wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 01:30 PM JST

PDB ID	:	7VUW
Title	:	Bovine heart cytochrome c oxidase in the cyanide-bound fully oxidized state at 50 K
Authors	:	Shimada, A.; Tsukihara, T.
Deposited on	:	2021-11-04
Resolution	:	1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

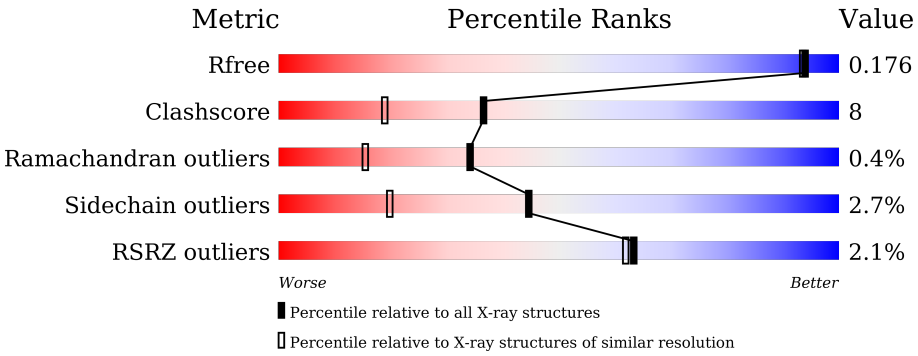
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	87% 12% •
1	N	514	89% 10% •
2	B	227	81% 17% •
2	O	227	% 81% 19%
3	C	259	94% 6%
3	P	259	86% 13% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	144	90% 9%
4	Q	144	88% 8%
5	E	105	90% 10%
5	R	105	95%
6	F	94	3% 87% 13%
6	S	94	4% 86% 13%
7	G	84	15% 77% 15% 7%
7	T	84	17% 77% 17% 5%
8	H	79	9% 84% 14%
8	U	79	8% 85% 13%
9	I	73	3% 89% 10%
9	V	73	4% 92% 8%
10	J	58	3% 86% 14%
10	W	58	7% 86% 14%
11	K	49	94% 6%
11	X	49	90% 10%
12	L	46	78% 20%
12	Y	46	76% 22%
13	M	43	7% 81% 14% 5%
13	Z	43	7% 79% 19%

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	609	-	-	X	-
20	EDO	A	623	-	-	X	-
20	EDO	A	626	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	627	-	-	X	-
20	EDO	A	633	-	-	X	-
20	EDO	B	312	-	-	X	-
20	EDO	B	321	-	-	X	-
20	EDO	C	325	-	-	X	-
20	EDO	D	202	-	-	X	-
20	EDO	D	209	-	-	X	-
20	EDO	D	214	-	-	-	X
20	EDO	L	110	-	-	X	-
20	EDO	O	314	-	-	X	-
20	EDO	Q	207	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 34951 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	35	0
			4152	2768	638	705	41			
1	N	513	Total	C	N	O	S	0	30	0
			4123	2751	632	701	39			

- 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	11	0
			1854	1202	283	349	20			
2	O	227	Total	C	N	O	S	0	12	0
			1857	1204	286	349	18			

- 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	9	0
			2138	1428	341	355	14			
3	P	259	Total	C	N	O	S	0	9	0
			2138	1428	341	355	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1207	786	199	218	4			
4	Q	138	Total	C	N	O	S	0	2	0
			1159	758	189	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total 854	C 546	N 144	O 162	S 2	0	1	0
5	R	105	Total 852	C 544	N 144	O 162	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total 718	C 445	N 127	O 140	S 6	0	1	0
6	S	94	Total 718	C 445	N 127	O 140	S 6	0	1	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0
7	T	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total 663	C 417	N 121	O 120	S 5	0	1	0
8	U	79	Total 663	C 417	N 121	O 120	S 5	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total 601	C 390	N 107	O 100	S 4	0	0	0
9	V	73	Total 613	C 398	N 109	O 102	S 4	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total 461	C 297	N 78	O 83	S 3	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			387	252	65	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			387	252	65	68	2			

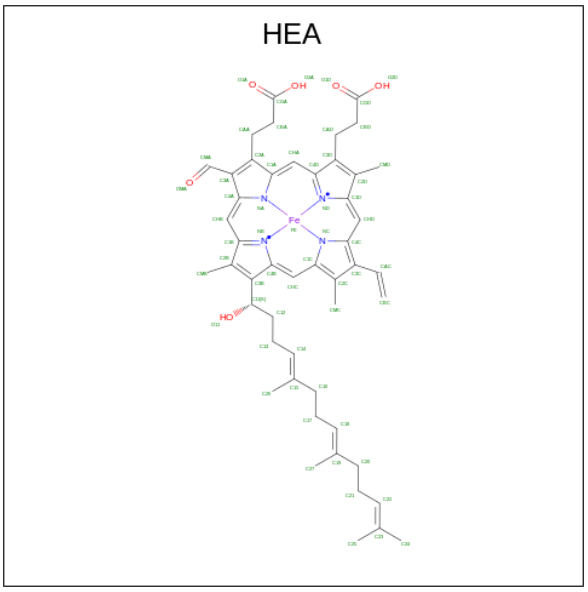
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			336	223	53	60			

- 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		

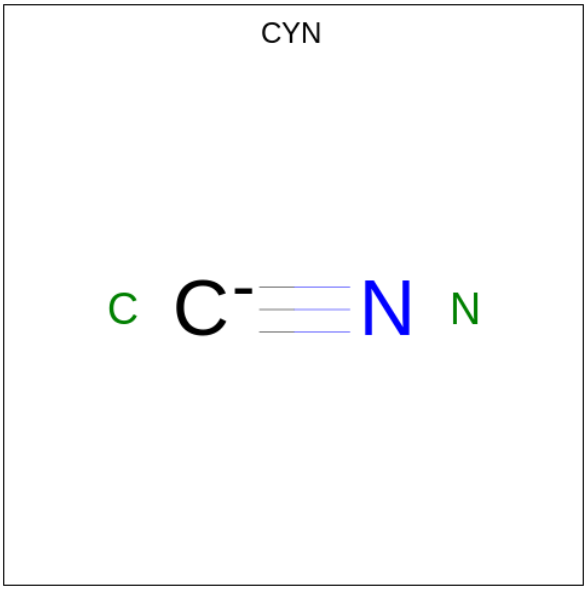
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

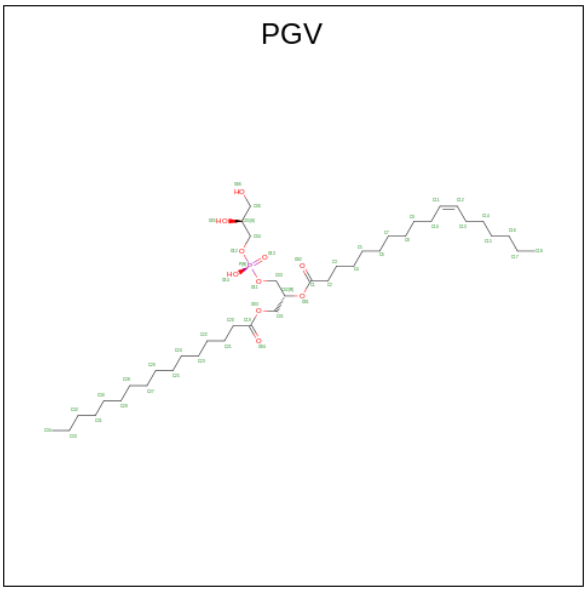
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is CYANIDE ION (three-letter code: CYN) (formula: CN).



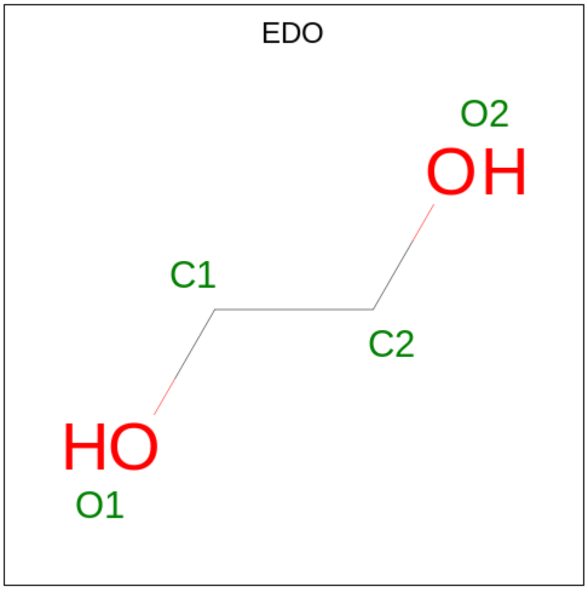
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C N 2 1 1	0	0
18	N	1	Total C N 2 1 1	0	0

- 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
			47	36	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			50	39	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			42	31	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		

- 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	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

Continued on next page...

Continued from previous page...

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	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	A	1	Total C O 3 1 2	0	1
20	B	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	B	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	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	B	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	B	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	B	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	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	C	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	C	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	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	C	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	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0
20	H	1	Total C O 4 2 2	0	0
20	H	1	Total C O 4 2 2	0	0
20	H	1	Total C O 4 2 2	0	0
20	H	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0
20	I	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	J	1	Total C O 4 2 2	0	0
20	J	1	Total C O 4 2 2	0	0
20	J	1	Total C O 4 2 2	0	0
20	K	1	Total C O 4 2 2	0	0
20	K	1	Total C O 4 2 2	0	0
20	K	1	Total C O 4 2 2	0	0
20	K	1	Total C O 4 2 2	0	0
20	K	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	L	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	L	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	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	M	1	Total C O 4 2 2	0	0
20	M	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	M	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	O	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	O	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	O	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	O	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	O	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

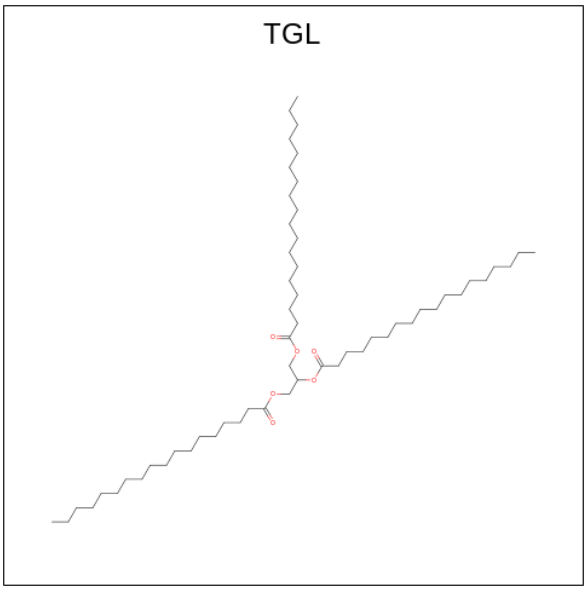
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

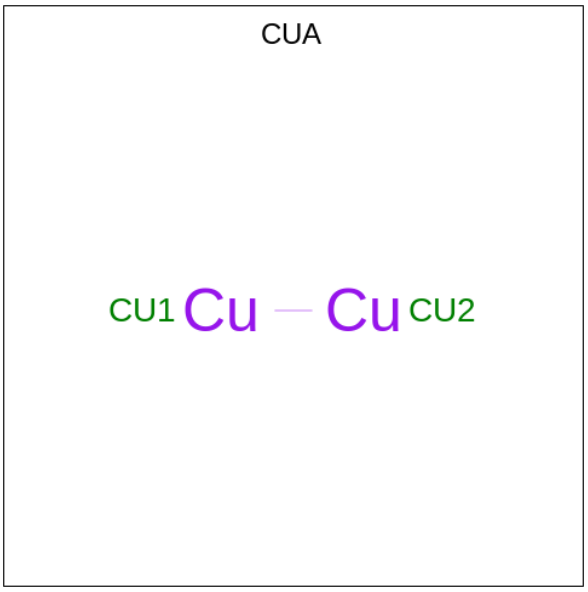
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	Y	1	Total C O 4 2 2	0	0
20	Y	1	Total C O 4 2 2	0	0
20	Y	1	Total C O 4 2 2	0	0
20	Z	1	Total C O 4 2 2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



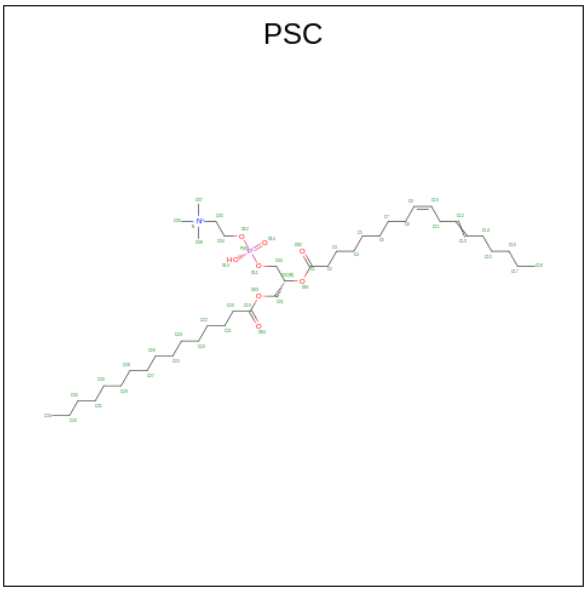
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C O 63 57 6	0	0
21	B	1	Total C O 62 56 6	0	0
21	L	1	Total C O 60 54 6	0	0
21	N	1	Total C O 63 57 6	0	0
21	Q	1	Total C O 63 57 6	0	0
21	Y	1	Total C O 60 54 6	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 23 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: $C_{42}H_{81}NO_8P$).



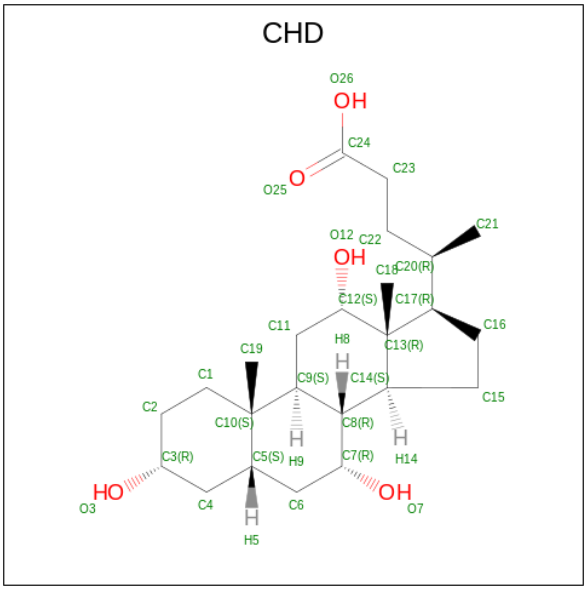
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C N O P 48 38 1 8 1	0	0

Continued on next page...

Continued from previous page...

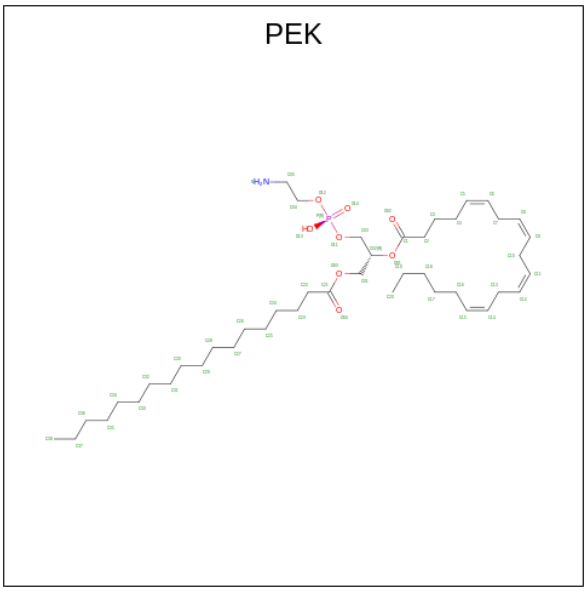
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	O	1	Total C O P 43 34 8 1	0	0

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



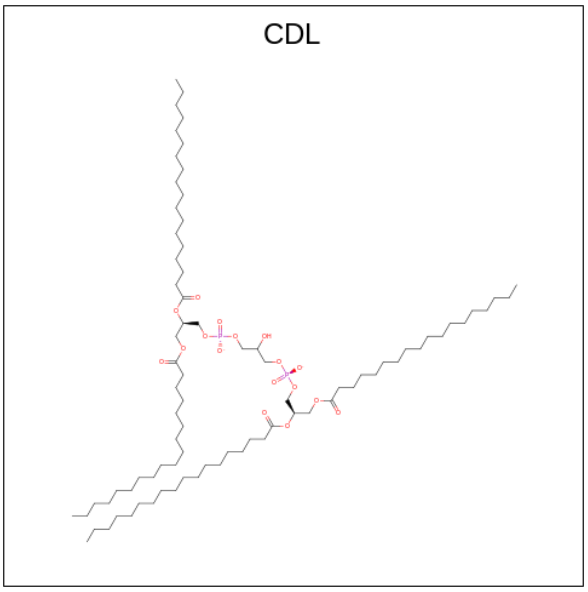
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	Y	1	Total C O 29 24 5	0	0

- 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: $C_{43}H_{78}NO_8P$).



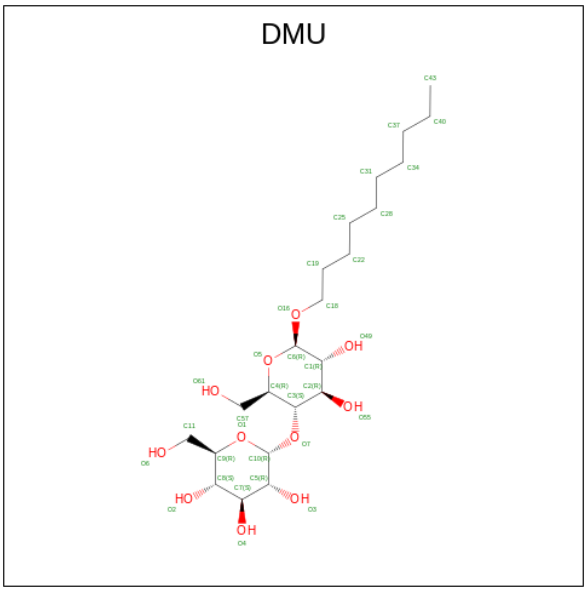
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			33	25	1	6	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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
			96	78	16	2		
26	G	1	Total	C	O	P	0	0
			90	74	14	2		
26	P	1	Total	C	O	P	0	0
			85	67	16	2		
26	T	1	Total	C	O	P	0	0
			92	75	15	2		

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

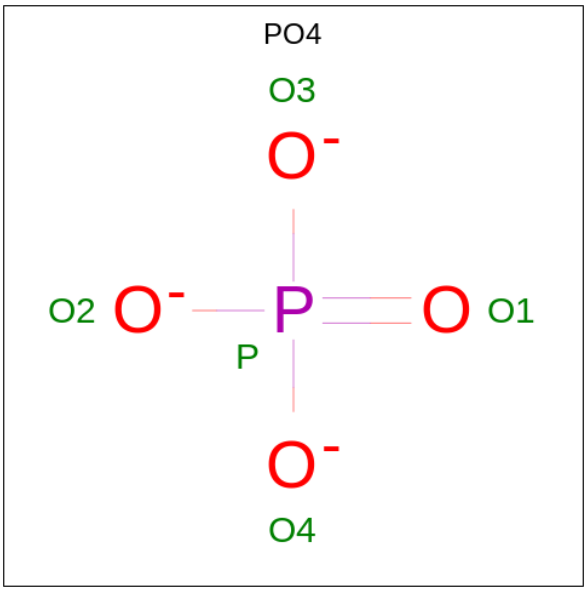


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 22 16 6	0	0
27	C	1	Total C O 33 22 11	0	0
27	J	1	Total C O 23 12 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	N	1	Total C O 17 15 2	0	0
27	O	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 21 16 5	0	0
27	X	1	Total C 10 10	0	0
27	X	1	Total C O 22 16 6	0	0
27	X	1	Total C O 33 22 11	0	0
27	X	1	Total C O 12 11 1	0	0
27	Z	1	Total C O 33 22 11	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
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	239	Total O 239 239	0	3
30	B	211	Total O 212 212	0	2
30	C	132	Total O 132 132	0	1
30	D	195	Total O 195 195	0	0
30	E	143	Total O 143 143	0	0
30	F	148	Total O 148 148	0	0
30	G	84	Total O 84 84	0	0
30	H	92	Total O 92 92	0	0
30	I	76	Total O 76 76	0	0
30	J	51	Total O 51 51	0	0

Continued on next page...

Continued from previous page...

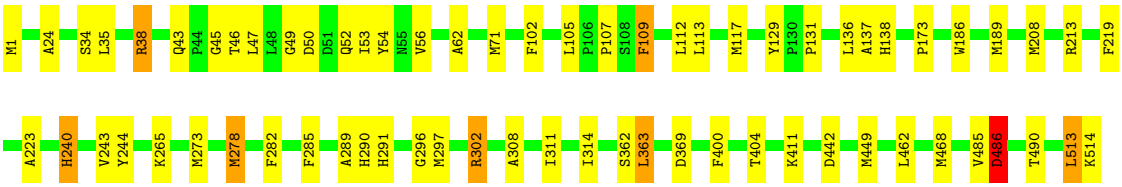
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	49	Total O 49 49	0	0
30	L	39	Total O 39 39	0	1
30	M	34	Total O 34 34	0	0
30	N	248	Total O 248 248	0	2
30	O	187	Total O 188 188	0	2
30	P	160	Total O 160 160	0	0
30	Q	118	Total O 118 118	0	0
30	R	105	Total O 105 105	0	0
30	S	136	Total O 136 136	0	0
30	T	68	Total O 68 68	0	0
30	U	82	Total O 82 82	0	0
30	V	64	Total O 64 64	0	0
30	W	43	Total O 43 43	0	0
30	X	41	Total O 41 41	0	0
30	Y	35	Total O 35 35	0	0
30	Z	23	Total O 23 23	0	0

3 Residue-property plots (i)

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

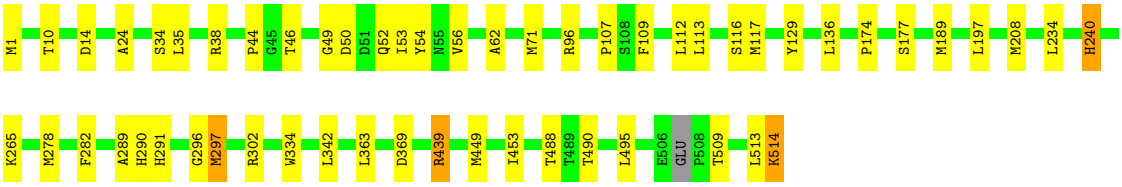
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



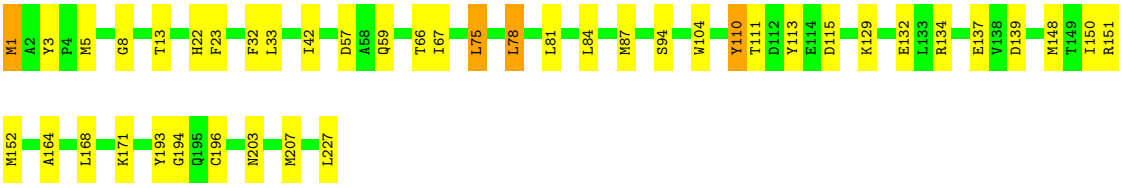
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



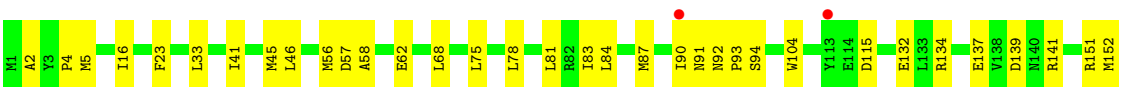
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



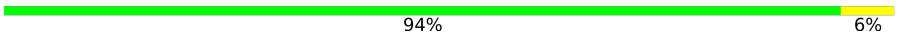
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



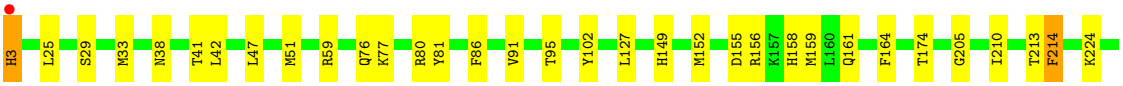
• Molecule 3: Cytochrome c oxidase subunit 3

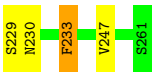
Chain C:



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:





• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:

• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

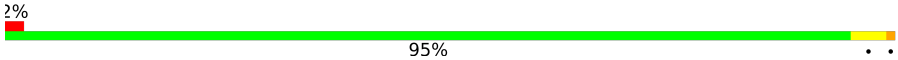
Chain Q:

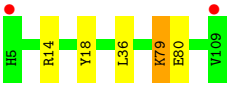
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:

• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

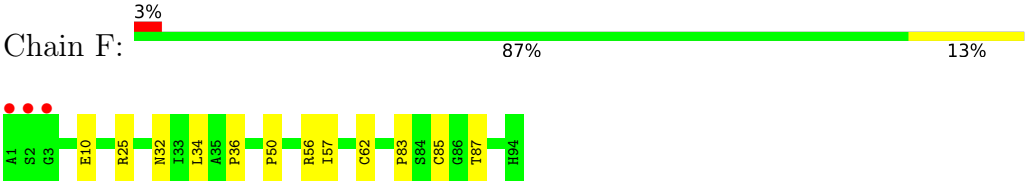
Chain R:





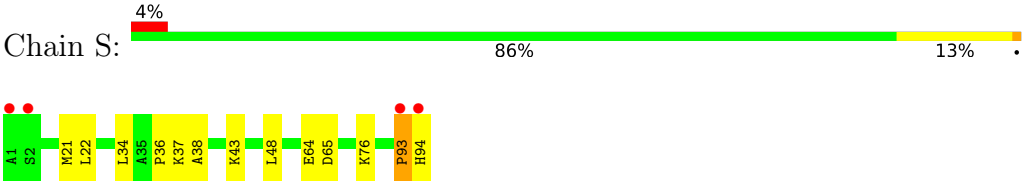
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



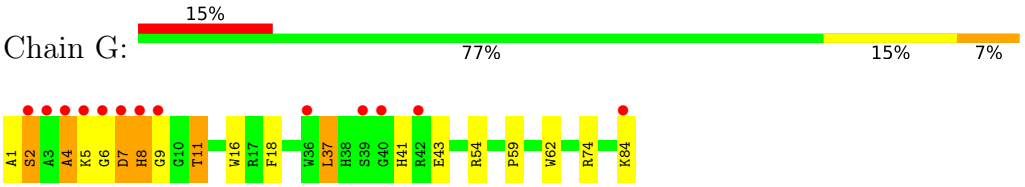
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



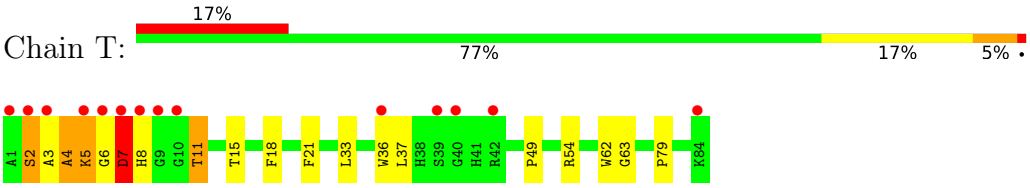
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



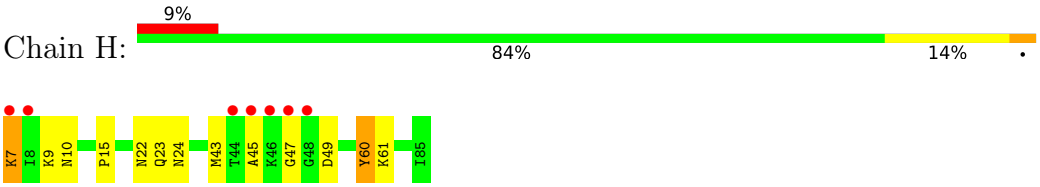
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



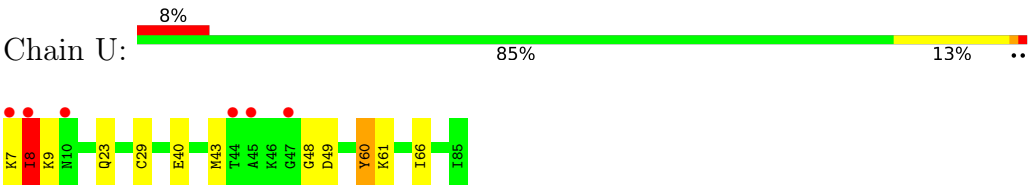
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



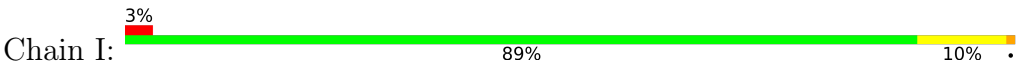
• Molecule 8: Cytochrome c oxidase subunit 6B1

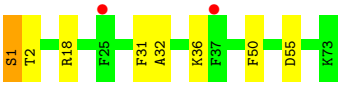
Chain U:



• Molecule 9: Cytochrome c oxidase subunit 6C

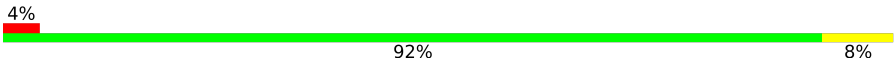
Chain I:

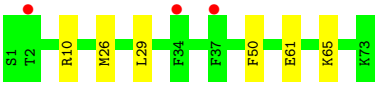




• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



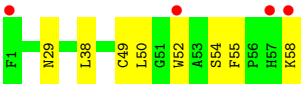


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:

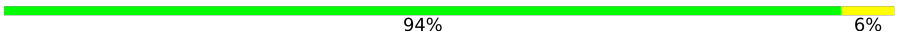
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

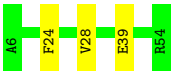
Chain W:



• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

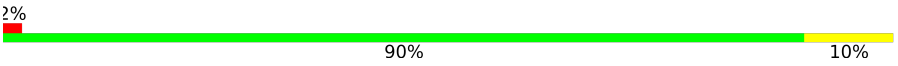
Chain K:

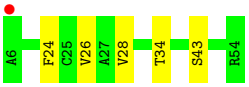




• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

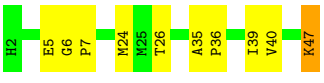
Chain X:





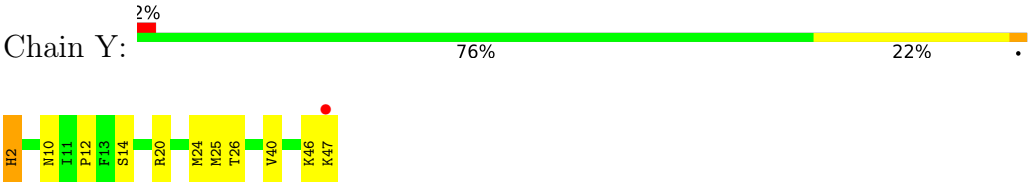
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



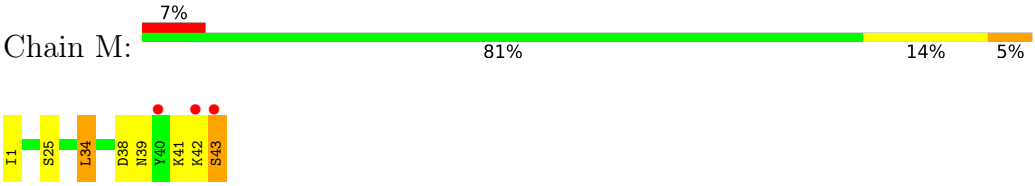
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



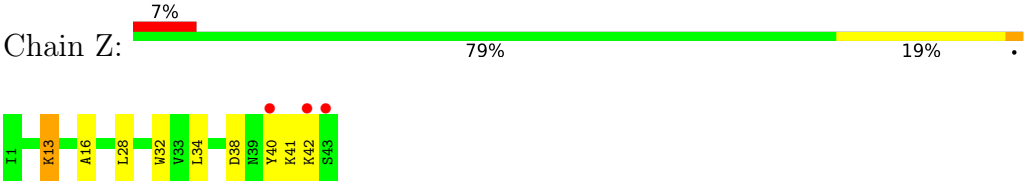
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	182.08Å 204.48Å 177.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 1.60 135.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.92-1.60) 99.7 (135.98-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.153 , 0.175 0.154 , 0.176	Depositor DCC
R_{free} test set	43213 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	34951	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.96	4/4426 (0.1%)	1.04	20/6039 (0.3%)
1	N	0.87	0/4373	0.92	7/5966 (0.1%)
2	B	0.85	1/1947 (0.1%)	1.03	5/2650 (0.2%)
2	O	0.76	0/1958	0.91	4/2665 (0.2%)
3	C	0.85	0/2278	0.83	1/3111 (0.0%)
3	P	0.82	0/2278	0.80	3/3111 (0.1%)
4	D	0.84	0/1259	0.88	3/1698 (0.2%)
4	Q	0.67	0/1204	0.75	2/1625 (0.1%)
5	E	0.79	0/878	0.87	1/1192 (0.1%)
5	R	0.64	0/871	0.73	1/1182 (0.1%)
6	F	0.83	0/740	0.84	0/1003
6	S	0.75	0/740	0.83	0/1003
7	G	0.80	0/691	0.86	0/937
7	T	0.69	0/691	0.86	1/937 (0.1%)
8	H	0.82	0/688	0.81	0/929
8	U	0.67	0/688	0.78	0/929
9	I	0.76	0/605	0.80	1/802 (0.1%)
9	V	0.62	0/622	0.79	1/825 (0.1%)
10	J	0.59	0/472	0.83	1/636 (0.2%)
10	W	0.54	0/472	0.71	0/636
11	K	0.74	0/406	0.76	0/556
11	X	0.57	0/406	0.66	0/556
12	L	0.94	0/401	0.80	0/536
12	Y	0.66	0/401	0.68	0/536
13	M	0.80	0/346	0.83	1/470 (0.2%)
13	Z	0.66	0/346	0.72	0/470
All	All	0.82	5/30187 (0.0%)	0.88	52/41000 (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	A	0	1
1	N	0	1
7	T	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362[A]	SER	CB-OG	-5.77	1.34	1.42
1	A	362[B]	SER	CB-OG	-5.77	1.34	1.42
1	A	34[A]	SER	CB-OG	-5.57	1.35	1.42
1	A	34[B]	SER	CB-OG	-5.57	1.35	1.42
2	B	110	TYR	CD2-CE2	5.03	1.46	1.39

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278[A]	MET	CG-SD-CE	-15.51	75.39	100.20
1	A	278[B]	MET	CG-SD-CE	-15.51	75.39	100.20
2	B	152[A]	MET	CG-SD-CE	-11.45	81.88	100.20
2	B	152[B]	MET	CG-SD-CE	-11.45	81.88	100.20
1	A	189[A]	MET	CG-SD-CE	-9.80	84.51	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
7	T	7	ASP	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	4152	0	4121	67	0
1	N	4123	0	4090	46	0
2	B	1854	0	1860	35	0
2	O	1857	0	1855	29	0
3	C	2138	0	2046	17	0
3	P	2138	0	2046	38	0
4	D	1207	0	1194	12	0
4	Q	1159	0	1146	9	0
5	E	854	0	850	8	0
5	R	852	0	845	3	0
6	F	718	0	698	11	0
6	S	718	0	698	14	0
7	G	676	0	644	10	0
7	T	676	0	643	12	0
8	H	663	0	624	9	0
8	U	663	0	624	10	0
9	I	601	0	613	7	0
9	V	613	0	627	3	0
10	J	461	0	459	6	0
10	W	461	0	459	7	0
11	K	387	0	371	2	0
11	X	387	0	371	5	0
12	L	382	0	381	14	0
12	Y	382	0	381	15	0
13	M	336	0	352	7	0
13	Z	336	0	352	4	0
14	A	129	0	88	3	0
14	N	129	0	88	3	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	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	98	0	141	2	0
19	C	101	0	147	9	0
19	N	93	0	128	4	0
19	P	102	0	152	11	0
20	A	115	0	168	44	0
20	B	76	0	114	16	0
20	C	64	0	96	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	84	0	126	18	0
20	E	52	0	78	5	0
20	F	32	0	48	5	0
20	G	12	0	18	3	0
20	H	16	0	24	6	0
20	I	24	0	36	4	0
20	J	12	0	18	1	0
20	K	20	0	30	0	0
20	L	40	0	60	7	0
20	M	20	0	30	3	0
20	N	100	0	150	16	0
20	O	64	0	96	16	0
20	P	68	0	102	8	0
20	Q	32	0	48	5	0
20	R	24	0	36	4	0
20	S	52	0	78	5	0
20	T	20	0	30	5	0
20	U	12	0	18	3	0
20	V	12	0	18	0	0
20	W	16	0	24	3	0
20	Y	24	0	36	0	0
20	Z	4	0	6	0	0
21	B	125	0	215	15	0
21	L	60	0	97	7	0
21	N	63	0	110	4	0
21	Q	63	0	110	9	0
21	Y	60	0	101	11	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	48	0	66	8	0
23	O	43	0	58	1	0
24	B	29	0	39	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	P	58	0	78	2	0
24	Y	29	0	39	2	0
25	C	155	0	220	11	0
25	P	138	0	189	9	0
26	C	96	0	150	6	0
26	G	90	0	138	8	0
26	P	85	0	122	11	0
26	T	92	0	141	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	55	0	73	5	0
27	J	23	0	21	2	0
27	M	33	0	42	0	0
27	N	17	0	22	0	0
27	O	33	0	42	0	0
27	P	66	0	84	9	0
27	T	21	0	27	3	0
27	X	77	0	113	4	0
27	Z	33	0	42	2	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	239	0	0	19	0
30	B	212	0	0	9	0
30	C	132	0	0	5	0
30	D	195	0	0	2	0
30	E	143	0	0	3	0
30	F	148	0	0	2	0
30	G	84	0	0	0	0
30	H	92	0	0	0	0
30	I	76	0	0	2	0
30	J	51	0	0	2	0
30	K	49	0	0	2	0
30	L	39	0	0	2	0
30	M	34	0	0	0	0
30	N	248	0	0	10	0
30	O	188	0	0	3	0
30	P	160	0	0	4	0
30	Q	118	0	0	4	0
30	R	105	0	0	0	0
30	S	136	0	0	10	0
30	T	68	0	0	3	0
30	U	82	0	0	4	0
30	V	64	0	0	3	0
30	W	43	0	0	0	0
30	X	41	0	0	0	0
30	Y	35	0	0	1	0
30	Z	23	0	0	1	0
All	All	34951	0	33038	511	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.

The worst 5 of 511 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)
20:A:609:EDO:H22	20:A:633:EDO:H22	1.41	1.01
12:L:6:GLY:H	20:L:110:EDO:H21	1.25	1.01
20:N:631:EDO:H11	20:S:105:EDO:H11	1.47	0.95
8:H:24:ASN:HD21	20:H:104:EDO:H12	1.40	0.87
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.57	0.86

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	547/514 (106%)	534 (98%)	13 (2%)	0	100	100
1	N	539/514 (105%)	523 (97%)	16 (3%)	0	100	100
2	B	236/227 (104%)	229 (97%)	7 (3%)	0	100	100
2	O	237/227 (104%)	230 (97%)	6 (2%)	1 (0%)	34	15
3	C	266/259 (103%)	260 (98%)	6 (2%)	0	100	100
3	P	266/259 (103%)	261 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
5	E	104/105 (99%)	104 (100%)	0	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	93/94 (99%)	92 (99%)	1 (1%)	0	100	100
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	81/84 (96%)	71 (88%)	5 (6%)	5 (6%)	1	0
7	T	81/84 (96%)	72 (89%)	4 (5%)	5 (6%)	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	78/79 (99%)	71 (91%)	5 (6%)	2 (3%)	5 0
8	U	78/79 (99%)	71 (91%)	6 (8%)	1 (1%)	12 2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
9	V	73/73 (100%)	72 (99%)	1 (1%)	0	100 100
10	J	56/58 (97%)	56 (100%)	0	0	100 100
10	W	56/58 (97%)	56 (100%)	0	0	100 100
11	K	48/49 (98%)	47 (98%)	1 (2%)	0	100 100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100 100
12	L	45/46 (98%)	42 (93%)	3 (7%)	0	100 100
12	Y	45/46 (98%)	43 (96%)	2 (4%)	0	100 100
13	M	41/43 (95%)	39 (95%)	2 (5%)	0	100 100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100 100
All	All	3609/3550 (102%)	3500 (97%)	95 (3%)	14 (0%)	34 15

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	T	3	ALA
7	T	4	ALA

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	460/426 (108%)	454 (99%)	6 (1%)	69 50
1	N	454/426 (107%)	448 (99%)	6 (1%)	69 50
2	B	221/210 (105%)	213 (96%)	8 (4%)	35 12
2	O	222/210 (106%)	213 (96%)	9 (4%)	30 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	233/224 (104%)	230 (99%)	3 (1%)	69 50
3	P	233/224 (104%)	229 (98%)	4 (2%)	60 38
4	D	131/128 (102%)	129 (98%)	2 (2%)	65 44
4	Q	124/128 (97%)	122 (98%)	2 (2%)	62 41
5	E	93/92 (101%)	91 (98%)	2 (2%)	52 27
5	R	92/92 (100%)	90 (98%)	2 (2%)	52 27
6	F	79/78 (101%)	78 (99%)	1 (1%)	69 50
6	S	79/78 (101%)	77 (98%)	2 (2%)	47 22
7	G	67/67 (100%)	59 (88%)	8 (12%)	5 0
7	T	67/67 (100%)	61 (91%)	6 (9%)	9 1
8	H	72/71 (101%)	70 (97%)	2 (3%)	43 18
8	U	72/71 (101%)	68 (94%)	4 (6%)	21 5
9	I	57/57 (100%)	55 (96%)	2 (4%)	36 13
9	V	59/57 (104%)	57 (97%)	2 (3%)	37 13
10	J	49/49 (100%)	48 (98%)	1 (2%)	55 31
10	W	49/49 (100%)	47 (96%)	2 (4%)	30 9
11	K	40/39 (103%)	40 (100%)	0	100 100
11	X	40/39 (103%)	40 (100%)	0	100 100
12	L	40/39 (103%)	39 (98%)	1 (2%)	47 22
12	Y	40/39 (103%)	38 (95%)	2 (5%)	24 6
13	M	37/37 (100%)	33 (89%)	4 (11%)	6 1
13	Z	37/37 (100%)	32 (86%)	5 (14%)	4 0
All	All	3147/3034 (104%)	3061 (97%)	86 (3%)	44 20

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	214	PHE
8	U	8	ILE
4	Q	20	ARG
7	T	2	SER
9	V	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	181	GLN
3	P	68	GLN
3	P	38	ASN
3	P	76	GLN
3	C	76	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.49	4 (50%)	7,9,11	2.06	3 (42%)
1	FME	N	1	1	8,9,10	0.48	0	7,9,11	1.65	2 (28%)
7	TPO	G	11	7	8,10,11	1.53	1 (12%)	10,14,16	1.05	1 (10%)
2	FME	O	1	2	8,9,10	0.84	0	7,9,11	1.27	0
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	10,14,16	1.11	1 (10%)
9	SAC	I	1	9	7,8,9	0.54	0	8,9,11	1.76	2 (25%)
1	FME	A	1	1	8,9,10	0.69	0	7,9,11	2.16	3 (42%)
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	1.35	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
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
9	SAC	I	1	9	-	6/7/8/10	-
1	FME	A	1	1	-	5/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	5.46	1.51	1.33
7	T	11	TPO	P-O1P	3.03	1.60	1.50
7	G	11	TPO	P-O1P	3.01	1.60	1.50
2	B	1	FME	CG-SD	-2.35	1.68	1.81
2	B	1	FME	O1-CN	-2.30	1.15	1.22

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	CA-N-CN	-4.04	116.60	122.82
7	T	11	TPO	CG2-CB-CA	3.04	119.16	113.16
9	I	1	SAC	CA-N-C1A	2.88	128.47	123.15
2	B	1	FME	CA-N-CN	-2.81	118.50	122.82
1	A	1	FME	O1-CN-N	-2.69	118.19	125.27

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	CB-CA-N-CN
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
7	T	11	TPO	1	0
9	I	1	SAC	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 316 ligands modelled in this entry, 8 are monoatomic - leaving 308 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	EDO	A	619	-	3,3,3	0.71	0	2,2,2	0.72	0
19	PGV	A	608	-	50,50,50	0.89	2 (4%)	53,56,56	1.12	3 (5%)
20	EDO	D	221	-	3,3,3	0.75	0	2,2,2	0.48	0
27	DMU	O	303	-	34,34,34	1.07	2 (5%)	45,45,45	1.57	10 (22%)
19	PGV	A	607	-	46,46,50	1.26	5 (10%)	49,52,56	2.11	13 (26%)
20	EDO	N	618	-	3,3,3	0.86	0	2,2,2	1.00	0
20	EDO	E	204	-	3,3,3	0.30	0	2,2,2	0.92	0
20	EDO	B	318	-	3,3,3	0.51	0	2,2,2	0.05	0
20	EDO	H	101	-	3,3,3	0.49	0	2,2,2	0.70	0
27	DMU	P	310	-	34,34,34	0.93	1 (2%)	45,45,45	1.33	5 (11%)
20	EDO	A	623	-	3,3,3	0.64	0	2,2,2	0.35	0
20	EDO	N	615	-	3,3,3	0.60	0	2,2,2	0.81	0
27	DMU	X	103	-	34,34,34	0.98	1 (2%)	45,45,45	1.93	16 (35%)
20	EDO	K	103	-	3,3,3	0.60	0	2,2,2	0.14	0
20	EDO	A	632	-	3,3,3	1.00	0	2,2,2	0.29	0
20	EDO	E	213	-	3,3,3	0.35	0	2,2,2	0.65	0
24	CHD	C	301	-	32,32,32	1.03	3 (9%)	51,51,51	1.46	9 (17%)
20	EDO	L	103	-	3,3,3	0.71	0	2,2,2	0.47	0
20	EDO	C	320	-	3,3,3	0.62	0	2,2,2	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	T	106	-	3,3,3	0.63	0	2,2,2	0.40	0
14	HEA	A	601[A]	-	57,67,67	1.55	12 (21%)	61,103,103	1.82	19 (31%)
20	EDO	F	105	-	3,3,3	0.57	0	2,2,2	0.31	0
20	EDO	D	201	-	3,3,3	0.49	0	2,2,2	0.41	0
27	DMU	M	101	-	34,34,34	0.67	1 (2%)	45,45,45	1.11	3 (6%)
20	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.33	0
20	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.16	0
20	EDO	W	102	-	3,3,3	0.33	0	2,2,2	0.36	0
20	EDO	A	637[A]	-	1,1,3	0.38	0	-		
20	EDO	C	314	-	3,3,3	0.52	0	2,2,2	0.11	0
20	EDO	D	212	-	3,3,3	0.68	0	2,2,2	0.97	0
20	EDO	B	306	-	3,3,3	0.59	0	2,2,2	0.20	0
20	EDO	Y	108	-	3,3,3	0.38	0	2,2,2	0.34	0
20	EDO	R	202	-	3,3,3	0.47	0	2,2,2	0.52	0
20	EDO	C	324	-	3,3,3	0.94	0	2,2,2	0.31	0
20	EDO	T	107	-	3,3,3	0.67	0	2,2,2	0.31	0
24	CHD	C	308	-	32,32,32	0.92	1 (3%)	51,51,51	2.53	22 (43%)
20	EDO	U	102	-	3,3,3	0.85	0	2,2,2	0.35	0
20	EDO	D	202	-	3,3,3	0.22	0	2,2,2	0.93	0
20	EDO	G	104	-	3,3,3	0.59	0	2,2,2	0.14	0
20	EDO	D	219	-	3,3,3	0.67	0	2,2,2	0.34	0
20	EDO	I	102	-	3,3,3	0.66	0	2,2,2	0.52	0
24	CHD	Y	102	-	32,32,32	0.85	2 (6%)	51,51,51	2.80	22 (43%)
20	EDO	C	311	-	3,3,3	1.00	0	2,2,2	0.13	0
24	CHD	P	301	-	32,32,32	0.94	1 (3%)	51,51,51	1.41	10 (19%)
20	EDO	C	322	-	3,3,3	0.72	0	2,2,2	0.15	0
20	EDO	B	315	-	3,3,3	0.50	0	2,2,2	0.29	0
20	EDO	P	311	-	3,3,3	0.26	0	2,2,2	1.42	0
20	EDO	I	103	-	3,3,3	0.67	0	2,2,2	0.63	0
20	EDO	K	101	-	3,3,3	0.76	0	2,2,2	0.16	0
20	EDO	B	312	-	3,3,3	0.63	0	2,2,2	0.18	0
20	EDO	O	306	-	3,3,3	0.57	0	2,2,2	0.25	0
25	PEK	C	303	-	52,52,52	0.67	1 (1%)	55,57,57	1.23	5 (9%)
20	EDO	Q	206	-	3,3,3	0.55	0	2,2,2	0.40	0
20	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.82	0
20	EDO	M	105	-	3,3,3	0.45	0	2,2,2	0.36	0
29	PO4	H	105	-	4,4,4	0.83	0	6,6,6	1.17	0
20	EDO	P	322	-	3,3,3	0.46	0	2,2,2	0.69	0
20	EDO	P	312	-	3,3,3	0.48	0	2,2,2	0.22	0
20	EDO	P	314	-	3,3,3	0.54	0	2,2,2	0.30	0
21	TGL	Y	101	-	59,59,62	1.29	3 (5%)	62,62,65	1.77	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	D	203	-	3,3,3	0.62	0	2,2,2	1.06	0
20	EDO	V	103	-	3,3,3	0.54	0	2,2,2	0.13	0
20	EDO	B	314	-	3,3,3	0.47	0	2,2,2	1.11	0
20	EDO	W	104	-	3,3,3	0.41	0	2,2,2	0.39	0
20	EDO	O	314	-	3,3,3	0.78	0	2,2,2	0.77	0
20	EDO	A	635	-	3,3,3	0.37	0	2,2,2	0.52	0
20	EDO	S	104	-	3,3,3	0.68	0	2,2,2	0.36	0
27	DMU	C	309	-	22,22,34	0.90	1 (4%)	27,27,45	1.66	6 (22%)
20	EDO	D	205	-	3,3,3	0.46	0	2,2,2	1.11	0
20	EDO	A	610	-	3,3,3	0.26	0	2,2,2	1.18	0
20	EDO	P	320	-	3,3,3	0.35	0	2,2,2	0.66	0
20	EDO	C	318	-	3,3,3	0.44	0	2,2,2	0.12	0
23	PSC	B	304	-	47,47,51	1.20	4 (8%)	50,52,59	1.55	6 (12%)
20	EDO	I	106	-	3,3,3	0.42	0	2,2,2	0.67	0
18	CYN	A	606	15	0,1,1	-	-	-		
20	EDO	V	102	-	3,3,3	0.50	0	2,2,2	0.32	0
21	TGL	B	302	-	61,61,62	1.16	3 (4%)	64,64,65	1.59	7 (10%)
22	CUA	O	301	2	0,1,1	-	-	-		
27	DMU	P	309	-	34,34,34	0.73	0	45,45,45	2.19	16 (35%)
20	EDO	N	633	-	3,3,3	1.07	0	2,2,2	0.20	0
20	EDO	R	204	-	3,3,3	0.69	0	2,2,2	0.72	0
20	EDO	D	220	-	3,3,3	0.51	0	2,2,2	0.18	0
20	EDO	Q	204	-	3,3,3	0.43	0	2,2,2	0.49	0
20	EDO	N	635	-	3,3,3	0.49	0	2,2,2	0.30	0
20	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.37	0
25	PEK	P	302	-	32,32,52	1.03	1 (3%)	34,36,57	1.38	4 (11%)
20	EDO	P	317	-	3,3,3	0.52	0	2,2,2	0.24	0
14	HEA	N	601[B]	-	57,67,67	1.33	10 (17%)	61,103,103	1.74	18 (29%)
20	EDO	S	110	-	3,3,3	0.43	0	2,2,2	0.74	0
20	EDO	K	104	-	3,3,3	0.42	0	2,2,2	0.60	0
20	EDO	F	103	-	3,3,3	0.91	0	2,2,2	0.32	0
20	EDO	K	105	-	3,3,3	0.46	0	2,2,2	0.76	0
27	DMU	N	610	-	17,17,34	0.77	0	17,18,45	1.26	3 (17%)
20	EDO	B	324	-	3,3,3	0.54	0	2,2,2	0.81	0
20	EDO	B	320	-	3,3,3	0.56	0	2,2,2	0.29	0
24	CHD	P	308	-	32,32,32	0.78	0	51,51,51	2.04	16 (31%)
20	EDO	S	111	-	3,3,3	0.62	0	2,2,2	0.28	0
18	CYN	N	606	15	0,1,1	-	-	-		
20	EDO	S	109	-	3,3,3	0.54	0	2,2,2	0.60	0
20	EDO	D	206	-	3,3,3	0.49	0	2,2,2	0.76	0
20	EDO	N	611	-	3,3,3	1.06	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	N	631	-	3,3,3	0.50	0	2,2,2	0.74	0
20	EDO	O	308	-	3,3,3	0.75	0	2,2,2	0.34	0
20	EDO	B	319	-	3,3,3	0.54	0	2,2,2	0.08	0
20	EDO	S	102	-	3,3,3	0.97	0	2,2,2	0.66	0
20	EDO	S	105	-	3,3,3	0.34	0	2,2,2	0.65	0
14	HEA	N	602	1	57,67,67	1.35	8 (14%)	61,103,103	1.80	18 (29%)
20	EDO	N	632	-	3,3,3	0.59	0	2,2,2	0.77	0
26	CDL	T	101	-	89,91,99	1.46	11 (12%)	94,100,111	1.92	23 (24%)
20	EDO	E	210	-	3,3,3	0.58	0	2,2,2	1.60	1 (50%)
20	EDO	M	106	-	3,3,3	0.91	0	2,2,2	0.92	0
20	EDO	C	313	-	3,3,3	0.54	0	2,2,2	0.17	0
20	EDO	A	613	-	3,3,3	1.32	0	2,2,2	0.97	0
20	EDO	I	101	-	3,3,3	0.56	0	2,2,2	0.83	0
20	EDO	Z	102	-	3,3,3	0.38	0	2,2,2	0.79	0
20	EDO	B	307	-	3,3,3	1.11	0	2,2,2	0.16	0
20	EDO	S	112	-	3,3,3	0.53	0	2,2,2	0.60	0
19	PGV	C	306	-	50,50,50	1.23	3 (6%)	53,56,56	1.44	7 (13%)
20	EDO	S	106	-	3,3,3	0.69	0	2,2,2	0.82	0
20	EDO	D	208	-	3,3,3	0.48	0	2,2,2	0.44	0
20	EDO	J	104	-	3,3,3	0.32	0	2,2,2	0.75	0
20	EDO	P	315	-	3,3,3	0.57	0	2,2,2	0.50	0
20	EDO	B	322	-	3,3,3	0.85	0	2,2,2	0.66	0
20	EDO	A	630	-	3,3,3	0.68	0	2,2,2	0.41	0
20	EDO	F	107	-	3,3,3	0.51	0	2,2,2	0.40	0
20	EDO	P	325	-	3,3,3	0.68	0	2,2,2	0.27	0
20	EDO	T	105	-	3,3,3	0.55	0	2,2,2	0.06	0
20	EDO	E	209	-	3,3,3	0.78	0	2,2,2	0.16	0
27	DMU	T	102	-	21,21,34	0.85	2 (9%)	25,25,45	1.08	0
20	EDO	C	319	-	3,3,3	0.42	0	2,2,2	0.43	0
19	PGV	C	305	-	49,49,50	0.75	1 (2%)	52,55,56	0.87	1 (1%)
20	EDO	J	103	-	3,3,3	0.88	0	2,2,2	0.21	0
21	TGL	B	301	-	62,62,62	1.15	3 (4%)	65,65,65	1.57	7 (10%)
19	PGV	P	306	-	50,50,50	1.12	2 (4%)	53,56,56	1.45	10 (18%)
20	EDO	O	318	-	3,3,3	0.83	0	2,2,2	0.37	0
25	PEK	P	304	-	51,51,52	1.15	2 (3%)	54,56,57	1.57	6 (11%)
20	EDO	B	323	-	3,3,3	0.50	0	2,2,2	0.65	0
20	EDO	A	631	-	3,3,3	0.64	0	2,2,2	0.30	0
20	EDO	H	102	-	3,3,3	0.44	0	2,2,2	0.04	0
20	EDO	Q	205	-	3,3,3	0.40	0	2,2,2	0.44	0
24	CHD	B	305	-	32,32,32	1.01	0	51,51,51	1.67	13 (25%)
20	EDO	Y	107	-	3,3,3	0.65	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	O	307	-	3,3,3	0.55	0	2,2,2	0.29	0
20	EDO	D	213	-	3,3,3	0.57	0	2,2,2	0.21	0
20	EDO	L	111	-	3,3,3	0.62	0	2,2,2	0.18	0
19	PGV	P	305	-	50,50,50	0.73	3 (6%)	53,56,56	1.10	5 (9%)
20	EDO	A	618	-	3,3,3	0.38	0	2,2,2	0.87	0
20	EDO	L	102	-	3,3,3	0.65	0	2,2,2	0.76	0
20	EDO	A	629	-	3,3,3	0.23	0	2,2,2	1.22	0
20	EDO	P	324	-	3,3,3	0.37	0	2,2,2	0.79	0
20	EDO	K	102	-	3,3,3	0.80	0	2,2,2	0.42	0
20	EDO	O	311	-	3,3,3	0.41	0	2,2,2	0.26	0
20	EDO	L	106	-	3,3,3	0.71	0	2,2,2	0.61	0
20	EDO	N	625	-	3,3,3	0.43	0	2,2,2	0.64	0
20	EDO	O	313	-	3,3,3	0.55	0	2,2,2	0.33	0
20	EDO	O	305	-	3,3,3	0.52	0	2,2,2	0.23	0
20	EDO	L	110	-	3,3,3	0.74	0	2,2,2	0.82	0
20	EDO	G	105	-	3,3,3	0.36	0	2,2,2	0.49	0
20	EDO	S	114	-	3,3,3	0.41	0	2,2,2	0.58	0
20	EDO	S	113	-	3,3,3	0.38	0	2,2,2	1.01	0
20	EDO	C	321	-	3,3,3	0.65	0	2,2,2	0.07	0
20	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.34	0
20	EDO	B	308	-	3,3,3	0.79	0	2,2,2	0.20	0
20	EDO	A	633	-	3,3,3	0.51	0	2,2,2	0.46	0
20	EDO	P	319	-	3,3,3	0.70	0	2,2,2	0.35	0
26	CDL	G	101	-	87,87,99	1.32	12 (13%)	89,94,111	1.47	14 (15%)
20	EDO	B	313	-	3,3,3	0.55	0	2,2,2	0.26	0
20	EDO	E	211	-	3,3,3	0.99	0	2,2,2	1.11	0
27	DMU	X	101	-	9,9,34	0.33	0	8,8,45	0.54	0
20	EDO	R	203	-	3,3,3	0.66	0	2,2,2	0.22	0
20	EDO	A	617	-	3,3,3	0.76	0	2,2,2	0.30	0
20	EDO	P	321	-	3,3,3	0.59	0	2,2,2	0.62	0
20	EDO	E	202	-	3,3,3	0.57	0	2,2,2	0.34	0
20	EDO	N	617	-	3,3,3	0.80	0	2,2,2	0.68	0
14	HEA	A	602	1	57,67,67	1.35	6 (10%)	61,103,103	1.90	14 (22%)
20	EDO	O	309	-	3,3,3	0.66	0	2,2,2	0.25	0
26	CDL	C	307	-	94,94,99	1.42	14 (14%)	102,104,111	1.68	22 (21%)
20	EDO	N	622	-	3,3,3	0.47	0	2,2,2	0.55	0
20	EDO	C	326	-	3,3,3	1.04	0	2,2,2	0.92	0
20	EDO	L	109	-	3,3,3	0.39	0	2,2,2	0.59	0
20	EDO	Y	103	-	3,3,3	0.66	0	2,2,2	0.40	0
20	EDO	C	317	-	3,3,3	0.77	0	2,2,2	0.20	0
20	EDO	F	102	-	3,3,3	0.65	0	2,2,2	0.50	0
20	EDO	R	205	-	3,3,3	0.64	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CUA	B	303	2	0,1,1	-	-	-		
20	EDO	D	204	-	3,3,3	0.74	0	2,2,2	0.09	0
21	TGL	L	101	-	58,58,62	1.30	3 (5%)	60,60,65	1.87	15 (25%)
20	EDO	O	317	-	3,3,3	0.42	0	2,2,2	0.74	0
20	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.77	0
20	EDO	D	214	-	3,3,3	0.70	0	2,2,2	0.12	0
27	DMU	Z	101	-	34,34,34	0.62	1 (2%)	45,45,45	1.06	2 (4%)
26	CDL	P	307	-	83,83,99	1.41	11 (13%)	91,93,111	1.79	22 (24%)
20	EDO	F	104	-	3,3,3	0.95	0	2,2,2	0.13	0
20	EDO	U	103	-	3,3,3	0.66	0	2,2,2	0.42	0
20	EDO	E	206	-	3,3,3	0.34	0	2,2,2	0.92	0
20	EDO	P	326	-	3,3,3	0.83	0	2,2,2	0.28	0
14	HEA	N	601[A]	-	57,67,67	1.31	10 (17%)	61,103,103	1.82	21 (34%)
20	EDO	F	109	-	3,3,3	0.70	0	2,2,2	0.76	0
20	EDO	D	216	-	3,3,3	0.67	0	2,2,2	0.51	0
20	EDO	N	620	-	3,3,3	0.65	0	2,2,2	0.41	0
20	EDO	A	636	-	3,3,3	0.42	0	2,2,2	0.49	0
20	EDO	L	107	-	3,3,3	0.39	0	2,2,2	0.66	0
29	PO4	U	104	-	4,4,4	0.74	0	6,6,6	0.72	0
20	EDO	T	104	-	3,3,3	0.75	0	2,2,2	0.70	0
20	EDO	P	323	-	3,3,3	0.84	0	2,2,2	0.32	0
19	PGV	N	609	-	50,50,50	1.04	4 (8%)	53,56,56	1.40	8 (15%)
20	EDO	E	203	-	3,3,3	0.56	0	2,2,2	0.38	0
20	EDO	N	634	-	3,3,3	0.34	0	2,2,2	1.13	0
19	PGV	N	608	-	41,41,50	1.09	2 (4%)	44,47,56	1.35	6 (13%)
20	EDO	R	206	-	3,3,3	0.61	0	2,2,2	0.64	0
20	EDO	A	611	-	3,3,3	0.52	0	2,2,2	0.65	0
20	EDO	N	628	-	3,3,3	0.49	0	2,2,2	0.56	0
27	DMU	C	310	-	34,34,34	0.88	1 (2%)	45,45,45	1.92	12 (26%)
20	EDO	O	304	-	3,3,3	0.44	0	2,2,2	0.59	0
20	EDO	N	619	-	3,3,3	0.43	0	2,2,2	0.75	0
20	EDO	D	209	-	3,3,3	0.38	0	2,2,2	0.59	0
20	EDO	A	615	-	3,3,3	0.88	0	2,2,2	0.46	0
23	PSC	O	302	-	42,42,51	1.25	4 (9%)	46,47,59	2.03	11 (23%)
20	EDO	E	207	-	3,3,3	0.48	0	2,2,2	0.52	0
20	EDO	F	106	-	3,3,3	0.58	0	2,2,2	0.21	0
27	DMU	J	101	-	24,24,34	0.55	0	35,35,45	1.55	10 (28%)
20	EDO	A	634	-	3,3,3	0.49	0	2,2,2	0.50	0
20	EDO	P	327	-	3,3,3	0.68	0	2,2,2	0.42	0
20	EDO	T	103	-	3,3,3	0.43	0	2,2,2	0.46	0
20	EDO	O	312	-	3,3,3	0.66	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	M	102	-	3,3,3	0.59	0	2,2,2	0.25	0
20	EDO	P	313	-	3,3,3	0.63	0	2,2,2	0.32	0
20	EDO	C	316	-	3,3,3	0.50	0	2,2,2	0.21	0
20	EDO	B	311	-	3,3,3	0.50	0	2,2,2	0.80	0
14	HEA	A	601[B]	-	57,67,67	1.56	12 (21%)	61,103,103	1.86	21 (34%)
20	EDO	C	325	-	3,3,3	0.68	0	2,2,2	0.28	0
20	EDO	H	104	-	3,3,3	0.43	0	2,2,2	0.55	0
20	EDO	Q	207	-	3,3,3	0.63	0	2,2,2	0.25	0
20	EDO	E	205	-	3,3,3	0.67	0	2,2,2	0.25	0
20	EDO	N	630	-	3,3,3	0.32	0	2,2,2	1.26	0
20	EDO	Y	106	-	3,3,3	0.68	0	2,2,2	0.47	0
20	EDO	D	218	-	3,3,3	0.87	0	2,2,2	0.36	0
20	EDO	R	201	-	3,3,3	0.23	0	2,2,2	1.03	0
20	EDO	D	210	-	3,3,3	0.39	0	2,2,2	0.50	0
24	CHD	G	102	-	32,32,32	0.95	1 (3%)	51,51,51	1.38	8 (15%)
20	EDO	G	103	-	3,3,3	0.66	0	2,2,2	0.69	0
20	EDO	N	623	-	3,3,3	0.53	0	2,2,2	0.20	0
20	EDO	Q	209	-	3,3,3	0.48	0	2,2,2	0.08	0
20	EDO	B	309	-	3,3,3	0.94	0	2,2,2	0.85	0
20	EDO	L	105	-	3,3,3	0.57	0	2,2,2	0.11	0
20	EDO	Q	208	-	3,3,3	0.58	0	2,2,2	0.31	0
20	EDO	O	319	-	3,3,3	0.40	0	2,2,2	0.37	0
20	EDO	A	614	-	3,3,3	0.39	0	2,2,2	0.49	0
25	PEK	C	302	-	48,48,52	1.23	2 (4%)	51,53,57	1.37	7 (13%)
20	EDO	C	312	-	3,3,3	0.78	0	2,2,2	0.50	0
20	EDO	L	108	-	3,3,3	0.55	0	2,2,2	0.15	0
20	EDO	S	107	-	3,3,3	0.54	0	2,2,2	0.13	0
20	EDO	B	321	-	3,3,3	0.31	0	2,2,2	1.01	0
20	EDO	E	201	-	3,3,3	0.87	0	2,2,2	2.08	1 (50%)
20	EDO	V	101	-	3,3,3	0.59	0	2,2,2	0.09	0
27	DMU	X	102	-	22,22,34	0.74	1 (4%)	27,27,45	1.01	1 (3%)
20	EDO	M	104	-	3,3,3	0.45	0	2,2,2	0.24	0
20	EDO	N	629	-	3,3,3	0.41	0	2,2,2	0.93	0
20	EDO	H	103	-	3,3,3	0.59	0	2,2,2	0.40	0
20	EDO	A	620	-	3,3,3	0.51	0	2,2,2	0.31	0
20	EDO	D	217	-	3,3,3	0.50	0	2,2,2	0.35	0
20	EDO	I	104	-	3,3,3	0.82	0	2,2,2	0.39	0
20	EDO	O	315	-	3,3,3	0.56	0	2,2,2	0.40	0
20	EDO	N	624	-	3,3,3	0.46	0	2,2,2	0.21	0
20	EDO	N	614	-	3,3,3	0.58	0	2,2,2	0.19	0
20	EDO	B	317	-	3,3,3	0.60	0	2,2,2	0.26	0
20	EDO	B	316	-	3,3,3	0.63	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	A	622	-	3,3,3	0.76	0	2,2,2	0.43	0
20	EDO	E	208	-	3,3,3	0.64	0	2,2,2	0.47	0
20	EDO	A	627	-	3,3,3	0.40	0	2,2,2	0.16	0
25	PEK	C	304	-	52,52,52	1.16	3 (5%)	55,57,57	1.43	7 (12%)
20	EDO	I	105	-	3,3,3	0.41	0	2,2,2	0.65	0
25	PEK	P	303	-	52,52,52	0.75	2 (3%)	55,57,57	2.27	12 (21%)
20	EDO	W	101	-	3,3,3	0.38	0	2,2,2	0.78	0
20	EDO	J	102	-	3,3,3	0.55	0	2,2,2	0.34	0
20	EDO	L	104	-	3,3,3	0.43	0	2,2,2	0.16	0
20	EDO	A	609	-	3,3,3	0.21	0	2,2,2	0.18	0
20	EDO	F	108	-	3,3,3	0.39	0	2,2,2	1.29	0
20	EDO	A	621	-	3,3,3	0.51	0	2,2,2	0.69	0
20	EDO	A	625	-	3,3,3	0.68	0	2,2,2	0.24	0
20	EDO	C	315	-	3,3,3	0.76	0	2,2,2	0.58	0
20	EDO	S	103	-	3,3,3	0.73	0	2,2,2	0.68	0
20	EDO	S	108	-	3,3,3	0.56	0	2,2,2	0.24	0
20	EDO	A	626	-	3,3,3	0.55	0	2,2,2	0.40	0
21	TGL	Q	201	-	62,62,62	1.07	3 (4%)	65,65,65	1.73	11 (16%)
20	EDO	O	316	-	3,3,3	0.47	0	2,2,2	0.20	0
20	EDO	N	627	-	3,3,3	0.79	0	2,2,2	0.36	0
20	EDO	D	207	-	3,3,3	0.68	0	2,2,2	0.37	0
20	EDO	Q	202	-	3,3,3	0.57	0	2,2,2	0.26	0
20	EDO	P	318	-	3,3,3	0.45	0	2,2,2	0.39	0
20	EDO	A	624	-	3,3,3	0.55	0	2,2,2	0.39	0
27	DMU	X	104	-	11,11,34	0.48	0	10,10,45	0.43	0
20	EDO	C	323	-	3,3,3	0.57	0	2,2,2	0.27	0
20	EDO	O	310	-	3,3,3	0.80	0	2,2,2	0.45	0
20	EDO	Y	105	-	3,3,3	0.75	0	2,2,2	0.41	0
20	EDO	N	621	-	3,3,3	0.31	0	2,2,2	0.37	0
20	EDO	Y	104	-	3,3,3	0.49	0	2,2,2	0.28	0
20	EDO	B	310	-	3,3,3	0.38	0	2,2,2	1.00	0
20	EDO	N	613	-	3,3,3	0.70	0	2,2,2	0.17	0
20	EDO	U	101	-	3,3,3	0.64	0	2,2,2	0.51	0
20	EDO	D	211	-	3,3,3	0.66	0	2,2,2	0.18	0
21	TGL	N	607	-	62,62,62	1.13	3 (4%)	65,65,65	1.30	8 (12%)
20	EDO	W	103	-	3,3,3	0.53	0	2,2,2	0.41	0
20	EDO	N	626	-	3,3,3	0.61	0	2,2,2	0.56	0
20	EDO	E	212	-	3,3,3	0.52	0	2,2,2	0.54	0
20	EDO	D	215	-	3,3,3	0.42	0	2,2,2	0.54	0
20	EDO	A	628	-	3,3,3	0.45	0	2,2,2	0.24	0
20	EDO	M	103	-	3,3,3	0.92	0	2,2,2	0.50	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
20	EDO	A	619	-	-	1/1/1/1	-
19	PGV	A	608	-	-	5/55/55/55	-
20	EDO	D	221	-	-	0/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	Q	209	-	-	1/1/1/1	-
20	EDO	V	102	-	-	1/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
21	TGL	B	302	-	-	37/64/64/65	-
19	PGV	A	607	-	-	27/51/51/55	-
27	DMU	O	303	-	-	8/19/59/59	0/2/2/2
20	EDO	L	110	-	-	0/1/1/1	-
20	EDO	B	309	-	-	1/1/1/1	-
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	E	204	-	-	1/1/1/1	-
20	EDO	L	105	-	-	1/1/1/1	-
27	DMU	P	309	-	-	6/19/59/59	0/2/2/2
20	EDO	Q	208	-	-	1/1/1/1	-
20	EDO	O	319	-	-	1/1/1/1	-
20	EDO	B	318	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	H	101	-	-	1/1/1/1	-
20	EDO	N	633	-	-	1/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
25	PEK	C	302	-	-	21/52/52/56	-
20	EDO	C	312	-	-	1/1/1/1	-
20	EDO	D	220	-	-	0/1/1/1	-
20	EDO	Q	204	-	-	1/1/1/1	-
20	EDO	S	114	-	-	1/1/1/1	-
20	EDO	N	635	-	-	1/1/1/1	-
27	DMU	P	310	-	-	5/19/59/59	0/2/2/2
20	EDO	S	113	-	-	1/1/1/1	-
20	EDO	A	623	-	-	0/1/1/1	-
20	EDO	C	321	-	-	0/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
25	PEK	P	302	-	-	16/34/34/56	-
20	EDO	P	317	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	L	108	-	-	0/1/1/1	-
20	EDO	S	107	-	-	0/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
20	EDO	B	321	-	-	1/1/1/1	-
20	EDO	N	615	-	-	1/1/1/1	-
27	DMU	X	103	-	-	7/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	4/32/76/76	-
20	EDO	B	308	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	V	101	-	-	1/1/1/1	-
20	EDO	K	103	-	-	1/1/1/1	-
20	EDO	A	632	-	-	0/1/1/1	-
20	EDO	S	110	-	-	0/1/1/1	-
20	EDO	A	633	-	-	0/1/1/1	-
27	DMU	X	102	-	-	10/13/33/59	0/1/1/2
20	EDO	P	319	-	-	0/1/1/1	-
20	EDO	E	213	-	-	0/1/1/1	-
20	EDO	M	104	-	-	0/1/1/1	-
26	CDL	G	101	-	-	42/90/90/110	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	EDO	K	104	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	K	105	-	-	1/1/1/1	-
20	EDO	B	313	-	-	0/1/1/1	-
20	EDO	N	629	-	-	1/1/1/1	-
20	EDO	E	211	-	-	1/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
27	DMU	N	610	-	-	9/11/19/59	0/1/1/2
27	DMU	X	101	-	-	2/7/7/59	-
20	EDO	B	324	-	-	0/1/1/1	-
20	EDO	C	320	-	-	0/1/1/1	-
20	EDO	R	203	-	-	1/1/1/1	-
20	EDO	H	103	-	-	0/1/1/1	-
20	EDO	T	106	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	8/32/76/76	-
20	EDO	B	320	-	-	1/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
20	EDO	D	201	-	-	0/1/1/1	-
20	EDO	A	620	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	E	202	-	-	1/1/1/1	-
14	HEA	A	602	1	-	4/32/76/76	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	O	309	-	-	0/1/1/1	-
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	D	217	-	-	0/1/1/1	-
24	CHD	P	308	-	-	5/9/74/74	0/4/4/4
26	CDL	C	307	-	-	55/98/98/110	-
20	EDO	I	104	-	-	0/1/1/1	-
27	DMU	M	101	-	-	5/19/59/59	0/2/2/2
20	EDO	S	111	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
20	EDO	O	315	-	-	1/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
20	EDO	P	316	-	-	1/1/1/1	-
20	EDO	N	622	-	-	0/1/1/1	-
20	EDO	C	326	-	-	0/1/1/1	-
20	EDO	D	206	-	-	0/1/1/1	-
20	EDO	S	109	-	-	1/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	L	109	-	-	0/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	N	631	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	R	205	-	-	1/1/1/1	-
20	EDO	O	308	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	B	317	-	-	1/1/1/1	-
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	B	316	-	-	1/1/1/1	-
20	EDO	B	319	-	-	0/1/1/1	-
20	EDO	D	204	-	-	1/1/1/1	-
21	TGL	L	101	-	-	34/59/59/65	-
20	EDO	D	212	-	-	1/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	O	317	-	-	1/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
20	EDO	Y	108	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	E	208	-	-	1/1/1/1	-
20	EDO	S	105	-	-	1/1/1/1	-
20	EDO	D	214	-	-	1/1/1/1	-
20	EDO	A	627	-	-	1/1/1/1	-
14	HEA	N	602	1	-	4/32/76/76	-
20	EDO	N	632	-	-	0/1/1/1	-
25	PEK	C	304	-	-	22/56/56/56	-
26	CDL	P	307	-	-	39/87/87/110	-
26	CDL	T	101	-	-	35/96/100/110	-
27	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	EDO	E	210	-	-	0/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	M	106	-	-	1/1/1/1	-
20	EDO	U	103	-	-	0/1/1/1	-
20	EDO	C	313	-	-	1/1/1/1	-
20	EDO	E	206	-	-	0/1/1/1	-
20	EDO	I	105	-	-	0/1/1/1	-
20	EDO	P	326	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	6/32/76/76	-
20	EDO	R	202	-	-	1/1/1/1	-
25	PEK	P	303	-	-	19/56/56/56	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	F	109	-	-	0/1/1/1	-
20	EDO	C	324	-	-	1/1/1/1	-
20	EDO	I	101	-	-	1/1/1/1	-
20	EDO	D	216	-	-	0/1/1/1	-
20	EDO	T	107	-	-	1/1/1/1	-
20	EDO	W	101	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	A	636	-	-	0/1/1/1	-
20	EDO	L	107	-	-	0/1/1/1	-
24	CHD	C	308	-	-	9/9/74/74	0/4/4/4
20	EDO	J	102	-	-	0/1/1/1	-
20	EDO	U	102	-	-	1/1/1/1	-
20	EDO	Z	102	-	-	0/1/1/1	-
20	EDO	D	202	-	-	0/1/1/1	-
20	EDO	G	104	-	-	1/1/1/1	-
20	EDO	T	104	-	-	0/1/1/1	-
20	EDO	D	219	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	F	108	-	-	1/1/1/1	-
20	EDO	I	102	-	-	1/1/1/1	-
20	EDO	P	323	-	-	0/1/1/1	-
20	EDO	S	112	-	-	1/1/1/1	-
20	EDO	A	621	-	-	1/1/1/1	-
20	EDO	A	625	-	-	0/1/1/1	-
24	CHD	Y	102	-	-	6/9/74/74	0/4/4/4
19	PGV	C	306	-	-	19/55/55/55	-
19	PGV	N	609	-	-	7/55/55/55	-
20	EDO	C	315	-	-	1/1/1/1	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	D	208	-	-	1/1/1/1	-
20	EDO	C	322	-	-	1/1/1/1	-
20	EDO	J	104	-	-	0/1/1/1	-
20	EDO	B	315	-	-	0/1/1/1	-
20	EDO	N	634	-	-	1/1/1/1	-
27	DMU	C	309	-	-	11/13/33/59	0/1/1/2
19	PGV	N	608	-	-	19/46/46/55	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	S	108	-	-	0/1/1/1	-
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	B	322	-	-	1/1/1/1	-
20	EDO	P	311	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	36/65/65/65	-
20	EDO	R	206	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	N	628	-	-	0/1/1/1	-
20	EDO	A	630	-	-	0/1/1/1	-
20	EDO	I	103	-	-	1/1/1/1	-
20	EDO	O	316	-	-	0/1/1/1	-
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	P	325	-	-	0/1/1/1	-
20	EDO	K	101	-	-	0/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	B	312	-	-	1/1/1/1	-
27	DMU	C	310	-	-	3/19/59/59	0/2/2/2
20	EDO	N	619	-	-	1/1/1/1	-
20	EDO	O	306	-	-	0/1/1/1	-
20	EDO	N	627	-	-	1/1/1/1	-
20	EDO	D	207	-	-	1/1/1/1	-
20	EDO	T	105	-	-	0/1/1/1	-
20	EDO	E	209	-	-	1/1/1/1	-
25	PEK	C	303	-	-	9/56/56/56	-
27	DMU	T	102	-	-	6/13/30/59	0/1/1/2
20	EDO	D	209	-	-	1/1/1/1	-
20	EDO	Q	202	-	-	0/1/1/1	-
20	EDO	P	318	-	-	1/1/1/1	-
20	EDO	Q	206	-	-	1/1/1/1	-
20	EDO	C	319	-	-	1/1/1/1	-
19	PGV	C	305	-	-	13/54/54/55	-
20	EDO	J	103	-	-	1/1/1/1	-
21	TGL	B	301	-	-	27/65/65/65	-
19	PGV	P	306	-	-	26/55/55/55	-
20	EDO	N	612	-	-	0/1/1/1	-
20	EDO	O	318	-	-	1/1/1/1	-
25	PEK	P	304	-	-	24/55/55/56	-
20	EDO	M	105	-	-	0/1/1/1	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	A	624	-	-	0/1/1/1	-
23	PSC	O	302	-	-	21/44/44/55	-
20	EDO	P	322	-	-	0/1/1/1	-
20	EDO	E	207	-	-	0/1/1/1	-
20	EDO	F	106	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
27	DMU	X	104	-	-	3/9/9/59	-
20	EDO	C	323	-	-	1/1/1/1	-
20	EDO	O	310	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	35/62/62/65	-
20	EDO	B	323	-	-	1/1/1/1	-
20	EDO	Y	105	-	-	1/1/1/1	-
20	EDO	A	631	-	-	1/1/1/1	-
20	EDO	D	203	-	-	1/1/1/1	-
20	EDO	H	102	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	621	-	-	1/1/1/1	-
20	EDO	Q	205	-	-	1/1/1/1	-
24	CHD	B	305	-	-	2/9/74/74	0/4/4/4
20	EDO	V	103	-	-	0/1/1/1	-
20	EDO	B	314	-	-	1/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
20	EDO	Y	107	-	-	1/1/1/1	-
27	DMU	J	101	-	-	1/8/48/59	0/2/2/2
20	EDO	O	307	-	-	0/1/1/1	-
20	EDO	A	634	-	-	0/1/1/1	-
20	EDO	A	635	-	-	1/1/1/1	-
20	EDO	O	314	-	-	1/1/1/1	-
20	EDO	P	327	-	-	0/1/1/1	-
20	EDO	O	312	-	-	1/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
20	EDO	D	213	-	-	0/1/1/1	-
20	EDO	P	313	-	-	0/1/1/1	-
20	EDO	L	111	-	-	1/1/1/1	-
20	EDO	B	310	-	-	1/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	Y	104	-	-	0/1/1/1	-
19	PGV	P	305	-	-	7/55/55/55	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	B	311	-	-	1/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	L	102	-	-	0/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
20	EDO	A	629	-	-	1/1/1/1	-
14	HEA	A	601[B]	-	-	5/32/76/76	-
20	EDO	C	325	-	-	1/1/1/1	-
20	EDO	D	211	-	-	1/1/1/1	-
20	EDO	H	104	-	-	1/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	P	324	-	-	0/1/1/1	-
20	EDO	Q	207	-	-	0/1/1/1	-
20	EDO	K	102	-	-	1/1/1/1	-
20	EDO	W	103	-	-	0/1/1/1	-
21	TGL	N	607	-	-	30/65/65/65	-
20	EDO	E	205	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	A	610	-	-	1/1/1/1	-
20	EDO	E	212	-	-	1/1/1/1	-
20	EDO	L	106	-	-	1/1/1/1	-
20	EDO	O	311	-	-	0/1/1/1	-
20	EDO	D	215	-	-	1/1/1/1	-
20	EDO	N	630	-	-	0/1/1/1	-
20	EDO	Y	106	-	-	0/1/1/1	-
20	EDO	D	218	-	-	0/1/1/1	-
20	EDO	P	320	-	-	1/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	C	318	-	-	1/1/1/1	-
20	EDO	A	628	-	-	0/1/1/1	-
20	EDO	D	210	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	G	103	-	-	0/1/1/1	-
23	PSC	B	304	-	-	24/51/51/55	-
20	EDO	N	625	-	-	0/1/1/1	-
20	EDO	I	106	-	-	1/1/1/1	-
20	EDO	O	313	-	-	0/1/1/1	-

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	101	TGL	OG2-CB1	6.39	1.52	1.34
21	L	101	TGL	OG2-CB1	6.13	1.51	1.34
19	C	306	PGV	O01-C1	5.33	1.49	1.34
26	T	101	CDL	OB8-CB7	5.25	1.48	1.33
21	B	301	TGL	OG1-CA1	5.20	1.48	1.33

The worst 5 of 551 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	303	PEK	C2-C3-C4	11.82	134.29	113.23
24	C	308	CHD	C23-C22-C20	-8.32	99.32	114.52
19	A	607	PGV	O01-C1-O02	8.26	143.67	123.70
26	T	101	CDL	OA6-CA5-C11	7.58	127.84	111.50
21	B	301	TGL	OG2-CB1-CB2	7.36	127.37	111.50

There are no chirality outliers.

5 of 909 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
19	A	607	PGV	C03-O11-P-O13
19	A	607	PGV	C03-O11-P-O14
19	A	607	PGV	C04-C05-C06-O06

There are no ring outliers.

146 monomers are involved in 324 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	608	PGV	1	0
19	A	607	PGV	1	0
20	N	618	EDO	3	0
27	P	310	DMU	5	0
20	A	623	EDO	4	0
20	N	615	EDO	1	0
20	C	320	EDO	1	0
20	T	106	EDO	2	0
20	F	105	EDO	1	0
20	D	201	EDO	1	0
20	Q	203	EDO	1	0
20	P	316	EDO	3	0
20	W	102	EDO	1	0
20	A	637[A]	EDO	2	0
20	D	212	EDO	1	0
20	R	202	EDO	2	0
20	T	107	EDO	2	0
24	C	308	CHD	4	0
20	U	102	EDO	1	0
20	D	202	EDO	4	0
20	G	104	EDO	1	0
20	D	219	EDO	1	0
24	Y	102	CHD	2	0
20	B	315	EDO	1	0
20	I	103	EDO	3	0
20	B	312	EDO	6	0
25	C	303	PEK	3	0
20	Q	206	EDO	2	0
21	Y	101	TGL	11	0
20	D	203	EDO	1	0
20	W	104	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	314	EDO	5	0
20	A	635	EDO	3	0
27	C	309	DMU	1	0
23	B	304	PSC	8	0
21	B	302	TGL	10	0
27	P	309	DMU	4	0
20	R	204	EDO	1	0
20	N	635	EDO	1	0
25	P	302	PEK	2	0
14	N	601[B]	HEA	1	0
24	P	308	CHD	2	0
20	S	109	EDO	2	0
20	D	206	EDO	1	0
20	N	631	EDO	1	0
20	S	105	EDO	1	0
14	N	602	HEA	1	0
20	N	632	EDO	2	0
26	T	101	CDL	11	0
20	E	210	EDO	1	0
20	M	106	EDO	2	0
20	S	112	EDO	1	0
19	C	306	PGV	8	0
20	J	104	EDO	1	0
20	A	630	EDO	2	0
20	E	209	EDO	1	0
27	T	102	DMU	3	0
20	C	319	EDO	3	0
19	C	305	PGV	1	0
21	B	301	TGL	5	0
19	P	306	PGV	8	0
20	O	318	EDO	2	0
25	P	304	PEK	2	0
20	A	631	EDO	3	0
20	H	102	EDO	3	0
20	Q	205	EDO	1	0
20	D	213	EDO	1	0
19	P	305	PGV	3	0
20	A	618	EDO	2	0
20	L	102	EDO	1	0
20	A	629	EDO	2	0
20	P	324	EDO	1	0
20	O	311	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	625	EDO	1	0
20	O	305	EDO	2	0
20	L	110	EDO	5	0
20	G	105	EDO	2	0
20	A	633	EDO	4	0
26	G	101	CDL	8	0
20	B	313	EDO	1	0
27	X	101	DMU	2	0
20	A	617	EDO	1	0
20	P	321	EDO	2	0
14	A	602	HEA	2	0
26	C	307	CDL	6	0
20	C	326	EDO	1	0
20	L	109	EDO	1	0
21	L	101	TGL	7	0
20	O	317	EDO	1	0
20	A	616	EDO	1	0
27	Z	101	DMU	2	0
26	P	307	CDL	11	0
20	P	326	EDO	2	0
14	N	601[A]	HEA	1	0
20	F	109	EDO	2	0
20	A	636	EDO	2	0
19	N	609	PGV	1	0
20	N	634	EDO	1	0
19	N	608	PGV	3	0
20	N	628	EDO	1	0
27	C	310	DMU	4	0
20	D	209	EDO	4	0
23	O	302	PSC	1	0
20	F	106	EDO	2	0
27	J	101	DMU	2	0
20	T	103	EDO	1	0
14	A	601[B]	HEA	1	0
20	C	325	EDO	4	0
20	H	104	EDO	2	0
20	Q	207	EDO	1	0
20	E	205	EDO	1	0
20	N	630	EDO	1	0
20	D	218	EDO	3	0
20	R	201	EDO	2	0
20	N	623	EDO	2	0

Continued on next page...

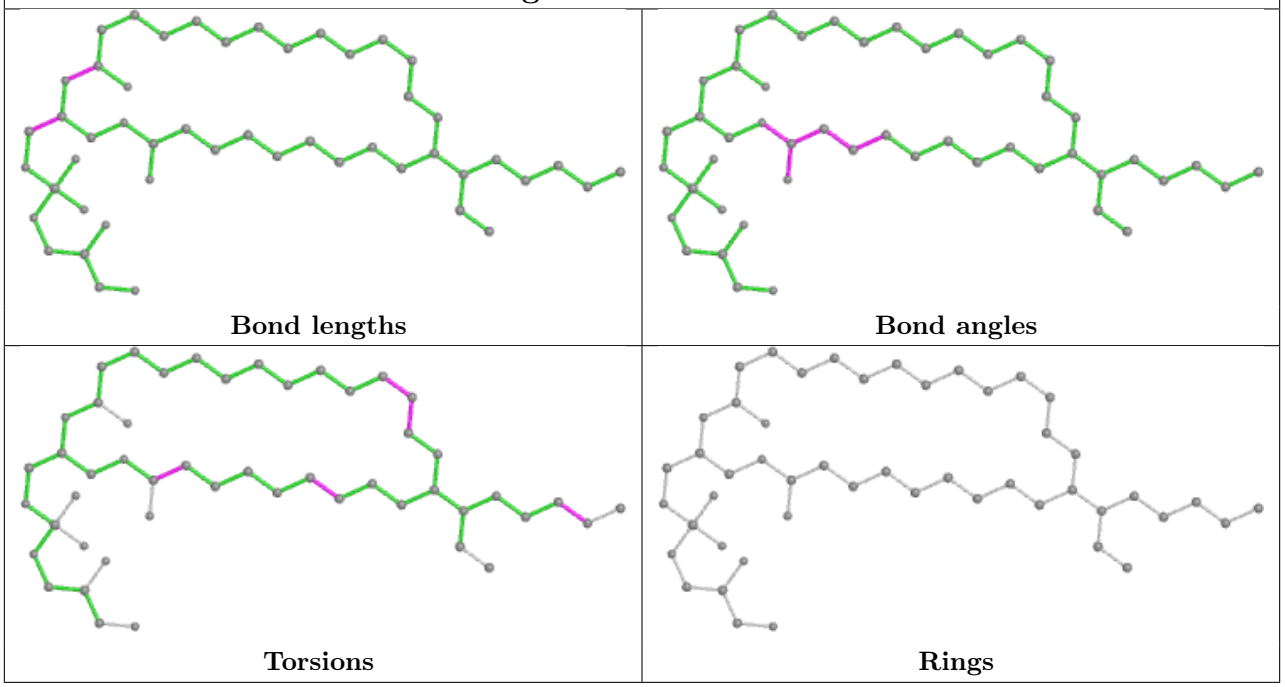
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	319	EDO	3	0
25	C	302	PEK	5	0
20	S	107	EDO	1	0
20	B	321	EDO	6	0
20	E	201	EDO	1	0
27	X	102	DMU	2	0
20	M	104	EDO	1	0
20	H	103	EDO	1	0
20	A	620	EDO	2	0
20	I	104	EDO	1	0
20	O	315	EDO	2	0
20	N	614	EDO	1	0
20	B	317	EDO	2	0
20	A	622	EDO	1	0
20	E	208	EDO	1	0
20	A	627	EDO	7	0
25	C	304	PEK	3	0
25	P	303	PEK	5	0
20	L	104	EDO	1	0
20	A	609	EDO	7	0
20	A	626	EDO	4	0
21	Q	201	TGL	9	0
20	O	316	EDO	2	0
20	N	627	EDO	1	0
20	D	207	EDO	1	0
20	P	318	EDO	2	0
20	N	621	EDO	1	0
20	U	101	EDO	2	0
21	N	607	TGL	4	0
20	W	103	EDO	1	0
20	D	215	EDO	1	0

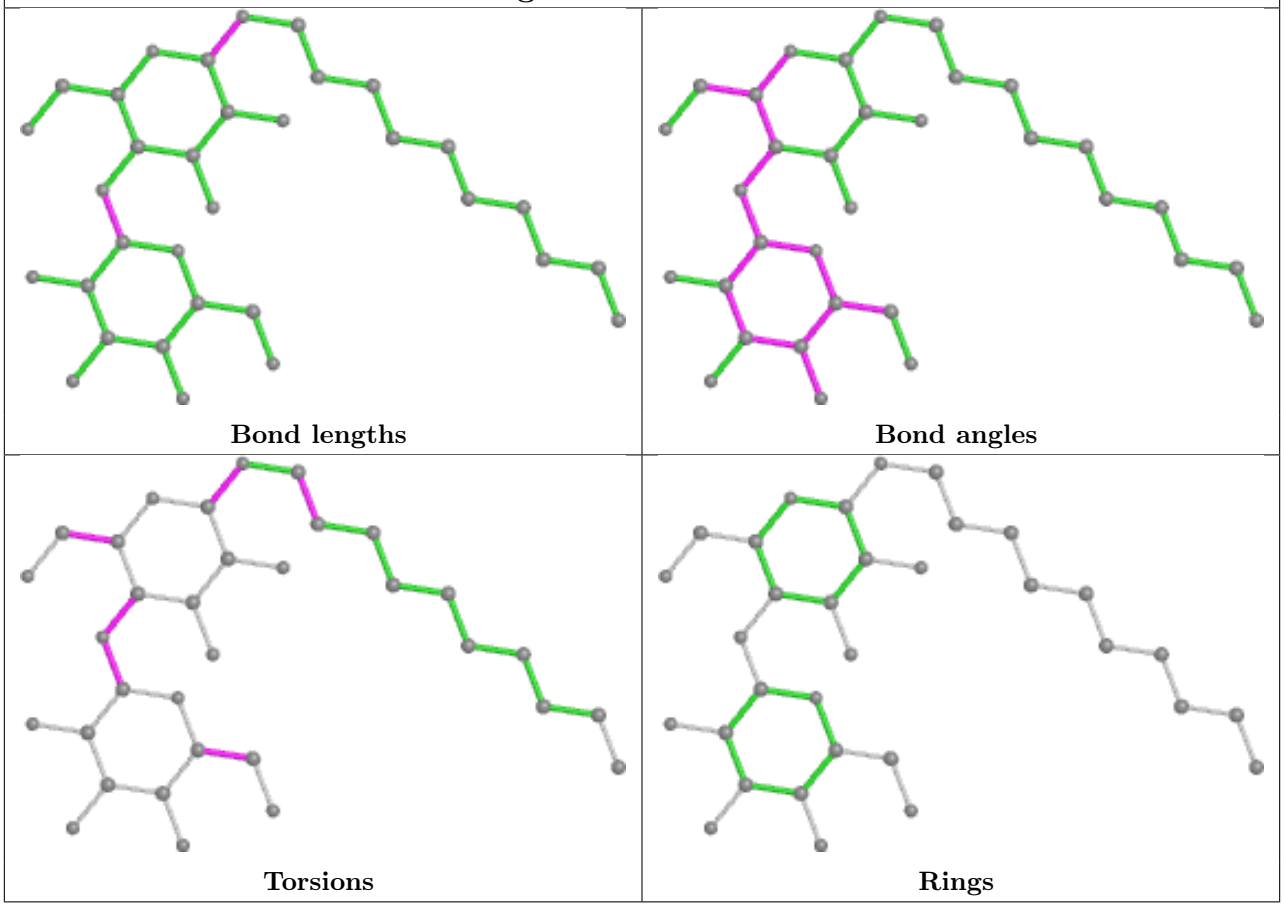
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

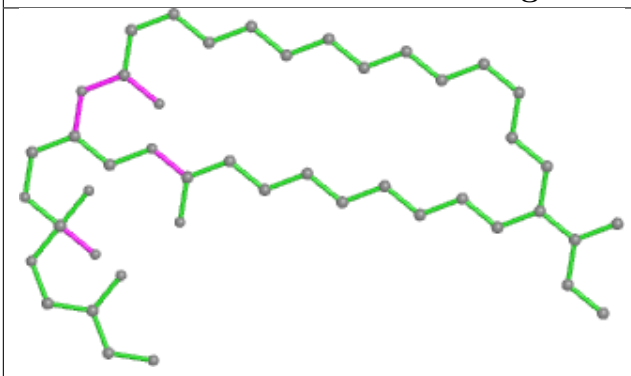
Ligand PGV A 608



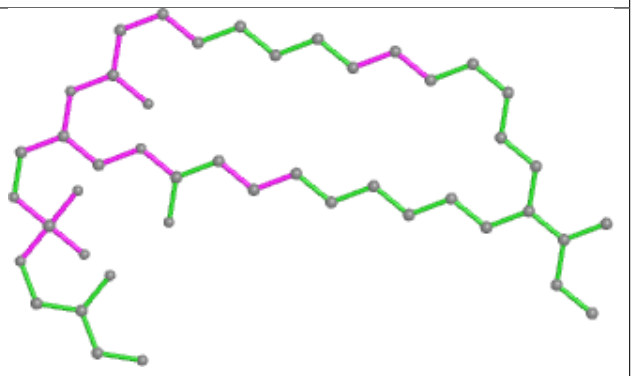
Ligand DMU O 303



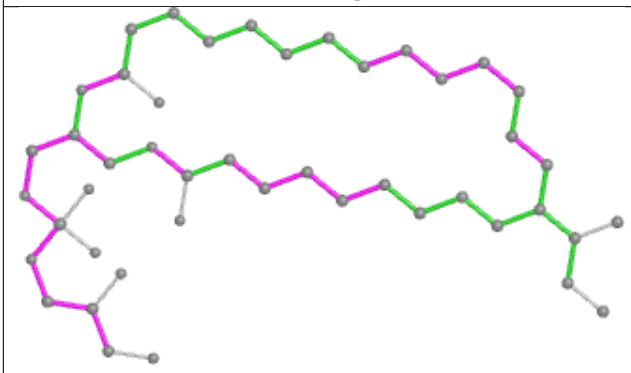
Ligand PGV A 607



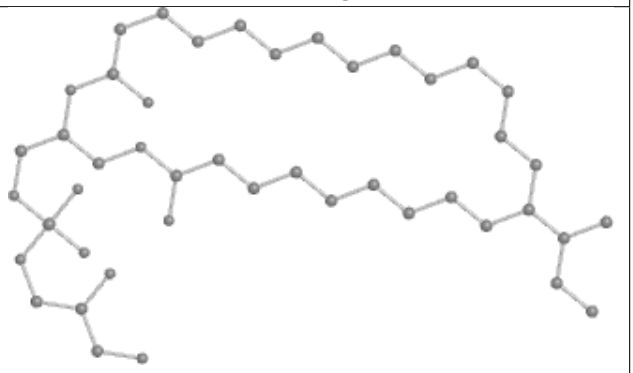
Bond lengths



Bond angles

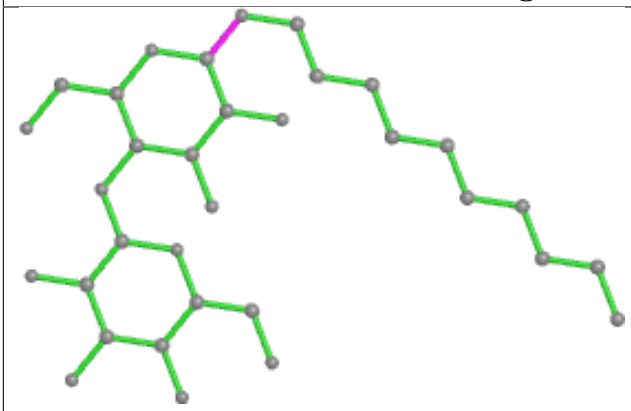


Torsions

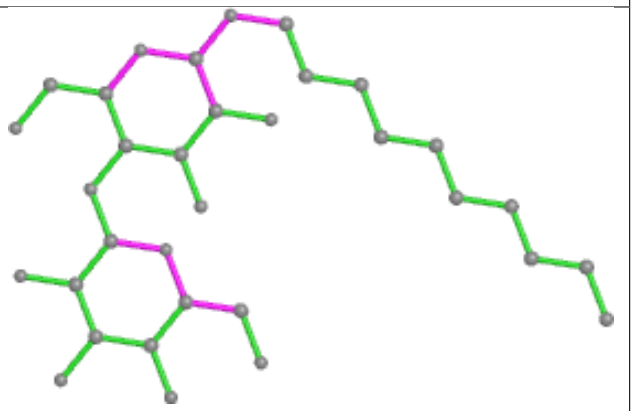


Rings

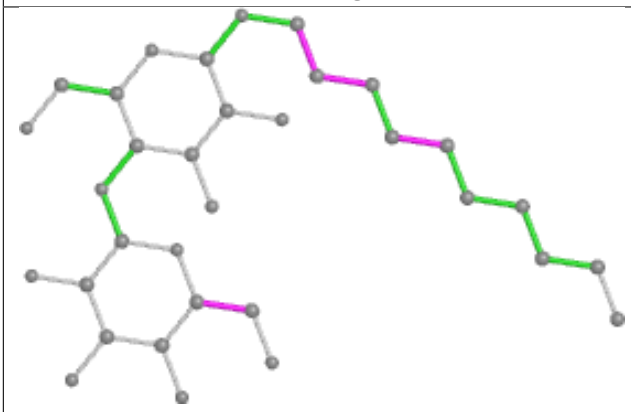
Ligand DMU P 310



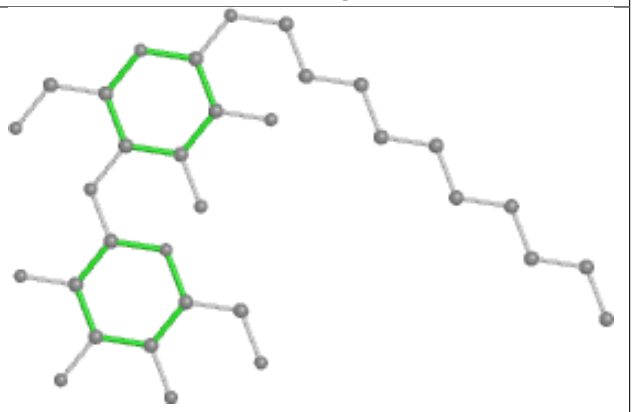
Bond lengths



Bond angles

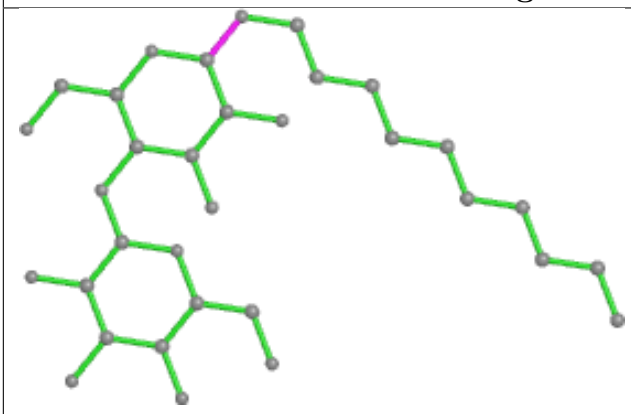


Torsions

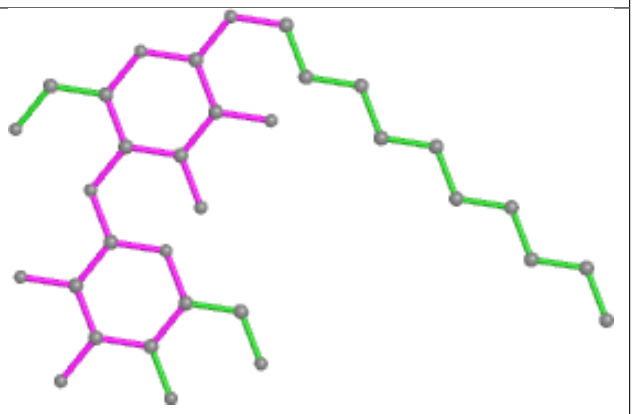


Rings

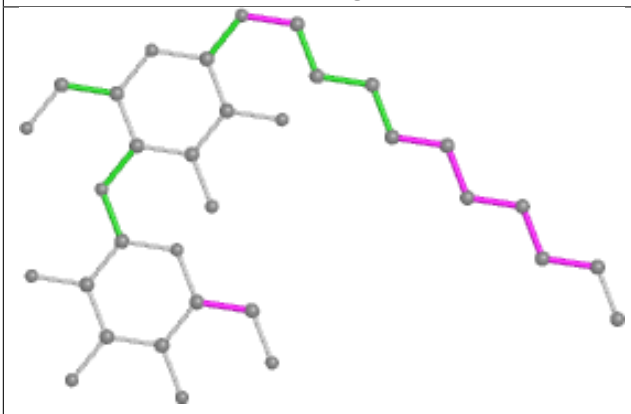
Ligand DMU X 103



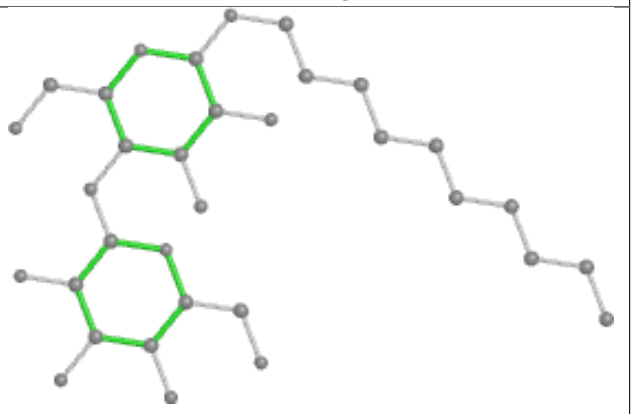
Bond lengths



Bond angles

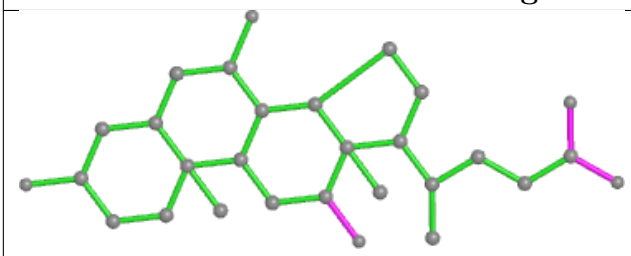


Torsions

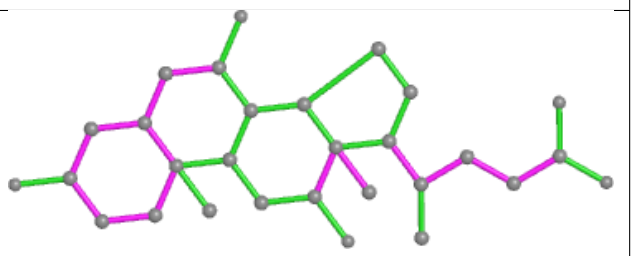


Rings

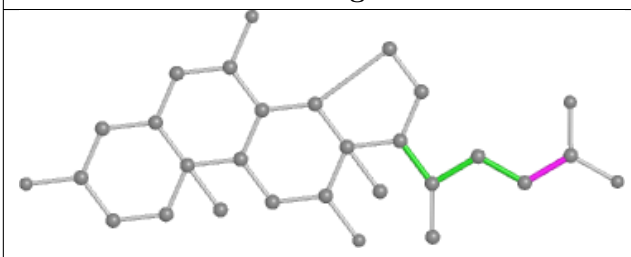
Ligand CHD C 301



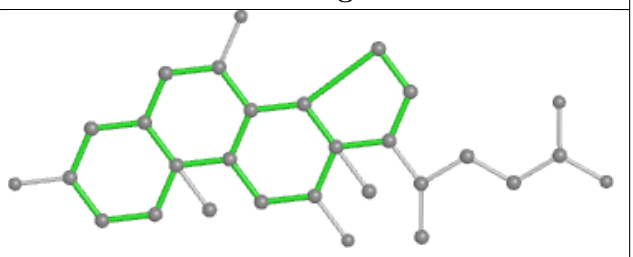
Bond lengths



Bond angles

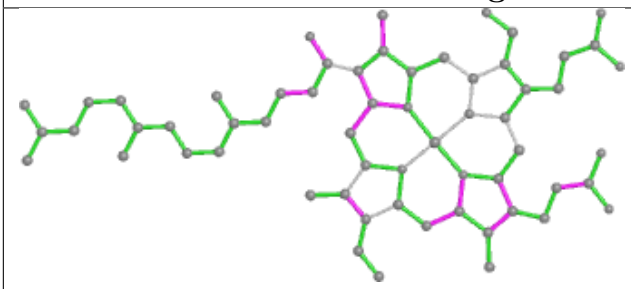


Torsions

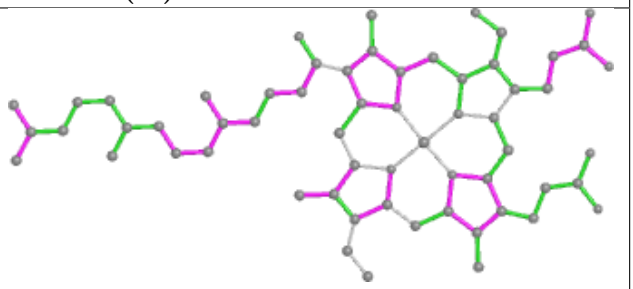


Rings

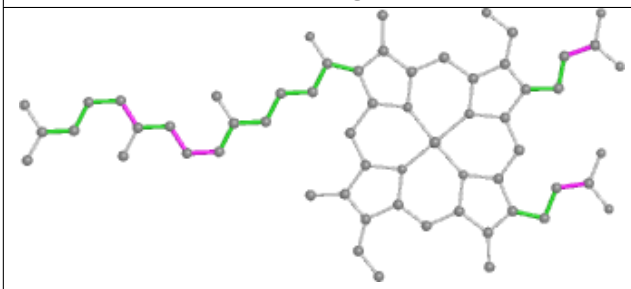
Ligand HEA A 601 (A)



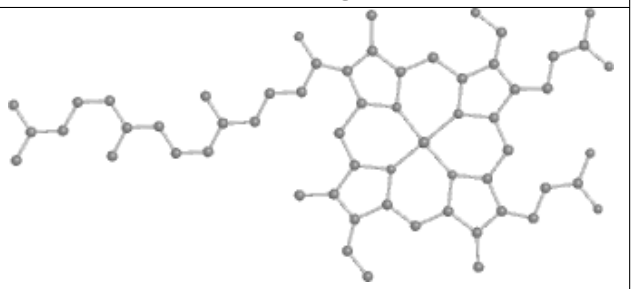
Bond lengths



Bond angles

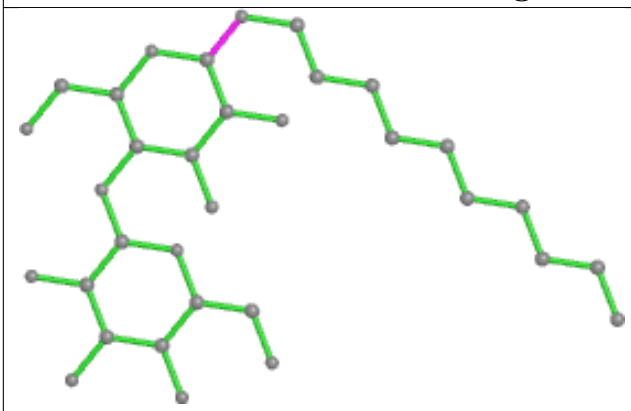


Torsions

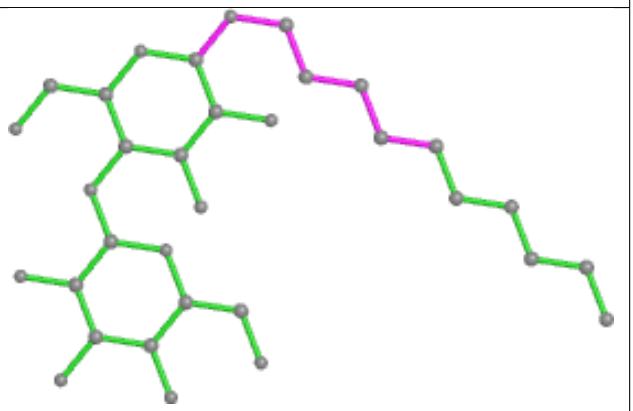


Rings

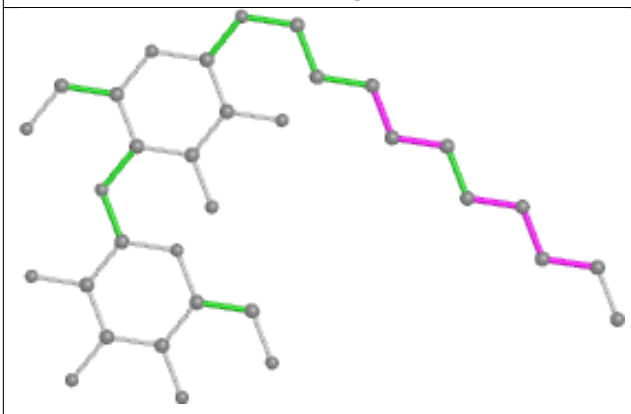
Ligand DMU M 101



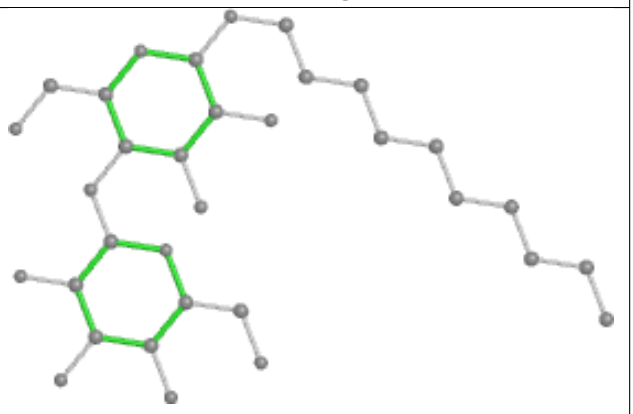
Bond lengths



Bond angles

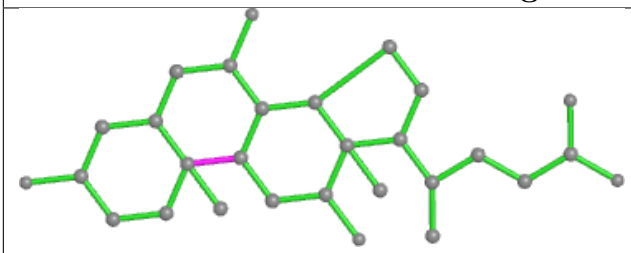


Torsions

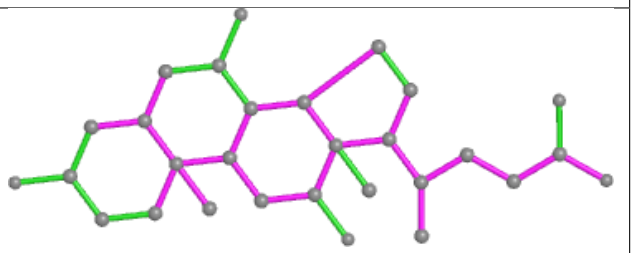


Rings

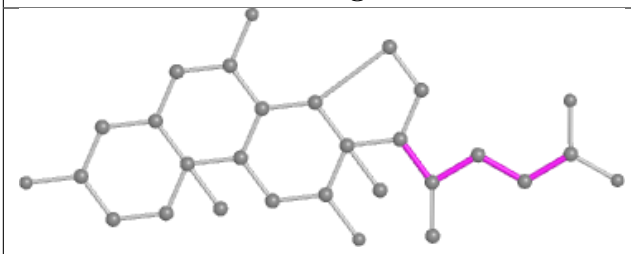
Ligand CHD C 308



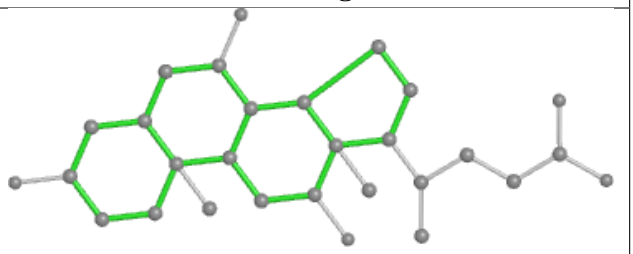
Bond lengths



Bond angles

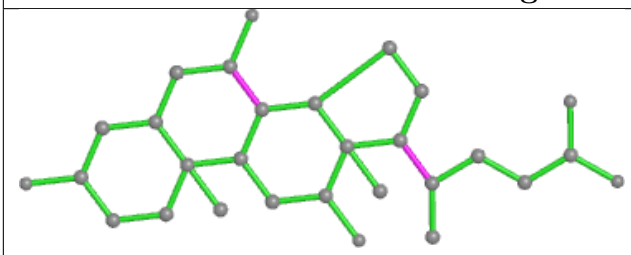


Torsions

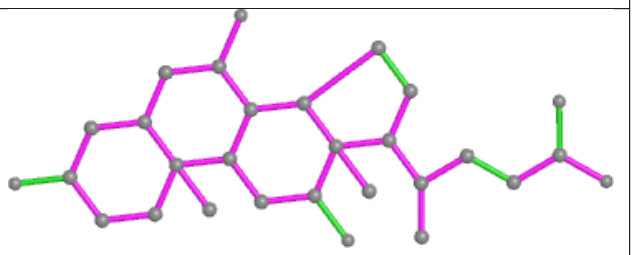


Rings

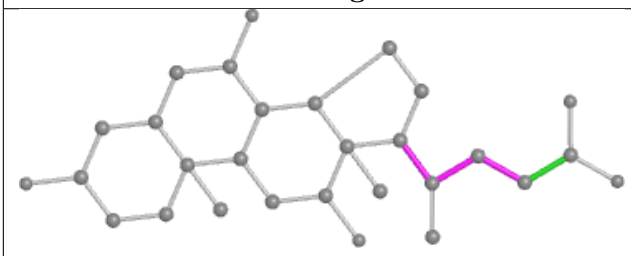
Ligand CHD Y 102



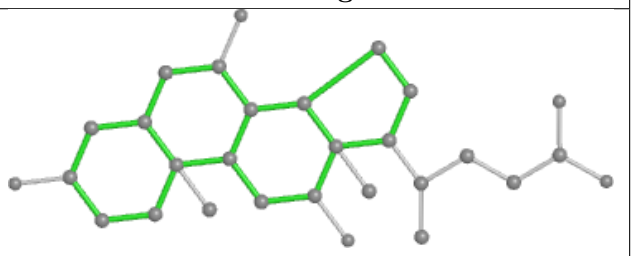
Bond lengths



Bond angles

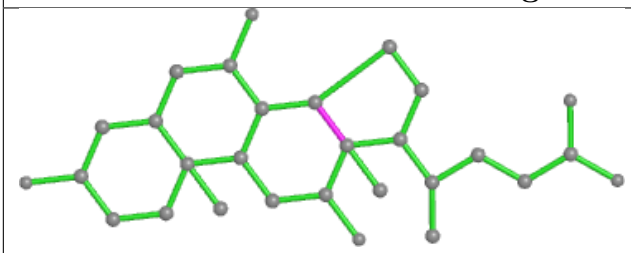


Torsions

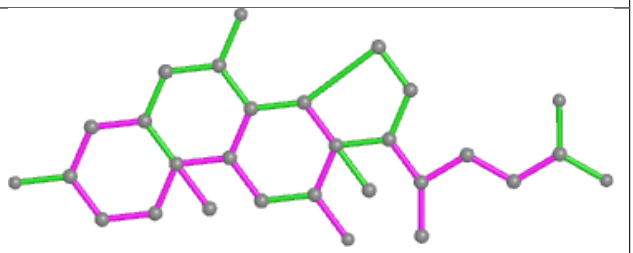


Rings

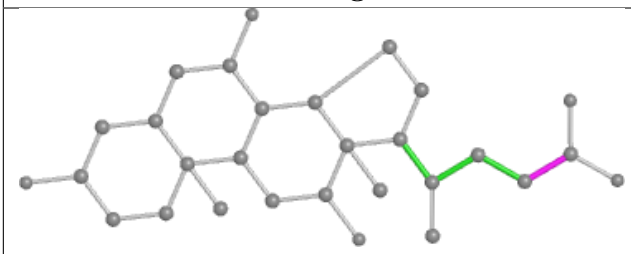
Ligand CHD P 301



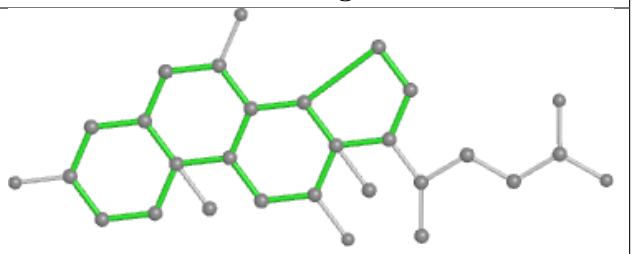
Bond lengths



Bond angles

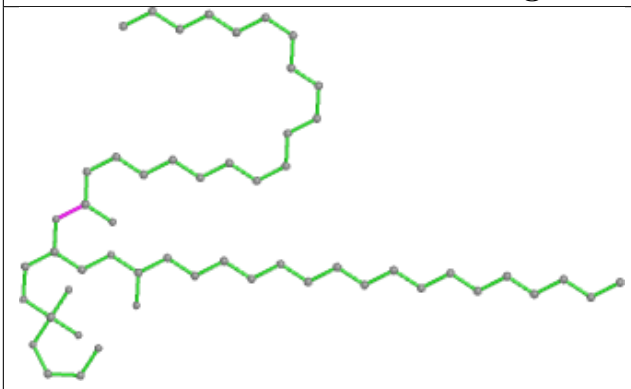


Torsions

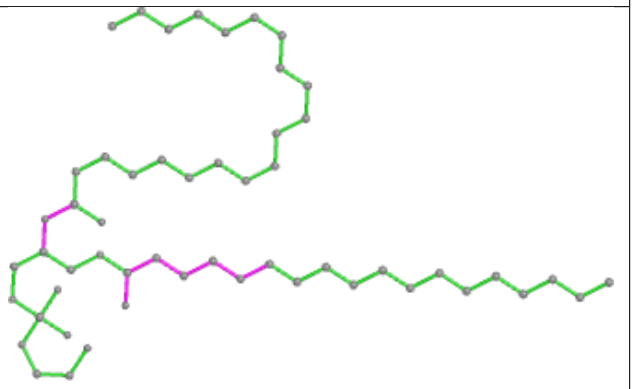


Rings

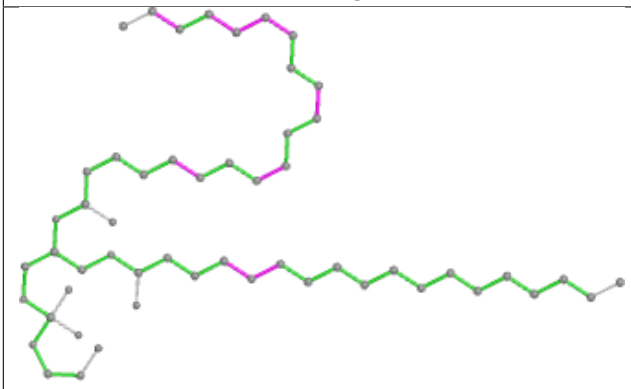
Ligand PEK C 303



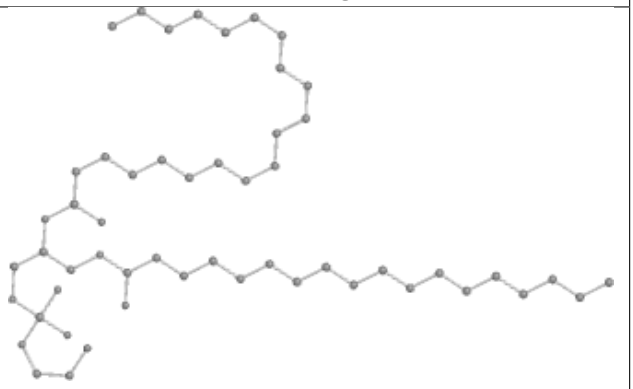
Bond lengths



Bond angles

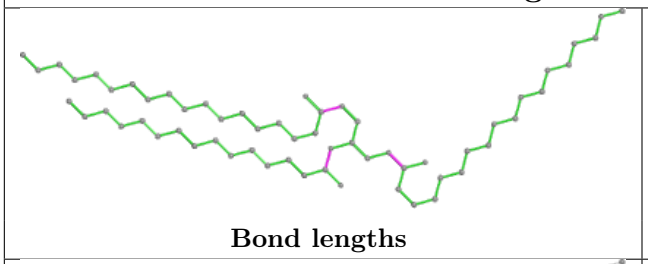


Torsions

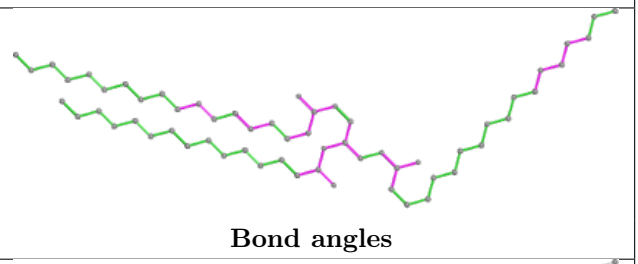


Rings

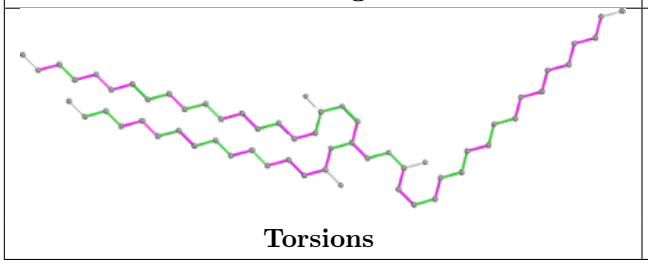
Ligand TGL Y 101



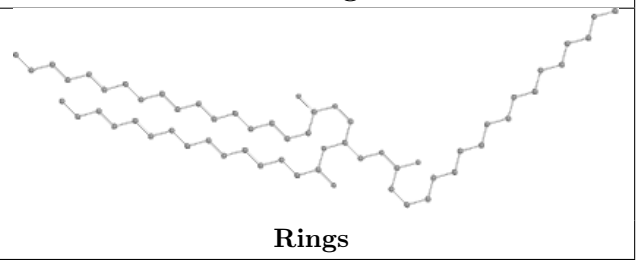
Bond lengths



Bond angles

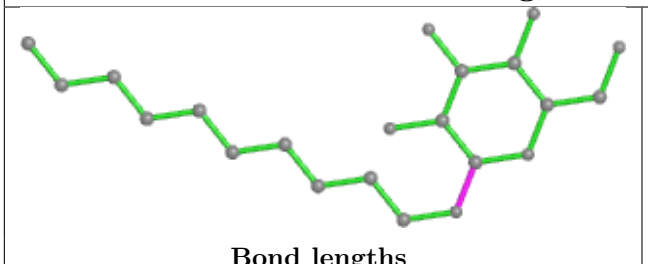


Torsions

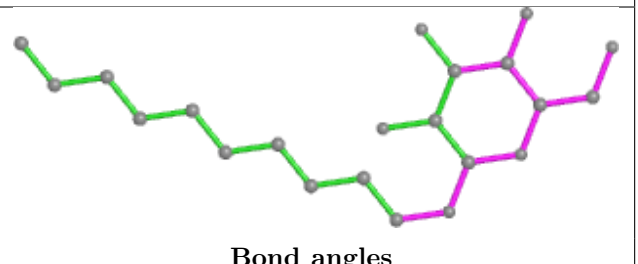


Rings

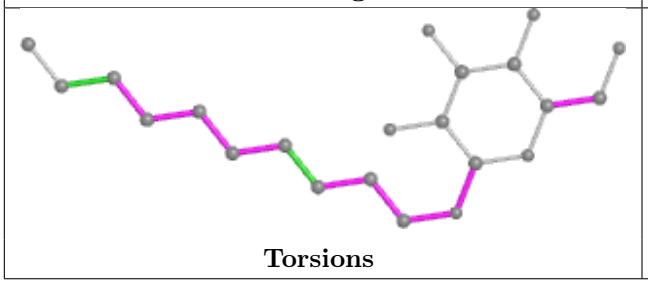
Ligand DMU C 309



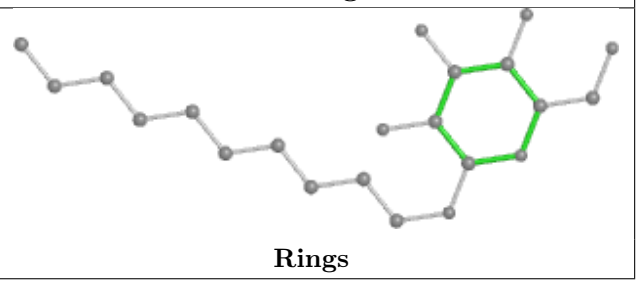
Bond lengths



Bond angles

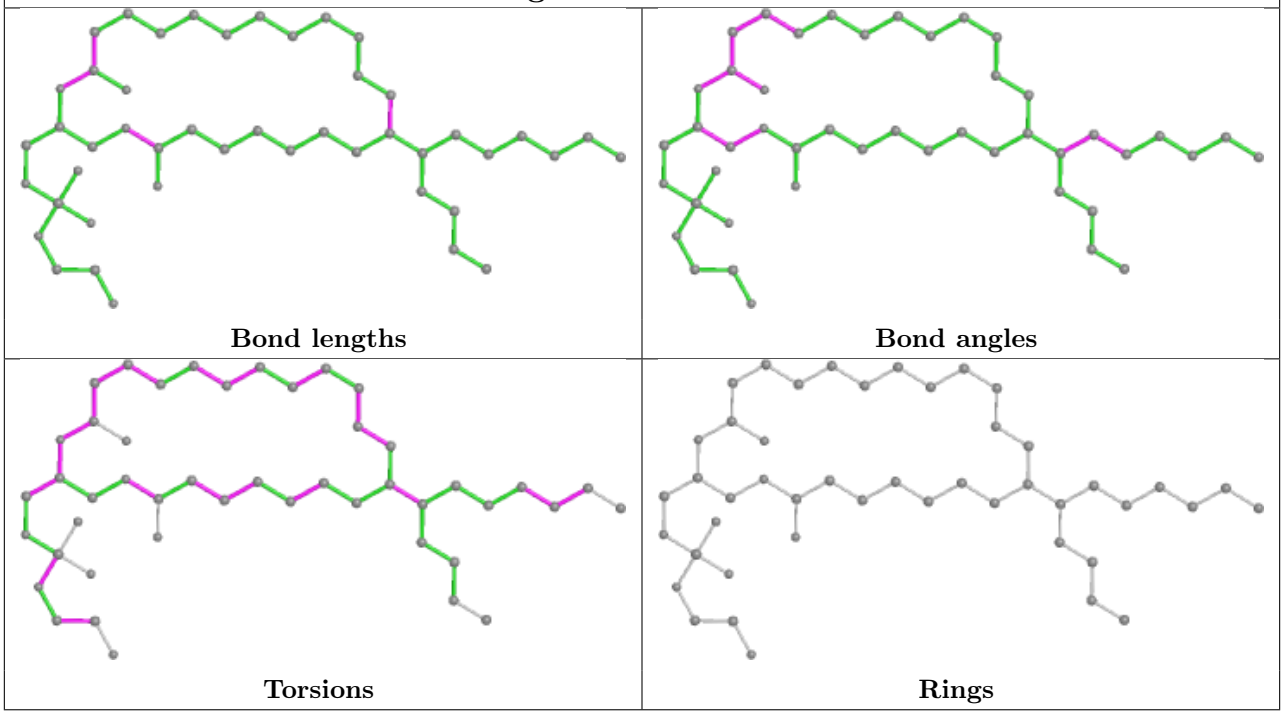


Torsions

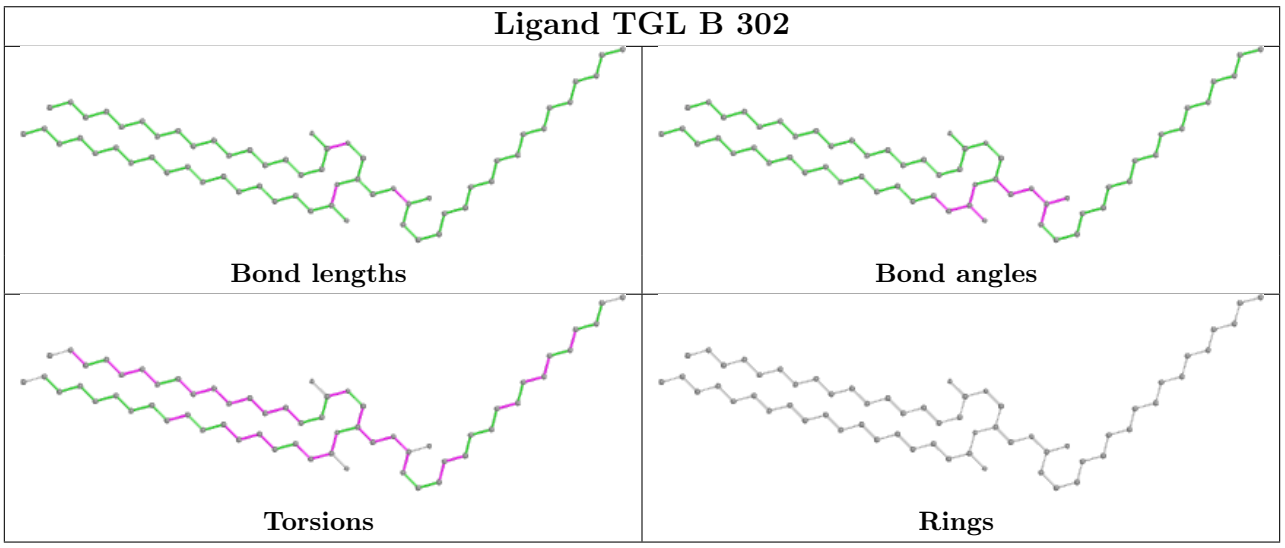


Rings

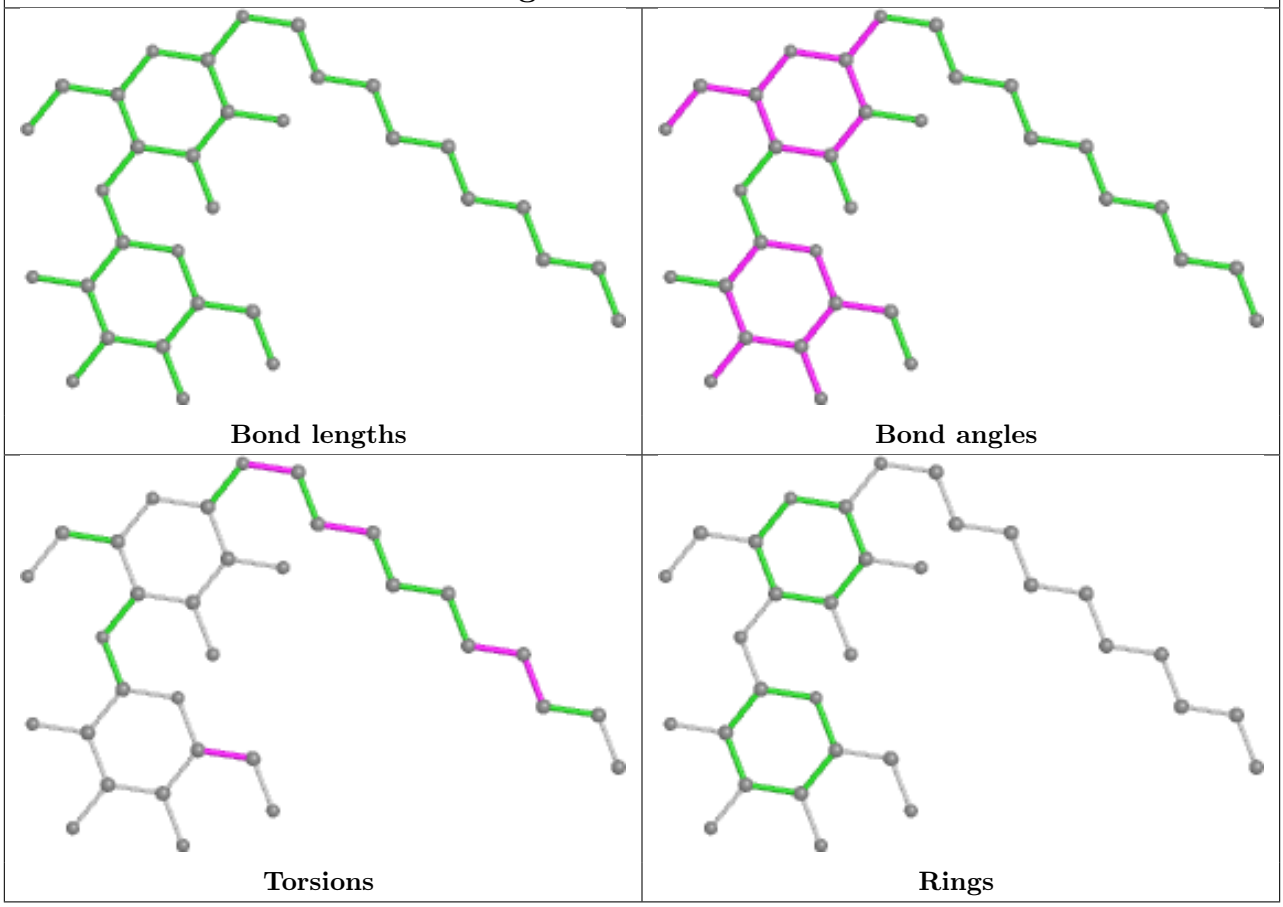
Ligand PSC B 304



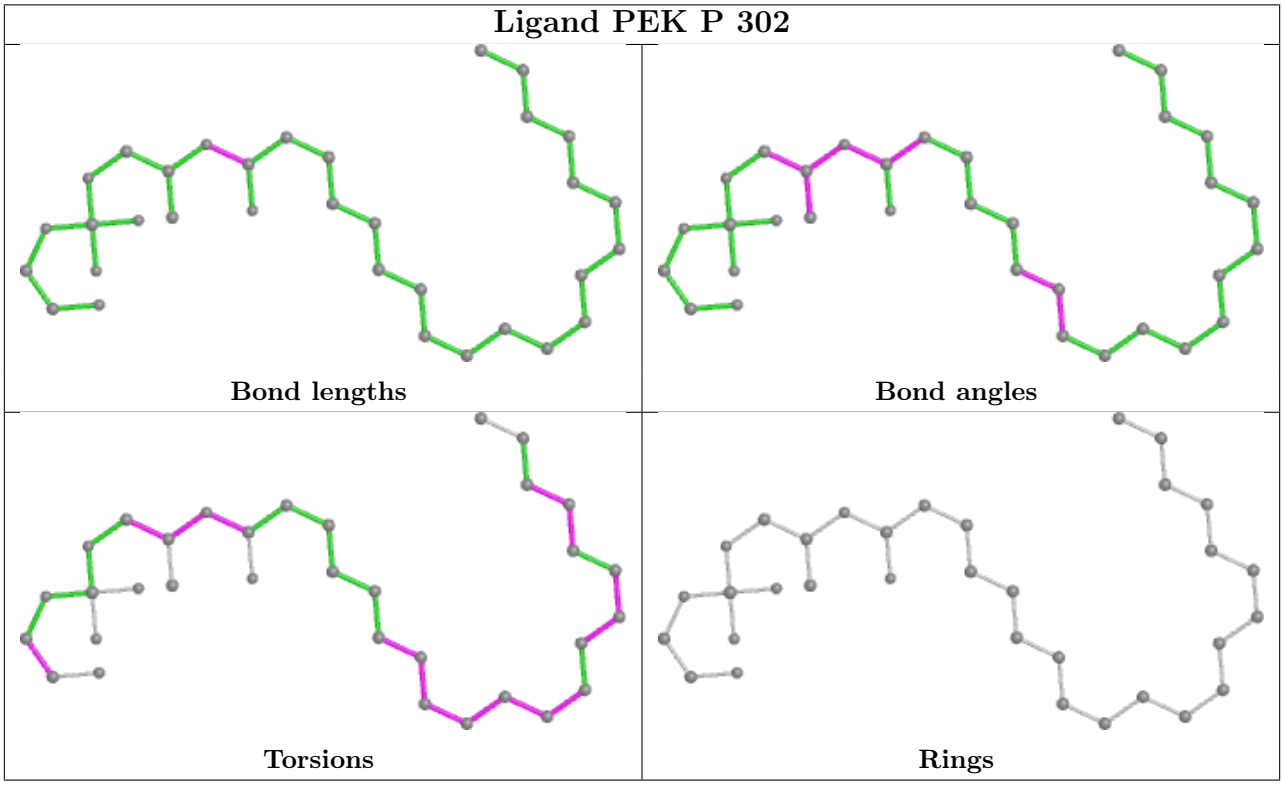
Ligand TGL B 302



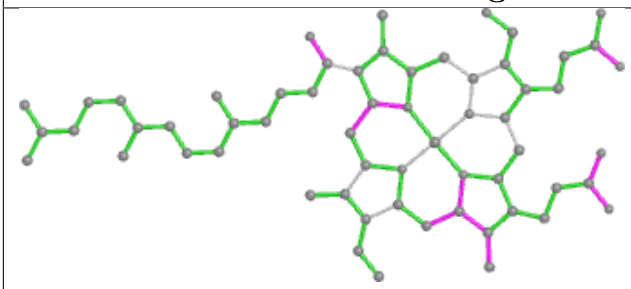
Ligand DMU P 309



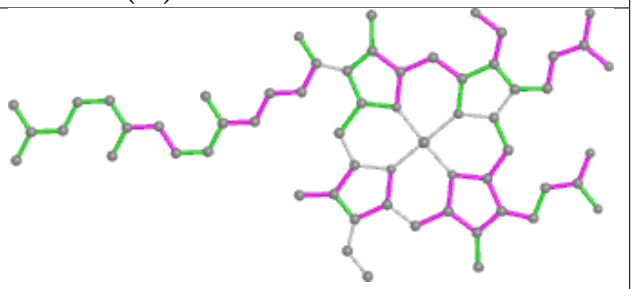
Ligand PEK P 302



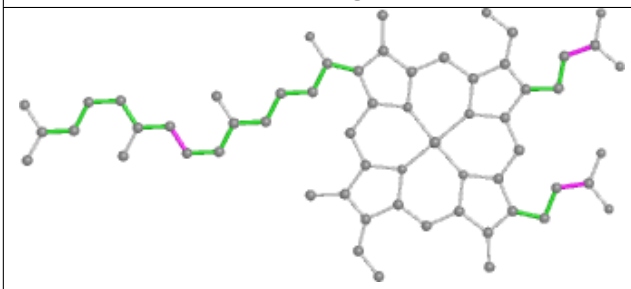
Ligand HEA N 601 (B)



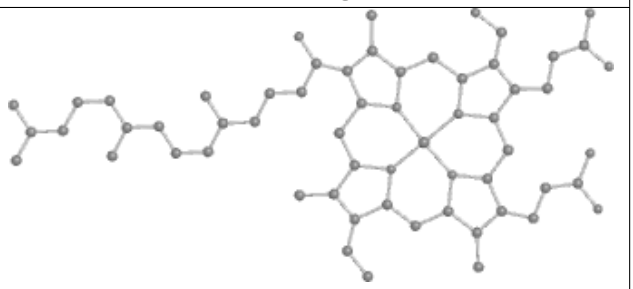
Bond lengths



Bond angles

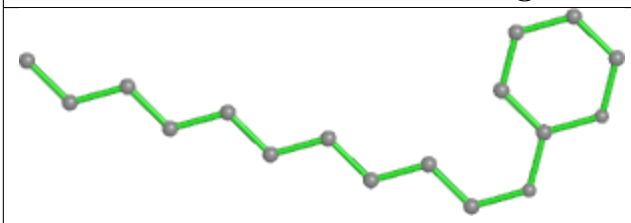


Torsions

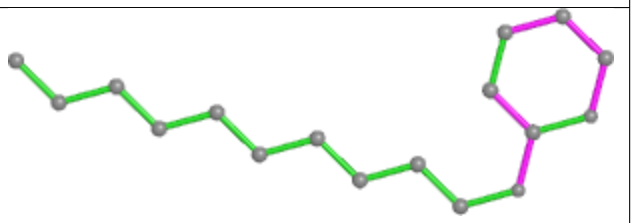


Rings

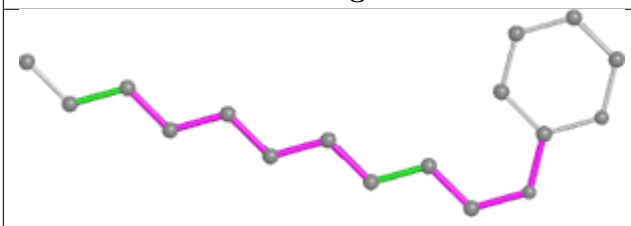
Ligand DMU N 610



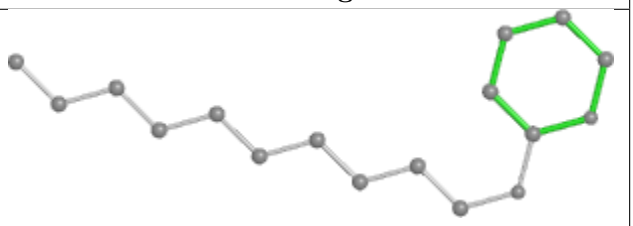
Bond lengths



Bond angles

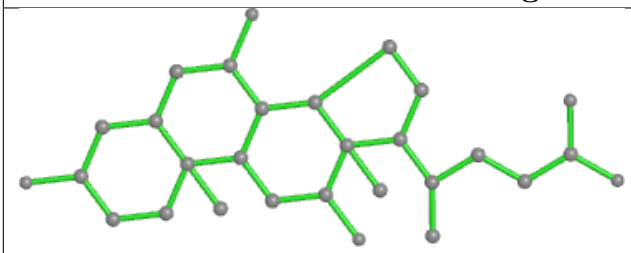


Torsions

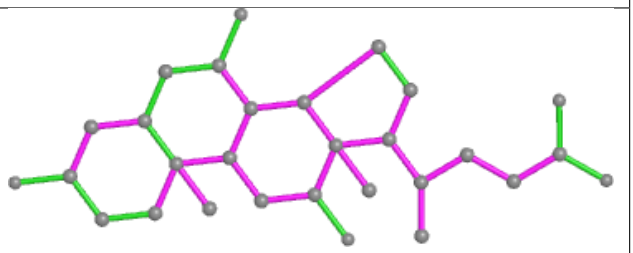


Rings

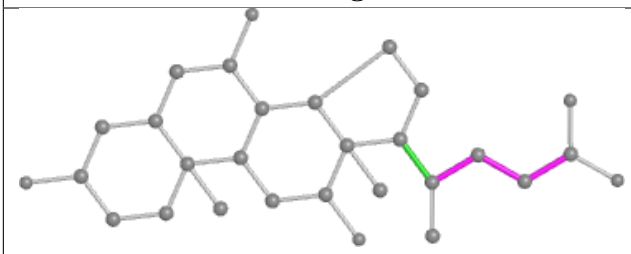
Ligand CHD P 308



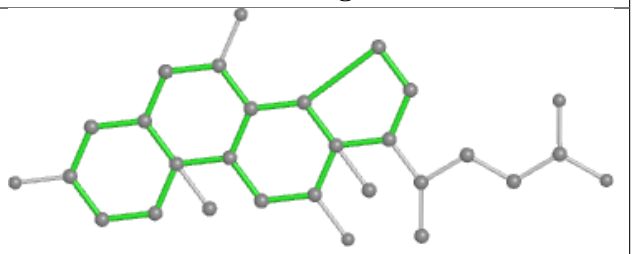
Bond lengths



Bond angles

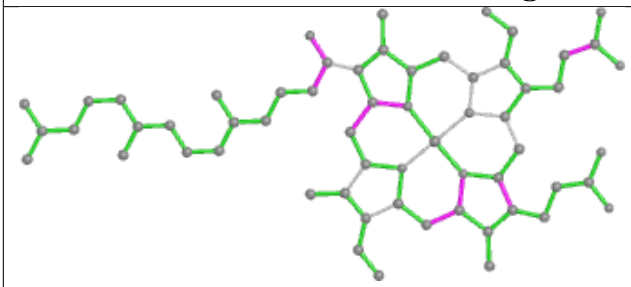


Torsions

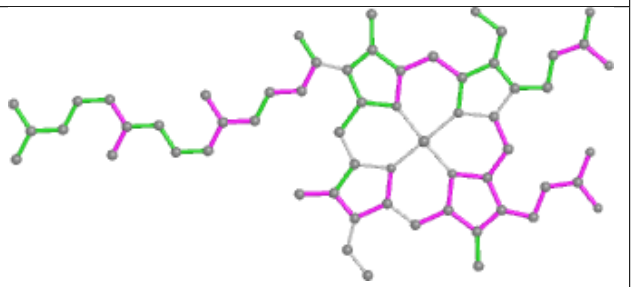


Rings

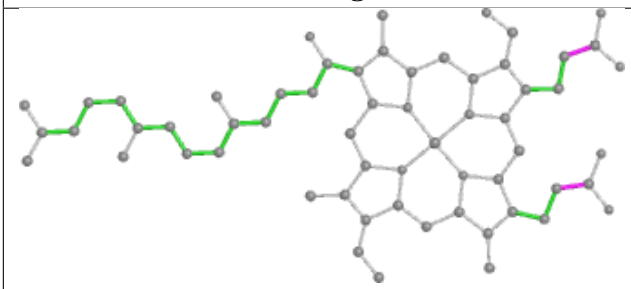
Ligand HEA N 602



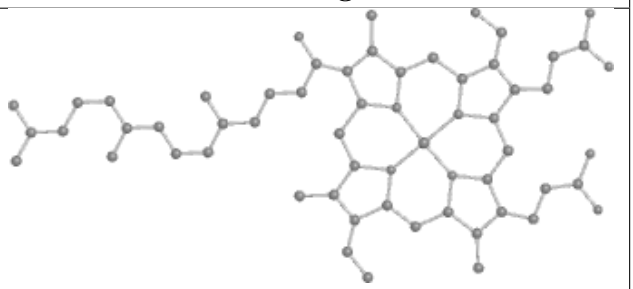
Bond lengths



Bond angles

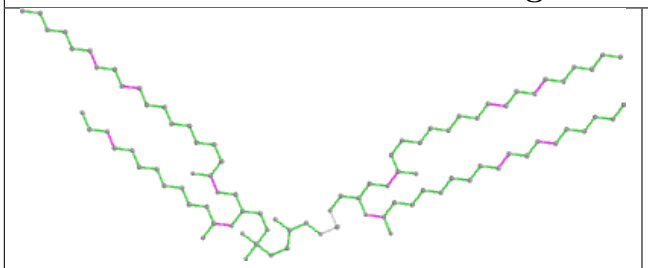


Torsions

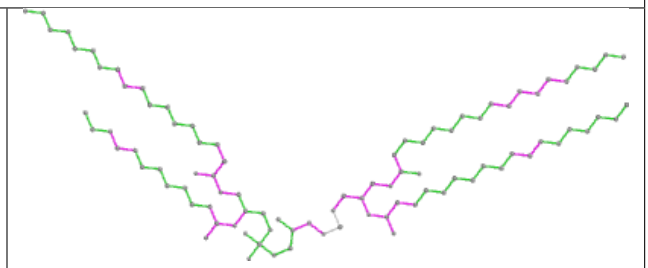


Rings

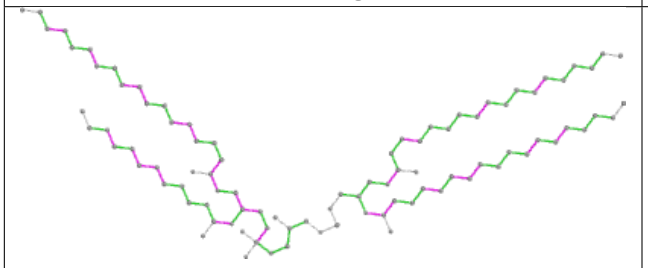
Ligand CDL T 101



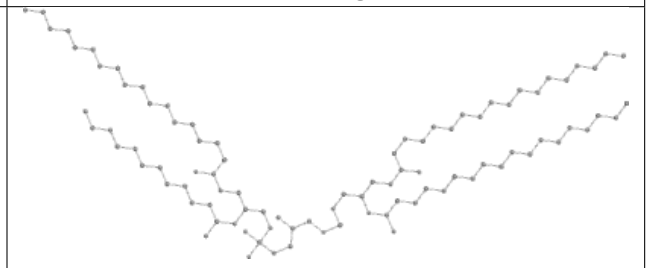
Bond lengths



Bond angles

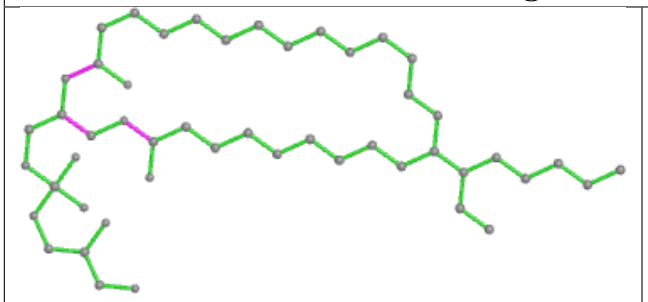


Torsions

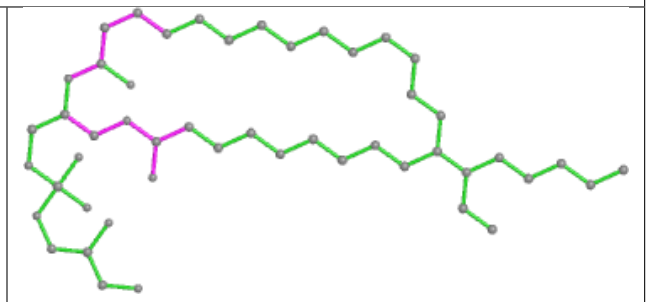


Rings

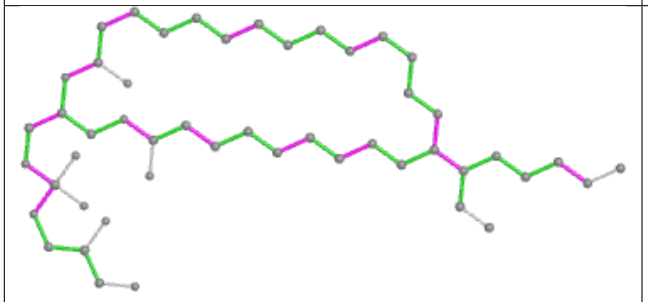
Ligand PGV C 306



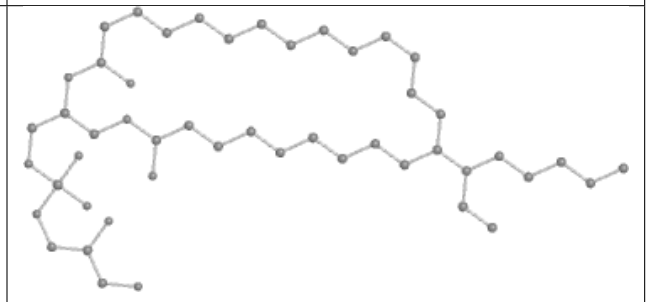
Bond lengths



Bond angles

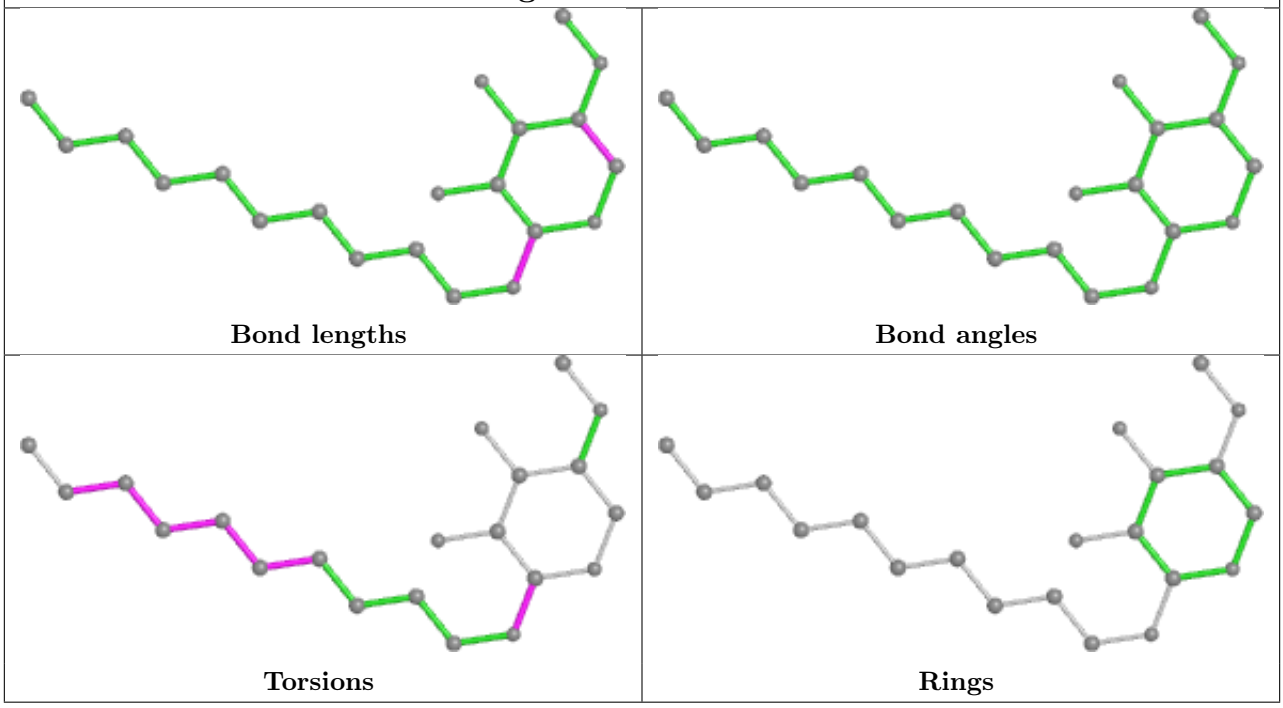


Torsions

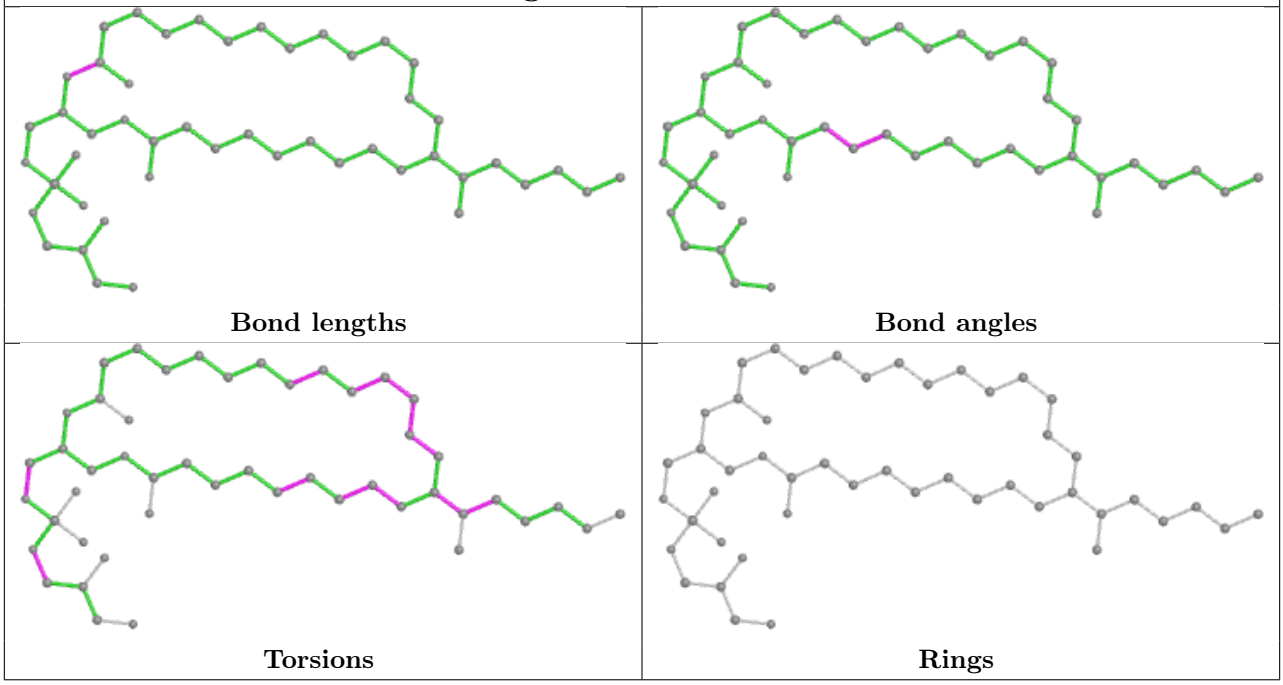


Rings

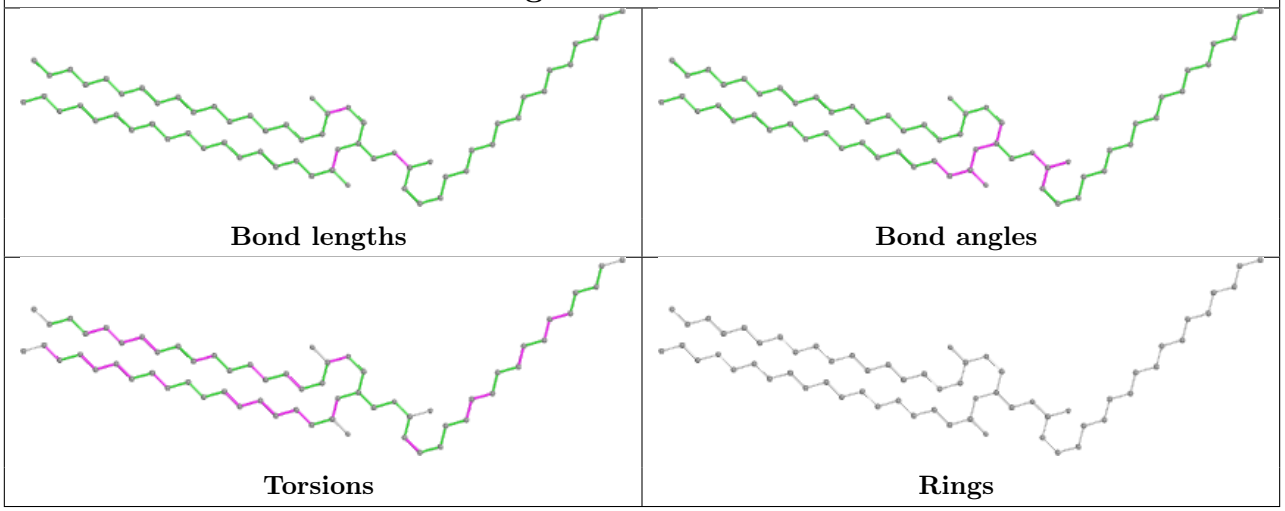
Ligand DMU T 102



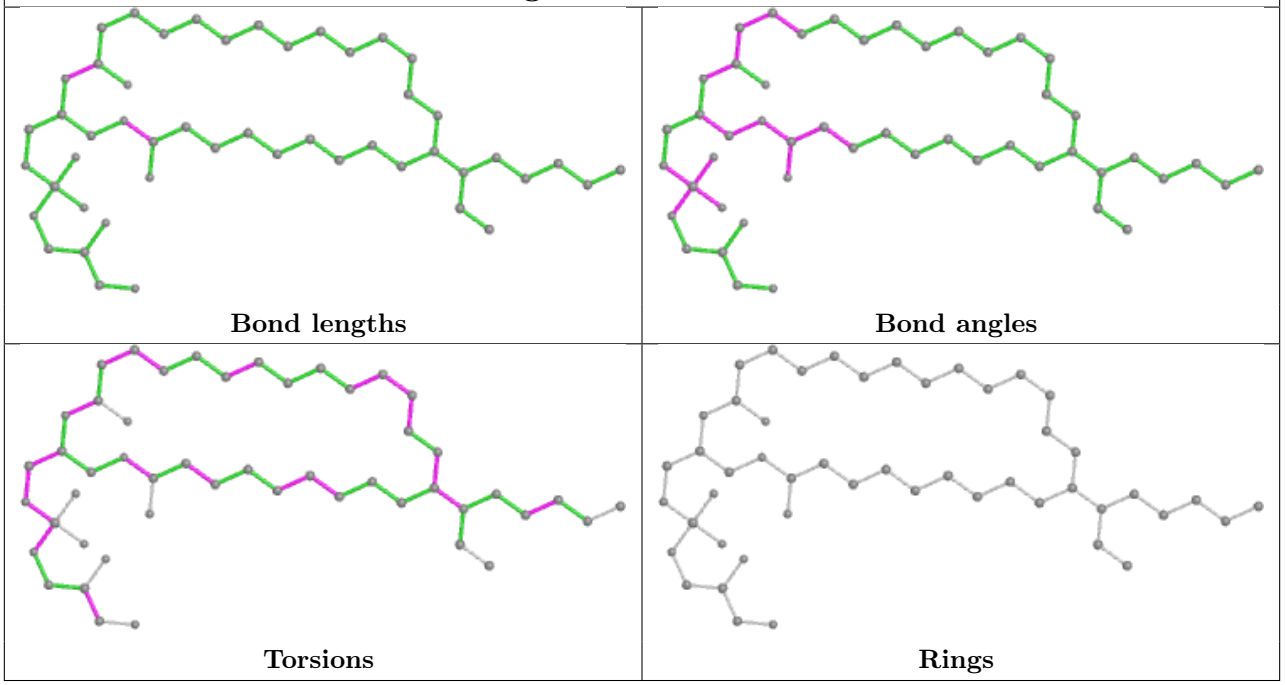
Ligand PGV C 305



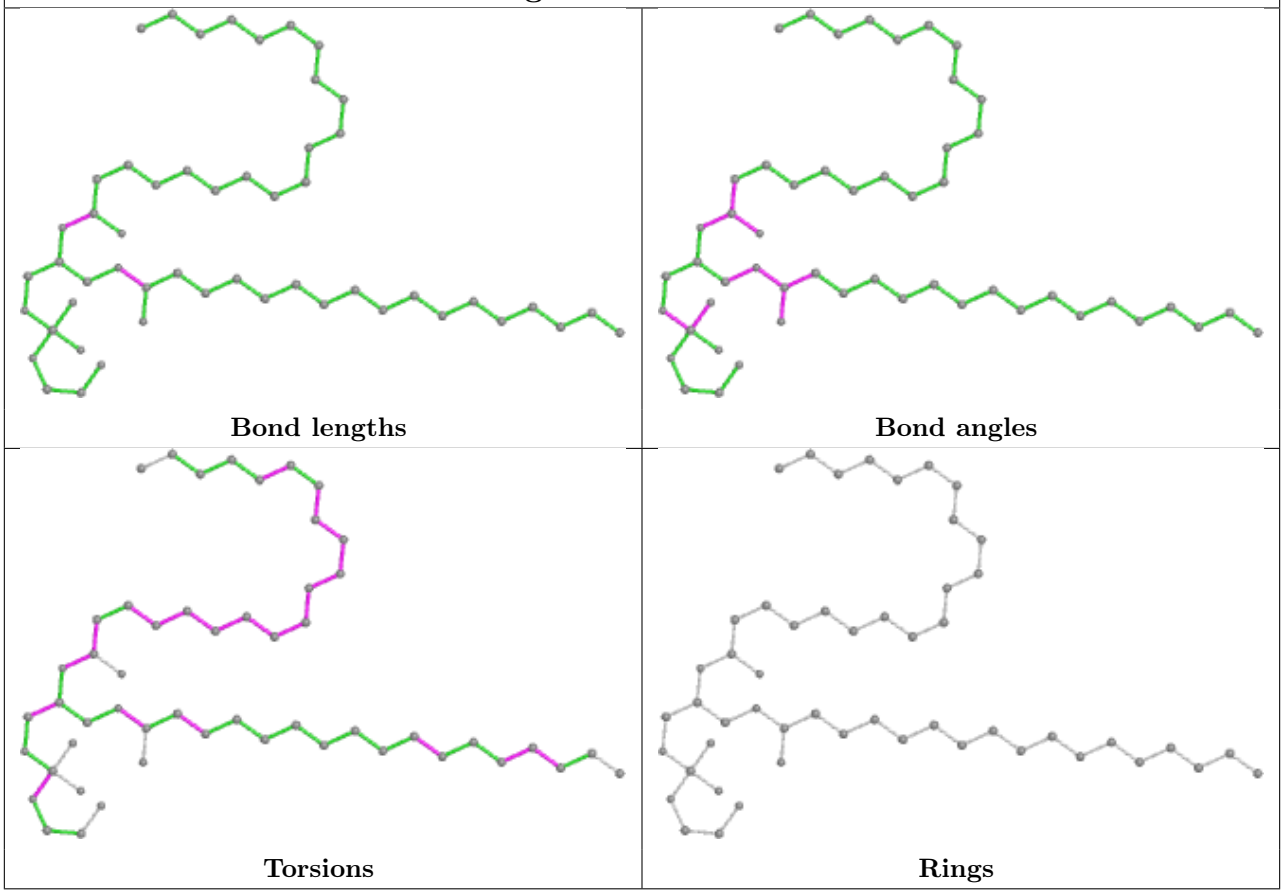
Ligand TGL B 301



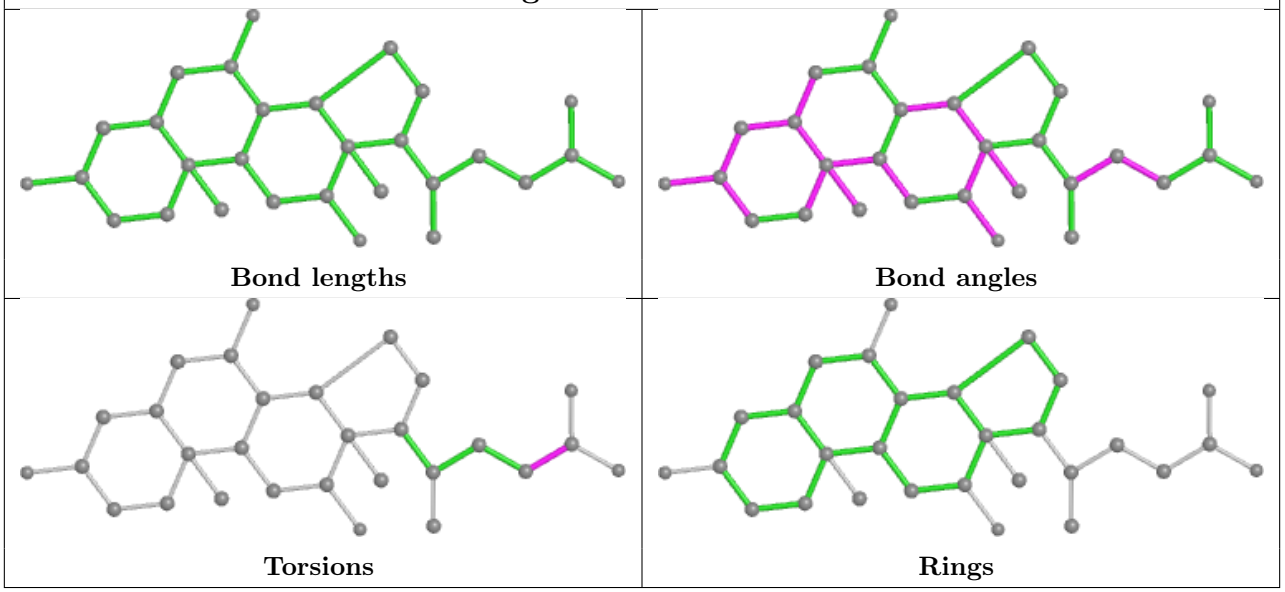
Ligand PGV P 306



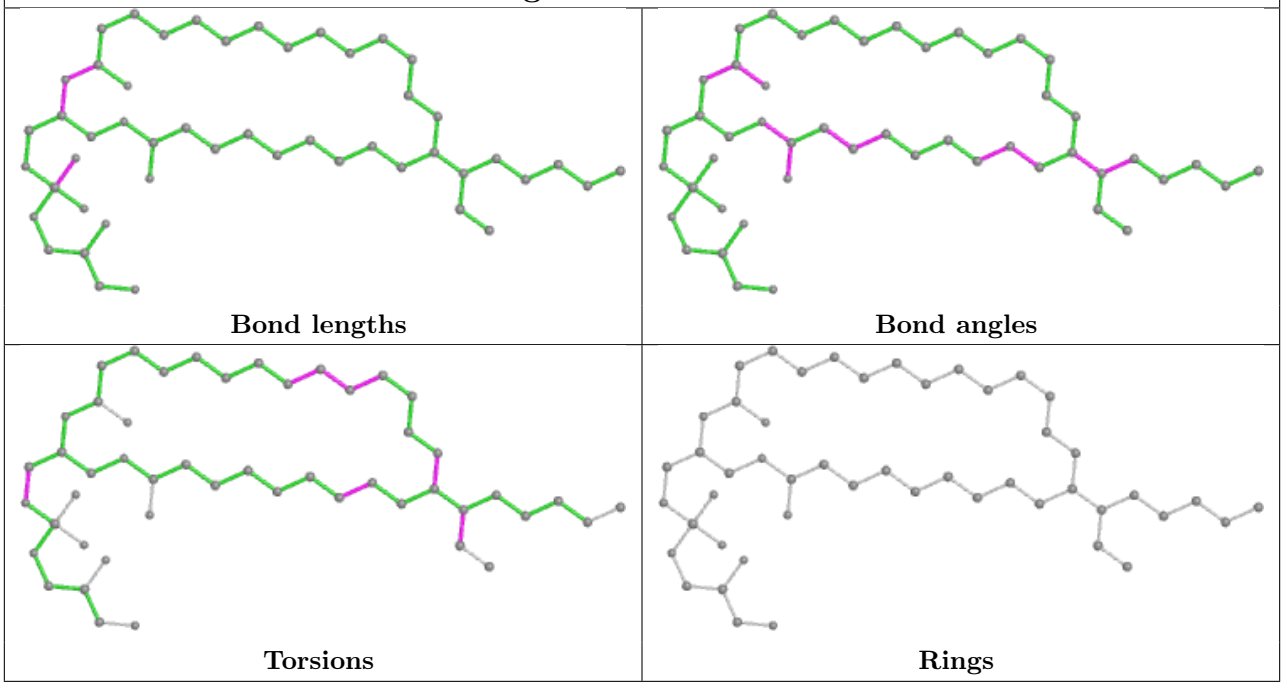
Ligand PEK P 304



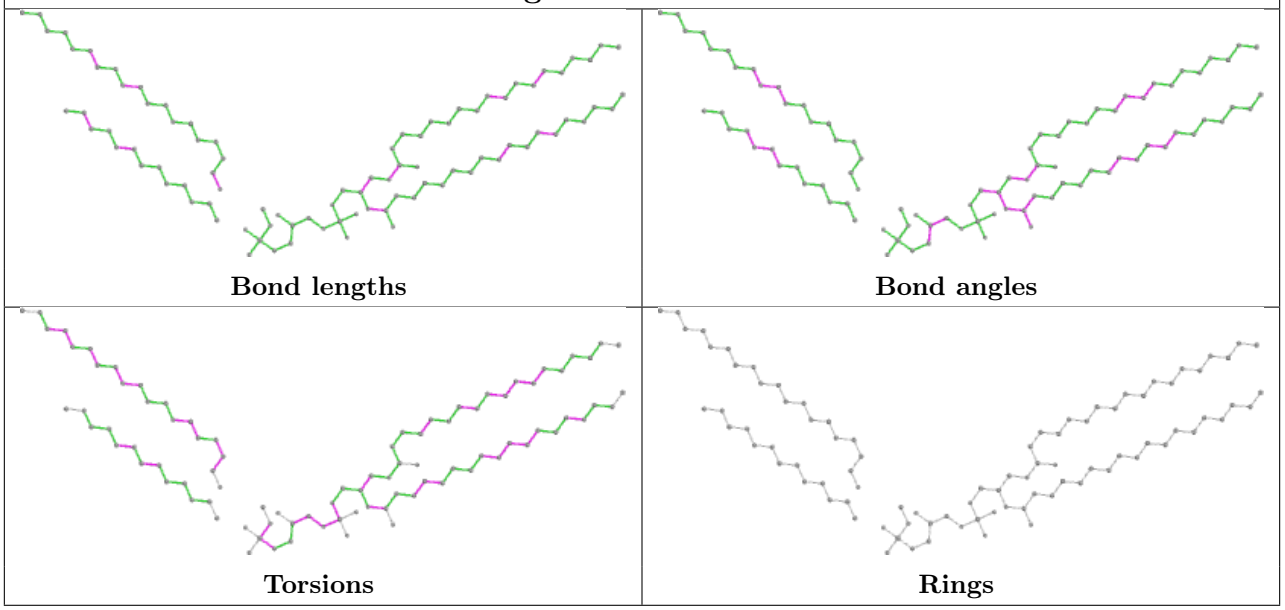
Ligand CHD B 305



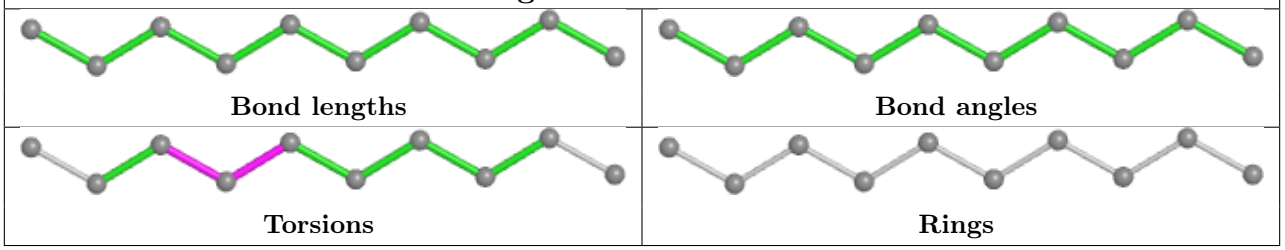
Ligand PGV P 305



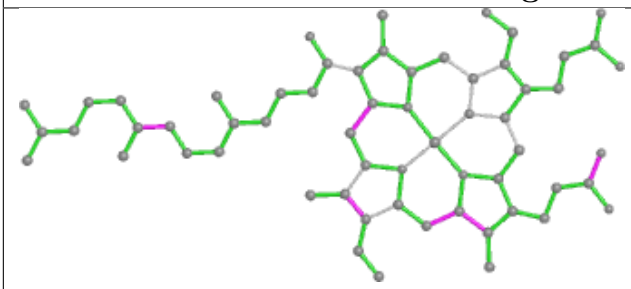
Ligand CDL G 101



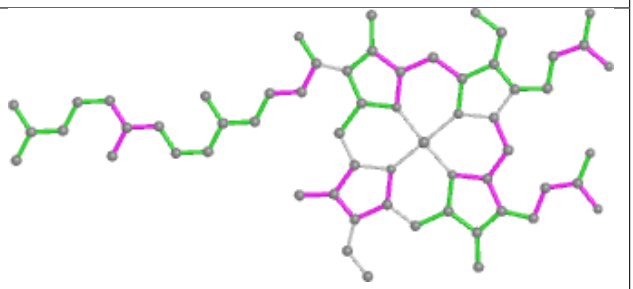
Ligand DMU X 101



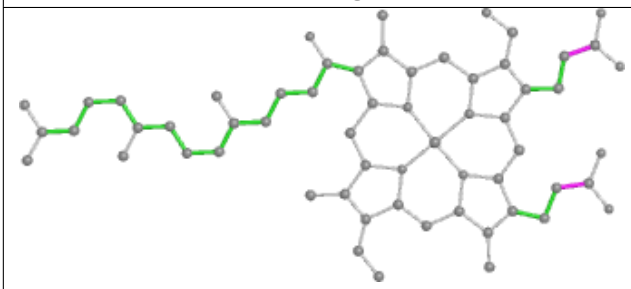
Ligand HEA A 602



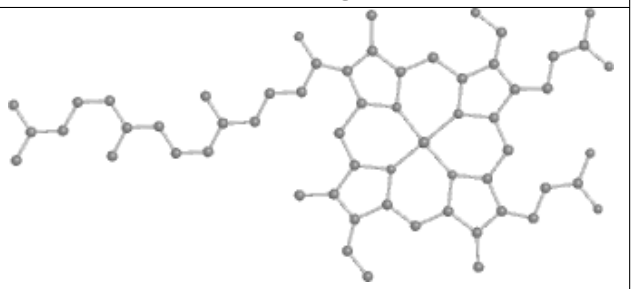
Bond lengths



Bond angles

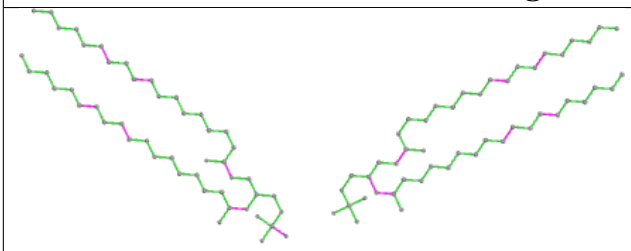


Torsions

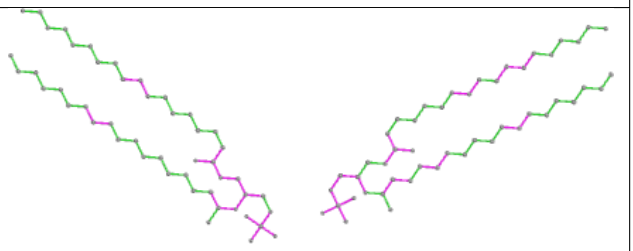


Rings

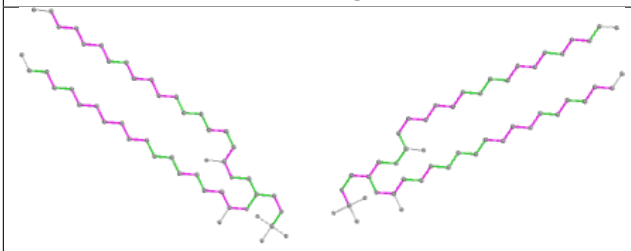
Ligand CDL C 307



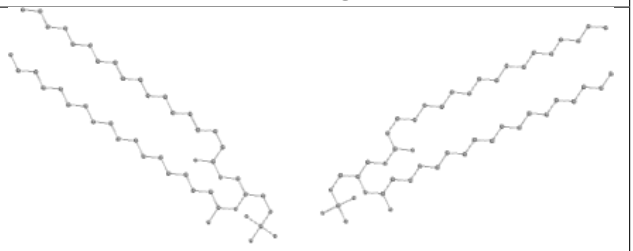
Bond lengths



Bond angles

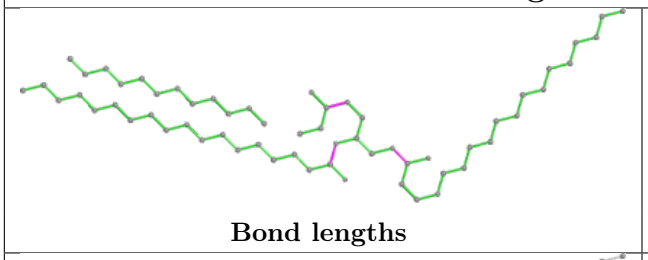


Torsions

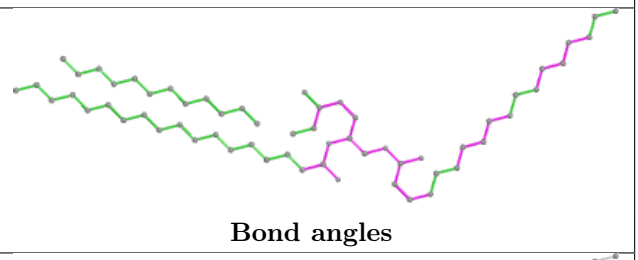


Rings

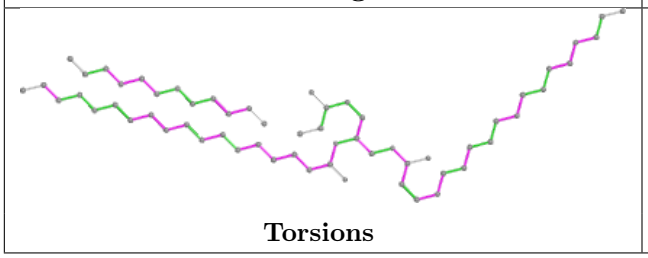
Ligand TGL L 101



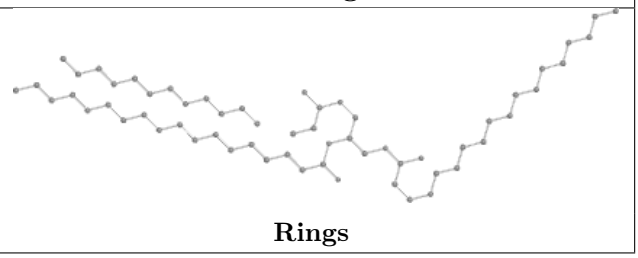
Bond lengths



Bond angles

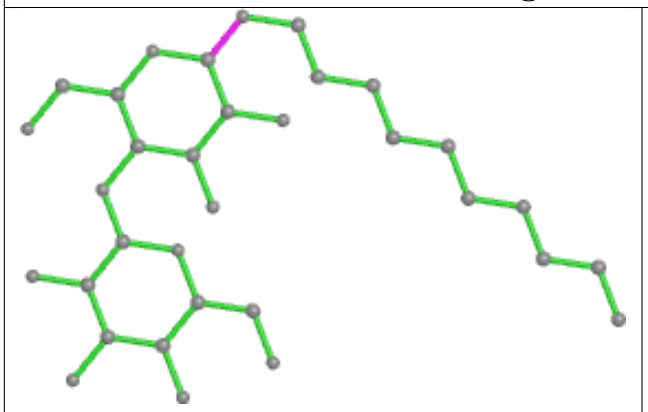


Torsions

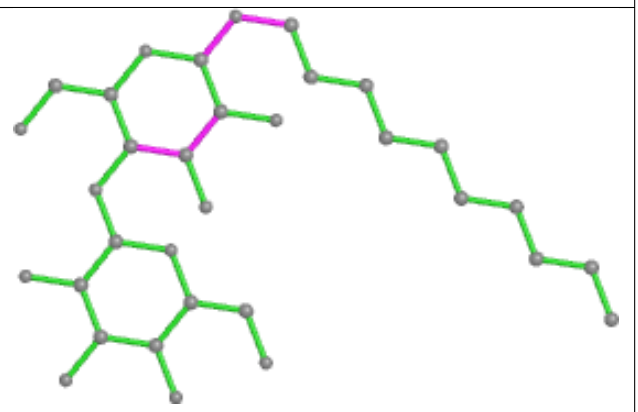


Rings

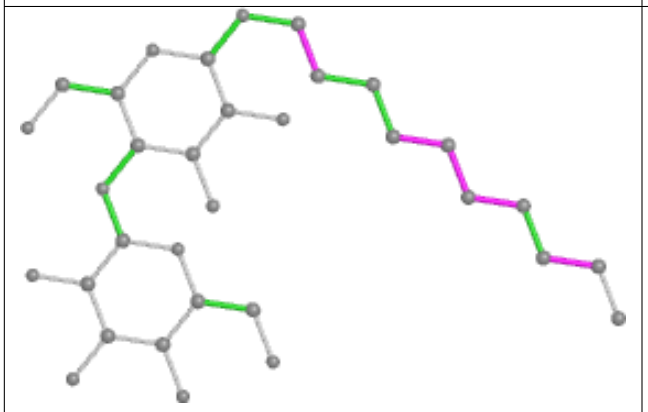
Ligand DMU Z 101



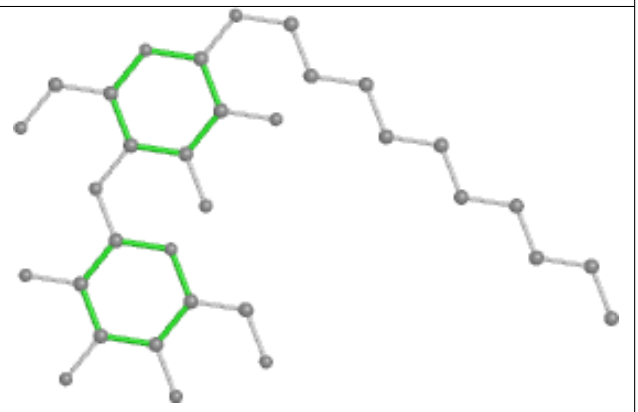
Bond lengths



Bond angles

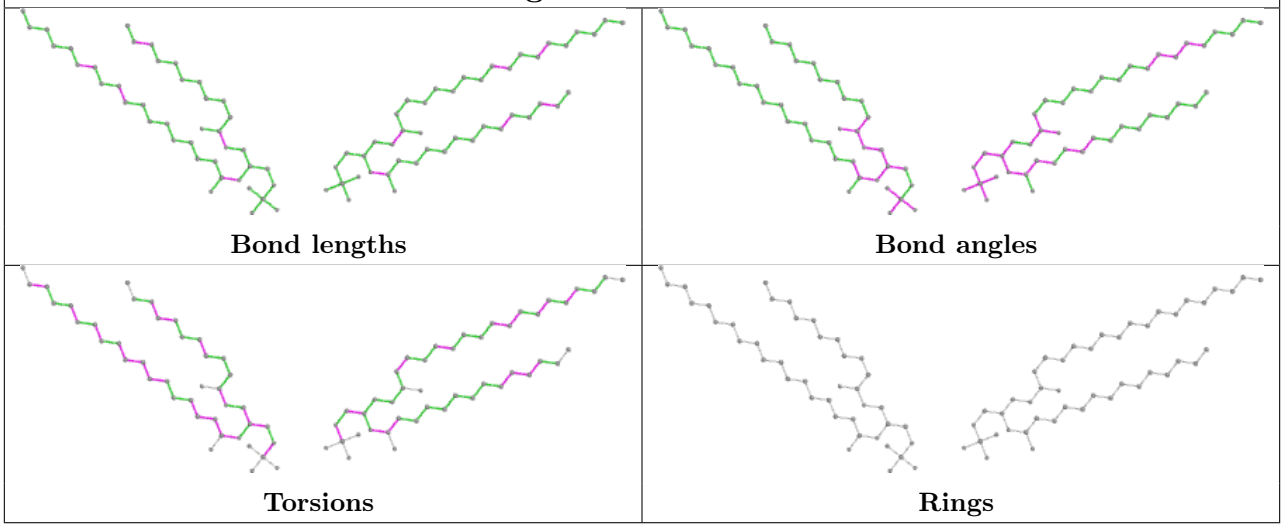


Torsions

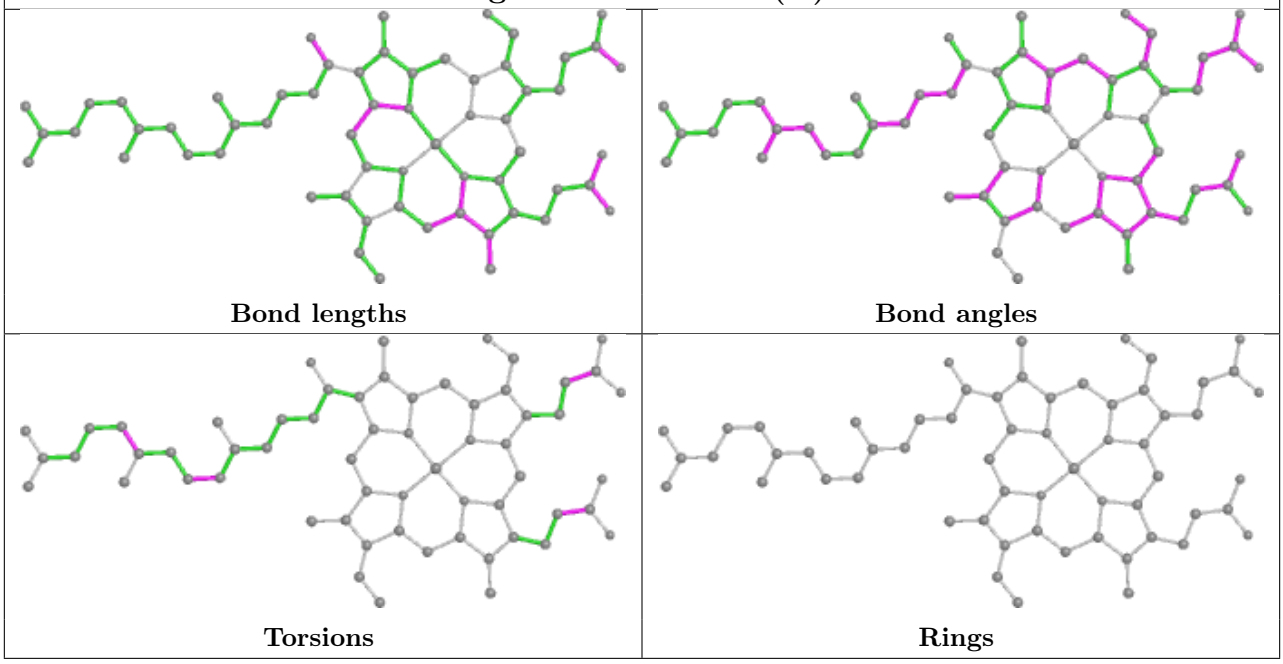


Rings

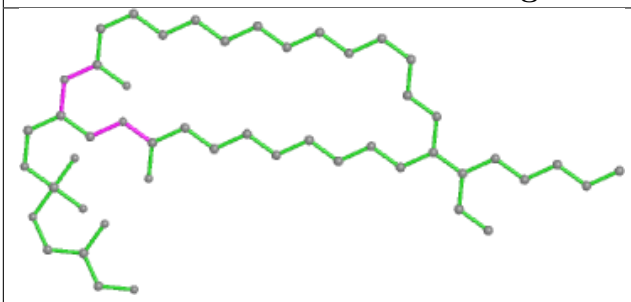
Ligand CDL P 307



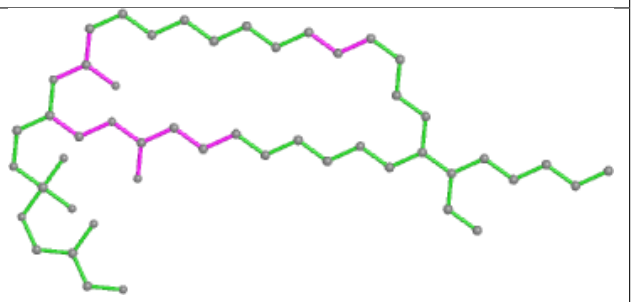
Ligand HEA N 601 (A)



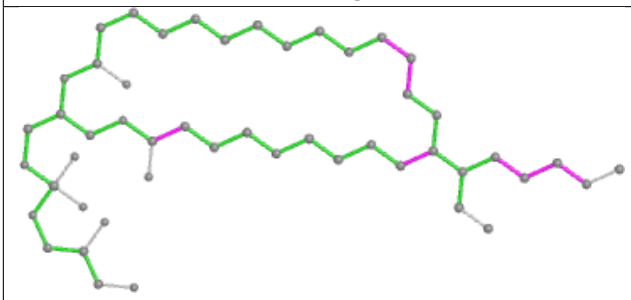
Ligand PGV N 609



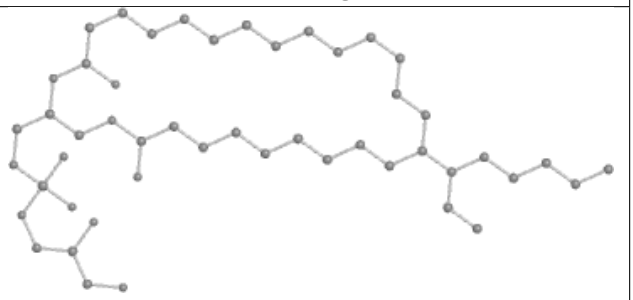
Bond lengths



Bond angles

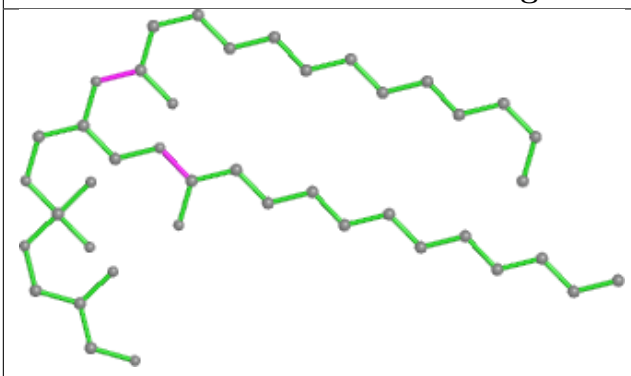


Torsions

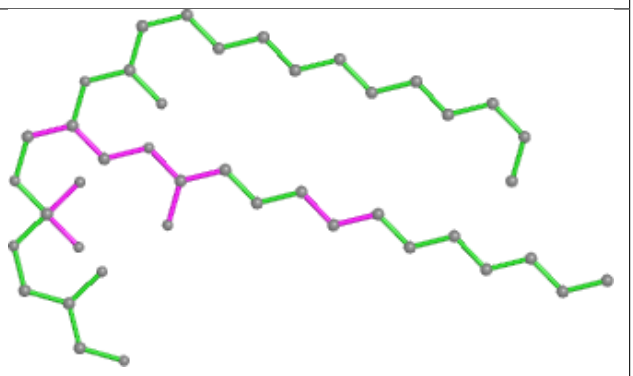


Rings

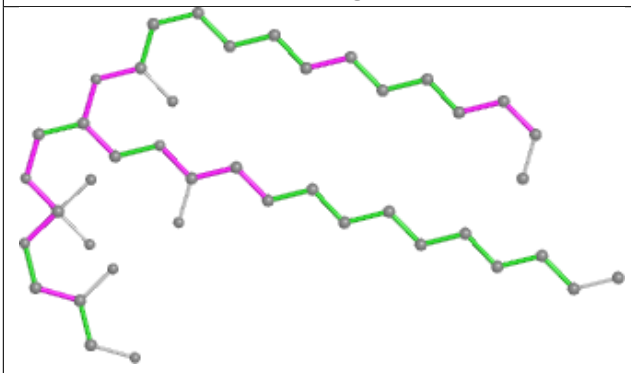
Ligand PGV N 608



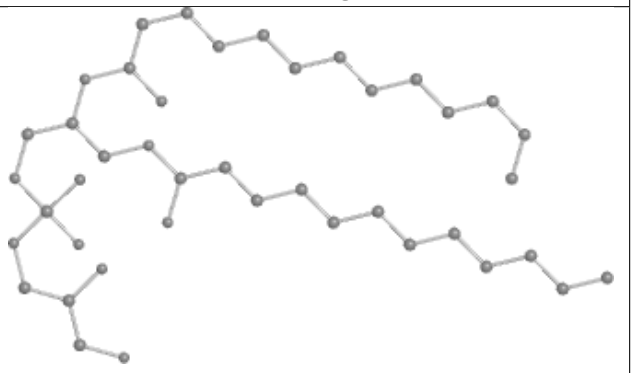
Bond lengths



Bond angles

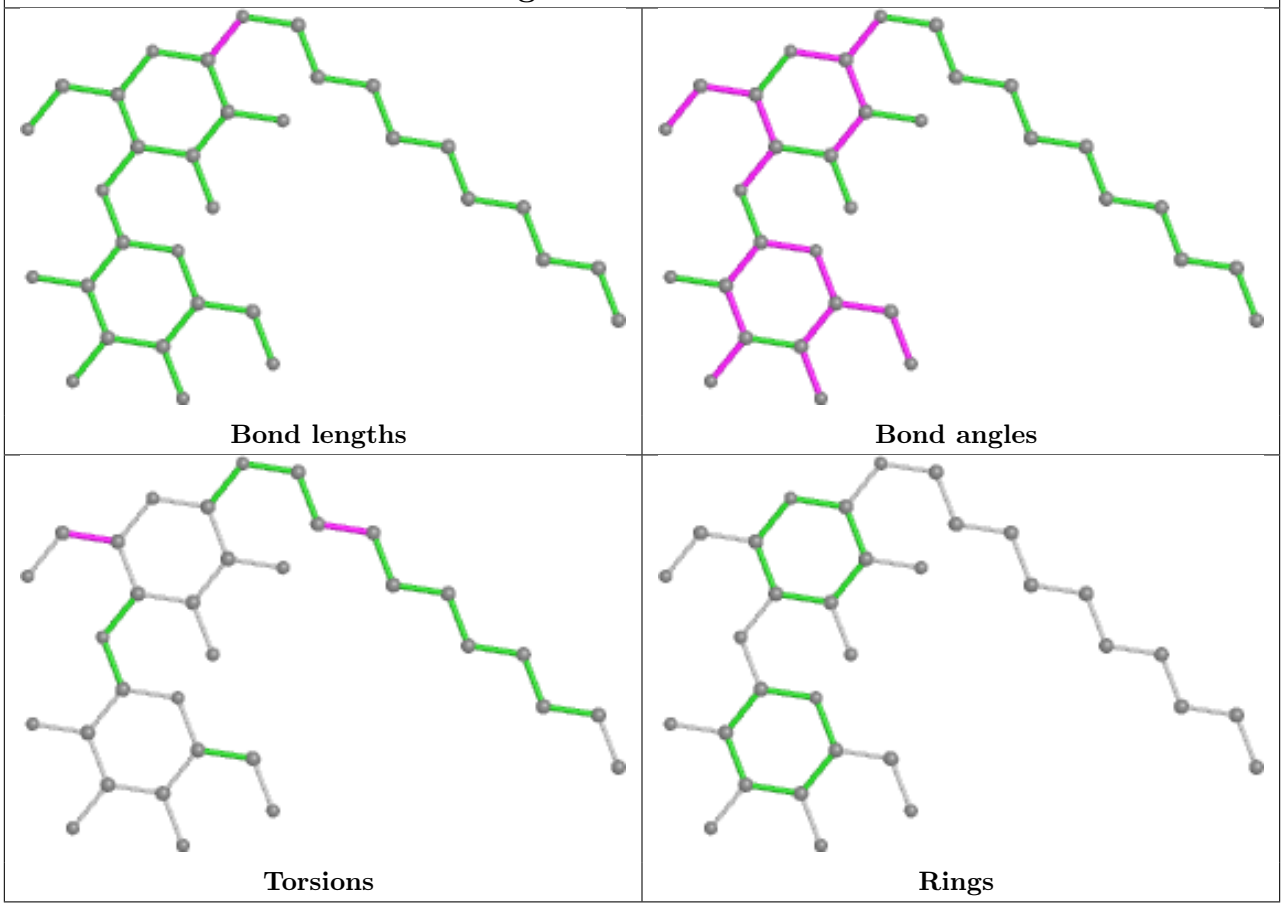


Torsions

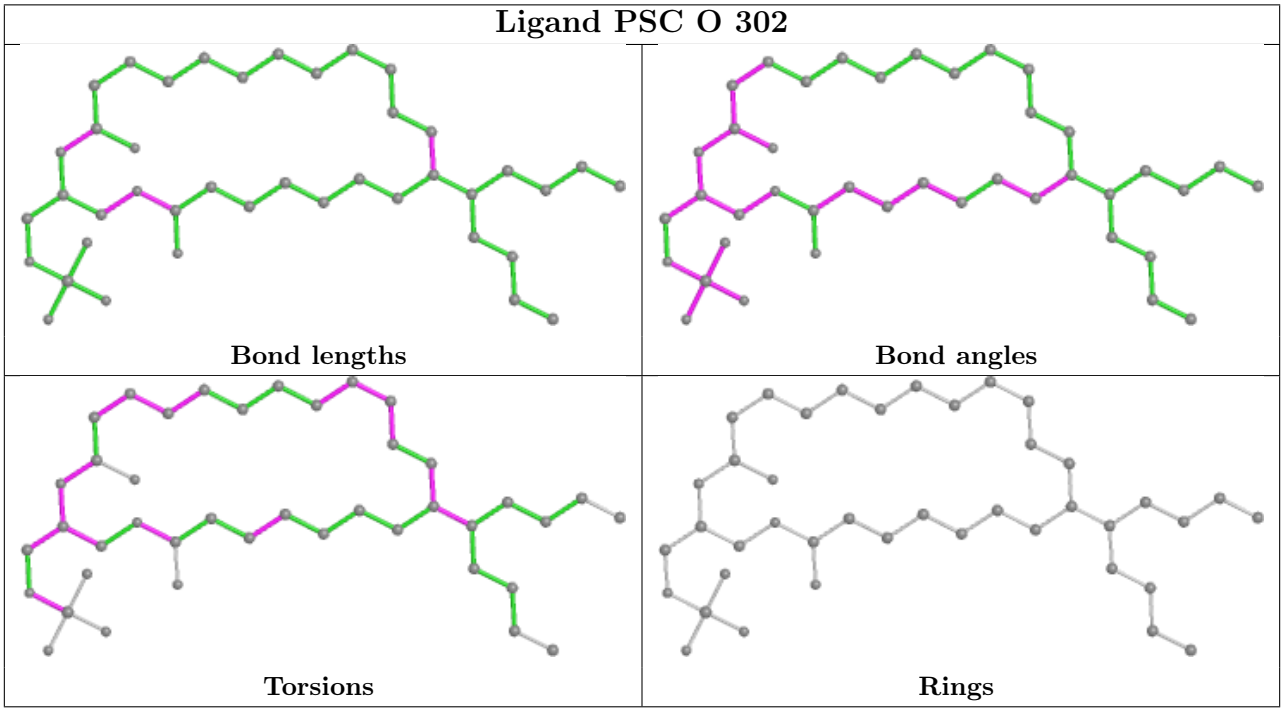


Rings

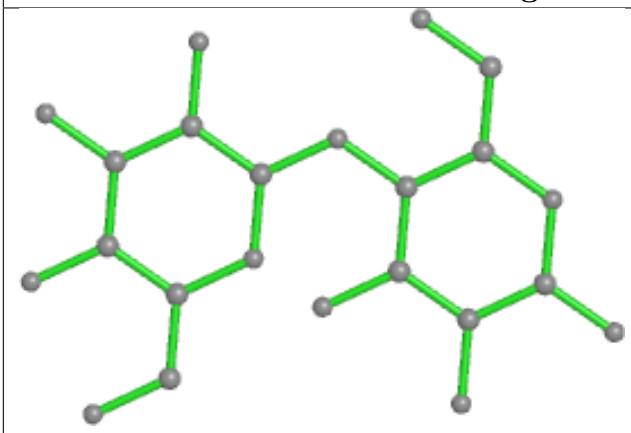
Ligand DMU C 310



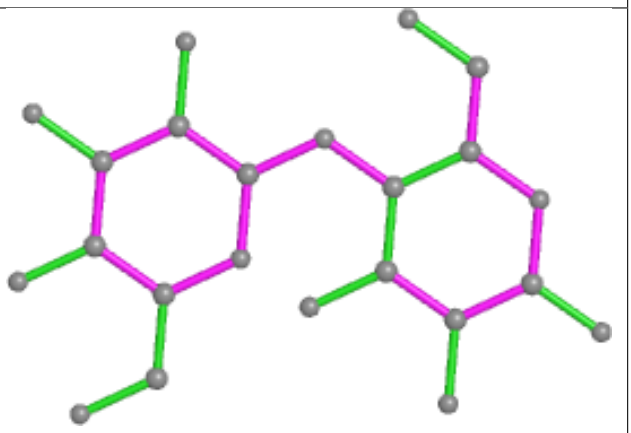
Ligand PSC O 302



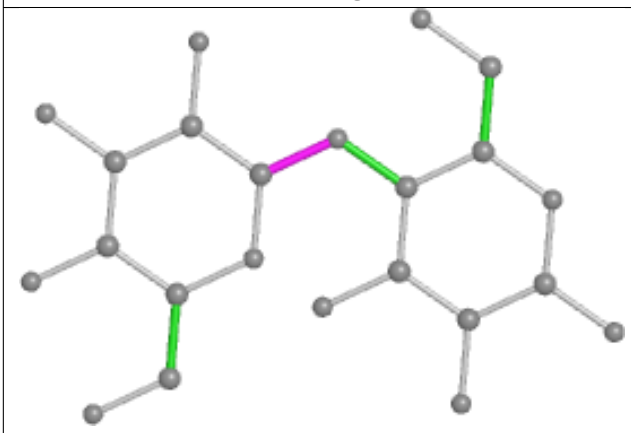
Ligand DMU J 101



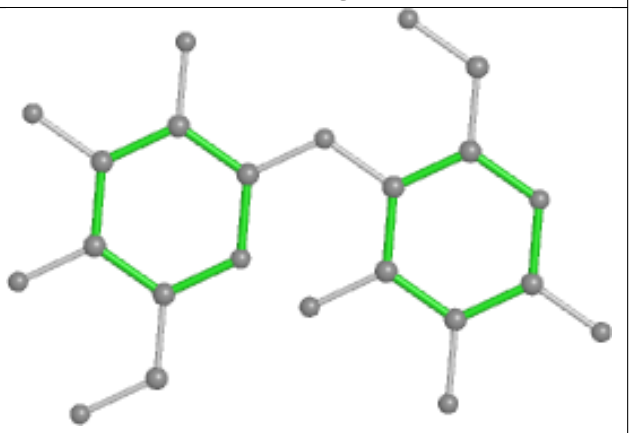
Bond lengths



Bond angles

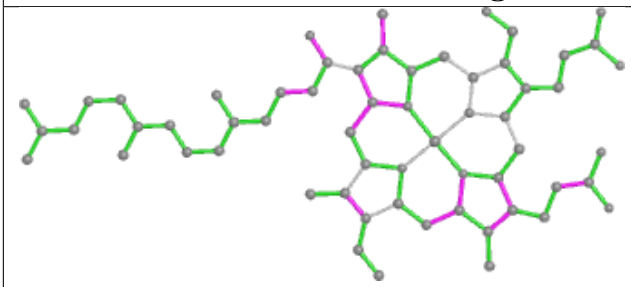


Torsions

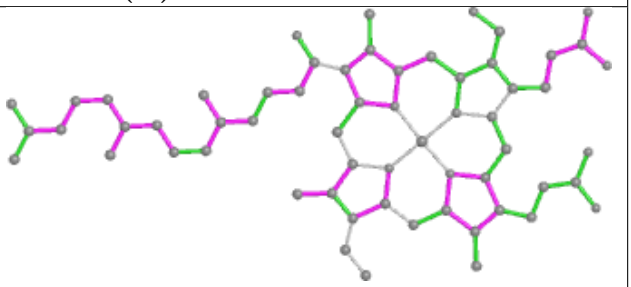


Rings

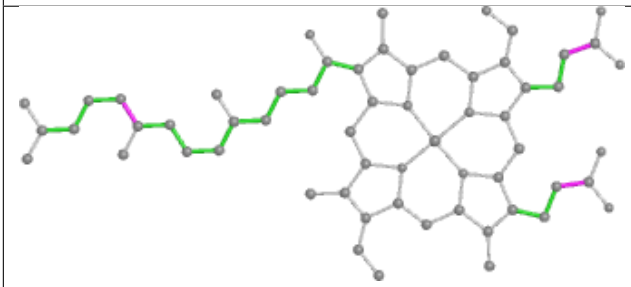
Ligand HEA A 601 (B)



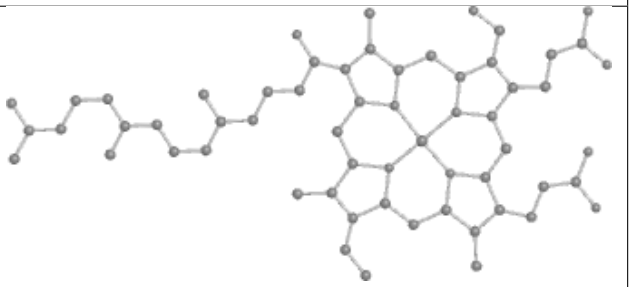
Bond lengths



Bond angles

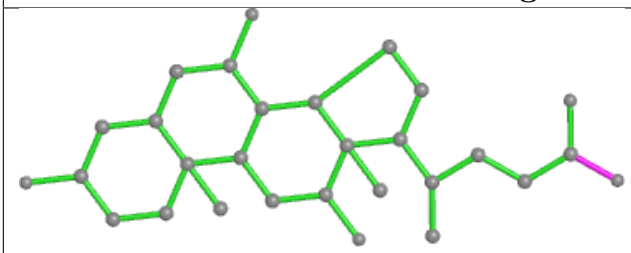


Torsions

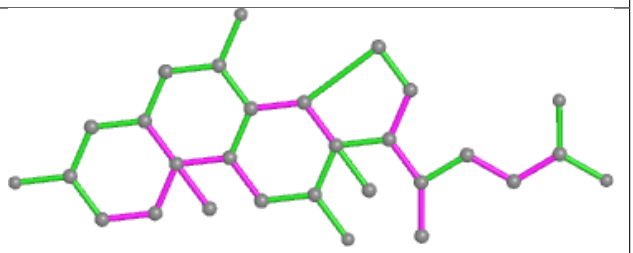


Rings

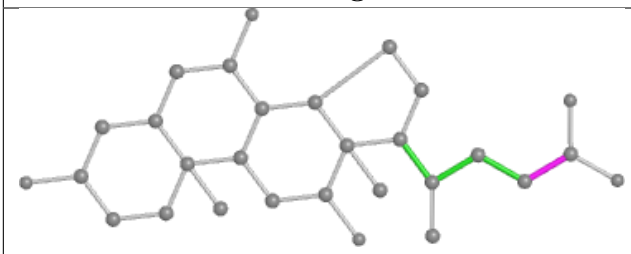
Ligand CHD G 102



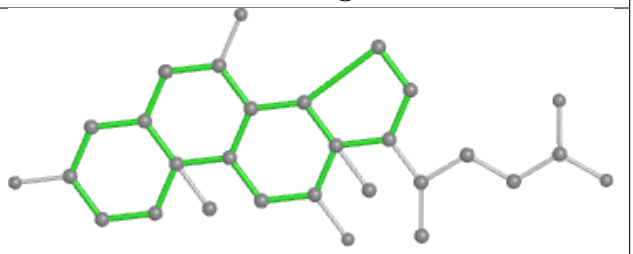
Bond lengths



Bond angles

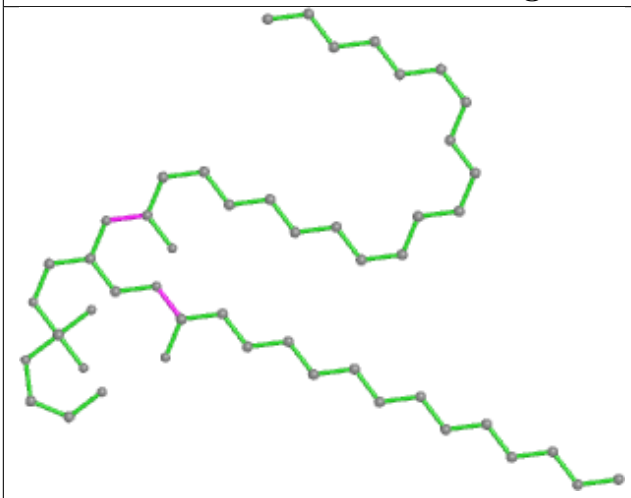


Torsions

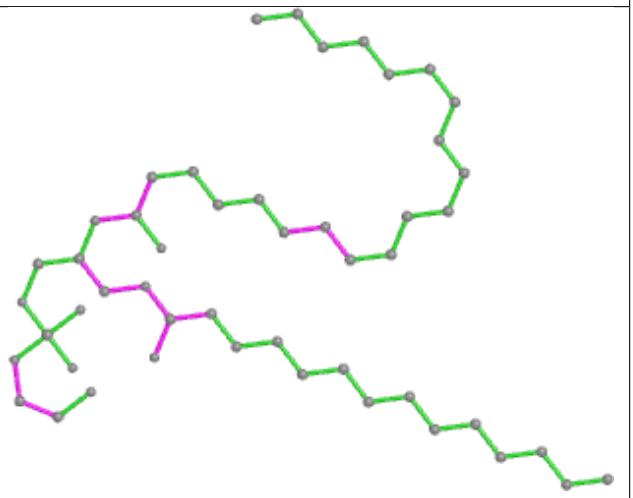


Rings

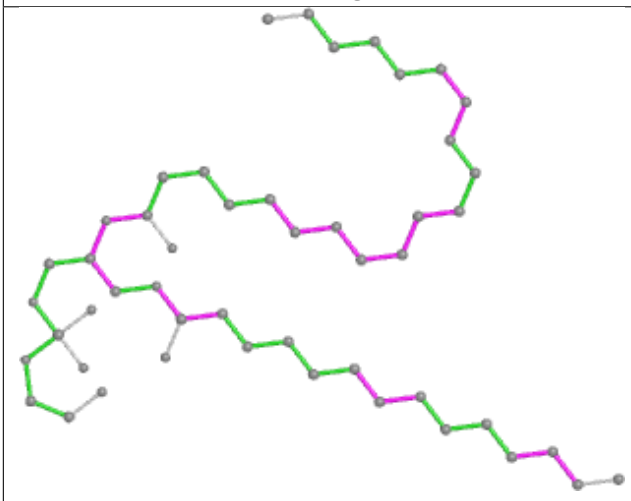
Ligand PEK C 302



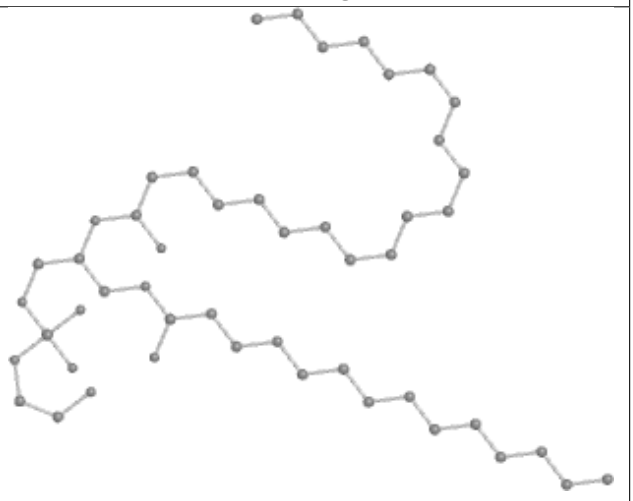
Bond lengths



Bond angles

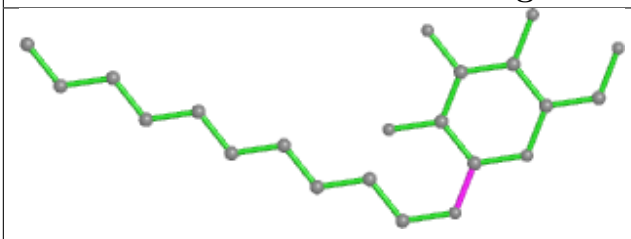


Torsions

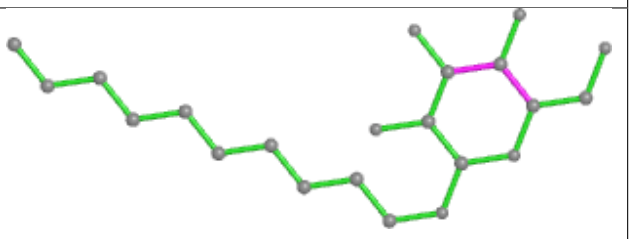


Rings

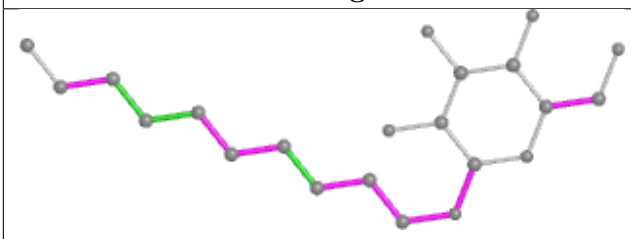
Ligand DMU X 102



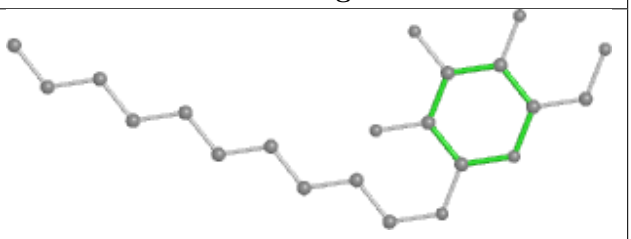
Bond lengths



Bond angles

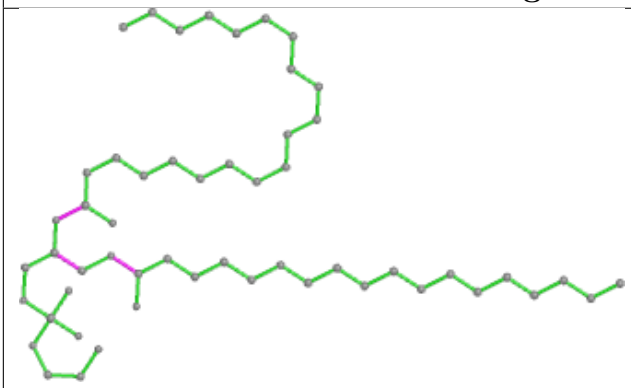


Torsions

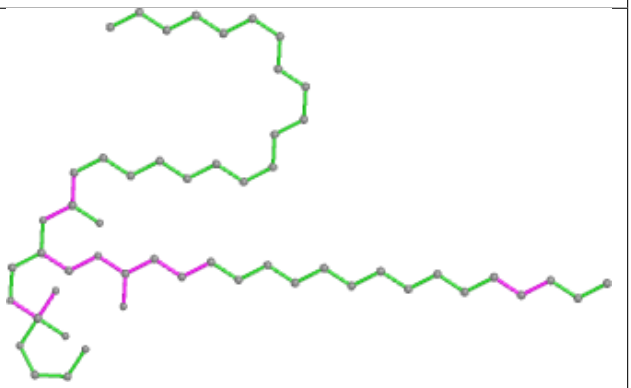


Rings

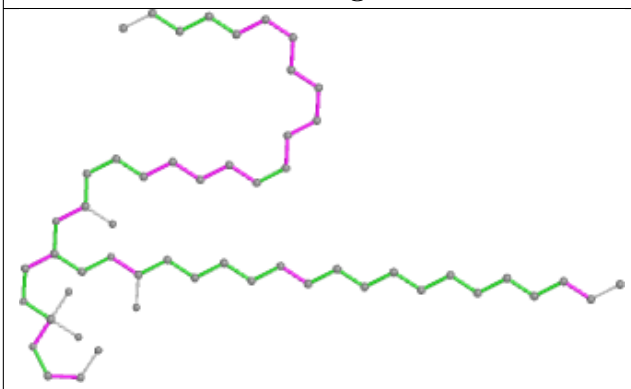
Ligand PEK C 304



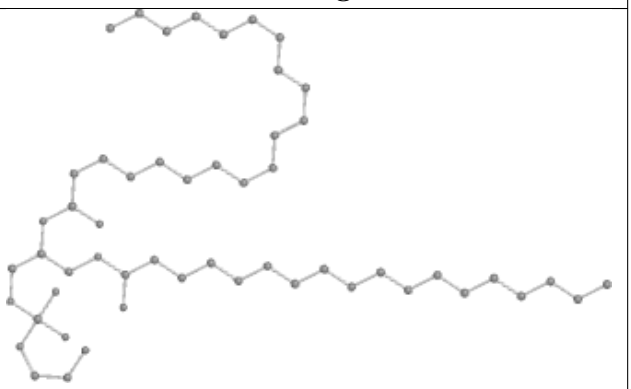
Bond lengths



Bond angles

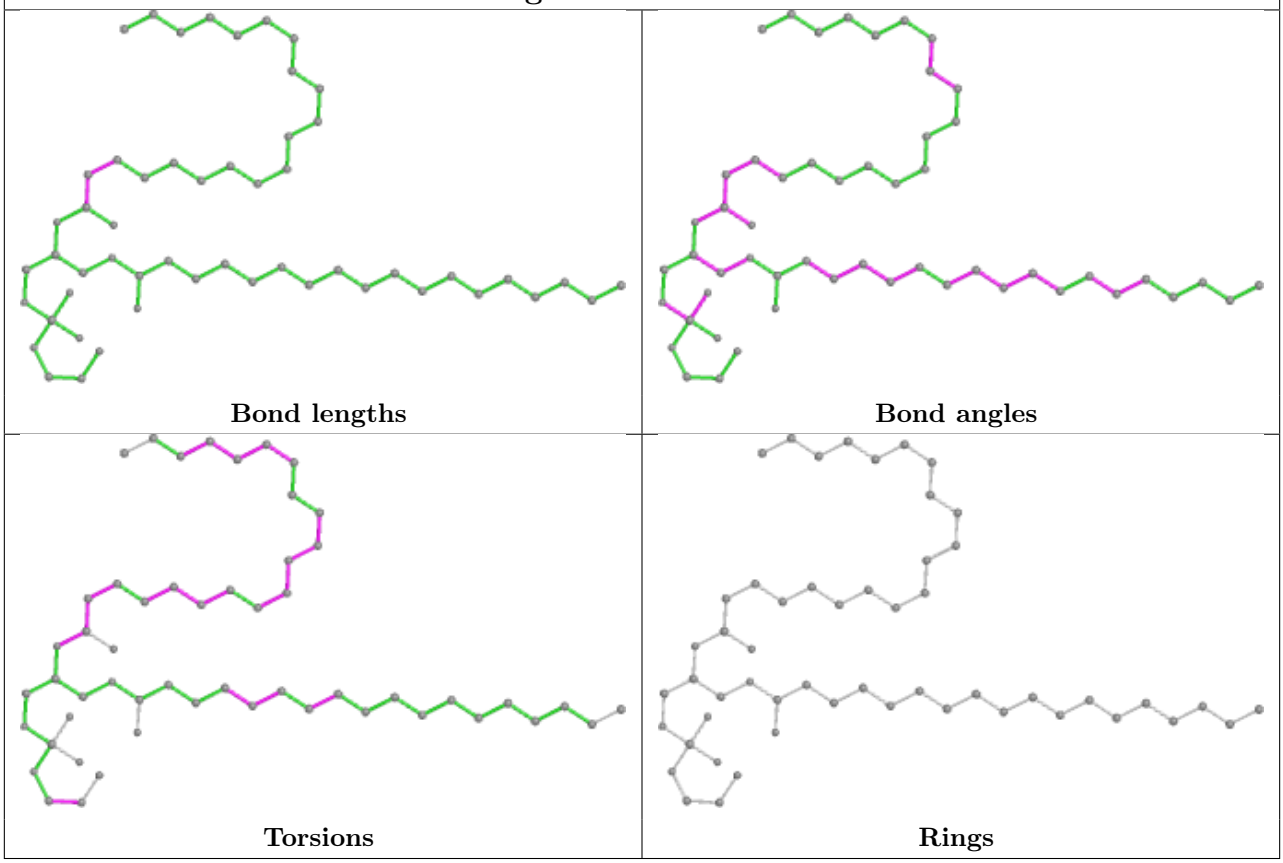


Torsions

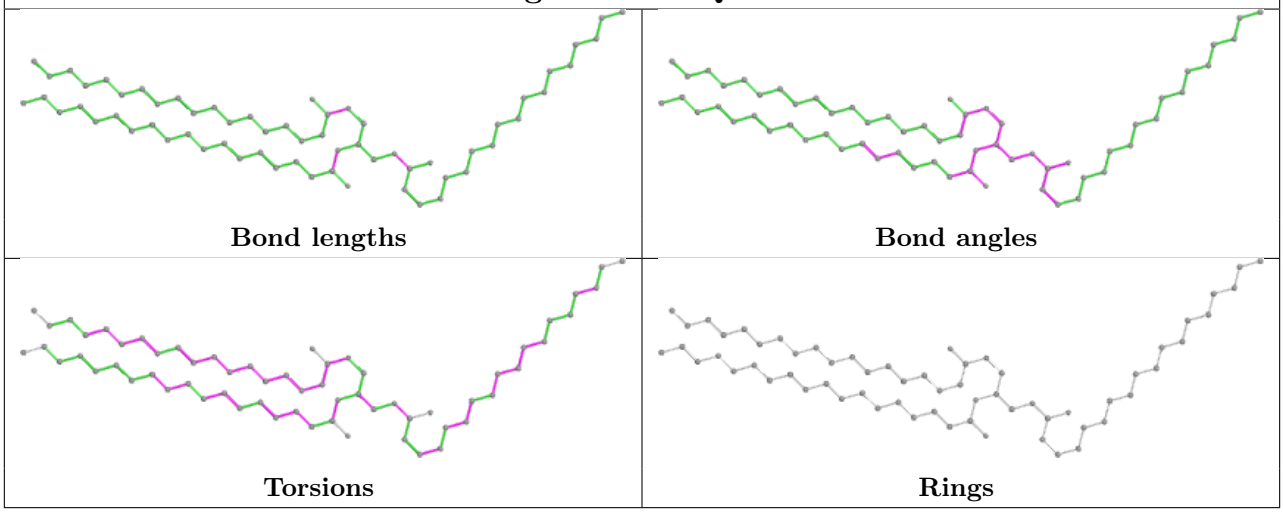


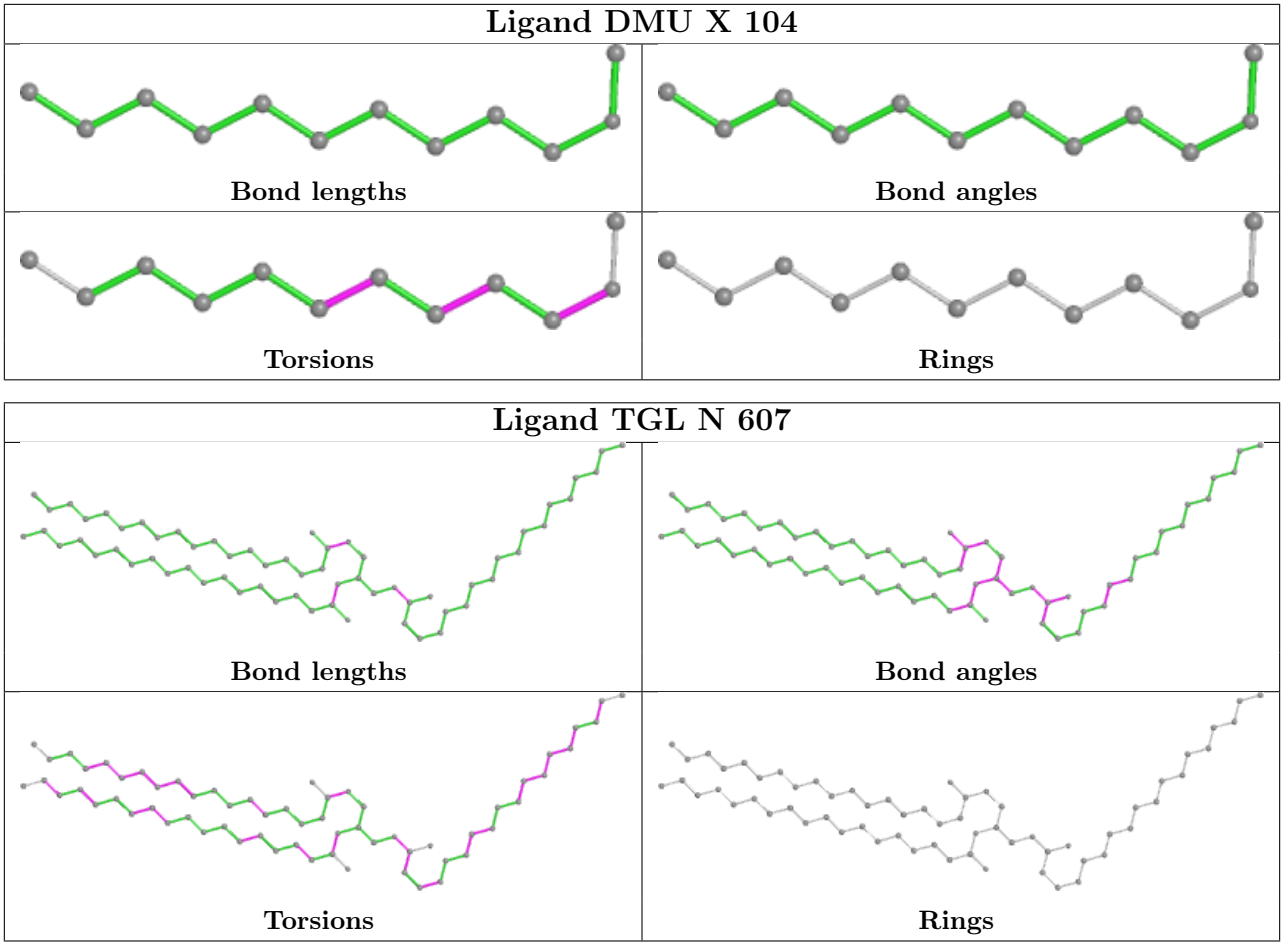
Rings

Ligand PEK P 303



Ligand TGL Q 201





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%)	-0.35	0 100 100	18, 22, 29, 77	0
1	N	512/514 (99%)	-0.41	0 100 100	19, 25, 34, 77	0
2	B	226/227 (99%)	-0.40	0 100 100	20, 28, 49, 91	0
2	O	226/227 (99%)	-0.37	2 (0%) 84 84	25, 34, 62, 102	0
3	C	259/259 (100%)	-0.39	0 100 100	20, 26, 37, 75	0
3	P	259/259 (100%)	-0.40	1 (0%) 92 92	21, 27, 40, 85	0
4	D	144/144 (100%)	-0.54	0 100 100	23, 30, 51, 83	0
4	Q	138/144 (95%)	-0.05	1 (0%) 87 87	30, 42, 74, 101	0
5	E	105/105 (100%)	-0.51	1 (0%) 82 82	24, 30, 56, 134	0
5	R	105/105 (100%)	-0.42	2 (1%) 66 65	26, 37, 63, 149	0
6	F	94/94 (100%)	-0.24	3 (3%) 47 44	21, 31, 63, 144	0
6	S	94/94 (100%)	-0.22	4 (4%) 35 32	22, 32, 60, 141	0
7	G	83/84 (98%)	0.45	13 (15%) 2 1	24, 34, 122, 164	0
7	T	83/84 (98%)	0.50	14 (16%) 1 1	23, 37, 114, 175	0
8	H	79/79 (100%)	0.14	7 (8%) 9 8	26, 35, 101, 127	0
8	U	79/79 (100%)	0.04	6 (7%) 13 12	31, 40, 108, 151	0
9	I	72/73 (98%)	-0.10	2 (2%) 53 50	27, 41, 71, 88	0
9	V	72/73 (98%)	0.01	3 (4%) 36 33	27, 49, 77, 156	0
10	J	58/58 (100%)	-0.14	2 (3%) 45 42	25, 36, 70, 142	0
10	W	58/58 (100%)	-0.19	4 (6%) 16 15	28, 39, 77, 170	0
11	K	49/49 (100%)	-0.42	0 100 100	27, 35, 51, 58	0
11	X	49/49 (100%)	-0.17	1 (2%) 65 64	35, 46, 73, 99	0
12	L	46/46 (100%)	-0.36	0 100 100	23, 27, 58, 87	0
12	Y	46/46 (100%)	-0.34	1 (2%) 62 60	28, 35, 62, 121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/43 (100%)	-0.10	3 (6%)	16	15	24, 28, 67, 122	0
13	Z	43/43 (100%)	-0.05	3 (6%)	16	15	32, 38, 82, 225	0
All	All	3535/3550 (99%)	-0.28	73 (2%)	63	62	18, 29, 65, 225	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	12.3
7	T	3	ALA	10.8
6	S	1	ALA	10.6
8	H	8	ILE	9.7
6	F	2	SER	9.0

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, 95th 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	0.34	0.34	188,205,220,225	0
7	TPO	G	11	11/12	0.69	0.30	61,113,143,248	0
7	TPO	T	11	11/12	0.75	0.31	66,125,184,270	0
9	SAC	I	1	9/10	0.78	0.28	94,112,142,154	0
1	FME	N	1	10/11	0.88	0.14	35,44,82,153	0
1	FME	A	1	10/11	0.94	0.10	34,43,84,159	0
2	FME	B	1	10/11	0.95	0.11	18,28,34,66	0
2	FME	O	1	10/11	0.98	0.08	32,35,40,95	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, 95th 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
27	DMU	O	303	33/33	0.25	0.34	64,83,90,92	0
20	EDO	A	622	4/4	0.30	0.36	59,70,82,92	0
27	DMU	N	610	17/33	0.35	0.34	68,77,89,90	0
20	EDO	E	211	4/4	0.35	0.18	52,60,66,70	0
20	EDO	K	102	4/4	0.37	0.17	60,65,68,71	0
20	EDO	Y	105	4/4	0.40	0.21	65,68,73,78	0
20	EDO	Q	203	4/4	0.45	0.17	62,62,66,70	0
20	EDO	L	106	4/4	0.45	0.14	49,65,74,75	0
20	EDO	V	103	4/4	0.46	0.30	66,79,84,85	0
20	EDO	D	212	4/4	0.46	0.22	59,68,73,78	0
20	EDO	N	623	4/4	0.47	0.28	72,78,84,92	0
27	DMU	C	310	33/33	0.47	0.26	63,80,88,93	0
20	EDO	D	207	4/4	0.52	0.23	66,68,71,76	0
27	DMU	P	310	33/33	0.53	0.30	39,78,84,87	0
20	EDO	D	213	4/4	0.57	0.19	74,75,78,80	0
20	EDO	J	102	4/4	0.57	0.12	61,69,75,83	0
20	EDO	D	221	4/4	0.58	0.27	50,66,71,82	0
20	EDO	O	308	4/4	0.60	0.24	62,66,67,68	0
25	PEK	C	302	49/53	0.60	0.37	46,72,108,213	0
27	DMU	T	102	21/33	0.61	0.21	56,74,95,104	0
27	DMU	X	103	33/33	0.61	0.32	66,80,88,96	0
20	EDO	A	637[A]	3/4	0.62	0.26	29,29,60,70	0
20	EDO	D	211	4/4	0.62	0.16	68,69,75,85	0
27	DMU	P	309	33/33	0.62	0.20	67,80,87,88	0
20	EDO	M	102	4/4	0.63	0.22	68,73,75,86	0
20	EDO	N	627	4/4	0.63	0.32	50,58,69,82	0
20	EDO	C	315	4/4	0.64	0.15	66,71,73,75	0
20	EDO	B	309	4/4	0.65	0.17	46,57,62,68	0
20	EDO	K	103	4/4	0.65	0.13	63,66,69,73	0
24	CHD	Y	102	29/29	0.66	0.34	72,81,86,89	0
20	EDO	N	615	4/4	0.66	0.22	61,63,64,70	0
27	DMU	C	309	22/33	0.66	0.19	53,68,95,98	0
20	EDO	N	633	4/4	0.66	0.29	45,45,45,50	0
27	DMU	X	102	22/33	0.66	0.33	75,83,87,98	0
20	EDO	B	320	4/4	0.66	0.17	63,64,76,91	0
20	EDO	P	316	4/4	0.67	0.14	41,60,70,80	0
25	PEK	C	304	53/53	0.68	0.24	35,67,94,199	0
25	PEK	P	302	33/53	0.68	0.23	48,69,94,166	0
25	PEK	P	304	52/53	0.68	0.27	36,67,109,179	0
26	CDL	T	101	92/100	0.69	0.26	46,72,99,186	0
20	EDO	U	101	4/4	0.69	0.37	45,54,59,81	0
19	PGV	N	608	42/51	0.69	0.27	43,66,100,164	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	H	101	4/4	0.69	0.17	58,63,69,71	0
20	EDO	Q	207	4/4	0.69	0.45	53,76,85,89	0
20	EDO	P	319	4/4	0.70	0.15	47,68,77,77	0
20	EDO	C	317	4/4	0.70	0.28	40,60,65,86	0
23	PSC	B	304	48/52	0.70	0.27	35,73,104,190	0
20	EDO	F	107	4/4	0.71	0.20	52,69,70,76	0
20	EDO	U	102	4/4	0.71	0.37	46,53,76,87	0
20	EDO	O	305	4/4	0.71	0.19	65,74,78,79	0
20	EDO	A	615	4/4	0.71	0.23	54,54,56,62	0
20	EDO	P	313	4/4	0.71	0.14	67,67,72,74	0
26	CDL	G	101	90/100	0.72	0.28	47,69,97,194	0
20	EDO	C	322	4/4	0.72	0.15	42,54,61,91	0
20	EDO	I	103	4/4	0.72	0.21	45,61,67,75	0
24	CHD	P	308	29/29	0.72	0.27	51,64,81,83	0
27	DMU	J	101	23/33	0.72	0.28	55,78,86,89	0
19	PGV	P	306	51/51	0.72	0.26	43,70,94,168	0
21	TGL	Y	101	60/63	0.73	0.22	39,62,90,109	0
20	EDO	D	204	4/4	0.73	0.30	45,63,84,94	0
19	PGV	C	306	51/51	0.73	0.24	39,69,92,152	0
20	EDO	P	327	4/4	0.73	0.16	50,63,64,69	0
27	DMU	X	101	10/33	0.74	0.16	57,77,79,81	0
20	EDO	R	204	4/4	0.74	0.16	38,59,60,65	0
21	TGL	Q	201	63/63	0.74	0.19	47,67,87,109	0
20	EDO	I	104	4/4	0.75	0.20	40,49,55,83	0
20	EDO	L	103	4/4	0.75	0.13	44,55,66,76	0
20	EDO	Q	208	4/4	0.75	0.17	50,68,70,75	0
20	EDO	N	614	4/4	0.76	0.12	62,64,73,87	0
20	EDO	O	309	4/4	0.76	0.12	48,53,60,69	0
20	EDO	D	214	4/4	0.77	0.50	48,50,64,77	0
21	TGL	B	302	62/63	0.77	0.18	36,62,84,94	0
20	EDO	B	319	4/4	0.77	0.21	59,64,73,89	0
27	DMU	X	104	12/33	0.77	0.21	72,78,81,86	0
23	PSC	O	302	43/52	0.78	0.20	34,67,94,178	0
20	EDO	C	320	4/4	0.78	0.12	44,60,64,71	0
20	EDO	C	314	4/4	0.78	0.10	55,57,67,69	0
20	EDO	A	630	4/4	0.79	0.24	38,42,72,79	0
20	EDO	B	311	4/4	0.79	0.27	49,60,76,83	0
20	EDO	Y	107	4/4	0.79	0.14	58,67,70,82	0
20	EDO	A	631	4/4	0.79	0.19	40,56,68,78	0
20	EDO	R	205	4/4	0.79	0.38	61,70,72,80	0
20	EDO	I	102	4/4	0.79	0.16	45,50,56,67	0
20	EDO	A	625	4/4	0.79	0.10	54,58,62,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	L	104	4/4	0.80	0.13	53,56,61,77	0
26	CDL	P	307	85/100	0.80	0.21	37,70,101,147	0
20	EDO	P	315	4/4	0.80	0.12	54,64,70,78	0
20	EDO	V	101	4/4	0.81	0.18	50,53,67,70	0
20	EDO	C	325	4/4	0.81	0.44	47,71,79,84	0
26	CDL	C	307	96/100	0.81	0.23	40,70,100,148	0
20	EDO	E	212	4/4	0.81	0.16	58,59,62,67	0
24	CHD	C	308	29/29	0.81	0.26	48,62,79,84	0
20	EDO	O	315	4/4	0.81	0.23	47,55,68,80	0
20	EDO	D	215	4/4	0.81	0.23	58,59,61,69	0
21	TGL	L	101	60/63	0.81	0.20	29,60,97,128	0
20	EDO	A	624	4/4	0.81	0.13	56,73,74,80	0
20	EDO	E	205	4/4	0.82	0.22	43,51,67,87	0
20	EDO	C	313	4/4	0.82	0.15	48,55,62,64	0
20	EDO	D	209	4/4	0.82	0.45	64,66,72,82	0
20	EDO	Y	104	4/4	0.82	0.10	59,65,70,72	0
20	EDO	M	103	4/4	0.82	0.22	44,49,66,67	0
20	EDO	S	111	4/4	0.82	0.28	40,52,67,76	0
20	EDO	M	105	4/4	0.82	0.11	54,58,64,78	0
20	EDO	N	629	4/4	0.83	0.13	64,70,72,75	0
20	EDO	T	107	4/4	0.83	0.34	48,51,66,80	0
20	EDO	A	634	4/4	0.83	0.17	41,51,56,63	0
20	EDO	Y	103	4/4	0.83	0.17	51,65,74,77	0
20	EDO	Q	206	4/4	0.84	0.34	49,69,79,82	0
20	EDO	D	202	4/4	0.84	0.13	47,57,64,76	0
20	EDO	D	203	4/4	0.84	0.28	44,50,53,98	0
20	EDO	E	208	4/4	0.84	0.23	50,51,83,89	0
20	EDO	E	209	4/4	0.84	0.13	34,52,58,59	0
20	EDO	B	312	4/4	0.84	0.31	41,44,46,64	0
20	EDO	C	323	4/4	0.84	0.09	56,59,65,75	0
19	PGV	A	607	47/51	0.84	0.21	26,61,97,181	0
20	EDO	G	105	4/4	0.84	0.12	47,61,74,76	0
20	EDO	N	630	4/4	0.84	0.12	57,63,68,79	0
20	EDO	D	218	4/4	0.84	0.34	43,48,57,89	0
20	EDO	L	105	4/4	0.85	0.10	55,63,73,78	0
20	EDO	S	112	4/4	0.85	0.20	45,52,70,86	0
20	EDO	S	114	4/4	0.85	0.17	55,65,65,68	0
20	EDO	T	105	4/4	0.85	0.21	51,60,72,75	0
20	EDO	I	105	4/4	0.85	0.21	60,65,68,73	0
21	TGL	N	607	63/63	0.85	0.19	42,68,82,87	0
20	EDO	L	102	4/4	0.85	0.23	41,43,54,70	0
20	EDO	D	201	4/4	0.85	0.09	50,63,65,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	A	621	4/4	0.85	0.22	39,51,55,62	0
20	EDO	O	311	4/4	0.85	0.23	79,80,83,86	0
20	EDO	S	103	4/4	0.85	0.14	39,41,54,54	0
20	EDO	H	104	4/4	0.86	0.26	37,42,56,62	0
20	EDO	J	103	4/4	0.86	0.23	48,52,53,84	0
20	EDO	K	104	4/4	0.86	0.10	61,68,75,91	0
20	EDO	P	312	4/4	0.86	0.10	50,55,68,69	0
20	EDO	N	624	4/4	0.86	0.33	55,57,57,83	0
20	EDO	U	103	4/4	0.86	0.31	49,52,68,75	0
20	EDO	K	105	4/4	0.86	0.17	60,75,75,83	0
27	DMU	Z	101	33/33	0.86	0.12	41,50,63,68	0
20	EDO	C	319	4/4	0.87	0.15	50,70,76,78	0
20	EDO	N	635	4/4	0.87	0.18	42,63,66,73	0
20	EDO	T	106	4/4	0.87	0.26	33,52,57,105	0
20	EDO	B	322	4/4	0.87	0.22	33,44,71,93	0
20	EDO	K	101	4/4	0.87	0.10	40,46,49,68	0
20	EDO	B	323	4/4	0.87	0.37	52,53,73,86	0
20	EDO	C	318	4/4	0.87	0.15	57,64,74,84	0
20	EDO	L	110	4/4	0.87	0.33	36,37,49,104	0
20	EDO	O	317	4/4	0.87	0.37	45,60,73,74	0
20	EDO	N	628	4/4	0.87	0.36	51,68,72,74	0
20	EDO	E	201	4/4	0.87	0.15	28,40,52,59	0
20	EDO	S	107	4/4	0.87	0.17	58,61,69,70	0
20	EDO	P	314	4/4	0.87	0.07	59,60,75,85	0
21	TGL	B	301	63/63	0.87	0.17	31,61,82,89	0
20	EDO	C	324	4/4	0.87	0.17	37,44,66,84	0
20	EDO	S	113	4/4	0.88	0.41	69,72,73,97	0
20	EDO	G	104	4/4	0.88	0.22	48,63,68,73	0
20	EDO	C	312	4/4	0.88	0.28	40,53,65,65	0
20	EDO	E	210	4/4	0.88	0.27	29,45,48,82	0
20	EDO	P	317	4/4	0.88	0.09	46,57,57,79	0
20	EDO	A	609	4/4	0.88	0.20	42,44,45,64	0
20	EDO	O	318	4/4	0.88	0.17	38,60,61,75	0
20	EDO	B	318	4/4	0.88	0.11	58,63,74,77	0
20	EDO	A	628	4/4	0.88	0.15	47,52,64,65	0
27	DMU	M	101	33/33	0.88	0.10	33,40,53,62	0
20	EDO	I	101	4/4	0.89	0.19	47,47,54,75	0
20	EDO	A	635	4/4	0.89	0.58	50,58,61,66	0
20	EDO	F	108	4/4	0.89	0.40	45,66,67,87	0
20	EDO	N	618	4/4	0.89	0.16	30,42,51,77	0
20	EDO	R	203	4/4	0.89	0.12	39,40,51,53	0
20	EDO	H	103	4/4	0.89	0.26	43,49,53,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	C	326	4/4	0.89	0.14	29,38,38,43	0
20	EDO	P	322	4/4	0.89	0.15	39,52,70,73	0
20	EDO	P	324	4/4	0.89	0.14	68,69,70,71	0
20	EDO	N	626	4/4	0.89	0.09	51,51,60,74	0
20	EDO	W	102	4/4	0.89	0.27	52,58,70,72	0
20	EDO	Q	202	4/4	0.89	0.23	58,67,68,68	0
20	EDO	P	326	4/4	0.90	0.31	35,54,67,73	0
20	EDO	O	312	4/4	0.90	0.22	39,45,58,85	0
20	EDO	O	304	4/4	0.90	0.17	53,55,71,86	0
20	EDO	S	108	4/4	0.90	0.36	43,68,69,77	0
20	EDO	O	316	4/4	0.90	0.49	49,64,85,98	0
20	EDO	C	316	4/4	0.90	0.06	64,68,68,81	0
20	EDO	D	217	4/4	0.90	0.19	46,56,67,92	0
20	EDO	P	321	4/4	0.90	0.32	51,64,70,71	0
20	EDO	T	103	4/4	0.90	0.09	46,70,82,83	0
20	EDO	A	610	4/4	0.90	0.20	56,58,63,70	0
20	EDO	D	219	4/4	0.90	0.18	34,59,69,79	0
20	EDO	N	619	4/4	0.91	0.25	56,61,73,76	0
20	EDO	O	313	4/4	0.91	0.41	42,62,72,86	0
20	EDO	N	620	4/4	0.91	0.22	38,70,78,90	0
20	EDO	N	634	4/4	0.91	0.17	57,58,71,82	0
20	EDO	A	636	4/4	0.91	0.26	36,39,48,56	0
20	EDO	H	102	4/4	0.91	0.27	43,53,76,81	0
20	EDO	E	206	4/4	0.91	0.25	53,56,64,65	0
20	EDO	E	207	4/4	0.91	0.16	58,60,69,72	0
20	EDO	I	106	4/4	0.91	0.36	41,54,72,76	0
20	EDO	A	623	4/4	0.91	0.27	36,73,79,80	0
20	EDO	R	202	4/4	0.92	0.18	53,58,71,81	0
20	EDO	O	314	4/4	0.92	0.31	38,54,61,77	0
20	EDO	A	613	4/4	0.92	0.10	25,25,28,31	0
20	EDO	D	208	4/4	0.92	0.20	36,52,85,98	0
20	EDO	B	313	4/4	0.92	0.26	47,56,57,60	0
20	EDO	L	111	4/4	0.92	0.14	38,62,63,74	0
20	EDO	D	210	4/4	0.92	0.30	63,66,88,89	0
20	EDO	S	109	4/4	0.92	0.41	43,50,54,69	0
24	CHD	C	301	29/29	0.92	0.07	23,27,32,33	0
20	EDO	W	101	4/4	0.92	0.12	47,63,63,65	0
20	EDO	C	321	4/4	0.92	0.19	36,56,61,71	0
20	EDO	B	317	4/4	0.92	0.30	46,57,74,87	0
20	EDO	M	106	4/4	0.92	0.29	38,40,61,78	0
20	EDO	D	206	4/4	0.92	0.12	48,48,53,74	0
20	EDO	Y	106	4/4	0.92	0.23	39,60,74,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	E	203	4/4	0.92	0.09	44,46,53,57	0
20	EDO	Z	102	4/4	0.92	0.22	66,71,77,83	0
20	EDO	N	622	4/4	0.93	0.19	36,61,75,79	0
20	EDO	D	220	4/4	0.93	0.21	36,50,64,75	0
20	EDO	P	325	4/4	0.93	0.23	41,53,75,93	0
20	EDO	L	108	4/4	0.93	0.15	35,53,72,83	0
20	EDO	N	625	4/4	0.93	0.08	43,58,61,66	0
20	EDO	N	611	4/4	0.93	0.10	35,38,38,42	0
20	EDO	W	103	4/4	0.93	0.22	44,48,72,88	0
20	EDO	A	620	4/4	0.93	0.17	37,60,63,67	0
20	EDO	Q	205	4/4	0.93	0.15	52,58,65,71	0
20	EDO	B	306	4/4	0.93	0.09	34,41,44,52	0
20	EDO	B	307	4/4	0.93	0.11	27,41,45,46	0
20	EDO	F	105	4/4	0.93	0.18	42,43,59,71	0
20	EDO	Y	108	4/4	0.93	0.12	55,56,62,64	0
20	EDO	N	632	4/4	0.93	0.17	33,41,45,65	0
20	EDO	P	320	4/4	0.93	0.08	56,70,71,85	0
20	EDO	M	104	4/4	0.93	0.10	55,59,66,68	0
29	PO4	U	104	5/5	0.93	0.34	54,56,61,69	0
25	PEK	P	303	53/53	0.94	0.13	27,48,81,88	0
20	EDO	L	107	4/4	0.94	0.17	48,53,74,85	0
20	EDO	B	316	4/4	0.94	0.11	48,53,53,78	0
20	EDO	Q	204	4/4	0.94	0.14	54,57,59,73	0
20	EDO	A	626	4/4	0.94	0.26	34,37,70,89	0
20	EDO	T	104	4/4	0.94	0.08	29,32,37,37	0
20	EDO	A	632	4/4	0.94	0.20	31,33,62,80	0
20	EDO	O	306	4/4	0.94	0.19	49,52,55,56	0
20	EDO	O	307	4/4	0.94	0.14	42,50,53,59	0
20	EDO	R	201	4/4	0.94	0.10	45,62,62,78	0
20	EDO	A	617	4/4	0.94	0.17	41,45,46,72	0
20	EDO	A	618	4/4	0.94	0.17	40,53,60,63	0
20	EDO	D	205	4/4	0.94	0.12	45,52,57,65	0
20	EDO	V	102	4/4	0.94	0.30	56,65,68,77	0
20	EDO	E	213	4/4	0.94	0.19	42,43,70,81	0
20	EDO	F	104	4/4	0.94	0.09	32,35,41,46	0
20	EDO	B	314	4/4	0.94	0.09	37,39,41,60	0
20	EDO	B	315	4/4	0.94	0.20	36,49,52,63	0
20	EDO	W	104	4/4	0.94	0.18	48,52,61,65	0
20	EDO	D	216	4/4	0.94	0.12	35,59,61,89	0
20	EDO	G	103	4/4	0.94	0.07	29,30,34,34	0
20	EDO	O	319	4/4	0.95	0.50	44,50,74,103	0
24	CHD	P	301	29/29	0.95	0.06	23,28,32,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	P	311	4/4	0.95	0.10	28,33,40,54	0
20	EDO	F	106	4/4	0.95	0.16	36,43,68,82	0
20	EDO	S	110	4/4	0.95	0.13	30,44,53,57	0
20	EDO	E	204	4/4	0.95	0.20	37,49,53,69	0
20	EDO	A	633	4/4	0.95	0.17	30,35,36,47	0
18	CYN	N	606	2/2	0.95	0.11	17,17,17,29	0
20	EDO	A	627	4/4	0.95	0.41	36,50,50,82	0
20	EDO	A	616	4/4	0.95	0.10	49,53,62,74	0
20	EDO	P	318	4/4	0.95	0.27	42,70,82,83	0
20	EDO	R	206	4/4	0.95	0.09	36,36,38,41	0
20	EDO	B	310	4/4	0.95	0.12	42,62,63,65	0
29	PO4	H	105	5/5	0.95	0.26	55,55,64,66	0
20	EDO	S	105	4/4	0.95	0.13	37,51,64,77	0
20	EDO	L	109	4/4	0.96	0.28	44,44,78,80	0
20	EDO	B	324	4/4	0.96	0.10	30,32,44,63	0
20	EDO	P	323	4/4	0.96	0.17	34,37,37,41	0
25	PEK	C	303	53/53	0.96	0.11	25,41,74,96	0
20	EDO	N	616	4/4	0.96	0.12	27,50,57,61	0
20	EDO	F	109	4/4	0.96	0.19	28,32,60,95	0
20	EDO	C	311	4/4	0.96	0.07	31,32,32,32	0
20	EDO	J	104	4/4	0.96	0.25	44,55,57,59	0
18	CYN	A	606	2/2	0.96	0.11	14,14,14,25	0
20	EDO	S	102	4/4	0.96	0.08	28,28,29,33	0
17	NA	N	605	1/1	0.96	0.09	29,29,29,29	0
20	EDO	A	619	4/4	0.96	0.11	29,37,44,72	0
20	EDO	A	612	4/4	0.96	0.12	37,38,42,48	0
20	EDO	N	612	4/4	0.96	0.10	23,26,28,30	0
20	EDO	A	629	4/4	0.97	0.18	28,36,37,75	0
20	EDO	N	621	4/4	0.97	0.13	34,34,51,61	0
20	EDO	N	613	4/4	0.97	0.10	36,38,41,42	0
20	EDO	O	310	4/4	0.97	0.06	29,30,31,32	0
19	PGV	N	609	51/51	0.97	0.10	23,31,61,77	0
20	EDO	S	104	4/4	0.97	0.07	32,34,39,41	0
19	PGV	P	305	51/51	0.97	0.10	21,30,73,85	0
20	EDO	B	321	4/4	0.97	0.22	30,53,63,69	0
20	EDO	Q	209	4/4	0.97	0.14	29,48,53,63	0
24	CHD	B	305	29/29	0.97	0.06	21,25,32,40	0
20	EDO	N	617	4/4	0.97	0.06	26,26,28,30	0
19	PGV	C	305	50/51	0.97	0.10	21,27,74,83	0
24	CHD	G	102	29/29	0.97	0.08	21,25,29,37	0
20	EDO	E	202	4/4	0.97	0.07	34,37,40,41	0
20	EDO	S	106	4/4	0.98	0.07	23,23,23,23	0

Continued on next page...

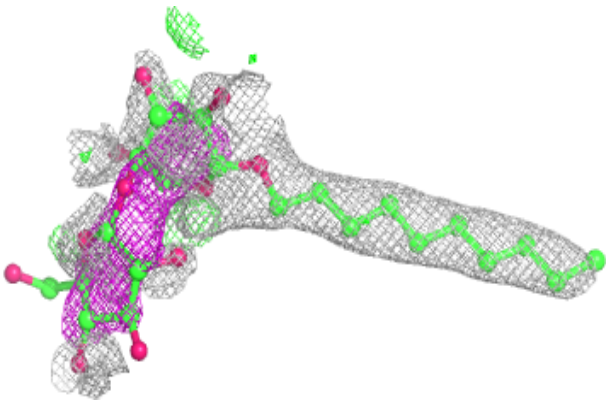
Continued from previous page...

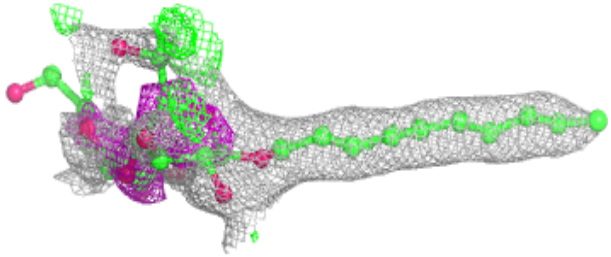
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	HEA	A	601[A]	60/60	0.98	0.08	17,19,31,39	9
20	EDO	A	614	4/4	0.98	0.12	28,36,74,76	0
14	HEA	A	601[B]	60/60	0.98	0.08	17,19,32,44	9
20	EDO	B	308	4/4	0.98	0.08	22,24,24,26	0
14	HEA	A	602	60/60	0.98	0.08	16,18,24,30	0
14	HEA	N	601[A]	60/60	0.98	0.08	21,24,35,43	9
19	PGV	A	608	51/51	0.98	0.10	21,28,64,68	0
20	EDO	F	102	4/4	0.98	0.11	28,29,30,32	0
14	HEA	N	601[B]	60/60	0.98	0.08	21,24,35,38	9
14	HEA	N	602	60/60	0.98	0.09	19,21,27,29	0
20	EDO	N	631	4/4	0.98	0.17	28,29,69,73	0
20	EDO	F	103	4/4	0.99	0.08	22,23,23,23	0
16	MG	N	604	1/1	0.99	0.08	25,25,25,25	0
17	NA	A	605	1/1	0.99	0.06	23,23,23,23	0
15	CU	N	603	1/1	0.99	0.13	21,21,21,21	0
20	EDO	A	611	4/4	0.99	0.08	21,22,24,25	0
16	MG	A	604	1/1	0.99	0.06	20,20,20,20	0
22	CUA	O	301	2/2	0.99	0.10	26,26,26,26	0
28	ZN	F	101	1/1	1.00	0.10	25,25,25,25	0
28	ZN	S	101	1/1	1.00	0.09	25,25,25,25	0
15	CU	A	603	1/1	1.00	0.13	19,19,19,19	0
22	CUA	B	303	2/2	1.00	0.13	21,21,21,21	0

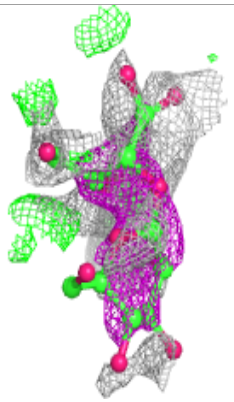
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU O 303:

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

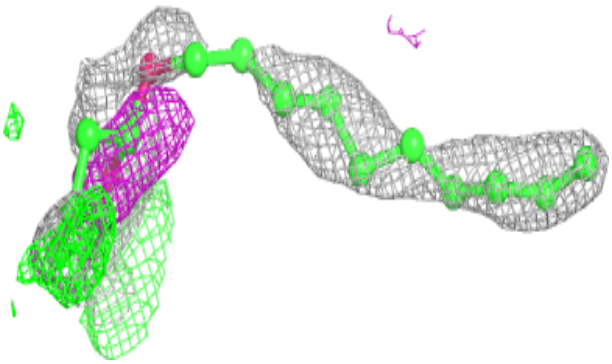


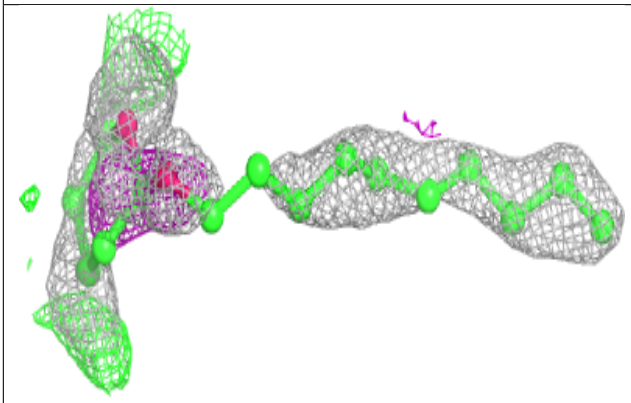


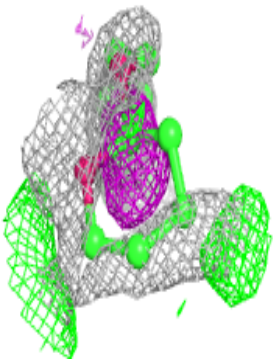


Electron density around DMU N 610:

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

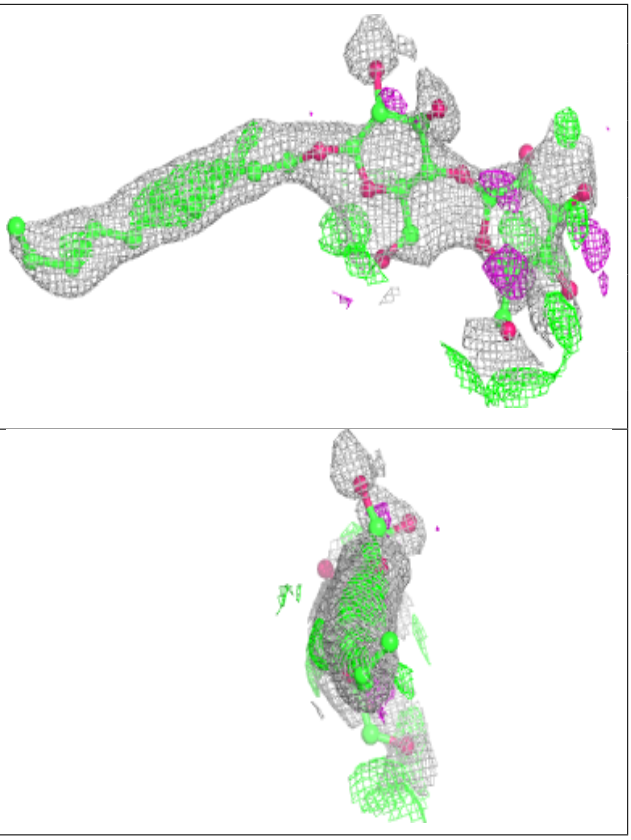






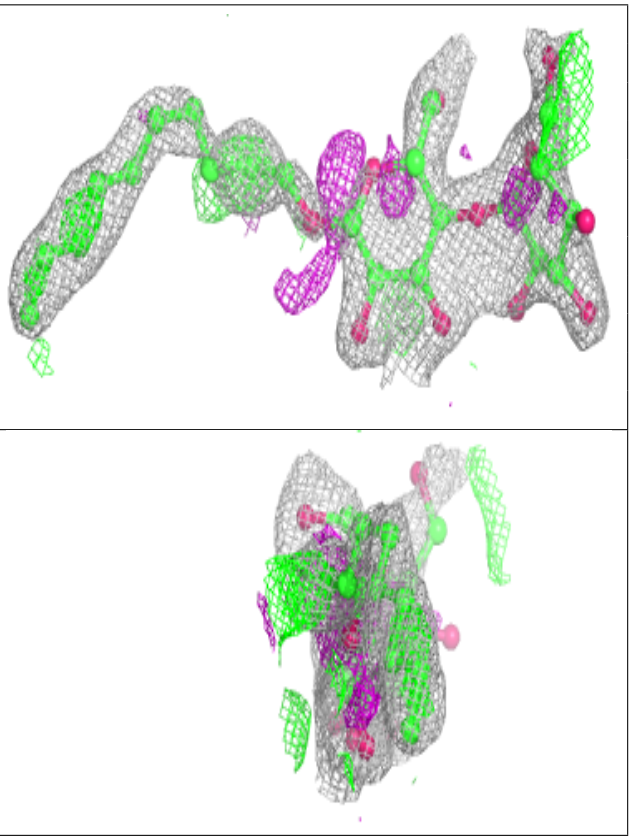
Electron density around DMU C 310:

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



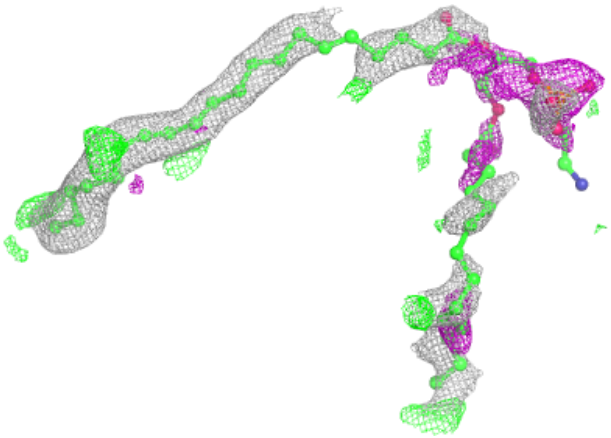
Electron density around DMU P 310:

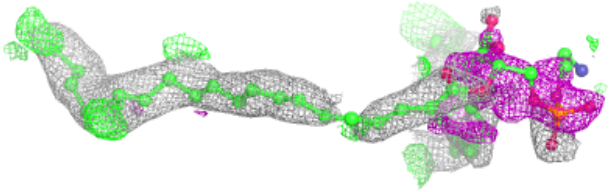
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

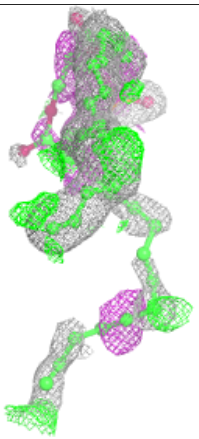


Electron density around PEK C 302:

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

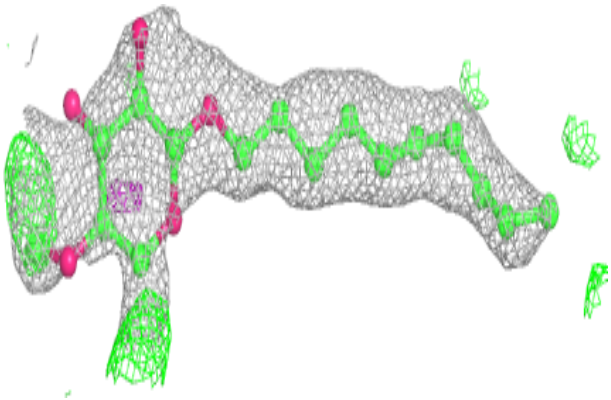


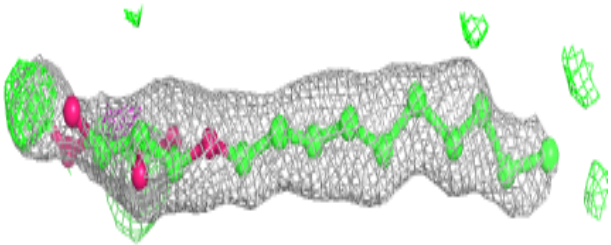


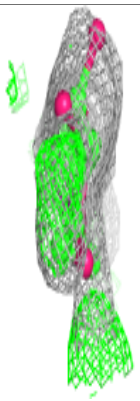


Electron density around DMU T 102:

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

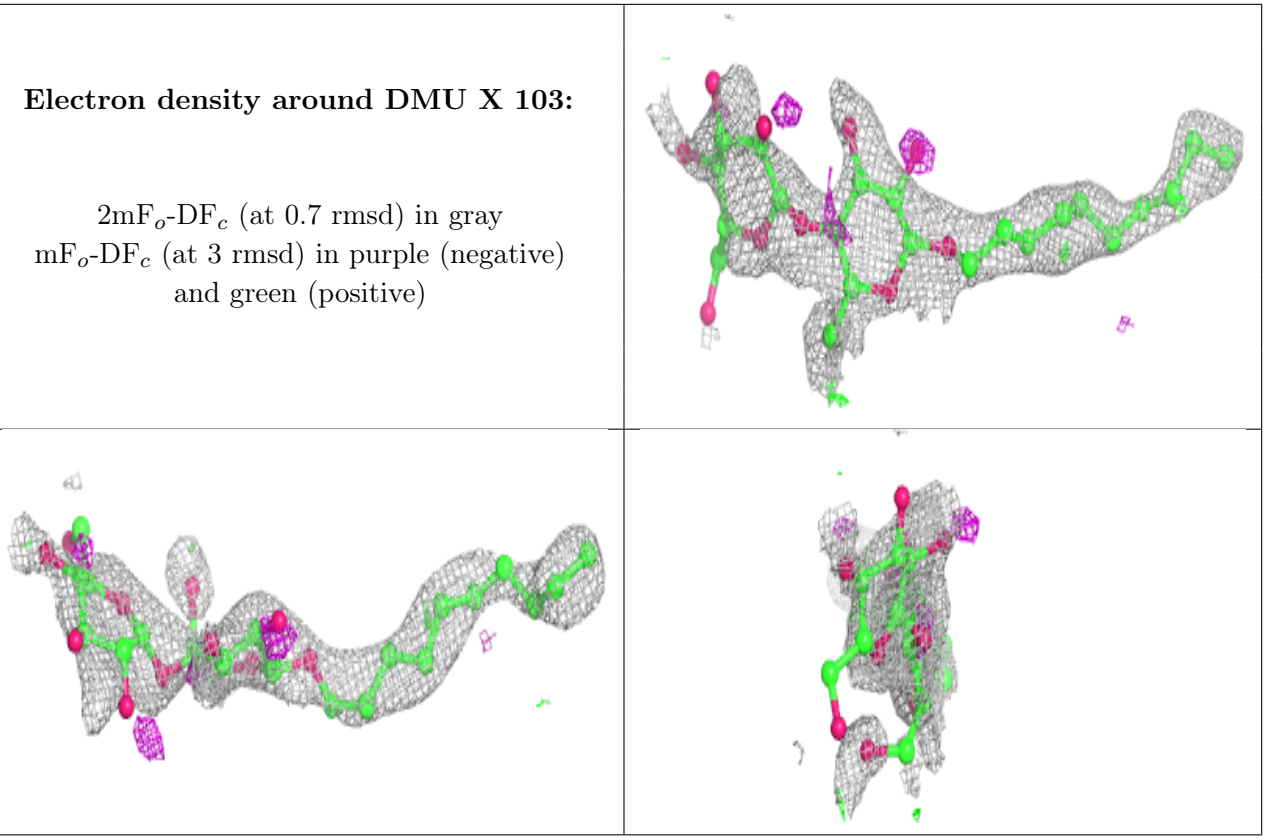






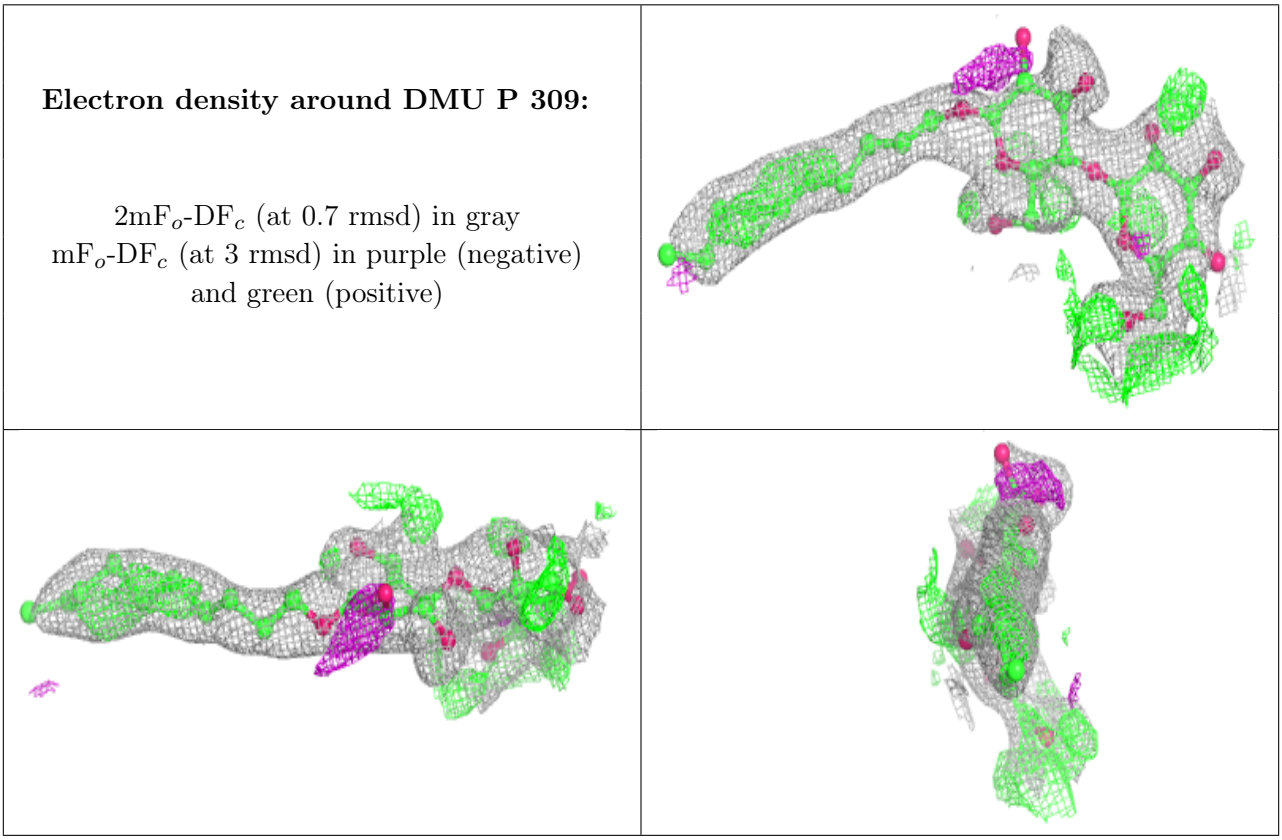
Electron density around DMU X 103:

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



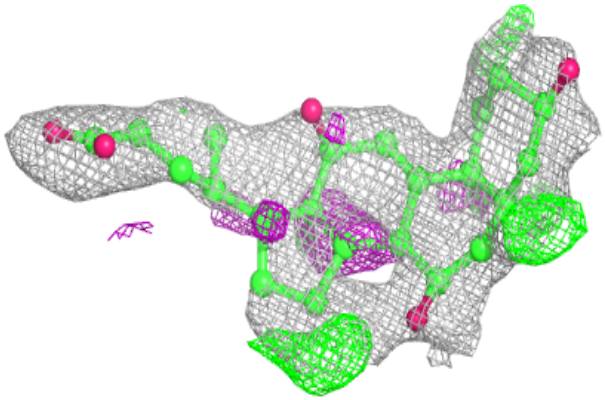
Electron density around DMU P 309:

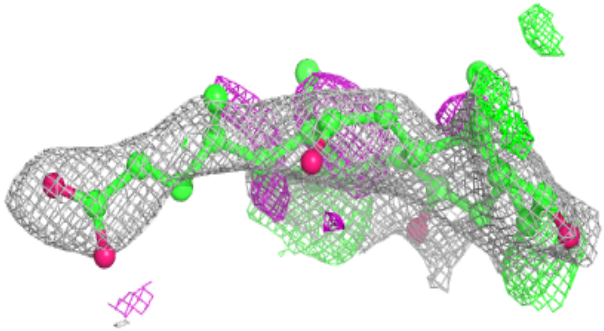
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

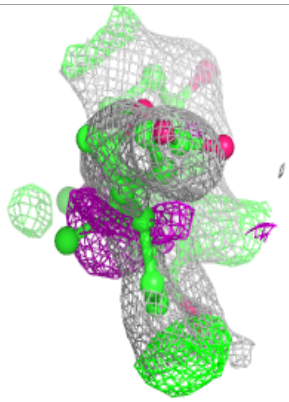


Electron density around CHD Y 102:

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

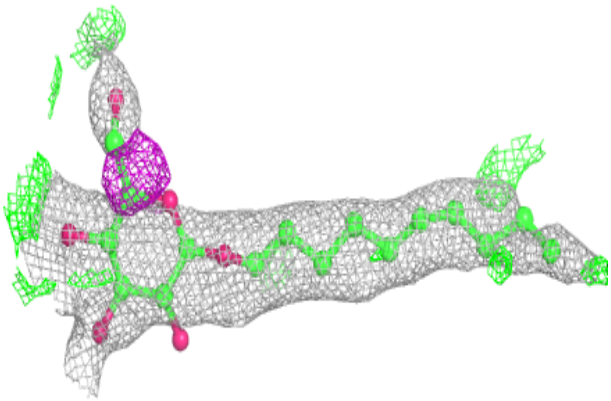


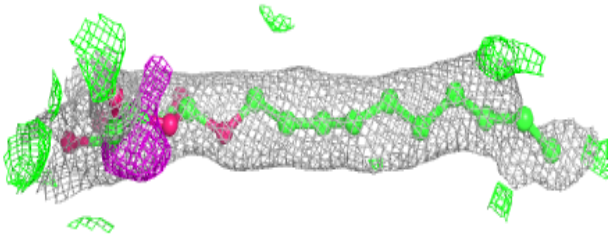


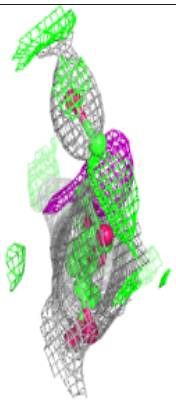


Electron density around DMU C 309:

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

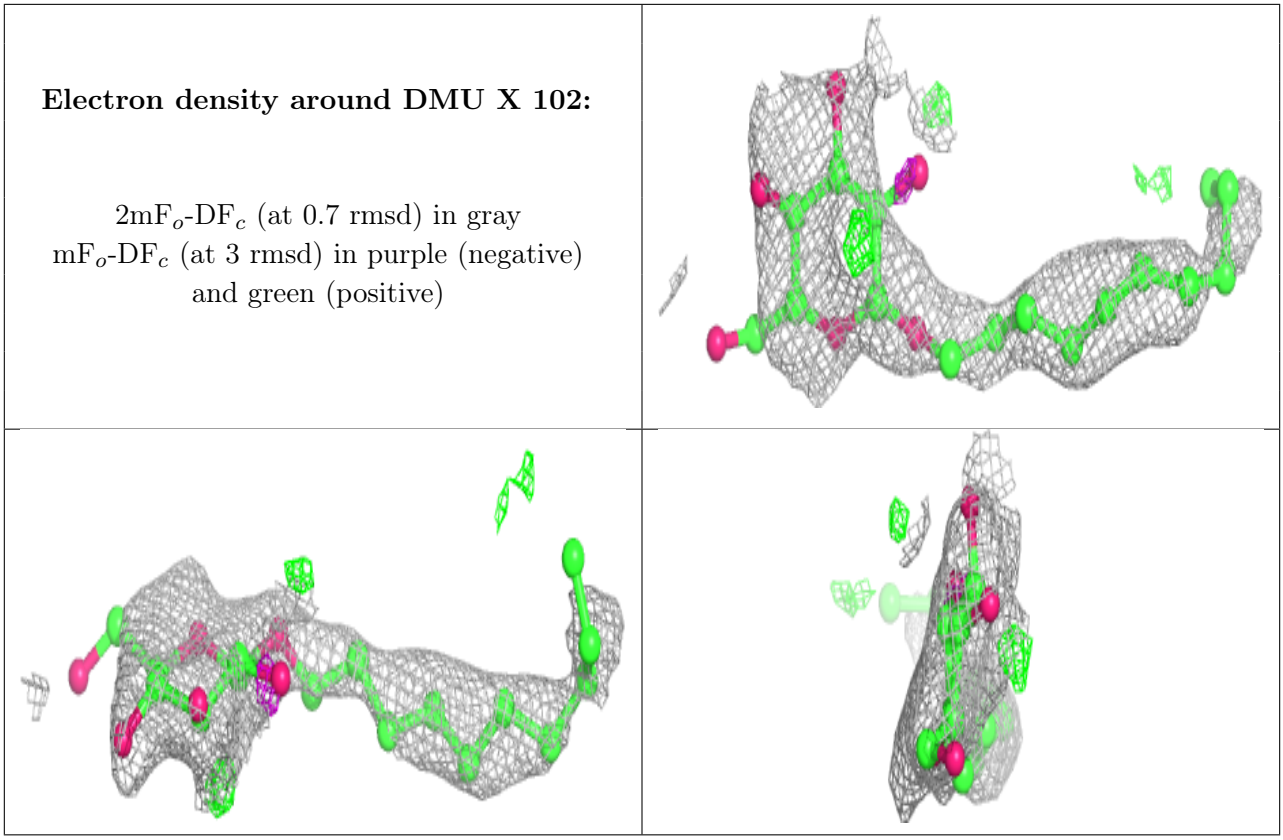






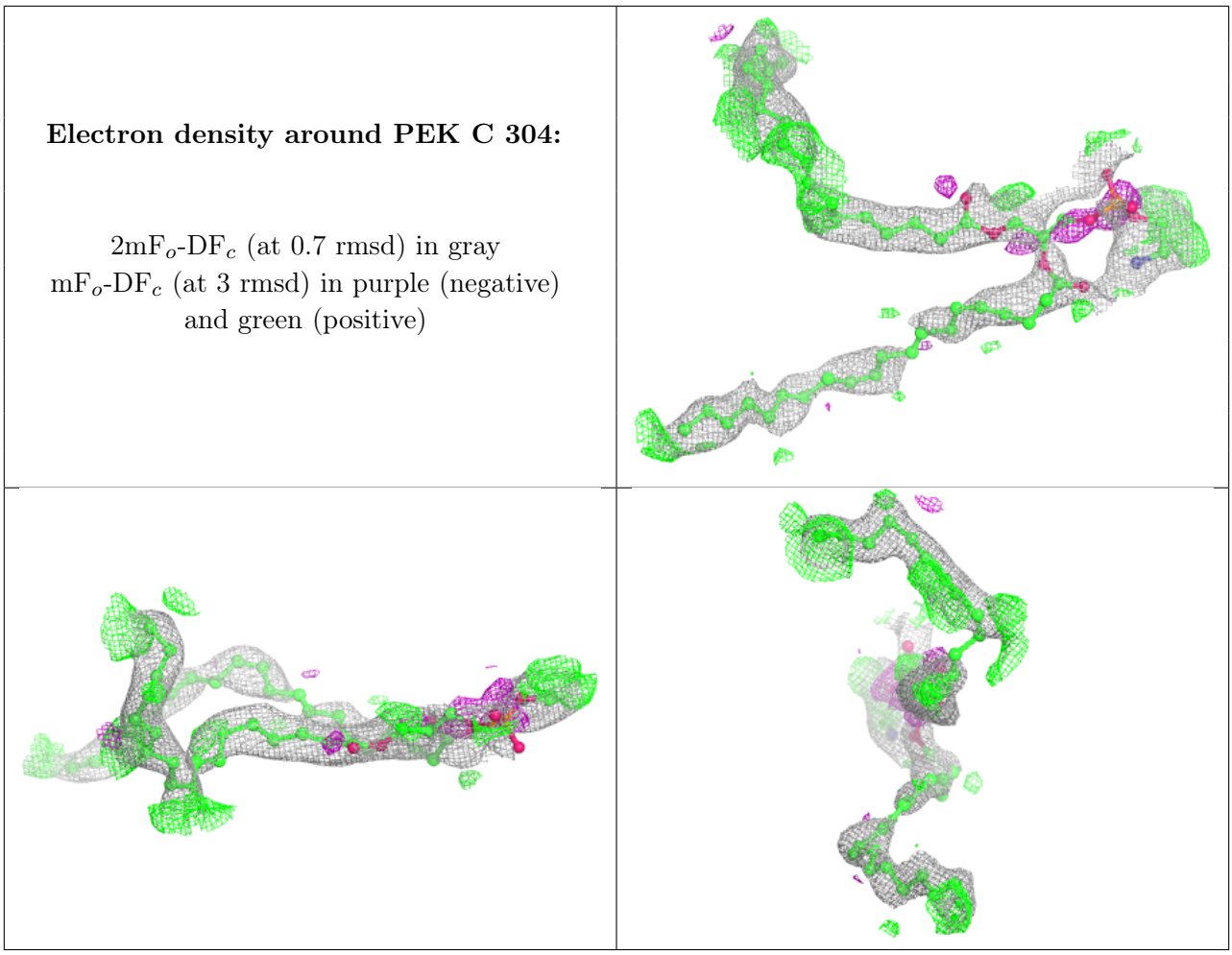
Electron density around DMU X 102:

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



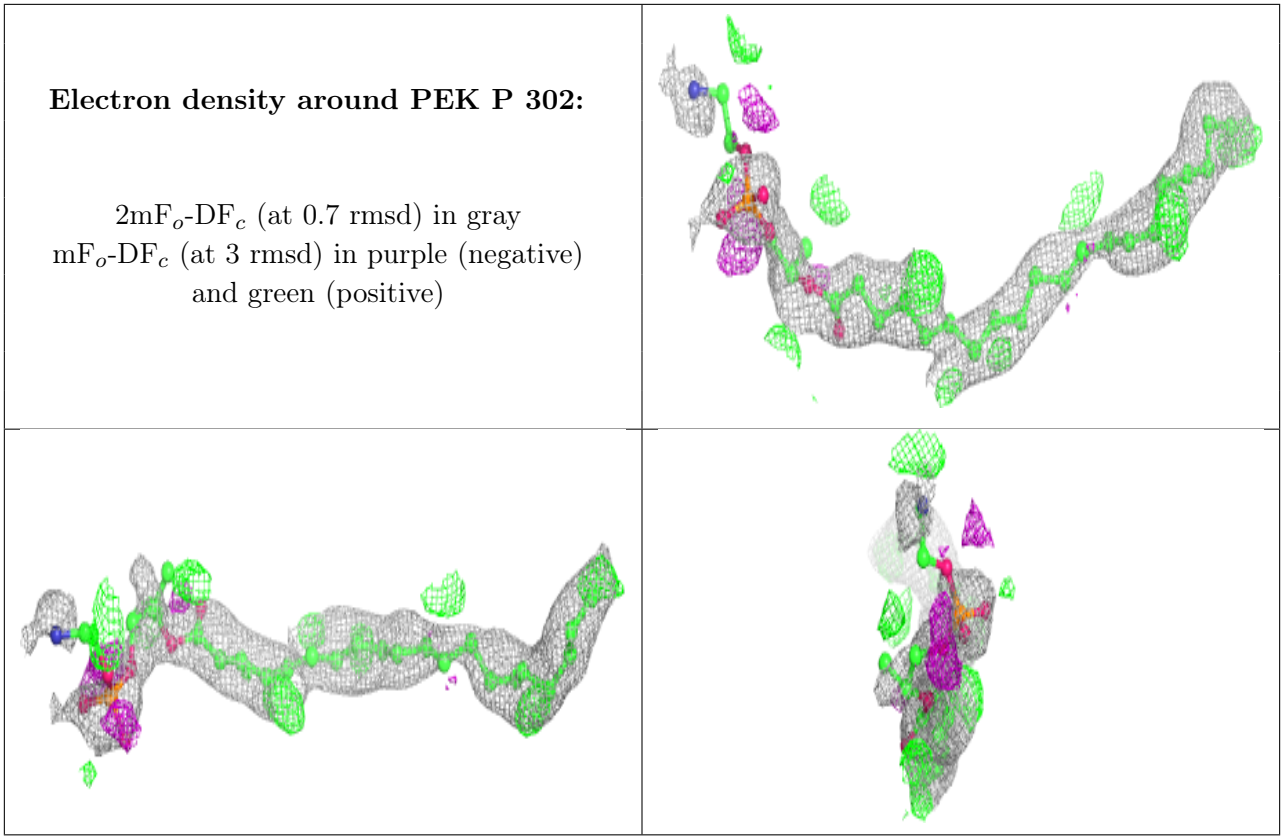
Electron density around PEK C 304:

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



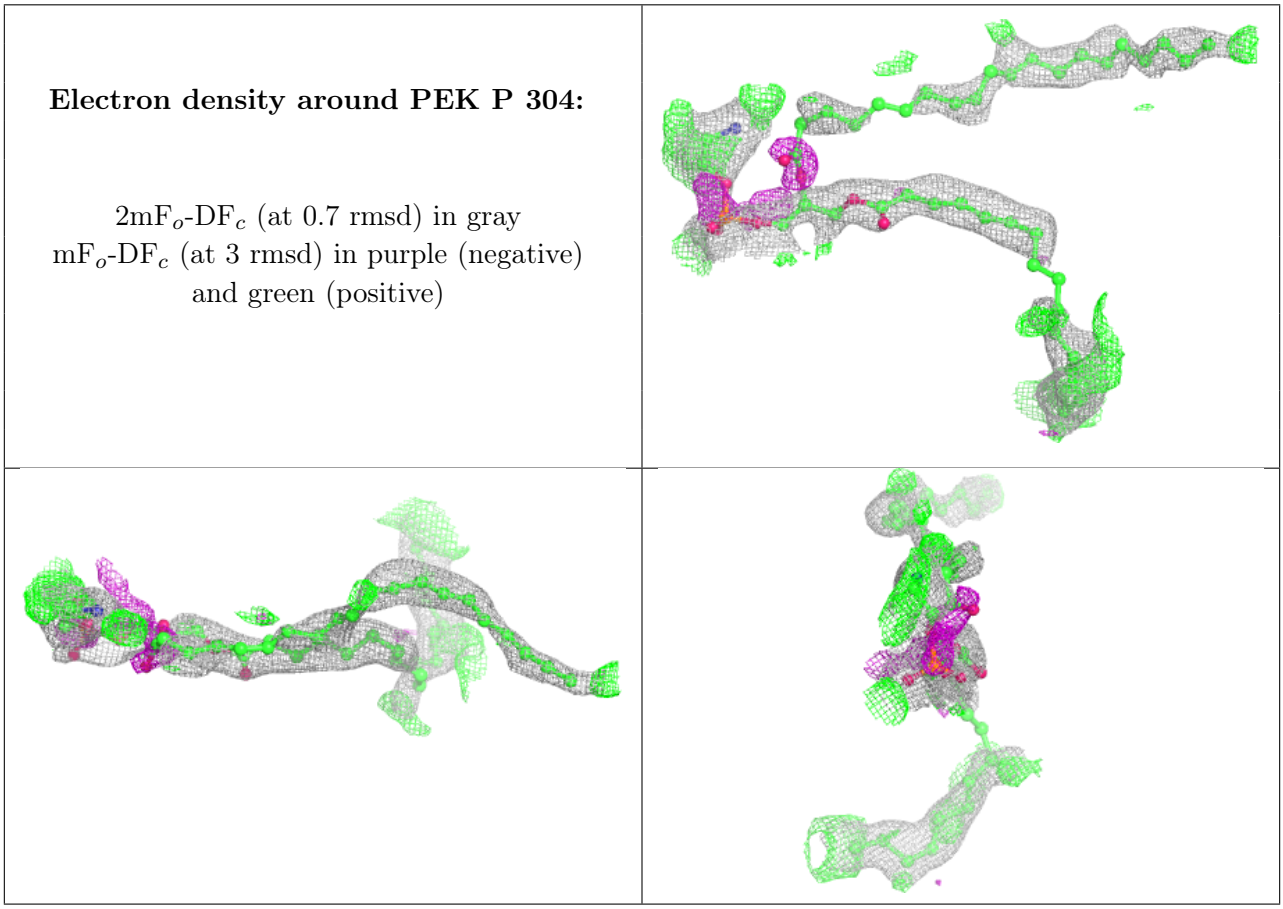
Electron density around PEK P 302:

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



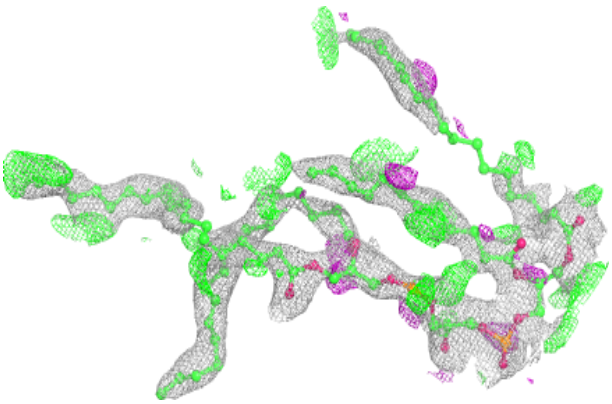
Electron density around PEK P 304:

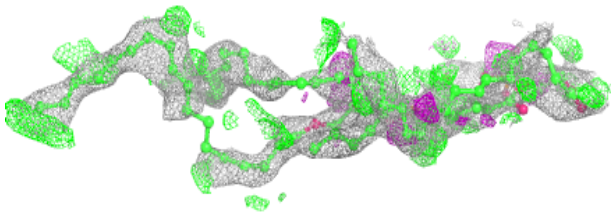
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

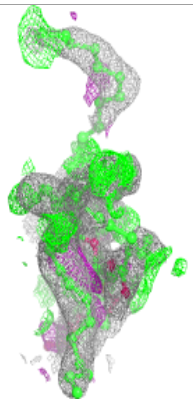


Electron density around CDL T 101:

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

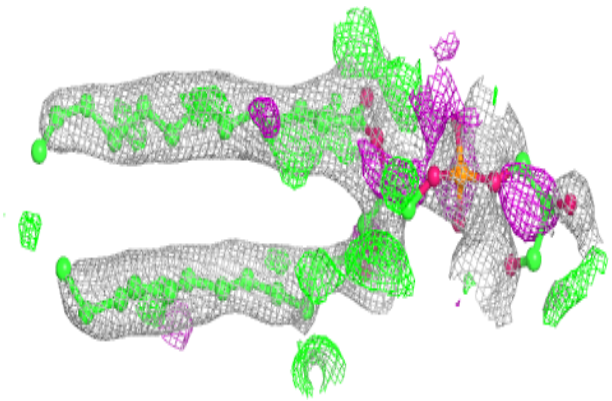


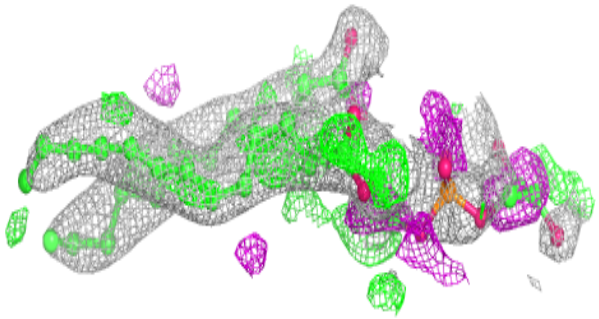


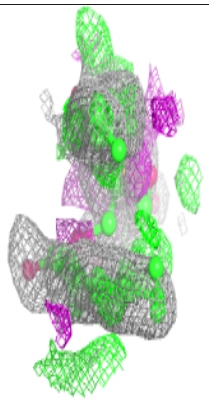


Electron density around PGV N 608:

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

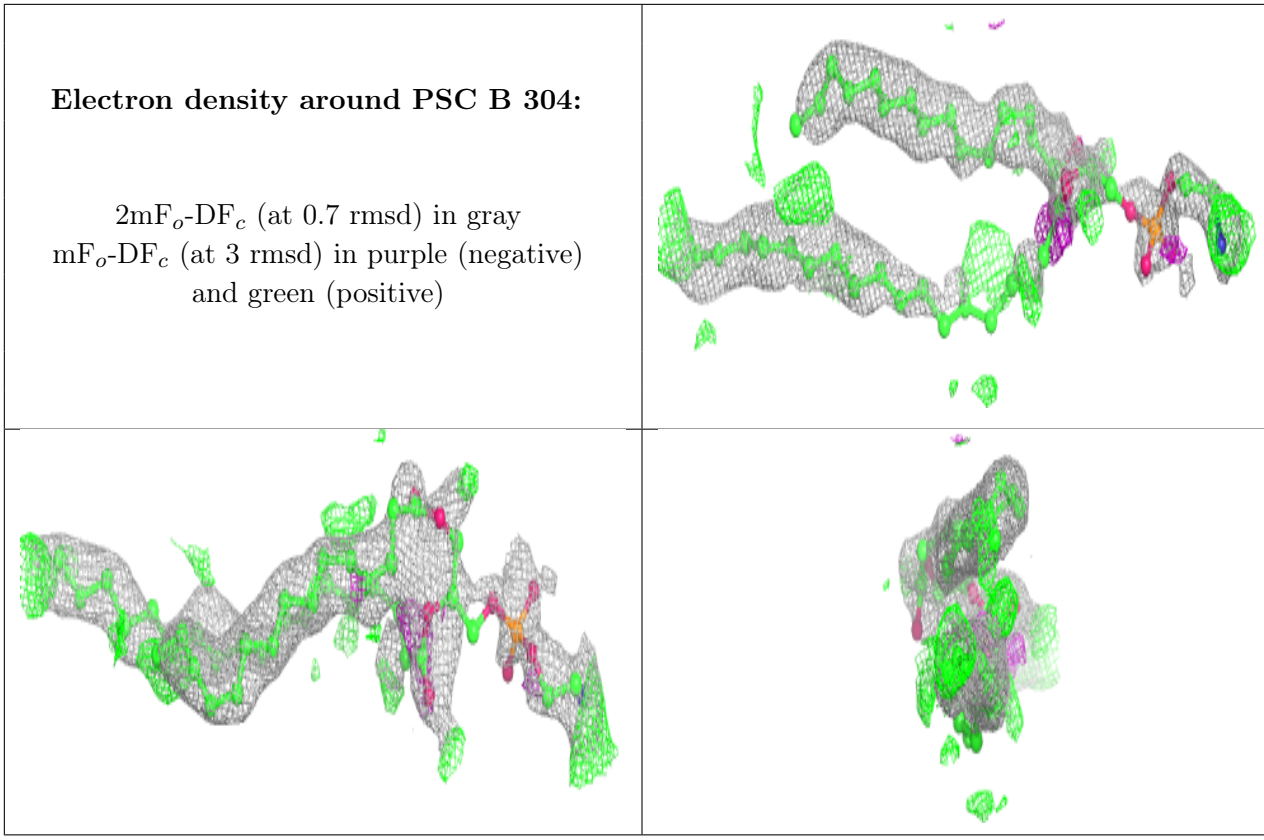






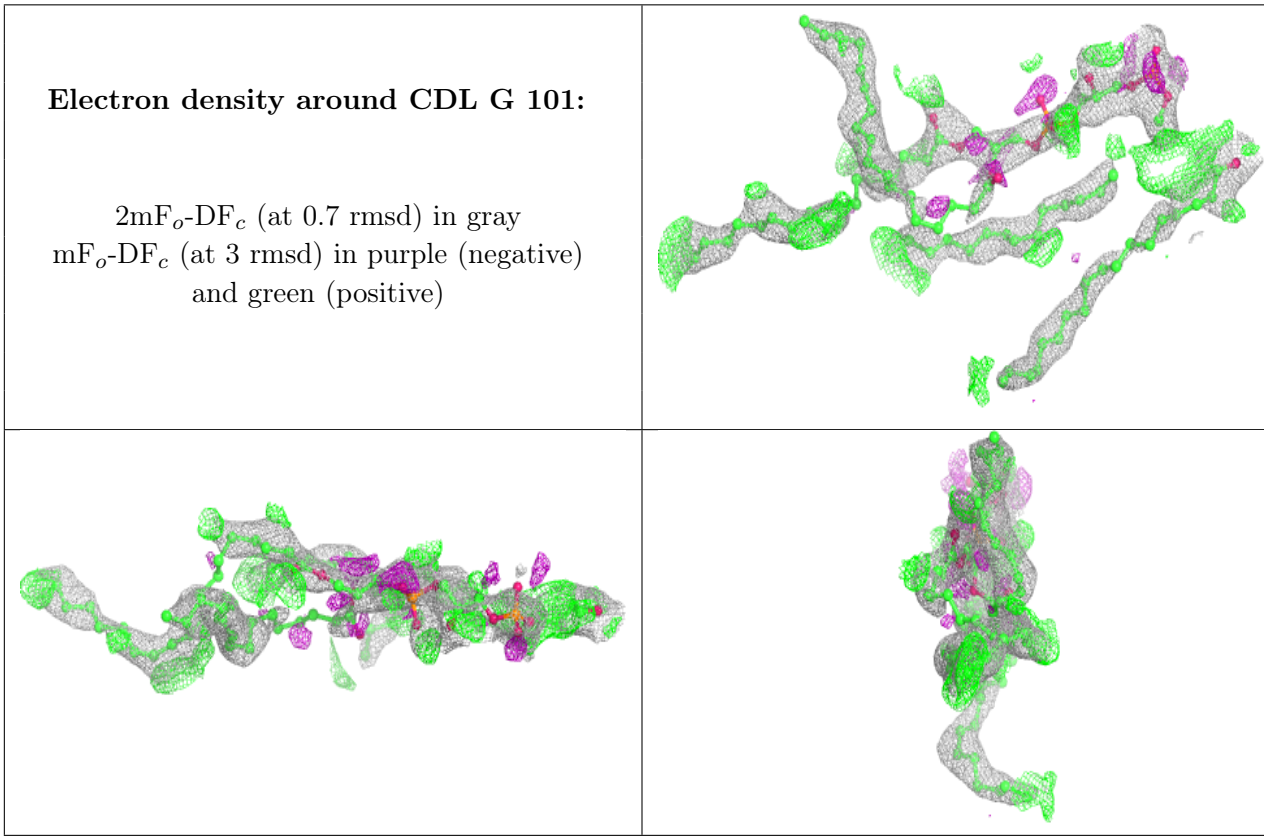
Electron density around PSC B 304:

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



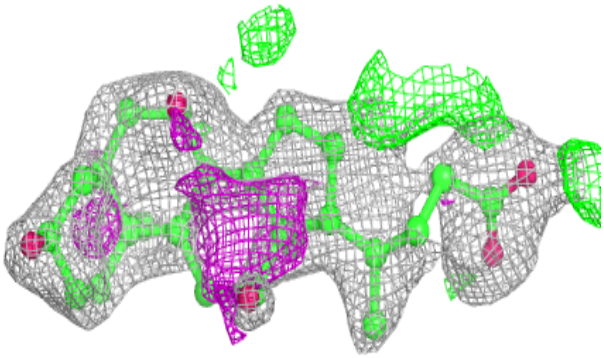
Electron density around CDL G 101:

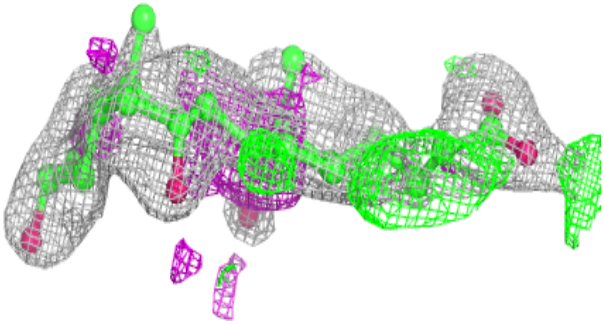
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

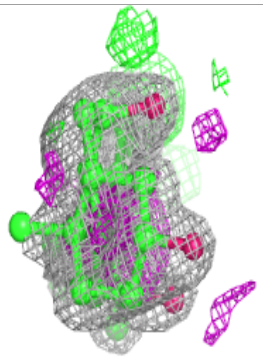


Electron density around CHD P 308:

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

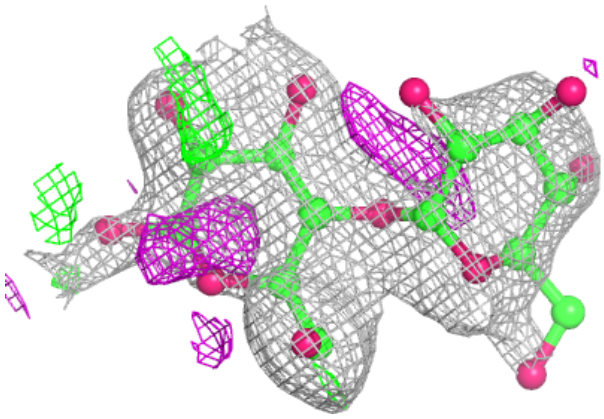


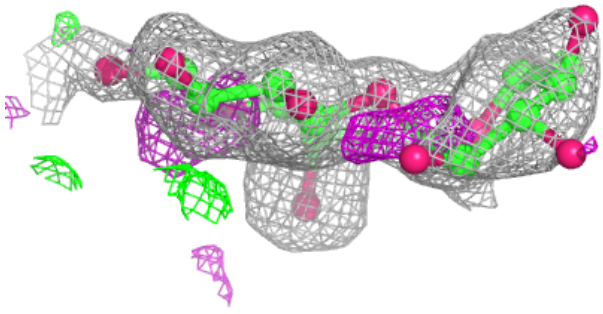


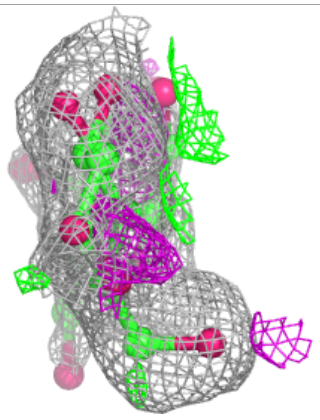


Electron density around DMU J 101:

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

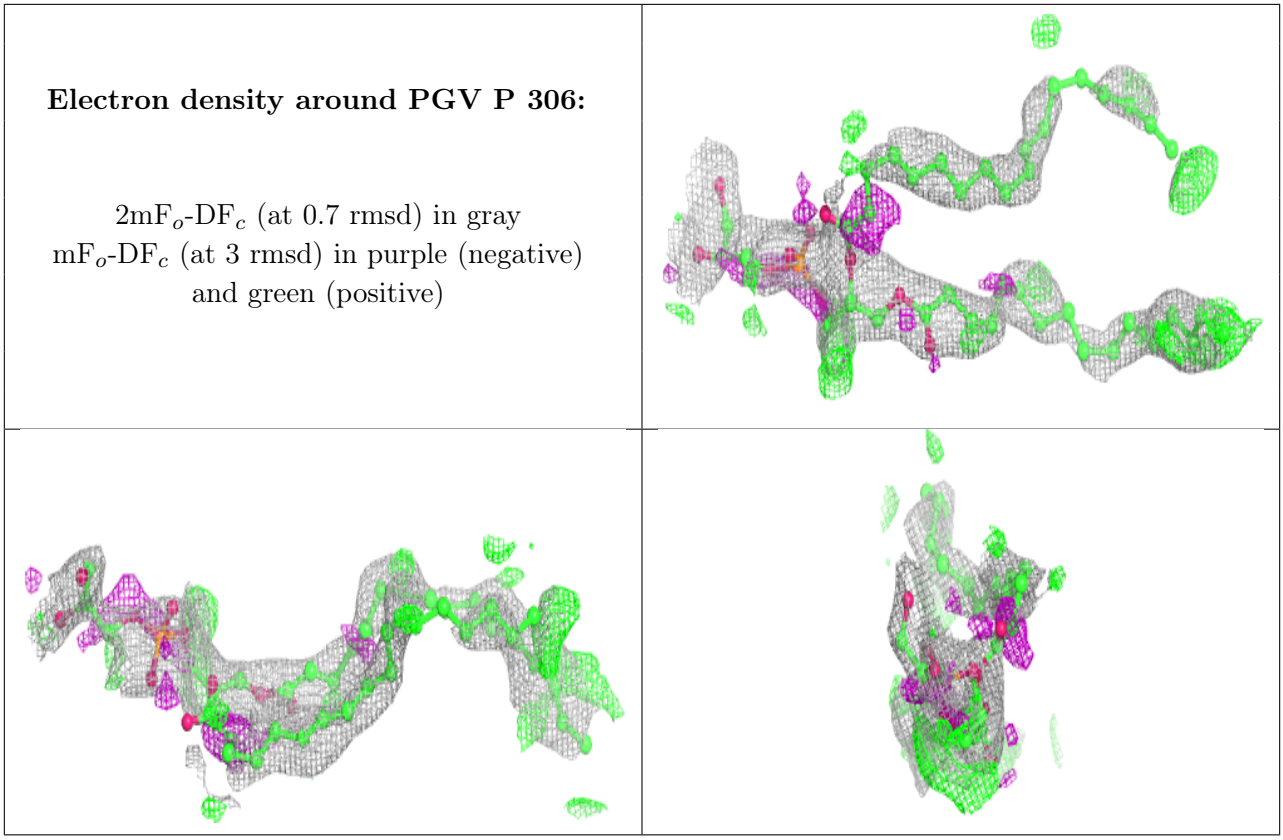






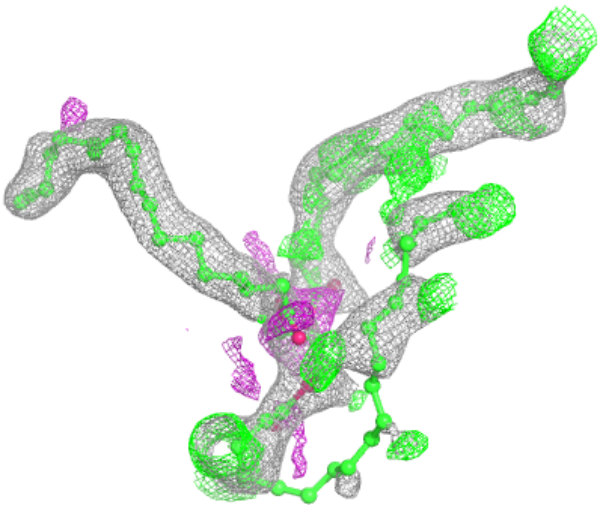
Electron density around PGV P 306:

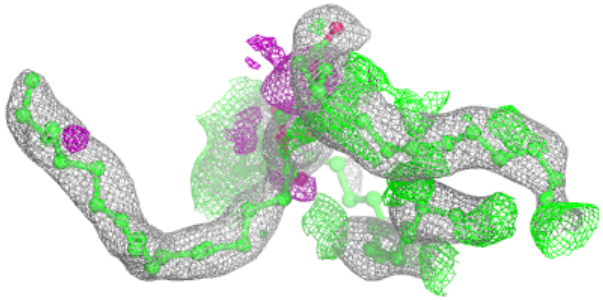
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

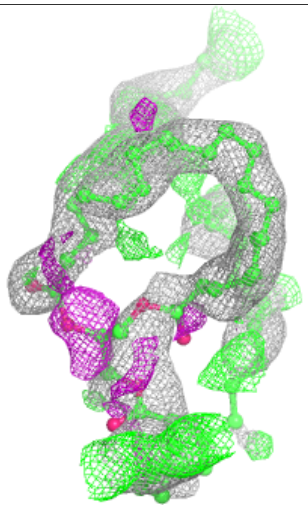


Electron density around TGL Y 101:

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

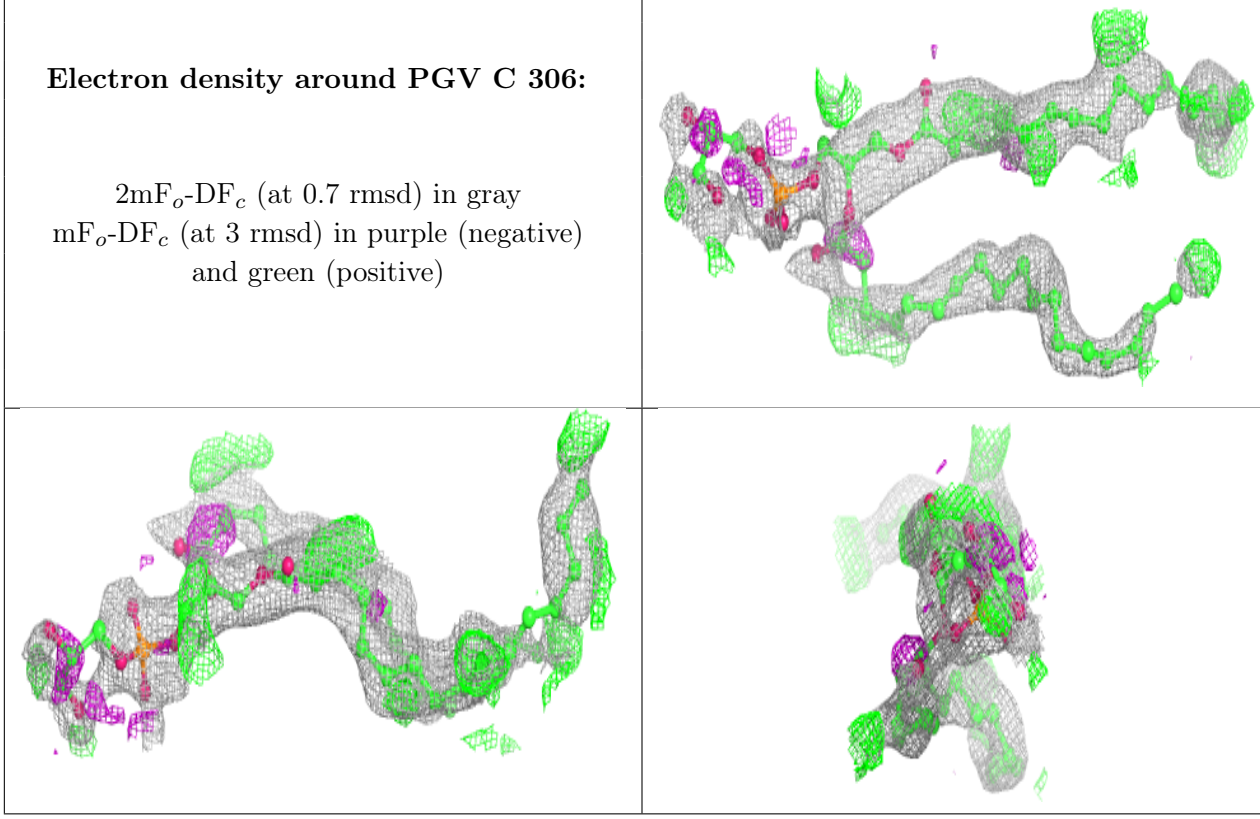






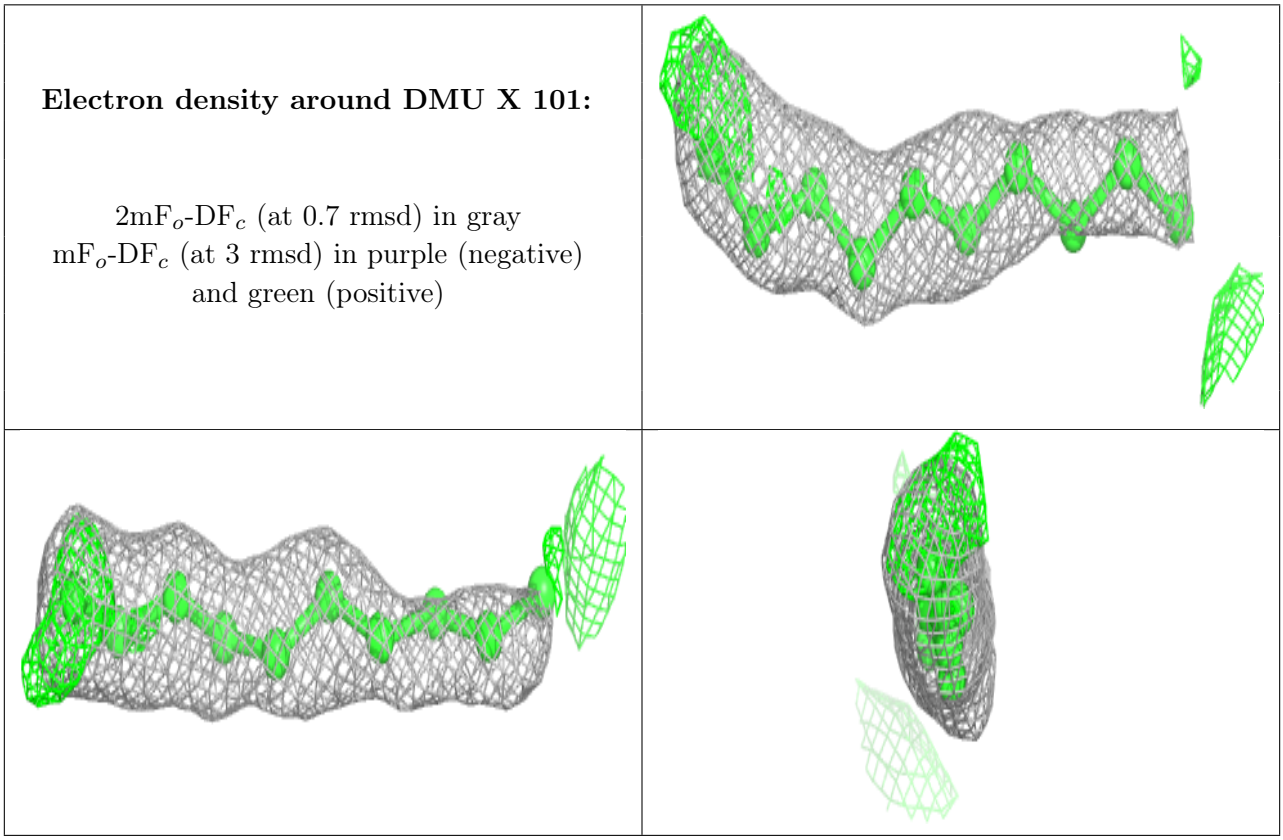
Electron density around PGV C 306:

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



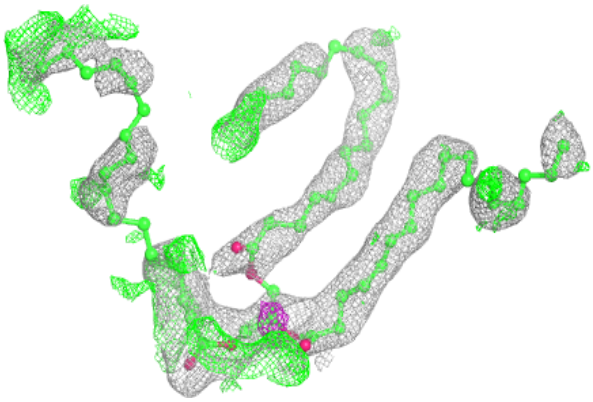
Electron density around DMU X 101:

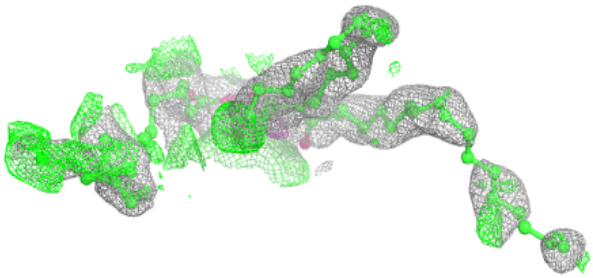
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

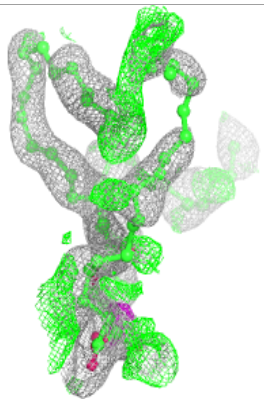


Electron density around TGL Q 201:

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

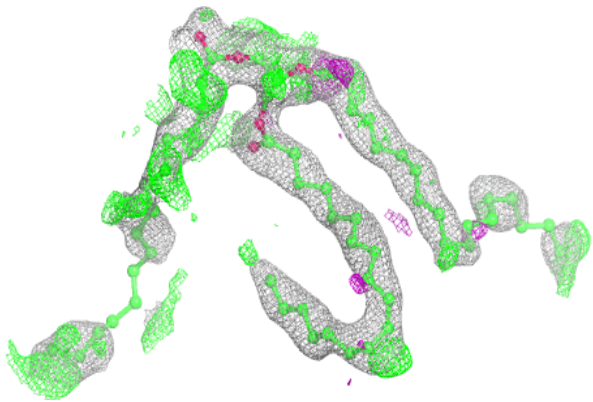


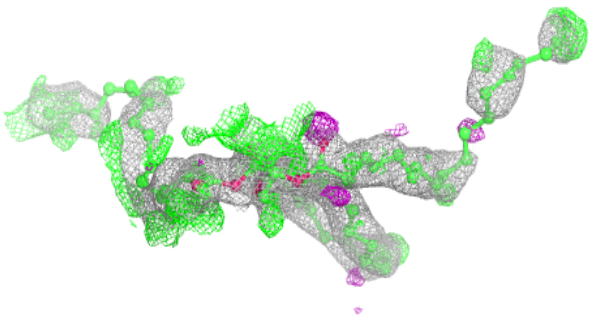


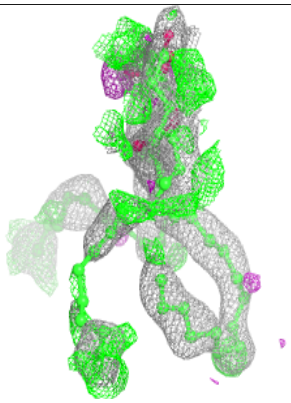


Electron density around TGL B 302:

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

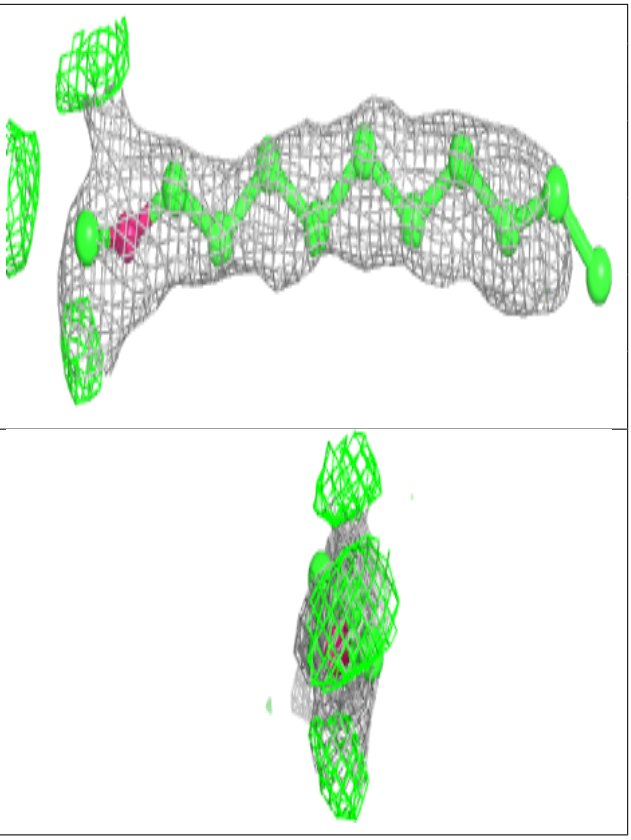






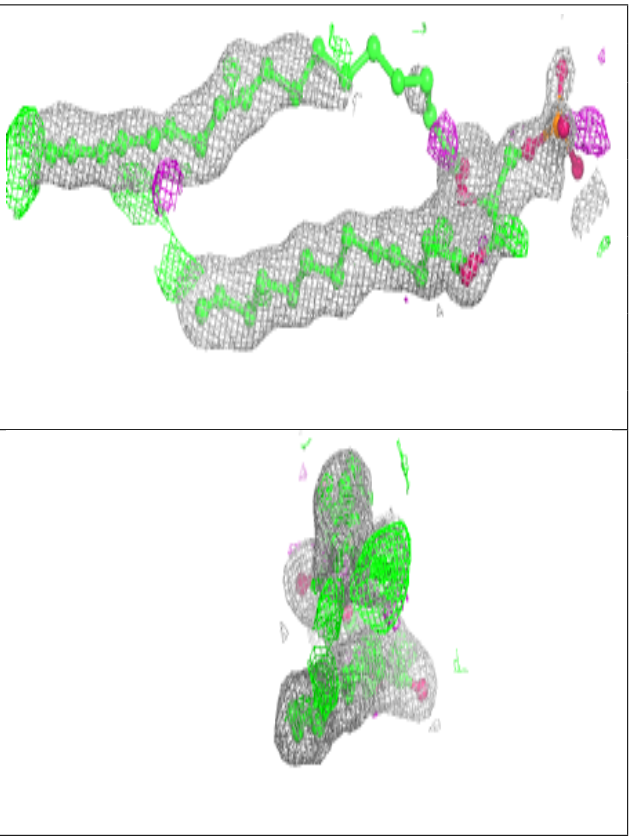
Electron density around DMU X 104:

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



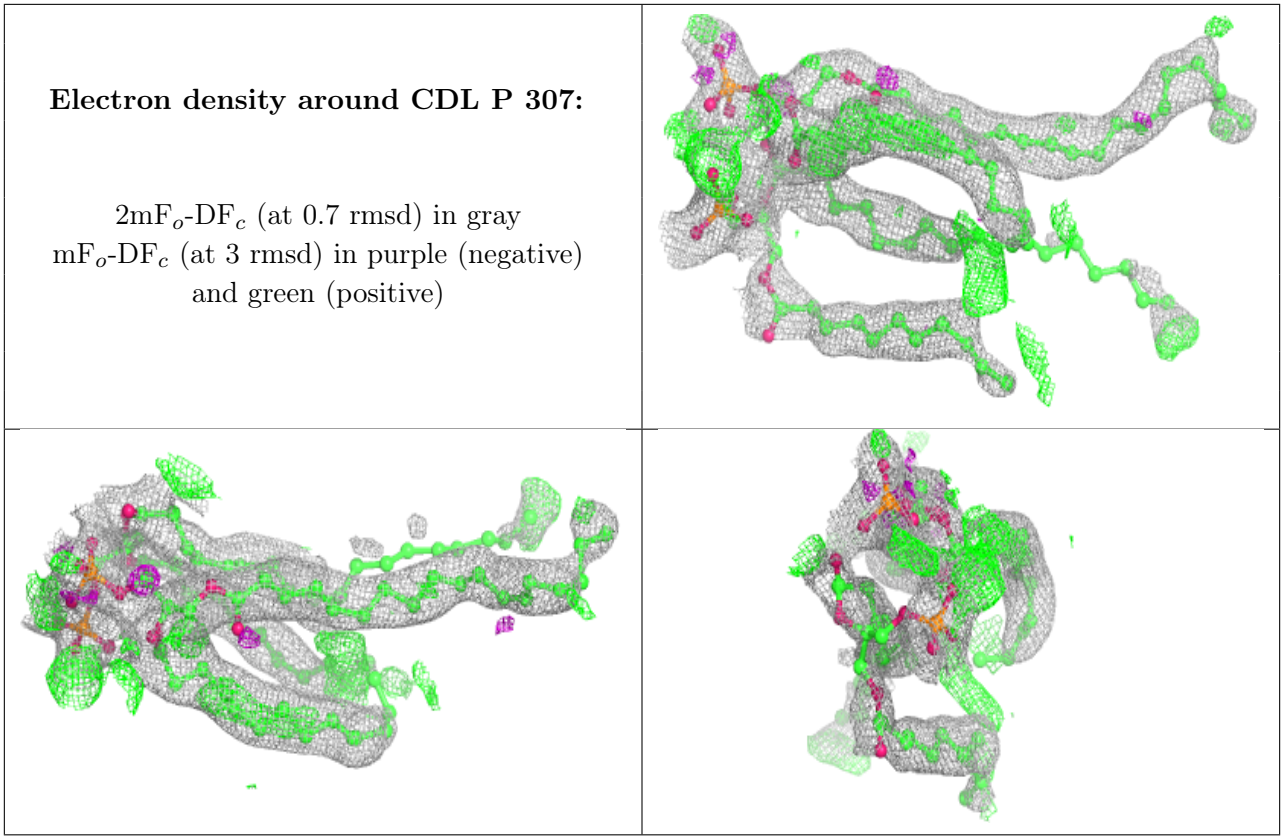
Electron density around PSC O 302:

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



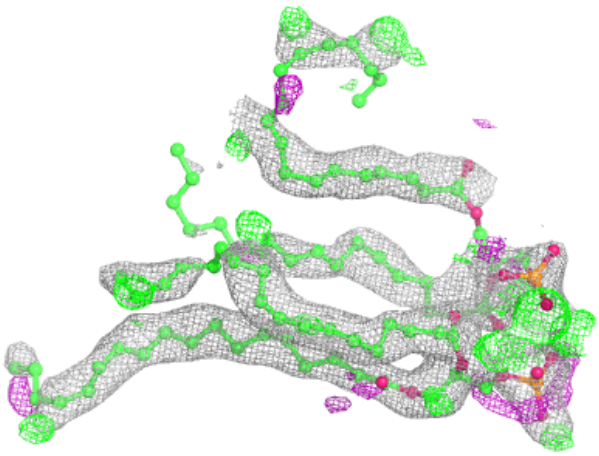
Electron density around CDL P 307:

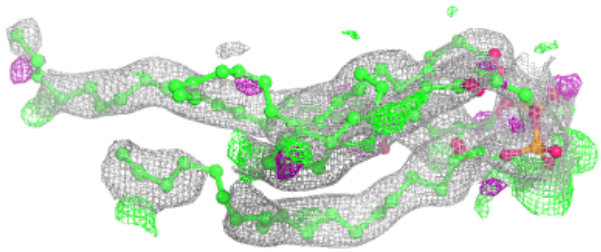
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

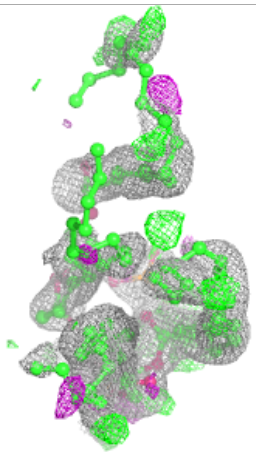


Electron density around CDL C 307:

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

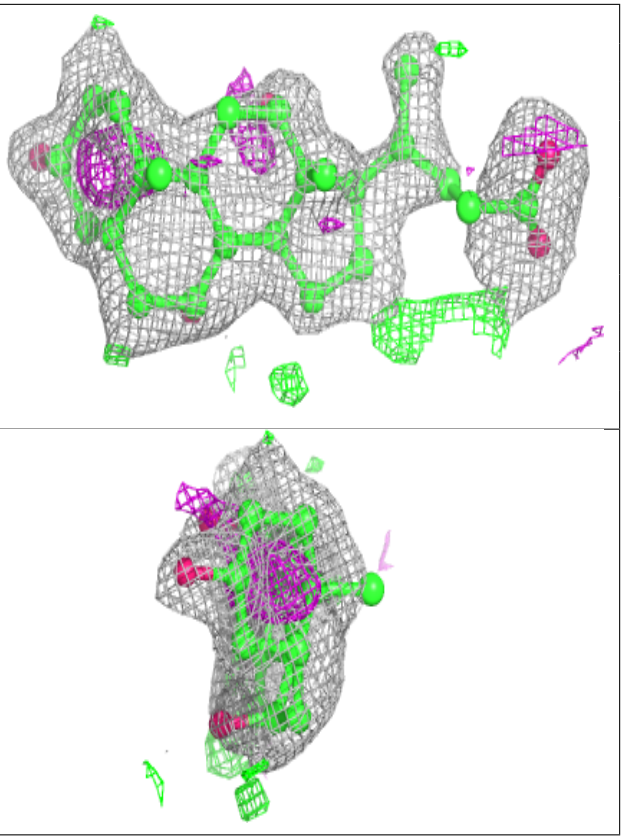






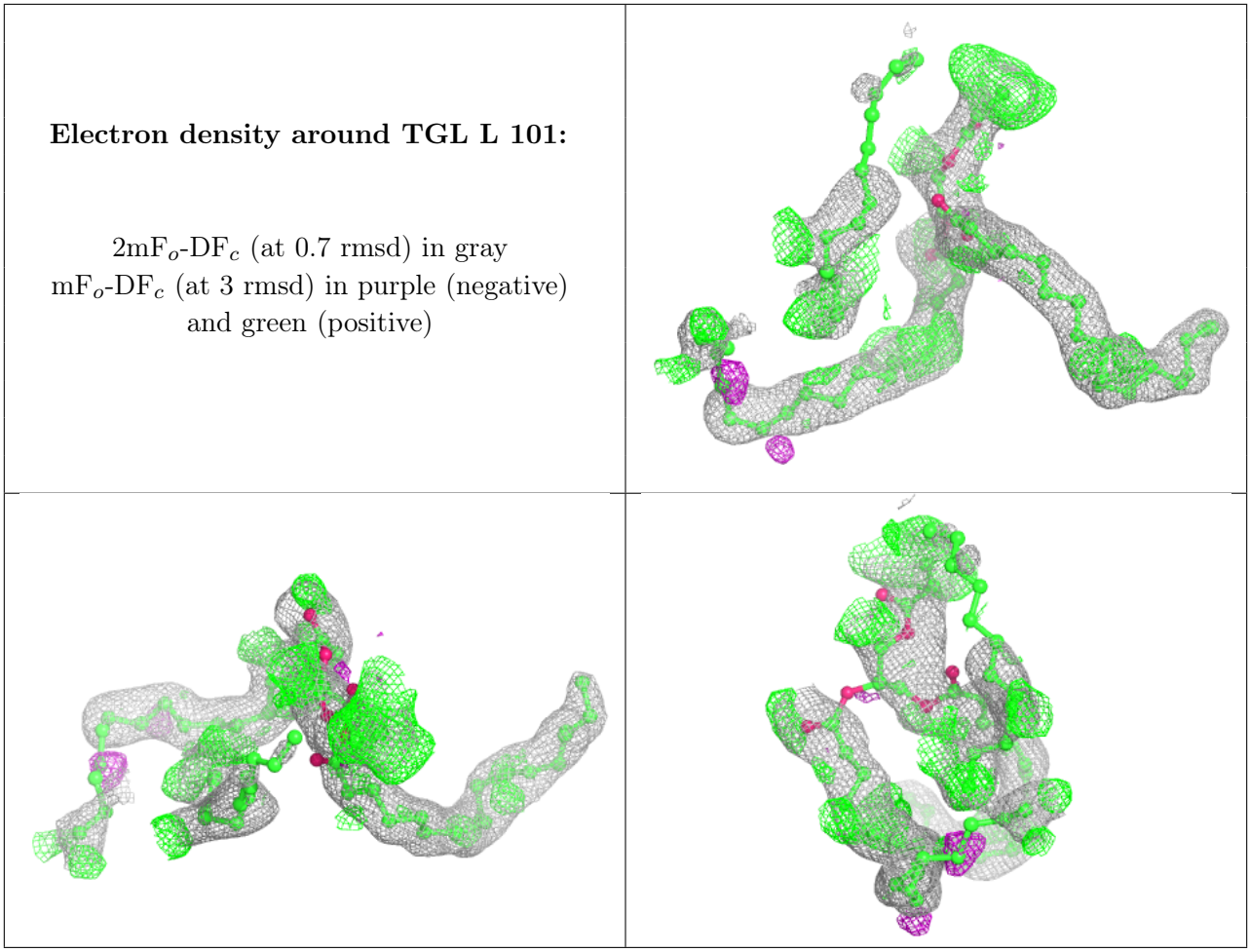
Electron density around CHD C 308:

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



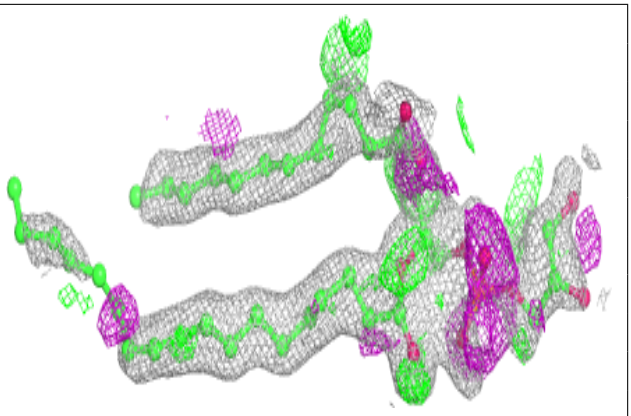
Electron density around TGL L 101:

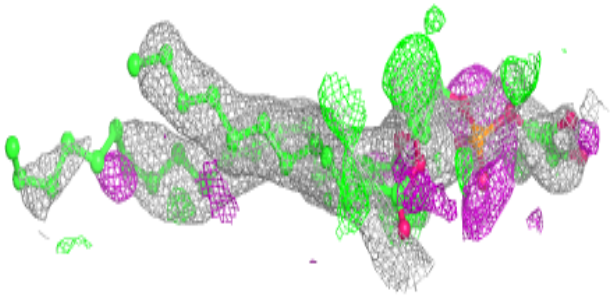
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

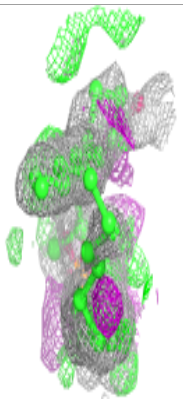


Electron density around PGV A 607:

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

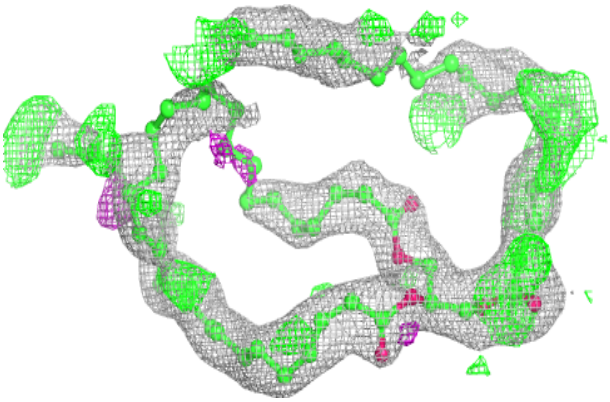


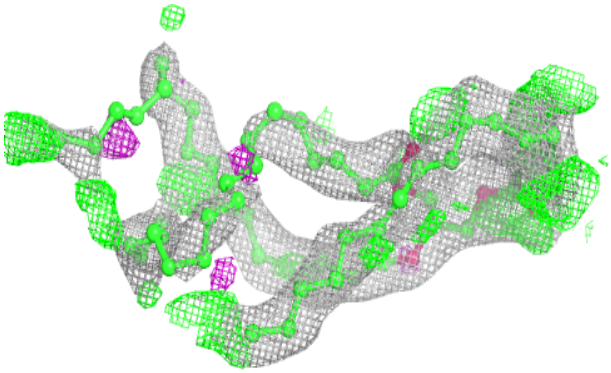


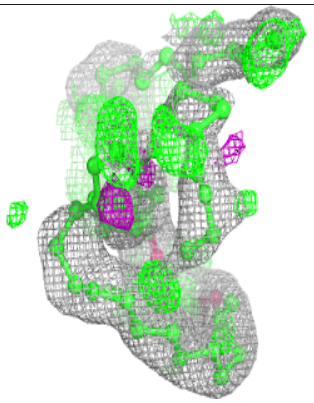


Electron density around TGL N 607:

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

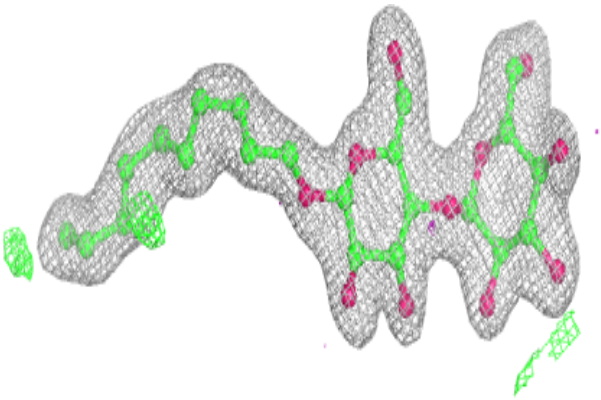


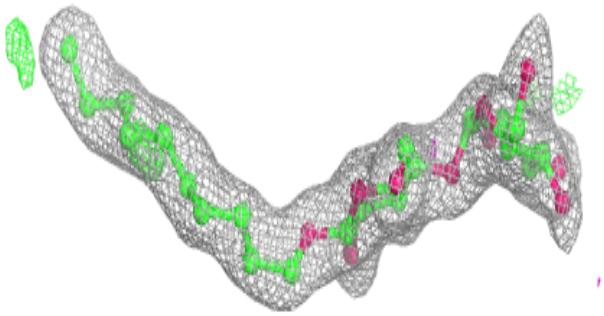


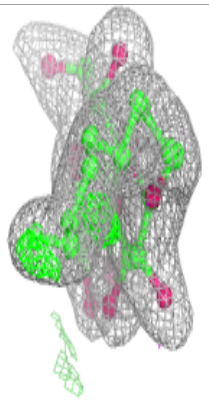


Electron density around DMU Z 101:

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

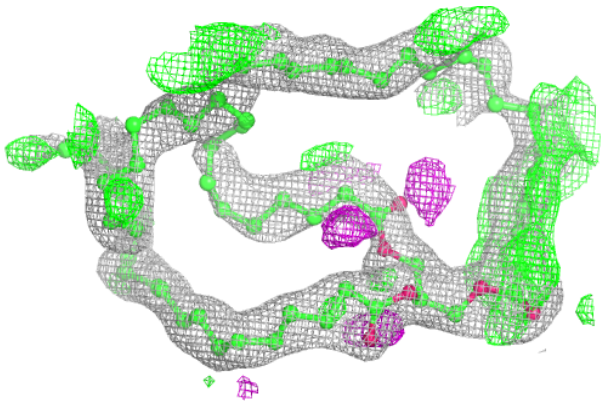


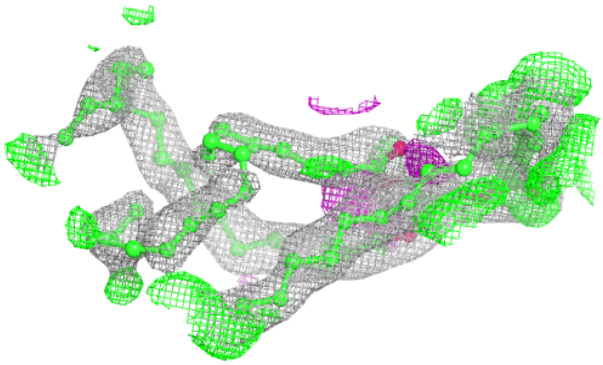


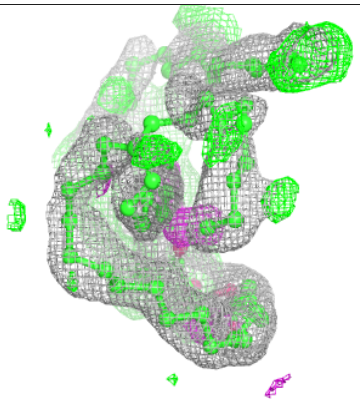


Electron density around TGL B 301:

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

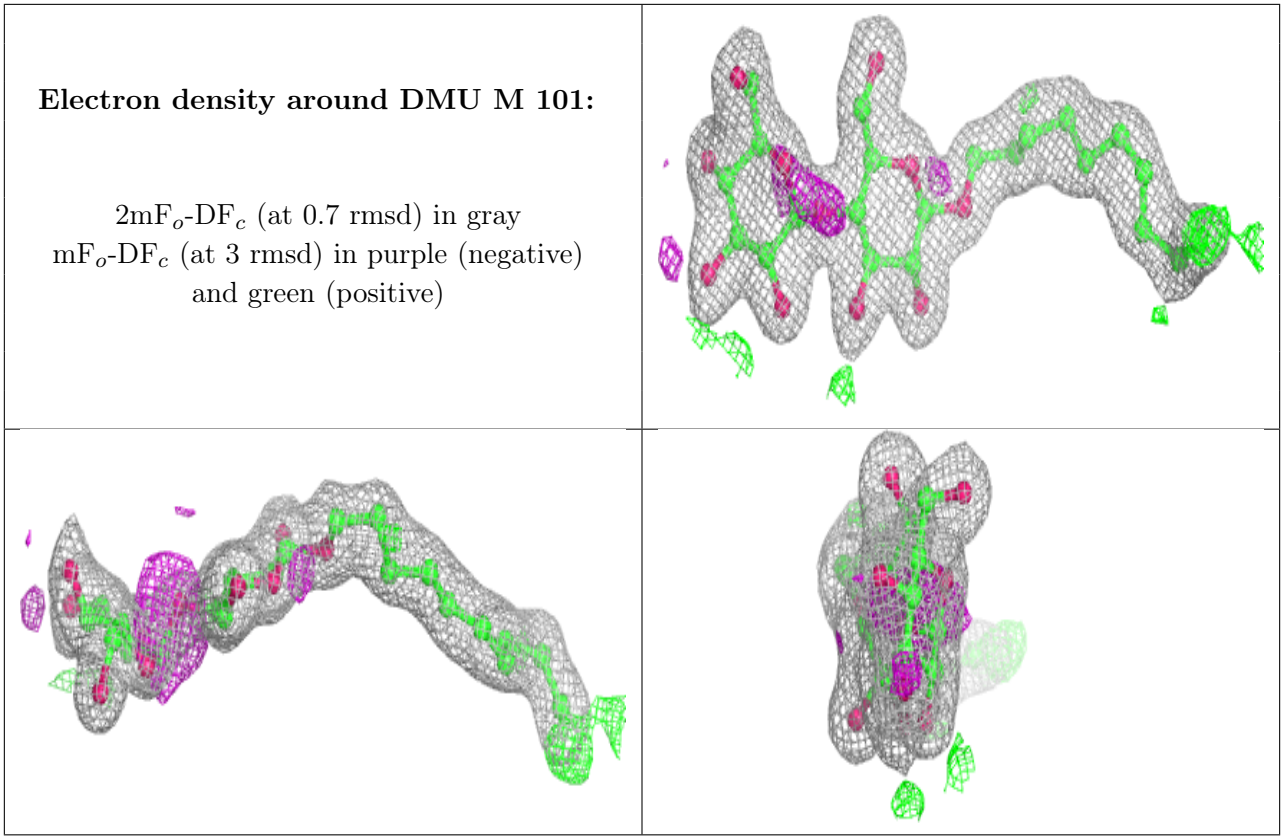






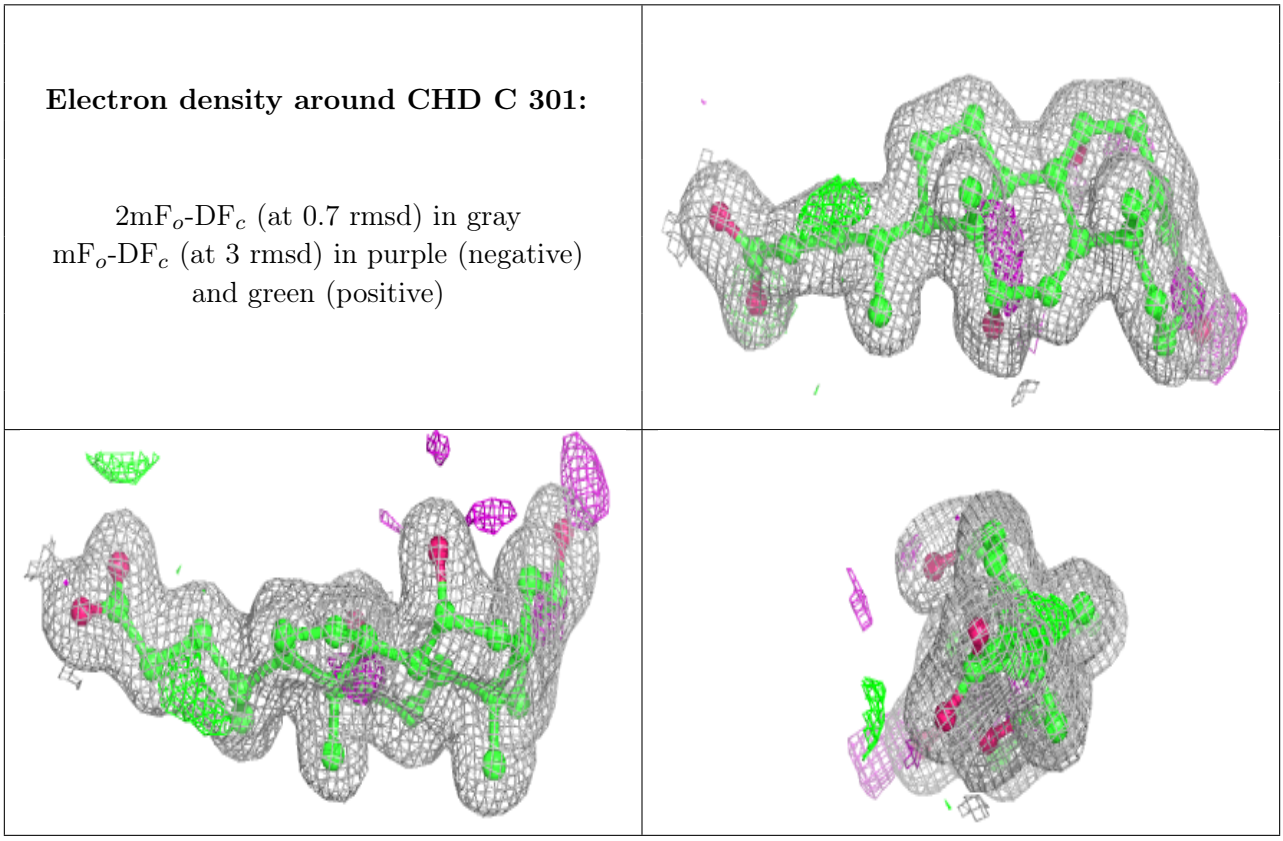
Electron density around DMU M 101:

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



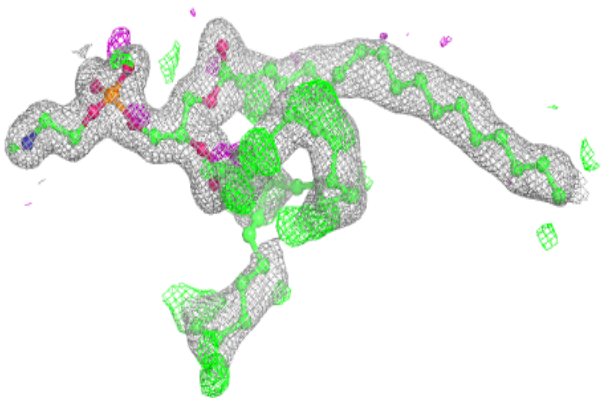
Electron density around CHD C 301:

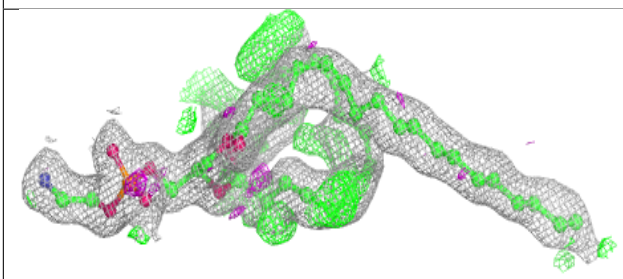
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

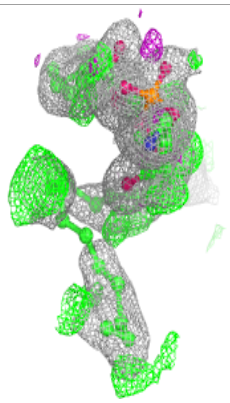


Electron density around PEK P 303:

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

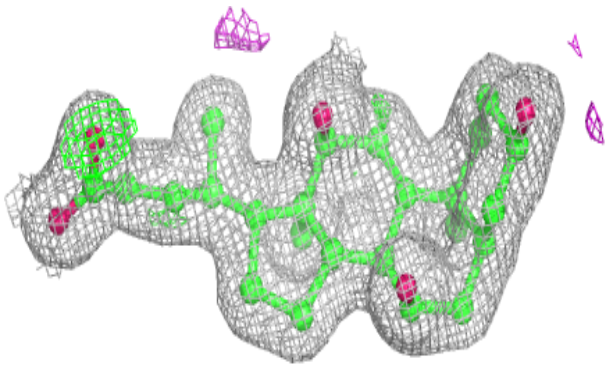


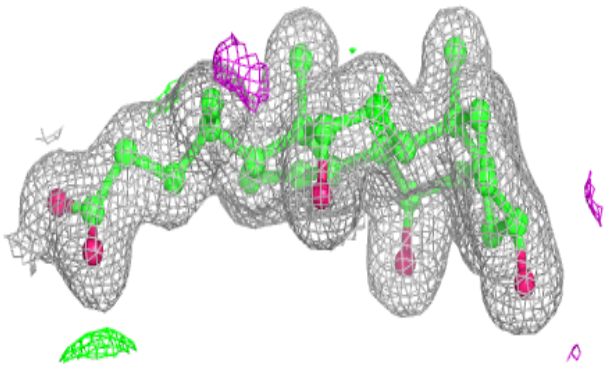




Electron density around CHD P 301:

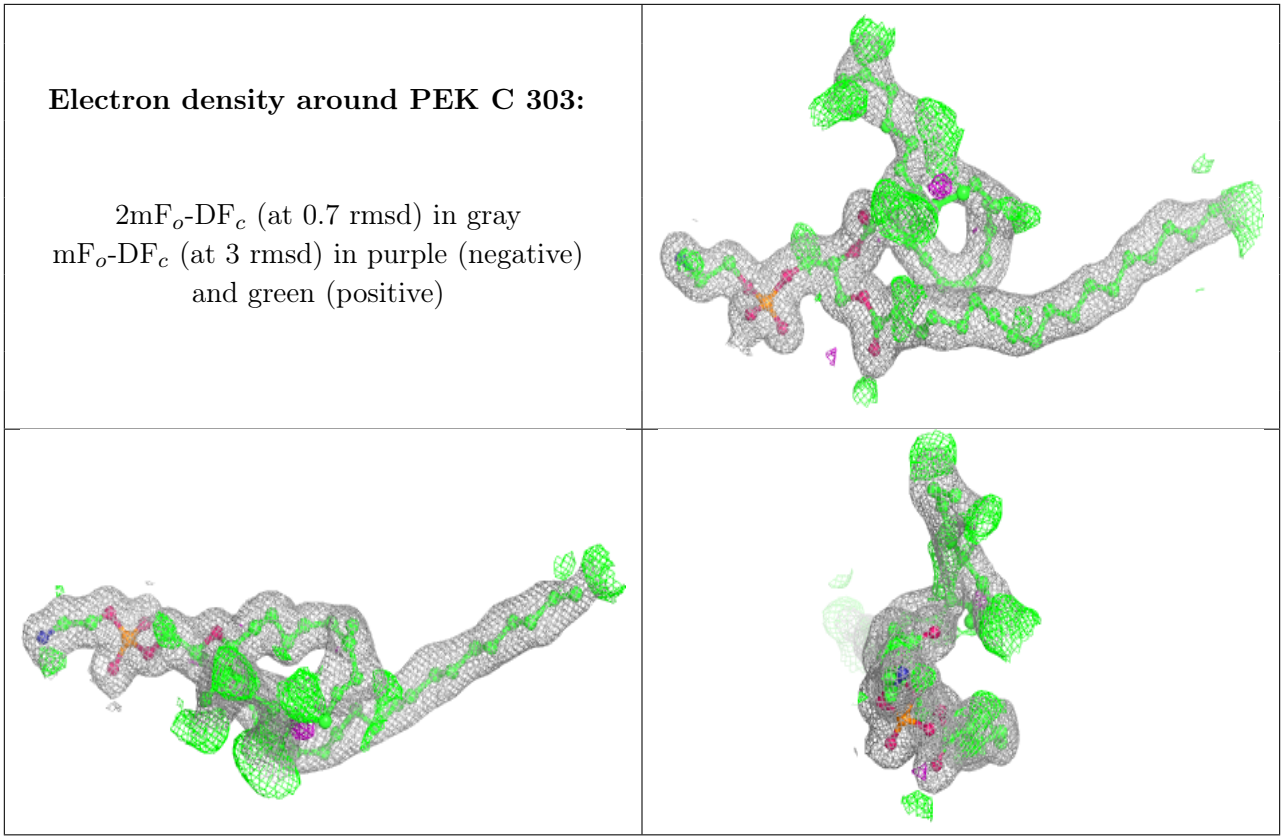
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





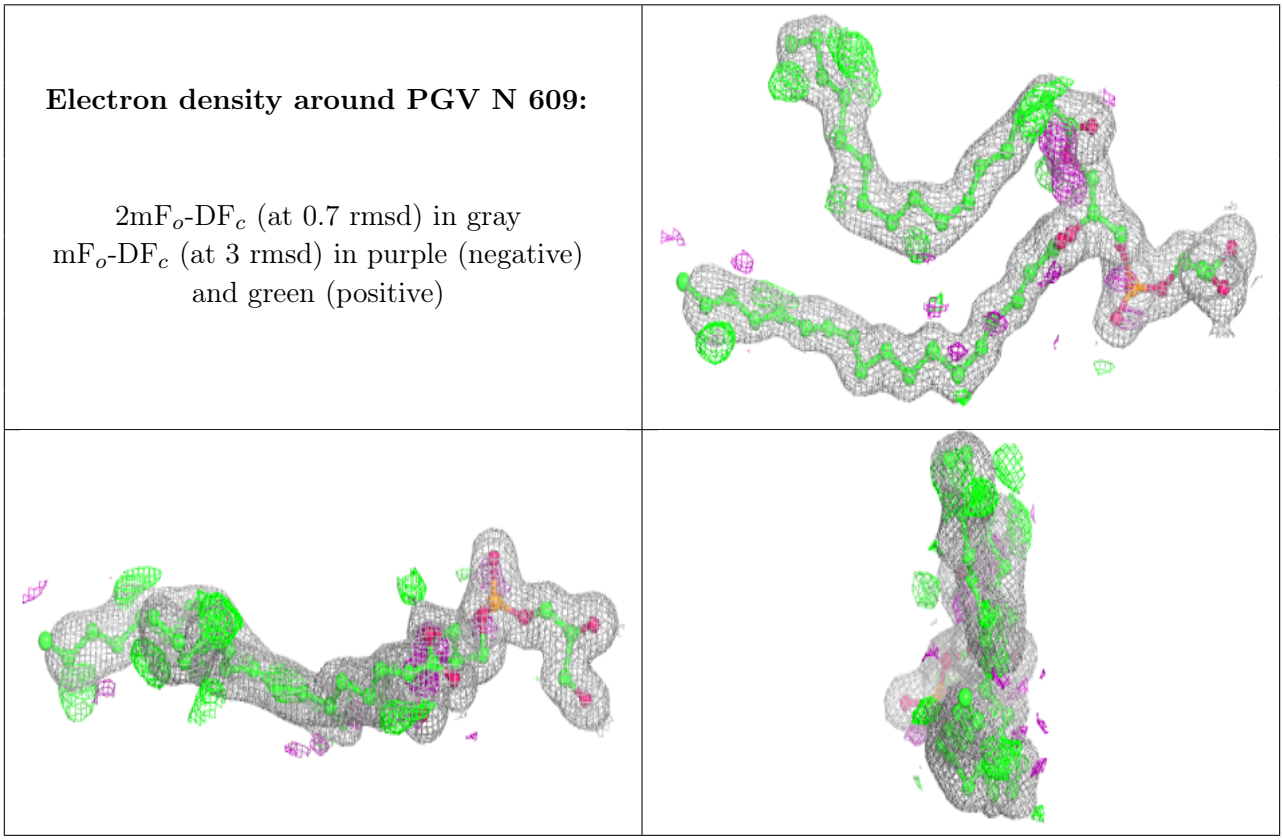
Electron density around PEK C 303:

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



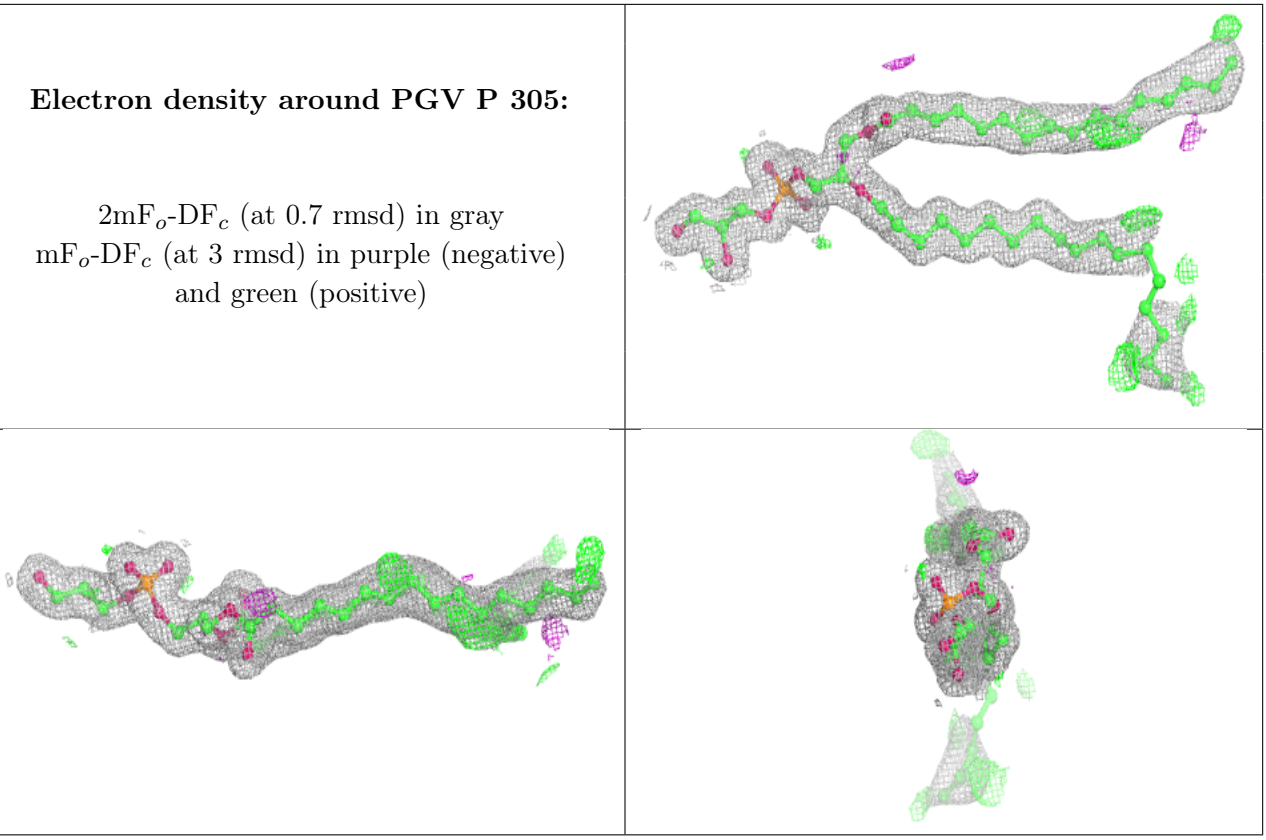
Electron density around PGV N 609:

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



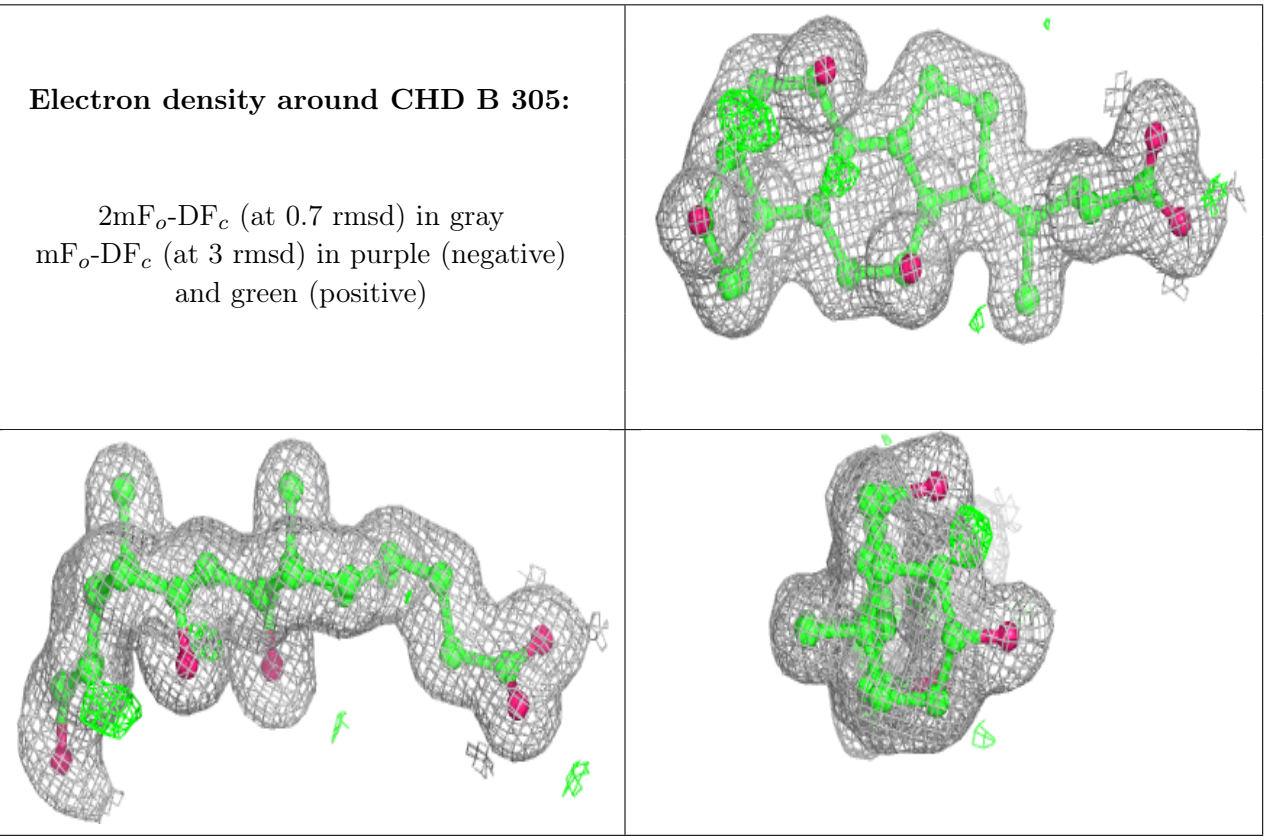
Electron density around PGV P 305:

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



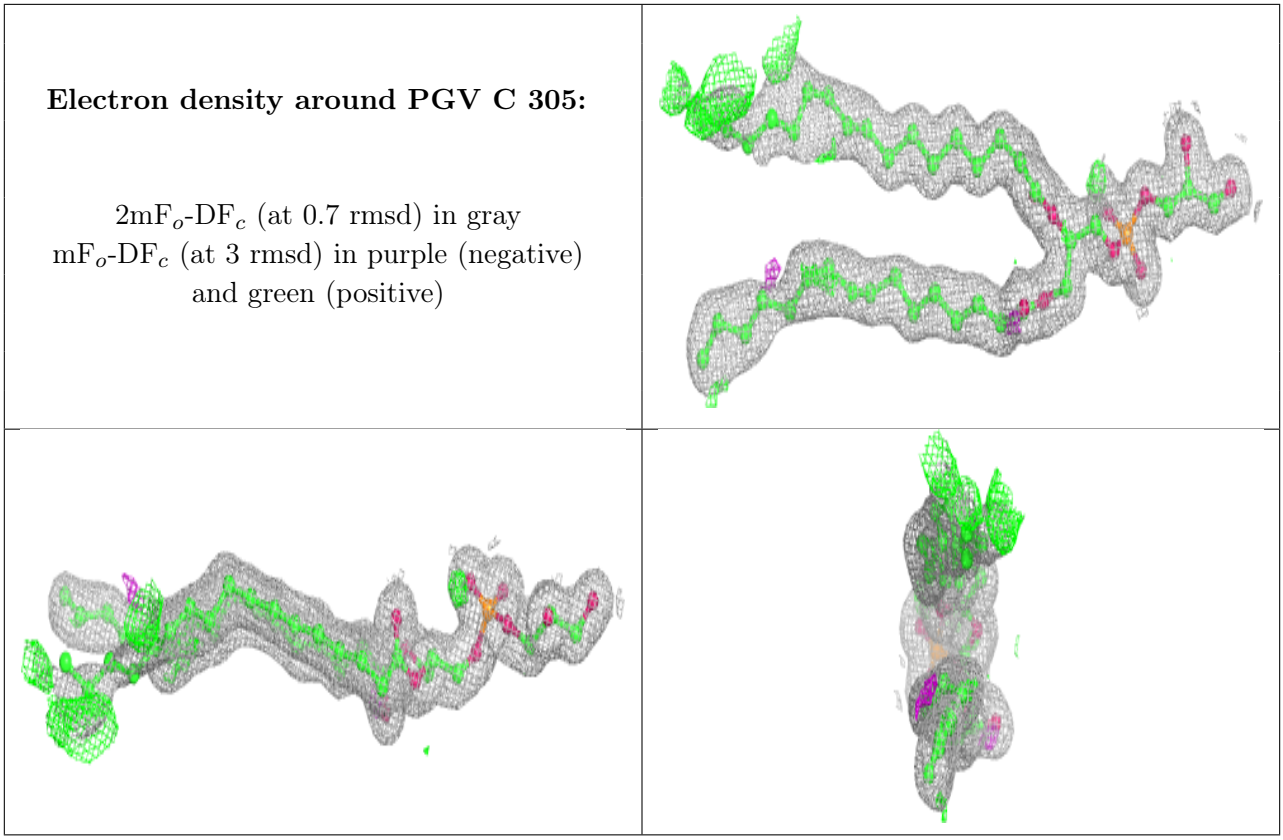
Electron density around CHD B 305:

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



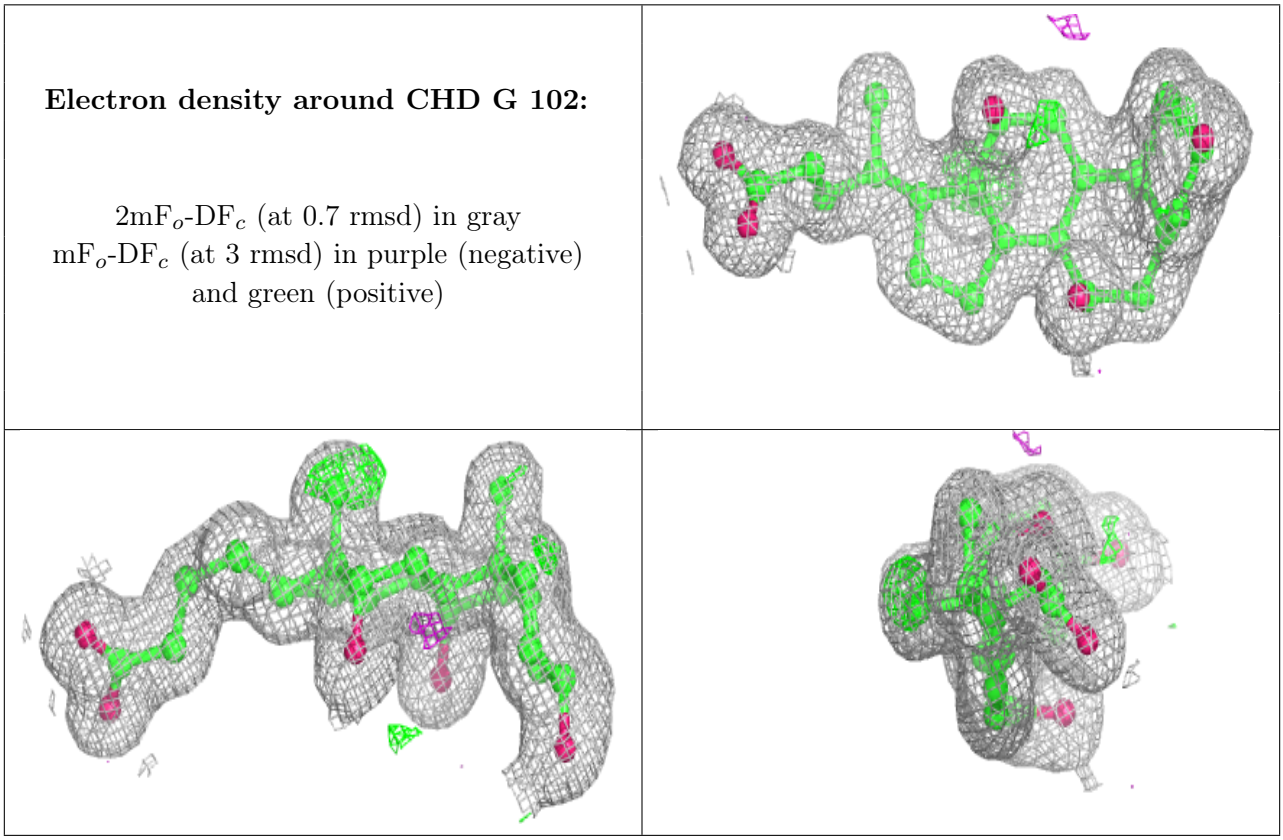
Electron density around PGV C 305:

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



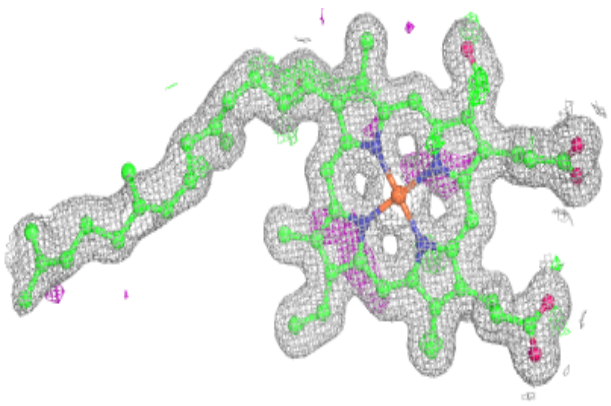
Electron density around CHD G 102:

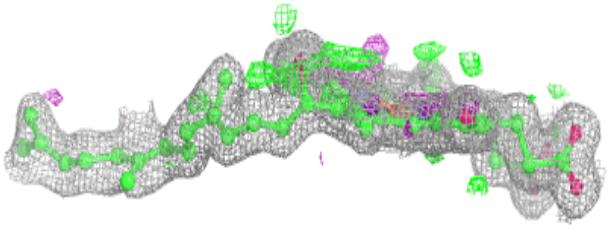
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

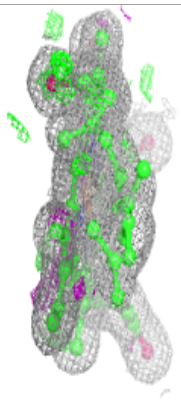


Electron density around HEA A 601 (A):

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

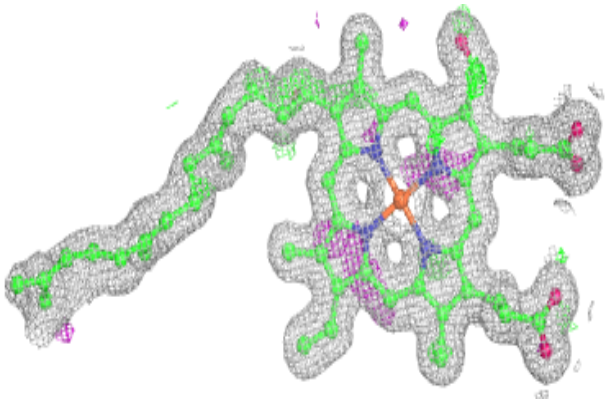


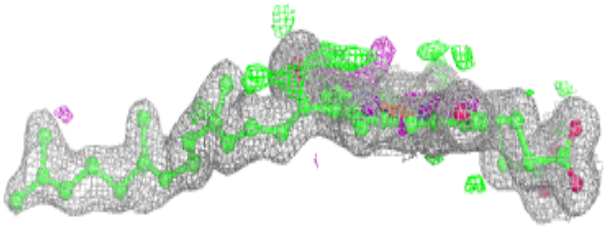


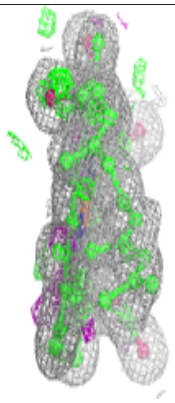


Electron density around HEA A 601 (B):

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

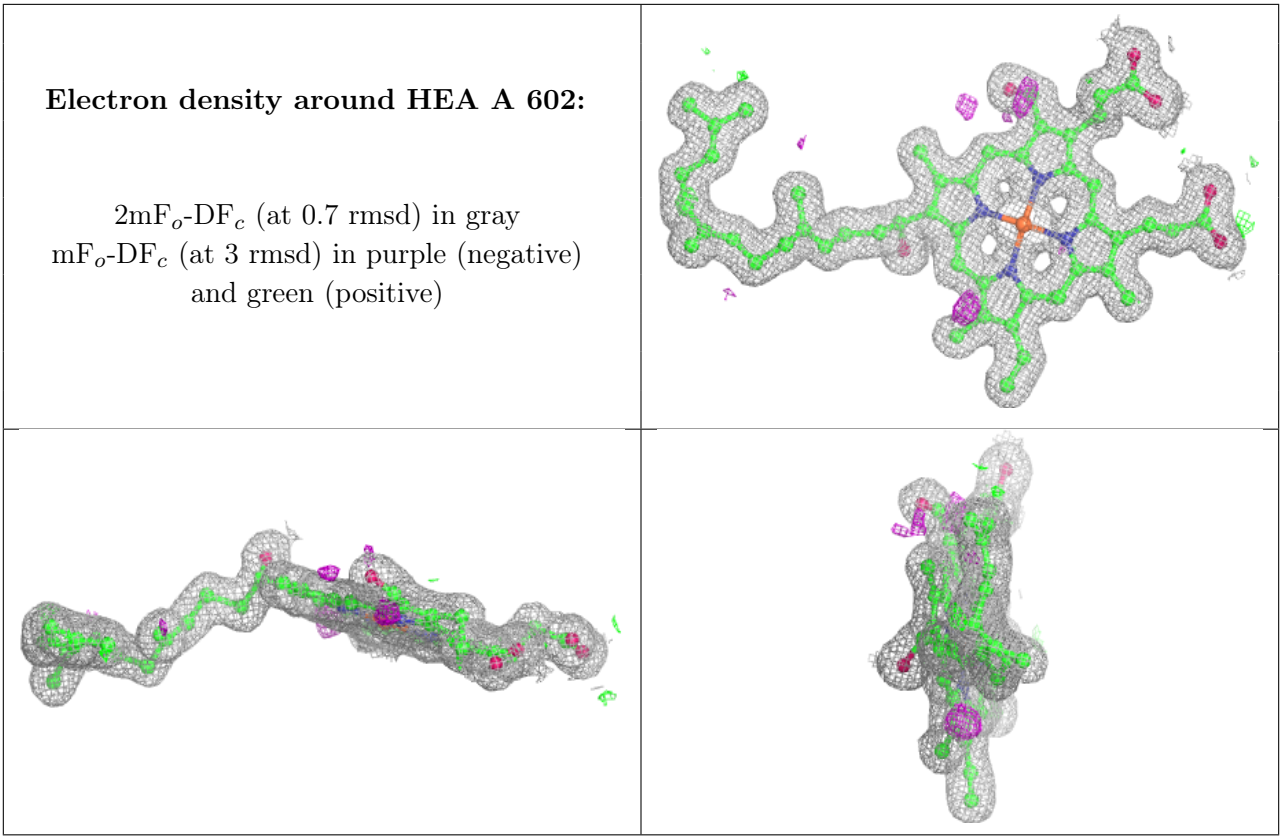






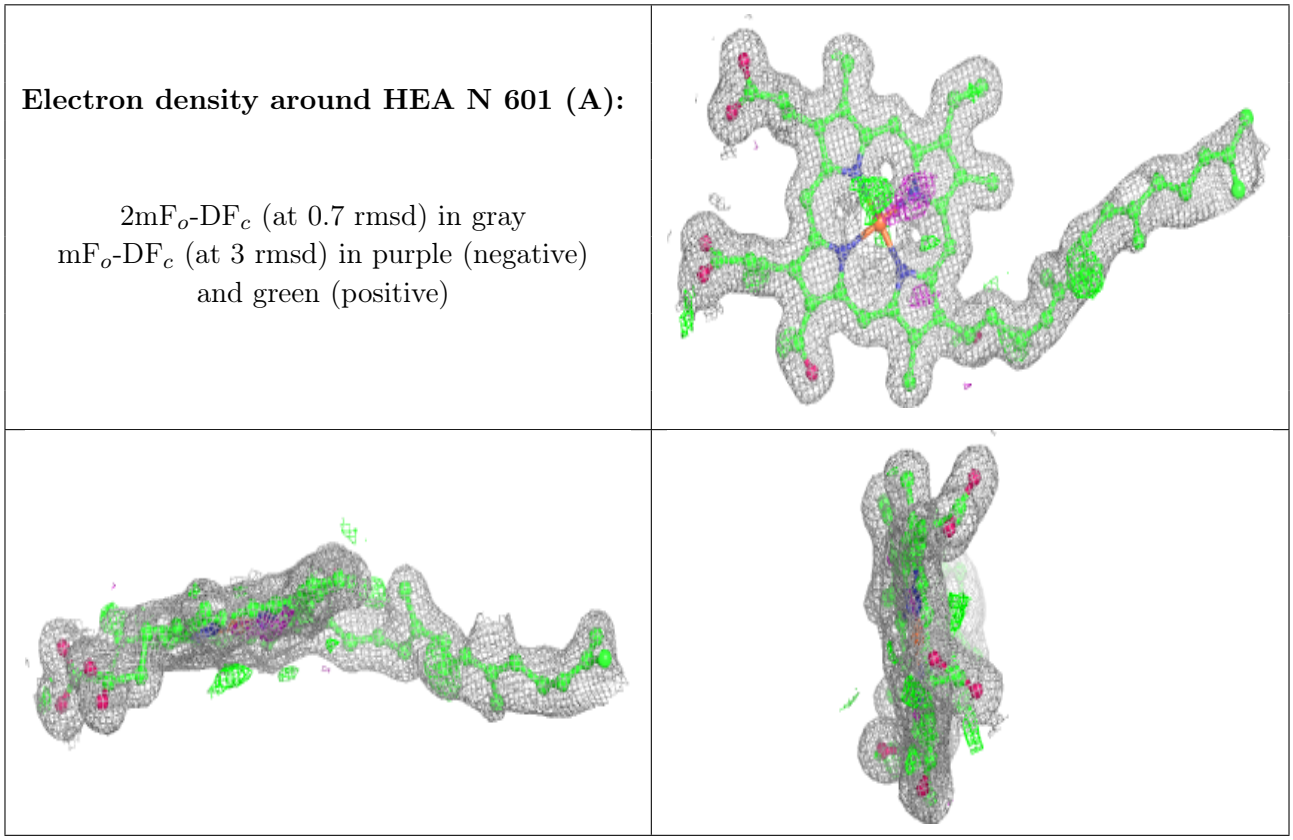
Electron density around HEA A 602:

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



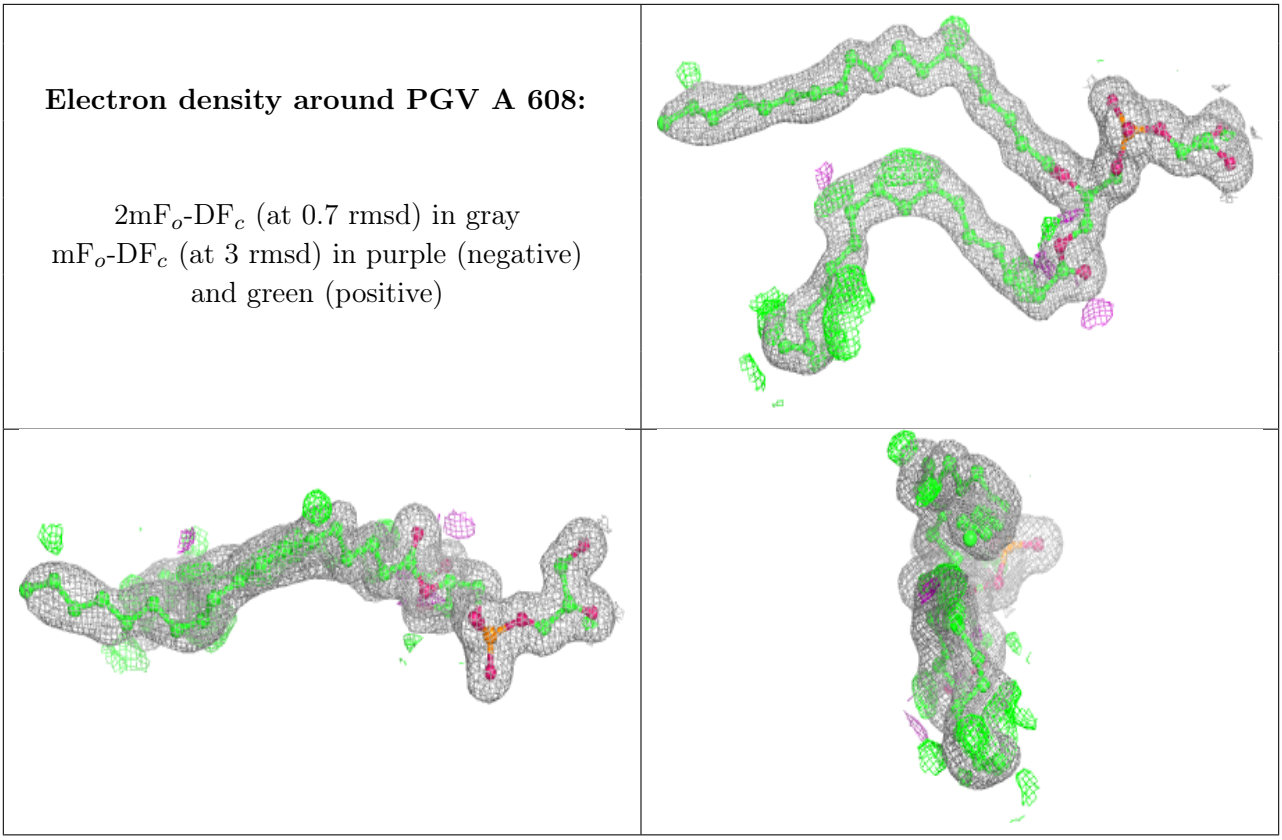
Electron density around HEA N 601 (A):

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



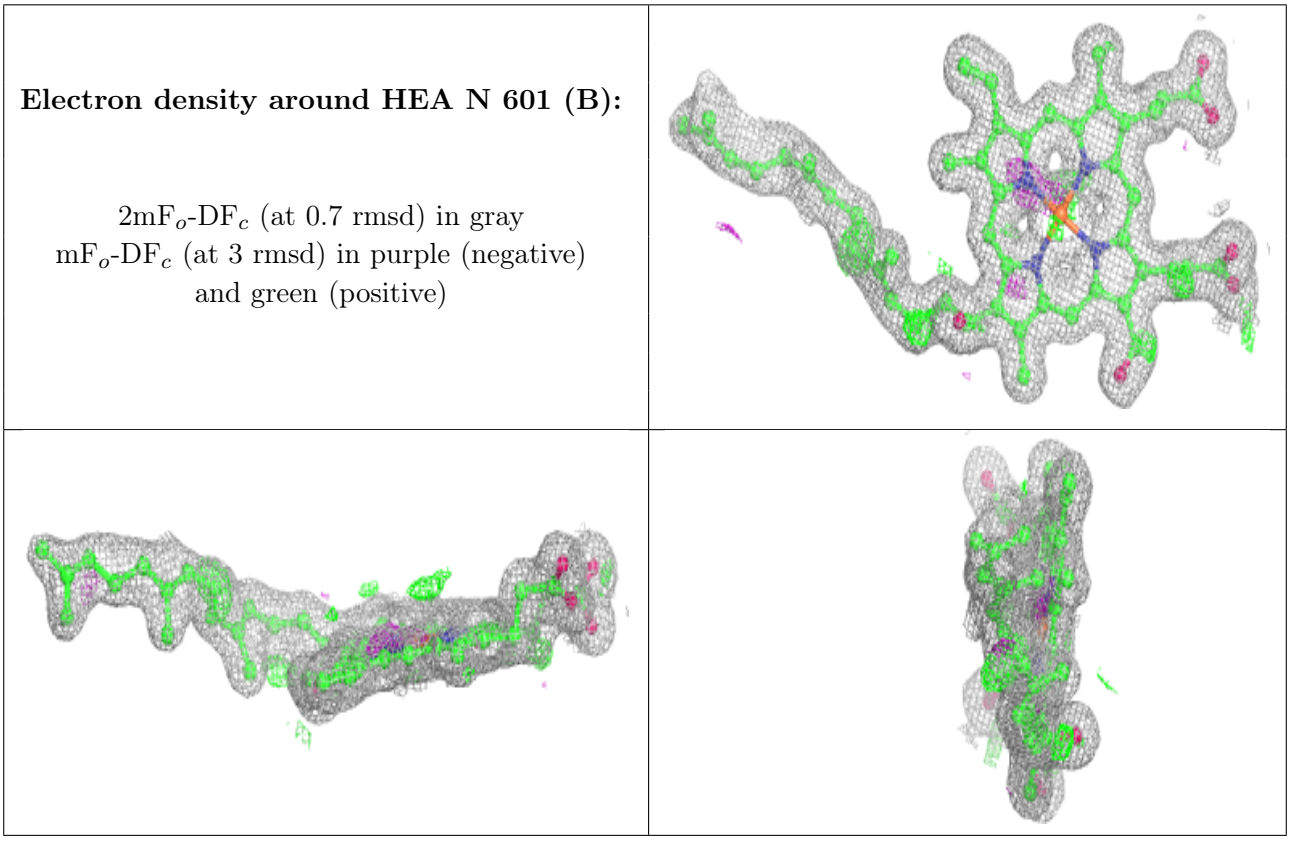
Electron density around PGV A 608:

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



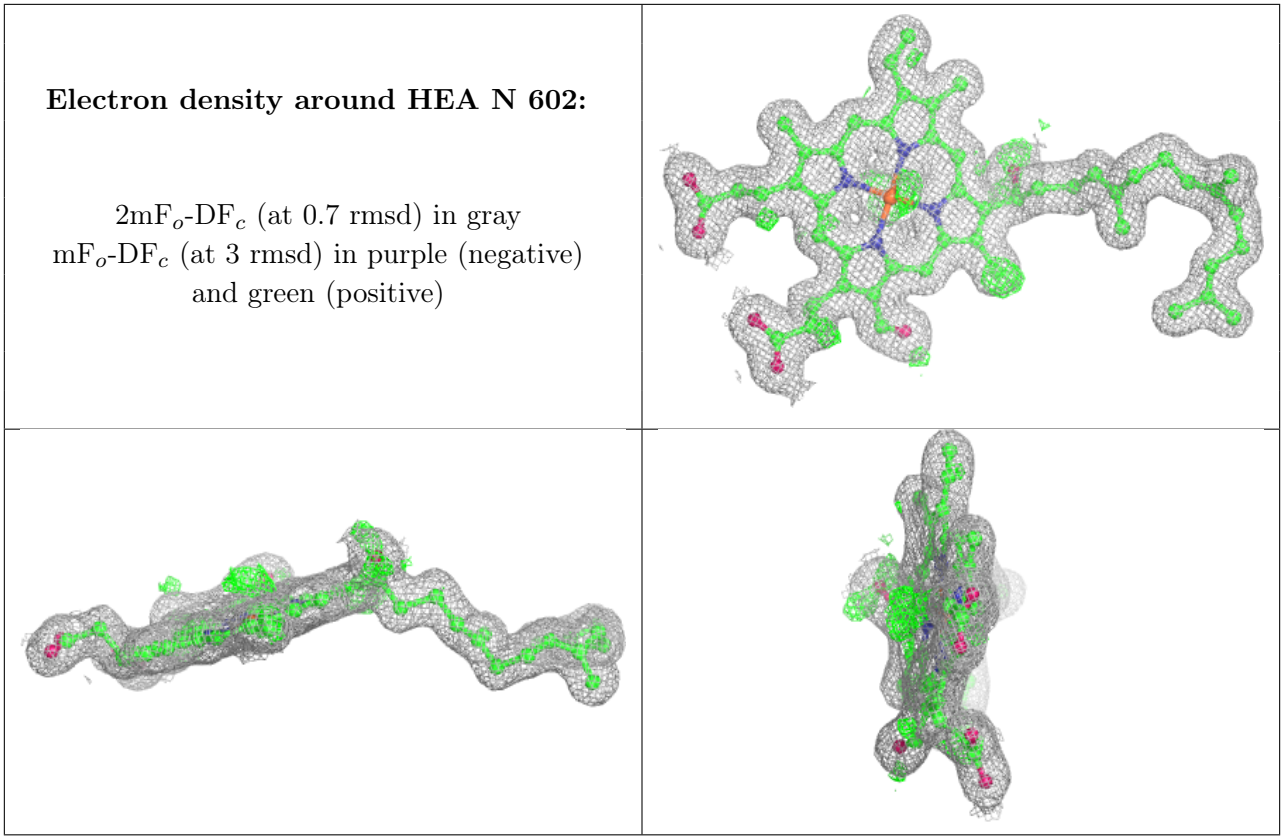
Electron density around HEA N 601 (B):

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.