2.69	121.05	124.38
14	A	601[B]	HEA	CHC-C4B-NB	-2.69	121.05	124.38
14	N	602	HEA	CHD-C1D-C2D	-2.68	119.30	126.72
25	C	302	PEK	O03-C21-O04	-2.67	116.85	123.59
14	N	601[A]	HEA	C13-C14-C15	-2.67	121.24	127.66
14	N	601[B]	HEA	C13-C14-C15	-2.67	121.24	127.66
21	X	101	DMU	O1-C10-C5	2.66	115.98	110.35
25	G	102	PEK	O03-C21-C22	2.66	120.26	111.91
25	C	309	PEK	C02-O01-C1	-2.66	111.25	117.79
26	P	306	CDL	CB2-C1-CA2	-2.66	104.97	112.79
26	G	101	CDL	OB6-CB5-OB7	-2.66	117.28	123.70
19	P	301	PGV	C01-O03-C19	-2.65	107.30	117.12
27	L	103	CHD	C19-C10-C9	-2.64	107.54	111.18
21	O	305	DMU	C6-O5-C4	-2.64	108.51	113.69
26	T	102	CDL	C45-C44-C43	-2.63	101.07	114.42
26	G	101	CDL	C40-C39-C38	2.62	127.73	114.42
21	B	306	DMU	O16-C6-C1	2.62	112.39	108.30
14	A	602	HEA	C4B-NB-C1B	-2.62	102.37	105.07
14	N	602	HEA	C26-C15-C16	2.61	119.67	115.27
22	Q	201	TGL	OG2-CB1-CB2	2.61	117.13	111.50
21	T	103	DMU	O1-C9-C8	2.60	114.42	109.69
27	J	101	CHD	C23-C22-C20	-2.60	109.76	114.52
27	C	305	CHD	C4-C5-C10	2.60	115.42	112.66
21	P	316	DMU	C8-C7-C5	-2.60	106.28	110.82
22	O	301	TGL	OG2-CB1-OB1	-2.60	117.42	123.70
27	J	101	CHD	C11-C9-C8	-2.60	107.08	110.88
21	K	106	DMU	C10-O7-C3	-2.59	111.54	117.96
27	T	101	CHD	C6-C5-C4	-2.59	108.21	111.19
27	J	101	CHD	C19-C10-C9	-2.59	107.62	111.18
22	Q	201	TGL	OG1-CA1-CA2	2.58	120.02	111.91
26	C	304	CDL	OB8-CB7-OB9	-2.58	117.07	123.59
27	W	101	CHD	C11-C9-C8	2.58	114.65	110.88
21	K	101	DMU	C10-C5-C7	2.57	115.36	110.00
22	L	101	TGL	CG2-OG2-CB1	2.57	124.13	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	306	DMU	O5-C6-C1	-2.57	104.91	110.35
22	D	201	TGL	OG1-CA1-CA2	2.57	119.97	111.91
14	A	602	HEA	C1D-ND-C4D	-2.56	102.42	105.07
21	B	306	DMU	O6-C11-C9	2.56	120.08	111.29
21	K	102	DMU	C7-C8-C9	-2.56	105.67	110.24
27	W	101	CHD	C13-C14-C8	-2.56	111.47	114.74
14	A	602	HEA	C26-C15-C16	2.56	119.57	115.27
19	A	607	PGV	O01-C1-C2	2.55	116.99	111.50
14	N	602	HEA	OMA-CMA-C3A	-2.54	119.38	124.91
21	T	103	DMU	O1-C9-C11	2.53	112.74	106.44
14	N	602	HEA	O2A-CGA-CBA	2.53	122.17	114.03
22	Y	101	TGL	OG3-CC1-OC1	-2.53	117.22	123.59
21	X	102	DMU	C6-C1-C2	2.52	115.24	110.00
21	K	104	DMU	C7-C8-C9	2.52	114.73	110.24
14	A	602	HEA	C2D-C1D-ND	2.51	112.82	109.84
19	P	302	PGV	O01-C1-O02	-2.51	117.63	123.70
26	C	304	CDL	OA8-CA7-C31	2.50	119.76	111.91
25	P	304	PEK	C3-C2-C1	-2.50	104.53	113.62
21	C	312	DMU	O5-C6-C1	2.50	115.64	110.35
26	T	102	CDL	OA8-CA7-C31	2.50	119.75	111.91
21	K	102	DMU	O1-C10-C5	2.49	115.62	110.35
14	N	601[A]	HEA	O1A-CGA-CBA	-2.49	115.08	123.08
14	N	601[B]	HEA	O1A-CGA-CBA	-2.49	115.08	123.08
25	G	102	PEK	C2-C3-C4	-2.49	108.79	113.23
14	N	601[A]	HEA	C2B-C1B-NB	2.48	112.86	109.88
14	N	601[B]	HEA	C2B-C1B-NB	2.48	112.86	109.88
14	A	601[A]	HEA	C2B-C1B-NB	2.48	112.85	109.88
14	A	601[B]	HEA	C2B-C1B-NB	2.48	112.85	109.88
19	P	302	PGV	C21-C20-C19	-2.48	104.60	113.62
26	C	304	CDL	OA6-CA4-CA3	2.48	117.38	108.40
25	C	307	PEK	C03-C02-C01	2.48	117.65	111.79
25	C	309	PEK	O03-C21-O04	-2.48	117.34	123.59
14	A	602	HEA	C13-C12-C11	-2.47	110.63	114.35
25	G	102	PEK	C8-C7-C6	-2.47	99.84	112.02
27	X	105	CHD	C11-C12-C13	-2.47	108.71	111.24
21	K	103	DMU	O1-C9-C11	2.47	112.57	106.44
21	Q	203	DMU	O5-C6-C1	2.47	115.57	110.35
21	P	314	DMU	O1-C9-C11	2.46	112.56	106.44
27	Y	102	CHD	C11-C9-C10	-2.46	111.19	113.73
27	T	101	CHD	C1-C10-C5	2.45	111.40	107.77
21	K	105	DMU	C18-O16-C6	-2.45	109.77	113.84
27	P	307	CHD	O25-C24-C23	-2.45	115.20	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	101	CHD	C5-C4-C3	2.45	116.36	112.76
27	Y	102	CHD	C21-C20-C22	-2.45	106.53	110.36
27	C	305	CHD	C14-C8-C9	-2.45	106.35	109.71
21	C	312	DMU	O1-C9-C8	2.45	114.14	109.69
21	K	102	DMU	C6-O5-C4	2.44	118.49	113.69
19	A	608	PGV	O03-C19-C20	2.44	119.56	111.91
19	N	607	PGV	C3-C2-C1	-2.44	104.75	113.62
14	N	601[A]	HEA	C2D-C1D-ND	2.44	112.73	109.84
14	N	601[B]	HEA	C2D-C1D-ND	2.44	112.73	109.84
14	A	602	HEA	CHB-C1B-NB	-2.43	121.79	124.43
21	X	101	DMU	O5-C6-C1	-2.43	105.20	110.35
27	P	308	CHD	C11-C9-C10	-2.43	111.22	113.73
21	K	106	DMU	O7-C10-C5	2.42	114.38	108.10
19	P	305	PGV	O03-C19-O04	-2.42	117.48	123.59
21	O	305	DMU	O5-C4-C57	2.42	112.45	106.44
21	L	102	DMU	O5-C4-C57	2.42	112.44	106.44
27	X	105	CHD	C5-C6-C7	-2.41	111.80	114.46
14	A	601[A]	HEA	O1A-CGA-CBA	-2.40	115.36	123.08
14	A	601[B]	HEA	O1A-CGA-CBA	-2.40	115.36	123.08
19	P	305	PGV	O01-C1-C2	2.40	116.68	111.50
27	J	101	CHD	C13-C14-C8	-2.40	111.67	114.74
21	T	103	DMU	C6-C1-C2	2.40	114.99	110.00
27	X	105	CHD	C1-C10-C5	2.39	111.31	107.77
27	Y	102	CHD	C22-C23-C24	-2.38	106.18	112.51
21	B	306	DMU	C18-O16-C6	2.38	117.79	113.84
21	X	102	DMU	C6-O5-C4	2.38	118.36	113.69
27	Y	102	CHD	C1-C2-C3	-2.38	107.42	110.47
27	C	306	CHD	C1-C2-C3	-2.37	107.43	110.47
21	Q	203	DMU	O1-C9-C11	2.37	112.32	106.44
27	J	101	CHD	C14-C8-C7	2.37	114.94	111.81
27	X	105	CHD	C1-C2-C3	2.36	113.50	110.47
24	B	303	PSC	O01-C1-O02	-2.36	118.00	123.70
14	A	601[A]	HEA	C13-C14-C15	-2.35	122.00	127.66
14	A	601[B]	HEA	C13-C14-C15	-2.35	122.00	127.66
14	N	601[A]	HEA	C4D-C3D-C2D	-2.35	103.47	106.90
14	N	601[B]	HEA	C4D-C3D-C2D	-2.35	103.47	106.90
22	Y	101	TGL	OG1-CA1-OA1	-2.35	117.67	123.59
21	K	104	DMU	O7-C3-C2	2.35	113.52	107.28
21	X	101	DMU	C1-C2-C3	2.34	115.03	109.68
19	P	305	PGV	O01-C1-O02	-2.34	118.05	123.70
21	K	105	DMU	C10-O1-C9	2.34	118.28	113.69
19	C	308	PGV	O01-C1-O02	-2.34	118.05	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	Q	203	DMU	O7-C3-C4	2.34	115.85	109.45
19	N	607	PGV	O03-C19-O04	-2.33	117.71	123.59
25	C	307	PEK	C2-C3-C4	-2.33	109.08	113.23
21	A	616	DMU	C10-O1-C9	2.33	118.26	113.69
27	P	308	CHD	C17-C13-C12	2.33	119.79	117.67
26	P	306	CDL	C21-C20-C19	-2.32	102.62	114.42
26	P	306	CDL	OB2-PB2-OB3	2.32	118.15	109.07
21	O	305	DMU	C8-C7-C5	2.32	114.88	110.82
21	O	305	DMU	O7-C10-C5	2.32	114.11	108.10
26	T	102	CDL	CB4-OB6-CB5	-2.32	112.08	117.79
27	Y	102	CHD	O25-C24-C23	-2.32	115.64	123.08
21	G	104	DMU	O7-C10-O1	-2.31	104.22	110.67
24	N	608	PSC	O01-C1-O02	-2.30	118.15	123.70
26	G	101	CDL	C39-C38-C37	2.29	126.05	114.42
21	P	316	DMU	C10-C5-C7	2.29	114.76	110.00
26	P	306	CDL	OB8-CB7-OB9	-2.29	117.82	123.59
19	A	608	PGV	C25-C24-C23	-2.29	102.81	114.42
14	A	601[A]	HEA	O2D-CGD-O1D	-2.29	117.60	123.30
14	A	601[B]	HEA	O2D-CGD-O1D	-2.29	117.60	123.30
21	Z	101	DMU	O49-C1-C2	-2.29	105.06	110.35
27	T	101	CHD	C21-C20-C22	-2.28	106.78	110.36
26	G	101	CDL	C45-C44-C43	-2.28	102.87	114.42
27	T	101	CHD	C14-C13-C12	-2.28	105.28	107.40
21	G	104	DMU	C10-O1-C9	2.27	118.15	113.69
21	K	101	DMU	C2-C3-C4	2.27	116.13	110.93
22	Y	101	TGL	OG2-CB1-OB1	-2.27	118.22	123.70
27	X	105	CHD	C14-C8-C7	2.27	114.81	111.81
21	C	312	DMU	C10-C5-C7	2.27	114.71	110.00
26	C	304	CDL	C61-C60-C59	-2.26	102.93	114.42
27	X	105	CHD	C22-C20-C17	2.26	114.95	110.28
26	P	306	CDL	OA8-CA7-OA9	-2.25	117.91	123.59
27	C	306	CHD	C22-C20-C17	-2.25	105.63	110.28
21	K	101	DMU	C8-C7-C5	2.25	114.75	110.82
21	K	101	DMU	O49-C1-C2	-2.24	105.17	110.35
14	A	601[A]	HEA	CHD-C1D-C2D	-2.24	120.53	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.24	120.53	126.72
21	D	202	DMU	O1-C9-C11	2.24	112.00	106.44
27	Y	102	CHD	O7-C7-C8	2.23	114.40	109.43
14	N	602	HEA	C21-C20-C19	2.22	120.28	112.98
14	N	602	HEA	O1A-CGA-CBA	-2.22	115.96	123.08
21	X	102	DMU	O5-C4-C57	2.21	111.94	106.44
27	J	101	CHD	C2-C1-C10	2.21	116.57	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	306	CHD	C15-C14-C8	-2.21	115.25	118.33
19	N	607	PGV	C26-C25-C24	-2.21	103.22	114.42
26	P	306	CDL	OB6-CB5-OB7	-2.20	118.38	123.70
25	C	302	PEK	C2-C3-C4	-2.20	109.31	113.23
27	G	103	CHD	C15-C14-C13	2.20	105.71	103.55
27	C	306	CHD	C18-C13-C17	-2.20	107.77	111.21
14	A	601[A]	HEA	C4A-CHB-C1B	2.20	125.46	122.56
14	A	601[B]	HEA	C4A-CHB-C1B	2.20	125.46	122.56
19	C	308	PGV	C21-C20-C19	-2.19	105.64	113.62
21	X	102	DMU	C3-C2-C1	2.19	114.65	110.82
14	A	602	HEA	C16-C15-C14	-2.19	116.68	121.12
21	K	101	DMU	C6-C1-C2	2.19	114.56	110.00
21	T	103	DMU	C1-C2-C3	2.19	114.68	109.68
22	Q	201	TGL	OG3-CC1-CC2	2.19	118.77	111.91
22	L	101	TGL	CC3-CC2-CC1	-2.18	105.69	113.62
25	C	307	PEK	C02-O01-C1	-2.18	112.42	117.79
25	C	302	PEK	C33-C32-C31	-2.18	103.36	114.42
21	M	101	DMU	O16-C6-C1	2.18	111.70	108.30
14	A	601[A]	HEA	CHA-C4D-ND	2.18	126.80	124.43
14	A	601[B]	HEA	CHA-C4D-ND	2.18	126.80	124.43
27	Y	102	CHD	C4-C3-C2	-2.18	107.95	110.55
21	K	104	DMU	C1-C2-C3	2.17	114.64	109.68
21	O	305	DMU	C2-C3-C4	2.17	115.90	110.93
24	N	608	PSC	C04-C05-N	-2.17	108.55	115.78
27	W	101	CHD	C6-C5-C4	-2.17	108.70	111.19
24	B	303	PSC	O01-C02-C03	2.16	116.24	108.40
21	Q	203	DMU	O2-C8-C7	-2.16	105.35	110.35
27	J	101	CHD	C15-C14-C8	2.16	121.35	118.33
27	C	305	CHD	C9-C8-C7	-2.16	109.29	111.88
27	P	307	CHD	C6-C7-C8	2.16	113.78	111.48
24	N	608	PSC	C26-C25-C24	-2.15	103.49	114.42
27	J	101	CHD	C11-C9-C10	-2.15	111.51	113.73
21	O	305	DMU	O1-C9-C8	2.15	113.61	109.69
21	O	305	DMU	O7-C3-C2	2.15	113.00	107.28
19	P	301	PGV	C03-C02-C01	-2.15	106.71	111.79
21	Z	101	DMU	O5-C4-C57	2.15	111.77	106.44
22	Q	201	TGL	OG3-CG3-CG2	2.14	114.67	108.43
19	N	607	PGV	C29-C28-C27	-2.14	103.55	114.42
27	C	306	CHD	C6-C5-C4	-2.14	108.73	111.19
14	N	602	HEA	C3C-C4C-NC	2.14	111.97	109.21
21	K	104	DMU	C6-C1-C2	2.14	114.45	110.00
26	G	101	CDL	PA1-OA5-CA3	2.13	134.19	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	103	CHD	C9-C11-C12	-2.13	111.48	114.30
27	P	307	CHD	C14-C8-C7	-2.13	108.98	111.81
21	M	101	DMU	C10-O7-C3	-2.13	112.70	117.96
19	P	302	PGV	O03-C19-O04	-2.13	118.22	123.59
14	A	602	HEA	OMA-CMA-C3A	-2.12	120.29	124.91
25	C	307	PEK	O11-P-O14	-2.12	100.79	109.07
19	P	302	PGV	C31-C30-C29	-2.12	103.68	114.42
27	X	105	CHD	C23-C22-C20	-2.12	110.65	114.52
27	W	101	CHD	C1-C10-C5	2.11	110.89	107.77
14	N	601[B]	HEA	C17-C18-C19	-2.11	122.57	127.66
25	C	302	PEK	C01-O03-C21	2.11	124.94	117.12
26	G	101	CDL	C61-C60-C59	-2.11	103.72	114.42
25	C	307	PEK	O13-P-O14	2.10	122.64	112.24
21	Z	101	DMU	C1-C2-C3	2.10	114.48	109.68
26	P	306	CDL	CA4-OA6-CA5	-2.10	112.62	117.79
21	P	314	DMU	O49-C1-C6	-2.10	104.95	110.05
14	N	602	HEA	O2D-CGD-O1D	-2.10	118.07	123.30
21	K	102	DMU	C6-C1-C2	-2.09	105.64	110.00
21	K	105	DMU	O5-C4-C3	2.09	114.16	109.75
27	J	101	CHD	O7-C7-C8	2.09	114.10	109.43
27	P	307	CHD	C14-C8-C9	-2.09	106.84	109.71
27	C	305	CHD	C19-C10-C1	-2.09	104.89	108.26
24	B	303	PSC	C07-N-C06	-2.09	103.61	108.97
22	O	301	TGL	CG3-OG3-CC1	2.08	124.83	117.12
19	C	303	PGV	O01-C1-O02	-2.08	118.68	123.70
27	W	101	CHD	C16-C17-C20	2.08	115.36	112.15
27	L	103	CHD	O25-C24-C23	-2.07	116.42	123.08
27	L	103	CHD	C22-C23-C24	-2.07	107.01	112.51
27	T	101	CHD	C11-C9-C8	-2.07	107.84	110.88
27	P	307	CHD	C17-C13-C12	2.07	119.56	117.67
27	X	105	CHD	O7-C7-C8	2.06	114.03	109.43
14	A	601[A]	HEA	CMD-C2D-C1D	2.05	128.17	125.04
14	A	601[B]	HEA	CMD-C2D-C1D	2.05	128.17	125.04
21	P	316	DMU	O5-C4-C57	-2.05	101.34	106.44
21	G	104	DMU	C6-O5-C4	2.05	117.71	113.69
21	M	101	DMU	C28-C25-C22	-2.04	104.05	114.42
26	C	304	CDL	C76-C75-C74	-2.04	104.05	114.42
21	C	312	DMU	C10-O7-C3	-2.04	112.91	117.96
19	A	607	PGV	C9-C10-C11	-2.04	100.74	112.43
21	T	103	DMU	C10-C5-C7	2.03	114.23	110.00
27	L	103	CHD	C15-C14-C8	2.03	121.17	118.33
14	A	602	HEA	C3B-C4B-NB	2.03	112.24	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	101	CHD	C19-C10-C5	-2.03	106.92	110.36
27	C	305	CHD	C5-C4-C3	-2.03	109.78	112.76
21	K	102	DMU	C8-C7-C5	-2.02	107.30	110.82
19	C	303	PGV	O03-C19-C20	2.02	118.24	111.91
21	K	101	DMU	C1-C2-C3	2.02	114.29	109.68
26	P	306	CDL	C57-C56-C55	-2.02	104.19	114.42
21	K	104	DMU	O16-C6-C1	2.02	111.45	108.30
26	T	102	CDL	CB6-CB4-CB3	-2.02	107.02	111.79
27	X	105	CHD	C14-C13-C12	2.01	109.28	107.40
26	P	306	CDL	C22-C21-C20	2.01	124.65	114.42
27	G	103	CHD	C6-C5-C4	2.01	113.51	111.19
21	K	103	DMU	C2-C3-C4	2.01	115.53	110.93
14	A	602	HEA	CHD-C1D-C2D	-2.01	121.16	126.72
14	N	601[A]	HEA	O2D-CGD-CBD	2.01	120.48	114.03
14	N	601[B]	HEA	O2D-CGD-CBD	2.01	120.48	114.03
27	C	305	CHD	C16-C17-C13	2.00	105.52	103.55

There are no chirality outliers.

All (948) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[B]	HEA	C18-C19-C20-C21
19	A	608	PGV	C04-O12-P-O14
19	A	608	PGV	C2-C1-O01-C02
19	A	608	PGV	O04-C19-O03-C01
19	A	608	PGV	C20-C19-O03-C01
19	C	308	PGV	C04-O12-P-O13
19	C	308	PGV	O01-C02-C03-O11
19	C	308	PGV	O04-C19-O03-C01
19	C	308	PGV	C20-C19-O03-C01
19	N	607	PGV	C04-O12-P-O13
19	N	607	PGV	O04-C19-O03-C01
19	N	607	PGV	C20-C19-O03-C01
19	N	607	PGV	C10-C11-C12-C13
19	P	302	PGV	C04-O12-P-O13
19	P	302	PGV	C10-C11-C12-C13
21	B	306	DMU	C19-C18-O16-C6
21	C	312	DMU	C1-C6-O16-C18
21	C	312	DMU	O5-C6-O16-C18
21	K	101	DMU	C1-C6-O16-C18
21	K	104	DMU	C1-C6-O16-C18
21	K	104	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
21	K	104	DMU	C19-C18-O16-C6
21	K	106	DMU	C19-C18-O16-C6
21	L	102	DMU	C1-C6-O16-C18
21	L	102	DMU	O5-C6-O16-C18
21	O	305	DMU	C1-C6-O16-C18
21	O	305	DMU	O5-C6-O16-C18
21	P	314	DMU	O5-C6-O16-C18
21	P	316	DMU	C19-C18-O16-C6
21	Q	203	DMU	C1-C6-O16-C18
21	Q	203	DMU	O5-C6-O16-C18
21	Q	203	DMU	C5-C10-O7-C3
21	X	102	DMU	O5-C6-O16-C18
21	X	102	DMU	C19-C18-O16-C6
21	X	103	DMU	C19-C18-O16-C6
22	L	101	TGL	CB2-CB1-OG2-CG2
22	L	101	TGL	OB1-CB1-OG2-CG2
22	Q	201	TGL	CC2-CC1-OG3-CG3
22	Y	101	TGL	OB1-CB1-OG2-CG2
24	B	303	PSC	C03-O11-P-O13
24	B	303	PSC	C04-O12-P-O11
24	B	303	PSC	C04-O12-P-O13
24	B	303	PSC	C04-O12-P-O14
24	B	303	PSC	C2-C1-O01-C02
24	B	303	PSC	C9-C10-C11-C12
24	N	608	PSC	C04-O12-P-O11
24	N	608	PSC	C04-O12-P-O13
24	N	608	PSC	C04-O12-P-O14
24	N	608	PSC	O12-C04-C05-N
24	N	608	PSC	O02-C1-O01-C02
24	N	608	PSC	C2-C1-O01-C02
25	C	302	PEK	C10-C11-C12-C13
25	C	307	PEK	C03-O11-P-O13
25	C	307	PEK	C04-O12-P-O13
25	C	307	PEK	C04-O12-P-O14
25	C	307	PEK	O04-C21-O03-C01
25	C	307	PEK	C22-C21-O03-C01
25	C	307	PEK	C11-C12-C13-C14
25	C	309	PEK	O04-C21-O03-C01
25	C	309	PEK	C22-C21-O03-C01
25	C	309	PEK	C7-C8-C9-C10
25	G	102	PEK	O04-C21-O03-C01
25	G	102	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
25	P	309	PEK	C04-O12-P-O13
25	P	309	PEK	O04-C21-O03-C01
25	P	309	PEK	C22-C21-O03-C01
25	P	309	PEK	C6-C7-C8-C9
25	P	309	PEK	C7-C8-C9-C10
25	P	309	PEK	C10-C11-C12-C13
26	C	304	CDL	CB2-C1-CA2-OA2
26	C	304	CDL	OA9-CA7-OA8-CA6
26	C	304	CDL	C31-CA7-OA8-CA6
26	C	304	CDL	CB2-OB2-PB2-OB4
26	C	304	CDL	CB3-OB5-PB2-OB3
26	C	304	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	CA2-OA2-PA1-OA4
26	G	101	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	C31-CA7-OA8-CA6
26	G	101	CDL	CB2-OB2-PB2-OB3
26	G	101	CDL	CB2-OB2-PB2-OB4
26	G	101	CDL	CB3-OB5-PB2-OB2
26	G	101	CDL	CB3-OB5-PB2-OB3
26	G	101	CDL	CB3-OB5-PB2-OB4
26	P	306	CDL	OA9-CA7-OA8-CA6
26	P	306	CDL	C31-CA7-OA8-CA6
26	P	306	CDL	CB2-OB2-PB2-OB4
26	P	306	CDL	CB3-OB5-PB2-OB2
26	P	306	CDL	CB3-OB5-PB2-OB3
26	P	306	CDL	CB3-OB5-PB2-OB4
26	T	102	CDL	CA2-OA2-PA1-OA4
26	T	102	CDL	C11-CA5-OA6-CA4
26	T	102	CDL	OA9-CA7-OA8-CA6
26	T	102	CDL	C31-CA7-OA8-CA6
26	T	102	CDL	CB2-OB2-PB2-OB4
26	T	102	CDL	CB3-OB5-PB2-OB2
26	T	102	CDL	CB3-OB5-PB2-OB3
26	T	102	CDL	CB3-OB5-PB2-OB4
27	J	101	CHD	C13-C17-C20-C21
27	J	101	CHD	C13-C17-C20-C22
27	J	101	CHD	C16-C17-C20-C21
27	J	101	CHD	C16-C17-C20-C22
27	W	101	CHD	C13-C17-C20-C22
27	X	105	CHD	C16-C17-C20-C21
21	D	202	DMU	C4-C3-O7-C10
21	L	102	DMU	C2-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
21	K	104	DMU	C2-C3-O7-C10
22	Q	201	TGL	OC1-CC1-OG3-CG3
21	A	616	DMU	O1-C10-O7-C3
21	B	306	DMU	O1-C10-O7-C3
21	X	101	DMU	O1-C10-O7-C3
21	B	306	DMU	C2-C3-O7-C10
21	K	106	DMU	C3-C4-C57-O61
21	K	102	DMU	O1-C10-O7-C3
21	Q	203	DMU	O1-C10-O7-C3
21	K	106	DMU	O6-C11-C9-C8
27	L	103	CHD	C16-C17-C20-C21
27	W	101	CHD	C16-C17-C20-C21
27	L	103	CHD	C13-C17-C20-C21
27	L	103	CHD	C16-C17-C20-C22
27	W	101	CHD	C16-C17-C20-C22
27	L	103	CHD	C13-C17-C20-C22
21	B	306	DMU	O6-C11-C9-C8
21	O	305	DMU	C5-C10-O7-C3
19	A	608	PGV	O02-C1-O01-C02
19	N	607	PGV	O02-C1-O01-C02
24	B	303	PSC	O02-C1-O01-C02
26	C	304	CDL	OA7-CA5-OA6-CA4
26	P	306	CDL	OA7-CA5-OA6-CA4
26	T	102	CDL	OA7-CA5-OA6-CA4
22	Y	101	TGL	CB2-CB1-OG2-CG2
26	C	304	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	C11-CA5-OA6-CA4
27	X	105	CHD	C13-C17-C20-C21
27	X	105	CHD	C16-C17-C20-C22
27	X	105	CHD	C13-C17-C20-C22
21	B	306	DMU	O5-C4-C57-O61
14	A	601[B]	HEA	C27-C19-C20-C21
21	K	105	DMU	O6-C11-C9-C8
22	O	301	TGL	CC2-CC1-OG3-CG3
24	N	608	PSC	C20-C19-O03-C01
21	O	305	DMU	O5-C4-C57-O61
19	C	303	PGV	C10-C11-C12-C13
19	P	305	PGV	C10-C11-C12-C13
24	N	608	PSC	C11-C12-C13-C14
25	C	307	PEK	C10-C11-C12-C13
25	C	307	PEK	C13-C14-C15-C16
22	D	201	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C77-C78-C79-C80
21	A	616	DMU	O5-C4-C57-O61
21	D	202	DMU	O6-C11-C9-O1
21	X	102	DMU	O5-C4-C57-O61
27	P	307	CHD	C17-C20-C22-C23
26	T	102	CDL	C40-C41-C42-C43
19	N	607	PGV	O12-C04-C05-O05
26	C	304	CDL	C60-C61-C62-C63
24	N	608	PSC	O04-C19-O03-C01
21	K	103	DMU	O5-C4-C57-O61
21	K	106	DMU	O5-C4-C57-O61
21	Q	203	DMU	O5-C4-C57-O61
21	T	103	DMU	O6-C11-C9-O1
19	N	607	PGV	C2-C1-O01-C02
21	L	102	DMU	O6-C11-C9-O1
21	Q	203	DMU	C4-C3-O7-C10
24	N	608	PSC	C20-C21-C22-C23
21	K	102	DMU	O5-C4-C57-O61
21	P	316	DMU	O6-C11-C9-O1
21	P	316	DMU	O6-C11-C9-C8
22	D	201	TGL	CC2-CC1-OG3-CG3
21	B	306	DMU	O6-C11-C9-O1
21	K	105	DMU	O6-C11-C9-O1
21	O	305	DMU	C3-C4-C57-O61
22	O	301	TGL	OC1-CC1-OG3-CG3
21	T	103	DMU	C2-C3-O7-C10
21	G	104	DMU	O5-C4-C57-O61
21	K	105	DMU	O5-C4-C57-O61
21	K	106	DMU	O6-C11-C9-O1
21	T	103	DMU	O5-C4-C57-O61
14	N	601[B]	HEA	C27-C19-C20-C21
21	K	103	DMU	C3-C4-C57-O61
21	X	102	DMU	C3-C4-C57-O61
14	N	601[B]	HEA	C18-C19-C20-C21
19	A	607	PGV	C26-C27-C28-C29
22	L	101	TGL	C11-C10-CB9-CB8
27	P	307	CHD	C21-C20-C22-C23
21	L	102	DMU	O6-C11-C9-C8
14	A	601[B]	HEA	C15-C16-C17-C18
26	T	102	CDL	C80-C81-C82-C83
22	L	101	TGL	CA2-CA1-OG1-CG1
26	P	306	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	O12-C04-C05-C06
19	N	607	PGV	O12-C04-C05-C06
26	P	306	CDL	CB2-C1-CA2-OA2
22	B	301	TGL	CC2-CC1-OG3-CG3
21	C	312	DMU	O5-C4-C57-O61
21	Q	203	DMU	O6-C11-C9-O1
27	C	305	CHD	C17-C20-C22-C23
21	B	306	DMU	C3-C4-C57-O61
21	G	104	DMU	C3-C4-C57-O61
21	K	102	DMU	C3-C4-C57-O61
21	T	103	DMU	C3-C4-C57-O61
26	P	306	CDL	O1-C1-CA2-OA2
21	Q	203	DMU	C2-C3-O7-C10
26	P	306	CDL	C37-C38-C39-C40
21	T	103	DMU	O6-C11-C9-C8
21	D	202	DMU	O6-C11-C9-C8
21	Q	203	DMU	C3-C4-C57-O61
19	C	308	PGV	C1-C2-C3-C4
25	C	307	PEK	C21-C22-C23-C24
27	C	305	CHD	C21-C20-C22-C23
22	Q	201	TGL	CB1-CB2-CB3-CB4
25	C	307	PEK	C4-C5-C6-C7
22	D	201	TGL	CB1-CB2-CB3-CB4
22	Y	101	TGL	CA1-CA2-CA3-CA4
25	C	307	PEK	C1-C2-C3-C4
26	P	306	CDL	C80-C81-C82-C83
21	T	103	DMU	C4-C3-O7-C10
22	B	301	TGL	CA1-CA2-CA3-CA4
22	B	301	TGL	CB1-CB2-CB3-CB4
24	B	303	PSC	C22-C23-C24-C25
21	K	105	DMU	C3-C4-C57-O61
27	W	101	CHD	C13-C17-C20-C21
26	C	304	CDL	C62-C63-C64-C65
22	B	301	TGL	OC1-CC1-OG3-CG3
21	A	616	DMU	C3-C4-C57-O61
21	K	101	DMU	O5-C6-O16-C18
14	N	601[B]	HEA	C15-C16-C17-C18
21	Q	203	DMU	O16-C18-C19-C22
21	Z	101	DMU	O16-C18-C19-C22
19	A	608	PGV	O12-C04-C05-O05
26	C	304	CDL	O1-C1-CA2-OA2
22	L	101	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
21	X	103	DMU	O16-C18-C19-C22
25	P	304	PEK	C7-C8-C9-C10
14	A	601[B]	HEA	C16-C17-C18-C19
19	C	308	PGV	C04-O12-P-O11
19	N	607	PGV	C04-O12-P-O11
19	P	302	PGV	C04-O12-P-O11
24	N	608	PSC	C03-O11-P-O12
25	C	307	PEK	C03-O11-P-O12
25	C	307	PEK	C04-O12-P-O11
25	P	309	PEK	C04-O12-P-O11
26	C	304	CDL	CB2-OB2-PB2-OB5
26	C	304	CDL	CB3-OB5-PB2-OB2
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CA3-OA5-PA1-OA2
26	G	101	CDL	CB2-OB2-PB2-OB5
26	T	102	CDL	CA2-OA2-PA1-OA5
26	T	102	CDL	CB2-OB2-PB2-OB5
26	G	101	CDL	CA5-C11-C12-C13
26	G	101	CDL	C80-C81-C82-C83
25	C	309	PEK	O02-C1-O01-C02
24	B	303	PSC	C04-C05-N-C06
24	B	303	PSC	C04-C05-N-C08
21	X	101	DMU	O6-C11-C9-C8
22	Q	201	TGL	CA6-CA7-CA8-CA9
25	C	309	PEK	C2-C1-O01-C02
26	C	304	CDL	C51-CB5-OB6-CB4
26	P	306	CDL	C51-CB5-OB6-CB4
19	A	608	PGV	C13-C14-C15-C16
21	B	306	DMU	C25-C28-C31-C34
21	G	104	DMU	C28-C31-C34-C37
21	L	102	DMU	C19-C22-C25-C28
22	D	201	TGL	CA3-CA4-CA5-CA6
22	L	101	TGL	CA3-CA4-CA5-CA6
22	O	301	TGL	CA5-CA6-CA7-CA8
22	O	301	TGL	C10-C11-C12-C13
24	N	608	PSC	C29-C30-C31-C32
21	K	101	DMU	C22-C25-C28-C31
21	K	102	DMU	C28-C31-C34-C37
21	K	106	DMU	C19-C22-C25-C28
22	D	201	TGL	C11-C12-C13-C14
22	D	201	TGL	C13-C14-C29-C30
22	D	201	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	O	301	TGL	CB4-CB5-CB6-CB7
22	O	301	TGL	C16-C15-CC9-CC8
22	O	301	TGL	C15-C16-C17-C18
22	O	301	TGL	C23-C24-C25-C26
22	Q	201	TGL	CC9-C15-C16-C17
26	P	306	CDL	C52-C53-C54-C55
26	P	306	CDL	C72-C73-C74-C75
19	N	607	PGV	C03-C02-O01-C1
26	C	304	CDL	OB7-CB5-OB6-CB4
26	P	306	CDL	OB7-CB5-OB6-CB4
22	L	101	TGL	CB1-CB2-CB3-CB4
22	Y	101	TGL	CB3-CB4-CB5-CB6
22	Y	101	TGL	C10-C11-C12-C13
25	P	304	PEK	C16-C17-C18-C19
26	P	306	CDL	C59-C60-C61-C62
26	T	102	CDL	OA5-CA3-CA4-OA6
22	L	101	TGL	CA6-CA7-CA8-CA9
22	L	101	TGL	CC3-CC4-CC5-CC6
22	L	101	TGL	C17-C18-C19-C33
26	P	306	CDL	C17-C18-C19-C20
21	M	101	DMU	C19-C22-C25-C28
21	X	101	DMU	O16-C18-C19-C22
22	B	301	TGL	C10-C11-C12-C13
26	C	304	CDL	C59-C60-C61-C62
19	C	308	PGV	C5-C6-C7-C8
19	P	302	PGV	C5-C6-C7-C8
21	O	305	DMU	C19-C22-C25-C28
22	O	301	TGL	C11-C10-CB9-CB8
22	Q	201	TGL	CB9-C10-C11-C12
26	P	306	CDL	C34-C35-C36-C37
26	T	102	CDL	C73-C74-C75-C76
27	J	101	CHD	C17-C20-C22-C23
19	C	303	PGV	C13-C14-C15-C16
21	K	105	DMU	C25-C28-C31-C34
22	O	301	TGL	CC2-CC3-CC4-CC5
22	Y	101	TGL	CC3-CC4-CC5-CC6
26	G	101	CDL	C17-C18-C19-C20
19	P	305	PGV	C7-C8-C9-C10
21	D	202	DMU	C22-C25-C28-C31
21	X	101	DMU	C19-C22-C25-C28
21	X	104	DMU	C31-C34-C37-C40
22	L	101	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	O	301	TGL	CB6-CB7-CB8-CB9
22	Q	201	TGL	CB5-CB6-CB7-CB8
22	Q	201	TGL	CC6-CC7-CC8-CC9
22	B	301	TGL	C11-C12-C13-C14
22	O	301	TGL	CC4-CC5-CC6-CC7
22	Q	201	TGL	C12-C13-C14-C29
25	C	307	PEK	C32-C33-C34-C35
25	G	102	PEK	O02-C1-O01-C02
25	G	102	PEK	C2-C1-O01-C02
21	G	104	DMU	C31-C34-C37-C40
22	Q	201	TGL	C19-C33-C34-C35
19	P	305	PGV	C1-C2-C3-C4
24	B	303	PSC	C19-C20-C21-C22
21	K	104	DMU	C25-C28-C31-C34
22	B	301	TGL	CC4-CC5-CC6-CC7
22	B	301	TGL	C16-C15-CC9-CC8
26	C	304	CDL	C34-C35-C36-C37
24	B	303	PSC	C04-C05-N-C07
22	D	201	TGL	C16-C15-CC9-CC8
22	D	201	TGL	C18-C19-C33-C34
22	O	301	TGL	CA4-CA5-CA6-CA7
26	T	102	CDL	C20-C21-C22-C23
19	C	303	PGV	C20-C21-C22-C23
21	K	104	DMU	C28-C31-C34-C37
21	Z	101	DMU	C22-C25-C28-C31
22	B	301	TGL	C22-C23-C24-C25
26	G	101	CDL	C20-C21-C22-C23
21	D	202	DMU	C31-C34-C37-C40
22	D	201	TGL	CA9-C20-C21-C22
22	O	301	TGL	C12-C13-C14-C29
21	T	103	DMU	C19-C18-O16-C6
22	B	301	TGL	C12-C13-C14-C29
22	D	201	TGL	CB9-C10-C11-C12
21	K	104	DMU	C31-C34-C37-C40
25	C	302	PEK	C25-C26-C27-C28
25	C	309	PEK	C4-C5-C6-C7
19	C	308	PGV	C20-C21-C22-C23
19	C	308	PGV	C27-C28-C29-C30
26	C	304	CDL	C22-C23-C24-C25
22	D	201	TGL	CC6-CC7-CC8-CC9
19	P	302	PGV	C20-C19-O03-C01
22	B	301	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
22	L	101	TGL	C13-C14-C29-C30
25	P	309	PEK	C33-C34-C35-C36
21	K	103	DMU	O1-C10-O7-C3
19	C	308	PGV	C30-C31-C32-C33
22	B	301	TGL	C17-C18-C19-C33
22	O	301	TGL	CB5-CB6-CB7-CB8
22	O	301	TGL	CC5-CC6-CC7-CC8
22	Y	101	TGL	CB2-CB3-CB4-CB5
25	C	309	PEK	C31-C32-C33-C34
19	P	302	PGV	O04-C19-O03-C01
22	Q	201	TGL	C16-C17-C18-C19
22	B	301	TGL	C16-C17-C18-C19
22	L	101	TGL	C24-C25-C26-C27
26	C	304	CDL	C80-C81-C82-C83
22	Q	201	TGL	OB1-CB1-OG2-CG2
21	K	102	DMU	C18-C19-C22-C25
22	D	201	TGL	C21-C22-C23-C24
19	N	607	PGV	C4-C5-C6-C7
21	A	616	DMU	C19-C22-C25-C28
22	B	301	TGL	CA6-CA7-CA8-CA9
22	Y	101	TGL	CB7-CB8-CB9-C10
20	C	311	EDO	O1-C1-C2-O2
20	F	104	EDO	O1-C1-C2-O2
20	L	104	EDO	O1-C1-C2-O2
20	N	616	EDO	O1-C1-C2-O2
20	N	617	EDO	O1-C1-C2-O2
20	N	620	EDO	O1-C1-C2-O2
20	O	304	EDO	O1-C1-C2-O2
20	W	102	EDO	O1-C1-C2-O2
21	C	312	DMU	C18-C19-C22-C25
21	K	105	DMU	C31-C34-C37-C40
22	Q	201	TGL	CC7-CC8-CC9-C15
22	Q	201	TGL	C21-C22-C23-C24
26	C	304	CDL	C36-C37-C38-C39
22	D	201	TGL	CC1-CC2-CC3-CC4
19	A	608	PGV	C7-C8-C9-C10
25	G	102	PEK	C25-C26-C27-C28
21	X	102	DMU	C18-C19-C22-C25
21	K	104	DMU	O5-C4-C57-O61
25	C	302	PEK	C22-C23-C24-C25
25	G	102	PEK	C10-C11-C12-C13
19	A	608	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	B	301	TGL	OB1-CB1-OG2-CG2
22	D	201	TGL	OB1-CB1-OG2-CG2
21	Z	101	DMU	C28-C31-C34-C37
27	L	103	CHD	C20-C22-C23-C24
27	X	105	CHD	C20-C22-C23-C24
22	Y	101	TGL	CA7-CA8-CA9-C20
22	Y	101	TGL	C11-C10-CB9-CB8
19	N	607	PGV	C20-C21-C22-C23
19	N	607	PGV	C19-C20-C21-C22
21	X	103	DMU	O5-C4-C57-O61
21	P	316	DMU	C19-C22-C25-C28
21	M	101	DMU	C22-C25-C28-C31
22	Y	101	TGL	C18-C19-C33-C34
22	B	301	TGL	CA5-CA6-CA7-CA8
22	D	201	TGL	CB2-CB1-OG2-CG2
22	O	301	TGL	CB2-CB1-OG2-CG2
22	Q	201	TGL	CB2-CB1-OG2-CG2
25	C	307	PEK	C2-C1-O01-C02
26	G	101	CDL	C11-CA5-OA6-CA4
26	G	101	CDL	C51-CB5-OB6-CB4
19	P	302	PGV	O01-C02-C03-O11
26	P	306	CDL	C57-C58-C59-C60
22	B	301	TGL	C15-C16-C17-C18
22	L	101	TGL	CB6-CB7-CB8-CB9
22	Y	101	TGL	CA9-C20-C21-C22
26	G	101	CDL	OA7-CA5-OA6-CA4
26	G	101	CDL	OB7-CB5-OB6-CB4
21	K	103	DMU	C2-C3-O7-C10
22	B	301	TGL	C21-C22-C23-C24
22	O	301	TGL	C14-C29-C30-C31
21	B	306	DMU	C1-C6-O16-C18
21	X	102	DMU	C1-C6-O16-C18
22	Q	201	TGL	C10-C11-C12-C13
19	N	607	PGV	C14-C15-C16-C17
22	Q	201	TGL	CC2-CC3-CC4-CC5
22	Y	101	TGL	C11-C12-C13-C14
21	X	103	DMU	C19-C22-C25-C28
25	G	102	PEK	C33-C34-C35-C36
19	P	302	PGV	C26-C27-C28-C29
21	P	314	DMU	O16-C18-C19-C22
21	K	101	DMU	O6-C11-C9-O1
22	Y	101	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C23-C24-C25-C26
21	A	616	DMU	C18-C19-C22-C25
22	O	301	TGL	OB1-CB1-OG2-CG2
25	C	307	PEK	O02-C1-O01-C02
26	T	102	CDL	C51-CB5-OB6-CB4
22	L	101	TGL	CB2-CB3-CB4-CB5
21	P	316	DMU	C18-C19-C22-C25
26	P	306	CDL	C74-C75-C76-C77
26	T	102	CDL	CB4-CB3-OB5-PB2
21	Q	203	DMU	C25-C28-C31-C34
22	D	201	TGL	CC7-CC8-CC9-C15
22	Q	201	TGL	C23-C24-C25-C26
19	C	308	PGV	C01-C02-C03-O11
26	P	306	CDL	OA5-CA3-CA4-CA6
22	Y	101	TGL	C24-C25-C26-C27
21	P	314	DMU	C28-C31-C34-C37
21	P	314	DMU	C31-C34-C37-C40
22	Y	101	TGL	C13-C14-C29-C30
26	P	306	CDL	C40-C41-C42-C43
21	A	616	DMU	C31-C34-C37-C40
25	P	309	PEK	C29-C30-C31-C32
26	G	101	CDL	C60-C61-C62-C63
21	K	104	DMU	O6-C11-C9-O1
21	X	102	DMU	C22-C25-C28-C31
26	P	306	CDL	C18-C19-C20-C21
26	T	102	CDL	C37-C38-C39-C40
21	D	202	DMU	C25-C28-C31-C34
19	C	303	PGV	C7-C8-C9-C10
19	C	308	PGV	O03-C01-C02-C03
22	B	301	TGL	OG1-CG1-CG2-CG3
22	L	101	TGL	OG1-CG1-CG2-CG3
26	P	306	CDL	C19-C20-C21-C22
24	B	303	PSC	C29-C30-C31-C32
27	X	105	CHD	C17-C20-C22-C23
21	K	106	DMU	C34-C37-C40-C43
19	C	308	PGV	C26-C27-C28-C29
19	A	608	PGV	C24-C25-C26-C27
21	O	305	DMU	O6-C11-C9-O1
19	P	301	PGV	C11-C10-C9-C8
21	K	101	DMU	O5-C4-C57-O61
21	K	102	DMU	O6-C11-C9-O1
21	P	314	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
22	Q	201	TGL	CB4-CB5-CB6-CB7
26	T	102	CDL	C56-C57-C58-C59
19	C	303	PGV	C19-C20-C21-C22
22	Q	201	TGL	CA1-CA2-CA3-CA4
21	P	316	DMU	C28-C31-C34-C37
27	P	307	CHD	C20-C22-C23-C24
26	C	304	CDL	C74-C75-C76-C77
21	C	312	DMU	O6-C11-C9-O1
21	X	101	DMU	O5-C4-C57-O61
22	Y	101	TGL	CA2-CA3-CA4-CA5
21	M	101	DMU	C25-C28-C31-C34
25	G	102	PEK	C7-C8-C9-C10
21	K	105	DMU	C28-C31-C34-C37
22	B	301	TGL	CA4-CA5-CA6-CA7
26	C	304	CDL	C18-C19-C20-C21
26	P	306	CDL	C41-C42-C43-C44
20	N	618	EDO	O1-C1-C2-O2
20	P	315	EDO	O1-C1-C2-O2
20	S	104	EDO	O1-C1-C2-O2
21	Q	203	DMU	C34-C37-C40-C43
25	C	302	PEK	C28-C29-C30-C31
21	B	306	DMU	C22-C25-C28-C31
21	P	314	DMU	C22-C25-C28-C31
21	Z	101	DMU	C25-C28-C31-C34
22	L	101	TGL	CB4-CB5-CB6-CB7
27	X	105	CHD	C21-C20-C22-C23
21	P	316	DMU	C1-C6-O16-C18
22	B	301	TGL	C23-C24-C25-C26
22	B	301	TGL	OG1-CG1-CG2-OG2
26	T	102	CDL	OB7-CB5-OB6-CB4
21	X	101	DMU	C18-C19-C22-C25
22	Y	101	TGL	C22-C23-C24-C25
25	C	302	PEK	C32-C33-C34-C35
26	C	304	CDL	C57-C58-C59-C60
21	K	103	DMU	C4-C3-O7-C10
21	P	316	DMU	C22-C25-C28-C31
26	G	101	CDL	C62-C63-C64-C65
22	Q	201	TGL	C25-C26-C27-C28
21	G	104	DMU	C25-C28-C31-C34
21	K	101	DMU	C34-C37-C40-C43
25	C	302	PEK	C27-C28-C29-C30
25	G	102	PEK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	C	309	PEK	C32-C33-C34-C35
26	C	304	CDL	C37-C38-C39-C40
19	P	301	PGV	C10-C11-C12-C13
25	C	302	PEK	C7-C8-C9-C10
25	C	302	PEK	C13-C14-C15-C16
25	P	304	PEK	C13-C14-C15-C16
21	X	104	DMU	C34-C37-C40-C43
26	P	306	CDL	C20-C21-C22-C23
19	P	302	PGV	C01-C02-C03-O11
26	T	102	CDL	OA5-CA3-CA4-CA6
26	P	306	CDL	CB5-C51-C52-C53
22	O	301	TGL	CA2-CA1-OG1-CG1
25	P	309	PEK	C35-C36-C37-C38
26	G	101	CDL	CB4-CB3-OB5-PB2
21	K	102	DMU	C19-C18-O16-C6
25	P	309	PEK	C1-C2-C3-C4
26	P	306	CDL	C61-C62-C63-C64
26	G	101	CDL	C58-C59-C60-C61
19	N	607	PGV	O03-C01-C02-C03
24	N	608	PSC	O03-C01-C02-C03
25	P	309	PEK	O03-C01-C02-C03
26	T	102	CDL	CA3-CA4-CA6-OA8
21	K	104	DMU	C22-C25-C28-C31
26	C	304	CDL	C78-C79-C80-C81
19	A	607	PGV	C10-C11-C12-C13
21	B	306	DMU	C4-C3-O7-C10
22	D	201	TGL	CA7-CA8-CA9-C20
21	K	102	DMU	C34-C37-C40-C43
19	P	302	PGV	C4-C5-C6-C7
24	B	303	PSC	C10-C11-C12-C13
24	N	608	PSC	C9-C10-C11-C12
25	C	302	PEK	C11-C12-C13-C14
25	C	307	PEK	C6-C7-C8-C9
25	C	307	PEK	C11-C10-C9-C8
25	C	307	PEK	C9-C10-C11-C12
25	C	307	PEK	C12-C13-C14-C15
25	C	309	PEK	C5-C6-C7-C8
25	C	309	PEK	C6-C7-C8-C9
25	C	309	PEK	C9-C10-C11-C12
25	C	309	PEK	C12-C13-C14-C15
25	G	102	PEK	C5-C6-C7-C8
25	G	102	PEK	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	G	102	PEK	C9-C10-C11-C12
25	G	102	PEK	C12-C13-C14-C15
25	P	304	PEK	C9-C10-C11-C12
25	P	309	PEK	C5-C6-C7-C8
25	P	309	PEK	C11-C10-C9-C8
25	P	309	PEK	C11-C12-C13-C14
25	P	309	PEK	C12-C13-C14-C15
21	G	104	DMU	O1-C10-O7-C3
22	D	201	TGL	CB5-CB6-CB7-CB8
19	A	608	PGV	O01-C02-C03-O11
26	C	304	CDL	OA5-CA3-CA4-OA6
26	P	306	CDL	OB5-CB3-CB4-OB6
19	P	302	PGV	C1-C2-C3-C4
26	C	304	CDL	C41-C42-C43-C44
22	B	301	TGL	C29-C30-C31-C32
26	T	102	CDL	OA6-CA4-CA6-OA8
21	X	101	DMU	C25-C28-C31-C34
21	K	103	DMU	C28-C31-C34-C37
26	T	102	CDL	C24-C25-C26-C27
21	K	102	DMU	C31-C34-C37-C40
21	T	103	DMU	C18-C19-C22-C25
19	A	608	PGV	C20-C21-C22-C23
26	C	304	CDL	CA4-CA3-OA5-PA1
19	P	305	PGV	C24-C25-C26-C27
21	X	104	DMU	C22-C25-C28-C31
20	M	102	EDO	O1-C1-C2-O2
22	D	201	TGL	C23-C24-C25-C26
22	O	301	TGL	C22-C23-C24-C25
21	P	316	DMU	C5-C10-O7-C3
22	D	201	TGL	C19-C33-C34-C35
21	B	306	DMU	O16-C18-C19-C22
22	L	101	TGL	CA2-CA3-CA4-CA5
19	A	608	PGV	C01-C02-C03-O11
24	B	303	PSC	C01-C02-C03-O11
26	C	304	CDL	OA5-CA3-CA4-CA6
22	D	201	TGL	CA2-CA3-CA4-CA5
25	C	302	PEK	C17-C18-C19-C20
21	B	306	DMU	C28-C31-C34-C37
22	L	101	TGL	C16-C15-CC9-CC8
25	C	309	PEK	C29-C30-C31-C32
22	O	301	TGL	OA1-CA1-OG1-CG1
22	O	301	TGL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	O	301	TGL	CA3-CA4-CA5-CA6
22	B	301	TGL	CC9-C15-C16-C17
22	L	101	TGL	CC5-CC6-CC7-CC8
24	N	608	PSC	C31-C32-C33-C34
22	O	301	TGL	CB7-CB8-CB9-C10
19	C	303	PGV	C02-C03-O11-P
19	P	305	PGV	C02-C03-O11-P
22	Y	101	TGL	OG1-CG1-CG2-CG3
24	B	303	PSC	O03-C01-C02-C03
26	C	304	CDL	C72-C73-C74-C75
21	L	102	DMU	C22-C25-C28-C31
22	L	101	TGL	C21-C20-CA9-CA8
25	C	302	PEK	C24-C25-C26-C27
26	P	306	CDL	C36-C37-C38-C39
21	K	105	DMU	C18-C19-C22-C25
19	C	308	PGV	O03-C01-C02-O01
24	N	608	PSC	O03-C01-C02-O01
25	P	309	PEK	O03-C01-C02-O01
26	C	304	CDL	OB6-CB4-CB6-OB8
26	G	101	CDL	OB6-CB4-CB6-OB8
26	T	102	CDL	OB6-CB4-CB6-OB8
19	P	301	PGV	C31-C32-C33-C34
22	O	301	TGL	C21-C20-CA9-CA8
21	K	104	DMU	C19-C22-C25-C28
19	C	303	PGV	C31-C32-C33-C34
19	P	302	PGV	O02-C1-O01-C02
19	C	303	PGV	C27-C28-C29-C30
22	Q	201	TGL	CB7-CB8-CB9-C10
25	P	304	PEK	C1-C2-C3-C4
21	Q	203	DMU	C19-C22-C25-C28
22	Q	201	TGL	C13-C14-C29-C30
21	X	101	DMU	C5-C10-O7-C3
19	N	607	PGV	C25-C26-C27-C28
21	K	101	DMU	C28-C31-C34-C37
22	Y	101	TGL	C25-C26-C27-C28
19	A	608	PGV	C04-O12-P-O11
21	C	312	DMU	C34-C37-C40-C43
22	Y	101	TGL	CC9-C15-C16-C17
26	P	306	CDL	C53-C54-C55-C56
25	C	309	PEK	C27-C28-C29-C30
19	A	608	PGV	C05-C04-O12-P
26	T	102	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
19	C	308	PGV	C04-O12-P-O14
19	N	607	PGV	C04-O12-P-O14
19	P	302	PGV	C04-O12-P-O14
25	C	307	PEK	C03-O11-P-O14
25	P	309	PEK	C04-O12-P-O14
26	C	304	CDL	CB2-OB2-PB2-OB3
26	G	101	CDL	CA3-OA5-PA1-OA3
22	Y	101	TGL	C21-C22-C23-C24
20	P	312	EDO	O1-C1-C2-O2
19	C	308	PGV	O02-C1-O01-C02
25	P	309	PEK	C4-C5-C6-C7
26	C	304	CDL	C40-C41-C42-C43
24	N	608	PSC	C05-C04-O12-P
21	Q	203	DMU	C28-C31-C34-C37
26	C	304	CDL	C61-C62-C63-C64
21	X	104	DMU	O16-C18-C19-C22
26	P	306	CDL	OA5-CA3-CA4-OA6
22	Y	101	TGL	C33-C34-C35-C36
22	Q	201	TGL	CB6-CB7-CB8-CB9
22	Y	101	TGL	CB9-C10-C11-C12
19	C	303	PGV	C1-C2-C3-C4
21	K	106	DMU	C25-C28-C31-C34
22	D	201	TGL	OG2-CG2-CG3-OG3
22	L	101	TGL	OG2-CG2-CG3-OG3
22	Y	101	TGL	OG1-CG1-CG2-OG2
24	B	303	PSC	O03-C01-C02-O01
22	Y	101	TGL	C12-C13-C14-C29
22	L	101	TGL	CB3-CB4-CB5-CB6
22	Y	101	TGL	CB1-CB2-CB3-CB4
19	C	303	PGV	C14-C15-C16-C17
21	Z	101	DMU	C19-C22-C25-C28
26	T	102	CDL	C58-C59-C60-C61
21	X	104	DMU	C3-C4-C57-O61
22	L	101	TGL	OG1-CA1-CA2-CA3
24	N	608	PSC	C22-C23-C24-C25
26	G	101	CDL	C36-C37-C38-C39
26	P	306	CDL	C77-C78-C79-C80
26	G	101	CDL	C40-C41-C42-C43
24	B	303	PSC	C01-C02-O01-C1
26	C	304	CDL	C71-C72-C73-C74
19	P	302	PGV	C02-C03-O11-P
26	P	306	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C29-C30-C31-C32
21	A	616	DMU	O16-C18-C19-C22
21	P	316	DMU	C2-C3-O7-C10
21	C	312	DMU	C3-C4-C57-O61
21	K	103	DMU	O16-C18-C19-C22
19	A	608	PGV	C19-C20-C21-C22
24	N	608	PSC	C12-C13-C14-C15
27	C	305	CHD	C20-C22-C23-C24
21	G	104	DMU	C1-C6-O16-C18
19	N	607	PGV	O03-C01-C02-O01
22	L	101	TGL	OG1-CG1-CG2-OG2
21	K	103	DMU	C31-C34-C37-C40
22	Q	201	TGL	C21-C20-CA9-CA8
26	C	304	CDL	CA2-OA2-PA1-OA5
26	C	304	CDL	CA3-OA5-PA1-OA2
26	P	306	CDL	CA2-OA2-PA1-OA5
26	P	306	CDL	CA3-OA5-PA1-OA2
26	T	102	CDL	CA3-OA5-PA1-OA2
26	C	304	CDL	C83-C84-C85-C86
22	D	201	TGL	CG1-CG2-CG3-OG3
22	L	101	TGL	CG1-CG2-CG3-OG3
22	Q	201	TGL	OG1-CG1-CG2-CG3
26	C	304	CDL	CB3-CB4-CB6-OB8
19	N	607	PGV	C23-C24-C25-C26
24	N	608	PSC	C04-C05-N-C06
22	Y	101	TGL	C29-C30-C31-C32
26	G	101	CDL	C1-CB2-OB2-PB2
21	K	102	DMU	C22-C25-C28-C31
22	L	101	TGL	C12-C13-C14-C29
27	G	103	CHD	C22-C23-C24-O26
19	P	301	PGV	C23-C24-C25-C26
19	C	303	PGV	C26-C27-C28-C29
21	L	102	DMU	C18-C19-C22-C25
22	D	201	TGL	C17-C18-C19-C33
26	T	102	CDL	C75-C76-C77-C78
26	C	304	CDL	C20-C21-C22-C23
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
27	T	101	CHD	C22-C23-C24-O25
26	T	102	CDL	C12-C13-C14-C15
22	O	301	TGL	CC9-C15-C16-C17
25	C	309	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	OB6-CB4-CB6-OB8
21	O	305	DMU	C2-C3-O7-C10
19	A	608	PGV	C02-C03-O11-P
19	C	303	PGV	C22-C23-C24-C25
19	P	301	PGV	C27-C28-C29-C30
26	T	102	CDL	C60-C61-C62-C63
25	C	307	PEK	C14-C15-C16-C17
26	T	102	CDL	C61-C62-C63-C64
21	Q	203	DMU	C18-C19-C22-C25
24	B	303	PSC	C20-C21-C22-C23
24	N	608	PSC	C30-C31-C32-C33
27	P	307	CHD	C22-C23-C24-O26
20	A	609	EDO	O1-C1-C2-O2
20	N	613	EDO	O1-C1-C2-O2
26	G	101	CDL	C41-C42-C43-C44
27	W	101	CHD	C22-C23-C24-O25
14	N	602	HEA	CAA-CBA-CGA-O1A
25	P	309	PEK	C13-C14-C15-C16
21	G	104	DMU	O5-C6-O16-C18
21	P	316	DMU	O5-C6-O16-C18
14	A	602	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O1D
25	P	309	PEK	C21-C22-C23-C24
27	P	307	CHD	C22-C23-C24-O25
27	C	306	CHD	C22-C23-C24-O25
27	J	101	CHD	C22-C23-C24-O25
22	L	101	TGL	C23-C24-C25-C26
25	P	309	PEK	C14-C15-C16-C17
27	W	101	CHD	C22-C23-C24-O26
24	N	608	PSC	C10-C11-C12-C13
25	C	302	PEK	C11-C10-C9-C8
25	C	309	PEK	C11-C12-C13-C14
25	G	102	PEK	C6-C7-C8-C9
25	G	102	PEK	C11-C12-C13-C14
25	P	309	PEK	C9-C10-C11-C12
27	J	101	CHD	C22-C23-C24-O26
22	L	101	TGL	C25-C26-C27-C28
26	P	306	CDL	C22-C23-C24-C25
24	N	608	PSC	C2-C3-C4-C5
21	L	102	DMU	C34-C37-C40-C43
14	N	602	HEA	CAD-CBD-CGD-O2D
25	P	309	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	P	309	PEK	C32-C33-C34-C35
25	P	309	PEK	C01-C02-C03-O11
22	Q	201	TGL	CC5-CC6-CC7-CC8
27	G	103	CHD	C22-C23-C24-O25
21	P	314	DMU	C18-C19-C22-C25
25	C	307	PEK	C24-C25-C26-C27
19	P	301	PGV	C24-C25-C26-C27
21	X	102	DMU	C28-C31-C34-C37
14	A	602	HEA	C4D-C3D-CAD-CBD
27	P	308	CHD	C16-C17-C20-C22
14	A	602	HEA	CAD-CBD-CGD-O2D
24	B	303	PSC	C12-C13-C14-C15
19	A	608	PGV	O01-C1-C2-C3
21	M	101	DMU	C34-C37-C40-C43
21	X	103	DMU	C34-C37-C40-C43
21	X	101	DMU	C31-C34-C37-C40
19	N	607	PGV	C2-C3-C4-C5
21	Q	203	DMU	C31-C34-C37-C40
21	O	305	DMU	O1-C10-O7-C3
19	P	302	PGV	C24-C25-C26-C27
19	A	607	PGV	C11-C12-C13-C14
20	A	614	EDO	O1-C1-C2-O2
20	S	107	EDO	O1-C1-C2-O2
20	W	103	EDO	O1-C1-C2-O2
25	C	309	PEK	C13-C14-C15-C16
14	A	601[A]	HEA	C27-C19-C20-C21
22	Q	201	TGL	C11-C12-C13-C14
26	C	304	CDL	C56-C57-C58-C59
19	N	607	PGV	C9-C10-C11-C12
19	P	302	PGV	C11-C12-C13-C14
25	C	302	PEK	C14-C15-C16-C17
21	X	101	DMU	O6-C11-C9-O1
21	D	202	DMU	C18-C19-C22-C25
26	G	101	CDL	C42-C43-C44-C45
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
22	L	101	TGL	CC2-CC3-CC4-CC5
19	P	302	PGV	C2-C1-O01-C02
27	T	101	CHD	C22-C23-C24-O26
21	X	101	DMU	C28-C31-C34-C37
26	T	102	CDL	C36-C37-C38-C39
26	G	101	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
21	D	202	DMU	O16-C18-C19-C22
22	O	301	TGL	C29-C30-C31-C32
21	X	104	DMU	O5-C4-C57-O61
24	N	608	PSC	C7-C8-C9-C10
25	C	307	PEK	O03-C21-C22-C23
21	O	305	DMU	C34-C37-C40-C43
14	N	602	HEA	CAA-CBA-CGA-O2A
26	C	304	CDL	C16-C17-C18-C19
26	T	102	CDL	C12-C11-CA5-OA6
24	B	303	PSC	C7-C8-C9-C10
25	C	307	PEK	C3-C4-C5-C6
26	T	102	CDL	C17-C18-C19-C20
14	A	602	HEA	CAA-CBA-CGA-O1A
24	N	608	PSC	C3-C4-C5-C6
22	Q	201	TGL	CA5-CA6-CA7-CA8
21	K	103	DMU	C18-C19-C22-C25
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
27	C	305	CHD	C22-C23-C24-O26
27	C	306	CHD	C22-C23-C24-O26
19	A	607	PGV	O03-C19-C20-C21
26	C	304	CDL	C76-C77-C78-C79
19	C	303	PGV	C11-C12-C13-C14
19	P	302	PGV	C9-C10-C11-C12
26	G	101	CDL	CB3-CB4-CB6-OB8
26	P	306	CDL	CB3-CB4-CB6-OB8
26	G	101	CDL	OA5-CA3-CA4-OA6
26	C	304	CDL	C52-C51-CB5-OB6
21	K	106	DMU	O16-C18-C19-C22
21	C	312	DMU	C31-C34-C37-C40
22	Q	201	TGL	OG3-CC1-CC2-CC3
20	N	615	EDO	O1-C1-C2-O2
20	P	311	EDO	O1-C1-C2-O2
20	Q	202	EDO	O1-C1-C2-O2
27	C	305	CHD	C22-C23-C24-O25
25	P	309	PEK	C3-C4-C5-C6
21	P	316	DMU	O5-C4-C57-O61
27	P	308	CHD	C22-C23-C24-O25
26	G	101	CDL	C38-C39-C40-C41
24	B	303	PSC	C20-C19-O03-C01
22	L	101	TGL	CB9-C10-C11-C12
26	P	306	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
19	P	301	PGV	O03-C19-C20-C21
26	T	102	CDL	C32-C31-CA7-OA8
26	T	102	CDL	C57-C58-C59-C60
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
19	A	608	PGV	C9-C10-C11-C12
21	C	312	DMU	C4-C3-O7-C10
21	C	312	DMU	O16-C18-C19-C22
26	P	306	CDL	C62-C63-C64-C65
21	X	103	DMU	C18-C19-C22-C25
25	C	309	PEK	O03-C21-C22-C23
22	O	301	TGL	C24-C25-C26-C27
14	N	601[A]	HEA	CAA-CBA-CGA-O1A
14	N	601[B]	HEA	CAA-CBA-CGA-O1A
19	C	303	PGV	C9-C10-C11-C12
19	C	308	PGV	C9-C10-C11-C12
19	C	308	PGV	C11-C12-C13-C14
19	P	301	PGV	C11-C12-C13-C14
26	P	306	CDL	C21-C22-C23-C24
26	G	101	CDL	C12-C11-CA5-OA7
21	K	103	DMU	C5-C10-O7-C3
21	K	102	DMU	C2-C3-O7-C10
22	L	101	TGL	CA9-C20-C21-C22
19	C	308	PGV	C2-C1-O01-C02
19	N	607	PGV	C11-C12-C13-C14
14	A	602	HEA	CAA-CBA-CGA-O2A
25	C	309	PEK	O04-C21-C22-C23
22	B	301	TGL	C20-C21-C22-C23
22	B	301	TGL	C14-C29-C30-C31
22	Q	201	TGL	OC1-CC1-CC2-CC3
21	K	105	DMU	C19-C22-C25-C28
25	C	309	PEK	C3-C4-C5-C6
25	C	307	PEK	O04-C21-C22-C23
26	C	304	CDL	C52-C51-CB5-OB7
21	Q	203	DMU	C22-C25-C28-C31
26	T	102	CDL	CB3-CB4-CB6-OB8
26	P	306	CDL	CB2-OB2-PB2-OB5
21	P	316	DMU	C25-C28-C31-C34
26	T	102	CDL	C12-C11-CA5-OA7
25	C	309	PEK	C26-C27-C28-C29
24	B	303	PSC	O04-C19-O03-C01
19	A	608	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C04-O12-P-O13
24	B	303	PSC	C03-O11-P-O14
24	N	608	PSC	C03-O11-P-O13
24	N	608	PSC	C03-O11-P-O14
26	C	304	CDL	CA3-OA5-PA1-OA3
26	P	306	CDL	CA3-OA5-PA1-OA3
25	P	309	PEK	O01-C1-C2-C3
21	P	316	DMU	C4-C3-O7-C10
26	G	101	CDL	C73-C74-C75-C76
25	P	304	PEK	O12-C04-C05-N
26	T	102	CDL	C32-C31-CA7-OA9
19	A	607	PGV	C29-C30-C31-C32
21	G	104	DMU	C5-C10-O7-C3
21	A	616	DMU	C2-C3-O7-C10
21	K	104	DMU	C34-C37-C40-C43
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
19	C	308	PGV	C3-C4-C5-C6
24	N	608	PSC	O03-C19-C20-C21
22	B	301	TGL	CA9-C20-C21-C22
25	C	309	PEK	C14-C15-C16-C17
25	P	304	PEK	C14-C15-C16-C17
22	D	201	TGL	OG2-CB1-CB2-CB3
22	L	101	TGL	OB1-CB1-CB2-CB3
22	Y	101	TGL	CB4-CB5-CB6-CB7
22	L	101	TGL	OG2-CB1-CB2-CB3
25	C	302	PEK	O03-C21-C22-C23
21	B	306	DMU	C18-C19-C22-C25
14	A	602	HEA	C2D-C3D-CAD-CBD
25	P	309	PEK	O02-C1-C2-C3
26	G	101	CDL	C15-C16-C17-C18
14	A	601[A]	HEA	C18-C19-C20-C21
24	B	303	PSC	C30-C31-C32-C33
24	B	303	PSC	O01-C1-C2-C3
25	C	307	PEK	O01-C1-C2-C3
25	P	304	PEK	O02-C1-C2-C3
21	K	105	DMU	C34-C37-C40-C43
26	C	304	CDL	C73-C74-C75-C76
22	O	301	TGL	CB2-CB3-CB4-CB5
25	C	307	PEK	O02-C1-C2-C3
25	P	309	PEK	C2-C1-O01-C02
21	X	104	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
25	C	302	PEK	O04-C21-C22-C23
19	A	607	PGV	C9-C10-C11-C12
21	K	106	DMU	O1-C10-O7-C3

There are no ring outliers.

76 monomers are involved in 291 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	307	PEK	13	0
19	P	305	PGV	4	0
25	C	302	PEK	3	0
19	P	301	PGV	3	0
20	N	617	EDO	2	0
21	P	316	DMU	10	0
27	X	105	CHD	5	0
21	X	102	DMU	2	0
21	O	305	DMU	2	0
20	Q	202	EDO	1	0
21	K	101	DMU	3	0
27	C	305	CHD	1	0
20	M	102	EDO	1	0
20	W	102	EDO	3	0
27	Y	102	CHD	3	0
22	Q	201	TGL	6	0
26	G	101	CDL	21	0
20	A	611	EDO	1	0
22	L	101	TGL	12	0
27	J	101	CHD	4	0
19	N	607	PGV	6	0
26	T	102	CDL	19	0
20	W	103	EDO	2	0
21	K	106	DMU	1	0
19	A	608	PGV	8	0
24	N	608	PSC	12	0
21	K	103	DMU	3	0
20	Y	103	EDO	1	0
19	A	607	PGV	1	0
14	A	602	HEA	2	0
22	O	301	TGL	1	0
26	C	304	CDL	23	0
21	X	101	DMU	1	0
14	N	601[B]	HEA	1	0

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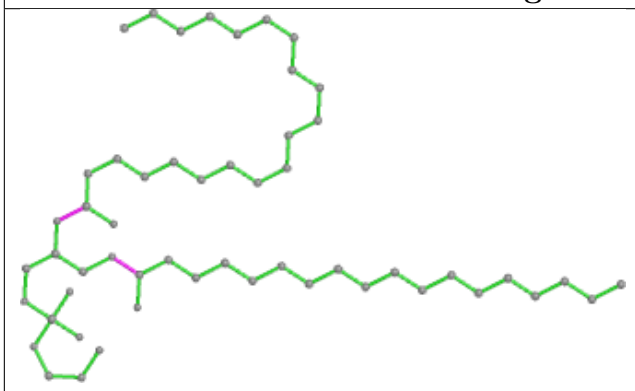
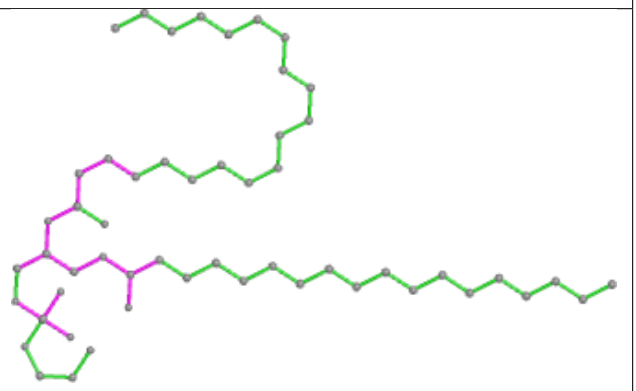
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	309	PEK	5	0
20	P	315	EDO	1	0
27	W	101	CHD	1	0
25	P	304	PEK	3	0
27	P	308	CHD	1	0
21	X	103	DMU	1	0
20	S	107	EDO	4	0
21	D	202	DMU	1	0
22	D	201	TGL	10	0
27	L	103	CHD	1	0
21	K	105	DMU	5	0
19	P	302	PGV	2	0
14	N	601[A]	HEA	1	0
20	A	612	EDO	4	0
21	M	101	DMU	1	0
20	N	613	EDO	4	0
21	Q	203	DMU	1	0
18	A	606	PER	1	0
20	C	311	EDO	1	0
22	B	301	TGL	6	0
19	C	303	PGV	2	0
14	A	601[B]	HEA	1	0
21	L	102	DMU	3	0
27	P	307	CHD	2	0
14	N	602	HEA	2	0
18	N	606	PER	1	0
21	K	104	DMU	1	0
22	Y	101	TGL	7	0
24	B	303	PSC	9	0
20	N	616	EDO	1	0
21	G	104	DMU	1	0
21	K	102	DMU	1	0
20	S	105	EDO	1	0
19	C	308	PGV	3	0
21	T	103	DMU	2	0
25	C	309	PEK	4	0
14	A	601[A]	HEA	1	0
25	G	102	PEK	4	0
26	P	306	CDL	18	0
21	A	616	DMU	1	0
20	N	618	EDO	1	0
20	N	612	EDO	1	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.

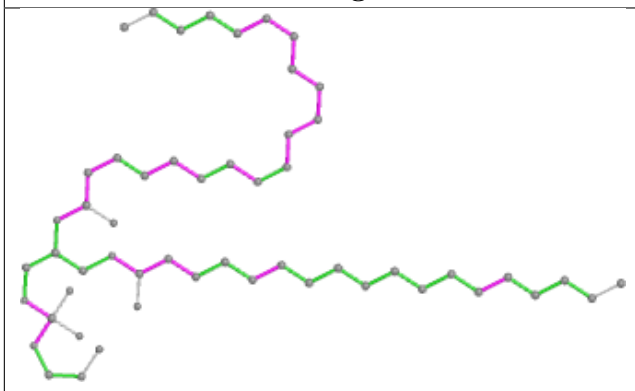
Ligand PEK C 307



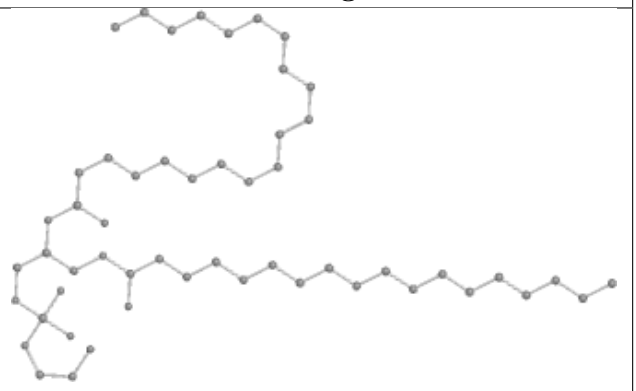
Bond lengths



Bond angles

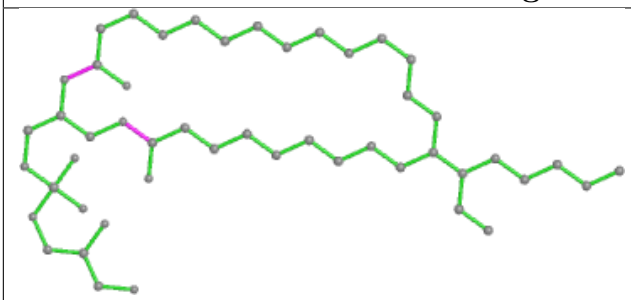


Torsions

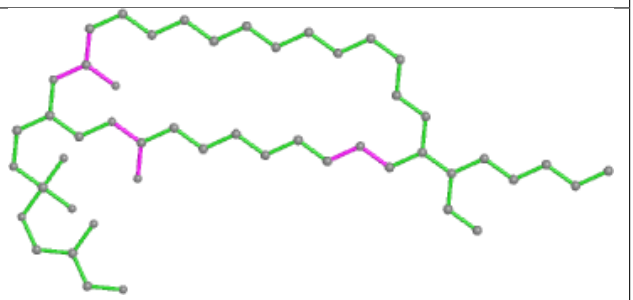


Rings

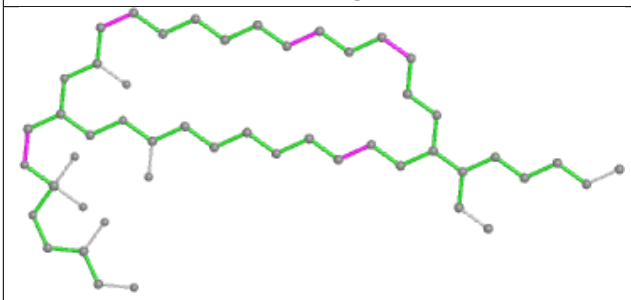
Ligand PGV P 305



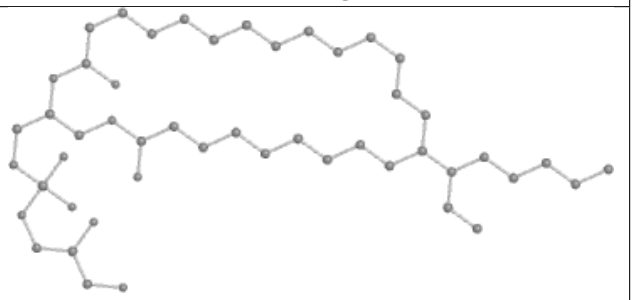
Bond lengths



Bond angles

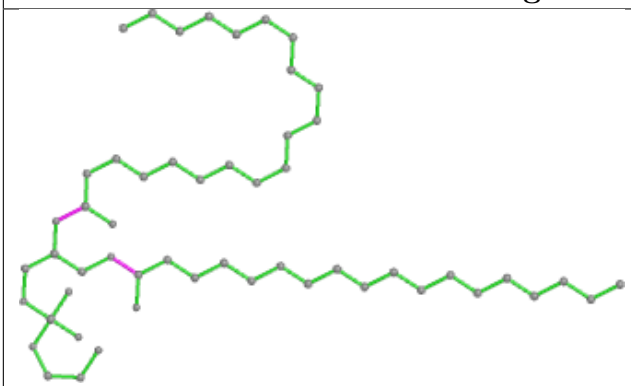


Torsions



Rings

Ligand PEK C 302



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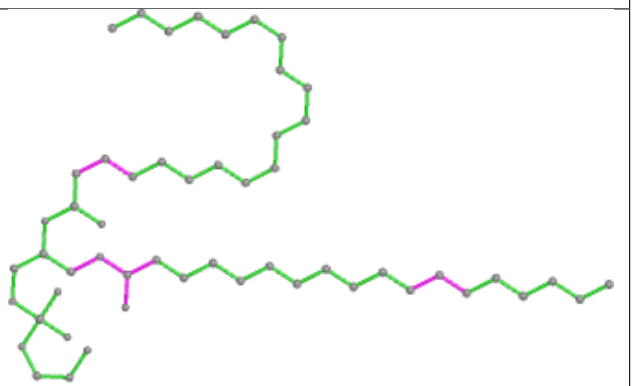
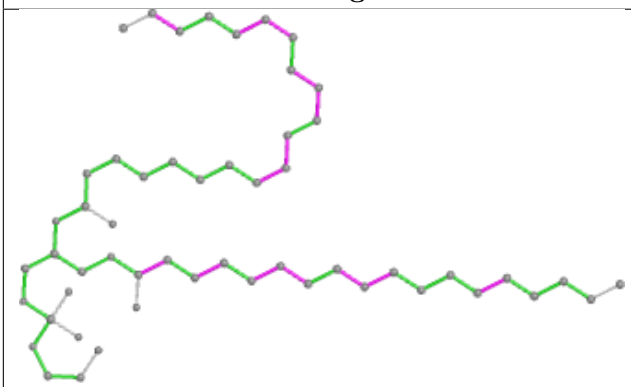
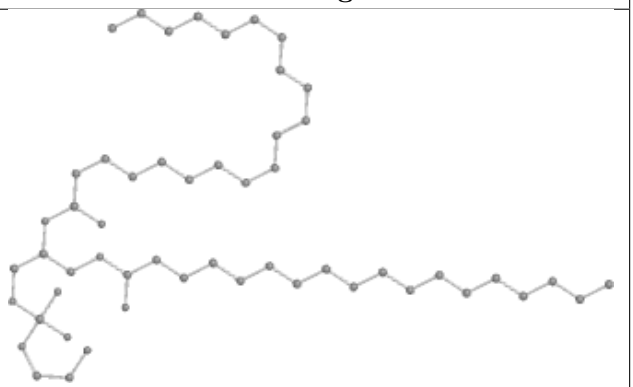


Bond angles

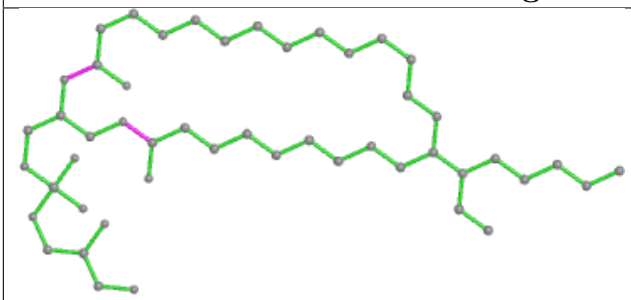


Torsions

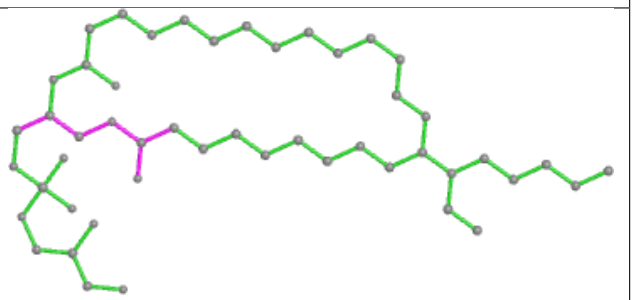


Rings

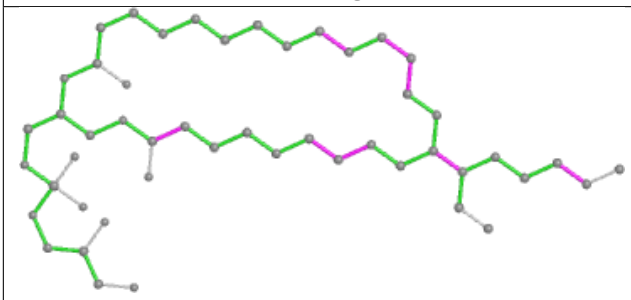
Ligand PGV P 301



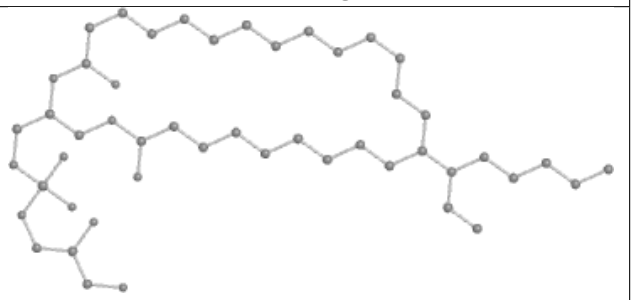
Bond lengths



Bond angles

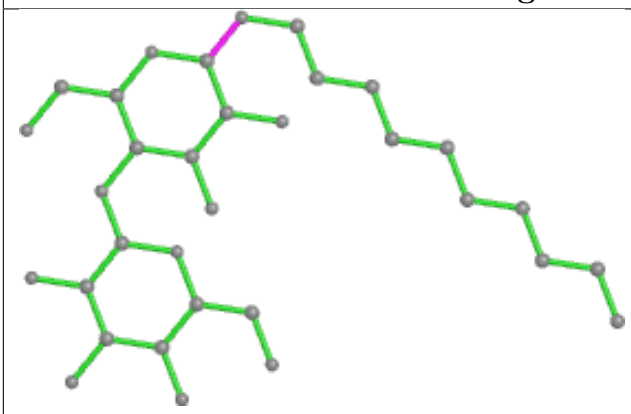


Torsions

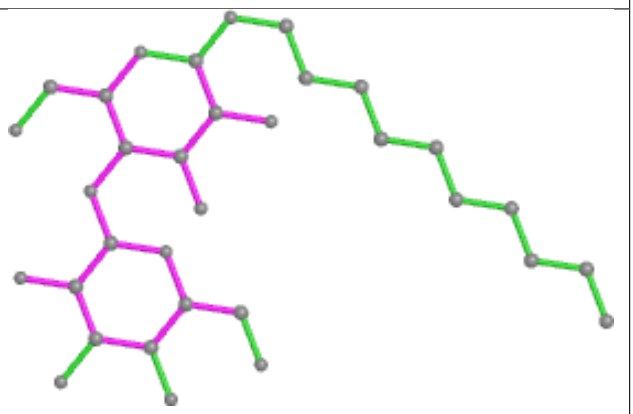


Rings

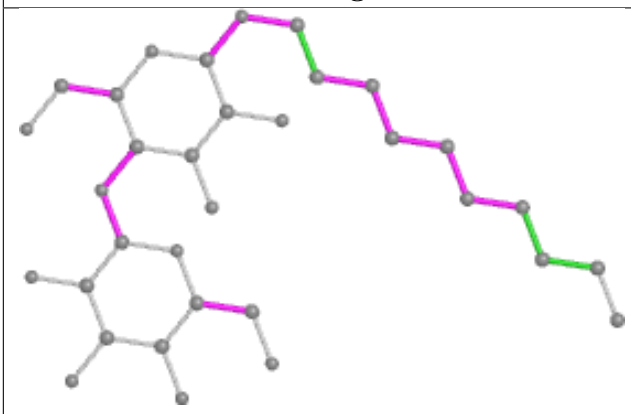
Ligand DMU P 316



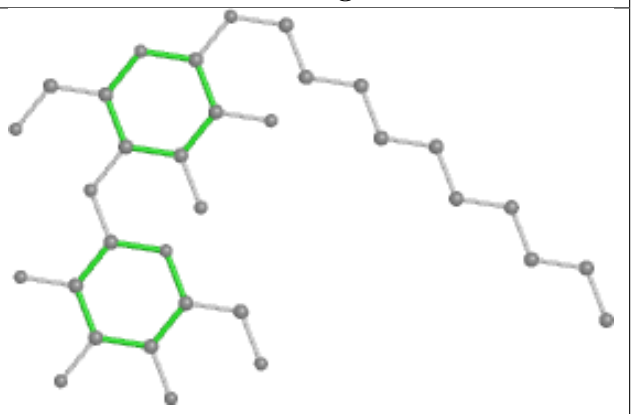
Bond lengths



Bond angles

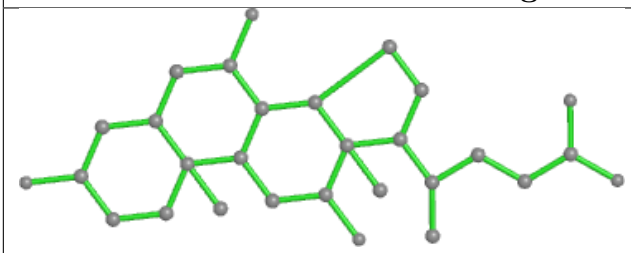


Torsions

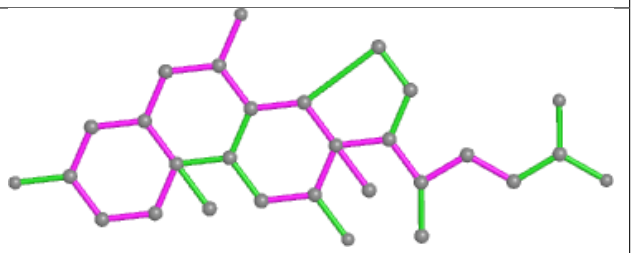


Rings

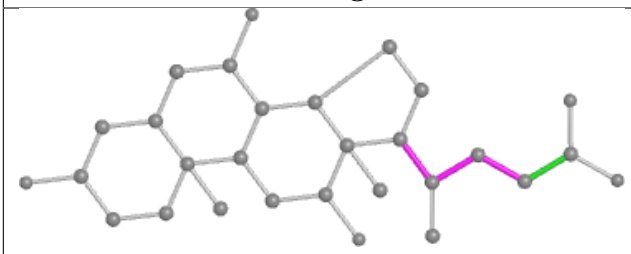
Ligand CHD X 105



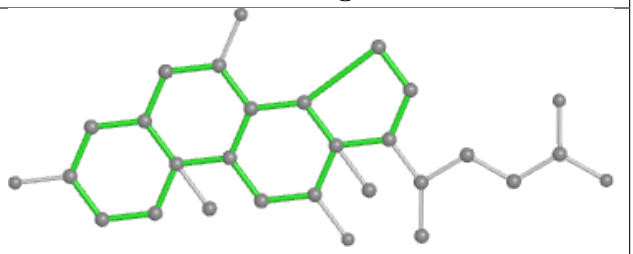
Bond lengths



Bond angles

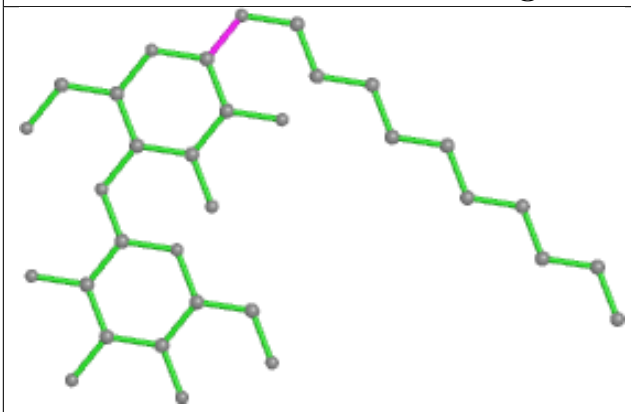


Torsions

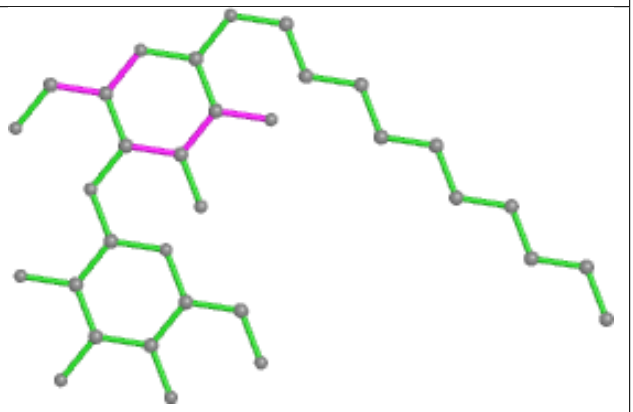


Rings

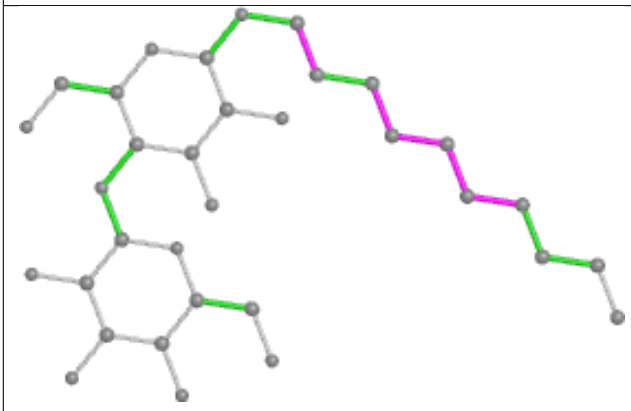
Ligand DMU Z 101



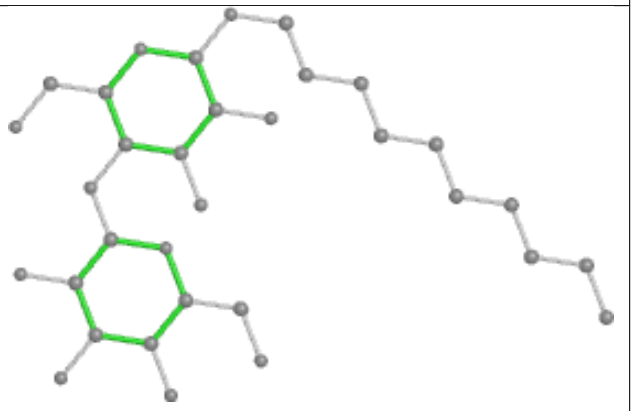
Bond lengths



Bond angles

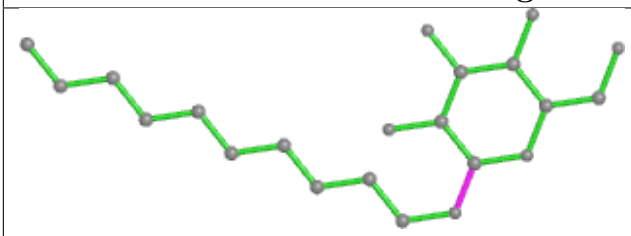


Torsions



Rings

Ligand DMU X 102



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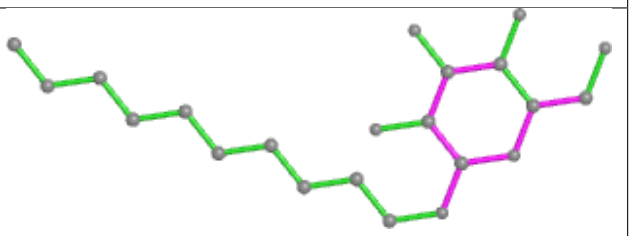
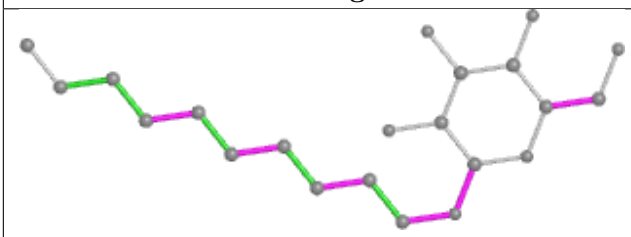
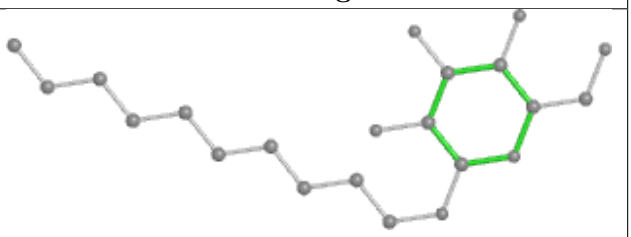


Bond angles

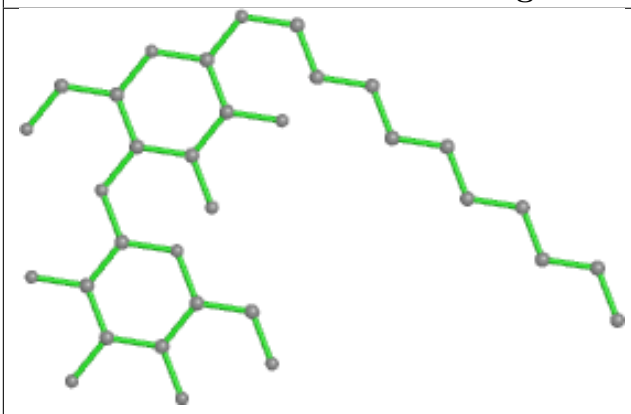


Torsions

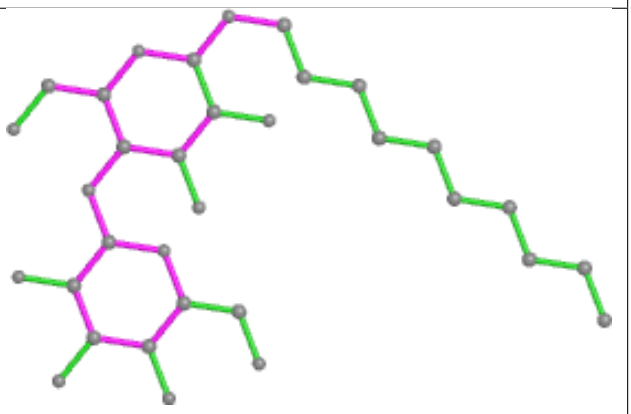


Rings

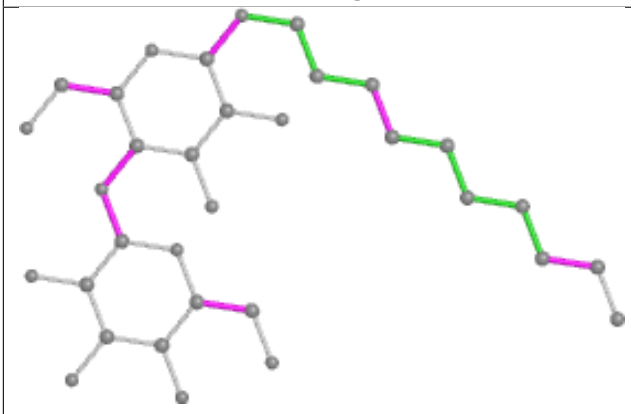
Ligand DMU O 305



Bond lengths



Bond angles



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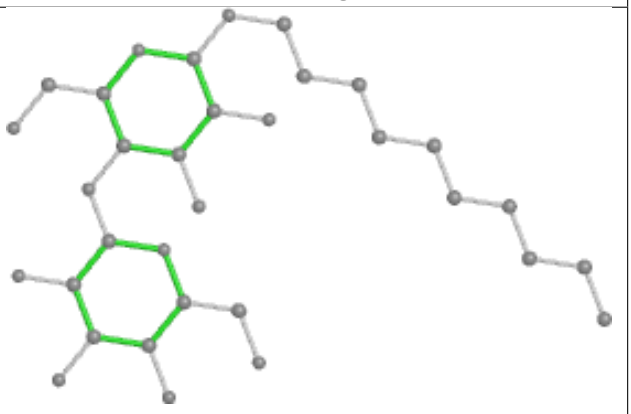
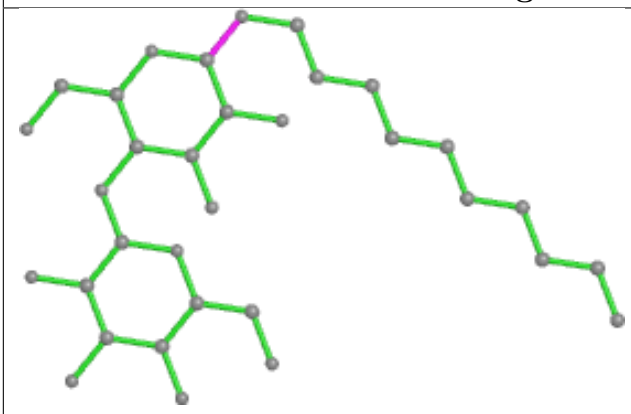


Rings

Ligand DMU K 101



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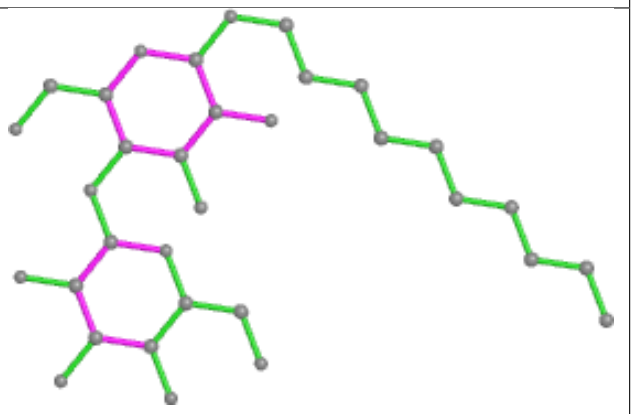
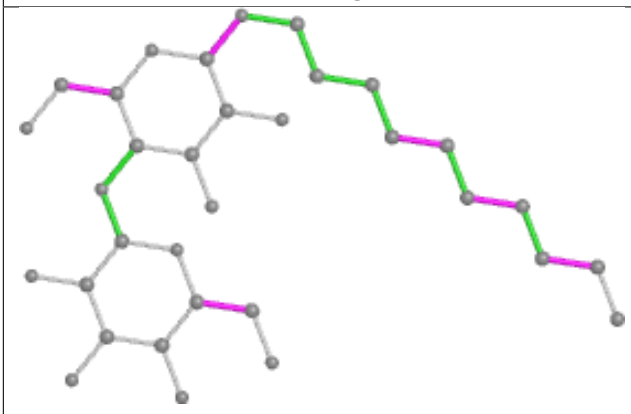


Bond angles



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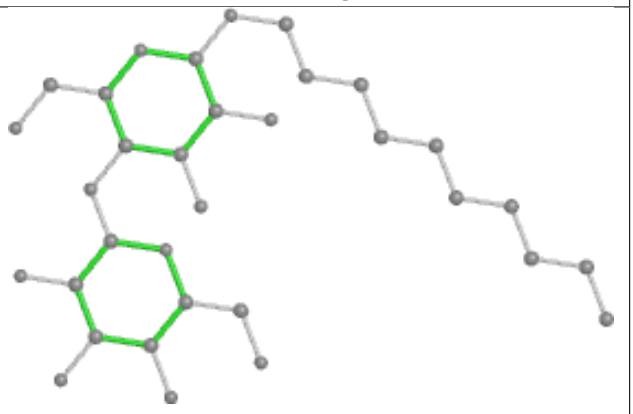
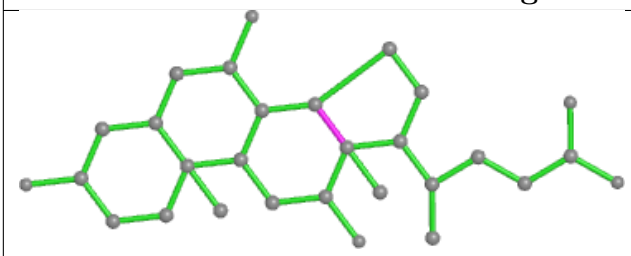
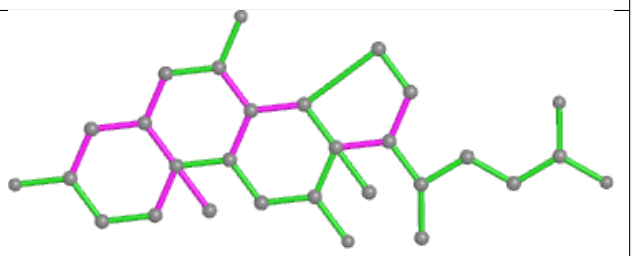


Rings

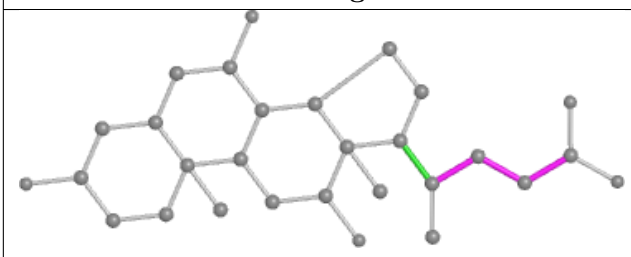
Ligand CHD C 305



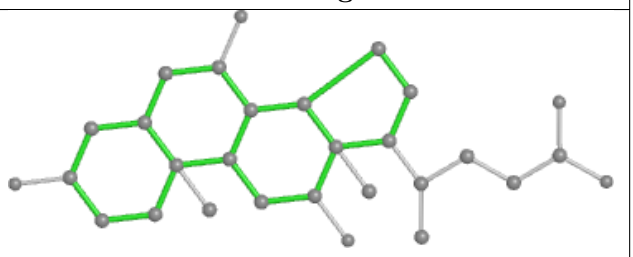
Bond lengths



Bond angles

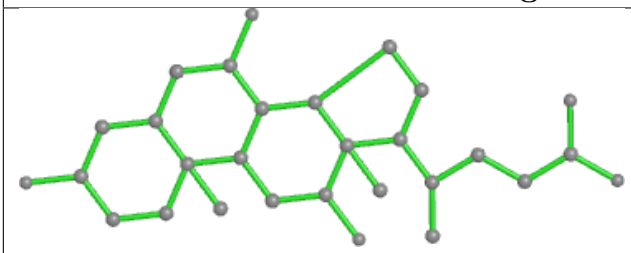


Torsions



Rings

Ligand CHD Y 102



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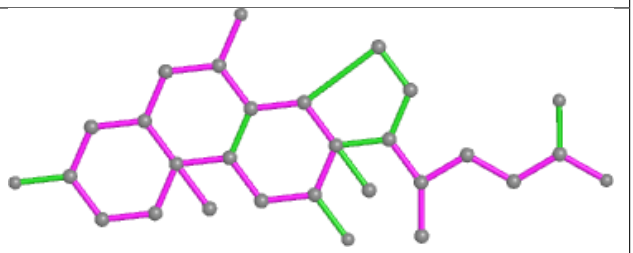
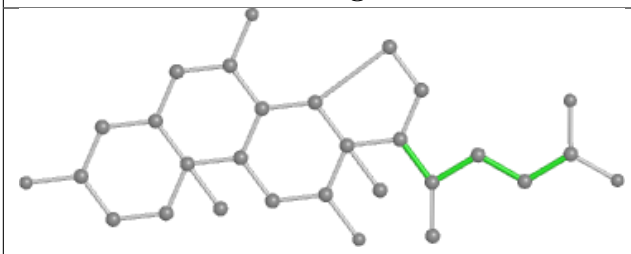


Bond angles



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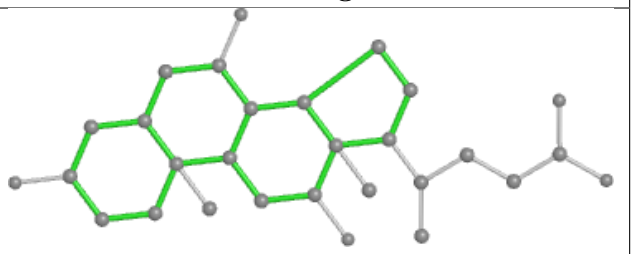
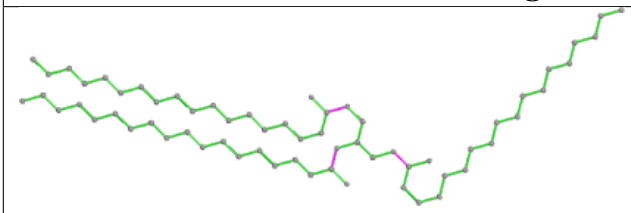
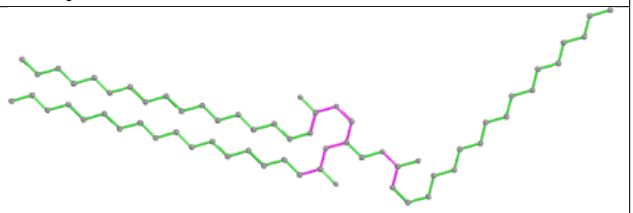


Rings

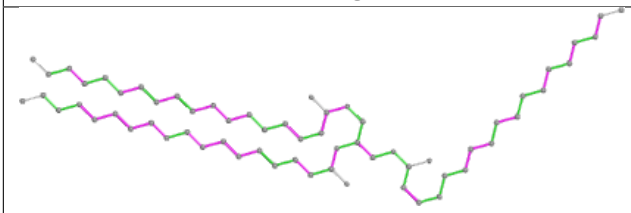
Ligand TGL Q 201



Bond lengths



Bond angles



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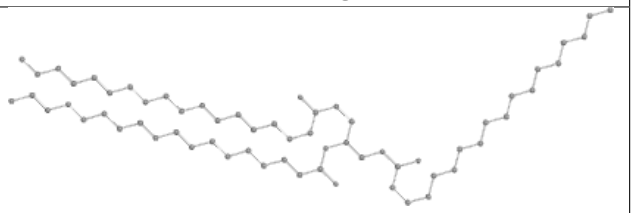
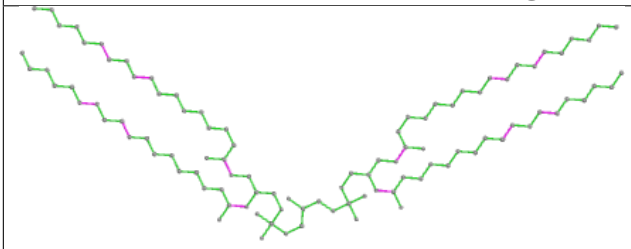
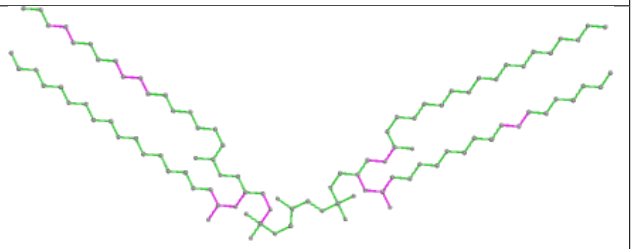


Rings

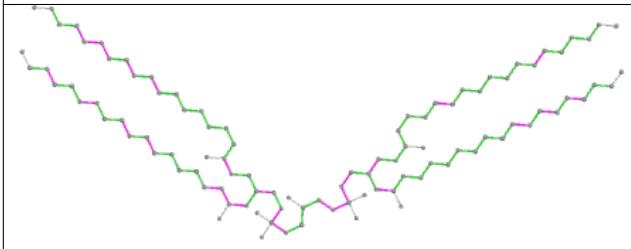
Ligand CDL G 101



Bond lengths



Bond angles



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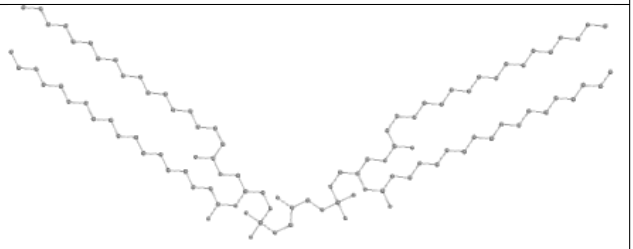
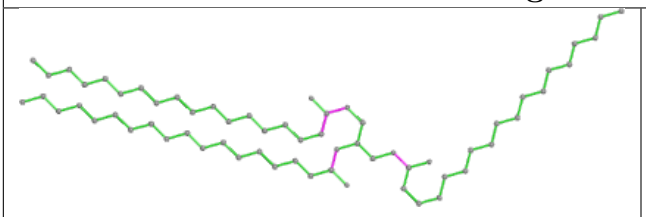
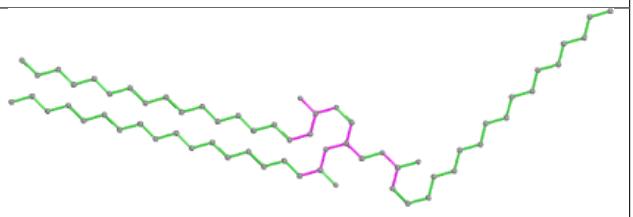


Rings

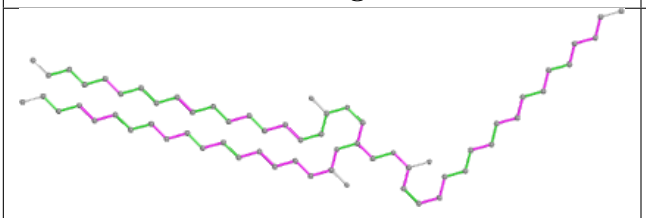
Ligand TGL L 101



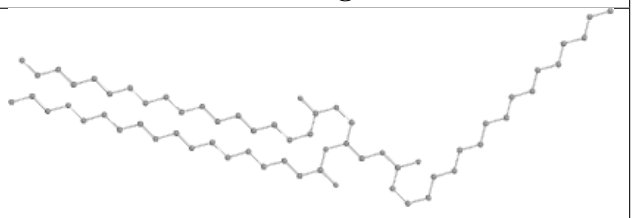
Bond lengths



Bond angles

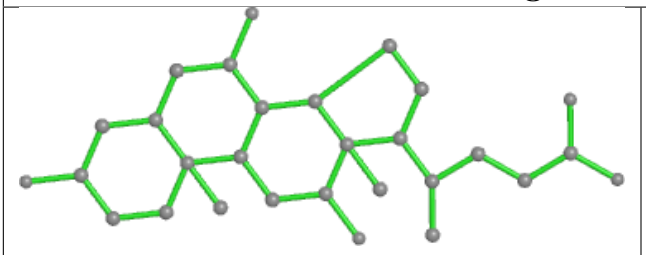


Torsions

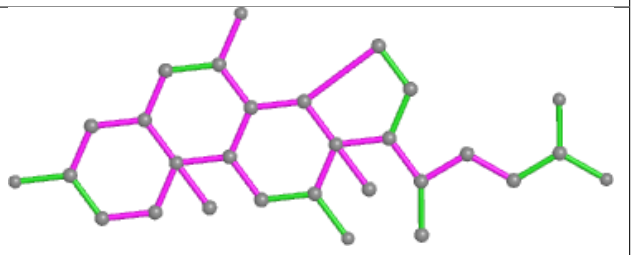


Rings

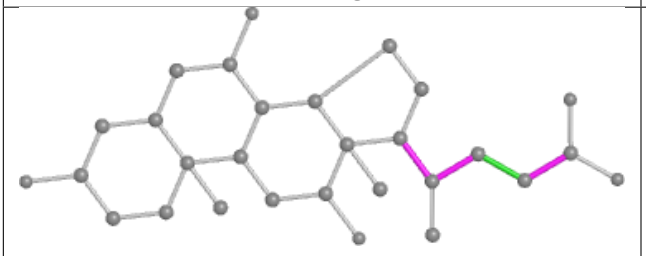
Ligand CHD J 101



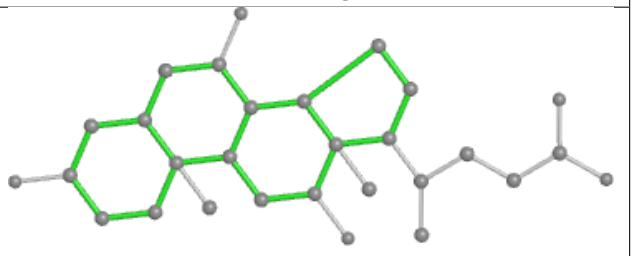
Bond lengths



Bond angles

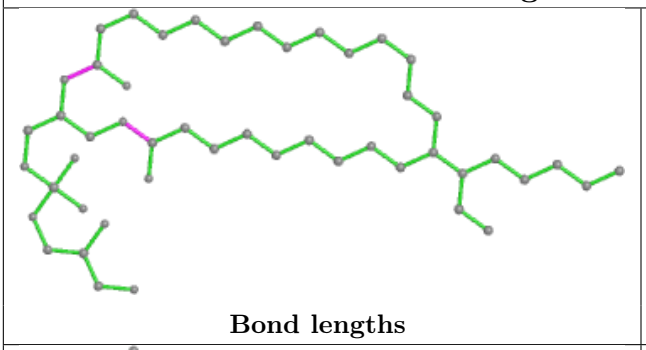


Torsions

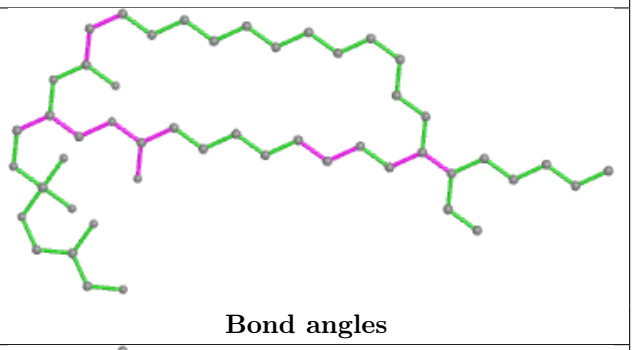


Rings

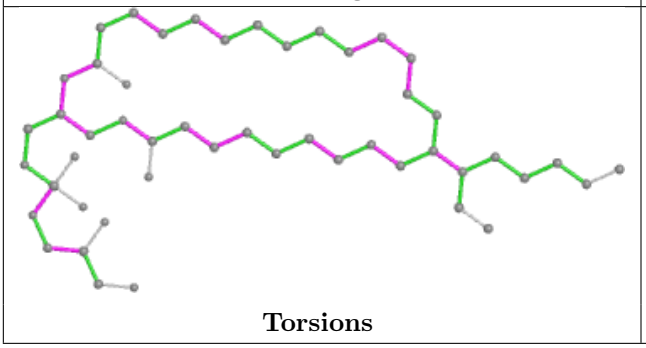
Ligand PGV N 607



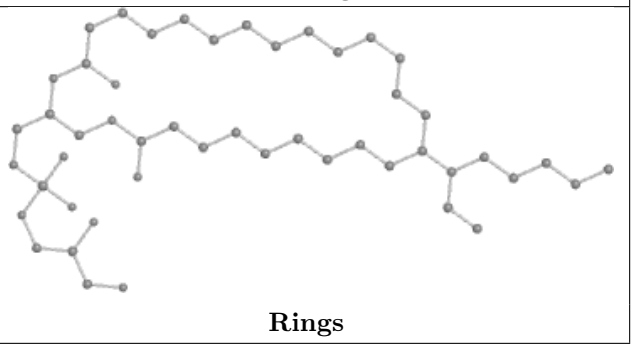
Bond lengths



Bond angles

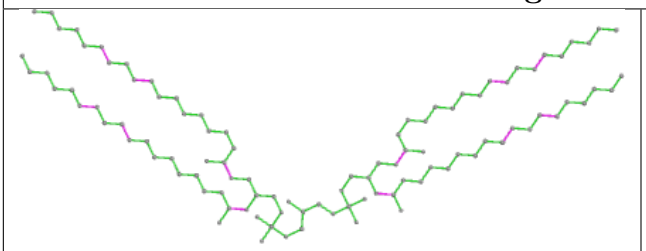


Torsions



Rings

Ligand CDL T 102



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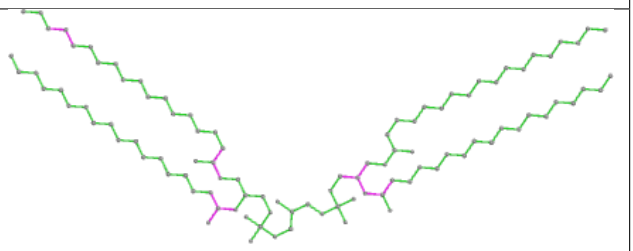
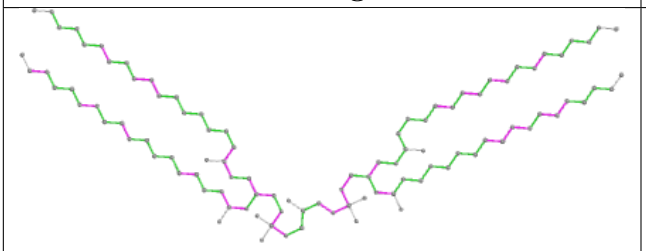
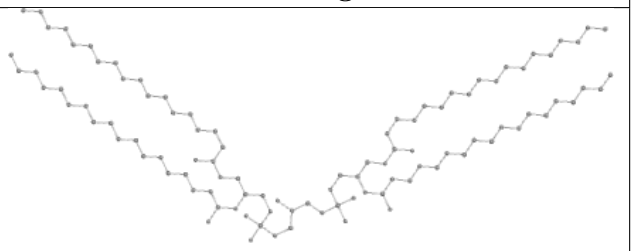


Bond angles

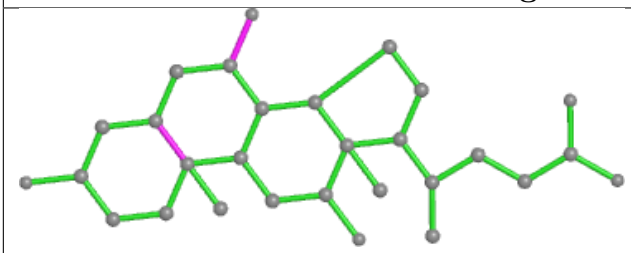


Torsions

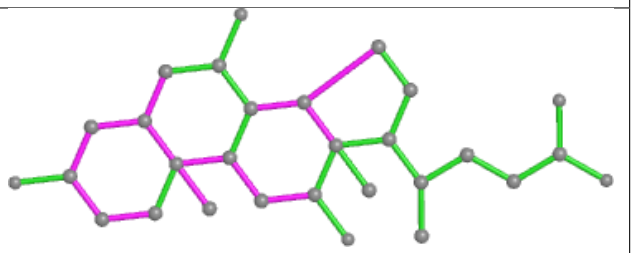


Rings

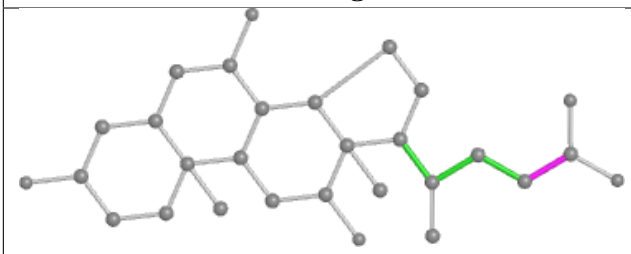
Ligand CHD G 103



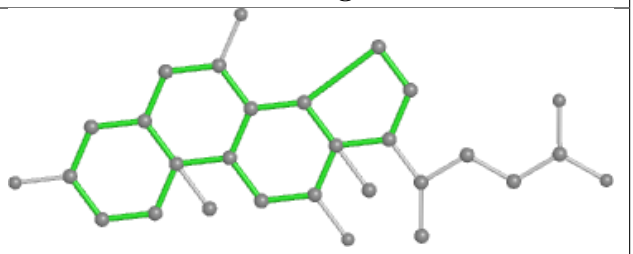
Bond lengths



Bond angles

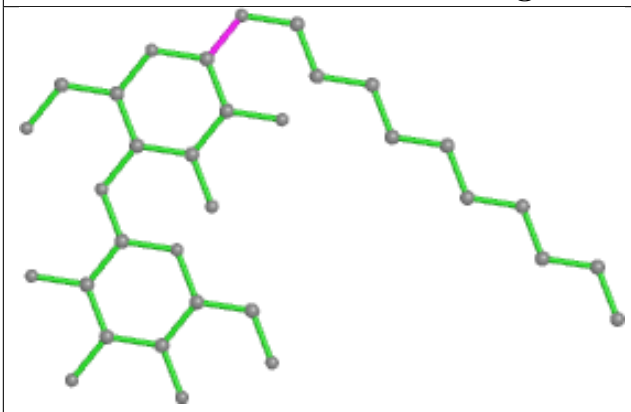


Torsions

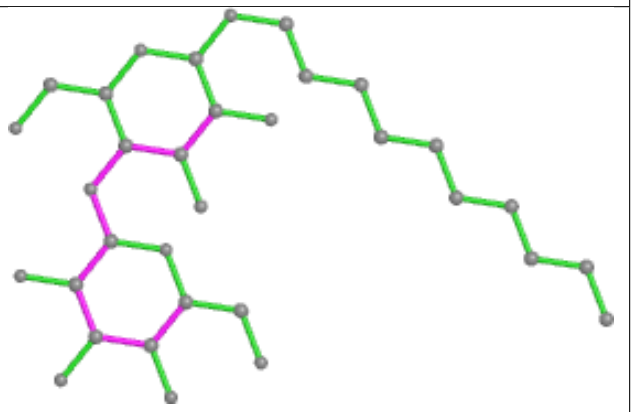


Rings

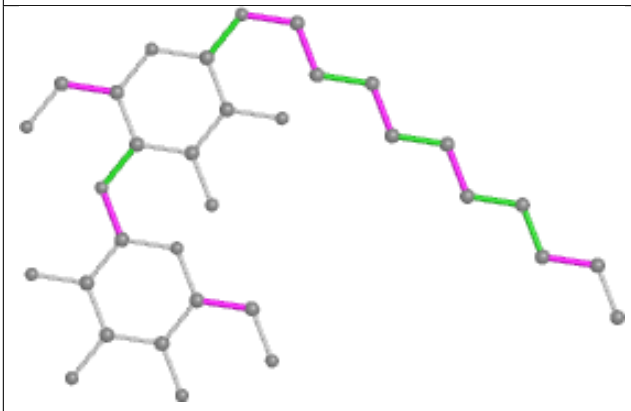
Ligand DMU K 106



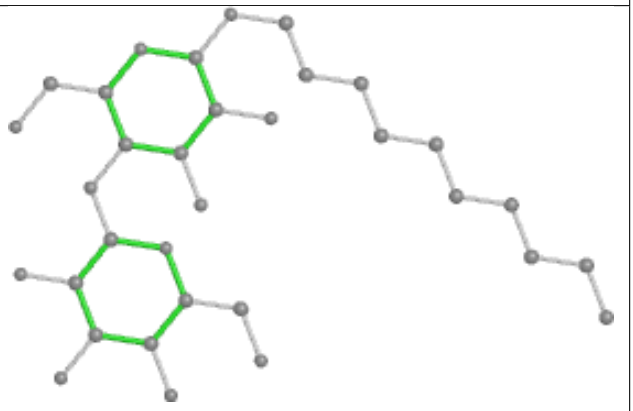
Bond lengths



Bond angles

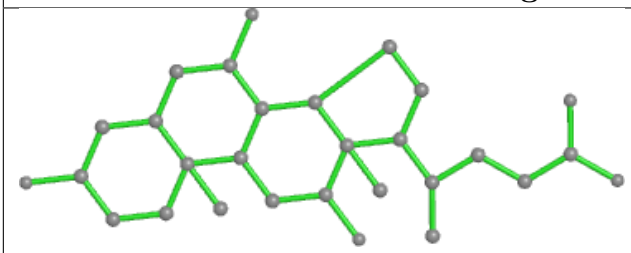


Torsions

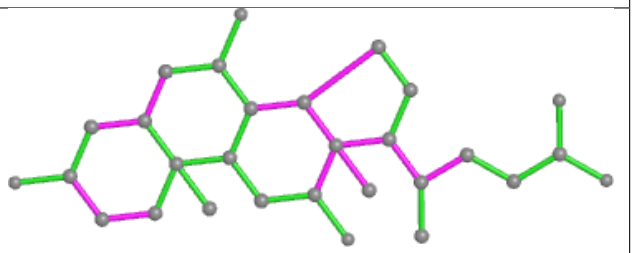


Rings

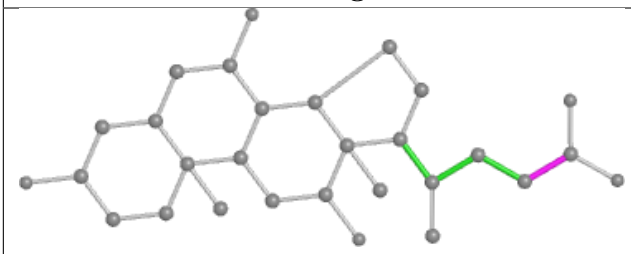
Ligand CHD C 306



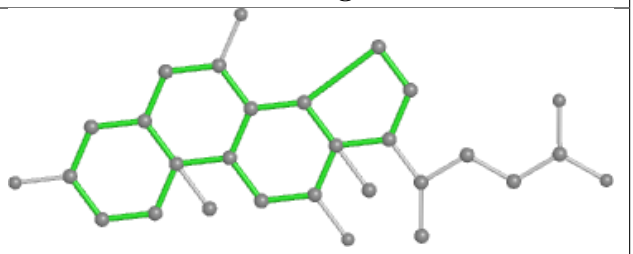
Bond lengths



Bond angles

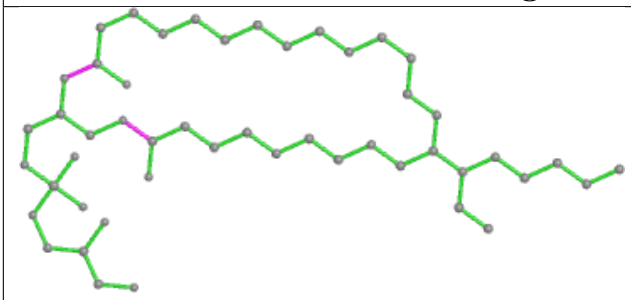


Torsions

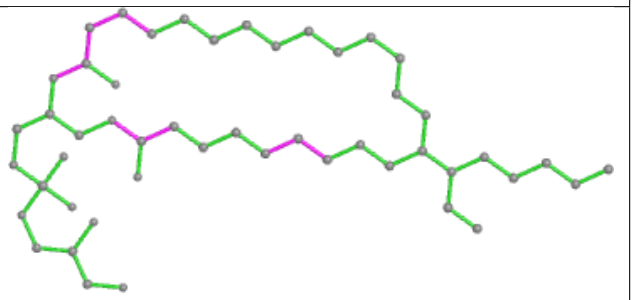


Rings

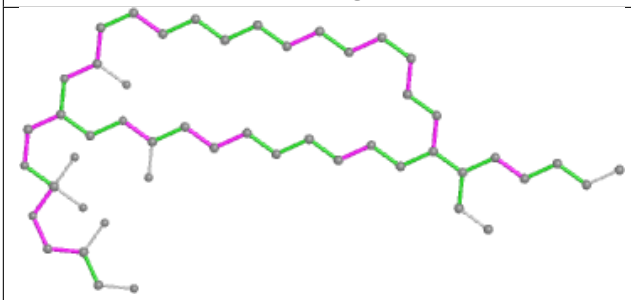
Ligand PGV A 608



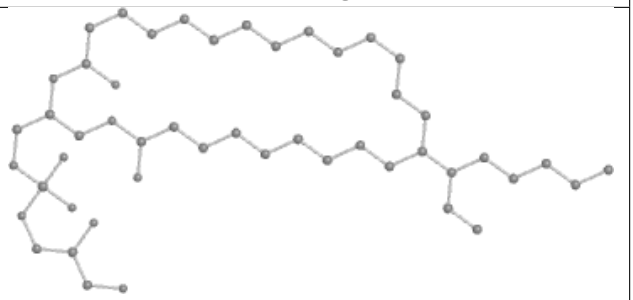
Bond lengths



Bond angles

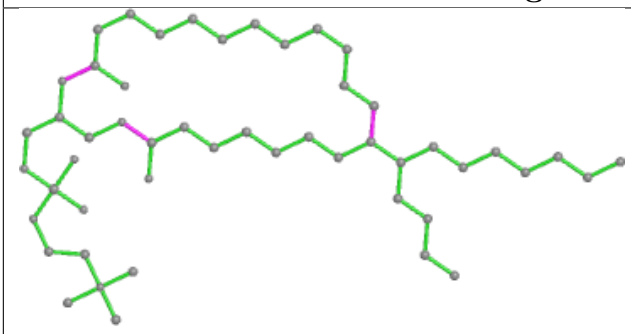


Torsions

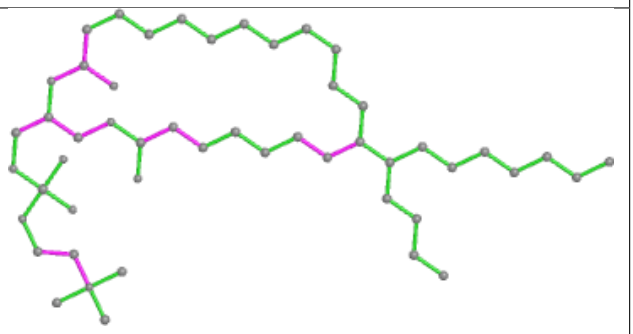


Rings

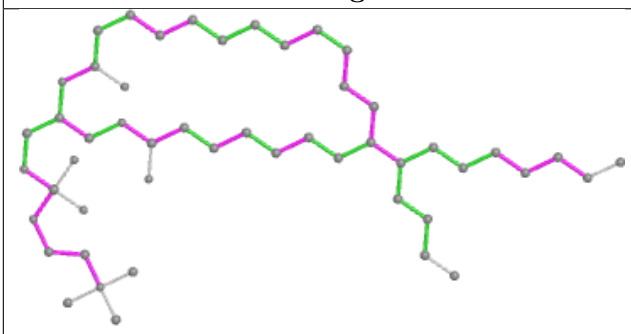
Ligand PSC N 608



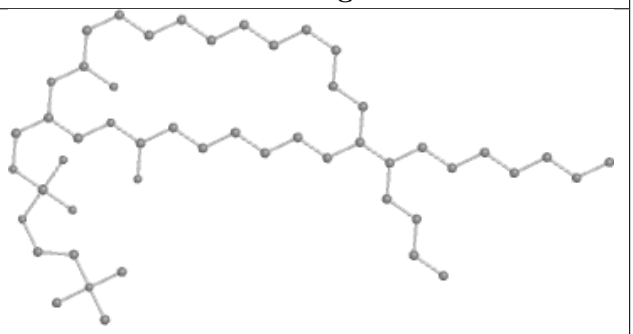
Bond lengths



Bond angles

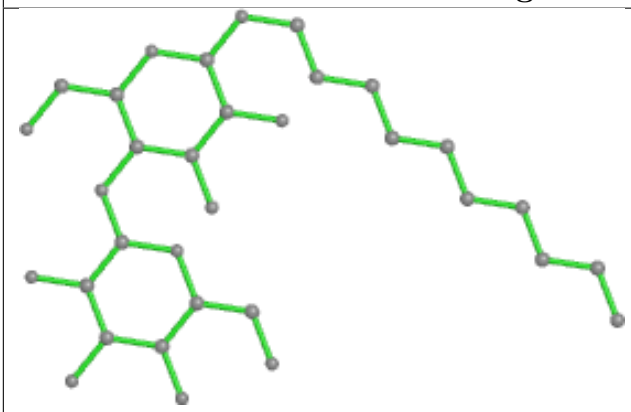


Torsions

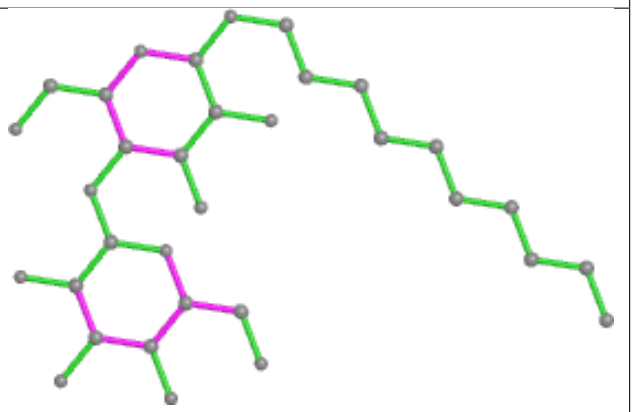


Rings

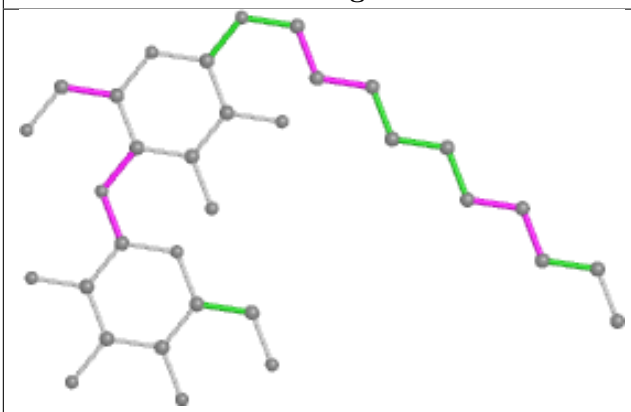
Ligand DMU K 103



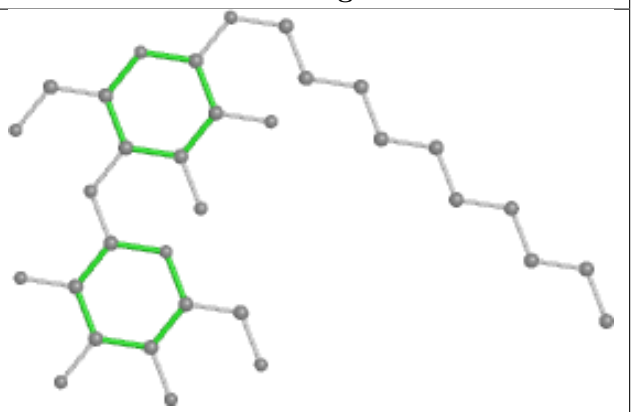
Bond lengths



Bond angles

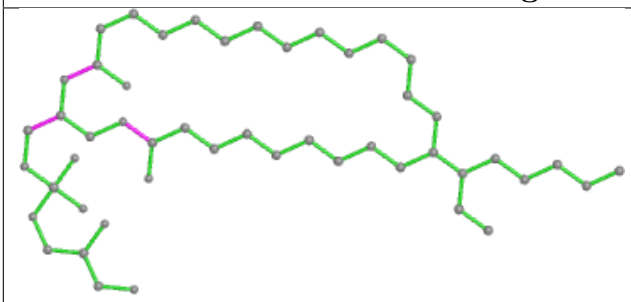


Torsions

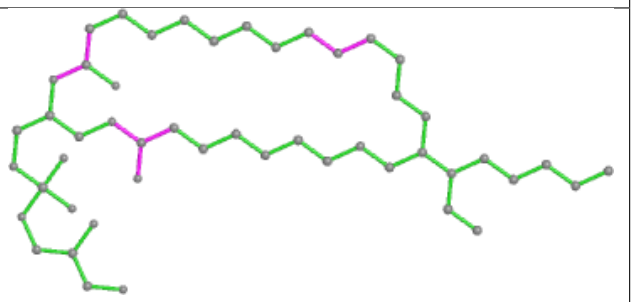


Rings

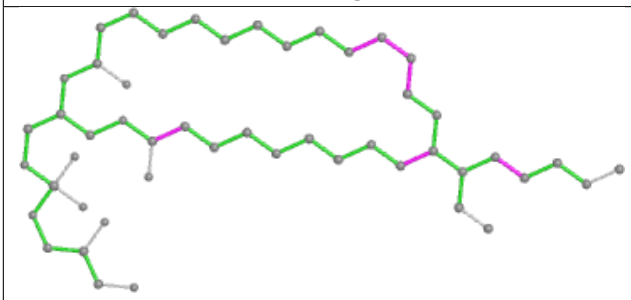
Ligand PGV A 607



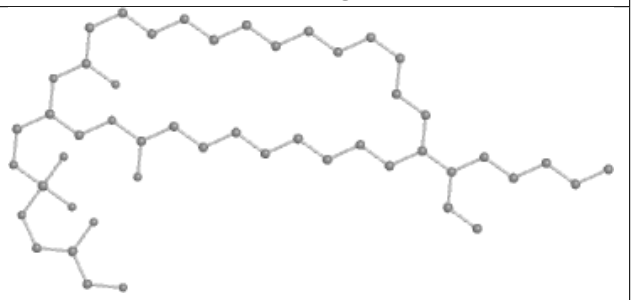
Bond lengths



Bond angles

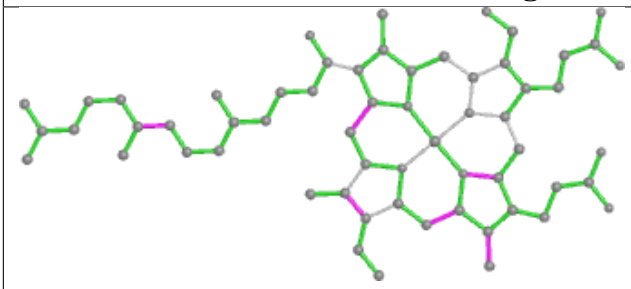


Torsions

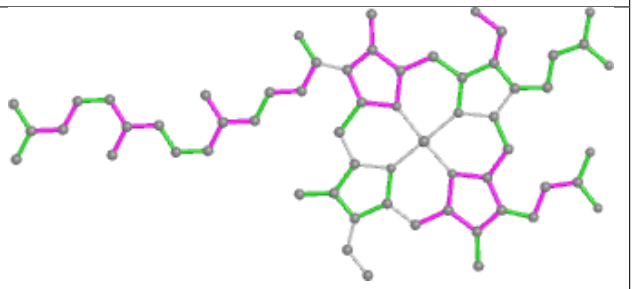


Rings

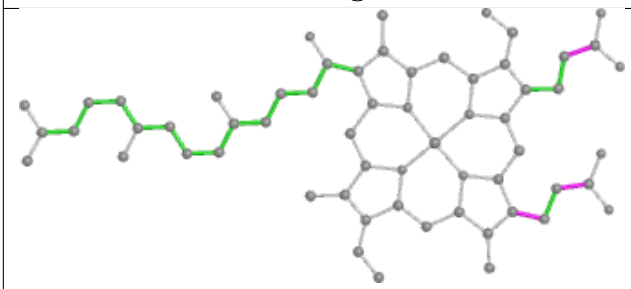
Ligand HEA A 602



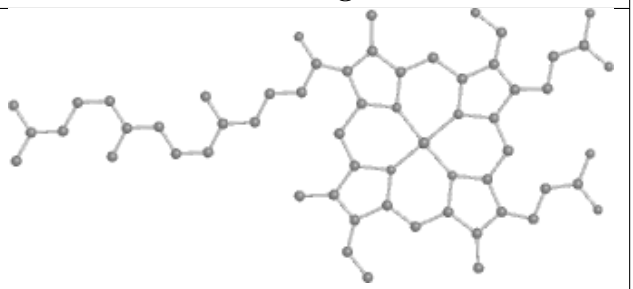
Bond lengths



Bond angles

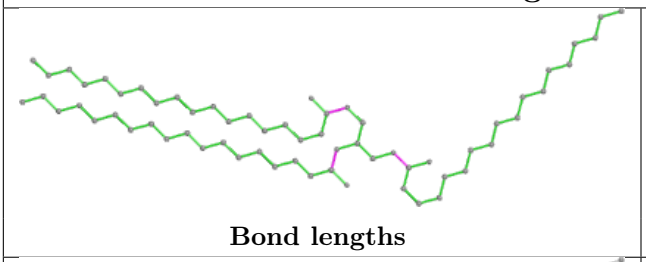


Torsions

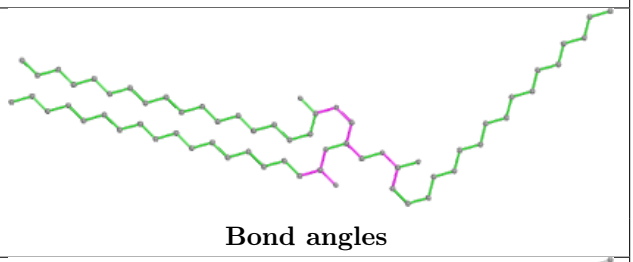


Rings

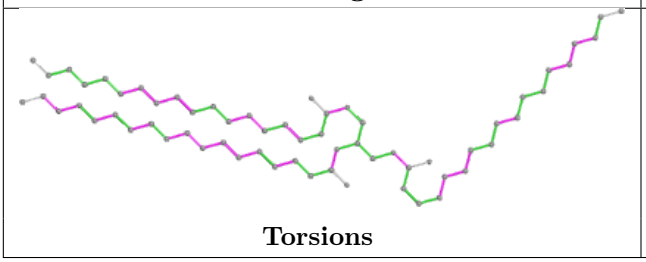
Ligand TGL O 301



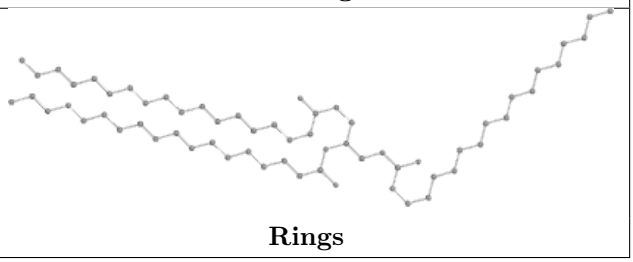
Bond lengths



Bond angles

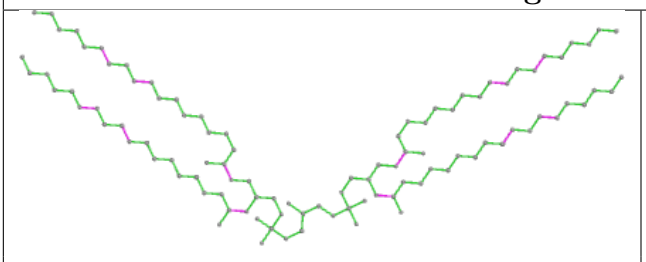


Torsions

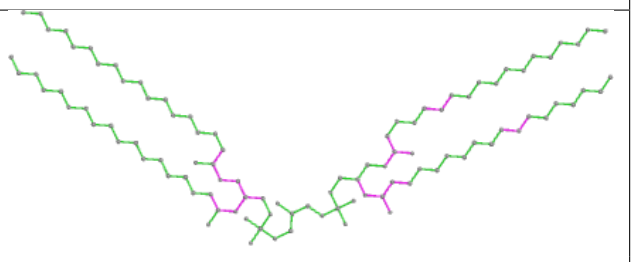


Rings

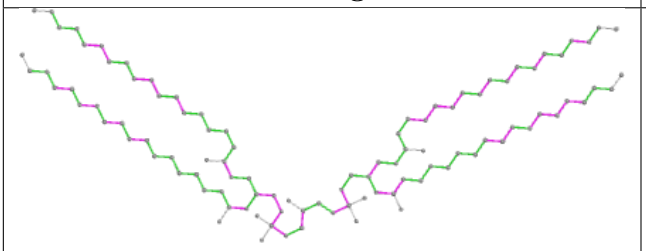
Ligand CDL C 304



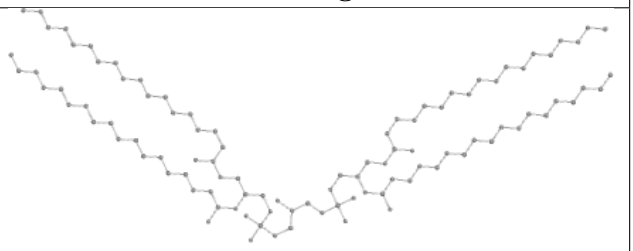
Bond lengths



Bond angles

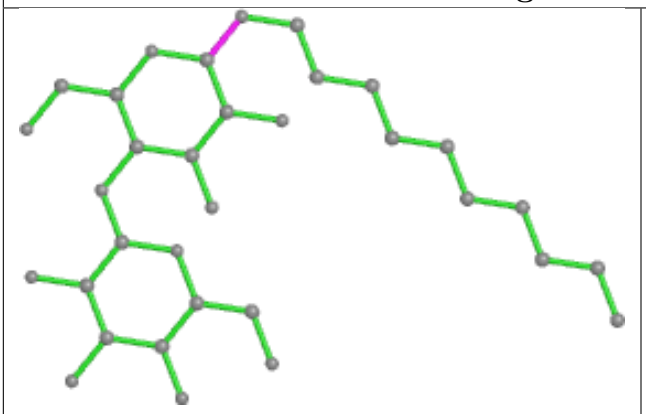


Torsions

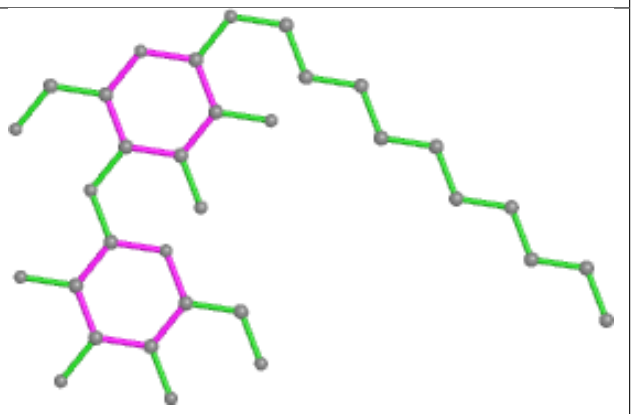


Rings

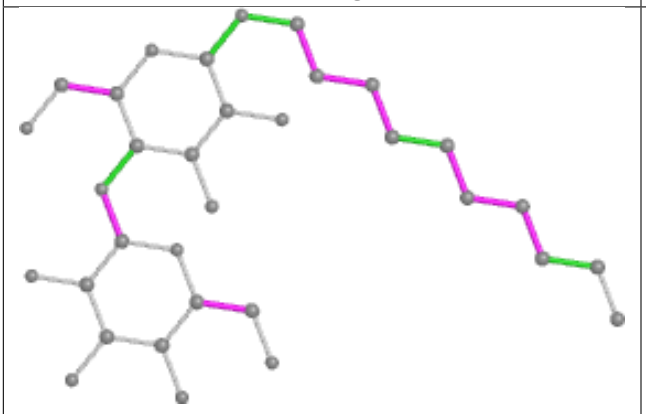
Ligand DMU X 101



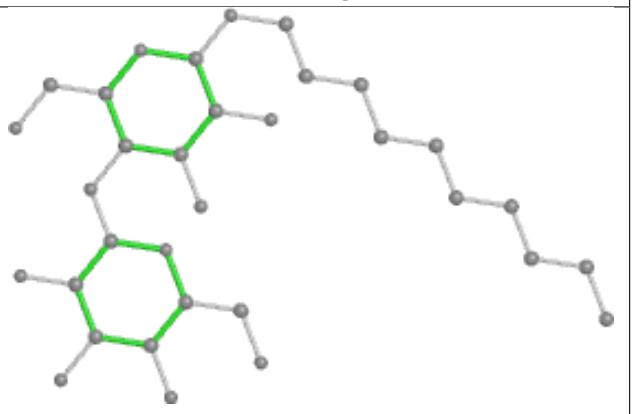
Bond lengths



Bond angles

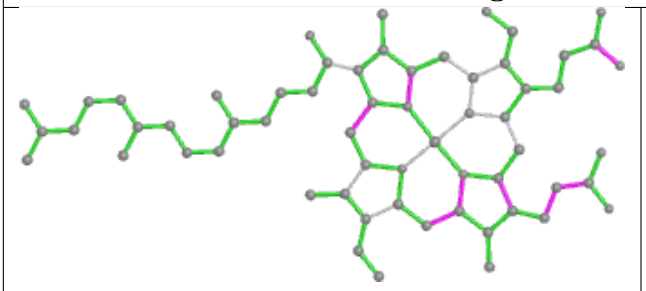


Torsions

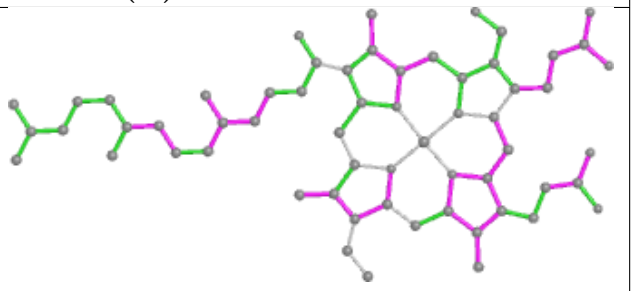


Rings

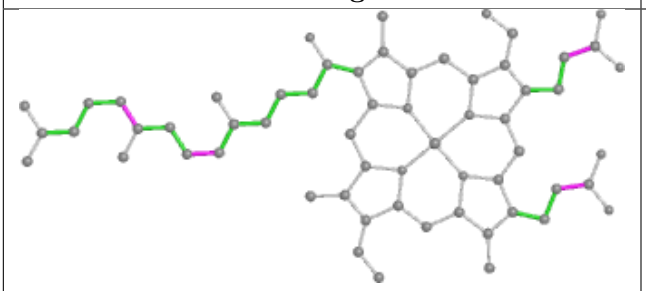
Ligand HEA N 601 (B)



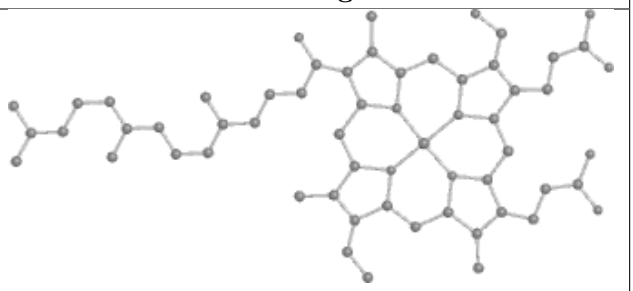
Bond lengths



Bond angles

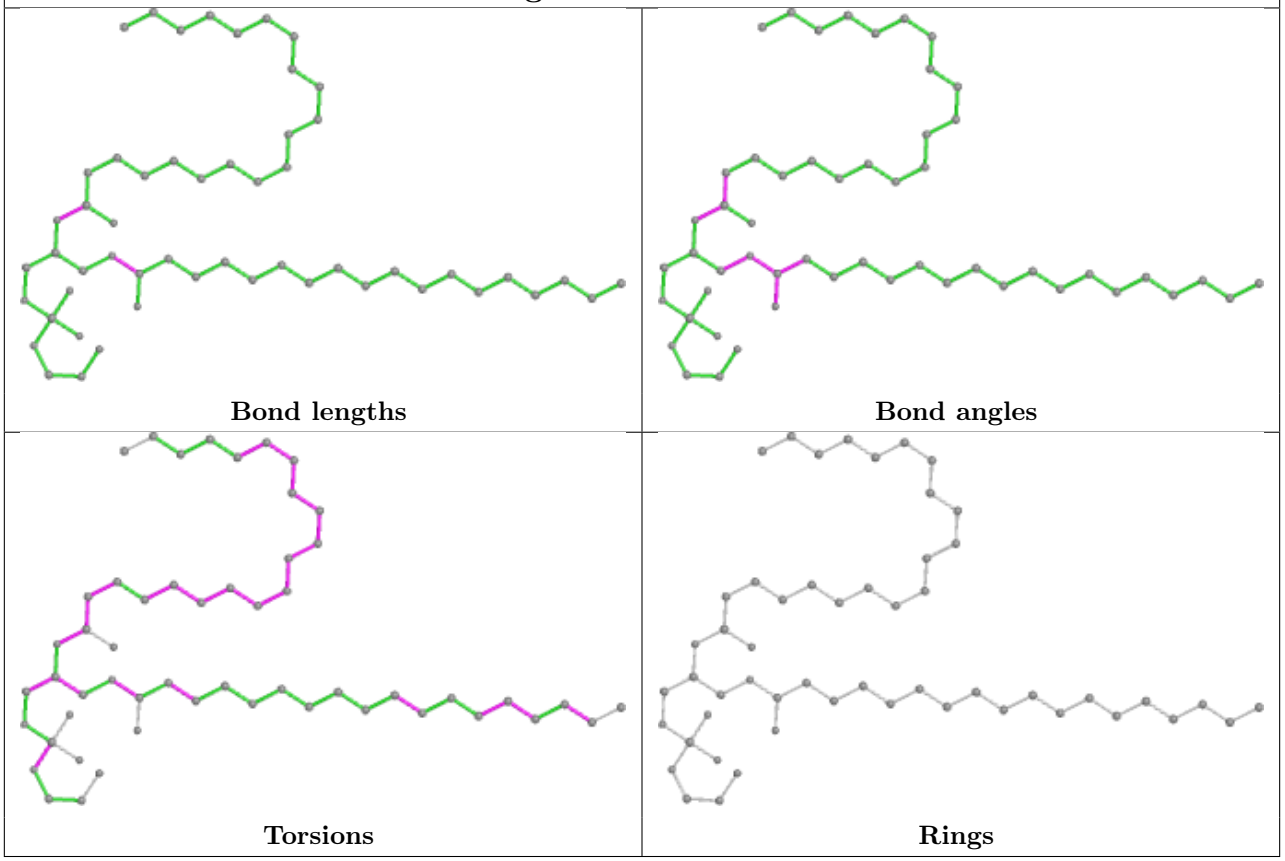


Torsions

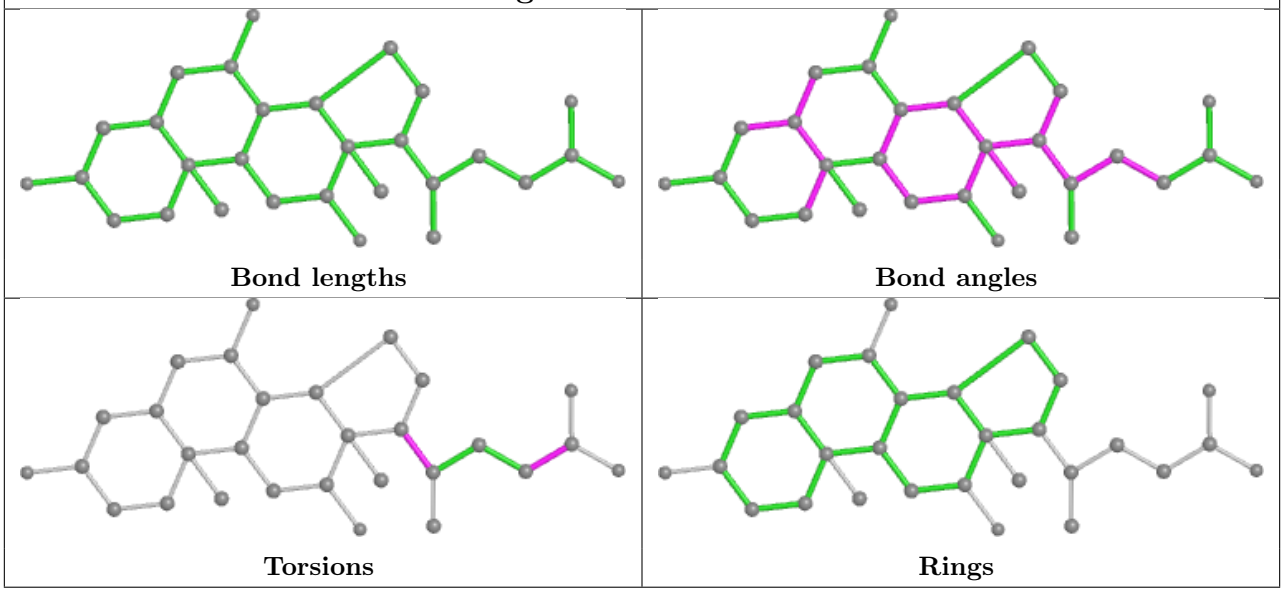


Rings

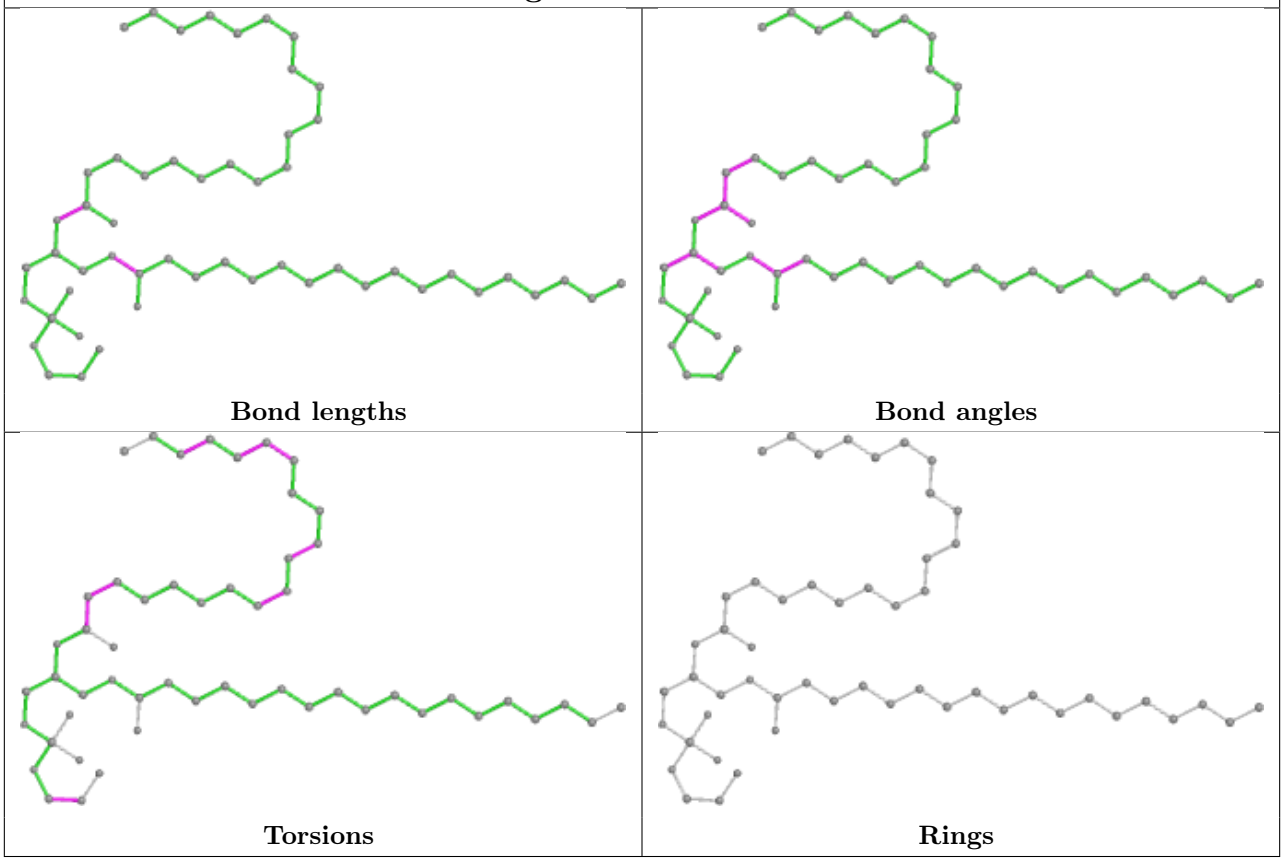
Ligand PEK P 309



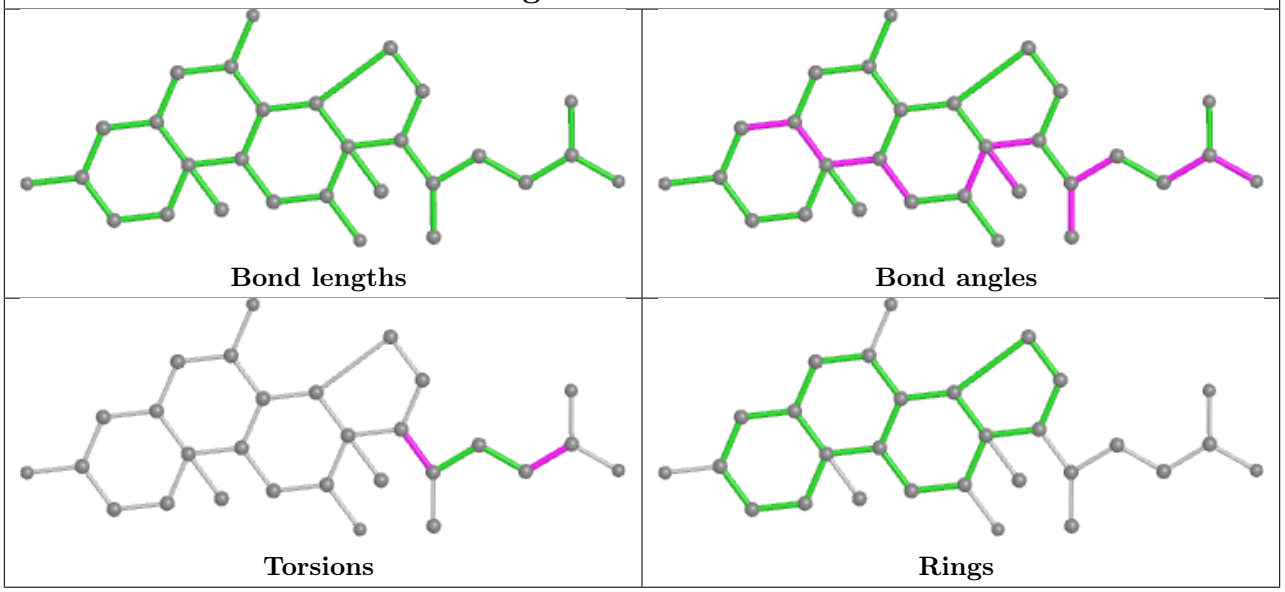
Ligand CHD W 101



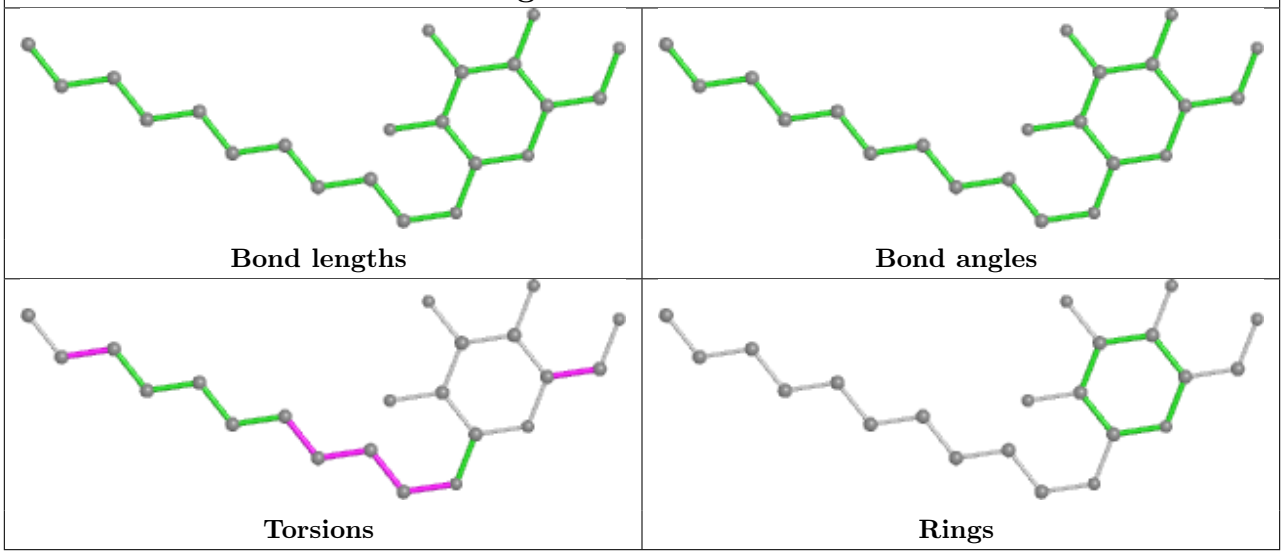
Ligand PEK P 304



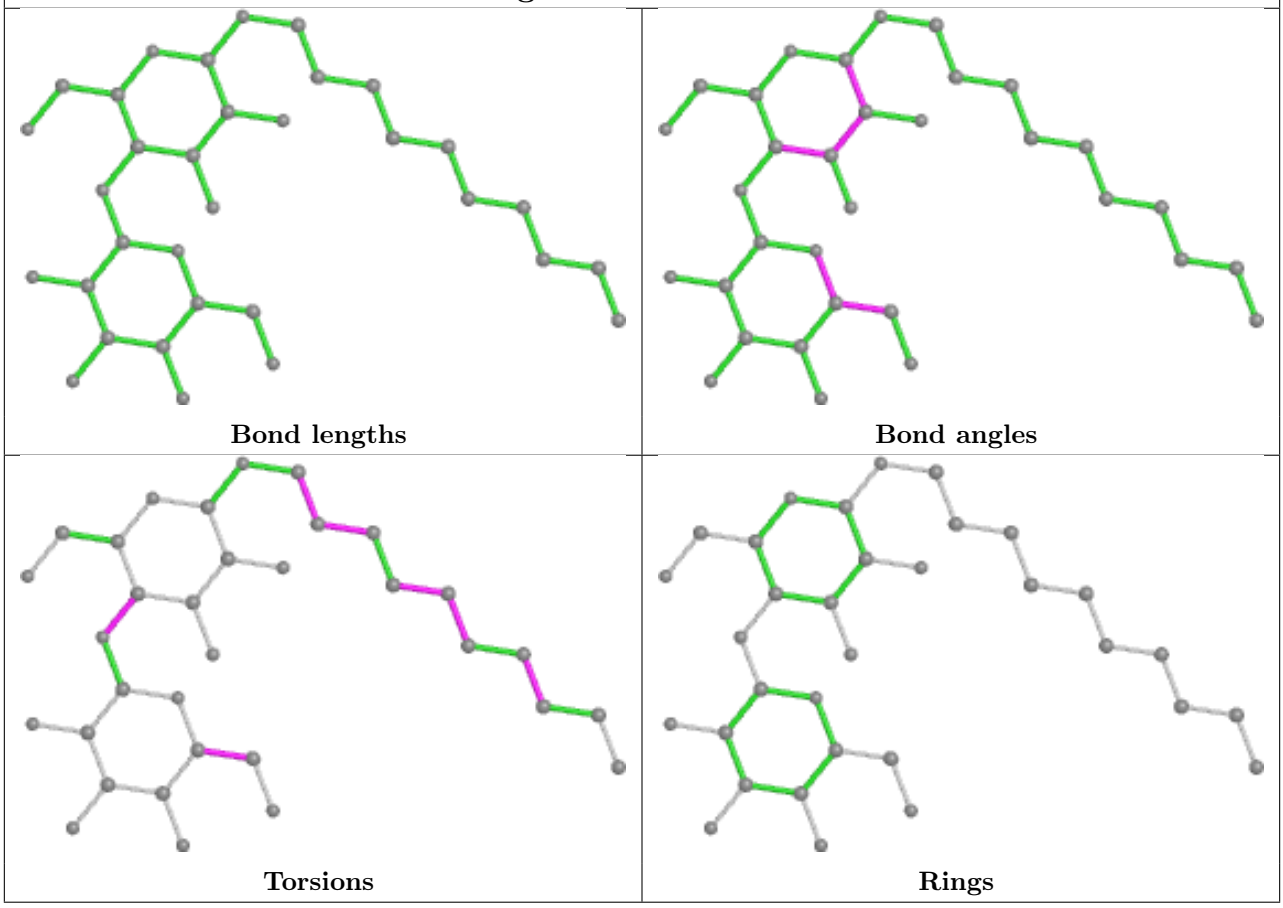
Ligand CHD P 308



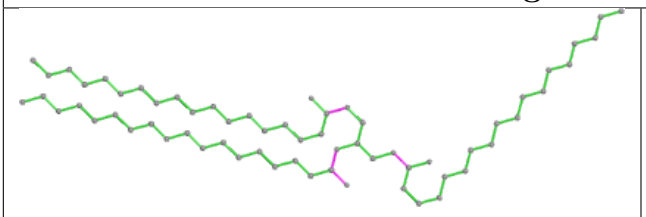
Ligand DMU X 103



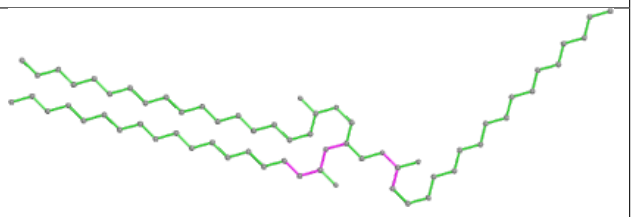
Ligand DMU D 202



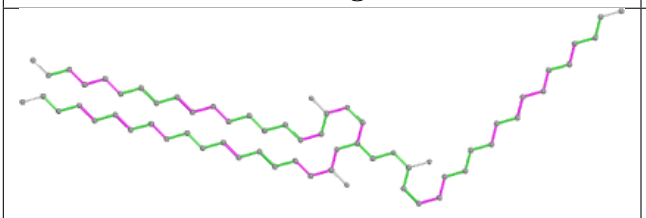
Ligand TGL D 201



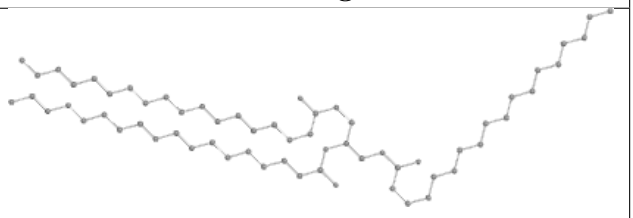
Bond lengths



Bond angles

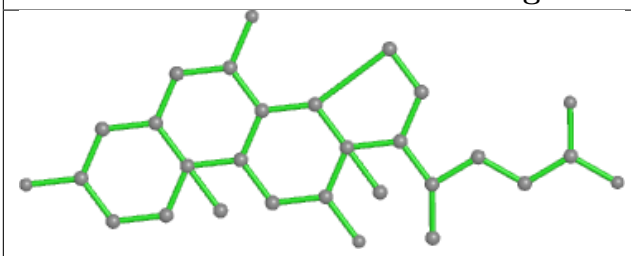


Torsions

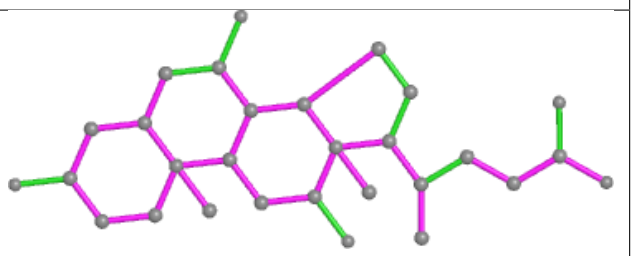


Rings

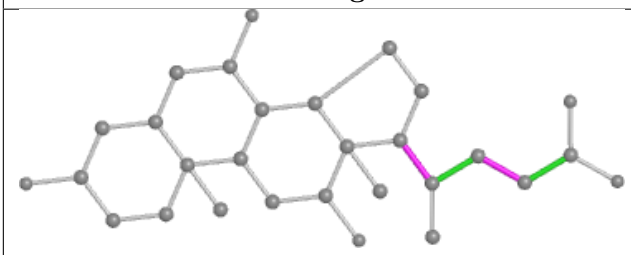
Ligand CHD L 103



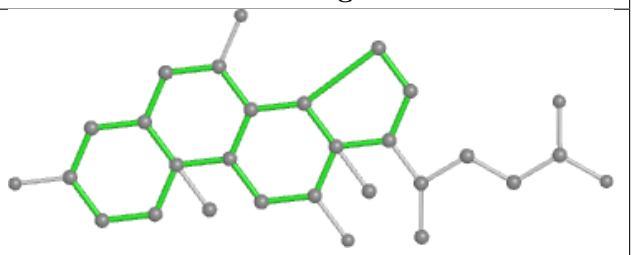
Bond lengths



Bond angles

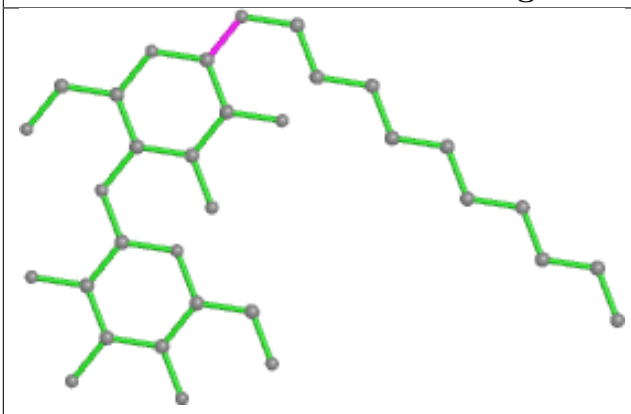


Torsions

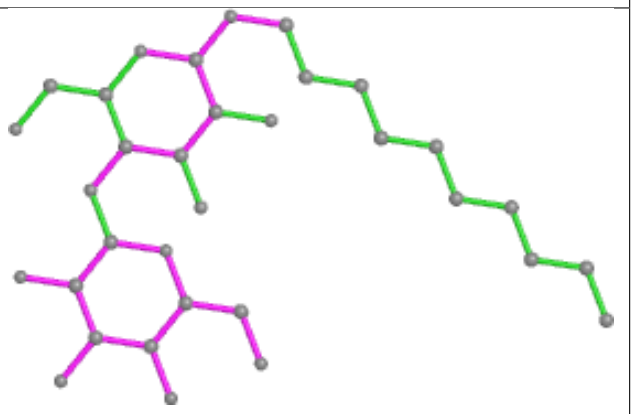


Rings

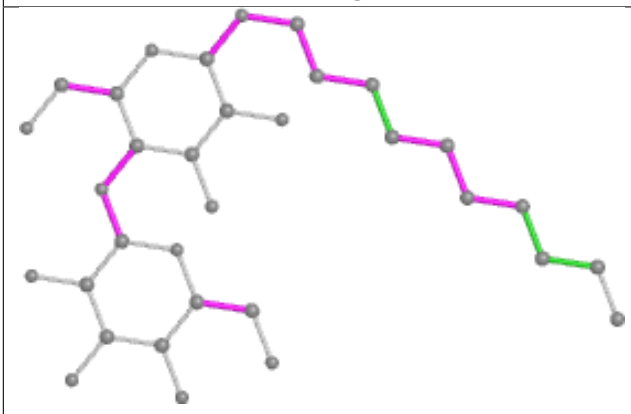
Ligand DMU B 306



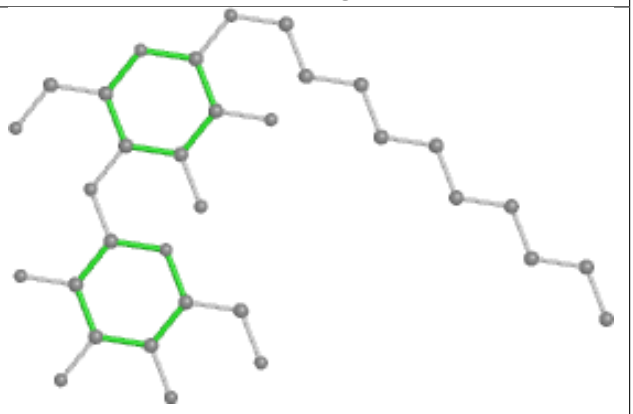
Bond lengths



Bond angles

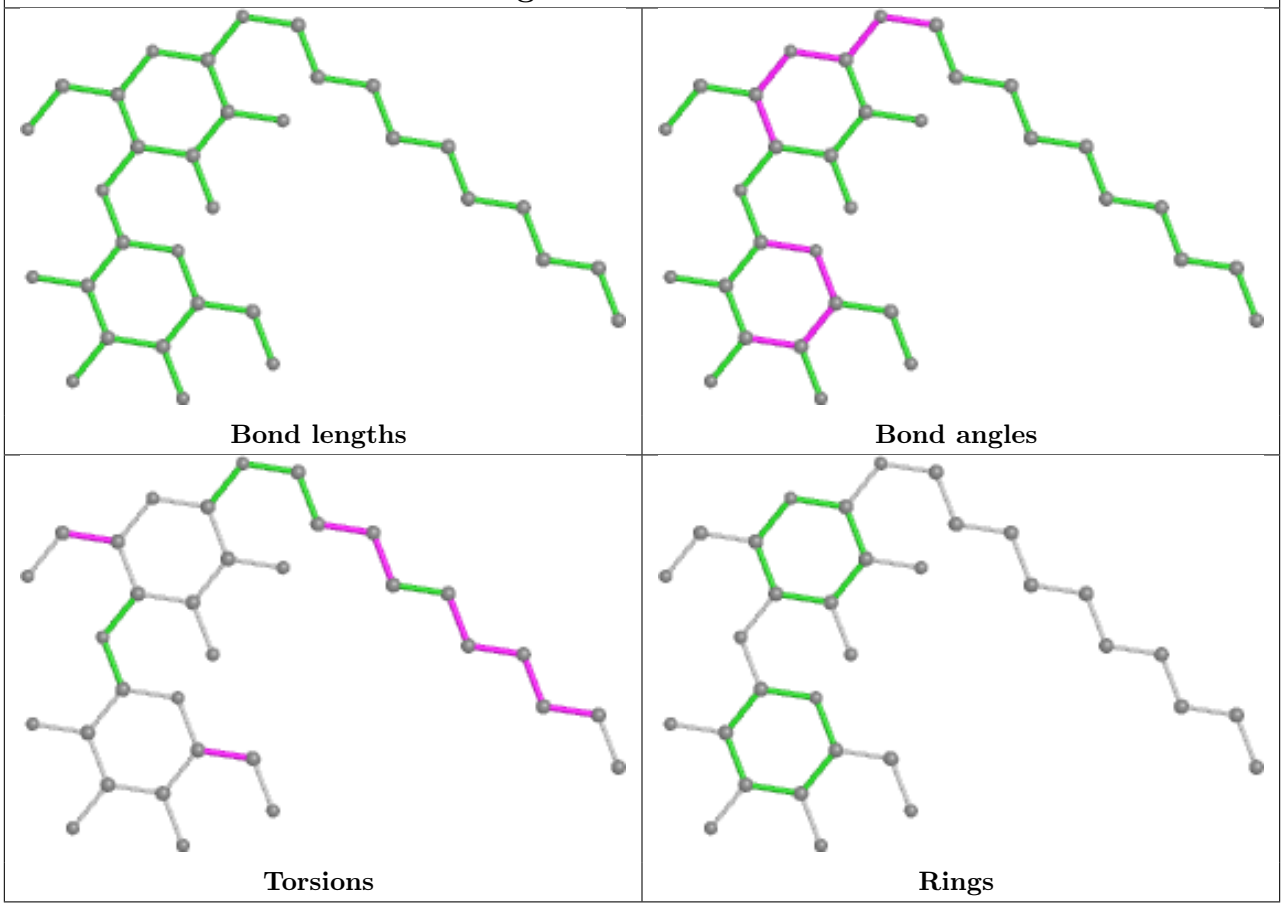


Torsions

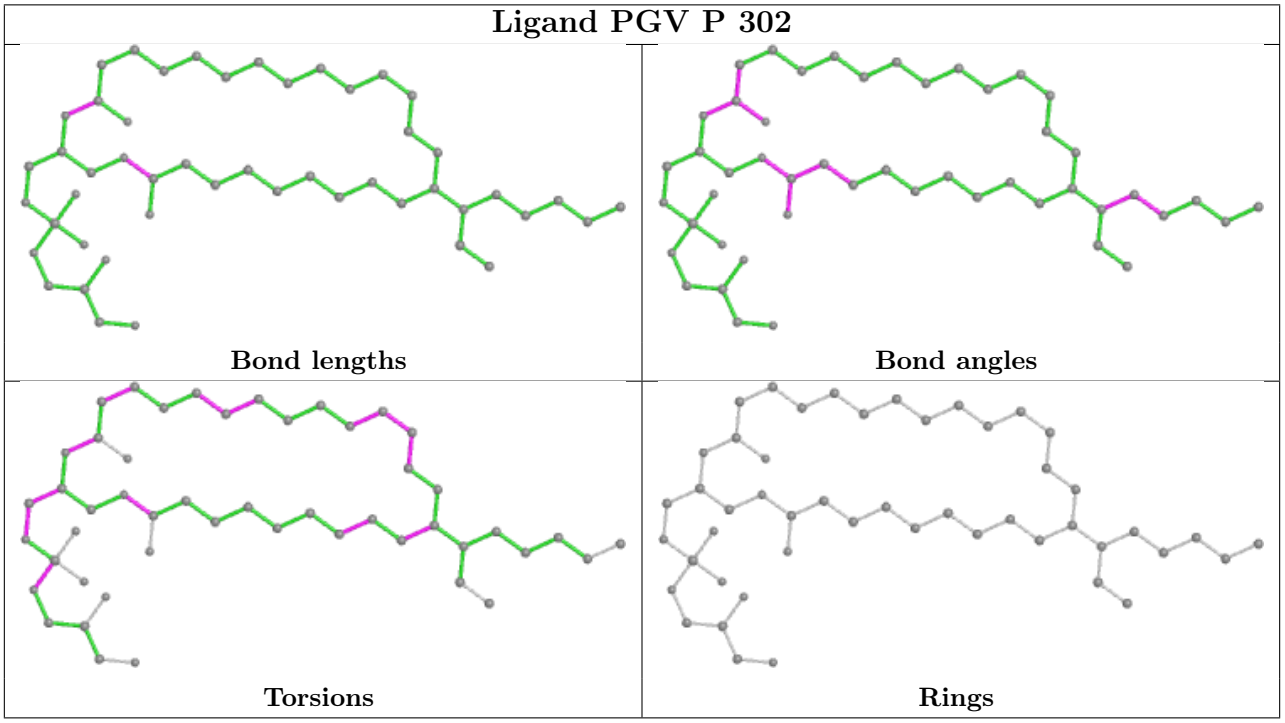


Rings

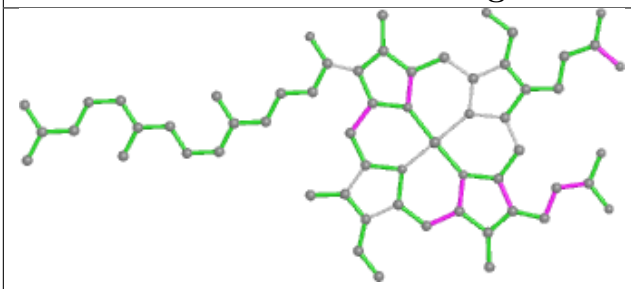
Ligand DMU K 105



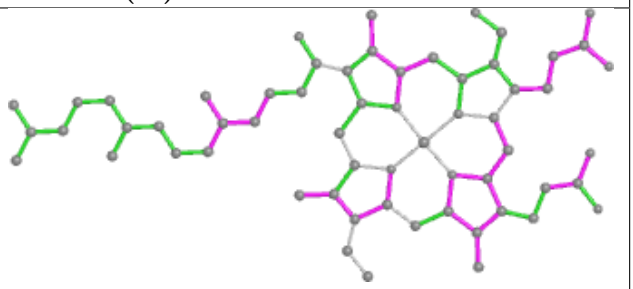
Ligand PGV P 302



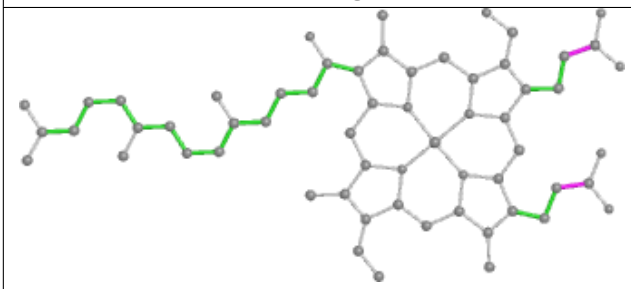
Ligand HEA N 601 (A)



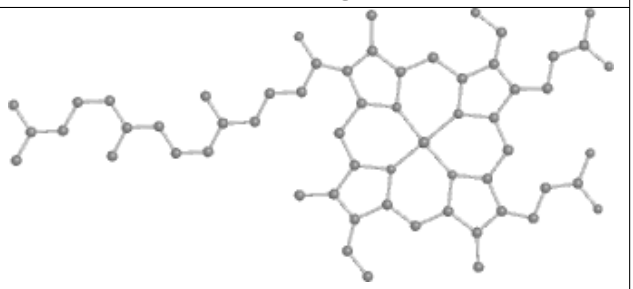
Bond lengths



Bond angles

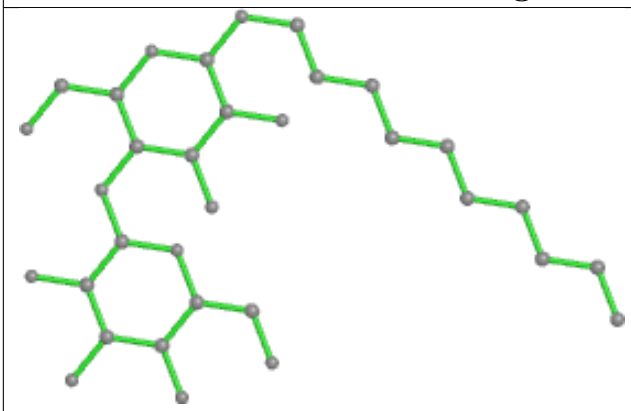


Torsions

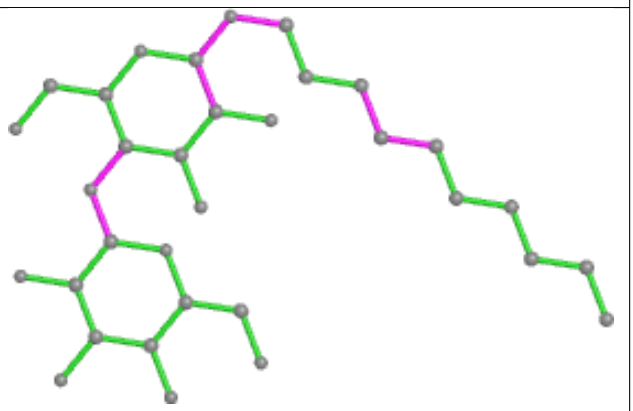


Rings

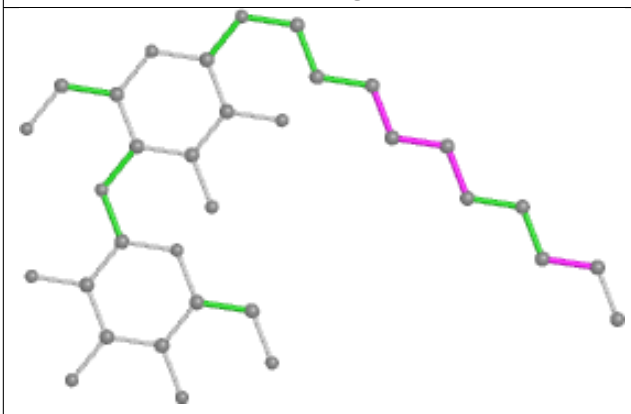
Ligand DMU M 101



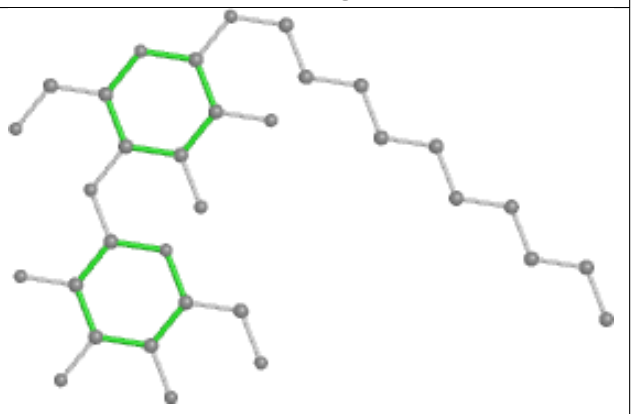
Bond lengths



Bond angles

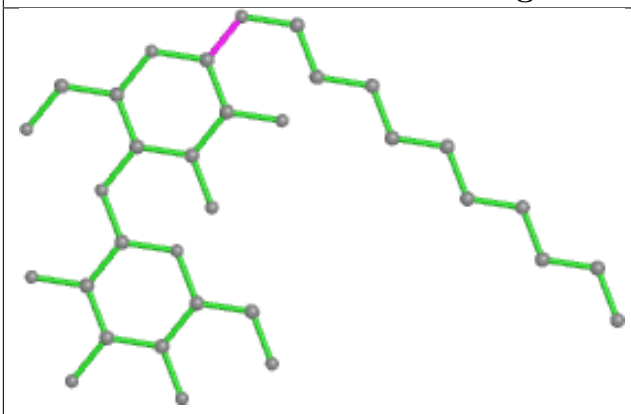


Torsions

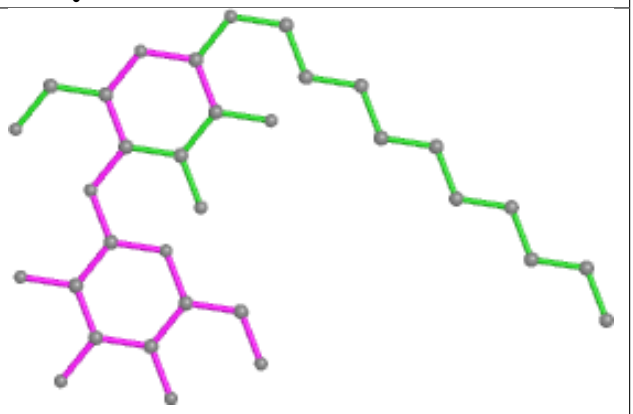


Rings

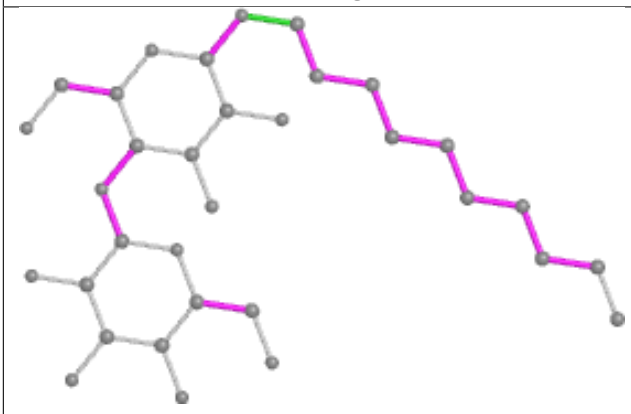
Ligand DMU Q 203



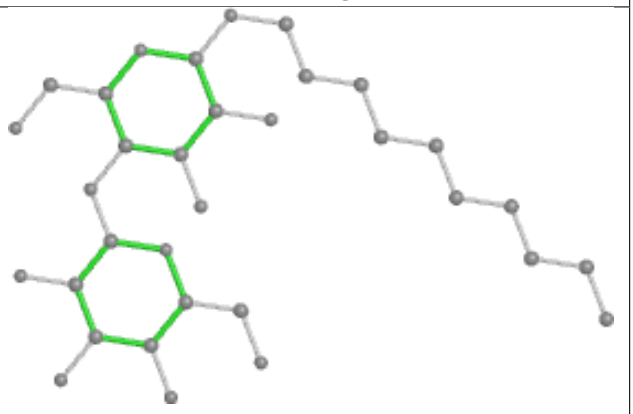
Bond lengths



Bond angles

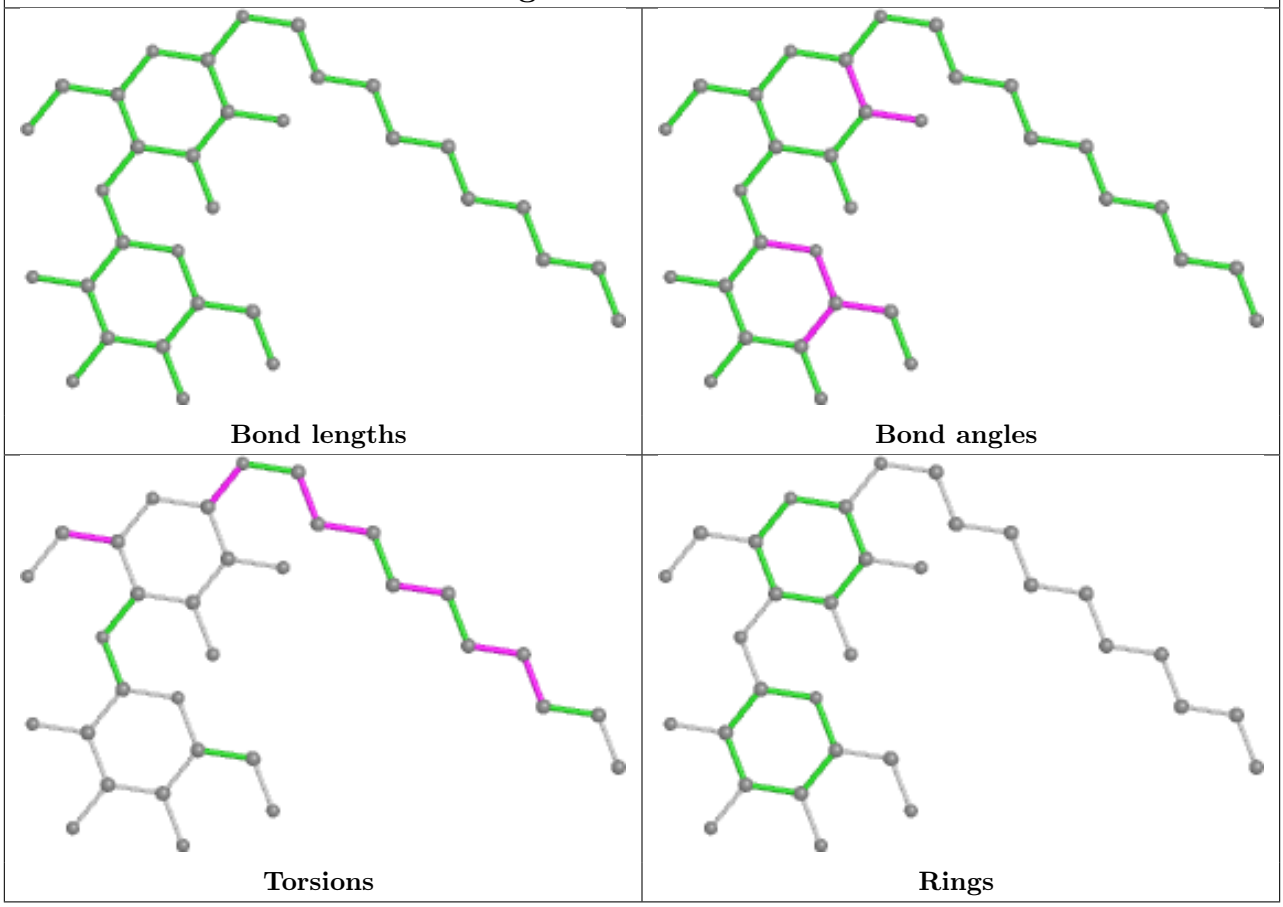


Torsions

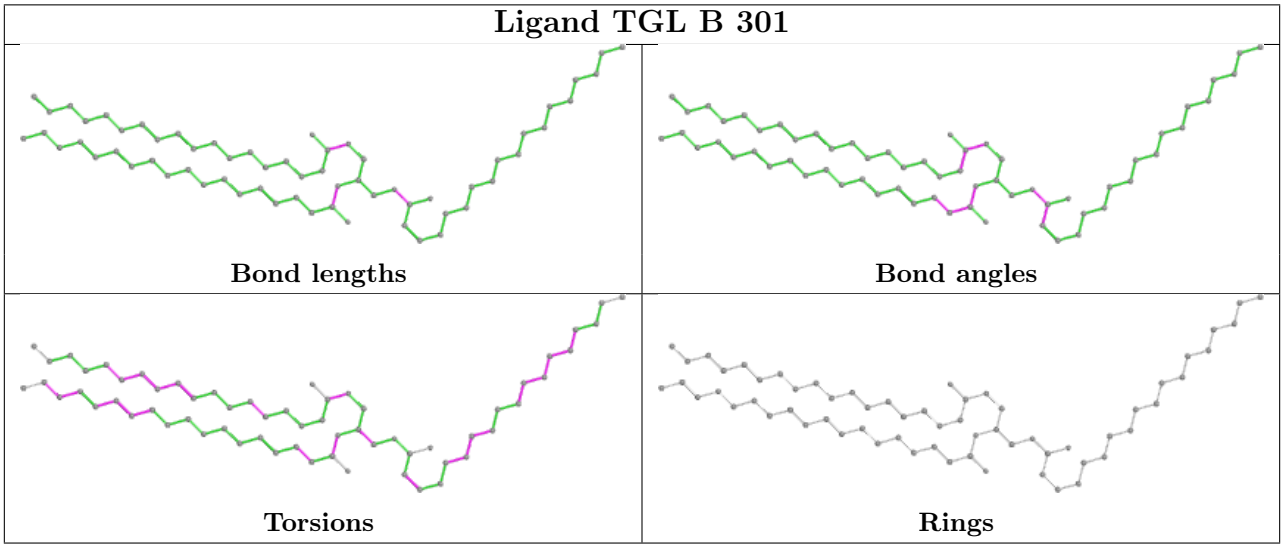


Rings

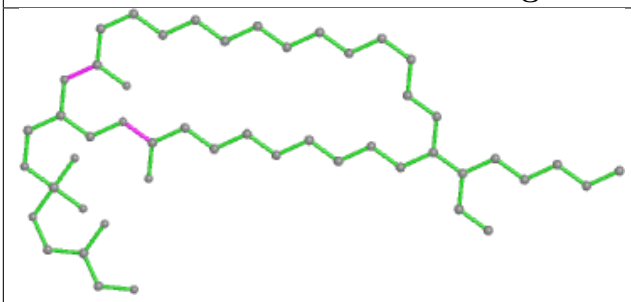
Ligand DMU P 314



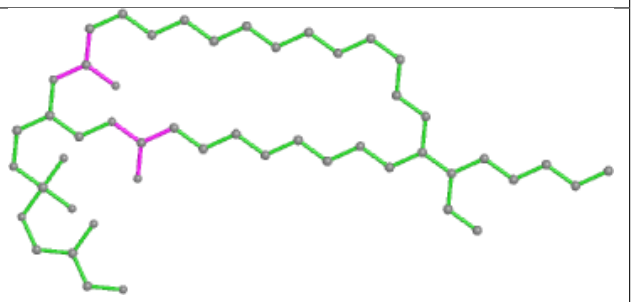
Ligand TGL B 301



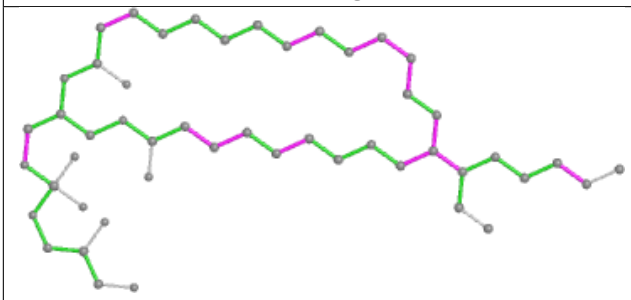
Ligand PGV C 303



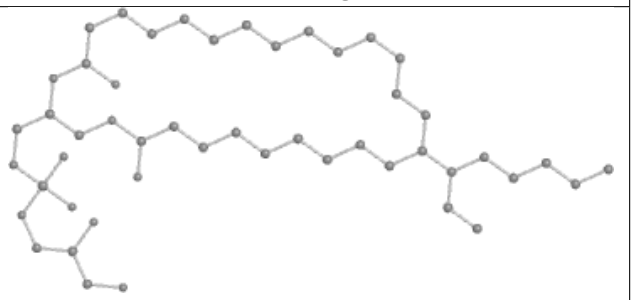
Bond lengths



Bond angles

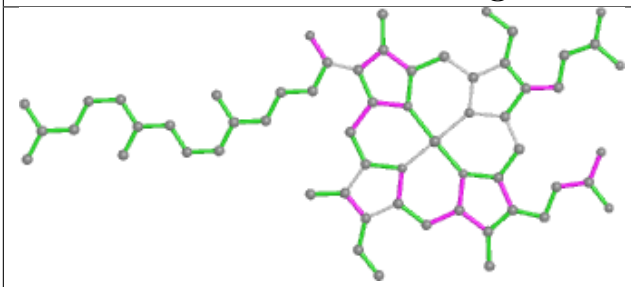


Torsions

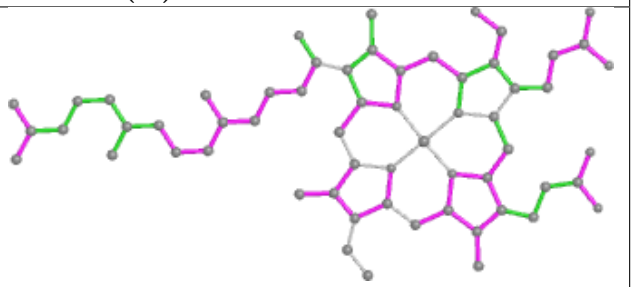


Rings

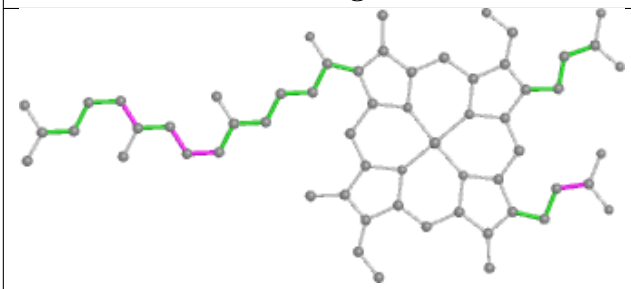
Ligand HEA A 601 (B)



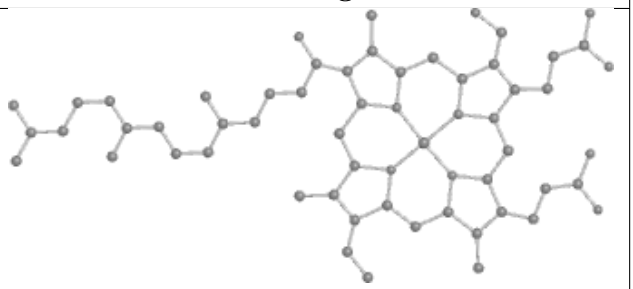
Bond lengths



Bond angles

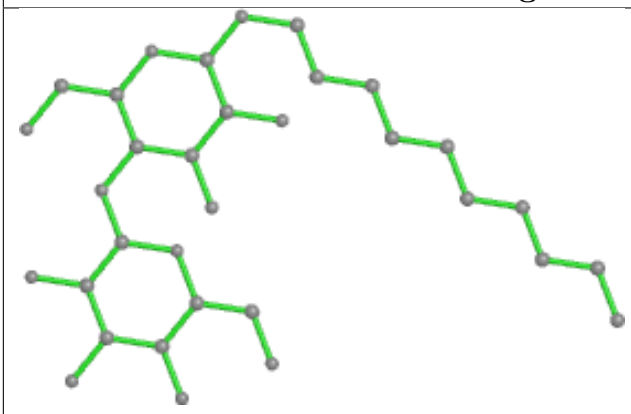


Torsions

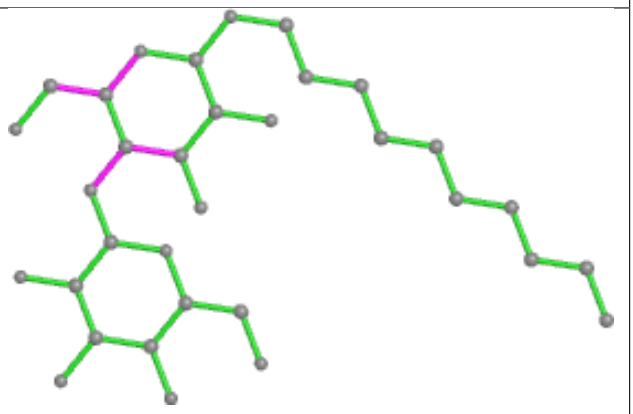


Rings

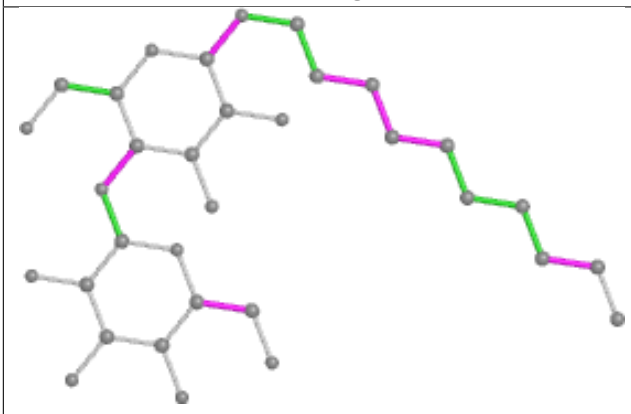
Ligand DMU L 102



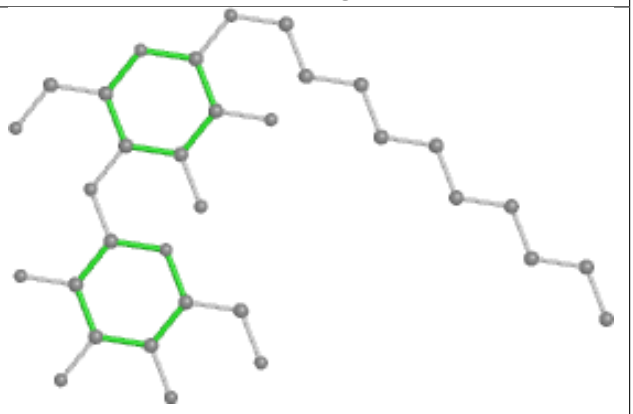
Bond lengths



Bond angles

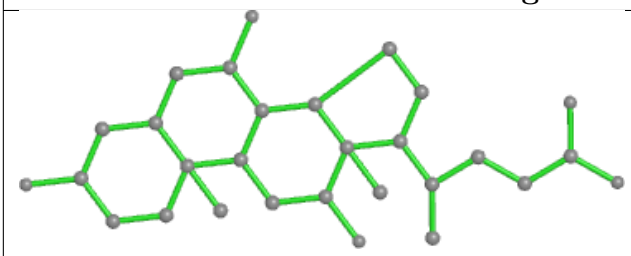


Torsions

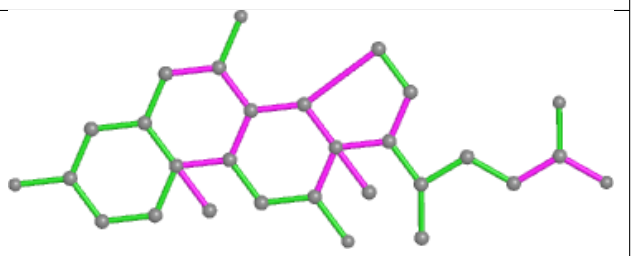


Rings

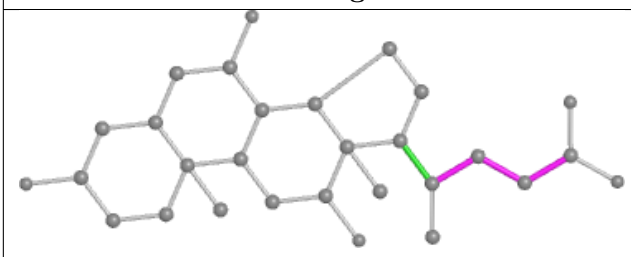
Ligand CHD P 307



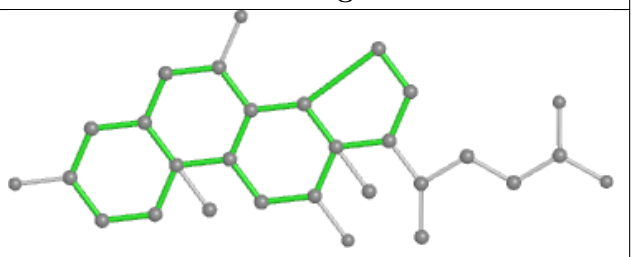
Bond lengths



Bond angles

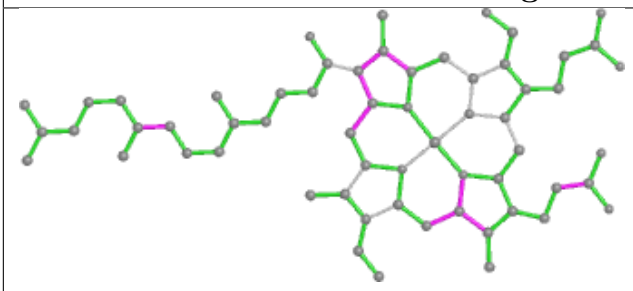


Torsions

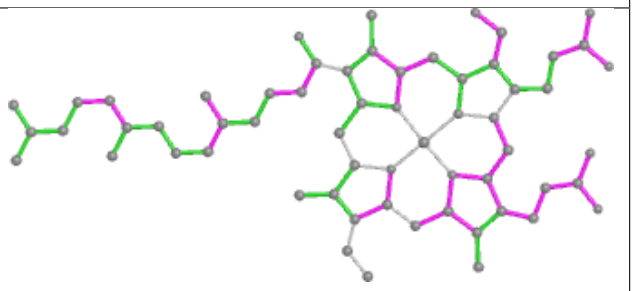


Rings

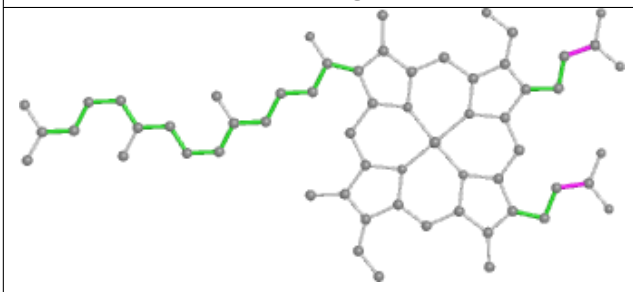
Ligand HEA N 602



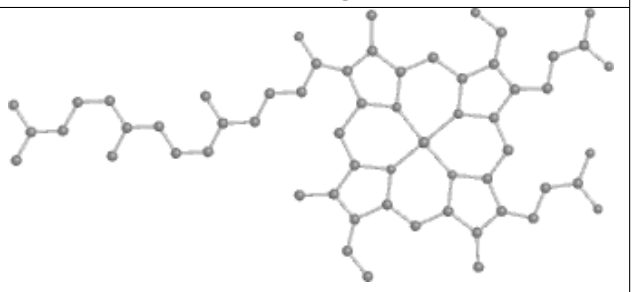
Bond lengths



Bond angles

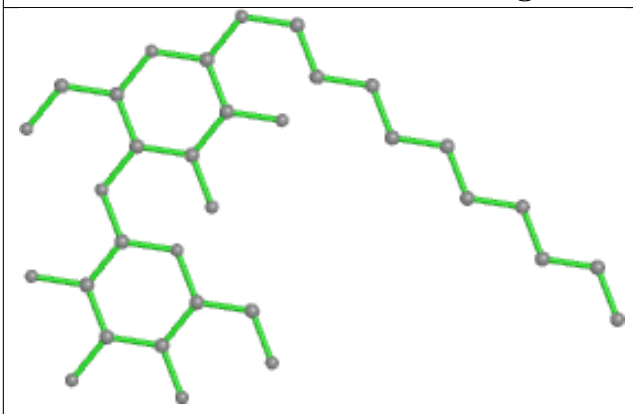


Torsions

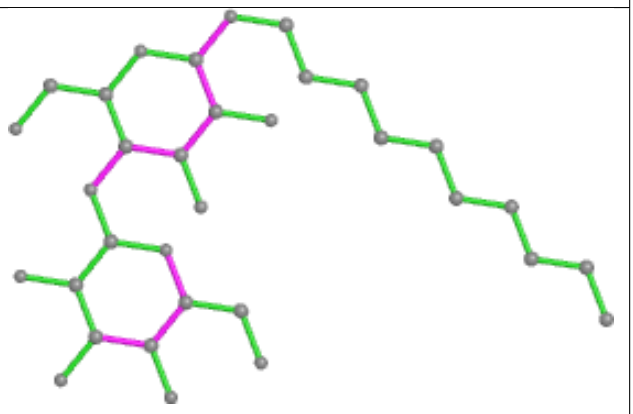


Rings

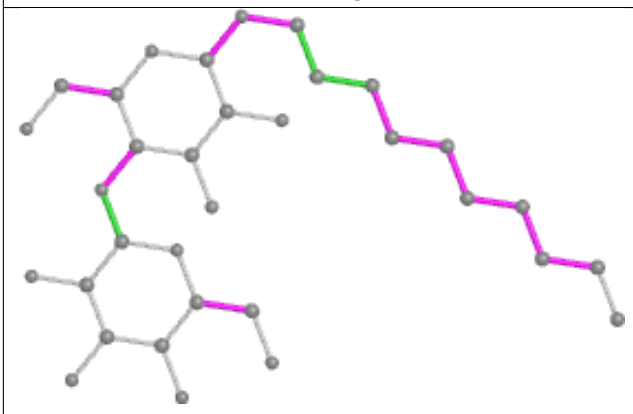
Ligand DMU K 104



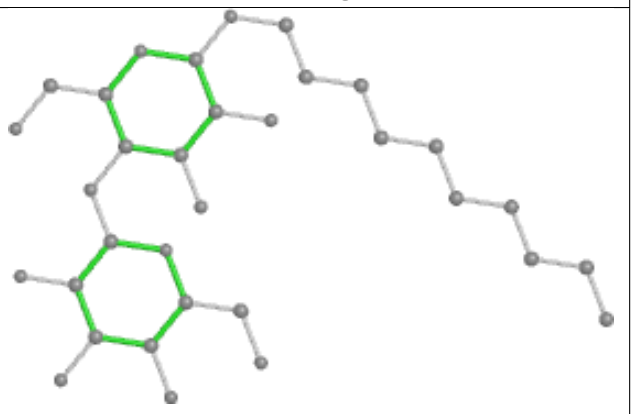
Bond lengths



Bond angles

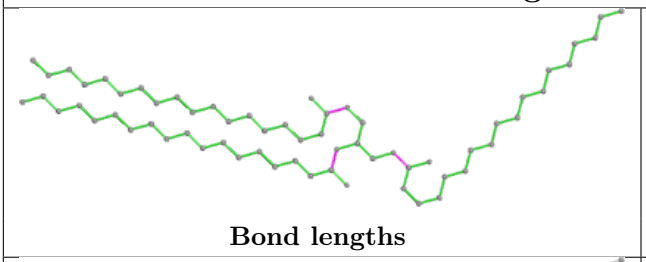


Torsions

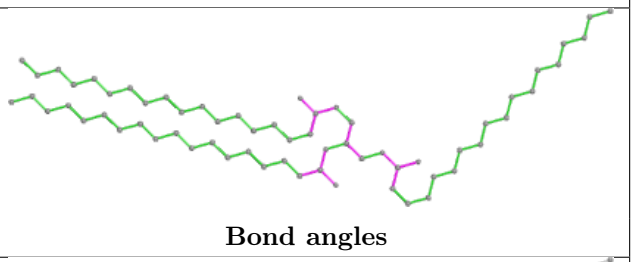


Rings

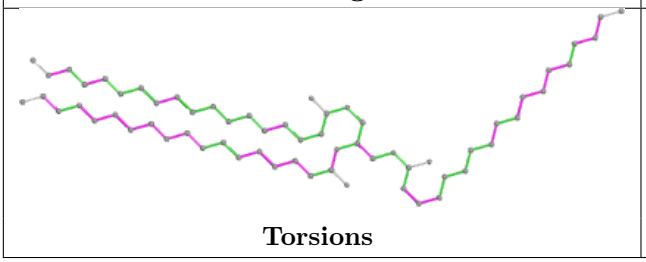
Ligand TGL Y 101



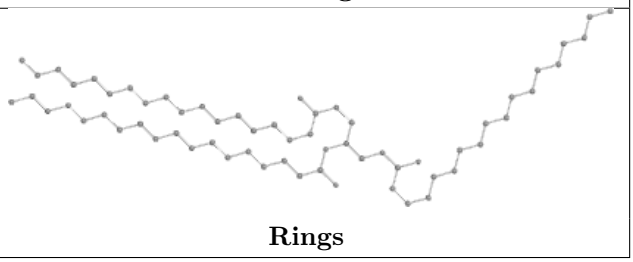
Bond lengths



Bond angles

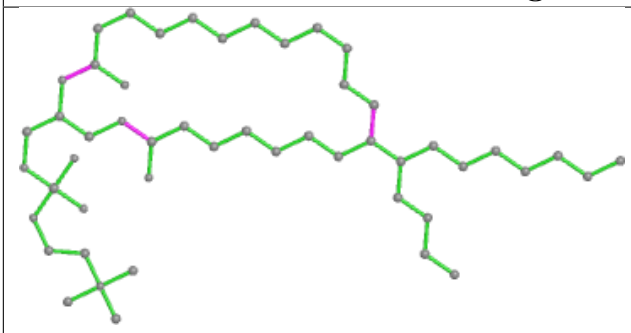


Torsions

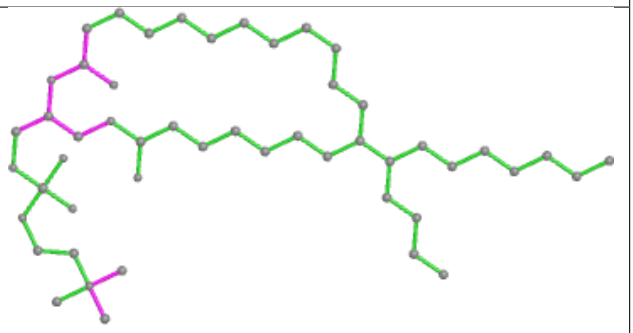


Rings

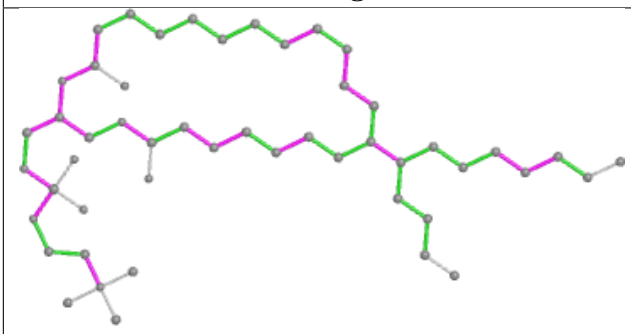
Ligand PSC B 303



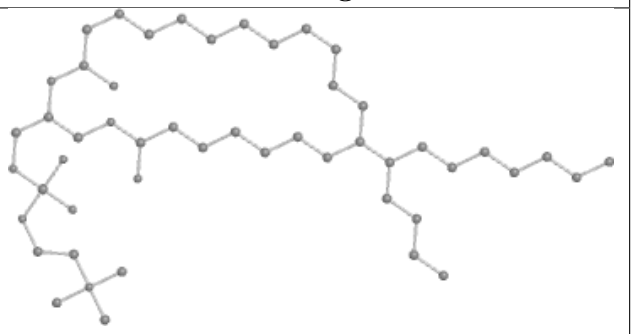
Bond lengths



Bond angles

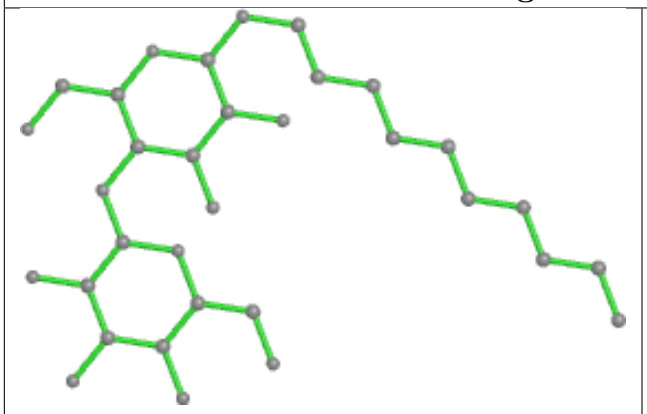


Torsions

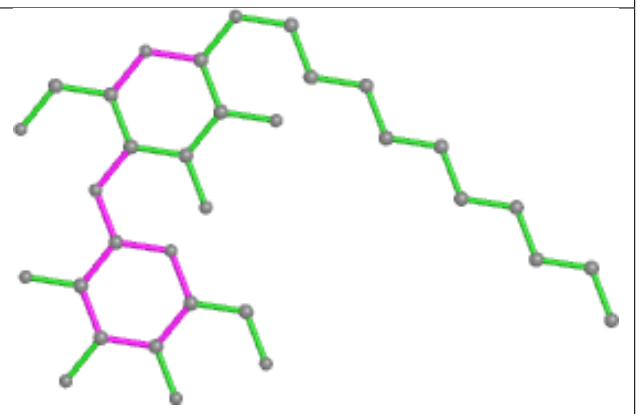


Rings

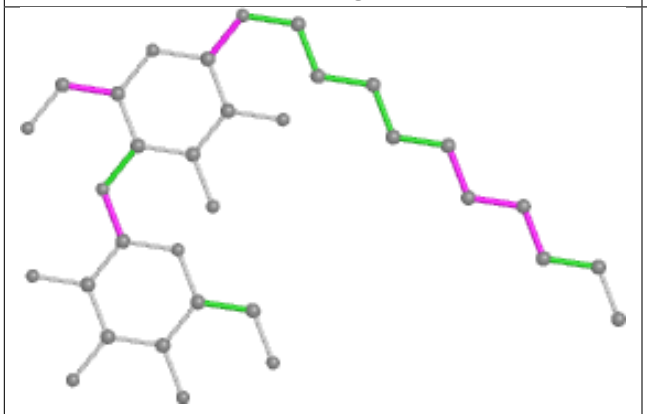
Ligand DMU G 104



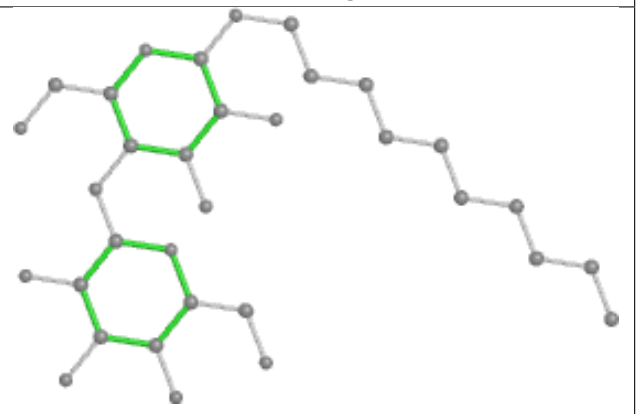
Bond lengths



Bond angles

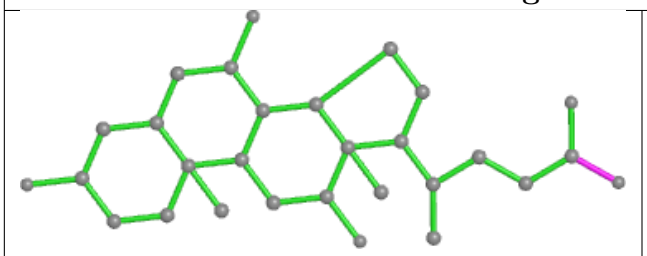


Torsions

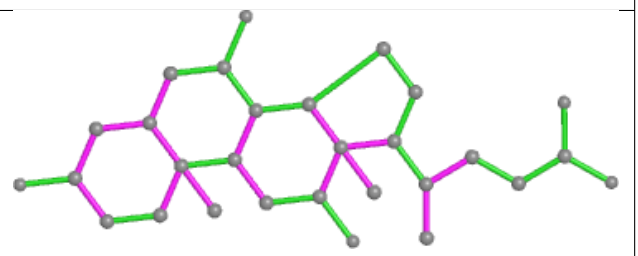


Rings

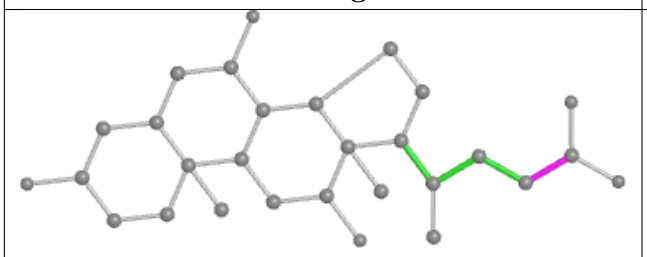
Ligand CHD T 101



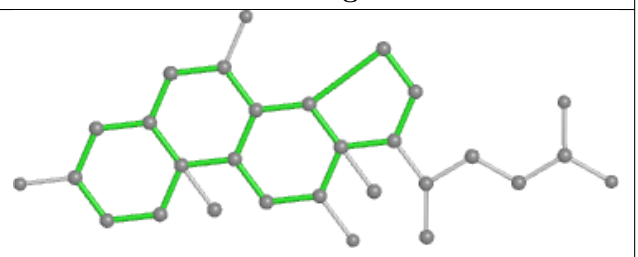
Bond lengths



Bond angles

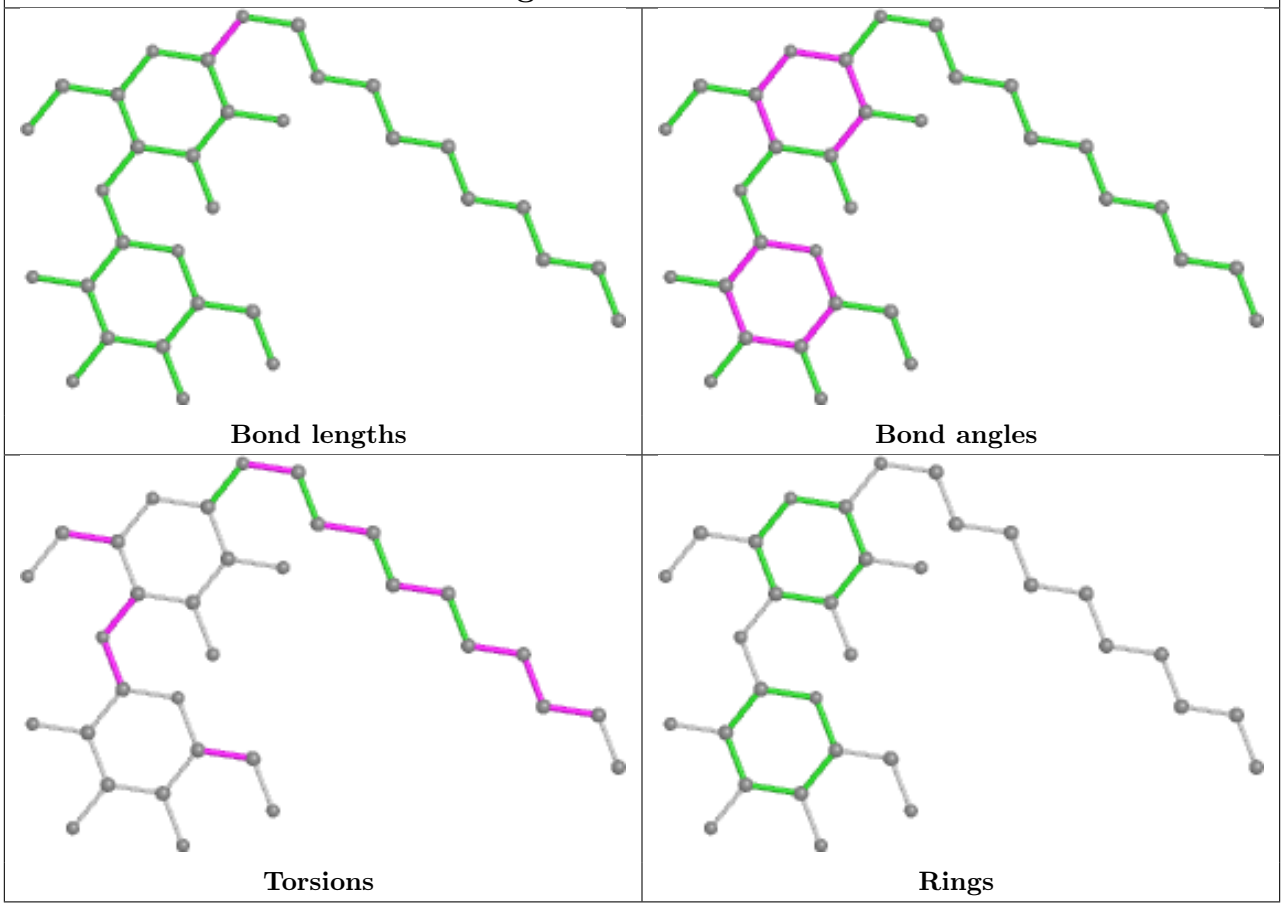


Torsions

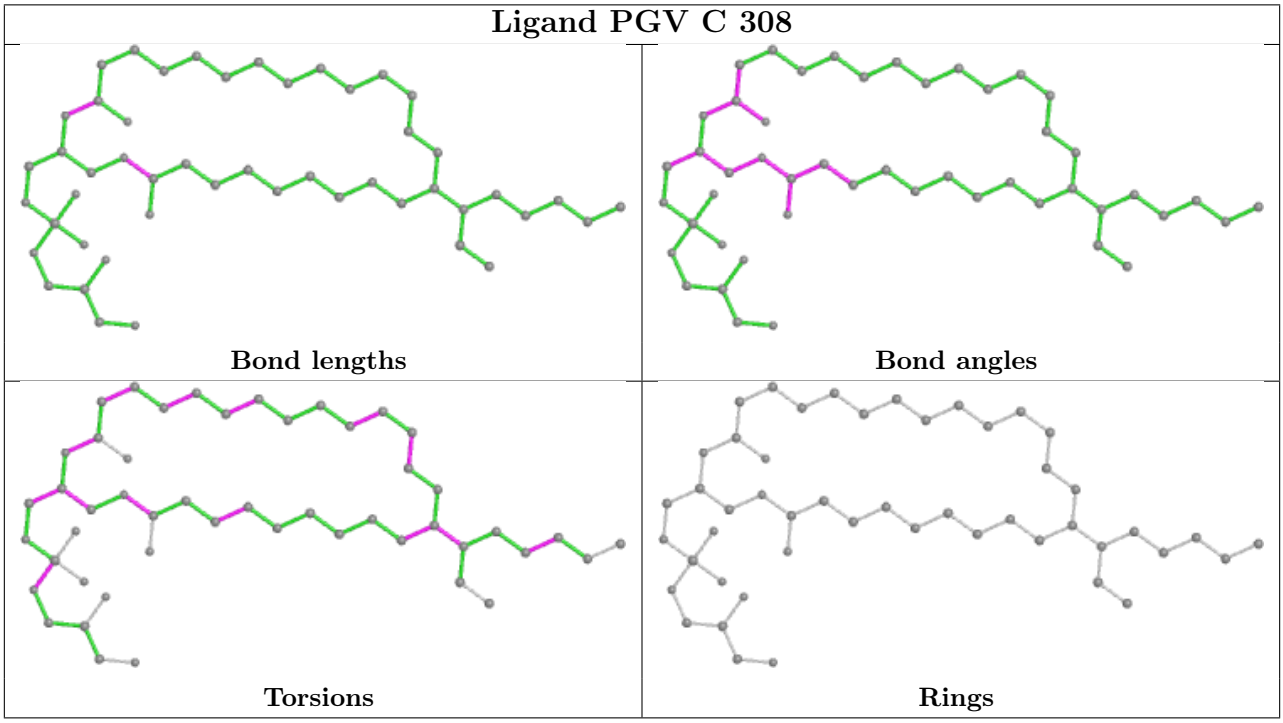


Rings

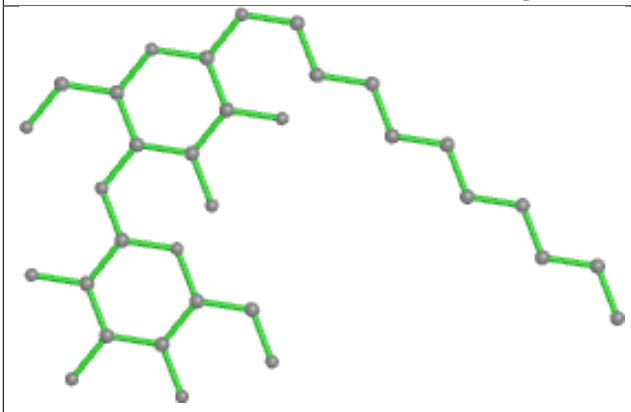
Ligand DMU K 102



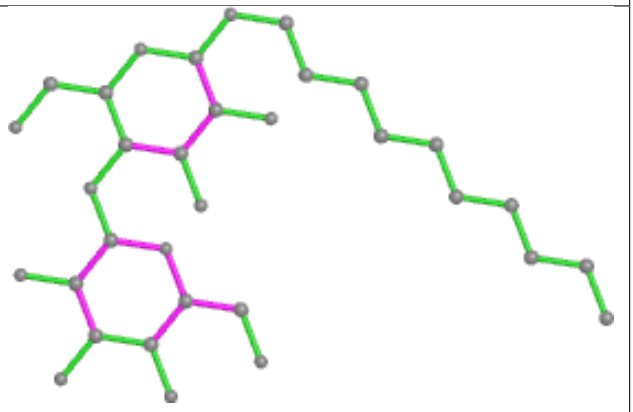
Ligand PGV C 308



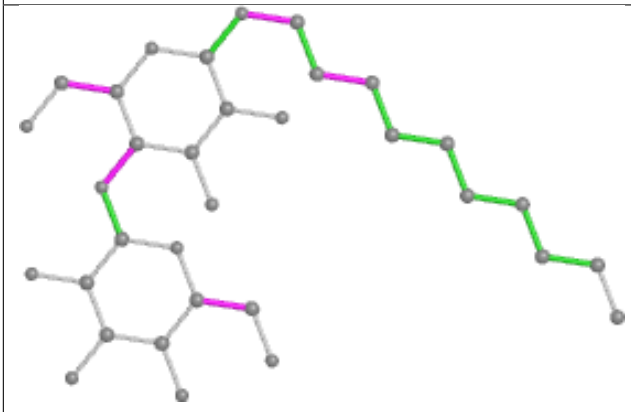
Ligand DMU T 103



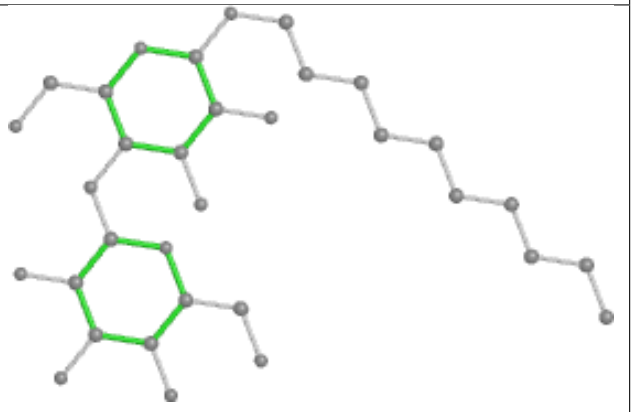
Bond lengths



Bond angles

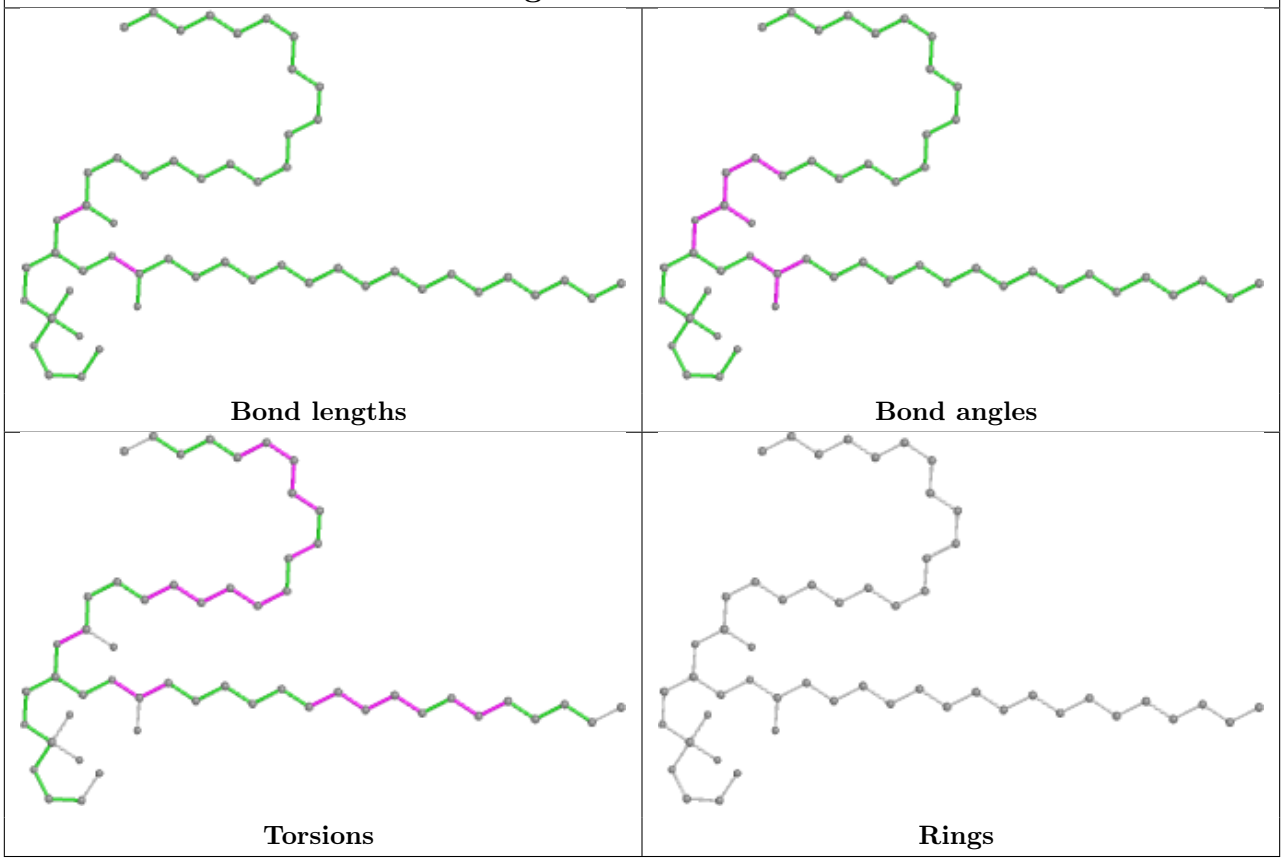


Torsions

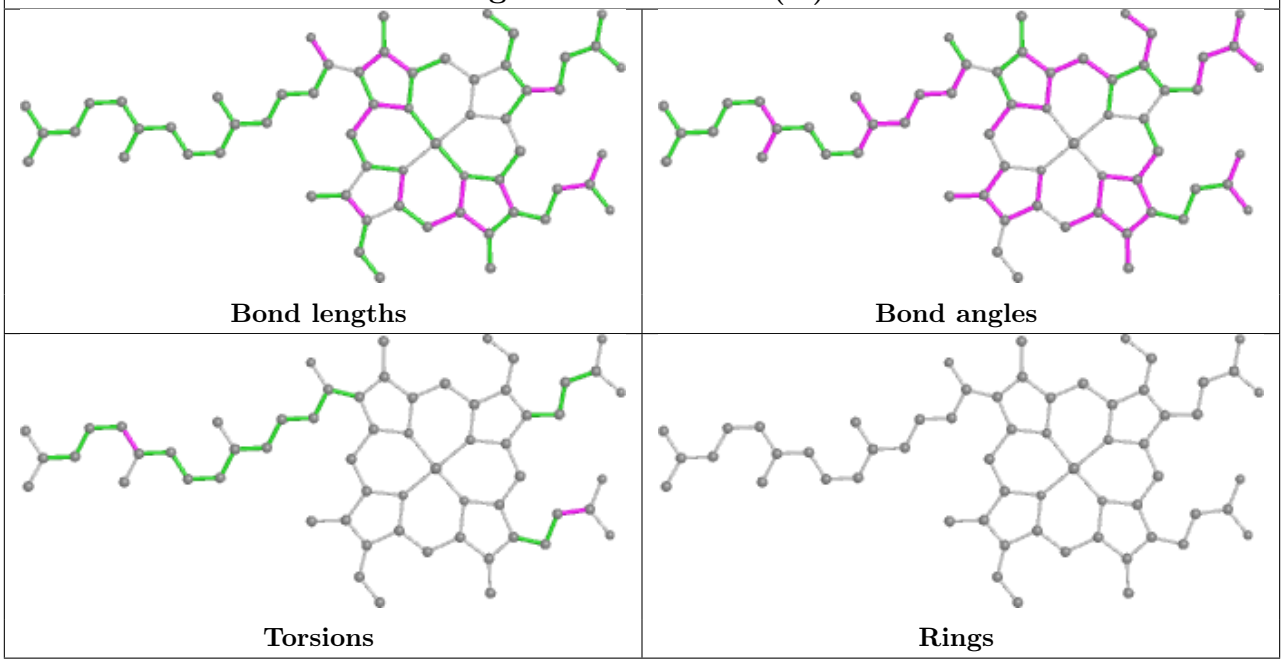


Rings

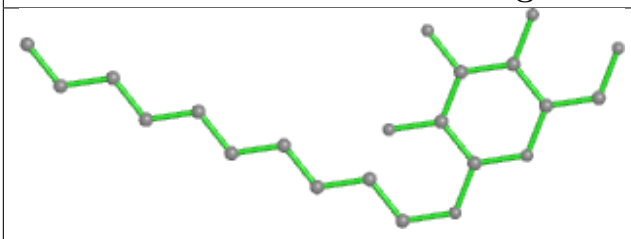
Ligand PEK C 309



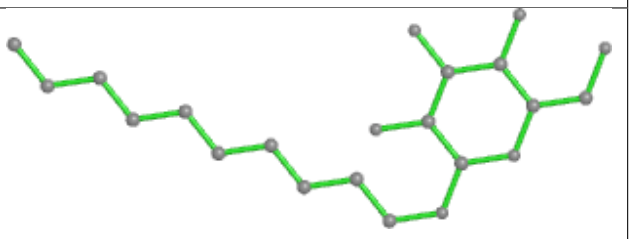
Ligand HEA A 601 (A)



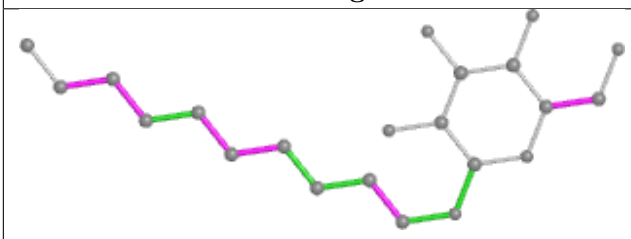
Ligand DMU X 104



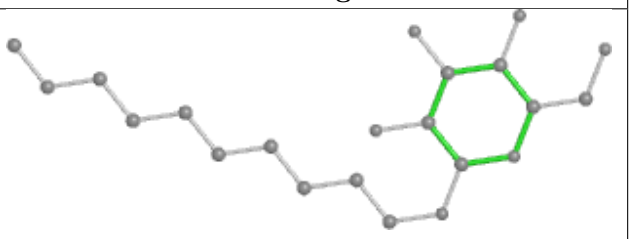
Bond lengths



Bond angles

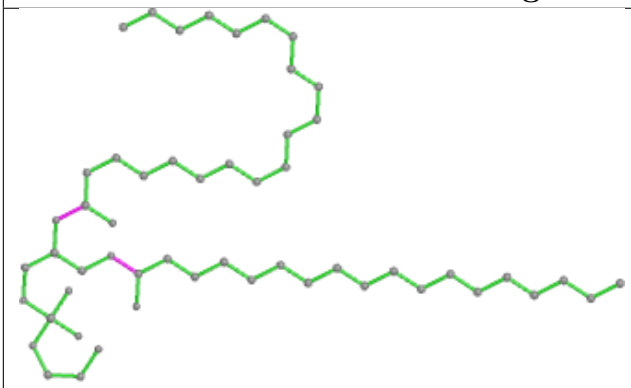


Torsions

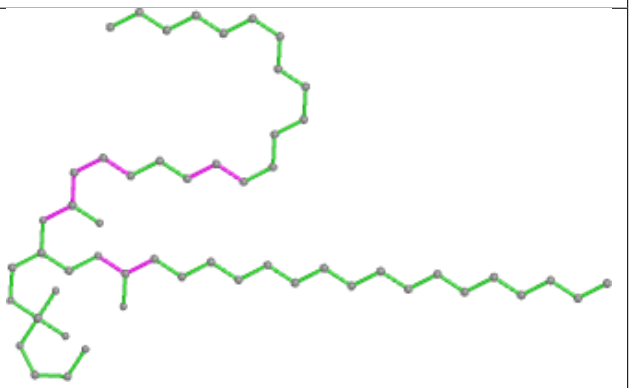


Rings

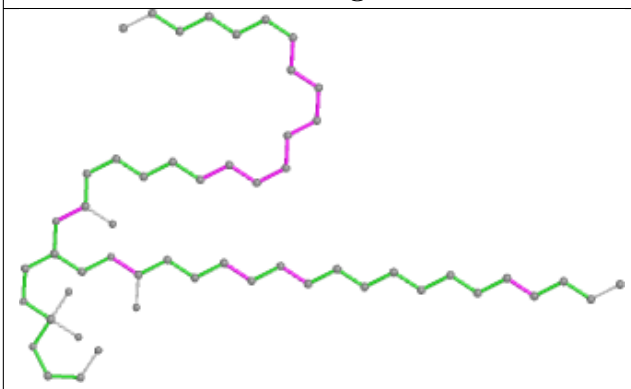
Ligand PEK G 102



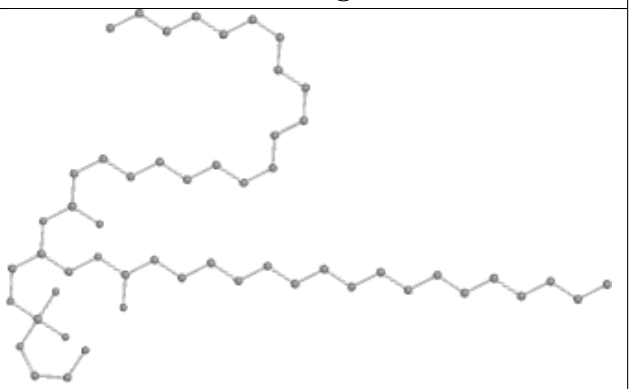
Bond lengths



Bond angles

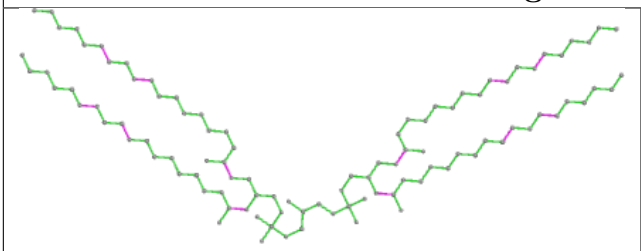


Torsions

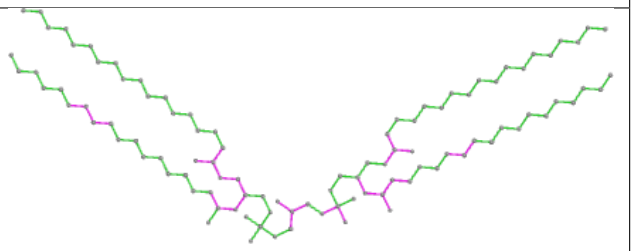


Rings

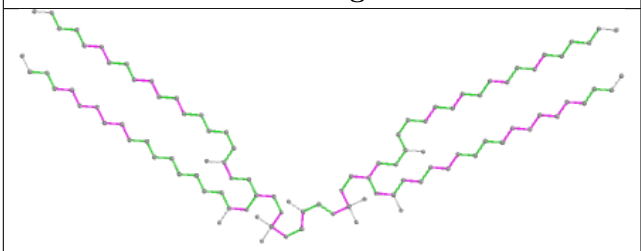
Ligand CDL P 306



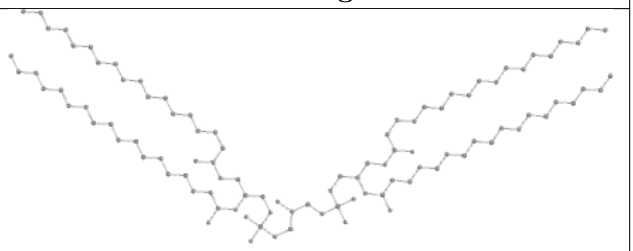
Bond lengths



Bond angles

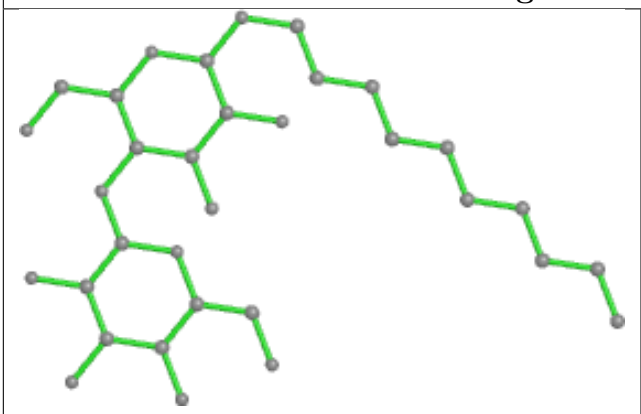


Torsions

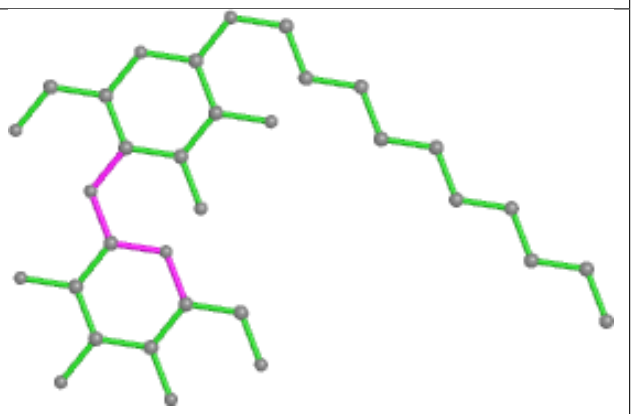


Rings

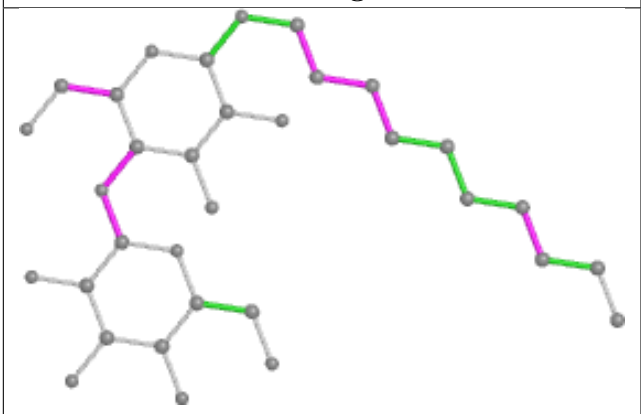
Ligand DMU A 616



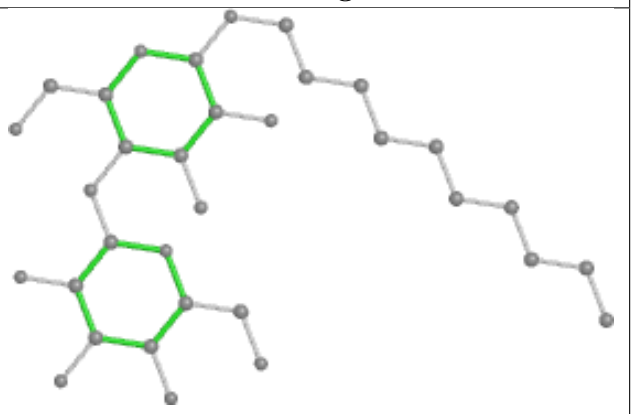
Bond lengths



Bond angles

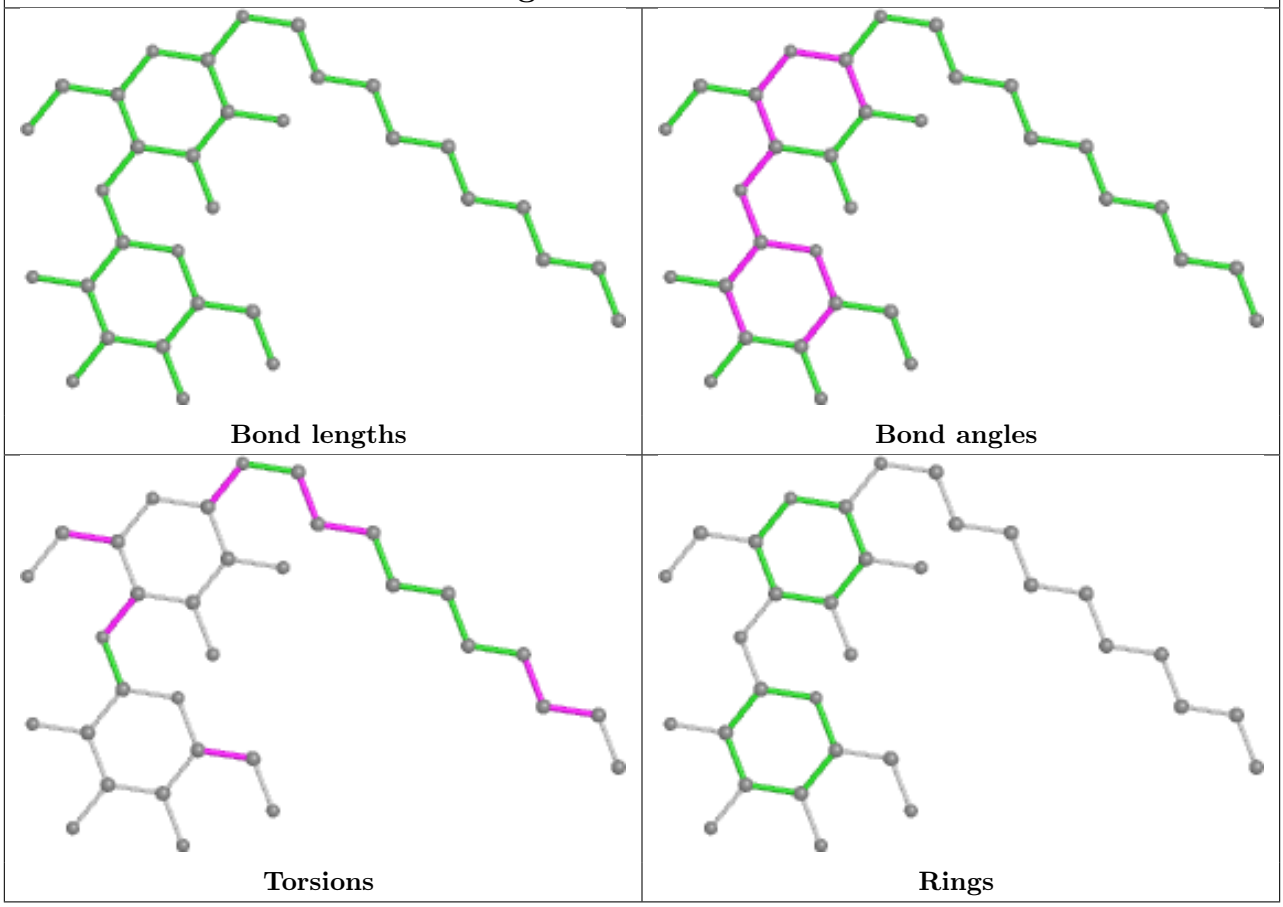


Torsions



Rings

Ligand DMU C 312



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	A	513/514 (99%)	-0.12	4 (0%) 86 87	13, 19, 29, 75	0
1	N	513/514 (99%)	-0.07	8 (1%) 72 74	15, 22, 33, 67	0
2	B	226/227 (99%)	0.22	12 (5%) 26 29	17, 26, 52, 93	0
2	O	226/227 (99%)	0.41	20 (8%) 10 11	22, 32, 68, 124	0
3	C	259/261 (99%)	0.01	5 (1%) 66 69	17, 23, 37, 79	0
3	P	259/261 (99%)	-0.04	1 (0%) 92 93	17, 24, 41, 80	0
4	D	144/147 (97%)	0.19	6 (4%) 36 39	19, 28, 50, 95	0
4	Q	144/147 (97%)	1.27	30 (20%) 1 1	26, 42, 87, 227	0
5	E	105/109 (96%)	0.49	13 (12%) 4 4	19, 28, 57, 141	0
5	R	105/109 (96%)	0.99	21 (20%) 1 1	24, 36, 61, 137	0
6	F	98/98 (100%)	0.62	10 (10%) 6 8	18, 29, 105, 151	0
6	S	98/98 (100%)	0.60	12 (12%) 4 4	19, 28, 94, 185	0
7	G	83/85 (97%)	1.03	19 (22%) 0 0	20, 32, 124, 163	0
7	T	83/85 (97%)	1.30	20 (24%) 0 0	20, 34, 114, 165	0
8	H	79/85 (92%)	0.85	12 (15%) 2 2	23, 35, 106, 153	0
8	U	79/85 (92%)	1.05	19 (24%) 0 0	27, 38, 131, 184	0
9	I	72/73 (98%)	0.99	13 (18%) 1 1	26, 39, 70, 87	0
9	V	72/73 (98%)	1.50	18 (25%) 0 0	25, 50, 75, 134	0
10	J	58/59 (98%)	0.64	7 (12%) 4 4	23, 34, 69, 106	0
10	W	58/59 (98%)	0.76	7 (12%) 4 4	24, 37, 78, 157	0
11	K	49/56 (87%)	0.42	3 (6%) 21 24	24, 35, 58, 62	0
11	X	49/56 (87%)	1.07	9 (18%) 1 1	36, 44, 65, 82	0
12	L	46/47 (97%)	0.08	2 (4%) 35 38	20, 26, 47, 94	0
12	Y	46/47 (97%)	0.40	4 (8%) 10 11	23, 32, 69, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.57	7 (16%)	1 1	20, 26, 68, 101	0
13	Z	43/46 (93%)	1.17	9 (20%)	1 1	29, 36, 86, 126	0
All	All	3550/3614 (98%)	0.36	291 (8%)	11 13	13, 27, 67, 227	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.1
8	H	8	ILE	12.9
6	F	96	LEU	12.3
4	Q	4	SER	11.6
4	Q	5	VAL	11.0
8	U	8	ILE	10.7
6	S	98	HIS	10.6
7	G	10	GLY	10.4
7	T	39	SER	10.0
4	Q	8	SER	9.9
7	T	8	HIS	9.9
7	T	1	ALA	9.9
7	T	40	GLY	9.1
5	R	5	HIS	9.0
9	V	37	PHE	8.5
2	O	90	ILE	8.4
9	I	37	PHE	8.4
8	H	44	THR	8.3
2	B	90	ILE	7.9
8	H	45	ALA	7.8
8	U	10	ASN	7.6
9	V	2	THR	7.6
8	U	44	THR	7.5
7	T	9	GLY	7.4
7	G	40	GLY	7.4
8	H	10	ASN	7.2
13	M	42	LYS	7.0
11	X	6	ALA	6.9
4	Q	35	ALA	6.9
10	J	58	LYS	6.9
10	W	57	HIS	6.8
4	D	4	SER	6.8
7	T	36	TRP	6.5
12	Y	47	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
13	Z	39	ASN	6.2
6	F	95	GLN	6.2
6	S	95	GLN	6.1
6	F	1	ALA	6.1
9	I	33	THR	5.9
5	E	5	HIS	5.9
11	K	6	ALA	5.8
7	G	2	SER	5.7
13	Z	42	LYS	5.7
5	R	7	THR	5.5
6	S	94	HIS	5.5
10	W	1	PHE	5.4
6	S	2	SER	5.4
4	D	5	VAL	5.4
13	M	43	SER	5.2
6	S	1	ALA	5.2
9	V	30	GLY	5.2
9	V	33	THR	5.1
7	T	10	GLY	5.1
2	B	60	GLU	5.1
11	K	7	PRO	5.0
4	Q	7	LYS	4.9
7	T	42	ARG	4.9
2	O	224	ALA	4.9
7	G	84	LYS	4.9
10	W	58	LYS	4.9
6	F	97	ALA	4.9
7	T	41	HIS	4.9
9	V	25	PHE	4.8
9	V	34	PHE	4.8
9	I	25	PHE	4.8
2	O	227	LEU	4.8
8	U	46	LYS	4.7
6	S	96	LEU	4.7
4	Q	53	ILE	4.7
7	G	38	HIS	4.6
5	R	109	VAL	4.6
8	U	7	LYS	4.6
5	E	7	THR	4.5
7	G	37	LEU	4.5
9	V	29	LEU	4.5
5	E	109	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
6	F	98	HIS	4.4
4	Q	147	LYS	4.4
7	T	38	HIS	4.3
5	R	6	GLU	4.3
9	V	26	MET	4.3
9	V	3	ALA	4.3
7	G	8	HIS	4.3
12	L	2	HIS	4.3
7	G	9	GLY	4.3
6	F	2	SER	4.3
10	W	56	PRO	4.3
6	F	94	HIS	4.2
12	L	47	LYS	4.2
4	Q	39	ALA	4.0
13	Z	43	SER	4.0
8	U	18	SER	4.0
7	G	42	ARG	4.0
6	F	3	GLY	4.0
5	R	10	GLU	4.0
7	G	39	SER	4.0
7	G	41	HIS	4.0
6	S	97	ALA	4.0
7	T	46	ALA	3.9
1	N	36	LEU	3.9
9	I	30	GLY	3.9
2	O	60	GLU	3.8
4	Q	33	LEU	3.8
8	H	7	LYS	3.8
7	G	3	ALA	3.8
6	S	3	GLY	3.7
8	H	9	LYS	3.7
10	J	52	TRP	3.7
9	I	26	MET	3.7
7	T	3	ALA	3.7
2	B	59	GLN	3.7
4	Q	36	SER	3.7
4	Q	50	SER	3.7
4	Q	32	ASN	3.7
8	H	47	GLY	3.7
10	W	2	GLU	3.6
10	J	57	HIS	3.6
8	U	9	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
7	G	43	GLU	3.6
5	R	13	ALA	3.6
2	O	59	GLN	3.6
8	U	11	TYR	3.5
11	X	7	PRO	3.5
9	I	29	LEU	3.5
5	E	10	GLU	3.5
9	I	22	VAL	3.5
7	T	43	GLU	3.4
4	Q	34	SER	3.4
13	Z	38	ASP	3.4
9	I	32	ALA	3.4
4	Q	31	LYS	3.4
2	O	113	TYR	3.4
4	Q	58	GLU	3.4
2	O	221	LYS	3.4
8	U	49	ASP	3.4
13	M	39	ASN	3.3
3	P	235	PHE	3.3
7	G	7	ASP	3.3
13	Z	37	LEU	3.3
8	U	51	SER	3.3
7	G	6	GLY	3.3
4	D	147	LYS	3.3
9	I	18	ARG	3.3
2	B	67	ILE	3.2
4	Q	52	SER	3.2
2	O	91	ASN	3.2
5	R	67	ILE	3.2
11	K	8	ASP	3.2
13	Z	40	TYR	3.2
2	O	89	GLU	3.2
4	Q	46	ALA	3.2
12	Y	27	LEU	3.2
6	S	93	PRO	3.2
2	O	217	LYS	3.2
5	R	70	VAL	3.2
7	G	36	TRP	3.1
13	M	38	ASP	3.1
5	R	9	GLU	3.1
9	I	19	PHE	3.1
5	R	23	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
13	Z	32	TRP	3.1
10	W	25	GLY	3.1
5	R	17	THR	3.0
5	E	6	GLU	3.0
11	X	13	TYR	3.0
13	M	37	LEU	3.0
9	I	23	GLY	3.0
4	Q	51	LEU	3.0
3	C	188	ILE	3.0
7	T	12	GLY	3.0
7	T	35	SER	3.0
9	V	19	PHE	3.0
8	U	48	GLY	3.0
1	N	472	ILE	2.9
4	Q	38	LYS	2.9
8	H	11	TYR	2.9
10	J	14	GLU	2.9
5	E	11	PHE	2.9
5	E	68	LEU	2.9
5	R	68	LEU	2.9
5	R	108	LYS	2.9
7	T	2	SER	2.9
13	Z	41	LYS	2.9
9	V	57	MET	2.9
10	W	52	TRP	2.8
2	O	86	MET	2.8
8	H	43	MET	2.8
4	Q	54	ASP	2.8
5	E	67	ILE	2.8
4	Q	73	ARG	2.8
5	R	14[A]	ARG	2.8
9	V	52	ARG	2.8
3	C	235	PHE	2.8
4	Q	42	GLU	2.8
9	V	53	ASN	2.7
2	O	32[A]	PHE	2.7
8	U	63	LEU	2.7
5	R	98	ILE	2.7
3	C	186	PHE	2.7
10	J	1	PHE	2.7
7	T	45	PRO	2.7
2	B	91	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
5	R	52	LEU	2.7
8	H	48	GLY	2.7
6	F	26	LYS	2.7
2	O	88	ASP	2.7
10	J	56	PRO	2.7
4	Q	10	ASP	2.6
8	U	52	VAL	2.6
1	A	113[A]	LEU	2.6
2	O	153	LEU	2.6
4	Q	9	GLU	2.6
5	E	9	GLU	2.6
8	U	45	ALA	2.6
6	S	27	GLY	2.6
6	F	44	GLU	2.6
2	O	68	LEU	2.5
7	T	37	LEU	2.5
5	R	89	LEU	2.5
8	U	77	ALA	2.5
12	Y	45	LEU	2.5
2	B	89	GLU	2.5
2	B	191	LEU	2.5
5	R	93	LEU	2.5
7	G	46	ALA	2.5
1	N	405	LEU	2.5
1	N	476	PHE	2.5
7	G	35	SER	2.4
4	D	143	ASN	2.4
1	N	37	ILE	2.4
9	I	52	ARG	2.4
9	V	28	SER	2.4
1	N	48	LEU	2.4
5	R	96	LEU	2.4
2	O	76	ILE	2.4
5	R	65	VAL	2.4
11	X	11	ASP	2.4
8	H	77	ALA	2.3
4	Q	75	THR	2.3
4	D	112	GLU	2.3
1	A	476	PHE	2.3
9	V	23	GLY	2.3
9	V	18	ARG	2.3
4	Q	30	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
8	U	42	ALA	2.2
9	I	2	THR	2.2
1	A	471	ILE	2.2
11	X	27	ALA	2.2
1	N	471	ILE	2.2
7	T	84	LYS	2.2
5	E	23	ASP	2.2
8	U	50	VAL	2.2
5	E	52	LEU	2.2
8	H	49	ASP	2.2
2	B	63	THR	2.2
7	G	5	LYS	2.2
13	Z	36	HIS	2.2
9	V	24	ALA	2.2
2	O	116	LEU	2.2
4	Q	140	TYR	2.2
13	M	40	TYR	2.2
2	B	153	LEU	2.1
11	X	12	LYS	2.1
2	B	92	ASN	2.1
2	O	57	ASP	2.1
4	D	87[A]	PHE	2.1
8	U	74	ASP	2.1
8	U	47	GLY	2.1
2	B	152[A]	MET	2.1
2	O	87[A]	MET	2.1
11	X	34	THR	2.1
5	E	108	LYS	2.1
3	C	39	SER	2.1
5	R	64	ALA	2.1
7	T	7	ASP	2.1
9	V	49	ASP	2.1
13	M	36	HIS	2.1
10	J	2	GLU	2.1
6	S	26	LYS	2.1
3	C	38	ASN	2.1
4	Q	144	GLU	2.1
2	O	184	LEU	2.1
11	X	14	GLY	2.1
12	Y	46	LYS	2.1
1	N	459	PHE	2.0
5	E	13	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
6	S	45	ASP	2.0
2	B	38	VAL	2.0
4	Q	139	ASP	2.0
1	A	472	ILE	2.0
11	X	38	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
9	SAC	V	1	9/10	0.40	0.81	168,196,204,213	0
7	TPO	G	11	11/12	0.62	0.47	102,138,168,184	0
7	TPO	T	11	11/12	0.82	0.31	37,90,131,149	0
9	SAC	I	1	9/10	0.84	0.40	64,103,134,151	0
1	FME	N	1	10/11	0.94	0.19	30,45,72,79	0
1	FME	A	1	10/11	0.96	0.20	30,35,87,99	0
2	FME	B	1	10/11	0.97	0.14	15,24,35,116	0
2	FME	O	1	10/11	0.98	0.19	25,35,45,96	0

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
21	DMU	B	306	33/33	-0.00	0.49	46,75,90,95	0
21	DMU	X	101	33/33	0.05	0.55	45,136,220,232	0
21	DMU	P	316	33/33	0.23	0.39	45,72,87,88	0
21	DMU	A	616	33/33	0.28	0.48	56,130,180,189	0
21	DMU	K	102	33/33	0.32	0.45	40,137,212,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	DMU	D	202	33/33	0.42	0.45	45,120,185,206	0
21	DMU	T	103	33/33	0.45	0.38	43,92,177,189	0
27	CHD	X	105	29/29	0.45	0.55	91,122,143,147	0
21	DMU	G	104	33/33	0.46	0.34	44,93,162,176	0
21	DMU	K	105	33/33	0.50	0.43	45,140,194,202	0
21	DMU	K	104	33/33	0.50	0.38	55,109,174,183	0
21	DMU	Q	203	33/33	0.50	0.37	50,70,87,89	0
21	DMU	K	103	33/33	0.53	0.43	46,125,193,196	0
24	PSC	B	303	52/52	0.54	0.37	29,85,150,174	0
21	DMU	C	312	33/33	0.54	0.26	40,102,147,166	0
27	CHD	J	101	29/29	0.55	0.36	36,97,125,132	0
21	DMU	K	106	33/33	0.56	0.34	37,128,202,207	0
21	DMU	X	103	22/33	0.57	0.24	44,114,175,179	0
27	CHD	W	101	29/29	0.58	0.42	48,87,120,129	0
25	PEK	P	309	53/53	0.59	0.30	31,69,134,199	0
21	DMU	K	101	33/33	0.60	0.28	41,96,158,172	0
25	PEK	G	102	53/53	0.60	0.32	35,84,135,144	0
22	TGL	Y	101	63/63	0.60	0.29	29,62,103,122	0
21	DMU	X	104	22/33	0.61	0.30	50,86,128,134	0
21	DMU	L	102	33/33	0.61	0.31	45,90,142,145	0
26	CDL	T	102	100/100	0.62	0.28	36,85,128,174	0
21	DMU	X	102	22/33	0.62	0.27	51,87,176,183	0
21	DMU	O	305	33/33	0.63	0.35	39,118,177,200	0
27	CHD	L	103	29/29	0.65	0.36	43,92,143,156	0
25	PEK	C	307	53/53	0.65	0.24	30,67,125,163	0
25	PEK	C	309	53/53	0.65	0.34	38,89,140,147	0
21	DMU	P	314	33/33	0.66	0.30	44,95,145,181	0
19	PGV	N	607	51/51	0.67	0.30	29,74,124,175	0
26	CDL	G	101	100/100	0.68	0.24	37,78,128,171	0
21	DMU	M	101	33/33	0.68	0.23	27,38,63,68	0
22	TGL	L	101	63/63	0.69	0.28	23,52,106,155	0
22	TGL	Q	201	63/63	0.70	0.24	34,64,99,123	0
24	PSC	N	608	52/52	0.70	0.29	26,80,141,151	0
21	DMU	Z	101	33/33	0.70	0.27	25,52,70,76	0
27	CHD	Y	102	29/29	0.71	0.36	51,96,128,136	0
19	PGV	C	308	51/51	0.73	0.27	38,73,130,148	0
19	PGV	A	608	51/51	0.76	0.24	24,62,119,169	0
22	TGL	D	201	63/63	0.76	0.21	25,56,92,141	0
20	EDO	N	619	4/4	0.77	0.16	45,52,58,70	0
26	CDL	P	306	100/100	0.77	0.24	21,78,136,154	0
26	CDL	C	304	100/100	0.79	0.23	15,70,122,136	0
19	PGV	P	302	51/51	0.81	0.19	39,75,131,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	S	105	4/4	0.82	0.29	50,56,81,100	0
20	EDO	M	102	4/4	0.82	0.12	44,46,46,67	0
22	TGL	O	301	63/63	0.82	0.18	29,69,101,117	0
22	TGL	B	301	63/63	0.82	0.18	26,59,100,113	0
27	CHD	P	307	29/29	0.83	0.21	37,57,80,101	0
27	CHD	C	305	29/29	0.84	0.25	38,56,79,104	0
20	EDO	P	310	4/4	0.87	0.36	36,41,65,76	0
20	EDO	O	304	4/4	0.88	0.11	40,61,63,67	0
20	EDO	W	103	4/4	0.88	0.11	45,47,50,68	0
20	EDO	P	313	4/4	0.88	0.15	28,43,51,66	0
20	EDO	Y	103	4/4	0.89	0.42	53,59,59,70	0
17	NA	P	303	1/1	0.90	0.11	42,42,42,42	0
20	EDO	A	613	4/4	0.90	0.17	30,42,53,62	0
20	EDO	N	618	4/4	0.91	0.10	49,51,55,101	0
20	EDO	F	105	4/4	0.91	0.19	45,45,75,75	0
29	PO4	U	101	5/5	0.91	0.19	48,52,113,186	0
20	EDO	N	614	4/4	0.92	0.20	38,46,50,53	0
20	EDO	L	105	4/4	0.92	0.14	45,52,55,62	0
27	CHD	P	308	29/29	0.93	0.10	17,25,33,42	0
20	EDO	P	312	4/4	0.93	0.13	40,50,56,61	0
20	EDO	S	107	4/4	0.93	0.18	45,51,52,55	0
25	PEK	P	304	53/53	0.93	0.19	22,39,106,120	0
20	EDO	N	615	4/4	0.93	0.25	28,52,52,53	0
20	EDO	N	617	4/4	0.94	0.26	44,48,53,81	0
25	PEK	C	302	53/53	0.94	0.20	19,37,81,96	0
27	CHD	C	306	29/29	0.94	0.08	18,26,33,37	0
27	CHD	G	103	29/29	0.94	0.10	16,21,28,36	0
20	EDO	R	201	4/4	0.94	0.13	45,45,50,50	0
20	EDO	B	304	4/4	0.94	0.12	31,56,61,72	0
20	EDO	F	103	4/4	0.94	0.08	33,33,38,51	0
20	EDO	N	620	4/4	0.94	0.18	45,47,56,72	0
20	EDO	O	303	4/4	0.94	0.20	20,21,27,32	0
20	EDO	N	610	4/4	0.94	0.15	24,25,31,40	0
20	EDO	F	104	4/4	0.94	0.16	45,45,67,73	0
20	EDO	A	609	4/4	0.94	0.07	34,65,68,70	0
14	HEA	N	601[A]	60/60	0.95	0.15	12,20,30,35	9
20	EDO	P	315	4/4	0.95	0.16	45,45,45,48	0
14	HEA	N	601[B]	60/60	0.95	0.15	12,21,47,59	9
20	EDO	G	105	4/4	0.95	0.23	45,45,45,45	0
20	EDO	S	106	4/4	0.95	0.09	34,35,46,54	0
20	EDO	L	104	4/4	0.95	0.09	45,45,51,58	0
20	EDO	A	614	4/4	0.95	0.13	37,41,48,59	0

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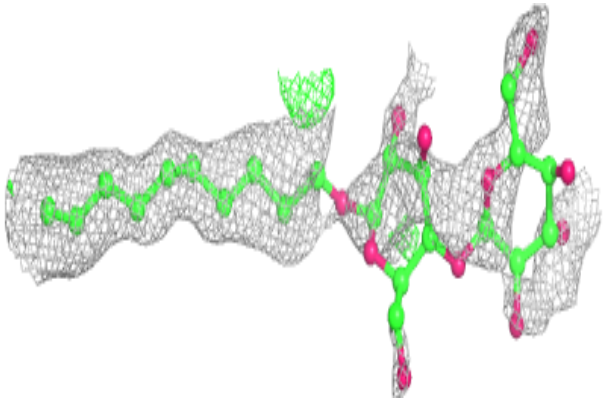
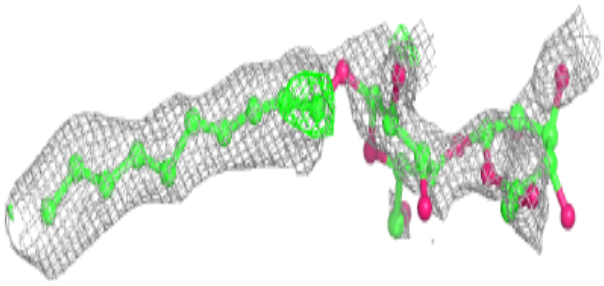
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	A	615	4/4	0.95	0.14	22,26,27,37	0
19	PGV	C	303	51/51	0.95	0.20	15,26,67,85	0
20	EDO	N	613	4/4	0.95	0.16	31,38,40,103	0
20	EDO	P	311	4/4	0.95	0.11	34,36,43,44	0
19	PGV	P	305	51/51	0.95	0.22	13,27,75,97	0
20	EDO	S	103	4/4	0.96	0.10	27,31,36,39	0
20	EDO	S	104	4/4	0.96	0.13	28,37,45,46	0
14	HEA	A	602	60/60	0.96	0.13	11,17,23,27	0
19	PGV	P	301	51/51	0.96	0.22	17,32,72,81	0
20	EDO	N	609	4/4	0.96	0.15	19,25,27,28	0
20	EDO	W	102	4/4	0.96	0.11	52,52,66,80	0
27	CHD	T	101	29/29	0.96	0.08	16,22,26,39	0
20	EDO	A	611	4/4	0.96	0.12	25,31,56,74	0
20	EDO	N	611	4/4	0.96	0.10	31,32,38,47	0
20	EDO	N	612	4/4	0.96	0.17	27,34,37,65	0
29	PO4	H	101	5/5	0.96	0.18	58,61,79,149	0
14	HEA	N	602	60/60	0.96	0.13	13,18,27,30	0
20	EDO	N	616	4/4	0.97	0.09	32,38,39,48	0
14	HEA	A	601[A]	60/60	0.97	0.12	10,16,32,46	9
20	EDO	B	305	4/4	0.97	0.16	17,19,25,30	0
20	EDO	S	102	4/4	0.97	0.11	19,19,19,20	0
20	EDO	C	310	4/4	0.97	0.11	26,31,32,34	0
20	EDO	C	311	4/4	0.97	0.11	23,27,47,49	0
18	PER	N	606	2/2	0.97	0.07	17,17,17,18	0
20	EDO	A	612	4/4	0.97	0.20	24,26,62,82	0
19	PGV	A	607	51/51	0.97	0.20	17,30,63,68	0
14	HEA	A	601[B]	60/60	0.97	0.12	10,16,35,64	9
17	NA	C	301	1/1	0.97	0.13	58,58,58,58	0
16	MG	N	604	1/1	0.98	0.03	16,16,16,16	0
17	NA	N	605	1/1	0.98	0.06	25,25,25,25	0
18	PER	A	606	2/2	0.99	0.06	12,12,12,15	0
20	EDO	Q	202	4/4	0.99	0.09	25,35,53,70	0
17	NA	A	605	1/1	0.99	0.06	20,20,20,20	0
20	EDO	A	610	4/4	0.99	0.12	19,22,22,23	0
16	MG	A	604	1/1	0.99	0.03	13,13,13,13	0
20	EDO	F	102	4/4	0.99	0.11	16,18,21,21	0
15	CU	N	603	1/1	1.00	0.04	18,18,18,18	0
23	CUA	B	302	2/2	1.00	0.03	18,18,18,19	0
28	ZN	F	101	1/1	1.00	0.04	22,22,22,22	0
28	ZN	S	101	1/1	1.00	0.05	22,22,22,22	0
23	CUA	O	302	2/2	1.00	0.04	22,22,22,22	0
15	CU	A	603	1/1	1.00	0.04	17,17,17,17	0

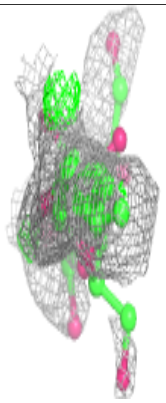
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU B 306:

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

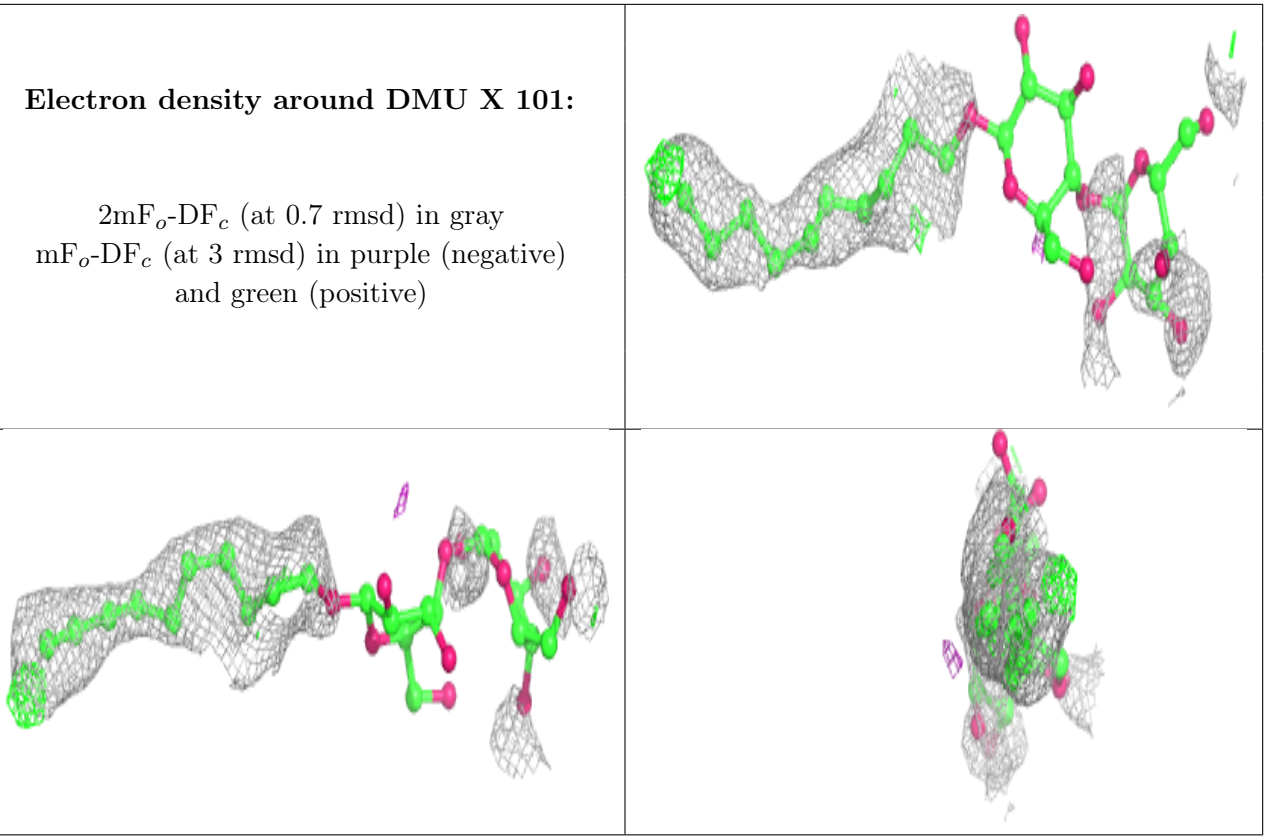






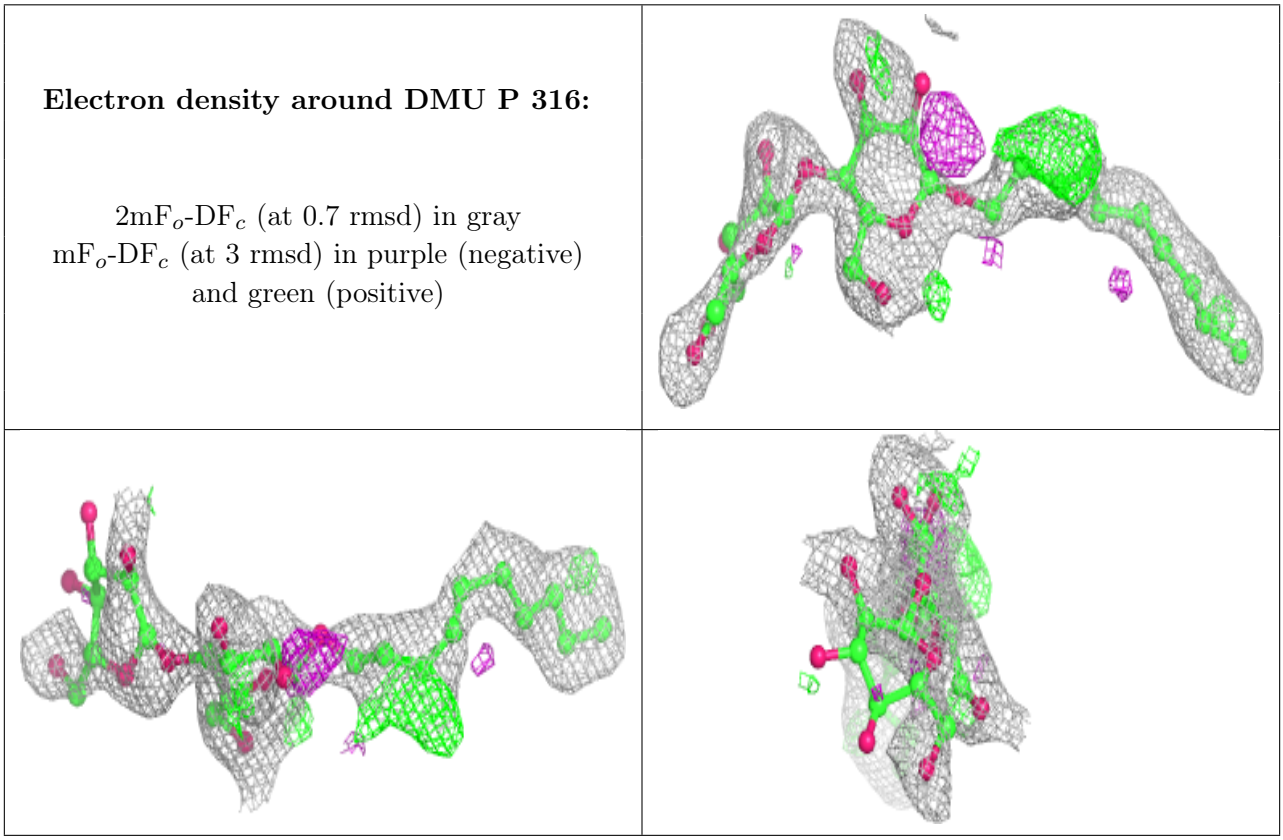
Electron density around DMU X 101:

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



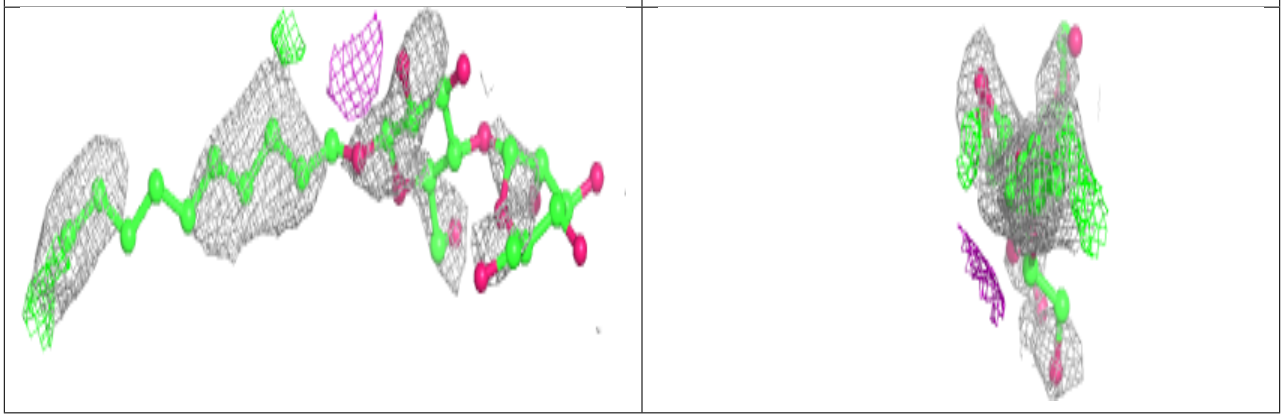
Electron density around DMU P 316:

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



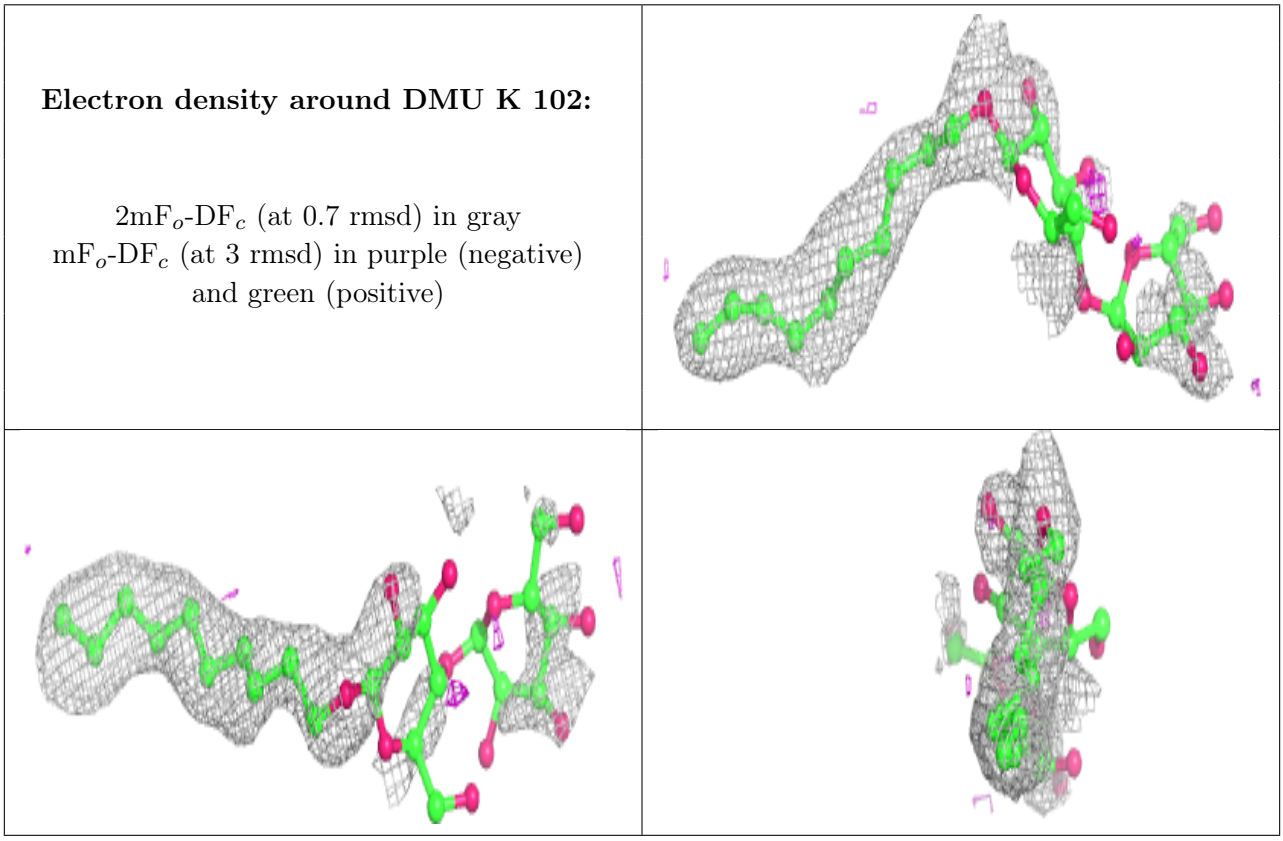
Electron density around DMU A 616:

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



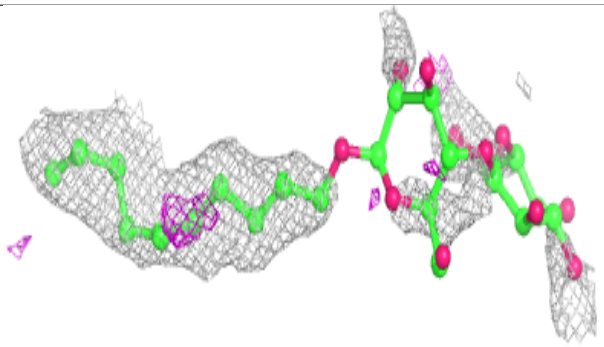
Electron density around DMU K 102:

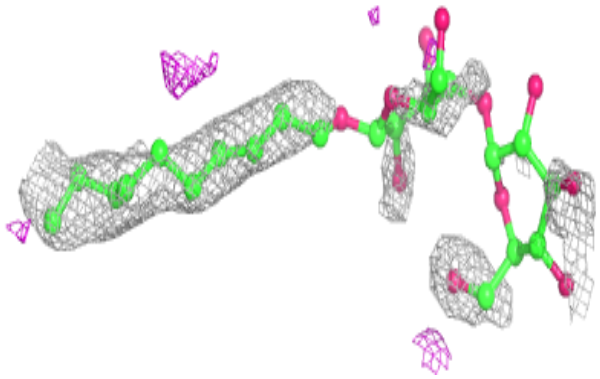
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

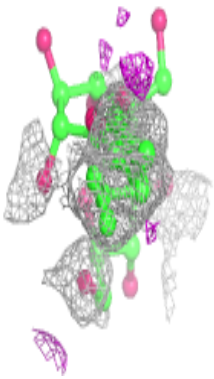


Electron density around DMU D 202:

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

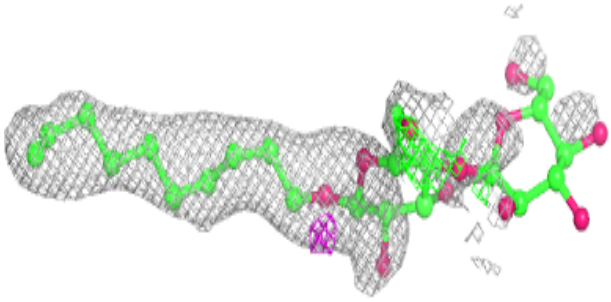


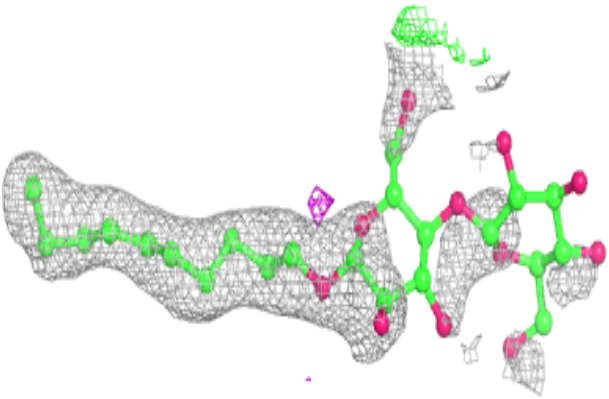


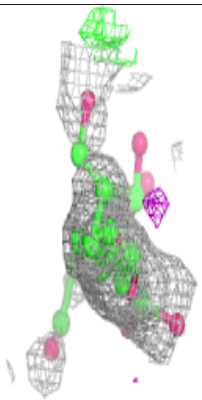


Electron density around DMU T 103:

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

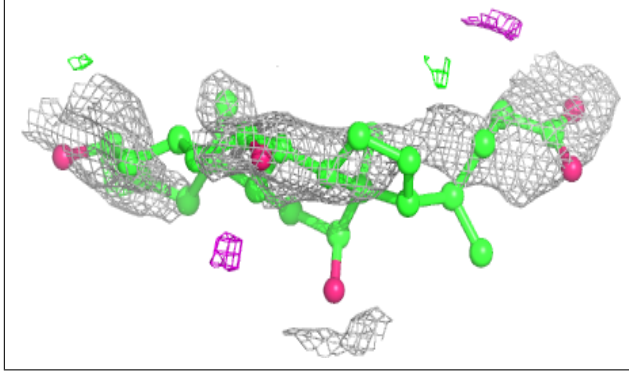


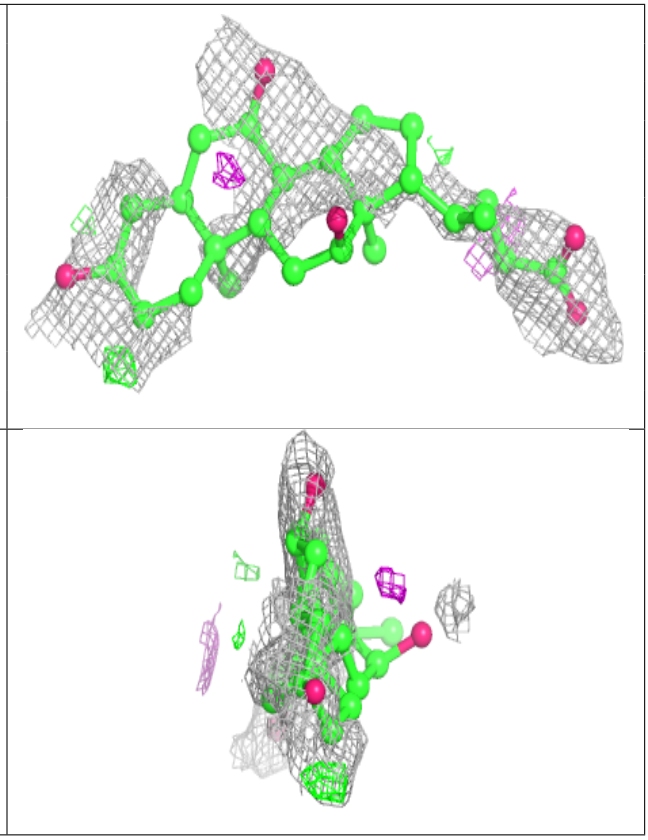




Electron density around CHD X 105:

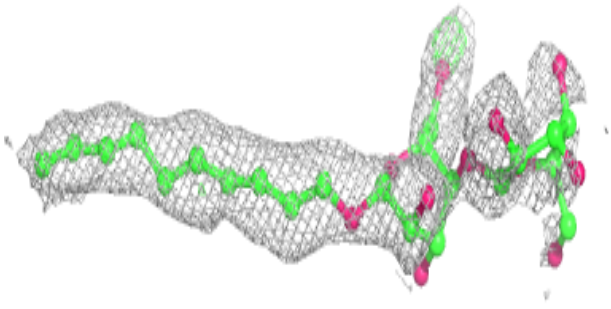
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

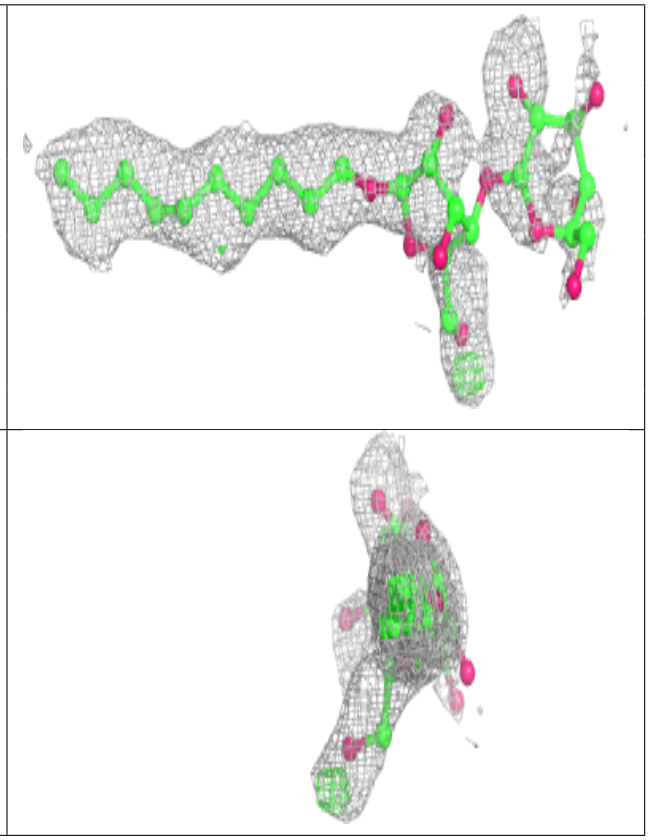




Electron density around DMU G 104:

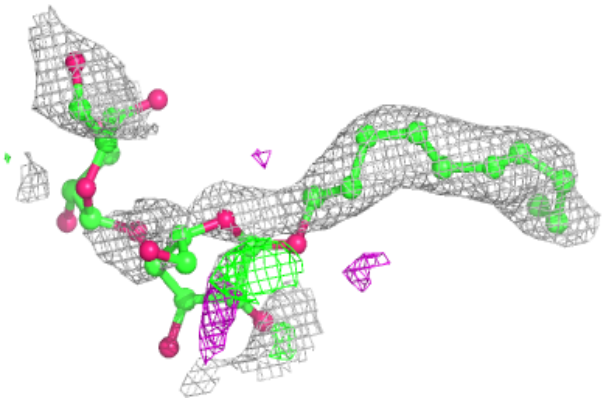
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

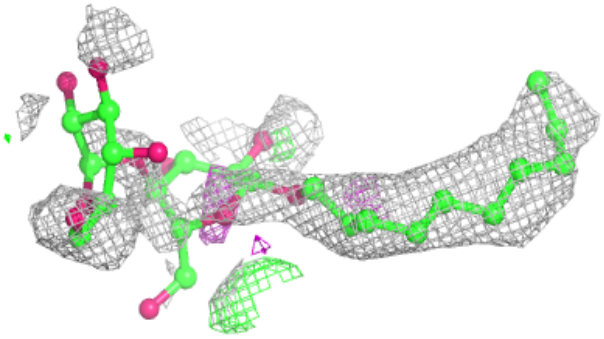


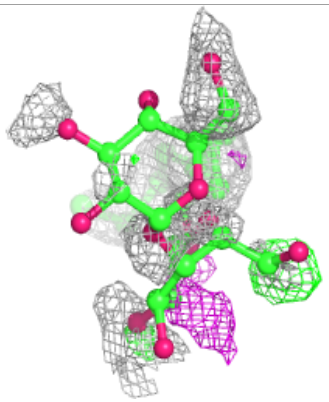


Electron density around DMU K 105:

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

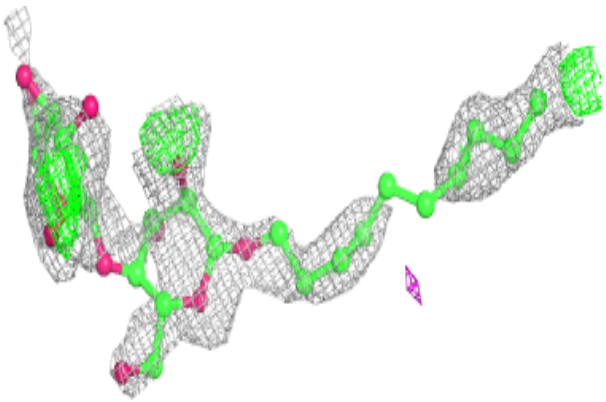


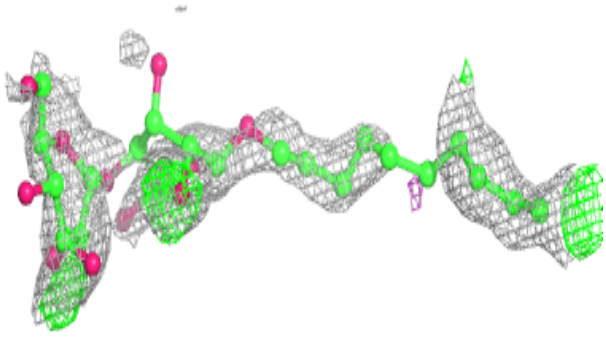


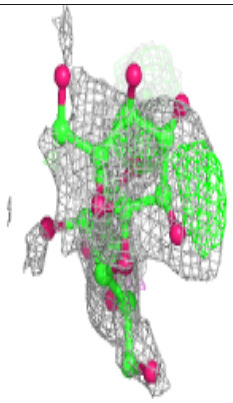


Electron density around DMU K 104:

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

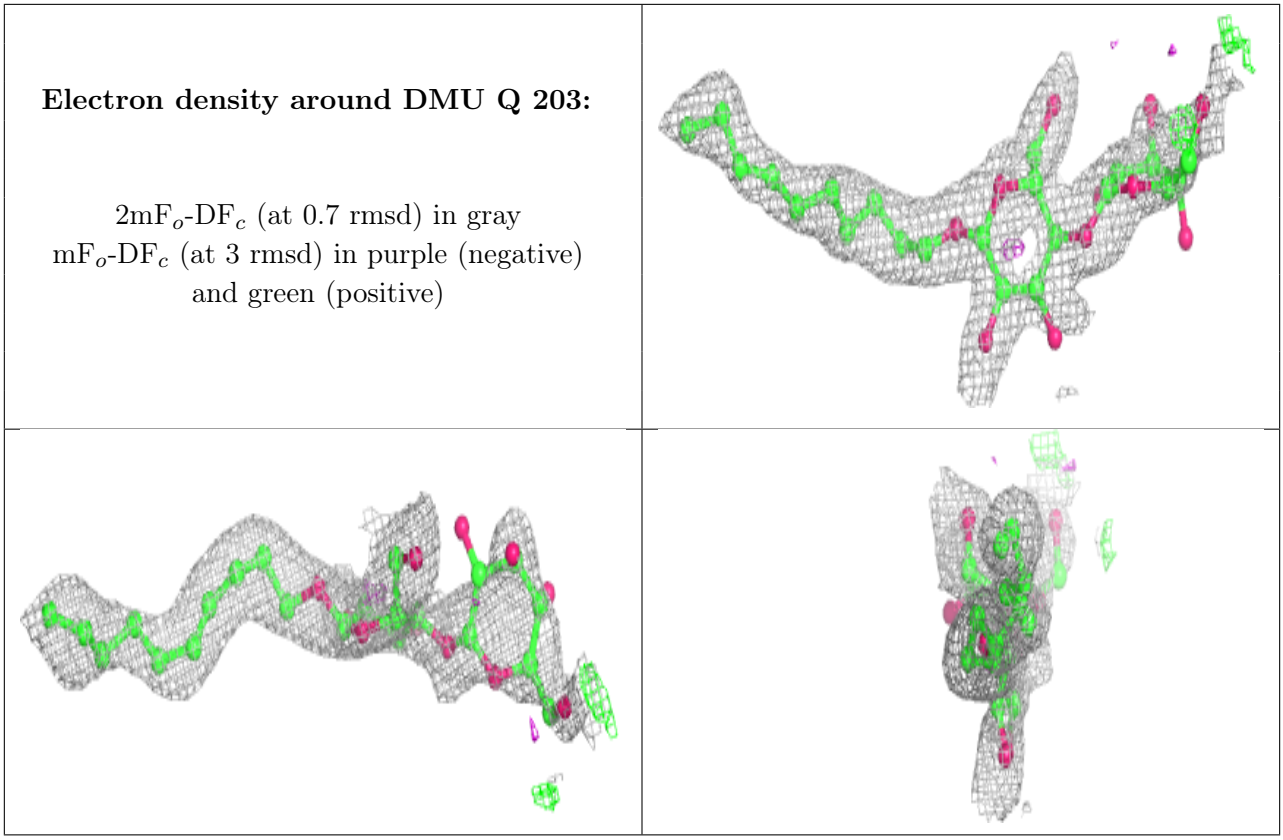






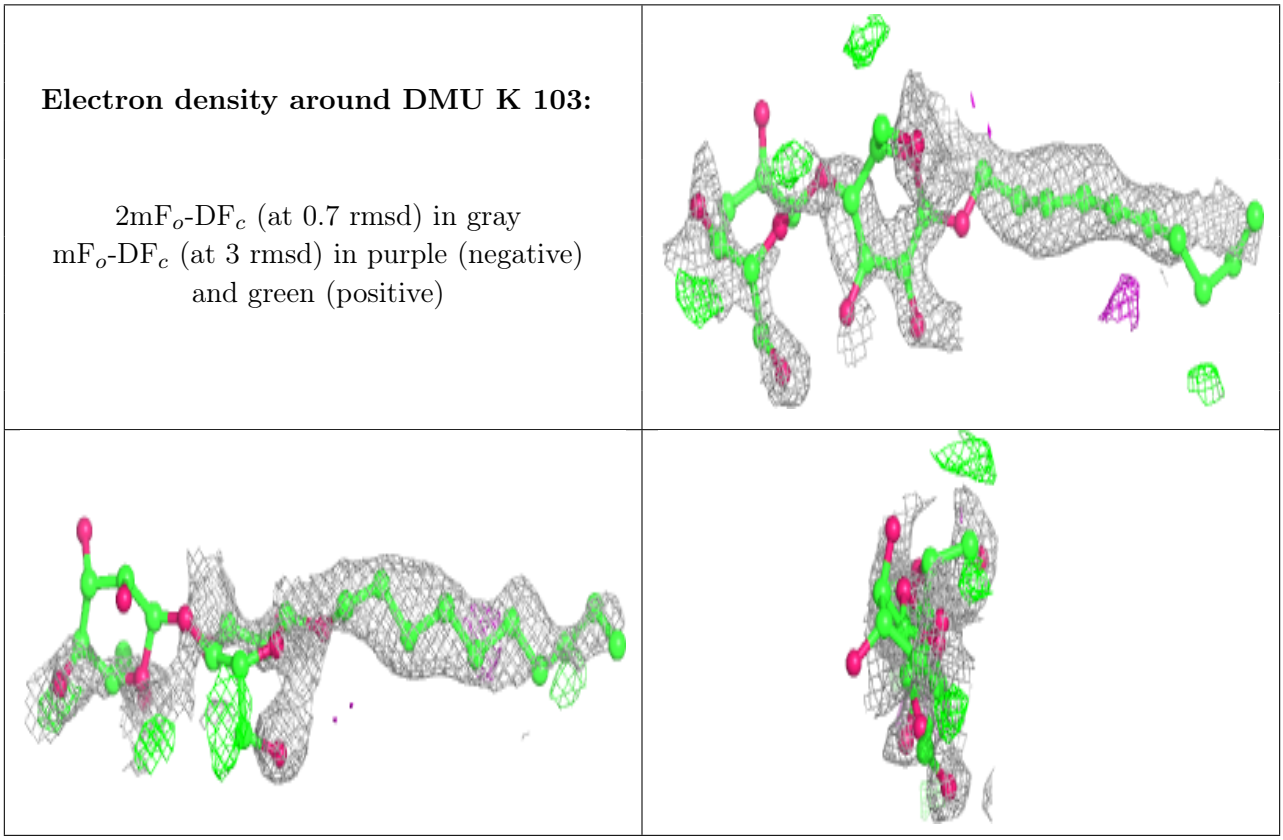
Electron density around DMU Q 203:

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



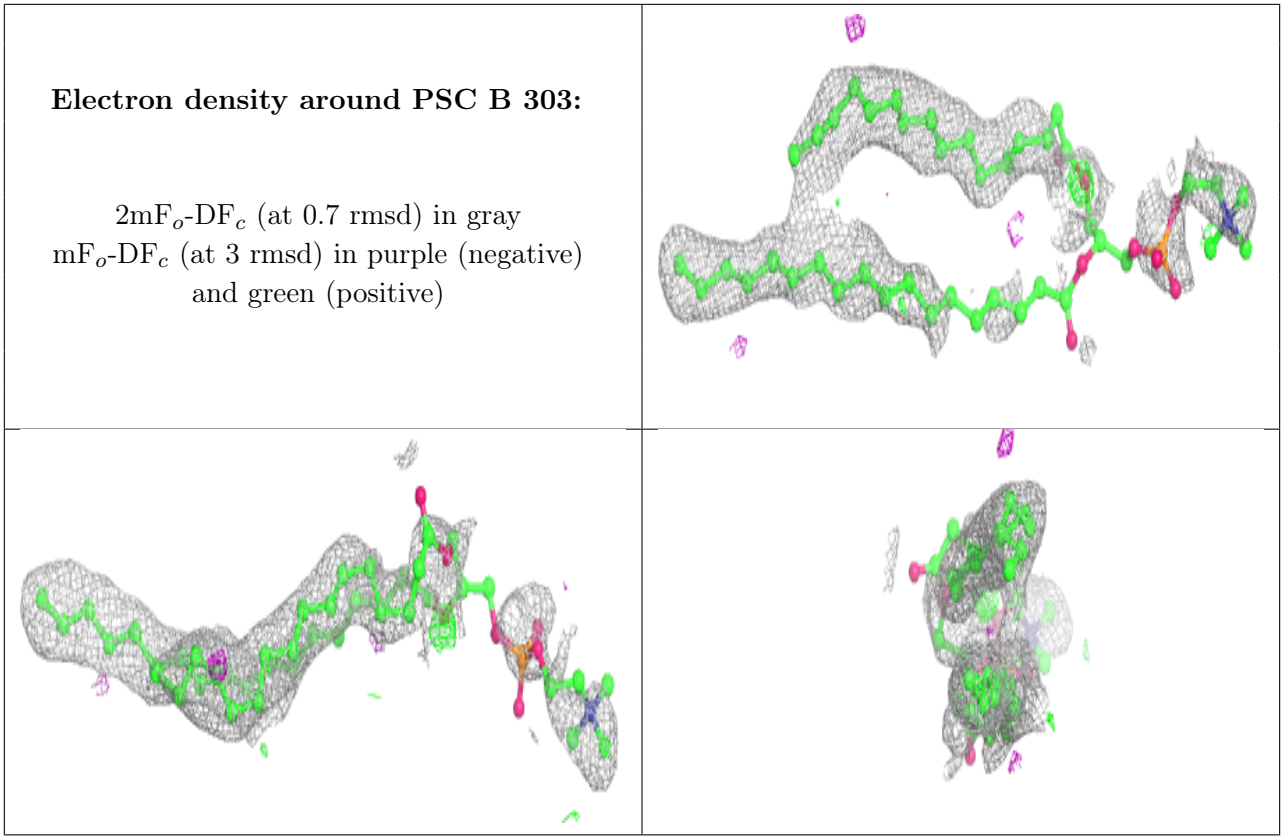
Electron density around DMU K 103:

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



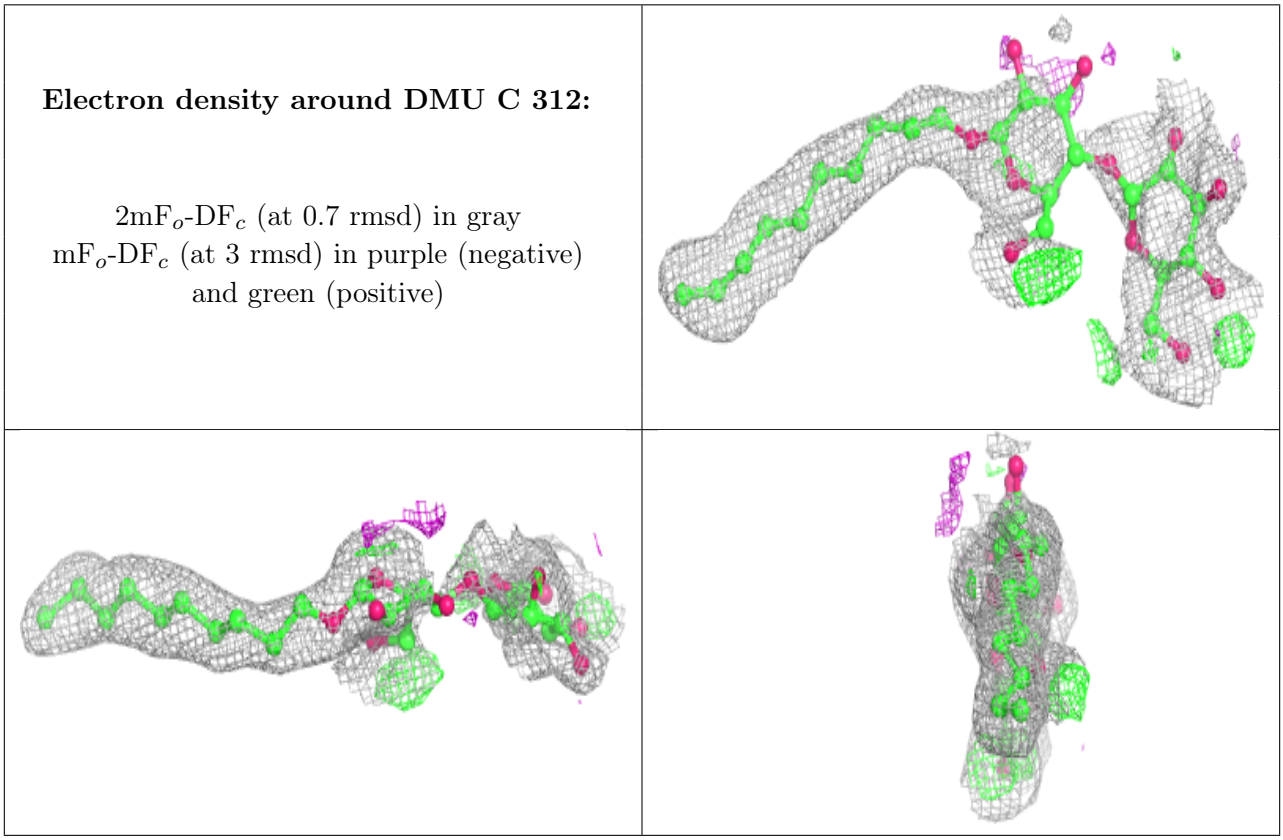
Electron density around PSC B 303:

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



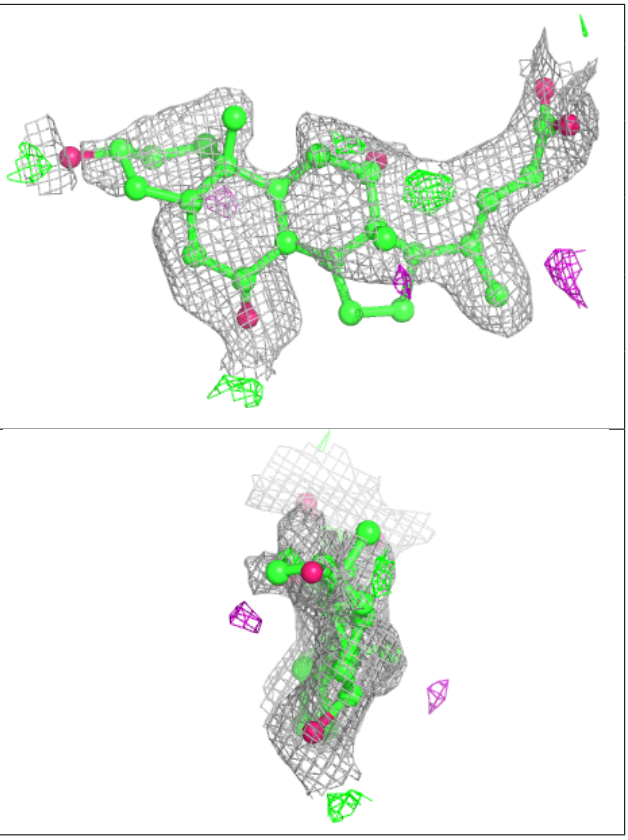
Electron density around DMU C 312:

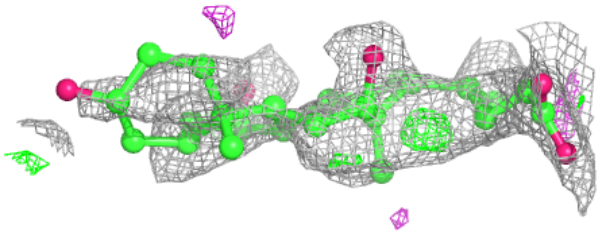
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CHD J 101:

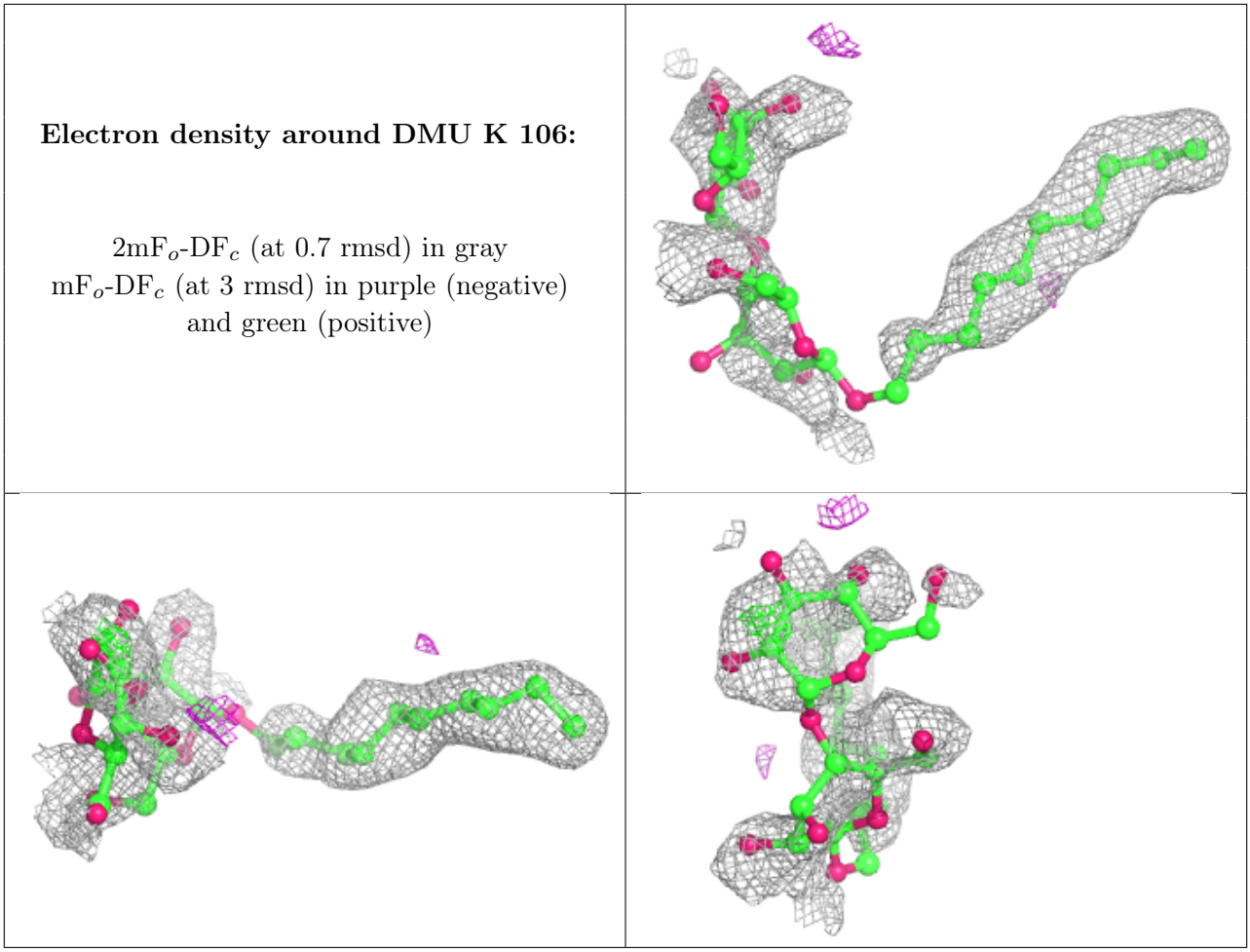
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





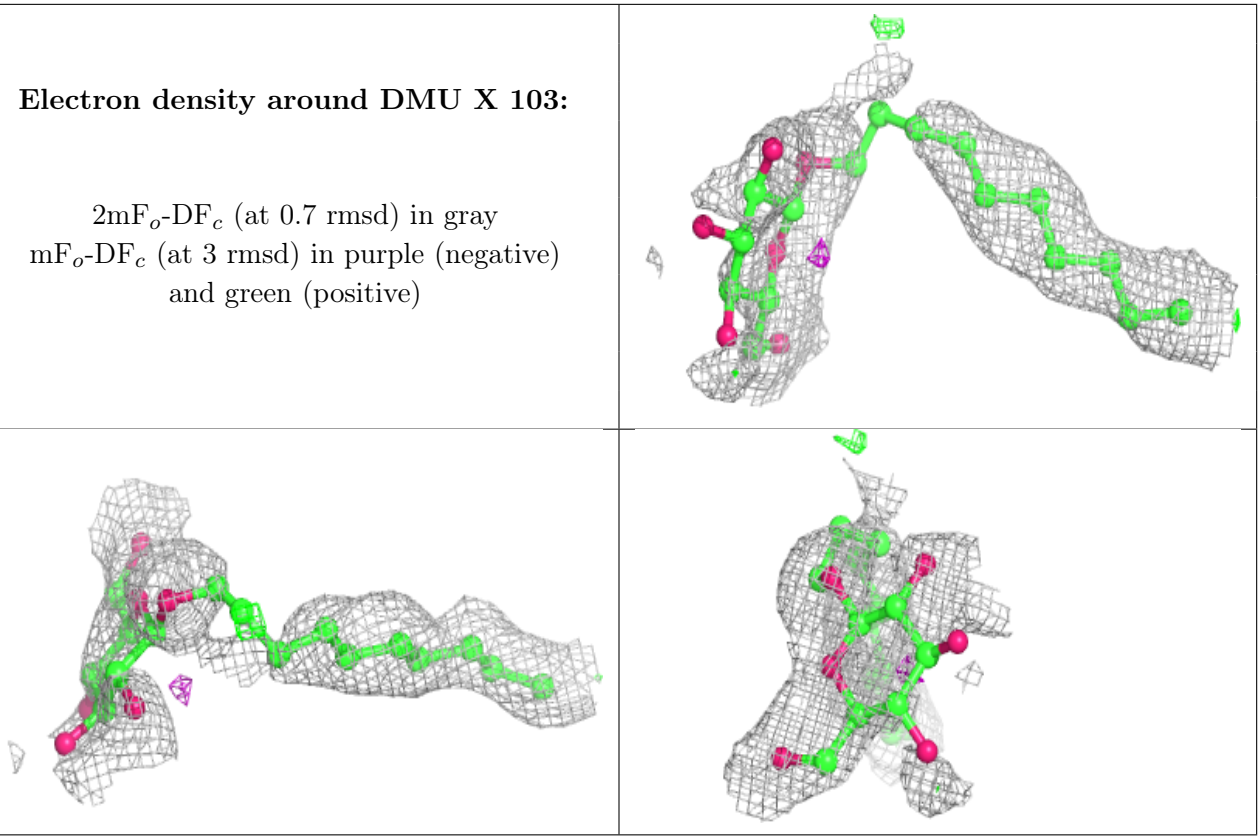
Electron density around DMU K 106:

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



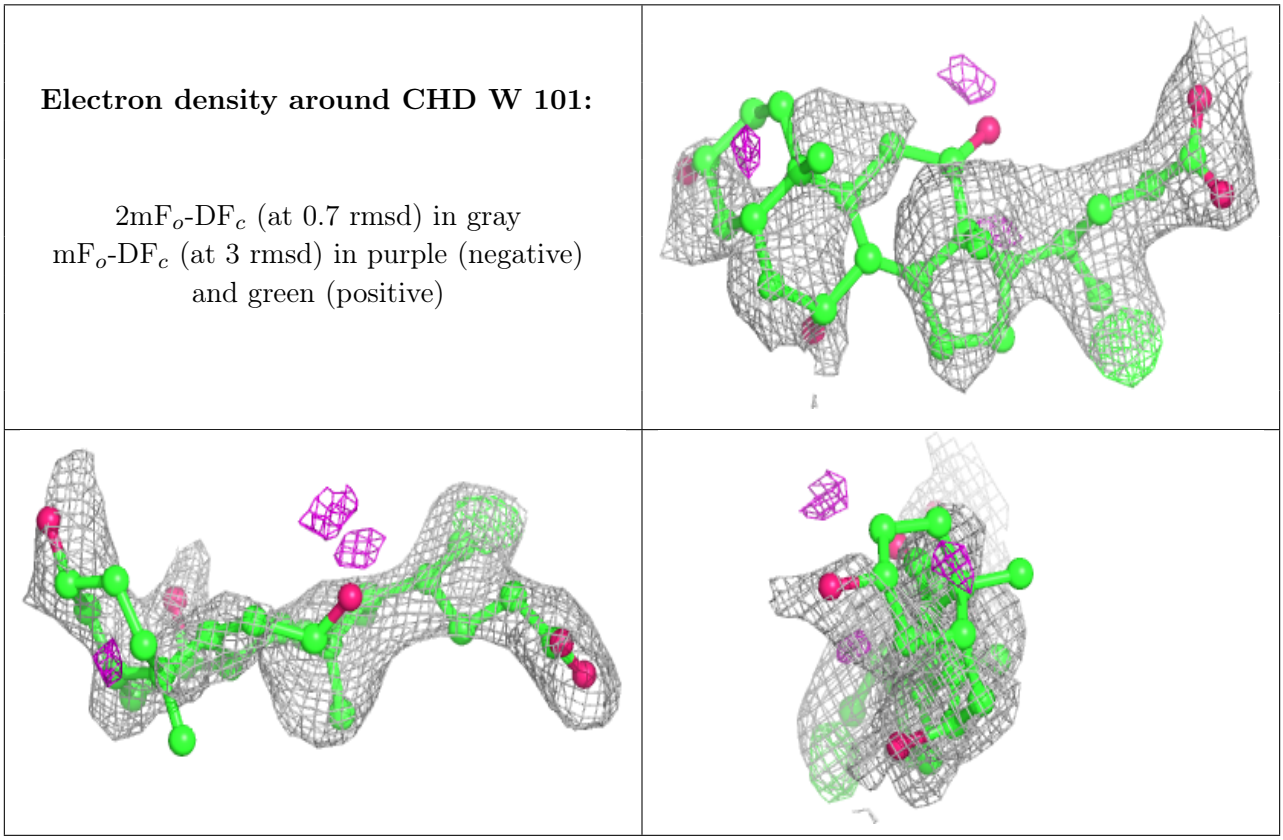
Electron density around DMU X 103:

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



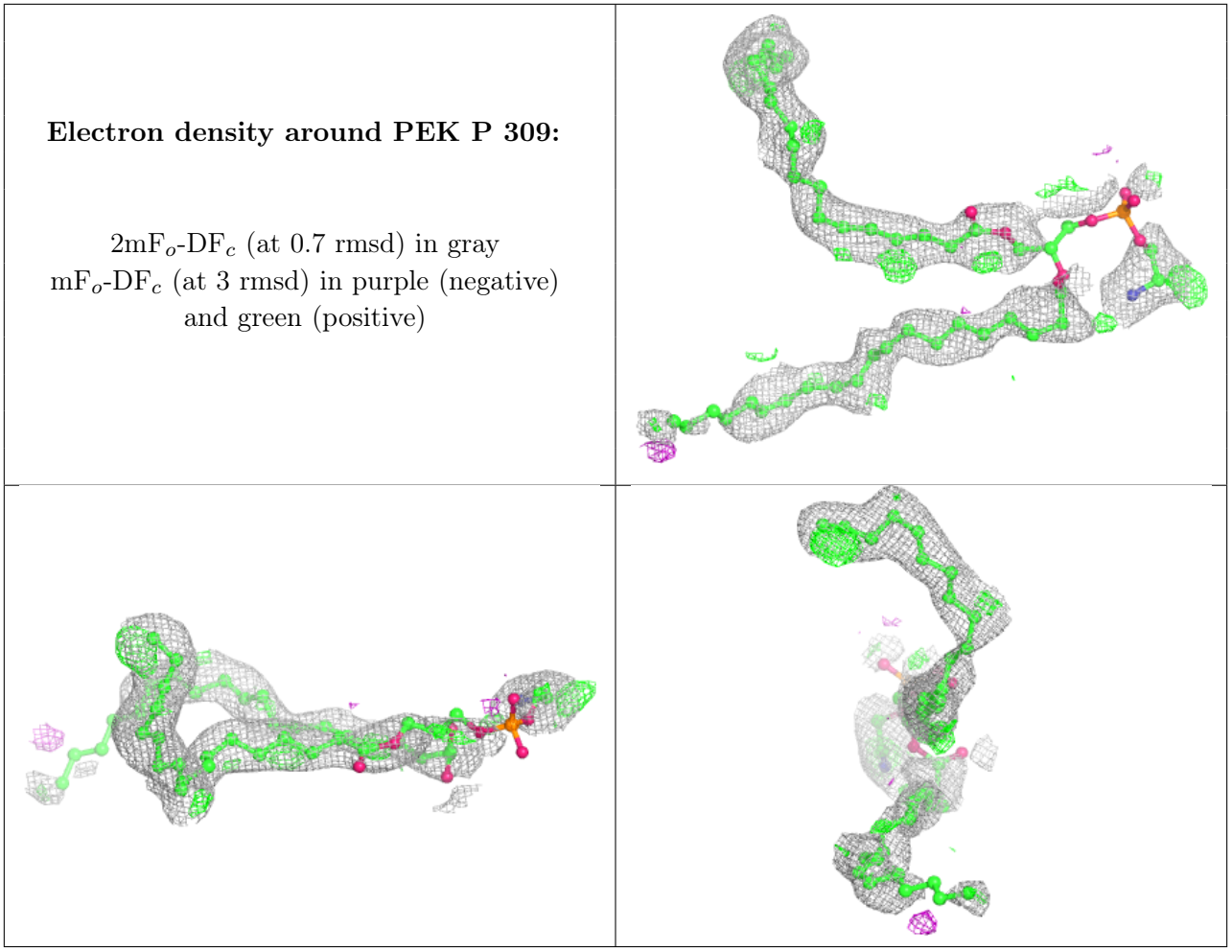
Electron density around CHD W 101:

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



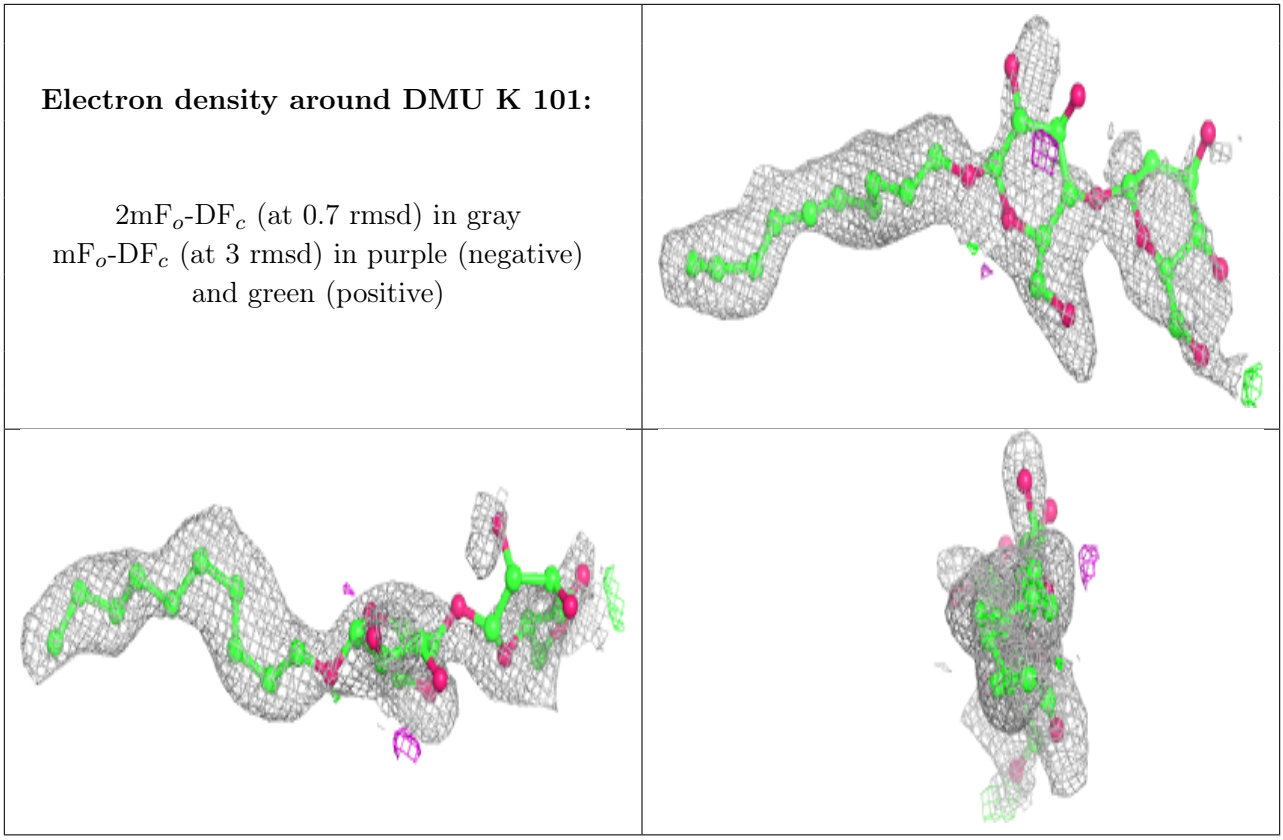
Electron density around PEK P 309:

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



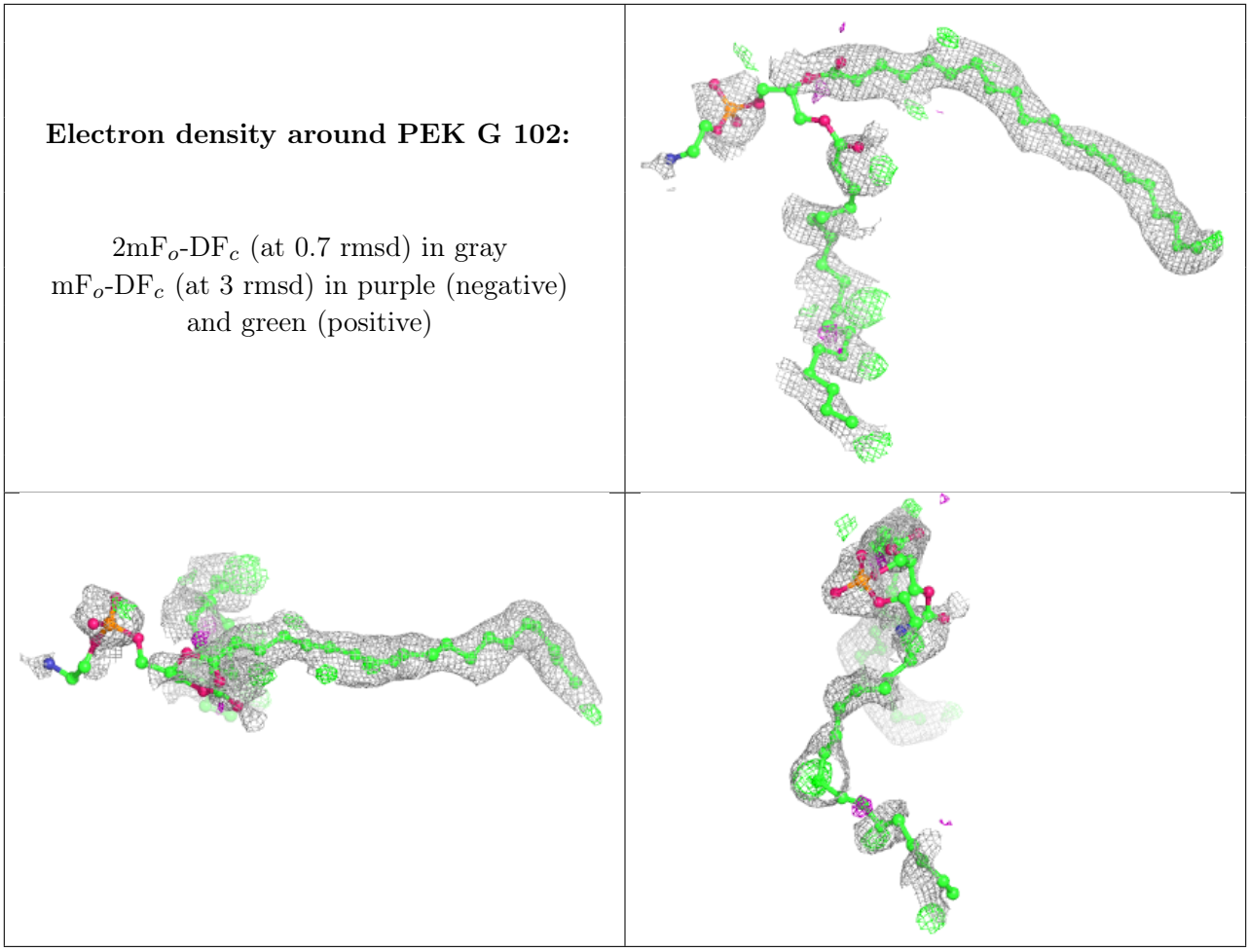
Electron density around DMU K 101:

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



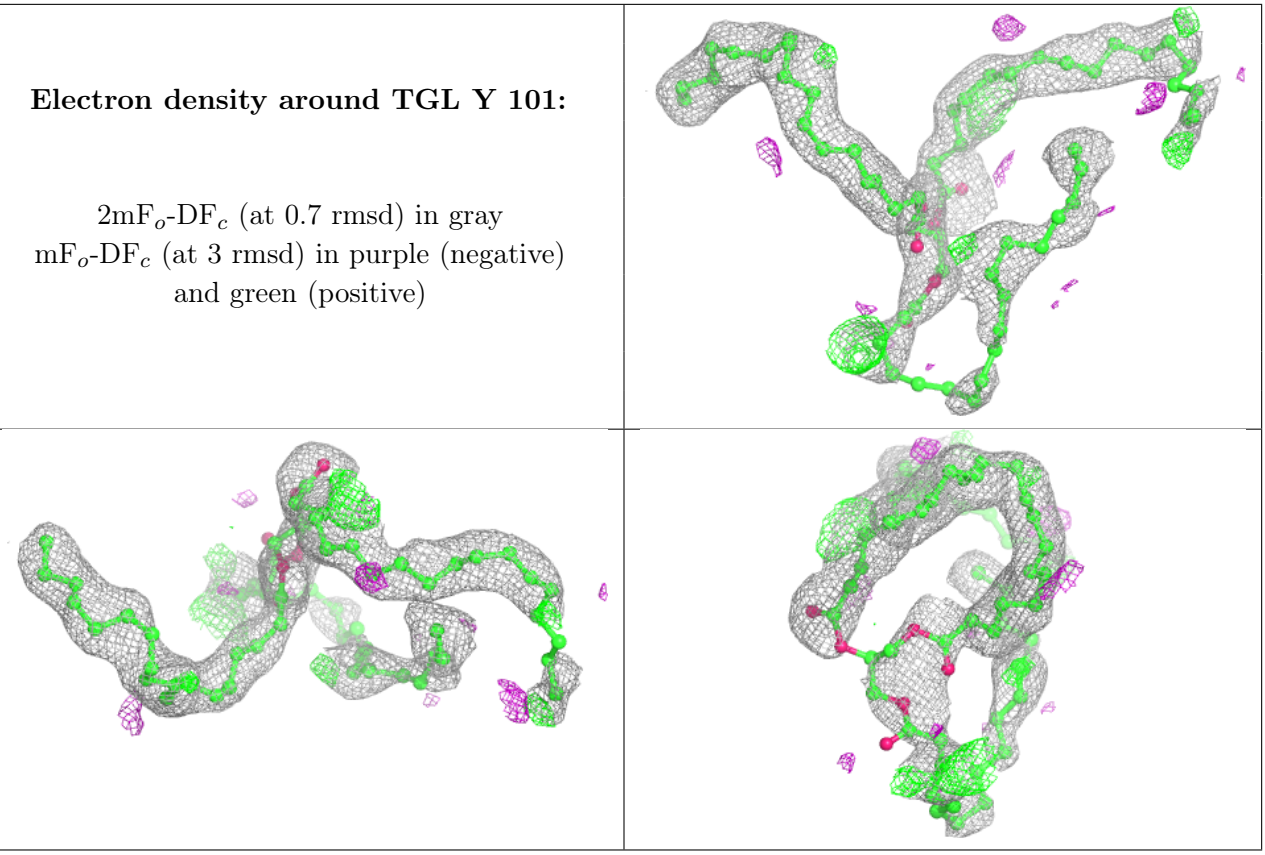
Electron density around PEK G 102:

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



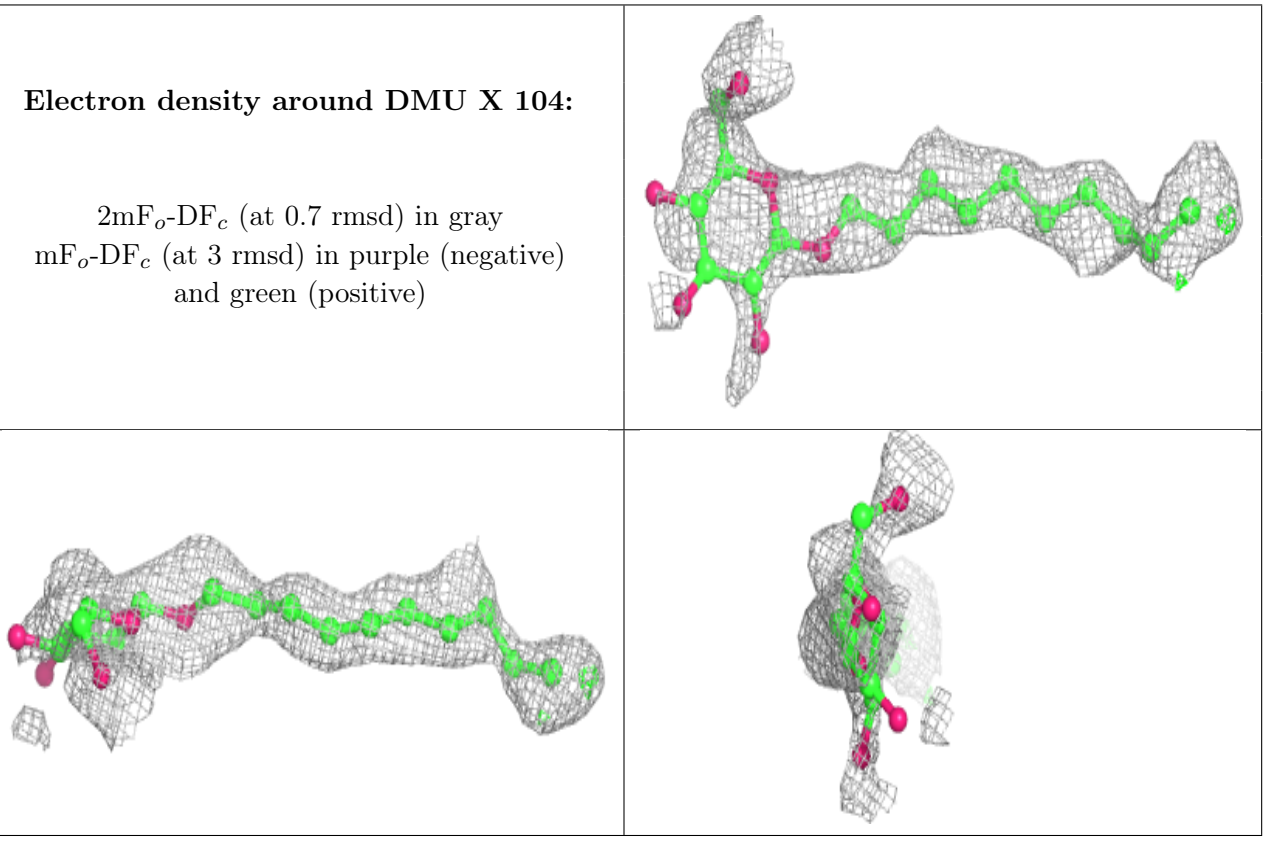
Electron density around TGL Y 101:

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



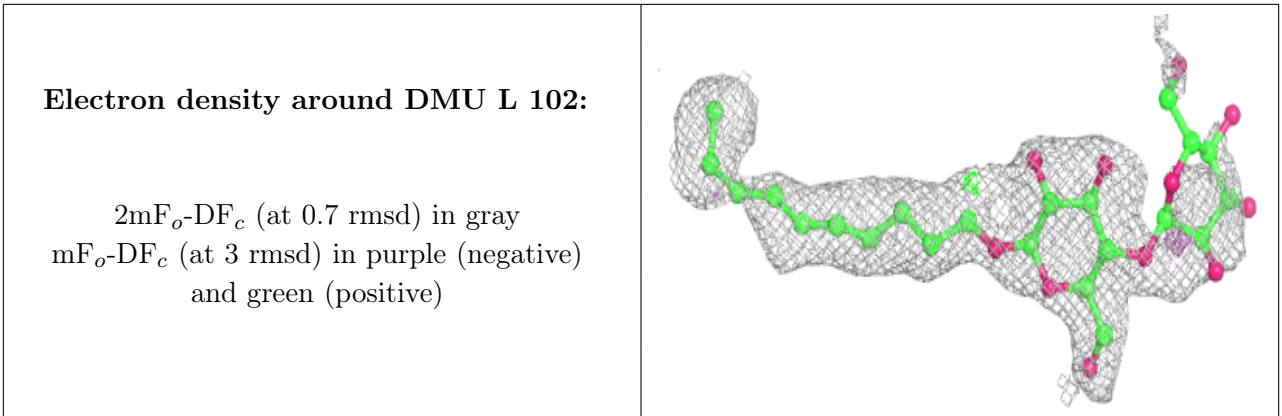
Electron density around DMU X 104:

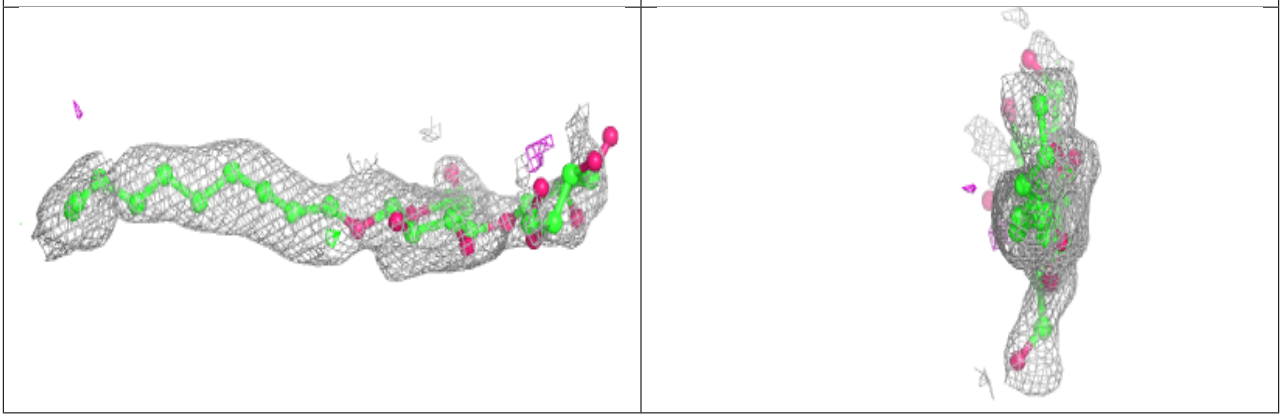
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DMU L 102:

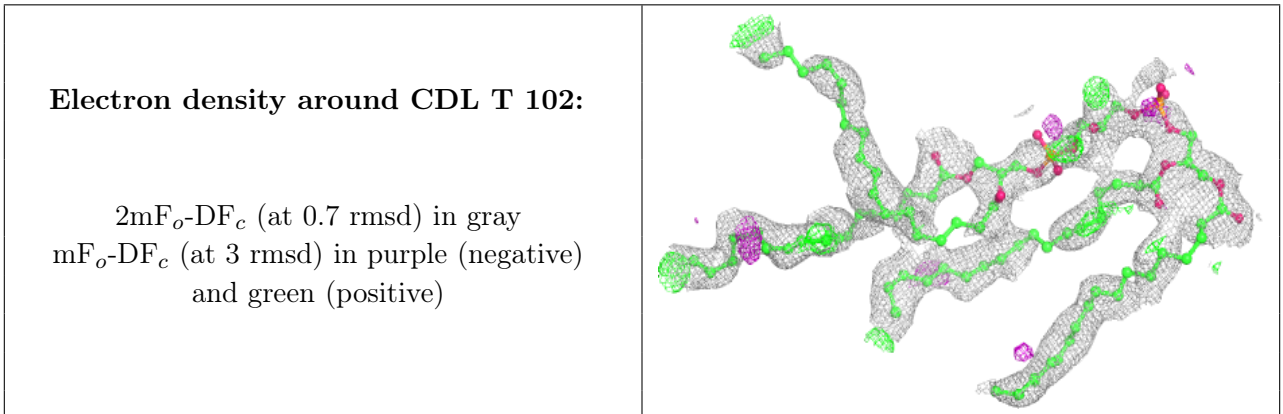
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

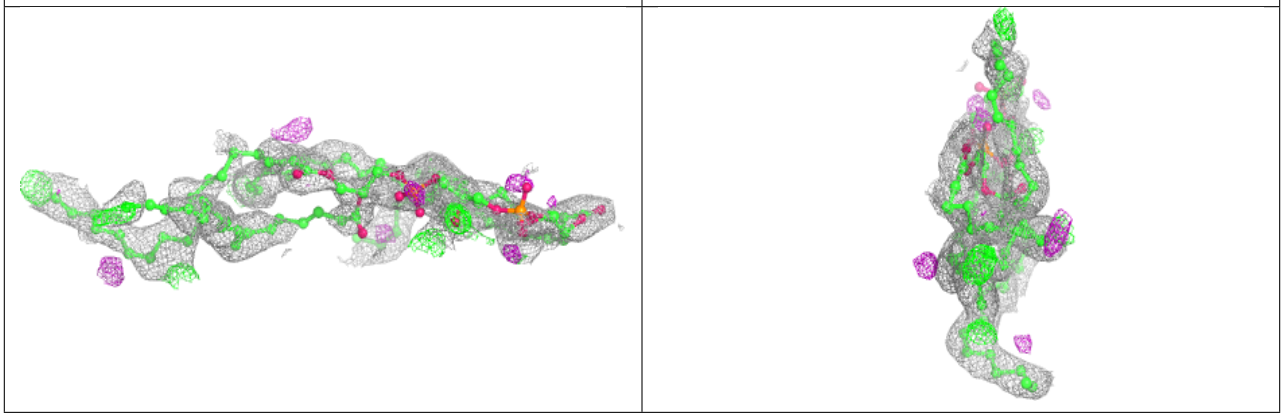




Electron density around CDL T 102:

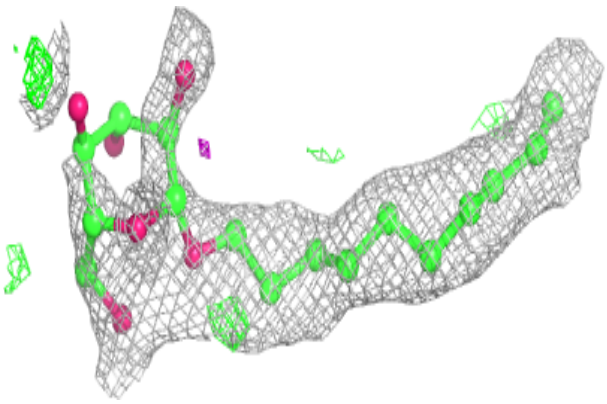
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

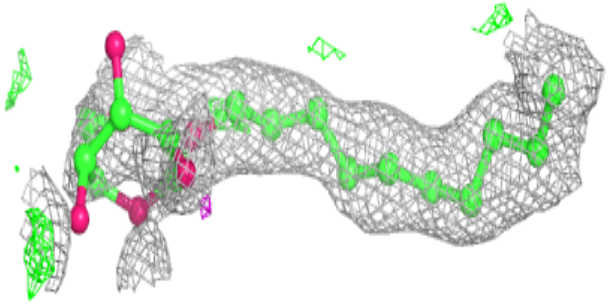


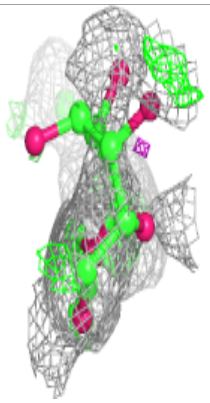


Electron density around DMU X 102:

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

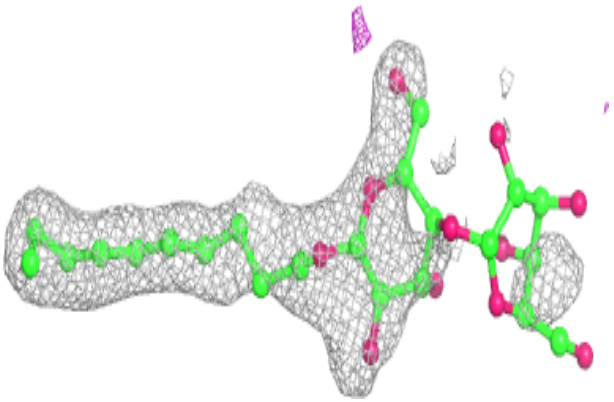


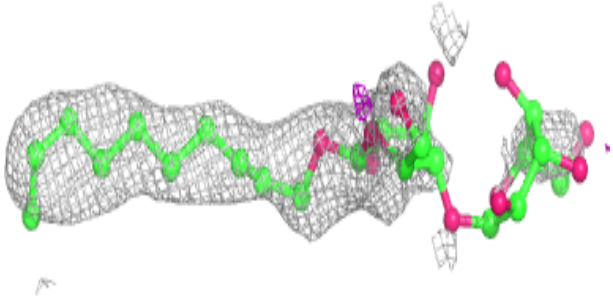


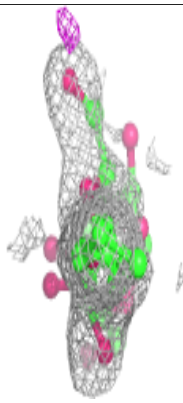


Electron density around DMU O 305:

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

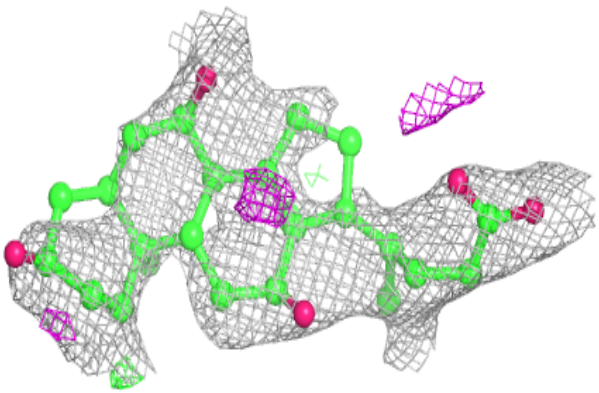


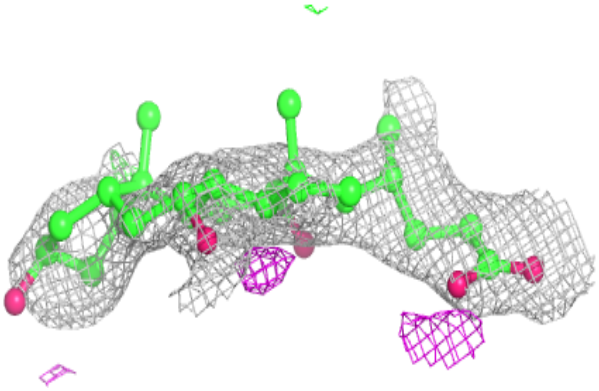


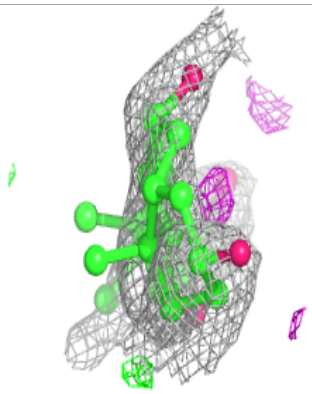


Electron density around CHD L 103:

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

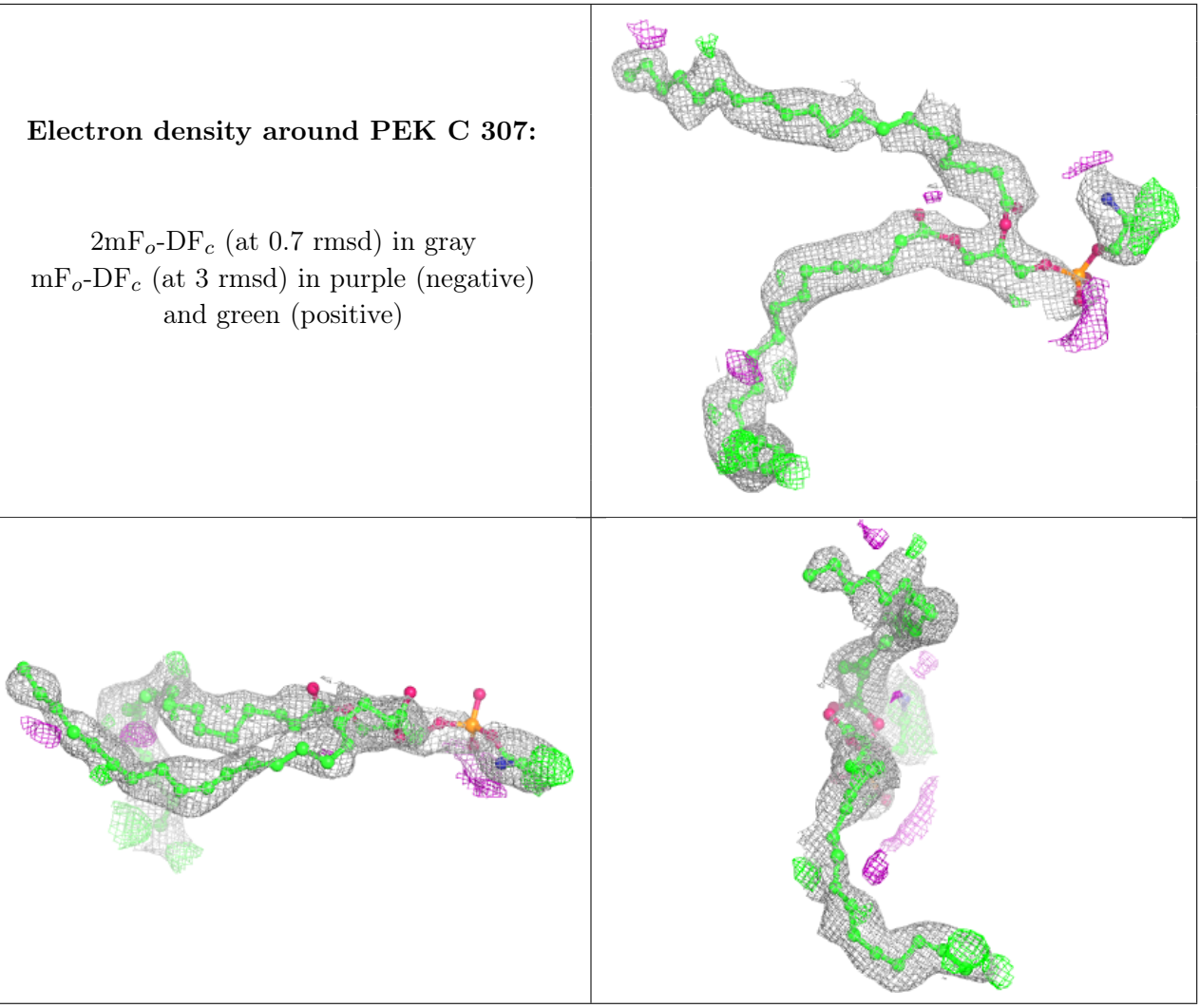






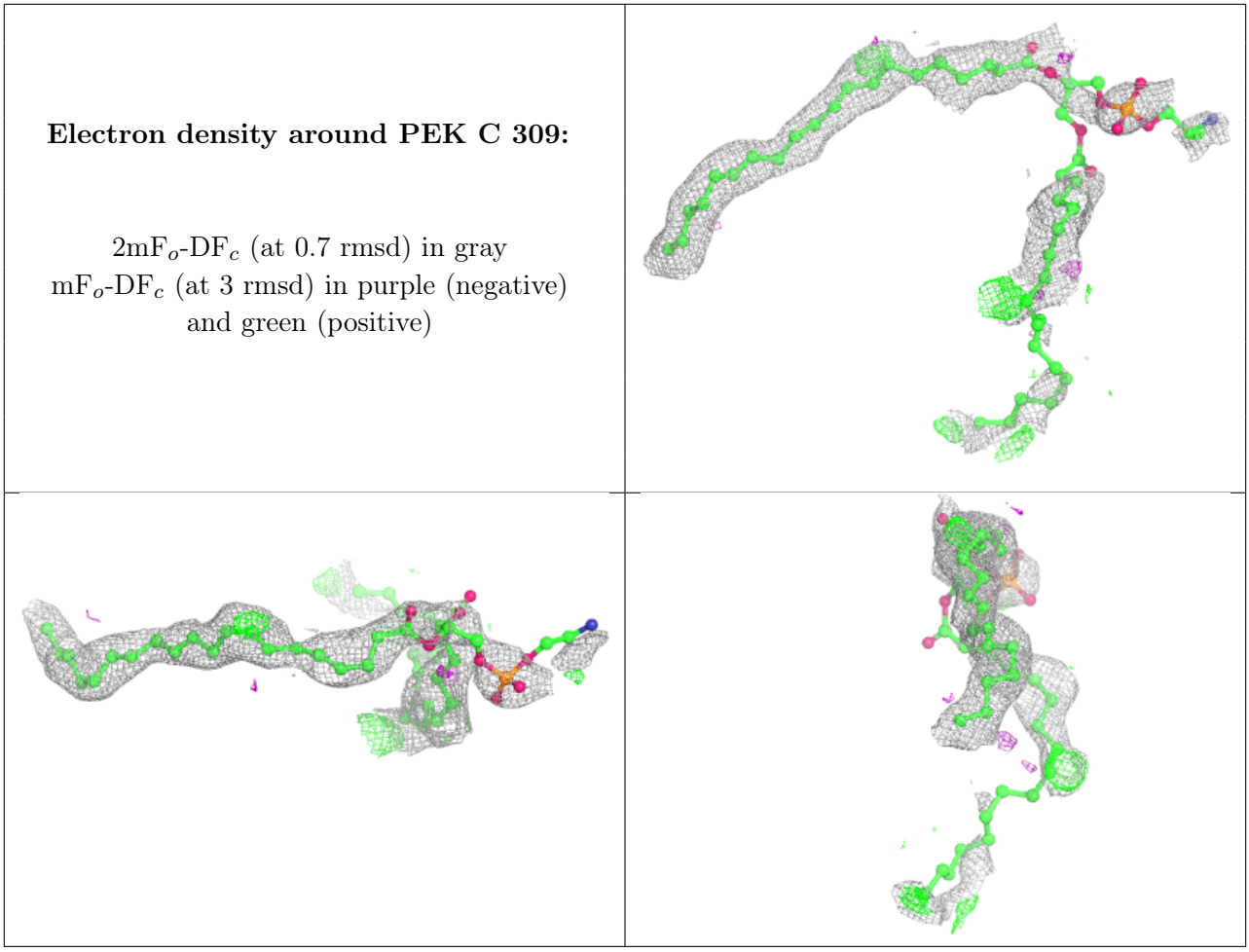
Electron density around PEK C 307:

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



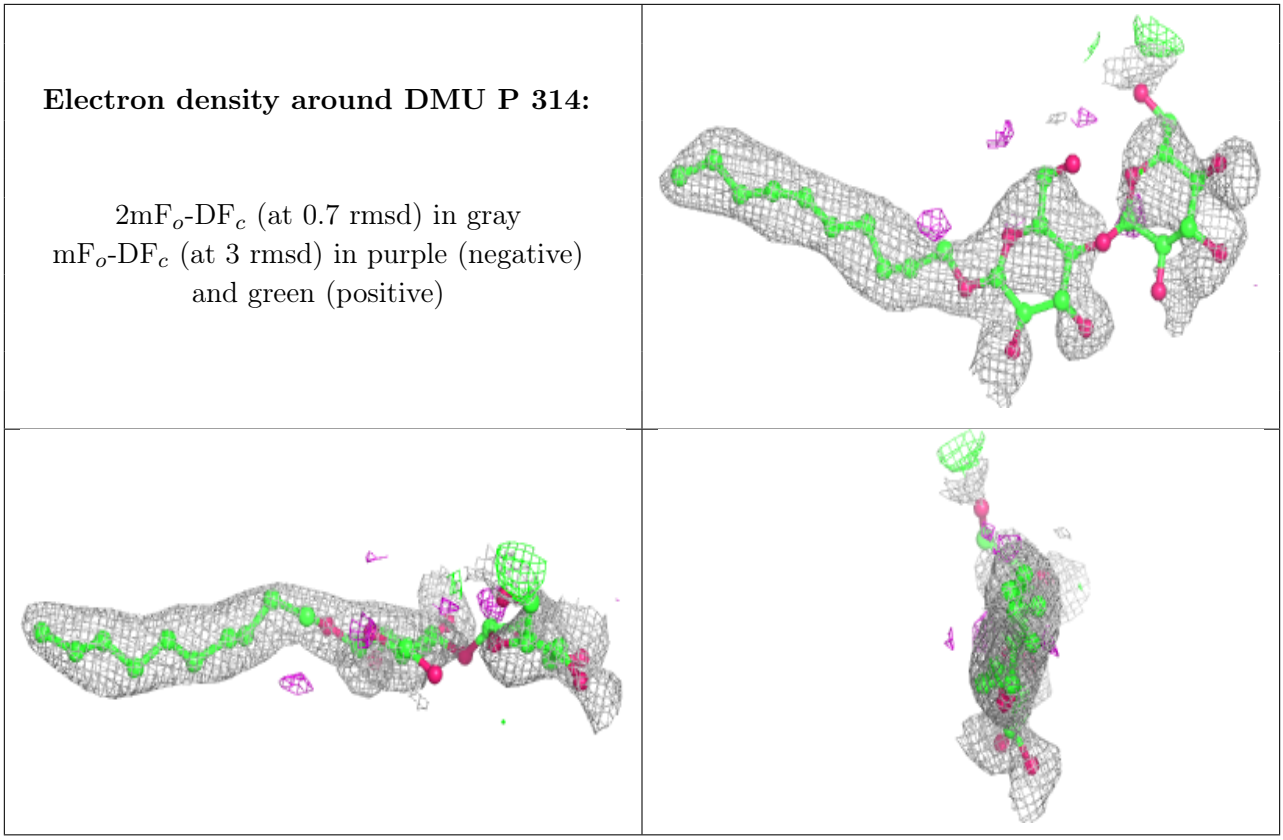
Electron density around PEK C 309:

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



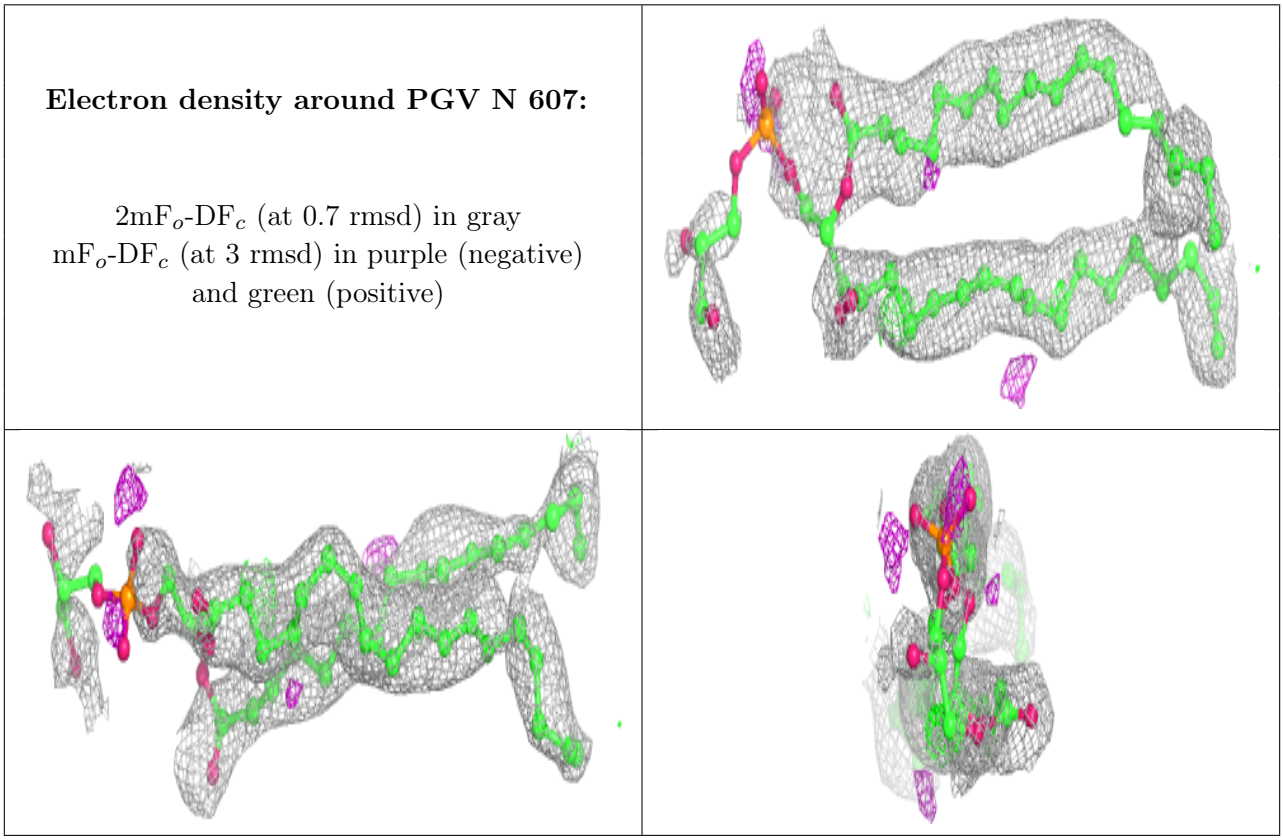
Electron density around DMU P 314:

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



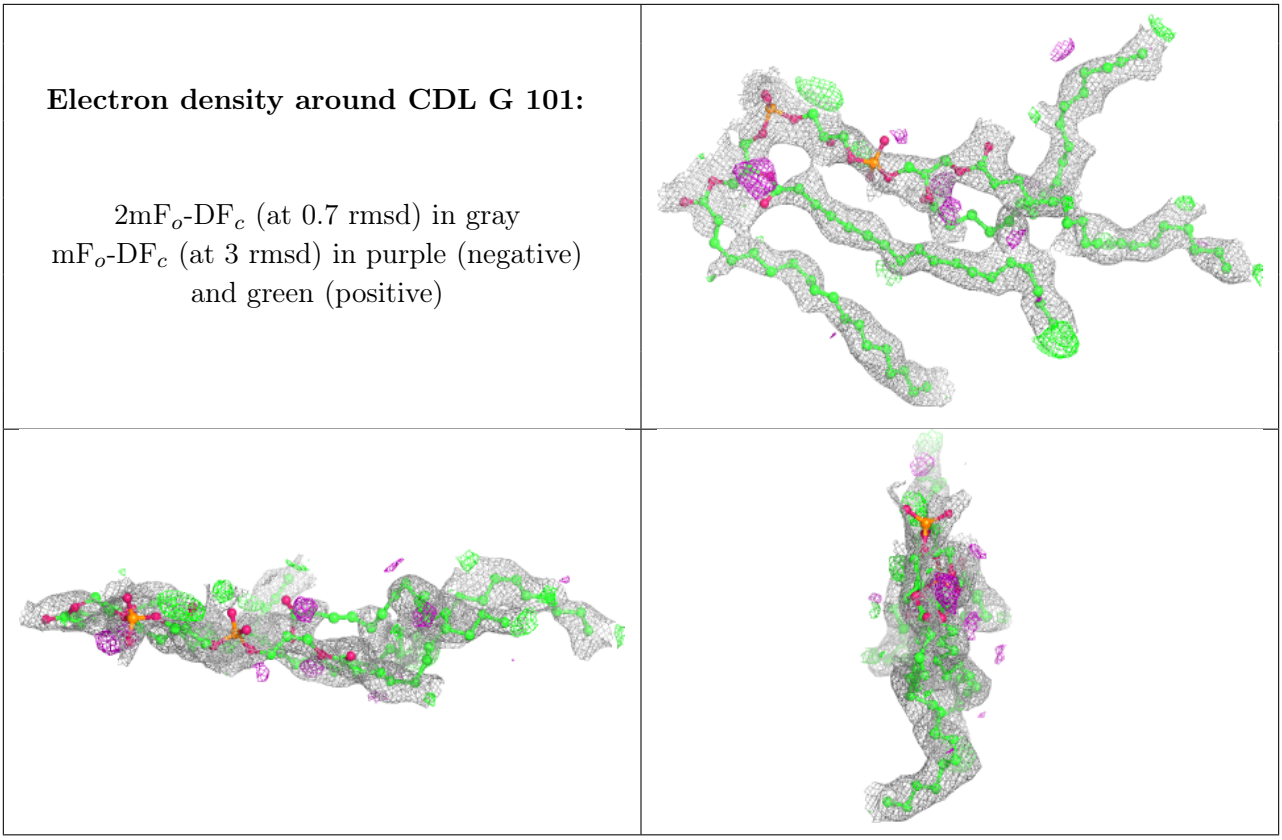
Electron density around PGV N 607:

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



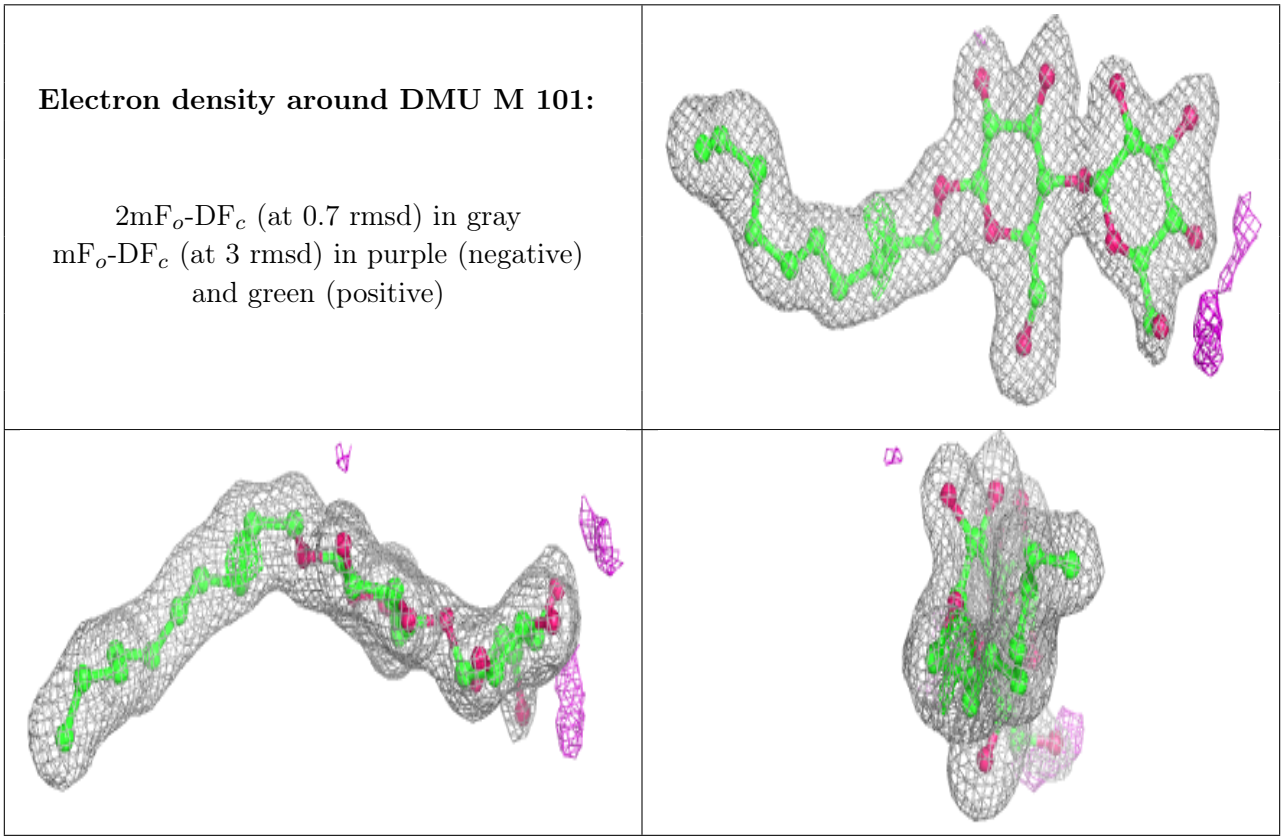
Electron density around CDL G 101:

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



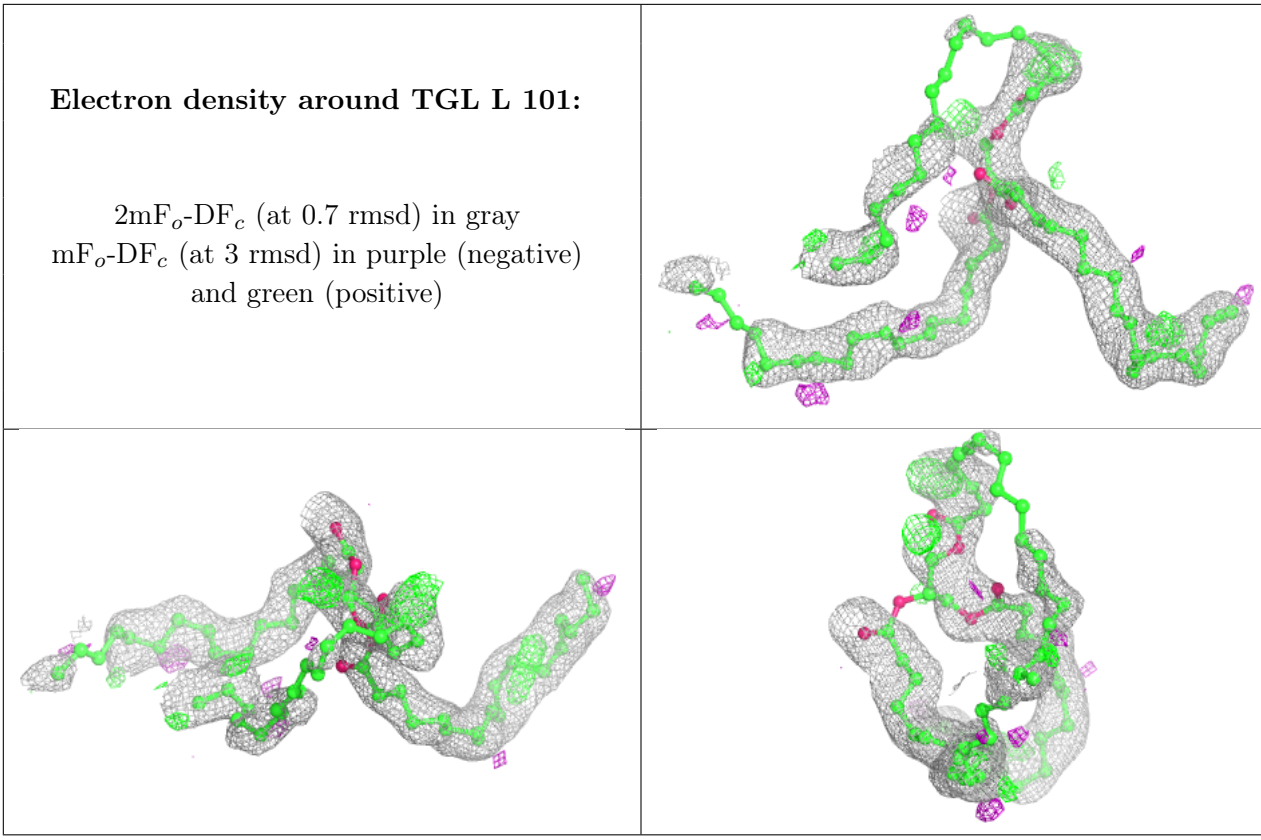
Electron density around DMU M 101:

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



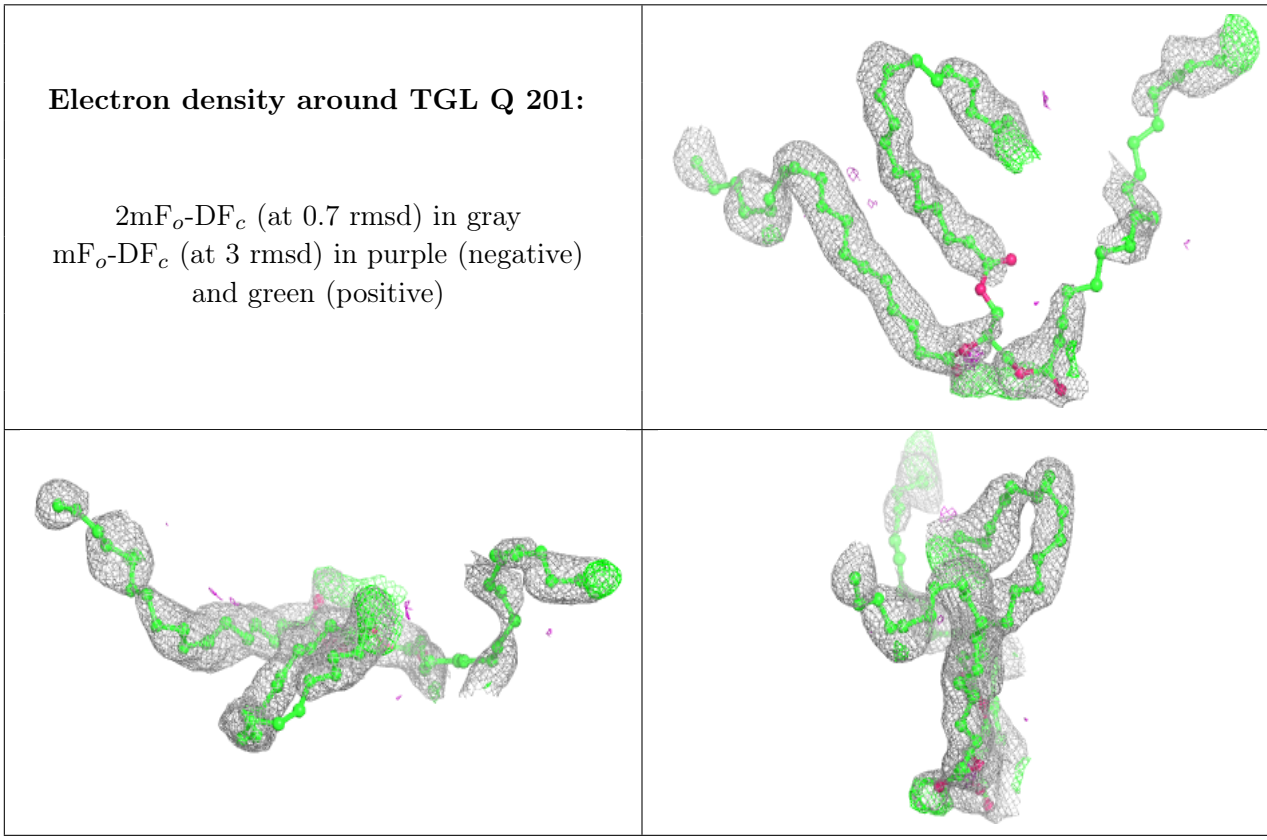
Electron density around TGL L 101:

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



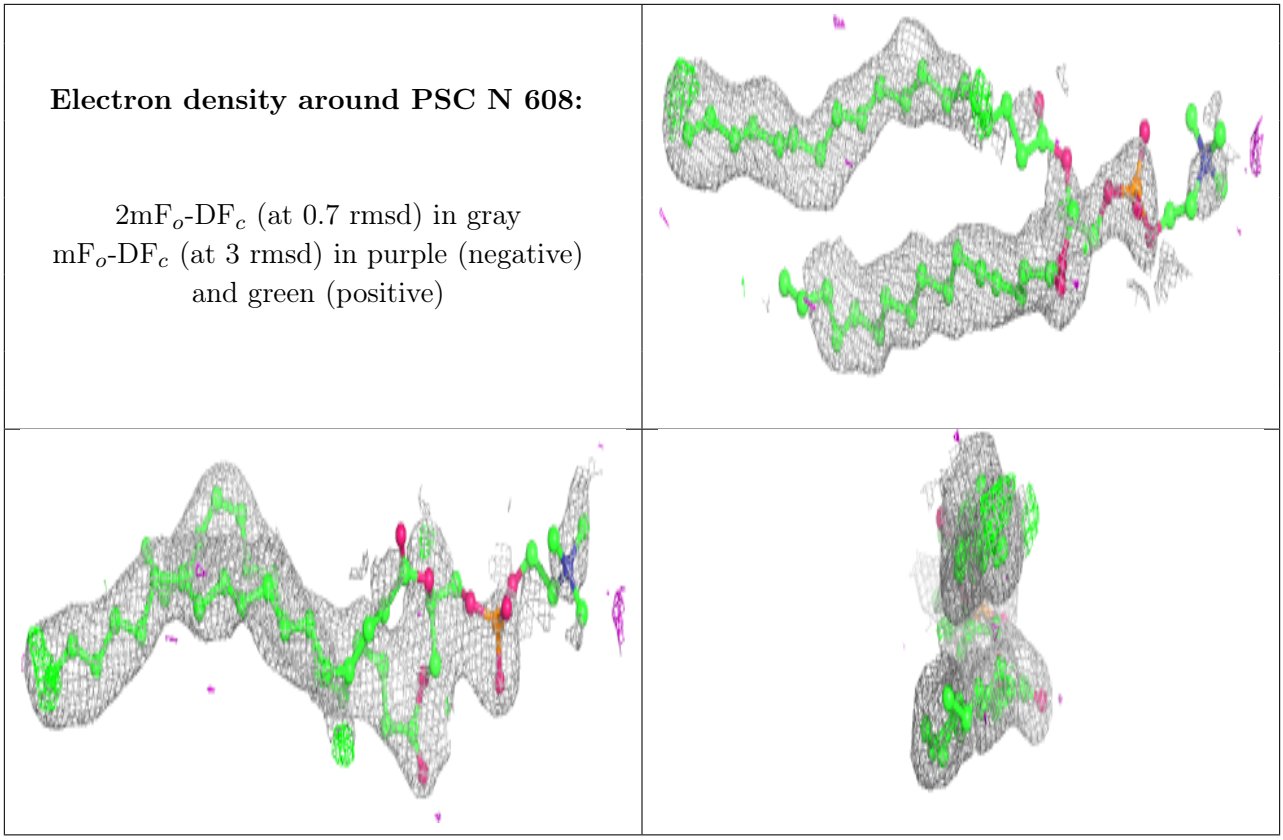
Electron density around TGL Q 201:

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



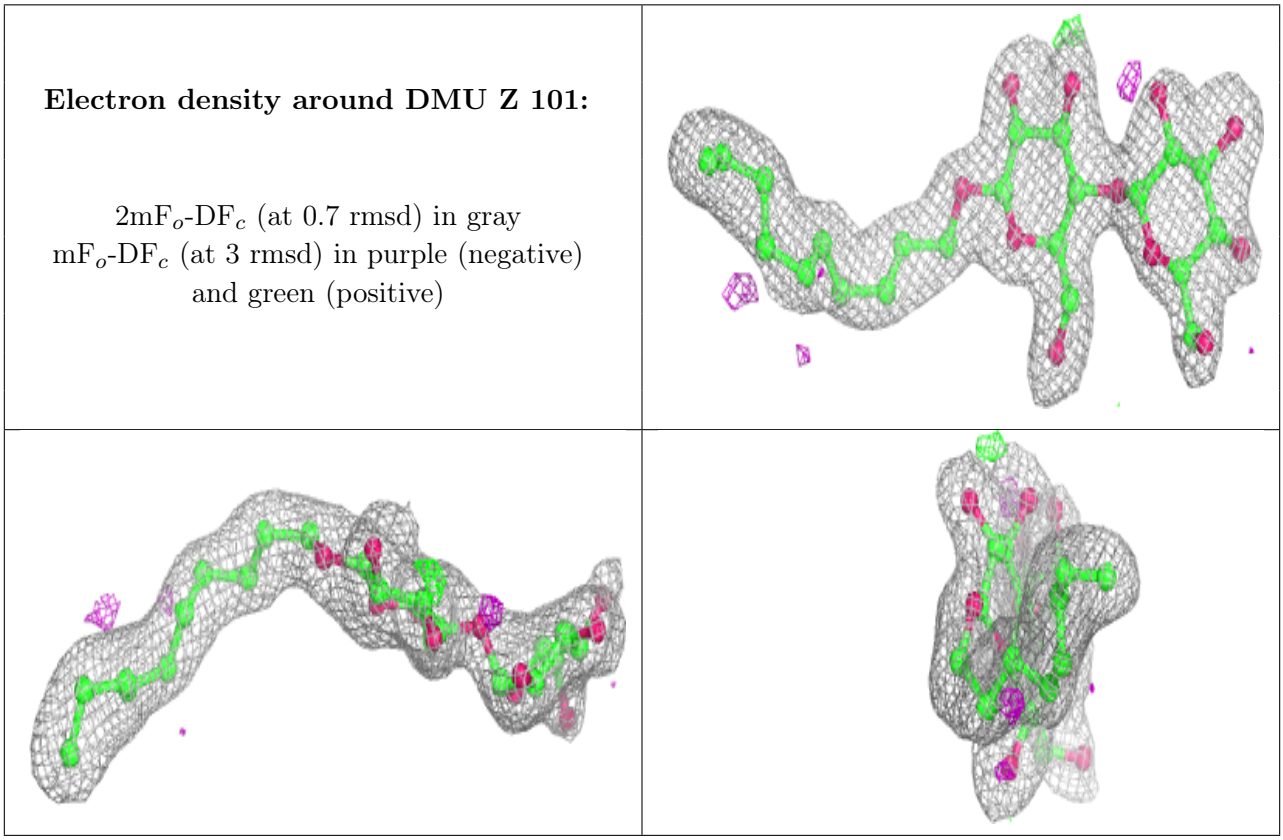
Electron density around PSC N 608:

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



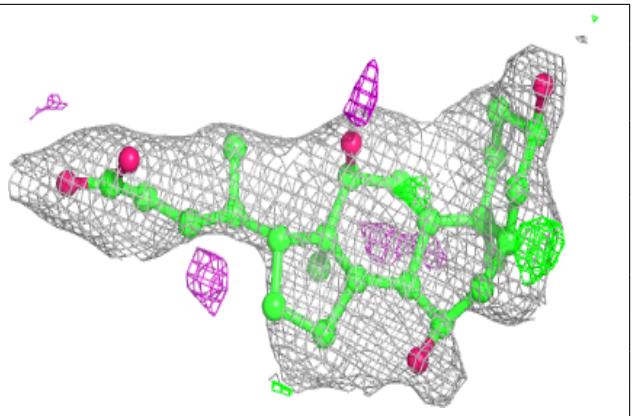
Electron density around DMU Z 101:

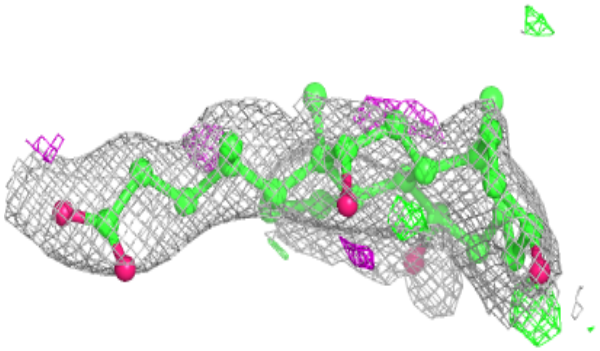
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

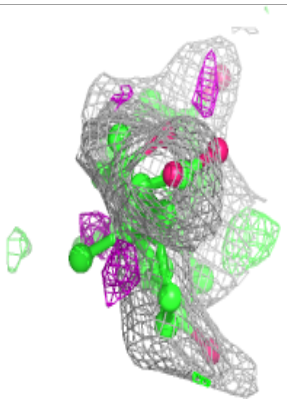


Electron density around CHD Y 102:

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

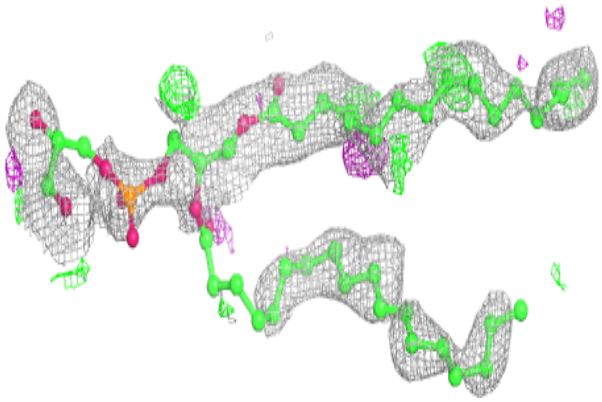


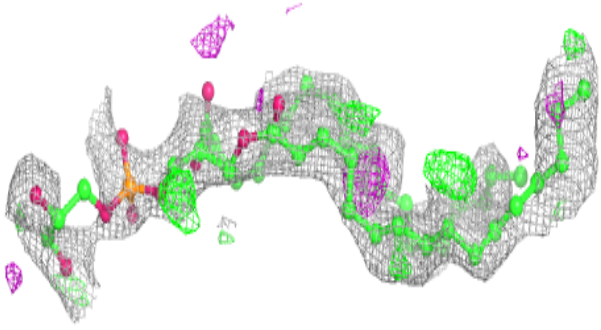


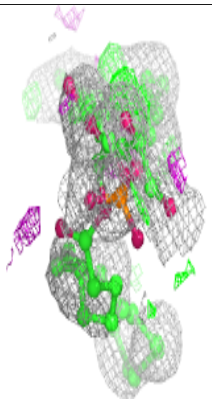


Electron density around PGV C 308:

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

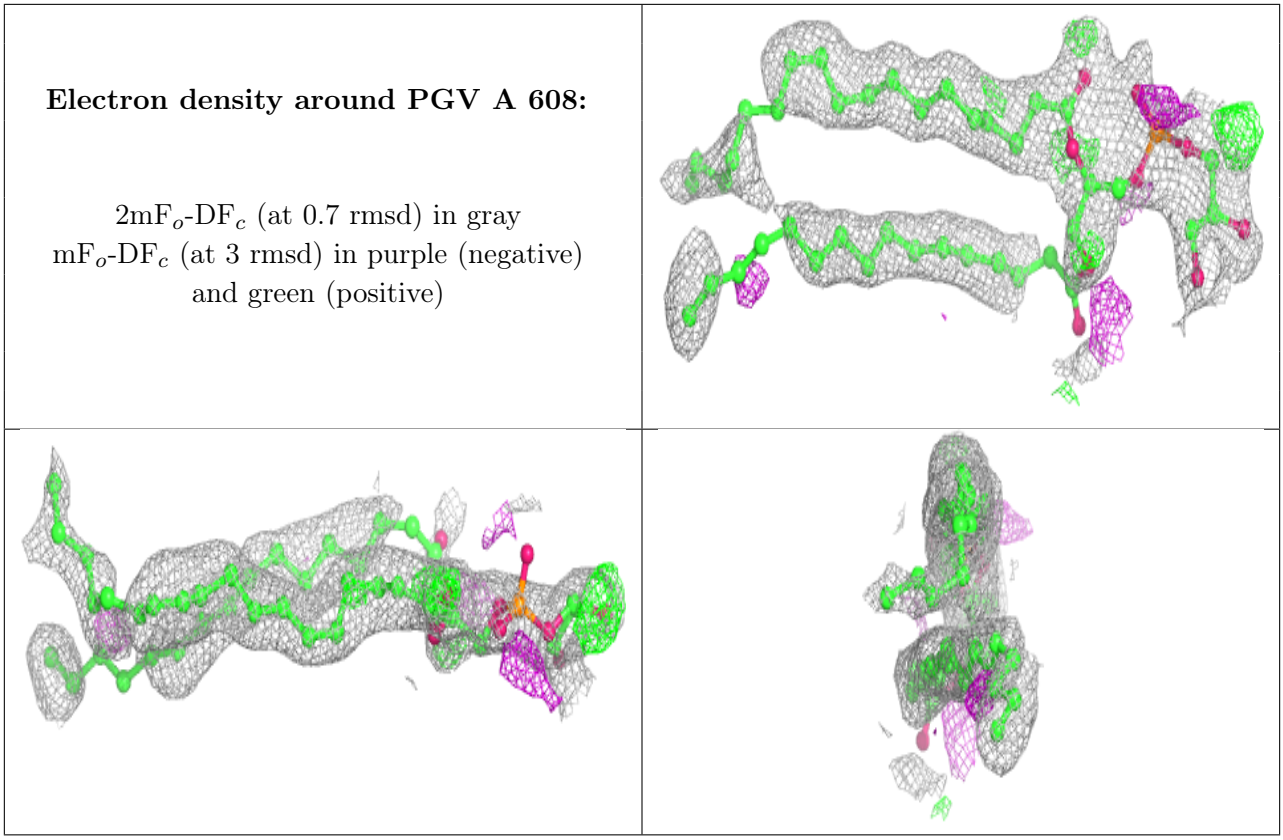






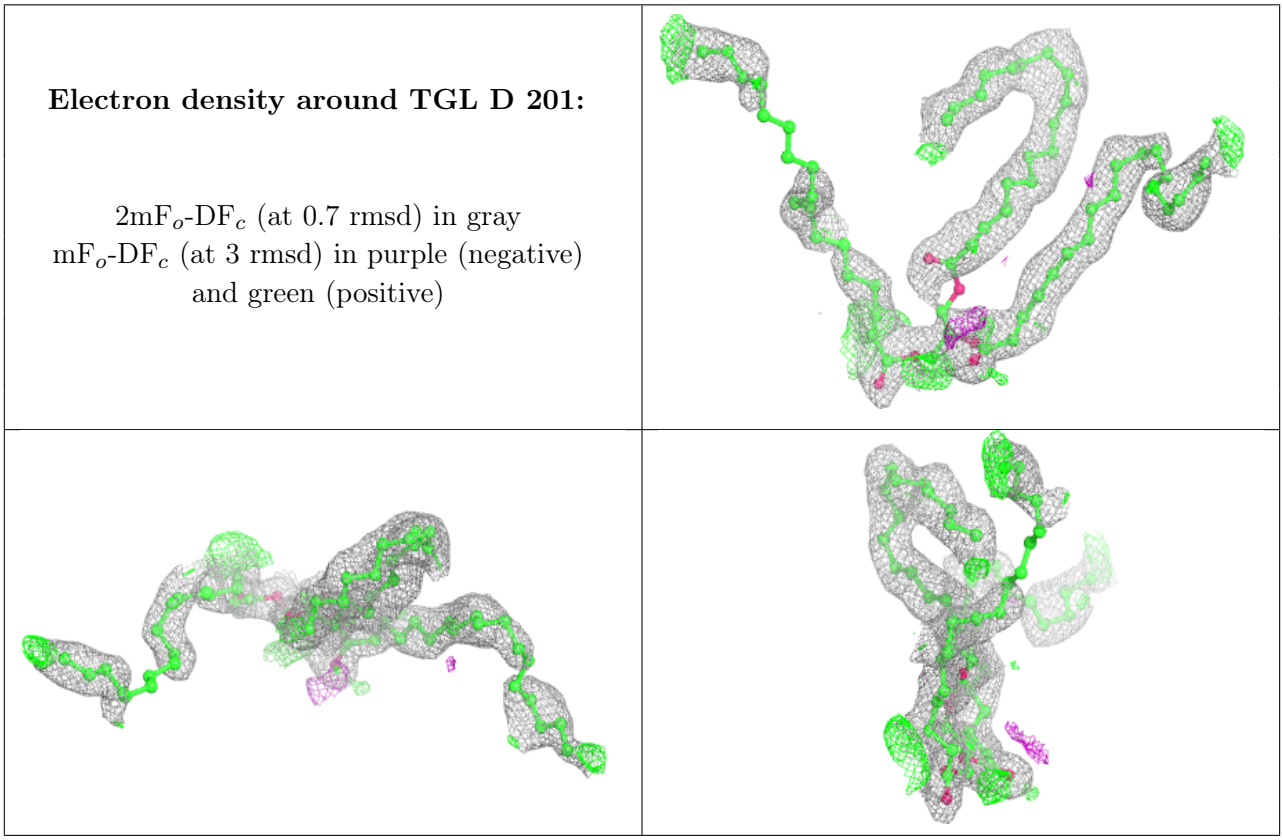
Electron density around PGV A 608:

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



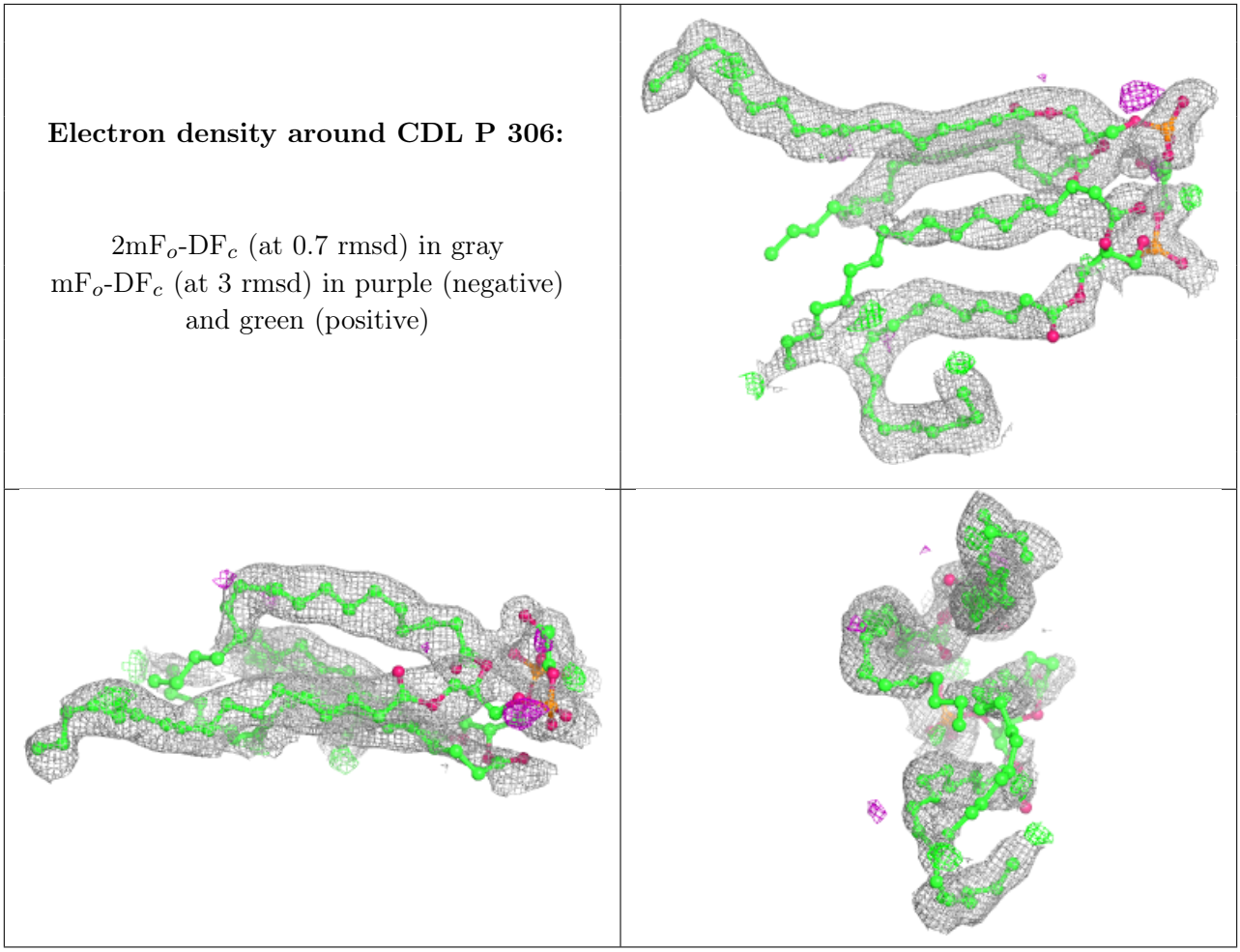
Electron density around TGL D 201:

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



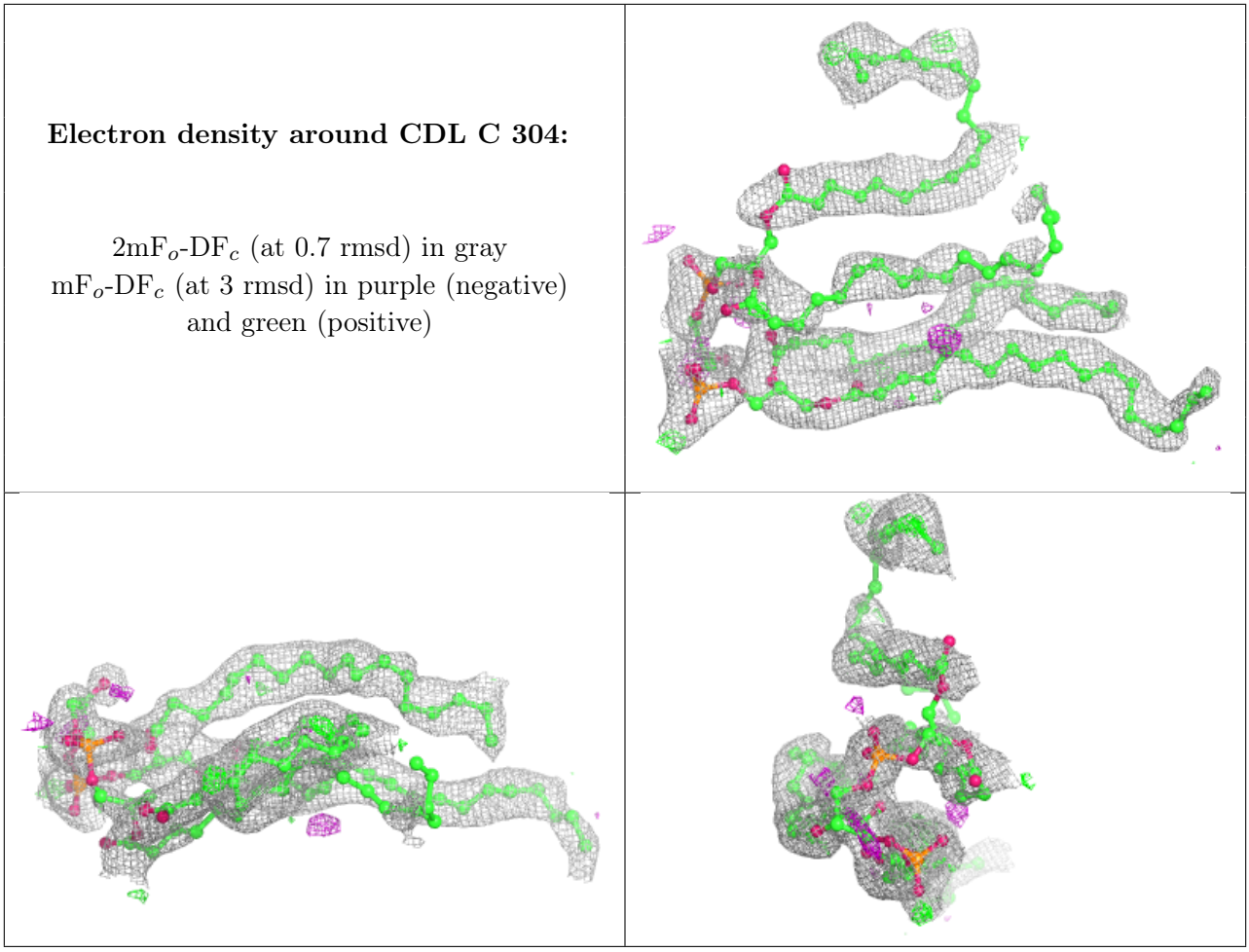
Electron density around CDL P 306:

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



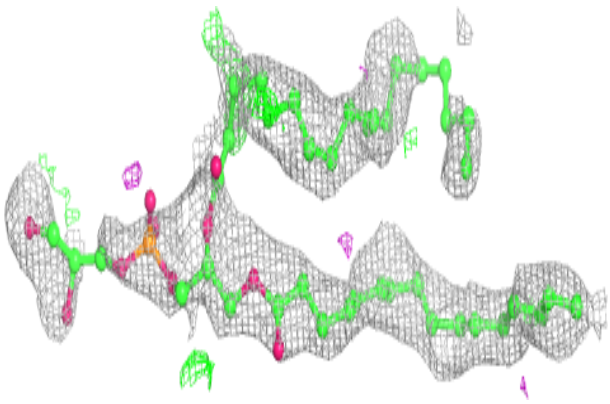
Electron density around CDL C 304:

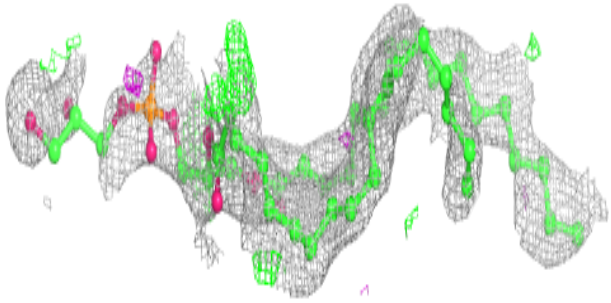
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

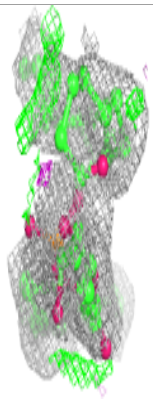


Electron density around PGV P 302:

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

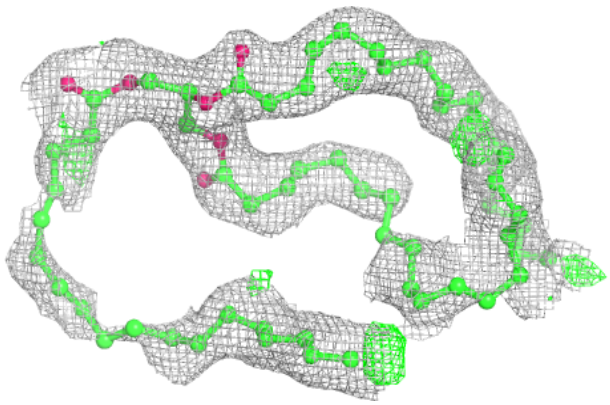


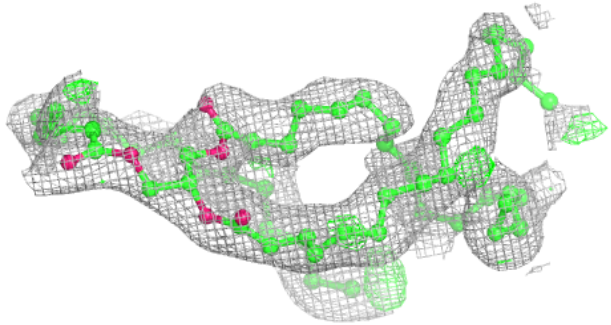


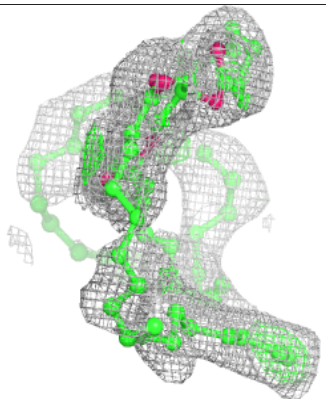


Electron density around TGL O 301:

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

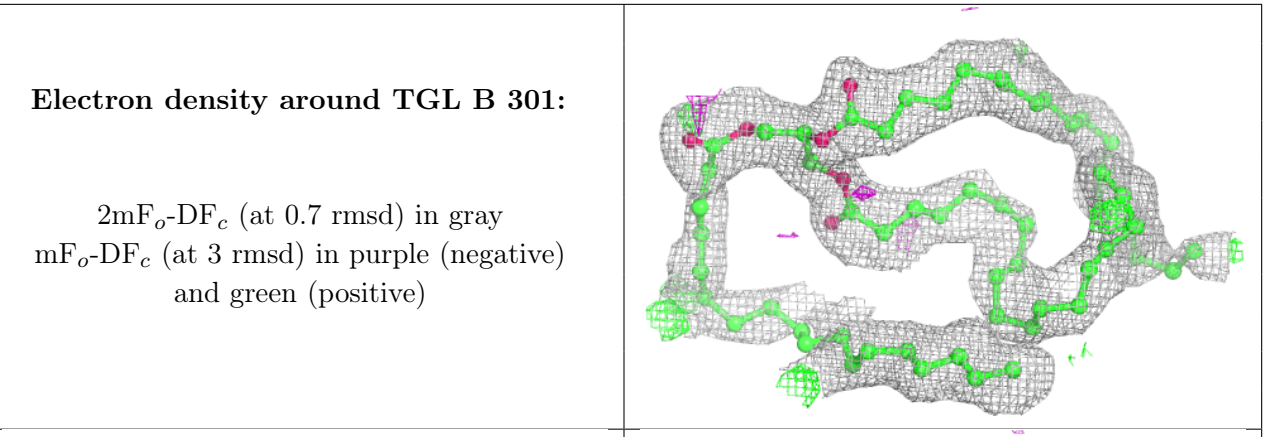






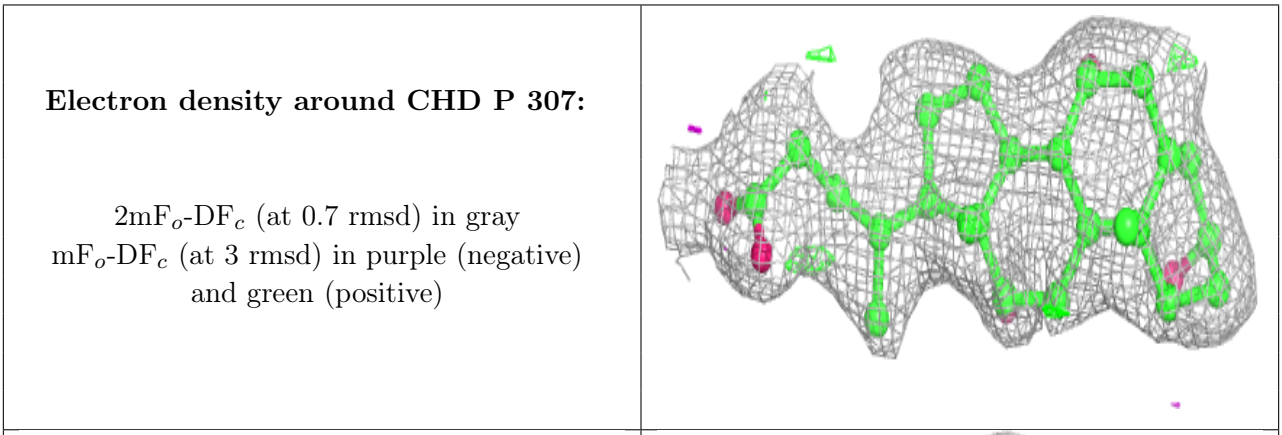
Electron density around TGL B 301:

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



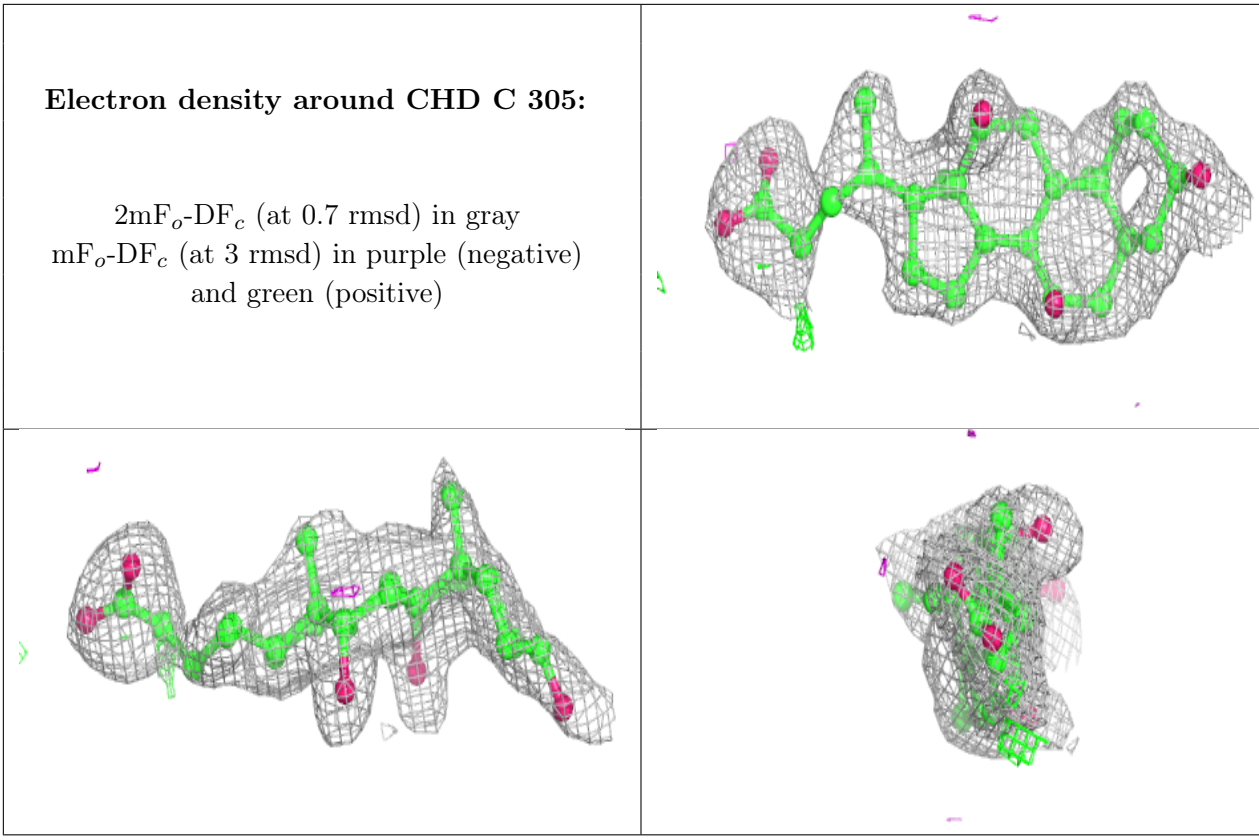
Electron density around CHD P 307:

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



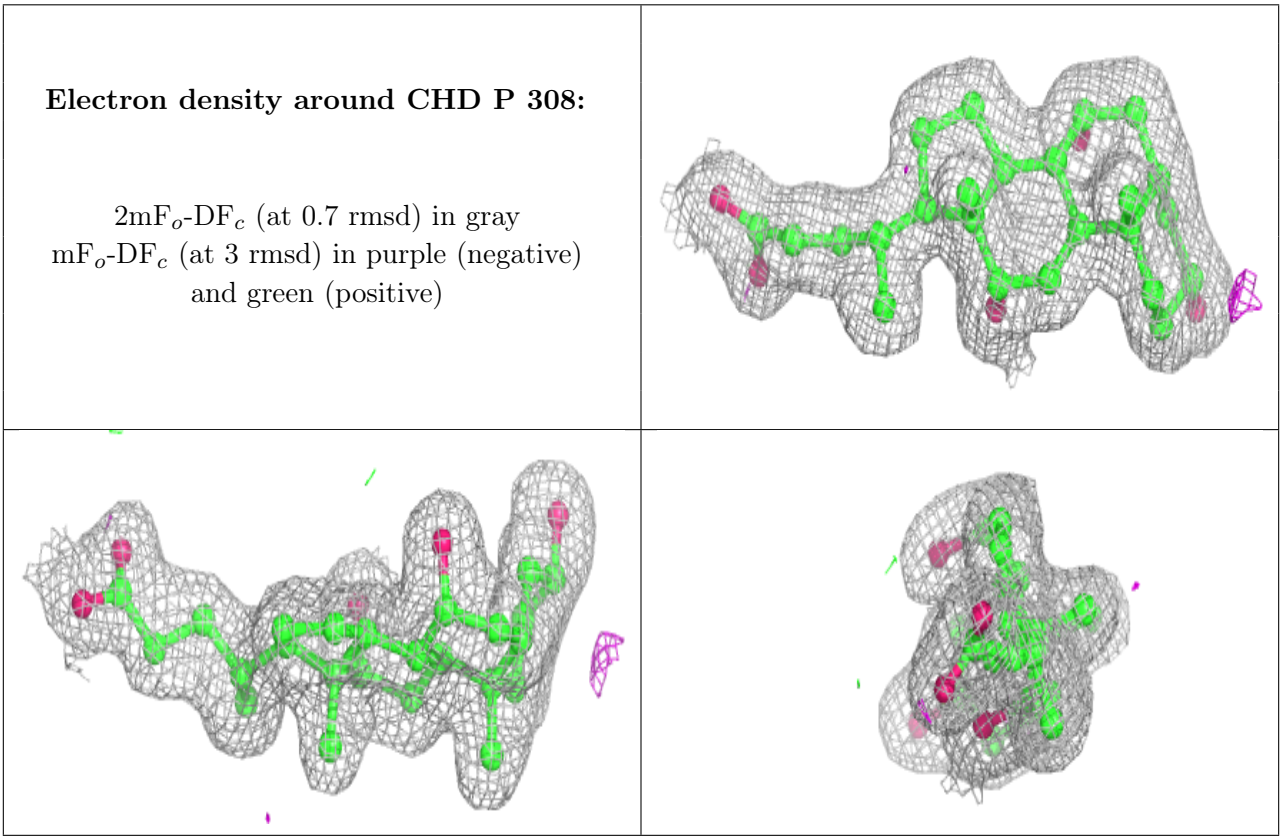
Electron density around CHD C 305:

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



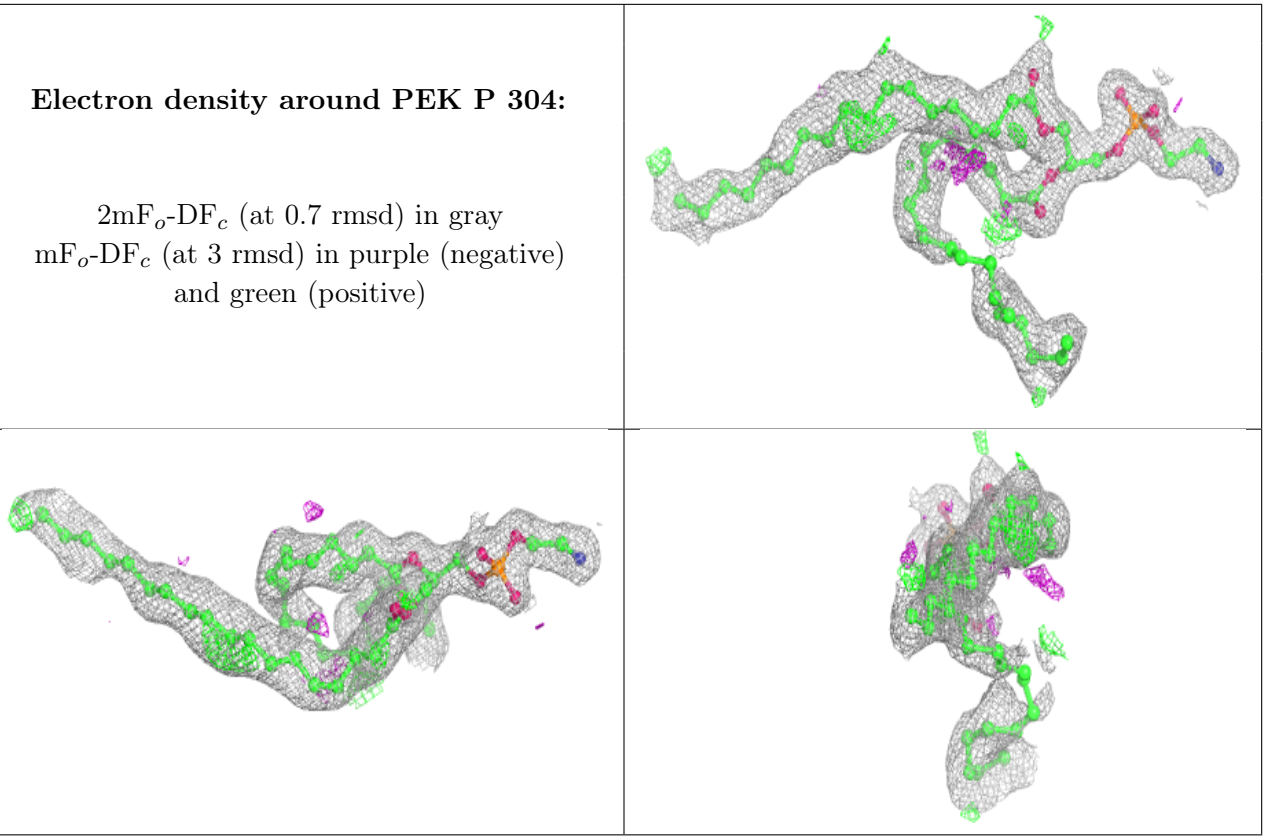
Electron density around CHD P 308:

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



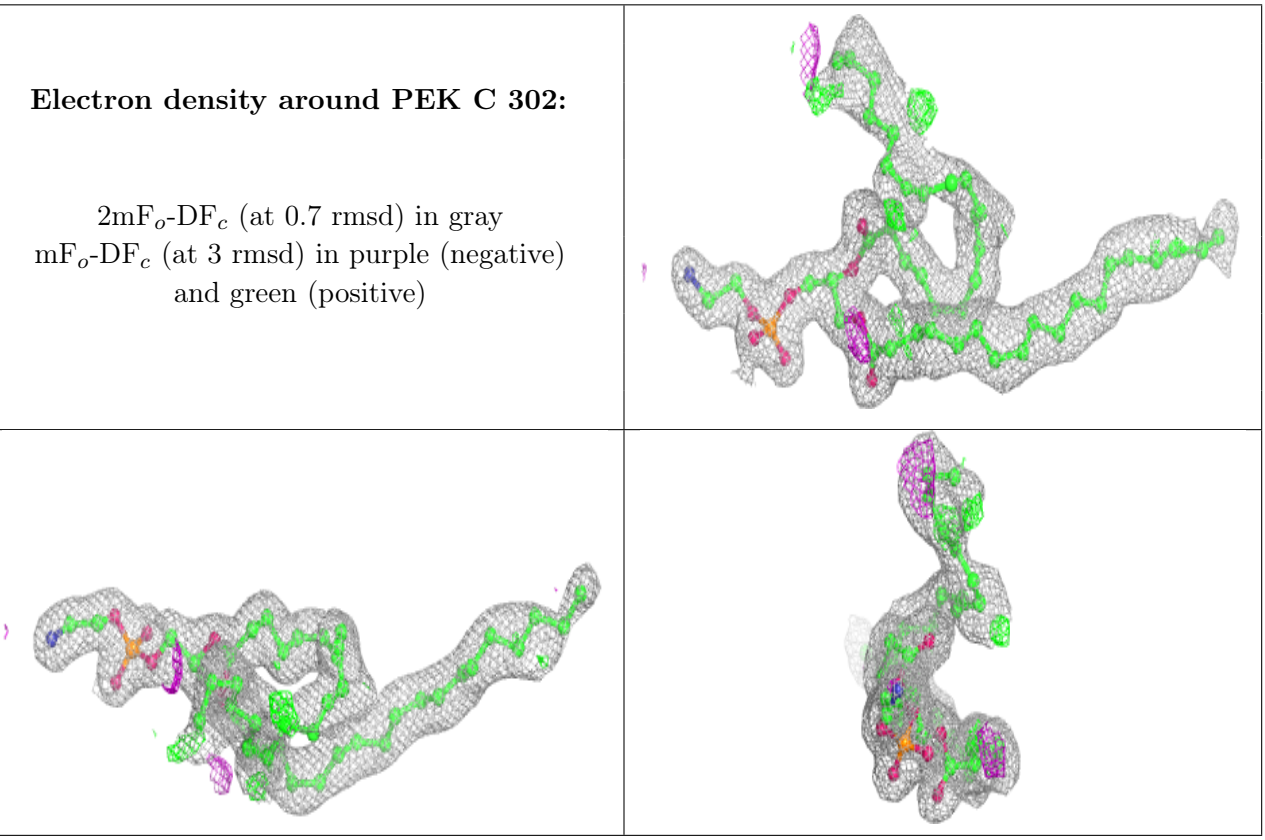
Electron density around PEK P 304:

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



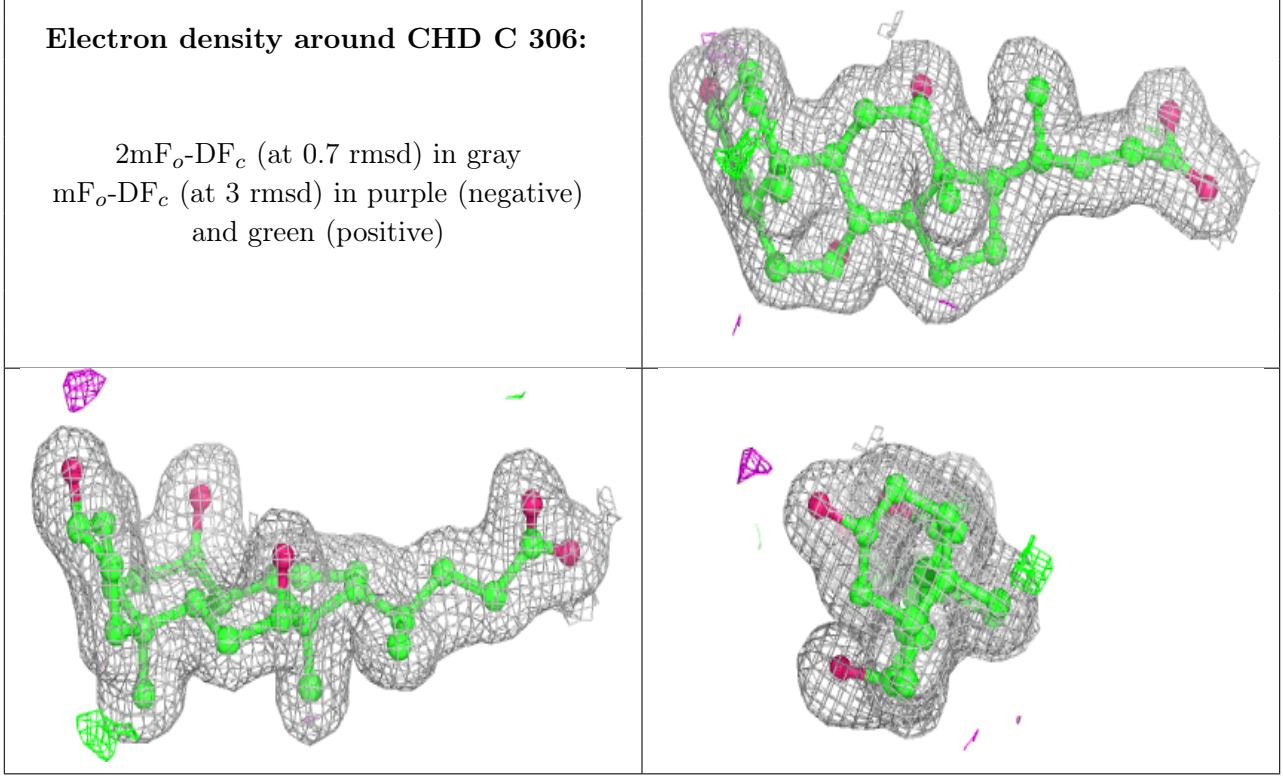
Electron density around PEK C 302:

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



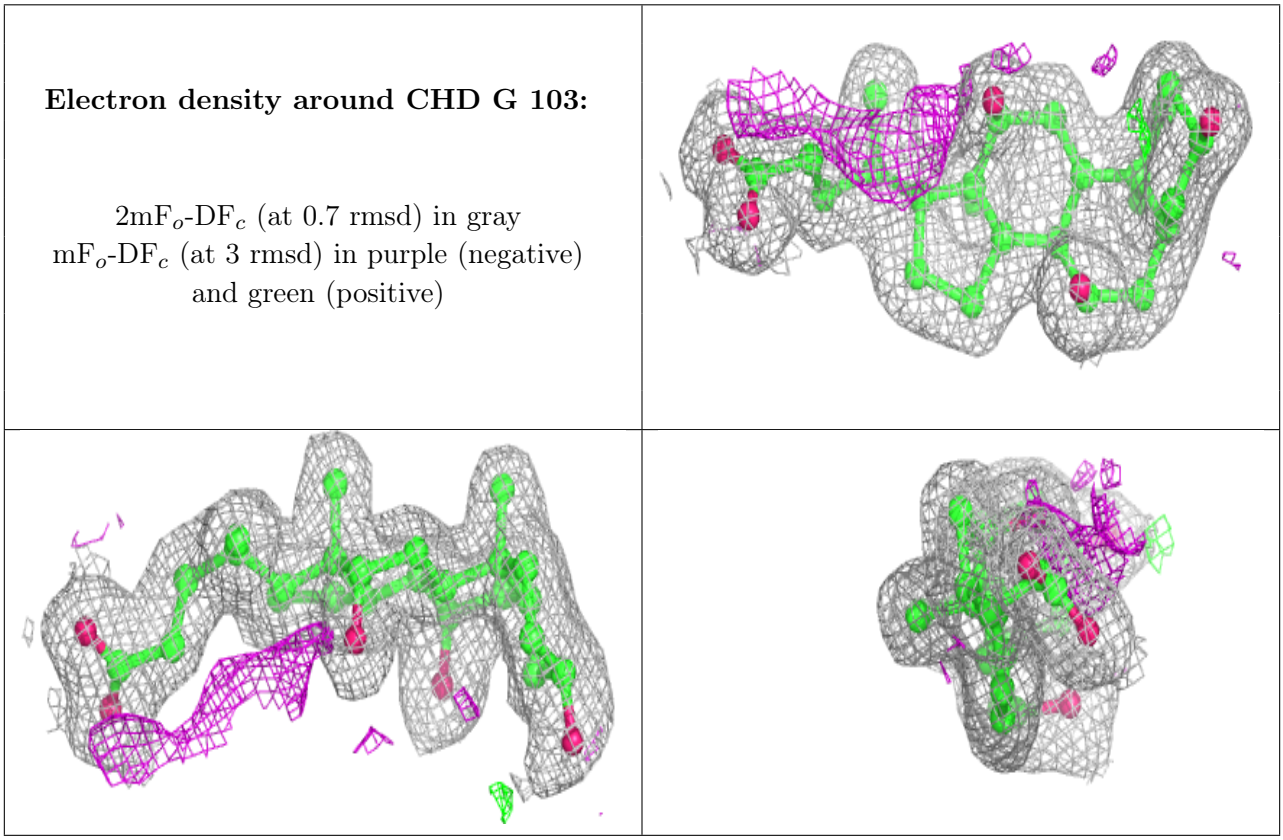
Electron density around CHD C 306:

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



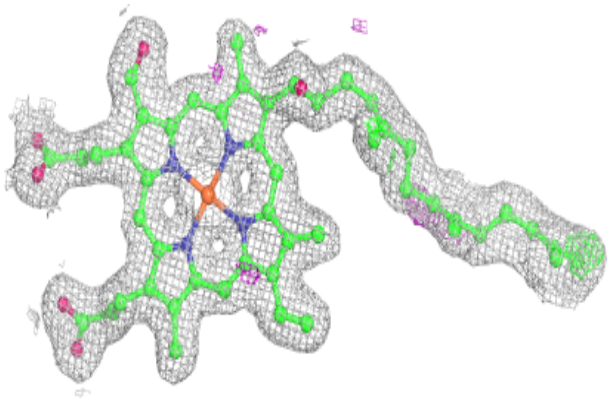
Electron density around CHD G 103:

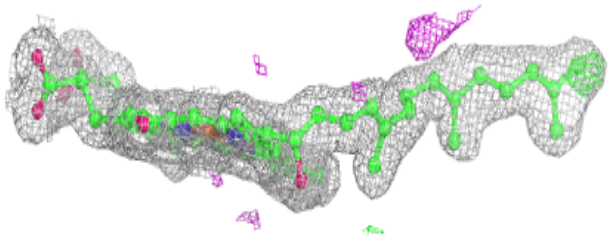
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

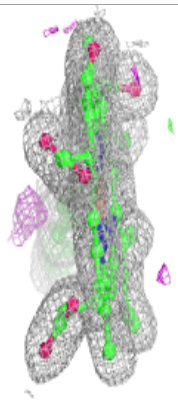


Electron density around HEA N 601 (A):

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

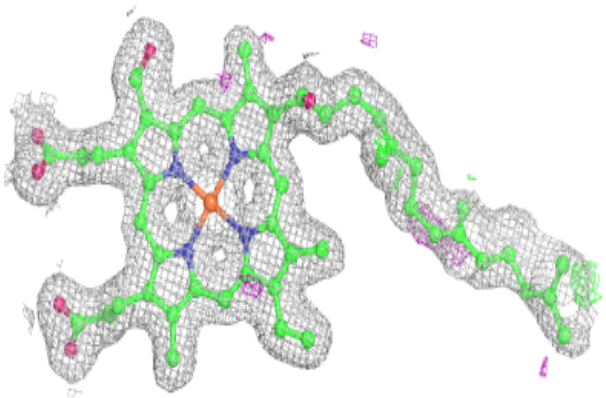


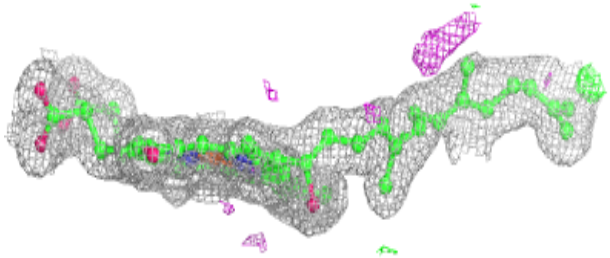


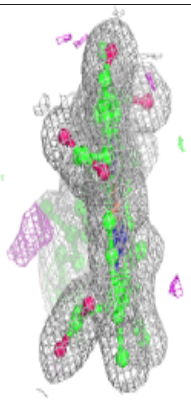


Electron density around HEA N 601 (B):

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

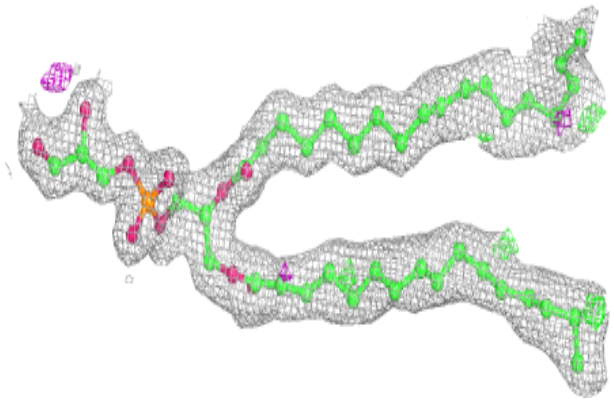


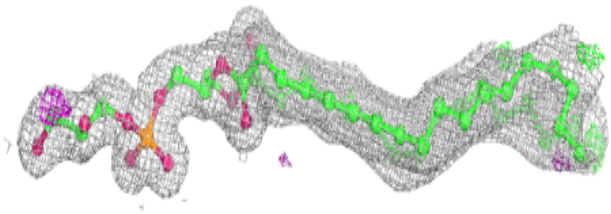


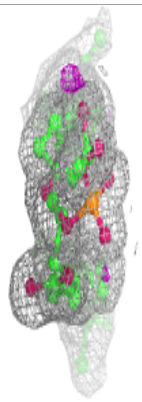


Electron density around PGV C 303:

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

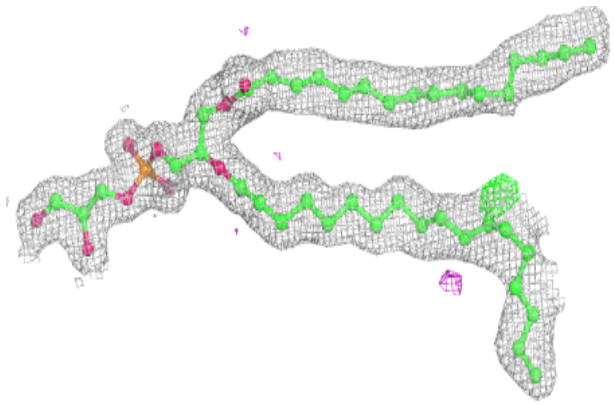


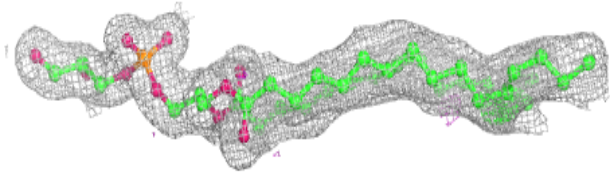


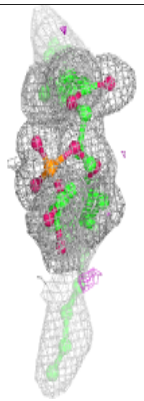


Electron density around PGV P 305:

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

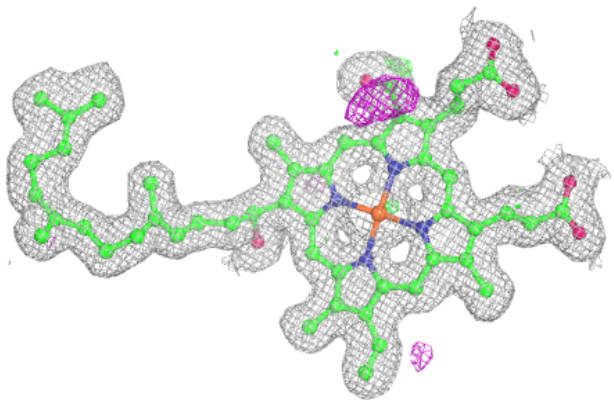


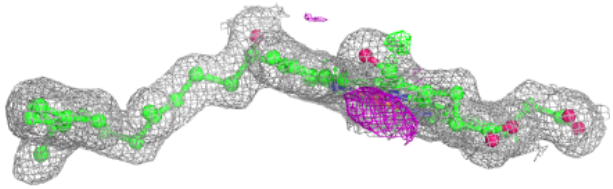


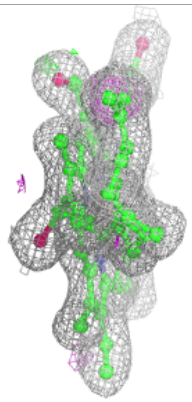


Electron density around HEA A 602:

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

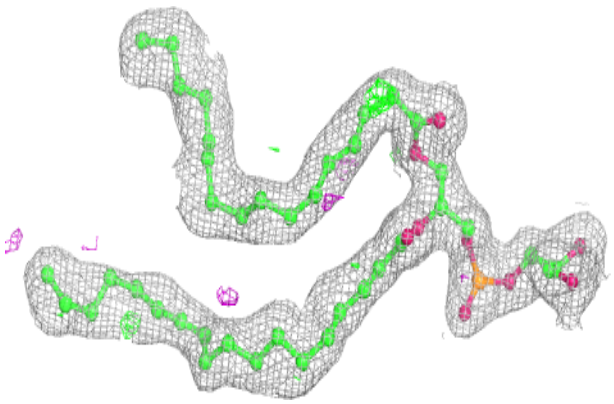


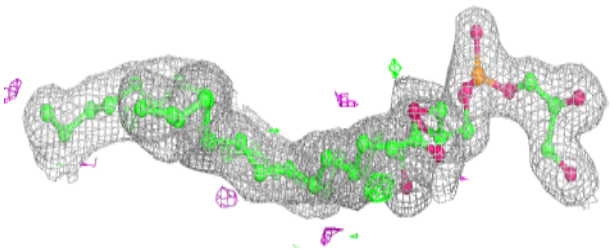


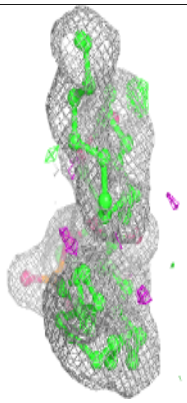


Electron density around PGV P 301:

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

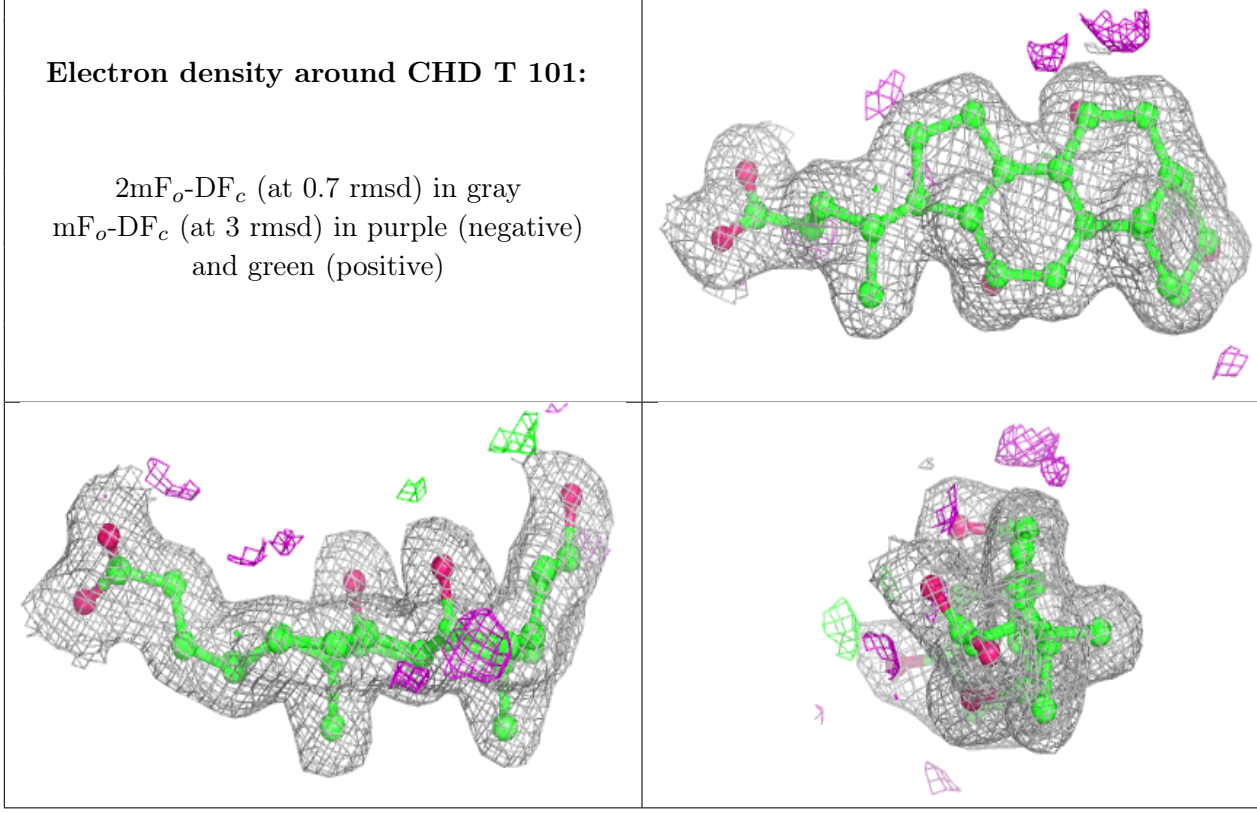






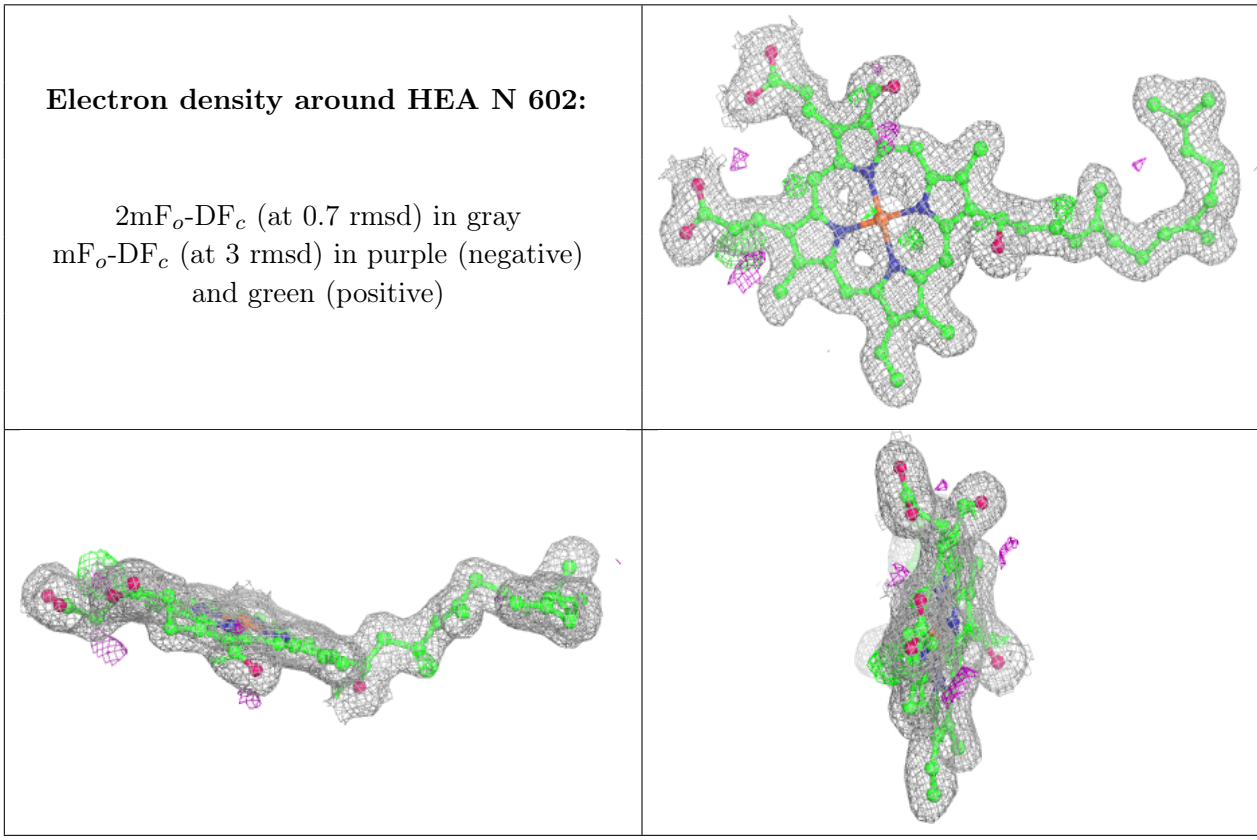
Electron density around CHD T 101:

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



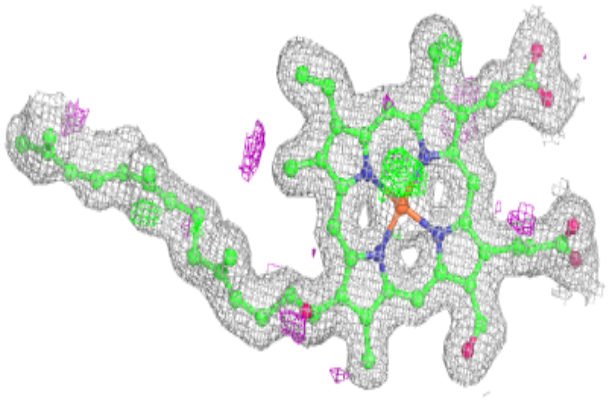
Electron density around HEA N 602:

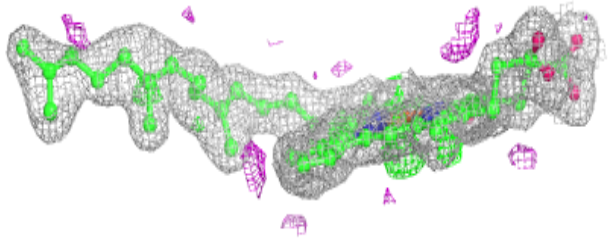
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

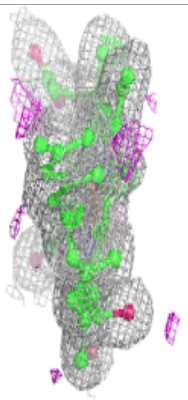


Electron density around HEA A 601 (A):

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

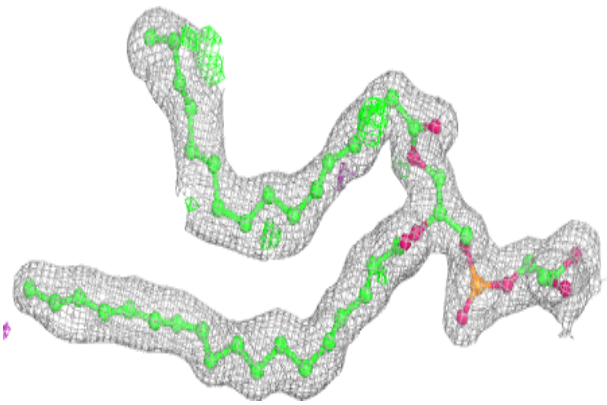


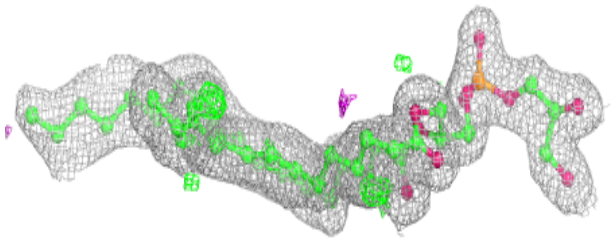


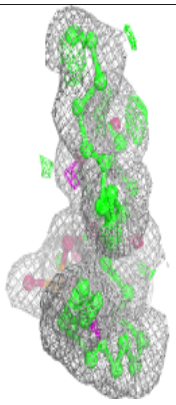


Electron density around PGV A 607:

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

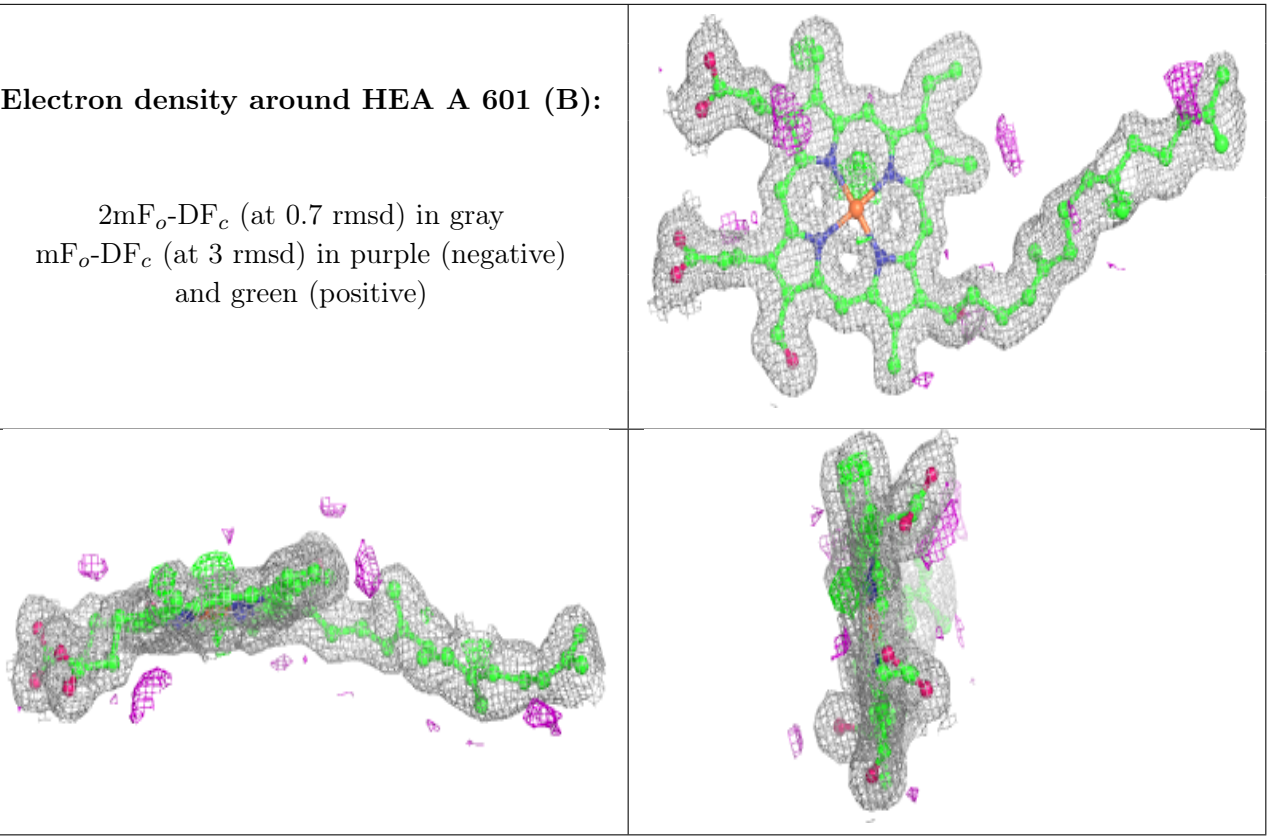






Electron density around HEA A 601 (B):

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



6.5 Other polymers (i)

There are no such residues in this entry.