wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 09:55 AM EDT

PDB ID	:	7THU
Title	:	Structure of reduced bovine cytochrome c oxidase at 1.93 Angstrom resolution obtained by synchrotron X-rays
Authors	:	Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on	:	2022-01-12
Resolution	:	1.93 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:

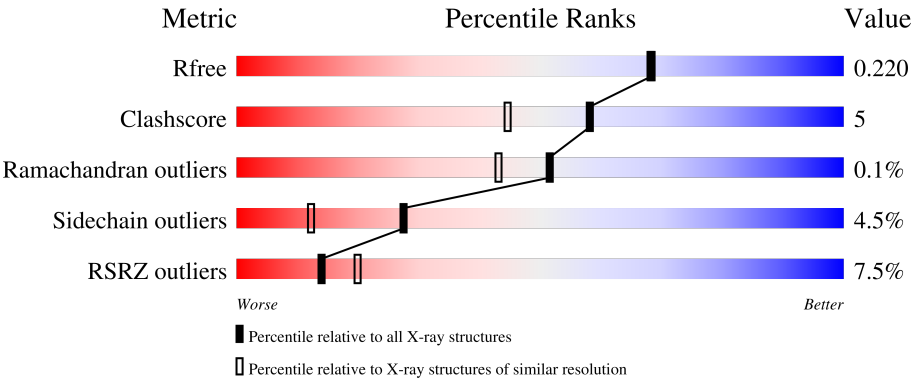
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	5% 89% 10%
1	N	514	4% 88% 11%
2	B	227	2% 87% 11%
2	O	227	4% 85% 15%
3	C	261	91% 8%

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Mol	Chain	Length	Quality of chain
3	P	261	2% 92% 7%
4	D	147	1% 93% 6%
4	Q	147	16% 90% 10%
5	E	109	5% 89% 5%
5	R	109	7% 92%
6	F	98	13% 94% 6%
6	S	98	8% 84% 15%
7	G	85	25% 75% 20%
7	T	85	28% 73% 21% 5%
8	H	85	18% 79% 11% 7%
8	U	85	16% 80% 11% 7%
9	I	73	12% 88% 10%
9	V	73	23% 85% 14%
10	J	59	14% 93% 5%
10	W	59	10% 92% 5%
11	K	56	5% 84% 9% 7%
11	X	56	16% 88% 5% 7%
12	L	47	4% 87% 11%
12	Y	47	4% 83% 15%
13	M	46	9% 76% 17% 7%
13	Z	46	17% 76% 17% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	606	X	-	-	-
18	HEA	A	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	606	X	-	-	-
18	HEA	N	607	X	-	-	-
19	EDO	N	614	-	-	X	-
23	DMU	C	301	-	-	-	X
28	SAC	V	101	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32695 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	0	0	0
			1214	788	201	221	4			
4	Q	147	Total	C	N	O	S	0	0	0
			1214	788	201	221	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			
11	X	52	Total	C	N	O	S	0	0	0
			413	266	72	73	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	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

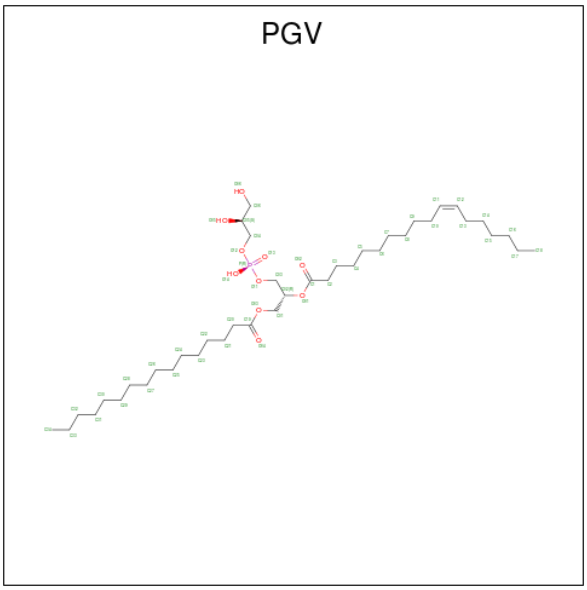
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

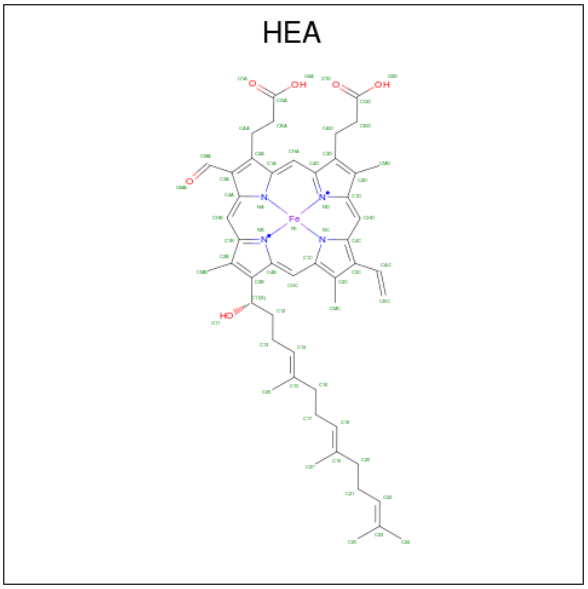
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



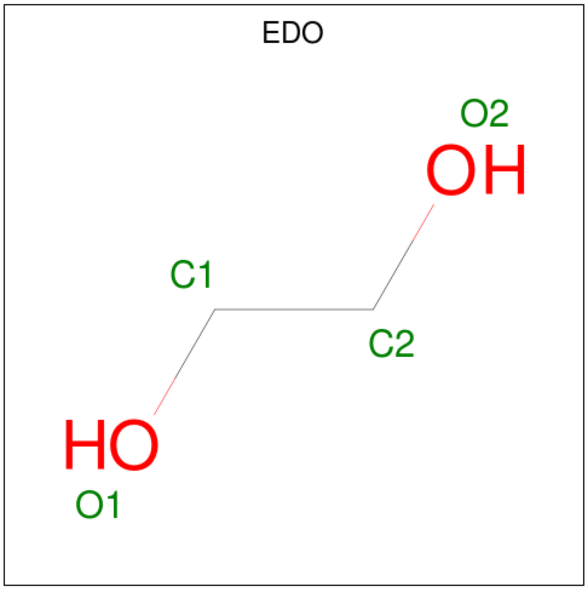
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C O P 51 40 10 1	0	0
17	A	1	Total C O P 51 40 10 1	0	0
17	C	1	Total C O P 51 40 10 1	0	0
17	N	1	Total C O P 51 40 10 1	0	0
17	N	1	Total C O P 51 40 10 1	0	0
17	P	1	Total C O P 51 40 10 1	0	0
17	T	1	Total C O P 51 40 10 1	0	0
17	Z	1	Total C O P 51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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total	C	O	0	0
			4	2	2		
19	F	1	Total	C	O	0	0
			4	2	2		
19	F	1	Total	C	O	0	0
			4	2	2		
19	F	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	I	1	Total	C	O	0	0
			4	2	2		
19	I	1	Total	C	O	0	0
			4	2	2		
19	J	1	Total	C	O	0	0
			4	2	2		
19	J	1	Total	C	O	0	0
			4	2	2		
19	J	1	Total	C	O	0	0
			4	2	2		
19	J	1	Total	C	O	0	0
			4	2	2		
19	K	1	Total	C	O	0	0
			4	2	2		
19	K	1	Total	C	O	0	0
			4	2	2		
19	L	1	Total	C	O	0	0
			4	2	2		
19	M	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		

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

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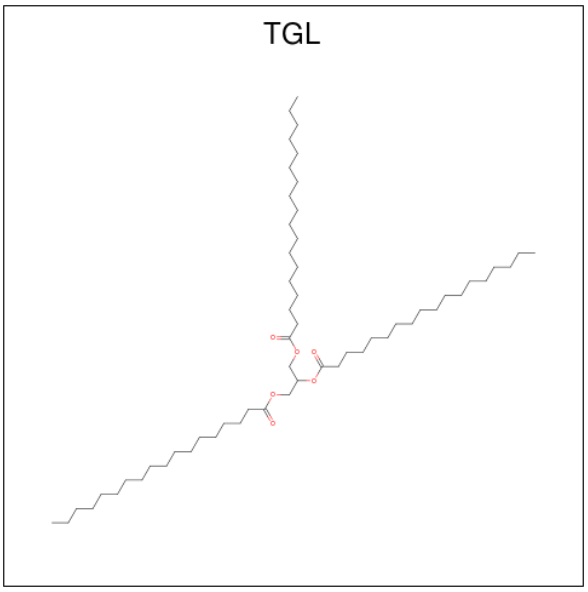
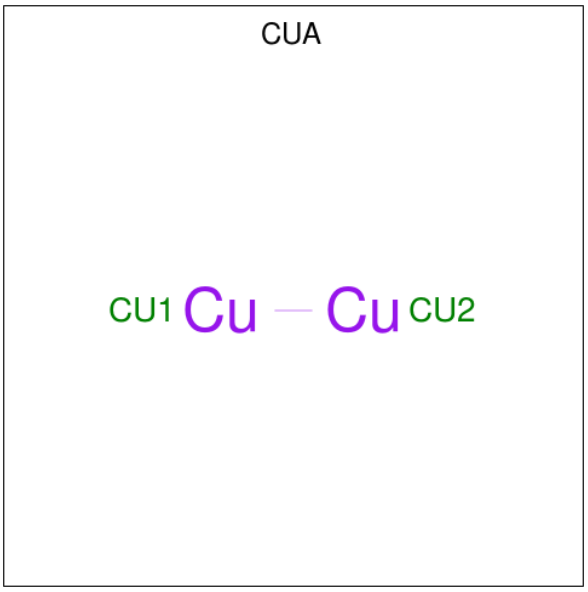
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	U	1	Total	C	O	0	0
			4	2	2		
19	V	1	Total	C	O	0	0
			4	2	2		
19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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$) (labeled as "Ligand of Interest" by depositor).



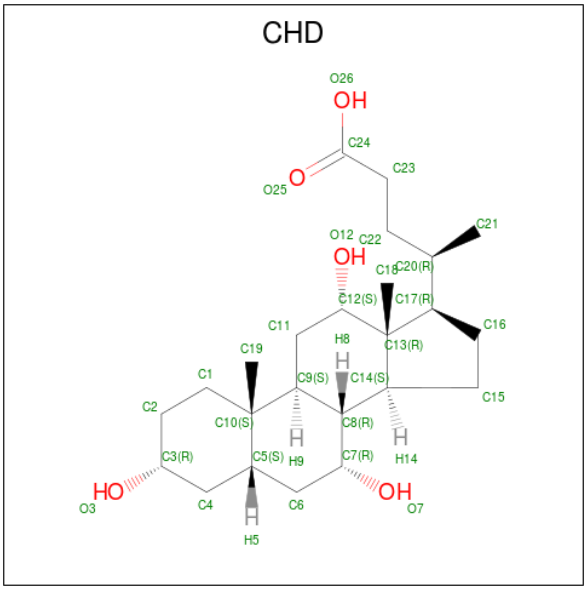
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 63 57 6	0	0
20	D	1	Total C O 63 57 6	0	0
20	L	1	Total C O 63 57 6	0	0
20	N	1	Total C O 63 57 6	0	0
20	Q	1	Total C O 63 57 6	0	0
20	Y	1	Total C O 63 57 6	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0

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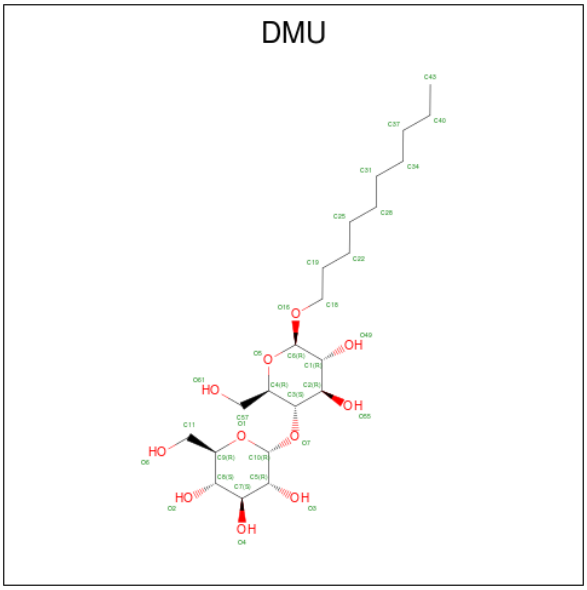
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	T	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0
22	Y	1	Total C O 29 24 5	0	0

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 33 22 11	0	0
23	C	1	Total C O 33 22 11	0	0
23	G	1	Total C O 33 22 11	0	0

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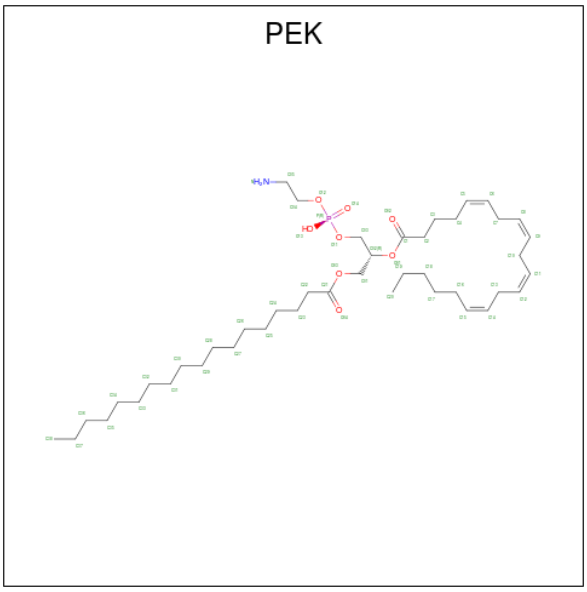
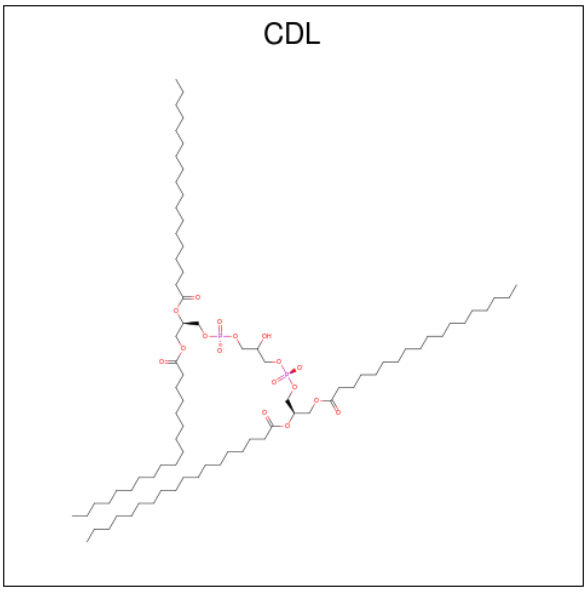
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	M	1	Total C O 33 22 11	0	0
23	P	1	Total C O 33 22 11	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 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: $C_{43}H_{78}NO_8P$).



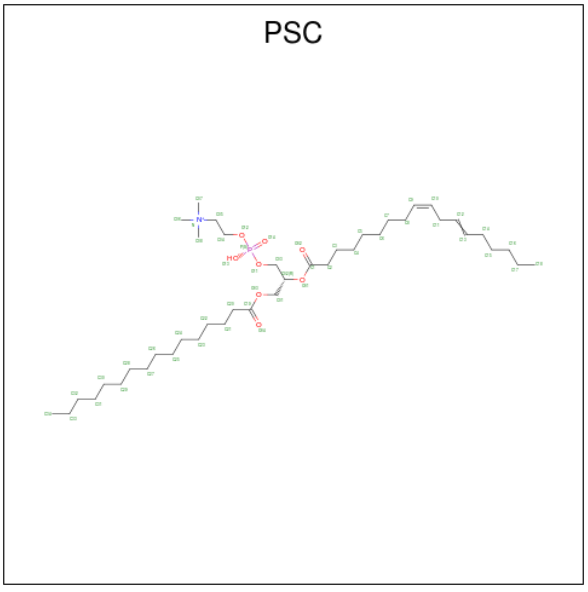
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 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: $C_{42}H_{81}NO_8P$).

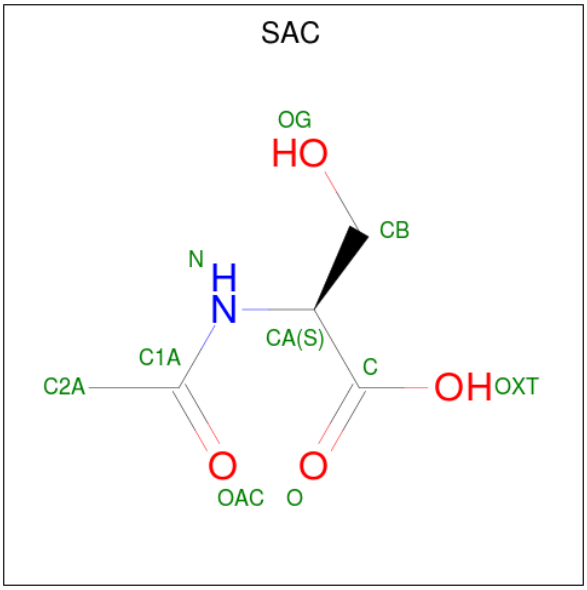


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	E	1	Total C N O P 52 42 1 8 1	0	0
26	O	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	F	1	Total Zn 1 1	0	0
27	S	1	Total Zn 1 1	0	0

- Molecule 28 is N-ACETYL-SERINE (three-letter code: SAC) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	I	1	Total C N O 9 5 1 3	0	0
28	V	1	Total C N O 9 5 1 3	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	190	Total O 190 190	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	125	Total O 125 125	0	0
29	C	96	Total O 96 96	0	0
29	D	68	Total O 68 68	0	0
29	E	53	Total O 53 53	0	0
29	F	70	Total O 70 70	0	0
29	G	35	Total O 35 35	0	0
29	H	39	Total O 39 39	0	0
29	I	24	Total O 24 24	0	0
29	J	17	Total O 17 17	0	0
29	K	9	Total O 9 9	0	0
29	L	21	Total O 21 21	0	0
29	M	14	Total O 14 14	0	0
29	N	179	Total O 179 179	0	0
29	O	85	Total O 85 85	0	0
29	P	80	Total O 80 80	0	0
29	Q	46	Total O 46 46	0	0
29	R	46	Total O 46 46	0	0
29	S	64	Total O 64 64	0	0
29	T	23	Total O 23 23	0	0
29	U	30	Total O 30 30	0	0
29	V	16	Total O 16 16	0	0

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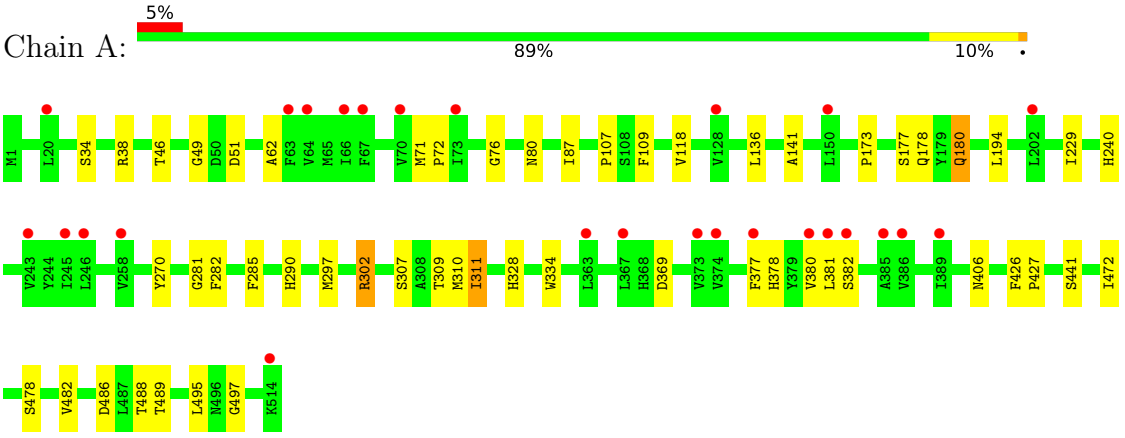
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	W	17	Total O 17 17	0	0
29	X	11	Total O 11 11	0	0
29	Y	18	Total O 18 18	0	0
29	Z	5	Total O 5 5	0	0

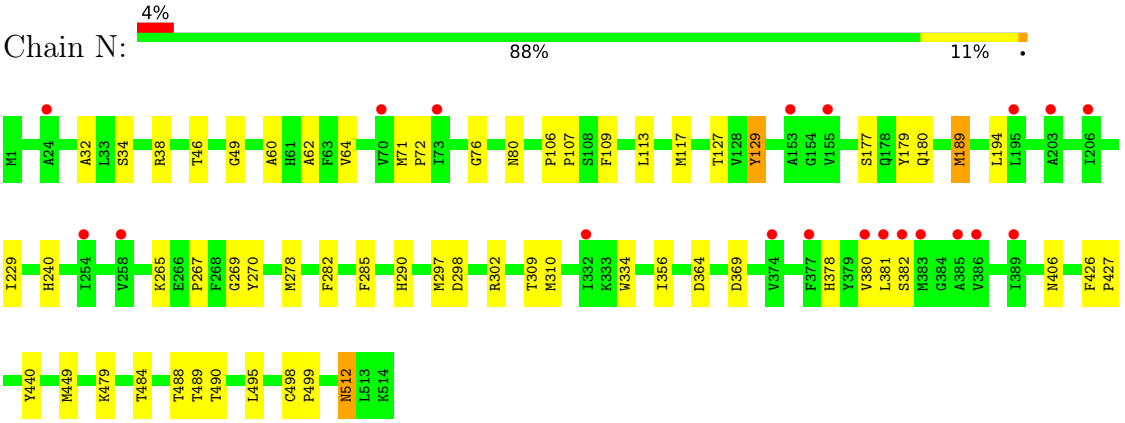
3 Residue-property plots (i)

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.

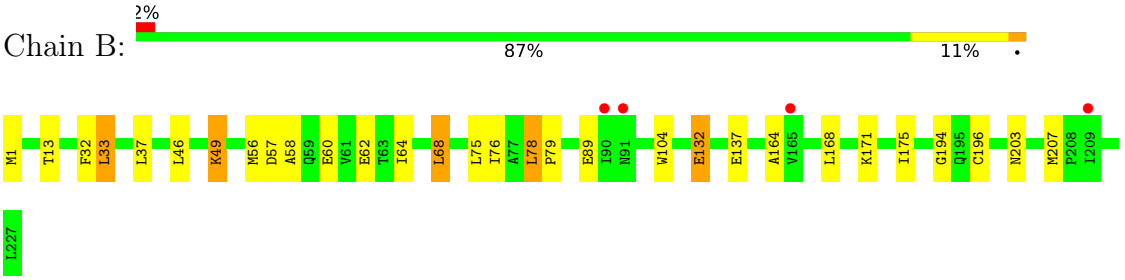
• Molecule 1: Cytochrome c oxidase subunit 1



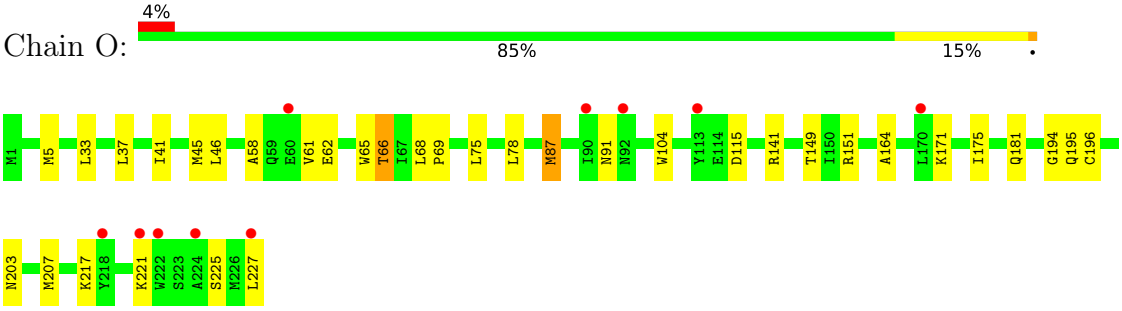
• Molecule 1: Cytochrome c oxidase subunit 1



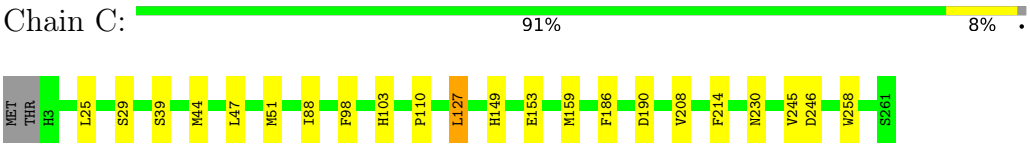
• Molecule 2: Cytochrome c oxidase subunit 2



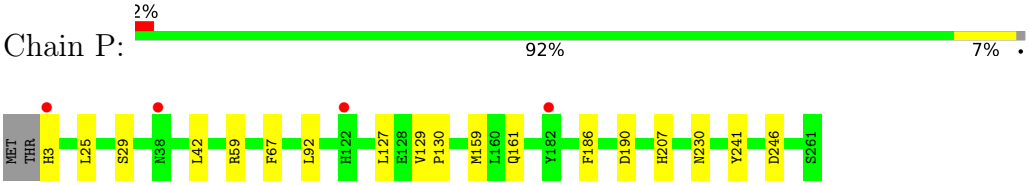
• Molecule 2: Cytochrome c oxidase subunit 2



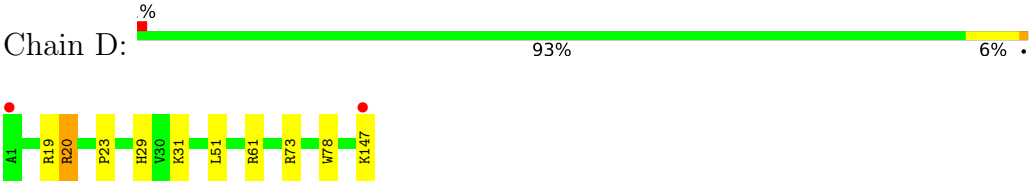
• Molecule 3: Cytochrome c oxidase subunit 3



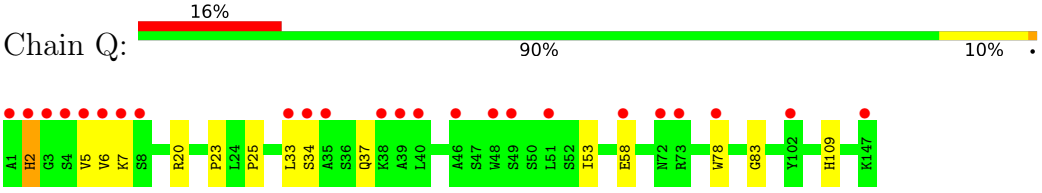
• Molecule 3: Cytochrome c oxidase subunit 3



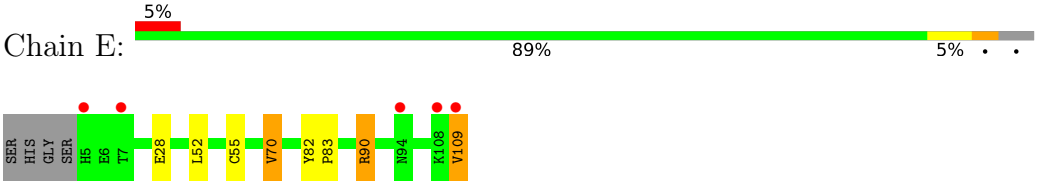
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

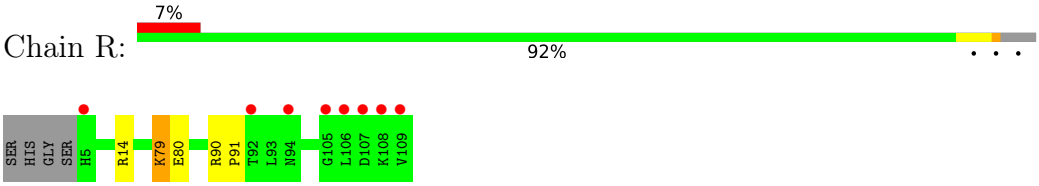


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



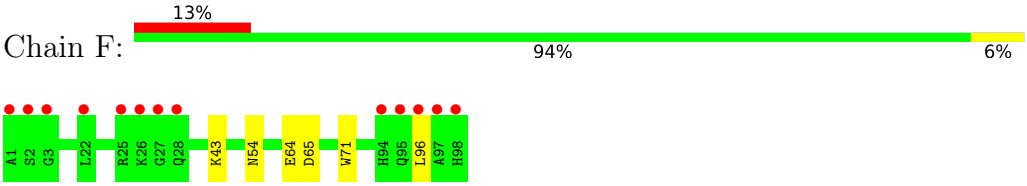
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



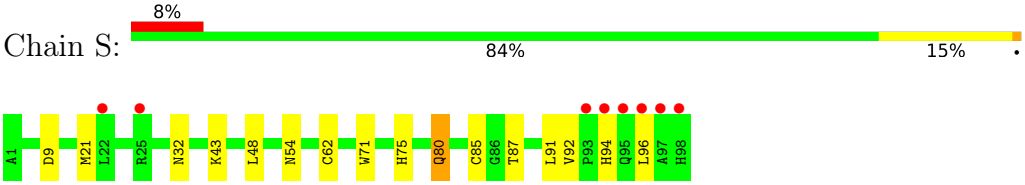
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



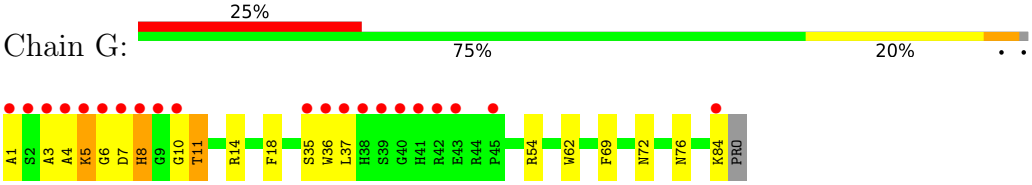
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



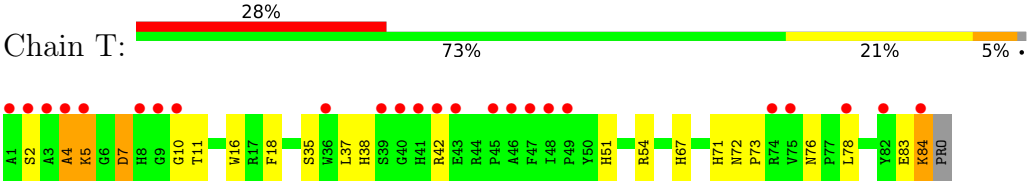
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



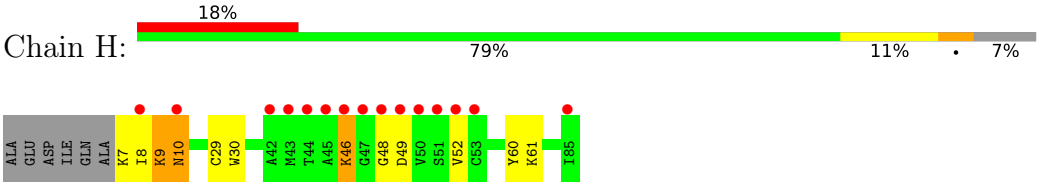
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



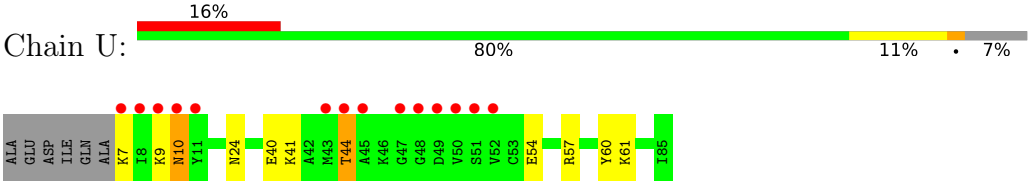
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



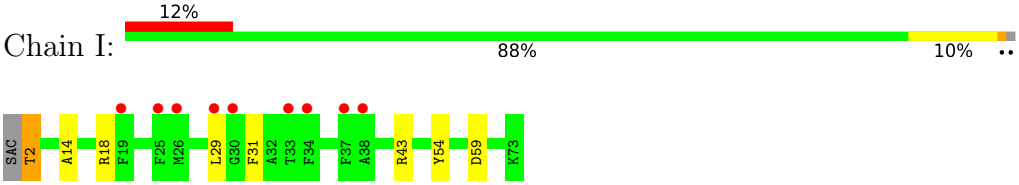
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



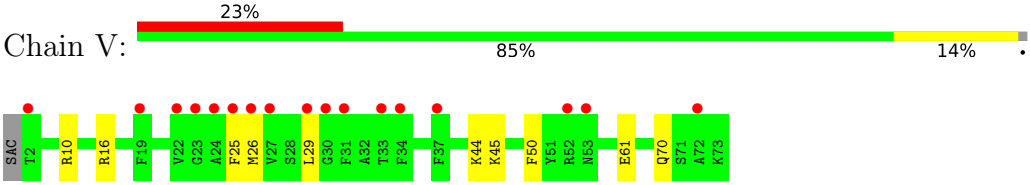
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



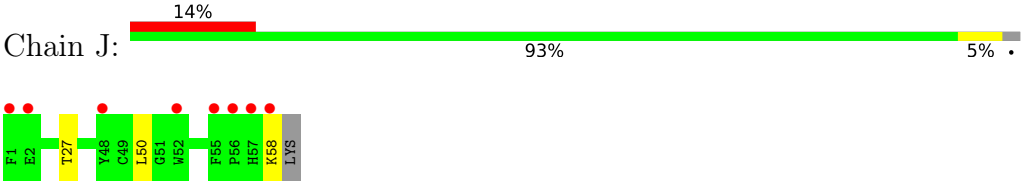
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



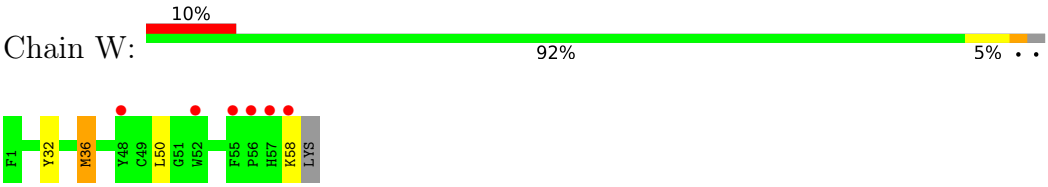
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



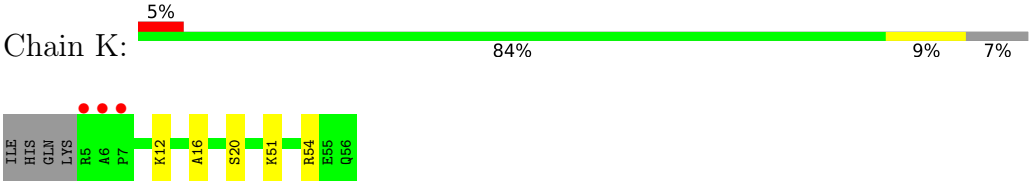
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



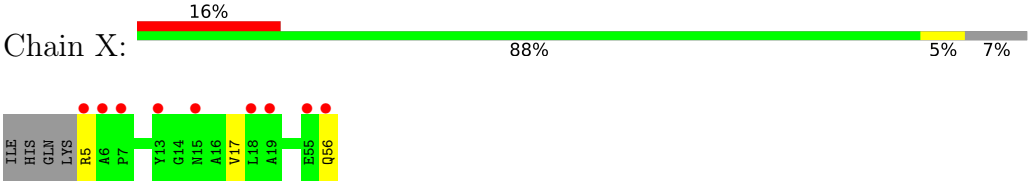
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



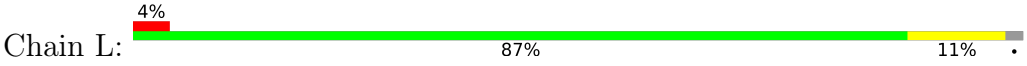
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

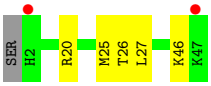
Chain X:



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

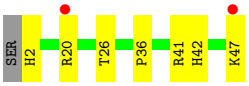
Chain L:





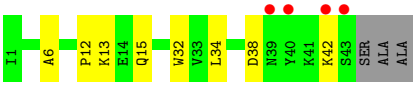
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



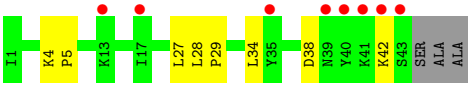
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	178.18Å 182.28Å 208.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93 39.97 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.93) 99.1 (39.97-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.184 , 0.212 0.194 , 0.220	Depositor DCC
R_{free} test set	24681 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32695	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PGV, CUA, EDO, TPO, FME, CU, CHD, NA, MG, TGL, HEA, ZN, PSC, CDL, DMU, SAC, PEK

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	0.70	0/4156	0.82	2/5678 (0.0%)
1	N	0.74	0/4156	0.79	2/5678 (0.0%)
2	B	0.77	1/1860 (0.1%)	0.90	0/2534
2	O	0.71	0/1860	0.86	0/2534
3	C	0.68	0/2197	0.76	0/3005
3	P	0.73	0/2197	0.74	0/3005
4	D	0.71	0/1249	0.82	3/1685 (0.2%)
4	Q	0.71	0/1249	0.77	1/1685 (0.1%)
5	E	0.72	0/871	0.78	0/1182
5	R	0.66	0/871	0.78	0/1182
6	F	0.70	0/765	0.86	0/1038
6	S	0.68	0/765	0.85	0/1038
7	G	0.66	0/690	0.83	0/937
7	T	0.66	0/690	0.80	0/937
8	H	0.70	0/682	0.88	0/921
8	U	0.67	0/682	0.83	0/921
9	I	0.68	0/605	0.86	0/802
9	V	0.67	0/605	0.79	0/802
10	J	0.64	0/471	0.81	0/636
10	W	0.73	0/471	0.74	0/636
11	K	0.70	0/427	0.79	0/584
11	X	0.70	0/427	0.72	0/584
12	L	0.65	0/393	0.85	0/526
12	Y	0.71	0/393	0.79	0/526
13	M	0.67	0/345	0.78	0/470
13	Z	0.68	0/345	0.78	0/470
All	All	0.71	1/29422 (0.0%)	0.81	8/39996 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	GLU	CD-OE2	5.50	1.31	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	20	ARG	NE-CZ-NH2	-7.15	116.73	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	N	240	HIS	CA-CB-CG	-5.73	103.85	113.60
4	D	20	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	302	ARG	NE-CZ-NH1	5.63	123.12	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4027	0	4001	43	0
1	N	4027	0	4001	58	0
2	B	1824	0	1833	20	0
2	O	1824	0	1833	18	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	13	0
4	D	1214	0	1201	10	0
4	Q	1214	0	1201	9	0
5	E	852	0	845	6	0
5	R	852	0	845	2	0
6	F	748	0	728	2	0
6	S	748	0	728	10	0
7	G	675	0	644	26	0
7	T	675	0	644	20	0
8	H	662	0	623	8	0
8	U	662	0	623	6	0
9	I	592	0	604	7	0
9	V	592	0	604	7	0
10	J	460	0	459	1	0
10	W	460	0	459	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	413	0	393	1	0
11	X	413	0	393	1	0
12	L	380	0	380	2	0
12	Y	380	0	380	3	0
13	M	335	0	352	5	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	102	0	152	4	0
17	C	51	0	76	0	0
17	N	102	0	152	2	0
17	P	51	0	76	0	0
17	T	51	0	76	1	0
17	Z	51	0	76	2	0
18	A	120	0	108	5	0
18	N	120	0	108	9	0
19	A	48	0	72	6	0
19	B	28	0	42	0	0
19	C	20	0	30	0	0
19	D	28	0	42	0	0
19	E	16	0	24	0	0
19	F	16	0	24	1	0
19	G	16	0	24	2	0
19	I	8	0	12	0	0
19	J	16	0	24	2	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	48	0	72	11	0
19	O	8	0	12	0	0
19	P	12	0	18	0	0
19	Q	12	0	18	0	0
19	R	8	0	12	0	0
19	S	24	0	36	4	0
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	4	0	6	0	0
20	A	63	0	110	1	0
20	D	63	0	110	7	0
20	L	63	0	110	2	0
20	N	63	0	110	0	0
20	Q	63	0	110	5	0
20	Y	63	0	110	2	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	G	29	0	39	1	0
22	J	29	0	39	0	0
22	P	58	0	78	1	0
22	T	29	0	39	7	0
22	W	29	0	39	0	0
22	Y	29	0	39	4	0
23	C	66	0	84	1	0
23	G	33	0	42	2	0
23	M	33	0	41	0	0
23	P	33	0	42	0	0
23	Z	33	0	42	1	0
24	C	159	0	231	8	0
24	P	159	0	231	6	0
25	C	200	0	312	15	0
25	P	100	0	156	4	0
25	T	100	0	156	3	0
26	E	52	0	80	5	0
26	O	52	0	80	5	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	2	0
28	V	9	0	8	1	0
29	A	190	0	0	0	0
29	B	125	0	0	0	0
29	C	96	0	0	7	0
29	D	68	0	0	0	0
29	E	53	0	0	0	0
29	F	70	0	0	0	0
29	G	35	0	0	0	0
29	H	39	0	0	1	0
29	I	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	J	17	0	0	0	0
29	K	9	0	0	0	0
29	L	21	0	0	2	0
29	M	14	0	0	0	0
29	N	179	0	0	7	0
29	O	85	0	0	3	0
29	P	80	0	0	1	0
29	Q	46	0	0	1	0
29	R	46	0	0	0	0
29	S	64	0	0	2	0
29	T	23	0	0	4	0
29	U	30	0	0	1	0
29	V	16	0	0	0	0
29	W	17	0	0	0	0
29	X	11	0	0	0	0
29	Y	18	0	0	1	0
29	Z	5	0	0	1	0
All	All	32695	0	32113	307	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 5.

The worst 5 of 307 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)
3:C:44:MET:HG3	29:C:496:HOH:O	1.38	1.19
9:I:2:THR:N	28:I:101:SAC:HG	1.47	1.12
1:A:270:TYR:H	19:A:614:EDO:H11	1.21	1.04
24:P:305:PEK:C38	25:T:102:CDL:H271	1.91	1.00
7:T:73:PRO:HG3	7:T:84:LYS:HE2	1.49	0.94

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	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
2	O	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	G	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
7	T	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	4
8	H	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	12	4
8	U	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3412 (97%)	100 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
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	426/426 (100%)	418 (98%)	8 (2%)	57	45
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	32
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	14
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	6
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	47
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	47
4	D	129/129 (100%)	126 (98%)	3 (2%)	50	38
4	Q	129/129 (100%)	124 (96%)	5 (4%)	32	17
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	24
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	24
6	F	81/81 (100%)	78 (96%)	3 (4%)	34	19
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	6
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	0
7	T	67/68 (98%)	56 (84%)	11 (16%)	2	0
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	1
8	U	71/75 (95%)	64 (90%)	7 (10%)	8	1
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	4
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	4
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	15
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	6
11	K	42/46 (91%)	39 (93%)	3 (7%)	14	4
11	X	42/46 (91%)	40 (95%)	2 (5%)	25	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	39/40 (98%)	36 (92%)	3 (8%)	13 3
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7 1
13	M	37/38 (97%)	33 (89%)	4 (11%)	6 1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6 1
All	All	3048/3082 (99%)	2910 (96%)	138 (4%)	27 12

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	9	LYS
8	U	60	TYR
12	Y	2	HIS
9	I	29	LEU
9	I	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	101	HIS
7	T	76	ASN
4	Q	109	HIS
6	S	80	GLN
9	V	70	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)

6 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	$\#\|Z\|>2$
1	FME	A	1	1	8,9,10	0.30	0	7,9,11	0.83	0
7	TPO	T	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.93	0
1	FME	N	1	1	8,9,10	0.59	0	7,9,11	1.09	0
2	FME	B	1	2	8,9,10	0.80	0	7,9,11	1.26	2 (28%)
2	FME	O	1	2	8,9,10	0.43	0	7,9,11	0.91	0
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	1.25	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	7/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.12	1.65	1.59
7	T	11	TPO	P-OG1	2.10	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	11	TPO	P-OG1-CB	3.02	132.33	123.21
2	B	1	FME	CG-CB-CA	-2.12	107.05	112.95
2	B	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 149 ligands modelled in this entry, 8 are monoatomic - leaving 141 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	$\#\|Z\| > 2$
19	EDO	M	102	-	3,3,3	0.13	0	2,2,2	0.13	0
24	PEK	C	303	-	52,52,52	0.49	0	55,57,57	0.79	0
18	HEA	A	607	1	57,67,67	1.77	12 (21%)	61,103,103	2.76	21 (34%)
19	EDO	W	301	-	3,3,3	0.18	0	2,2,2	0.42	0
19	EDO	A	609	-	3,3,3	0.20	0	2,2,2	0.12	0
23	DMU	G	1302	-	34,34,34	1.85	10 (29%)	45,45,45	1.43	7 (15%)
19	EDO	W	304	-	3,3,3	0.18	0	2,2,2	0.24	0
25	CDL	P	307	-	99,99,99	0.34	0	105,111,111	0.51	1 (0%)
19	EDO	A	618	-	3,3,3	0.16	0	2,2,2	0.58	0
26	PSC	E	201	-	51,51,51	0.44	0	57,59,59	0.51	0
19	EDO	B	309	-	3,3,3	0.11	0	2,2,2	0.30	0
19	EDO	P	311	-	3,3,3	0.37	0	2,2,2	0.44	0
20	TGL	Y	101	-	62,62,62	0.32	0	65,65,65	0.52	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PEK	P	304	-	52,52,52	0.42	0	55,57,57	0.72	2 (3%)
19	EDO	A	616	-	3,3,3	0.08	0	2,2,2	0.23	0
17	PGV	A	604	-	50,50,50	1.18	2 (4%)	53,56,56	1.59	5 (9%)
23	DMU	C	301	-	34,34,34	1.54	5 (14%)	45,45,45	1.86	9 (20%)
19	EDO	A	611	-	3,3,3	0.14	0	2,2,2	0.10	0
19	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.24	0
17	PGV	T	101	-	50,50,50	1.14	2 (4%)	53,56,56	1.19	4 (7%)
19	EDO	V	104	-	3,3,3	0.37	0	2,2,2	0.48	0
19	EDO	N	619	-	3,3,3	0.11	0	2,2,2	0.20	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.55	2 (3%)
19	EDO	G	1306	-	3,3,3	0.12	0	2,2,2	0.25	0
19	EDO	G	1303	-	3,3,3	0.07	0	2,2,2	0.31	0
24	PEK	C	304	-	52,52,52	0.35	0	55,57,57	0.51	0
19	EDO	N	615	-	3,3,3	0.11	0	2,2,2	0.31	0
18	HEA	A	606	1	57,67,67	1.59	10 (17%)	61,103,103	2.47	21 (34%)
25	CDL	C	306	-	99,99,99	0.38	0	105,111,111	0.59	2 (1%)
25	CDL	T	102	-	99,99,99	0.36	0	105,111,111	0.46	0
19	EDO	B	305	-	3,3,3	0.13	0	2,2,2	0.31	0
19	EDO	C	309	-	3,3,3	0.03	0	2,2,2	0.21	0
26	PSC	O	302	-	51,51,51	0.40	0	57,59,59	0.42	0
19	EDO	L	102	-	3,3,3	0.25	0	2,2,2	0.42	0
19	EDO	A	610	-	3,3,3	0.26	0	2,2,2	0.18	0
19	EDO	R	202	-	3,3,3	0.14	0	2,2,2	0.28	0
22	CHD	P	308	-	32,32,32	0.59	0	51,51,51	1.09	2 (3%)
19	EDO	C	314	-	3,3,3	0.11	0	2,2,2	0.19	0
19	EDO	C	308	-	3,3,3	0.36	0	2,2,2	0.12	0
19	EDO	B	303	-	3,3,3	0.41	0	2,2,2	0.31	0
19	EDO	T	105	-	3,3,3	0.05	0	2,2,2	0.36	0
19	EDO	D	203	-	3,3,3	0.09	0	2,2,2	0.12	0
24	PEK	P	305	-	52,52,52	0.33	0	55,57,57	0.40	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.34	0
19	EDO	D	207	-	3,3,3	0.24	0	2,2,2	0.12	0
19	EDO	A	620	-	3,3,3	0.30	0	2,2,2	0.13	0
19	EDO	E	205	-	3,3,3	0.07	0	2,2,2	0.22	0
19	EDO	S	2206	-	3,3,3	0.19	0	2,2,2	0.12	0
20	TGL	A	615	-	62,62,62	0.35	0	65,65,65	0.48	1 (1%)
19	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.43	0
19	EDO	B	308	-	3,3,3	0.08	0	2,2,2	0.08	0
19	EDO	S	2205	-	3,3,3	0.11	0	2,2,2	0.08	0
22	CHD	Y	102	-	32,32,32	0.57	0	51,51,51	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	PGV	N	605	-	50,50,50	0.82	2 (4%)	53,56,56	1.29	4 (7%)
20	TGL	L	101	-	62,62,62	0.33	0	65,65,65	0.27	0
17	PGV	C	305	-	50,50,50	0.73	2 (4%)	53,56,56	0.82	1 (1%)
19	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.41	0
19	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.81	0
19	EDO	S	2204	-	3,3,3	0.32	0	2,2,2	0.48	0
19	EDO	F	702	-	3,3,3	0.17	0	2,2,2	0.13	0
19	EDO	D	205	-	3,3,3	0.31	0	2,2,2	0.33	0
19	EDO	D	206	-	3,3,3	0.19	0	2,2,2	0.33	0
17	PGV	P	306	-	50,50,50	0.76	2 (4%)	53,56,56	0.98	4 (7%)
19	EDO	D	204	-	3,3,3	0.09	0	2,2,2	0.15	0
19	EDO	F	701	-	3,3,3	0.14	0	2,2,2	0.44	0
19	EDO	P	310	-	3,3,3	0.32	0	2,2,2	0.31	0
19	EDO	S	2201	-	3,3,3	0.41	0	2,2,2	0.60	0
19	EDO	J	1103	-	3,3,3	0.09	0	2,2,2	0.15	0
23	DMU	Z	101	-	34,34,34	1.19	4 (11%)	45,45,45	1.55	7 (15%)
19	EDO	J	1105	-	3,3,3	0.23	0	2,2,2	0.43	0
19	EDO	N	617	-	3,3,3	0.04	0	2,2,2	0.24	0
19	EDO	P	309	-	3,3,3	0.17	0	2,2,2	0.32	0
23	DMU	M	101	-	34,34,34	1.11	3 (8%)	45,45,45	1.26	5 (11%)
28	SAC	I	101	-	7,8,9	0.52	0	8,9,11	1.04	1 (12%)
19	EDO	C	311	-	3,3,3	0.12	0	2,2,2	0.19	0
19	EDO	J	1104	-	3,3,3	0.49	0	2,2,2	0.73	0
20	TGL	Q	201	-	62,62,62	0.29	0	65,65,65	0.30	0
19	EDO	E	202	-	3,3,3	0.13	0	2,2,2	0.15	0
19	EDO	F	704	-	3,3,3	0.15	0	2,2,2	0.31	0
19	EDO	G	1304	-	3,3,3	0.17	0	2,2,2	0.39	0
19	EDO	S	2203	-	3,3,3	0.35	0	2,2,2	0.28	0
19	EDO	G	1301	-	3,3,3	0.22	0	2,2,2	0.51	0
19	EDO	C	310	-	3,3,3	0.08	0	2,2,2	0.16	0
19	EDO	N	608	-	3,3,3	0.25	0	2,2,2	0.46	0
19	EDO	N	610	-	3,3,3	0.38	0	2,2,2	0.77	0
19	EDO	Z	103	-	3,3,3	0.24	0	2,2,2	0.34	0
19	EDO	O	303	-	3,3,3	0.47	0	2,2,2	0.76	0
19	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.38	0
19	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.57	0
19	EDO	J	1101	-	3,3,3	0.47	0	2,2,2	0.29	0
22	CHD	C	302	-	32,32,32	0.64	1 (3%)	51,51,51	0.79	1 (1%)
17	PGV	A	605	-	50,50,50	0.84	2 (4%)	53,56,56	1.22	2 (3%)
23	DMU	P	302	-	34,34,34	1.12	2 (5%)	45,45,45	1.96	11 (24%)
19	EDO	T	103	-	3,3,3	0.37	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PEK	C	315	-	52,52,52	0.43	0	55,57,57	0.57	0
22	CHD	T	104	-	32,32,32	0.70	0	51,51,51	1.26	6 (11%)
19	EDO	S	2207	-	3,3,3	0.12	0	2,2,2	0.39	0
21	CUA	B	301	2	0,1,1	-	-	-		
19	EDO	A	612	-	3,3,3	0.20	0	2,2,2	0.19	0
19	EDO	K	101	-	3,3,3	0.09	0	2,2,2	0.22	0
19	EDO	N	609	-	3,3,3	0.18	0	2,2,2	0.16	0
22	CHD	B	302	-	32,32,32	0.60	0	51,51,51	0.85	1 (1%)
19	EDO	N	614	-	3,3,3	0.53	0	2,2,2	0.69	0
19	EDO	U	1501	-	3,3,3	0.27	0	2,2,2	0.54	0
19	EDO	D	208	-	3,3,3	0.16	0	2,2,2	0.16	0
22	CHD	C	307	-	32,32,32	0.60	0	51,51,51	0.78	0
19	EDO	A	617	-	3,3,3	0.15	0	2,2,2	0.20	0
21	CUA	O	301	2	0,1,1	-	-	-		
20	TGL	N	604	-	62,62,62	0.27	0	65,65,65	0.46	1 (1%)
19	EDO	N	620	-	3,3,3	0.34	0	2,2,2	0.55	0
18	HEA	N	607	1	57,67,67	2.03	14 (24%)	61,103,103	2.60	23 (37%)
19	EDO	A	608	-	3,3,3	0.31	0	2,2,2	0.34	0
24	PEK	P	301	-	52,52,52	0.32	0	55,57,57	0.49	0
19	EDO	V	103	-	3,3,3	0.16	0	2,2,2	0.36	0
22	CHD	P	303	-	32,32,32	0.68	1 (3%)	51,51,51	0.73	0
19	EDO	O	304	-	3,3,3	0.28	0	2,2,2	0.39	0
19	EDO	N	618	-	3,3,3	0.18	0	2,2,2	0.13	0
17	PGV	Z	102	-	50,50,50	1.09	2 (4%)	53,56,56	1.16	5 (9%)
19	EDO	N	612	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	B	306	-	3,3,3	0.22	0	2,2,2	0.30	0
19	EDO	I	103	-	3,3,3	0.17	0	2,2,2	0.43	0
19	EDO	W	303	-	3,3,3	0.40	0	2,2,2	0.49	0
19	EDO	I	102	-	3,3,3	0.10	0	2,2,2	0.24	0
19	EDO	N	611	-	3,3,3	0.18	0	2,2,2	0.09	0
19	EDO	E	204	-	3,3,3	0.11	0	2,2,2	0.24	0
22	CHD	G	1305	-	32,32,32	0.56	0	51,51,51	0.80	0
19	EDO	Q	204	-	3,3,3	0.22	0	2,2,2	0.06	0
23	DMU	C	313	-	34,34,34	1.81	7 (20%)	45,45,45	1.93	10 (22%)
28	SAC	V	101	-	7,8,9	0.49	0	8,9,11	1.10	1 (12%)
19	EDO	Q	202	-	3,3,3	0.18	0	2,2,2	0.24	0
19	EDO	F	705	-	3,3,3	0.33	0	2,2,2	0.39	0
19	EDO	D	202	-	3,3,3	0.12	0	2,2,2	0.21	0
25	CDL	C	312	-	99,99,99	0.37	0	105,111,111	0.45	0
18	HEA	N	606	1	57,67,67	1.68	14 (24%)	61,103,103	2.51	25 (40%)
19	EDO	K	102	-	3,3,3	0.11	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	EDO	B	304	-	3,3,3	0.22	0	2,2,2	0.28	0
19	EDO	Q	203	-	3,3,3	0.20	0	2,2,2	0.16	0
17	PGV	N	616	-	50,50,50	1.04	2 (4%)	53,56,56	1.04	3 (5%)
22	CHD	J	1102	-	32,32,32	0.63	1 (3%)	51,51,51	0.77	0
22	CHD	W	302	-	32,32,32	0.55	0	51,51,51	0.74	0
19	EDO	R	201	-	3,3,3	0.10	0	2,2,2	0.16	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
19	EDO	M	102	-	-	0/1/1/1	-
24	PEK	C	303	-	-	22/56/56/56	-
18	HEA	A	607	1	3/3/7/16	7/32/76/76	-
19	EDO	W	301	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
23	DMU	G	1302	-	-	11/19/59/59	0/2/2/2
19	EDO	W	304	-	-	1/1/1/1	-
25	CDL	P	307	-	-	49/110/110/110	-
19	EDO	A	618	-	-	0/1/1/1	-
26	PSC	E	201	-	-	27/55/55/55	-
19	EDO	B	309	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
20	TGL	Y	101	-	-	30/65/65/65	-
24	PEK	P	304	-	-	20/56/56/56	-
19	EDO	A	616	-	-	0/1/1/1	-
17	PGV	A	604	-	-	30/55/55/55	-
23	DMU	C	301	-	-	11/19/59/59	0/2/2/2
19	EDO	A	611	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
17	PGV	T	101	-	-	26/55/55/55	-
19	EDO	V	104	-	-	0/1/1/1	-
19	EDO	N	619	-	-	1/1/1/1	-
20	TGL	D	201	-	-	36/65/65/65	-
19	EDO	G	1306	-	-	1/1/1/1	-
19	EDO	G	1303	-	-	1/1/1/1	-
24	PEK	C	304	-	-	29/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	N	615	-	-	1/1/1/1	-
18	HEA	A	606	1	3/3/7/16	6/32/76/76	-
25	CDL	C	306	-	-	59/110/110/110	-
25	CDL	T	102	-	-	63/110/110/110	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
26	PSC	O	302	-	-	37/55/55/55	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	A	610	-	-	0/1/1/1	-
19	EDO	R	202	-	-	1/1/1/1	-
22	CHD	P	308	-	-	4/9/74/74	0/4/4/4
19	EDO	C	314	-	-	1/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-
19	EDO	B	303	-	-	0/1/1/1	-
19	EDO	T	105	-	-	1/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
24	PEK	P	305	-	-	31/56/56/56	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	D	207	-	-	1/1/1/1	-
19	EDO	A	620	-	-	0/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
19	EDO	S	2206	-	-	1/1/1/1	-
20	TGL	A	615	-	-	42/65/65/65	-
19	EDO	A	613	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	S	2205	-	-	0/1/1/1	-
22	CHD	Y	102	-	-	8/9/74/74	1/4/4/4
17	PGV	N	605	-	-	14/55/55/55	-
20	TGL	L	101	-	-	35/65/65/65	-
17	PGV	C	305	-	-	13/55/55/55	-
19	EDO	E	203	-	-	0/1/1/1	-
19	EDO	N	613	-	-	0/1/1/1	-
19	EDO	S	2204	-	-	1/1/1/1	-
19	EDO	F	702	-	-	0/1/1/1	-
19	EDO	D	205	-	-	1/1/1/1	-
19	EDO	D	206	-	-	1/1/1/1	-
17	PGV	P	306	-	-	9/55/55/55	-
19	EDO	D	204	-	-	1/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	P	310	-	-	0/1/1/1	-
19	EDO	S	2201	-	-	1/1/1/1	-
19	EDO	J	1103	-	-	0/1/1/1	-
23	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
19	EDO	J	1105	-	-	1/1/1/1	-
19	EDO	N	617	-	-	0/1/1/1	-
19	EDO	P	309	-	-	1/1/1/1	-
23	DMU	M	101	-	-	6/19/59/59	0/2/2/2
28	SAC	I	101	-	-	7/7/8/10	-
19	EDO	C	311	-	-	0/1/1/1	-
19	EDO	J	1104	-	-	0/1/1/1	-
20	TGL	Q	201	-	-	32/65/65/65	-
19	EDO	E	202	-	-	1/1/1/1	-
19	EDO	F	704	-	-	1/1/1/1	-
19	EDO	G	1304	-	-	1/1/1/1	-
19	EDO	S	2203	-	-	0/1/1/1	-
19	EDO	G	1301	-	-	0/1/1/1	-
19	EDO	C	310	-	-	1/1/1/1	-
19	EDO	N	608	-	-	1/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	Z	103	-	-	0/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
19	EDO	A	619	-	-	1/1/1/1	-
19	EDO	J	1101	-	-	0/1/1/1	-
22	CHD	C	302	-	-	2/9/74/74	0/4/4/4
17	PGV	A	605	-	-	15/55/55/55	-
23	DMU	P	302	-	-	6/19/59/59	0/2/2/2
19	EDO	T	103	-	-	1/1/1/1	-
24	PEK	C	315	-	-	27/56/56/56	-
22	CHD	T	104	-	-	6/9/74/74	1/4/4/4
19	EDO	S	2207	-	-	1/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	N	609	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	U	1501	-	-	0/1/1/1	-
19	EDO	D	208	-	-	0/1/1/1	-
22	CHD	C	307	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	A	617	-	-	1/1/1/1	-
20	TGL	N	604	-	-	33/65/65/65	-
19	EDO	N	620	-	-	1/1/1/1	-
18	HEA	N	607	1	3/3/7/16	4/32/76/76	-
19	EDO	A	608	-	-	0/1/1/1	-
24	PEK	P	301	-	-	29/56/56/56	-
19	EDO	V	103	-	-	0/1/1/1	-
22	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	O	304	-	-	0/1/1/1	-
19	EDO	N	618	-	-	0/1/1/1	-
17	PGV	Z	102	-	-	25/55/55/55	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	B	306	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	I	102	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
22	CHD	G	1305	-	-	2/9/74/74	0/4/4/4
19	EDO	Q	204	-	-	0/1/1/1	-
23	DMU	C	313	-	-	6/19/59/59	0/2/2/2
28	SAC	V	101	-	-	2/7/8/10	-
19	EDO	Q	202	-	-	1/1/1/1	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	D	202	-	-	0/1/1/1	-
25	CDL	C	312	-	-	63/110/110/110	-
18	HEA	N	606	1	3/3/7/16	4/32/76/76	-
19	EDO	K	102	-	-	1/1/1/1	-
19	EDO	B	304	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	1/1/1/1	-
17	PGV	N	616	-	-	24/55/55/55	-
22	CHD	J	1102	-	-	2/9/74/74	0/4/4/4
22	CHD	W	302	-	-	2/9/74/74	0/4/4/4
19	EDO	R	201	-	-	1/1/1/1	-

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C1D-ND	-5.88	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	1302	DMU	O16-C6	5.73	1.50	1.40
23	C	313	DMU	O16-C6	5.56	1.49	1.40
18	A	607	HEA	C1D-ND	-5.54	1.30	1.40
18	N	607	HEA	C4B-NB	-5.33	1.31	1.40

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	607	HEA	C16-C15-C14	9.20	139.74	121.12
18	A	607	HEA	C26-C15-C14	-8.38	102.19	123.68
23	P	302	DMU	C18-O16-C6	7.96	127.05	113.84
23	C	313	DMU	O1-C9-C11	7.14	124.19	106.44
18	A	606	HEA	C1D-C2D-C3D	-7.12	99.47	106.96

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	606	HEA	ND
18	A	606	HEA	NA
18	A	606	HEA	NB
18	A	607	HEA	ND
18	A	607	HEA	NA

5 of 980 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C03-O11-P-O14
17	A	604	PGV	C04-C05-C06-O06
17	A	604	PGV	O02-C1-O01-C02
17	A	604	PGV	C2-C1-O01-C02

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	T	104	CHD	C1-C10-C2-C3-C4-C5
22	Y	102	CHD	C1-C10-C2-C3-C4-C5

50 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	303	PEK	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	607	HEA	3	0
23	G	1302	DMU	2	0
25	P	307	CDL	4	0
26	E	201	PSC	5	0
20	Y	101	TGL	2	0
24	P	304	PEK	1	0
19	A	616	EDO	1	0
17	A	604	PGV	4	0
17	T	101	PGV	1	0
19	N	619	EDO	1	0
20	D	201	TGL	7	0
19	G	1303	EDO	2	0
24	C	304	PEK	2	0
18	A	606	HEA	2	0
25	C	306	CDL	2	0
25	T	102	CDL	3	0
26	O	302	PSC	5	0
22	P	308	CHD	1	0
24	P	305	PEK	5	0
19	S	2206	EDO	1	0
20	A	615	TGL	1	0
19	A	613	EDO	1	0
22	Y	102	CHD	4	0
17	N	605	PGV	1	0
20	L	101	TGL	2	0
19	N	613	EDO	1	0
19	F	702	EDO	1	0
19	S	2201	EDO	3	0
23	Z	101	DMU	1	0
28	I	101	SAC	2	0
19	J	1104	EDO	1	0
20	Q	201	TGL	5	0
19	A	614	EDO	3	0
19	J	1101	EDO	1	0
22	C	302	CHD	1	0
24	C	315	PEK	2	0
22	T	104	CHD	7	0
19	N	614	EDO	9	0
19	U	1501	EDO	3	0
18	N	607	HEA	4	0
19	A	608	EDO	1	0
19	V	103	EDO	1	0

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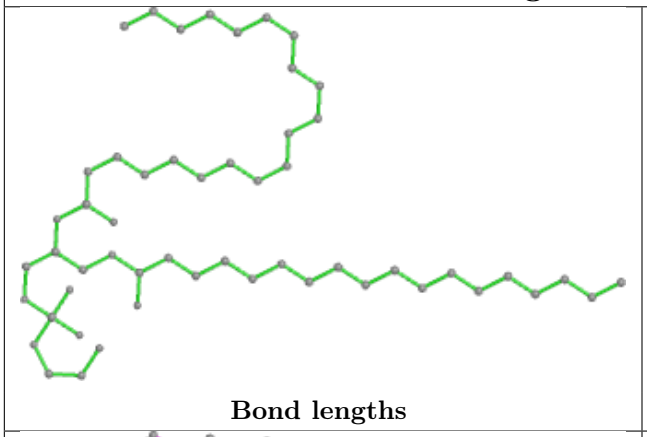
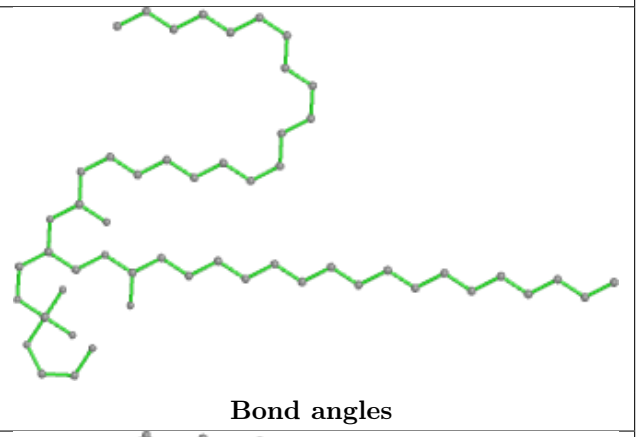
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Z	102	PGV	2	0
22	G	1305	CHD	1	0
23	C	313	DMU	1	0
28	V	101	SAC	1	0
25	C	312	CDL	13	0
18	N	606	HEA	5	0
17	N	616	PGV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

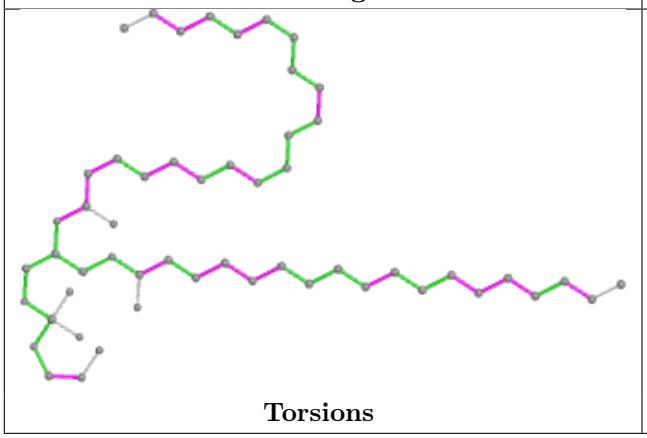
Ligand PEK C 303



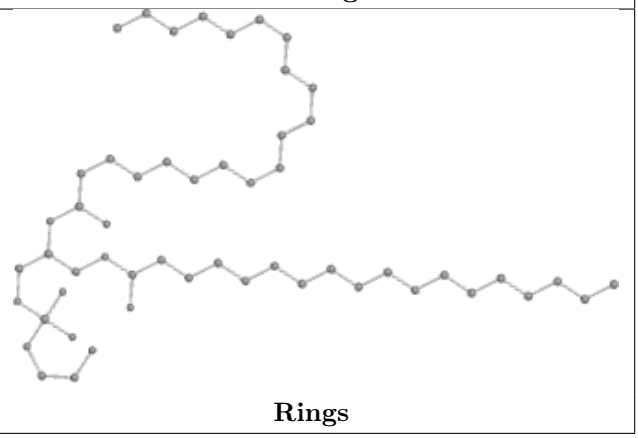
Bond lengths



Bond angles

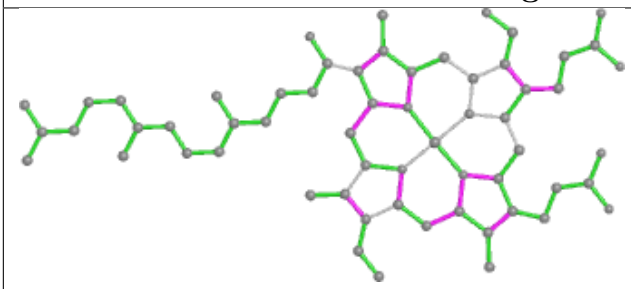


Torsions

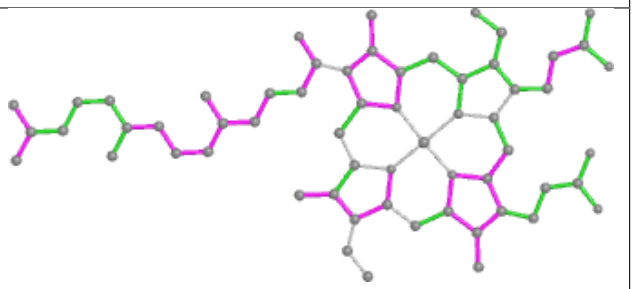


Rings

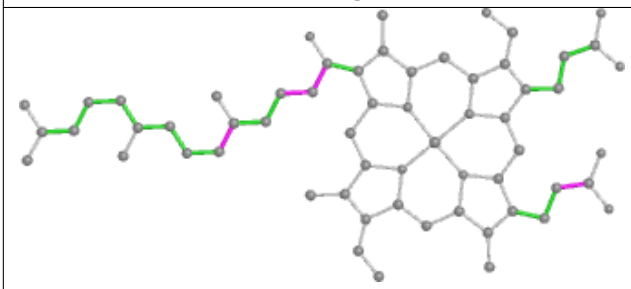
Ligand HEA A 607



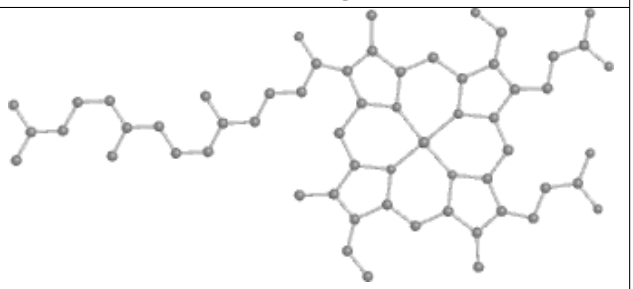
Bond lengths



Bond angles

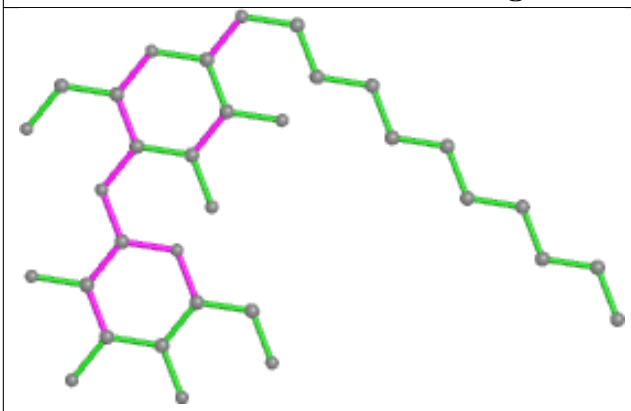


Torsions

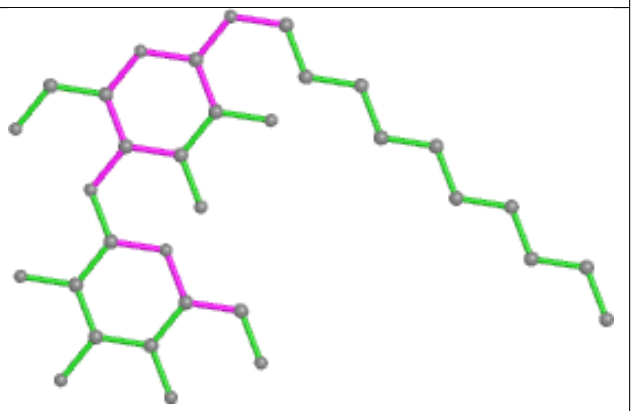


Rings

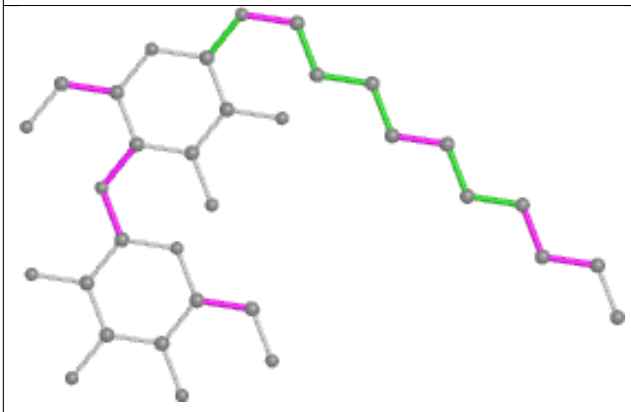
Ligand DMU G 1302



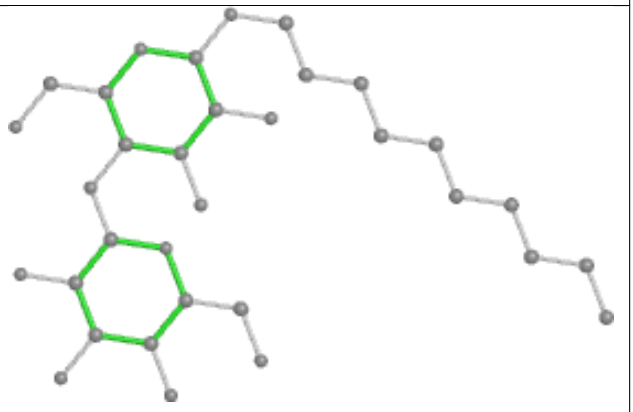
Bond lengths



Bond angles

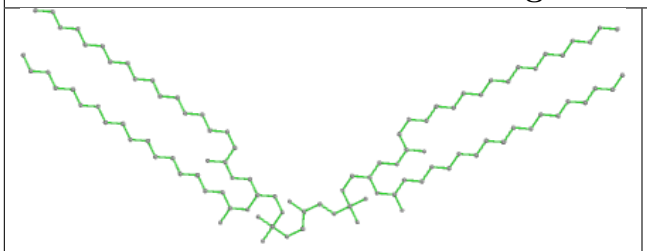


Torsions

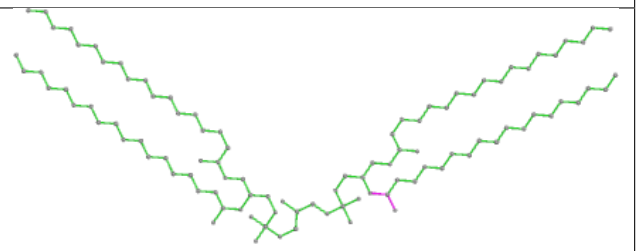


Rings

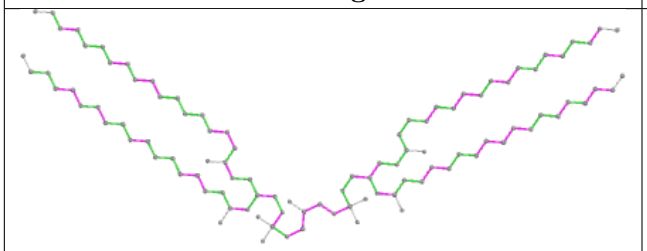
Ligand CDL P 307



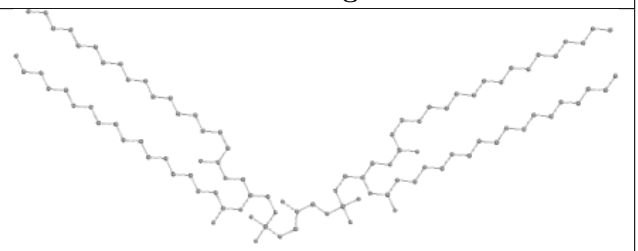
Bond lengths



Bond angles

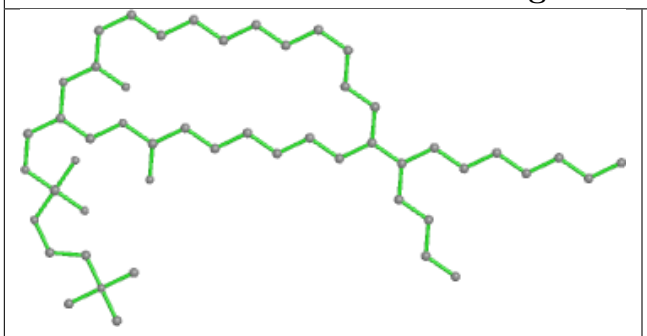


Torsions

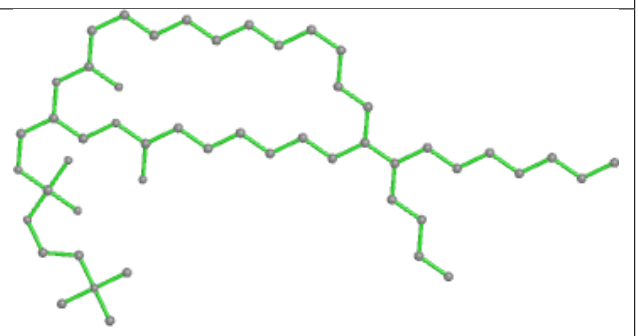


Rings

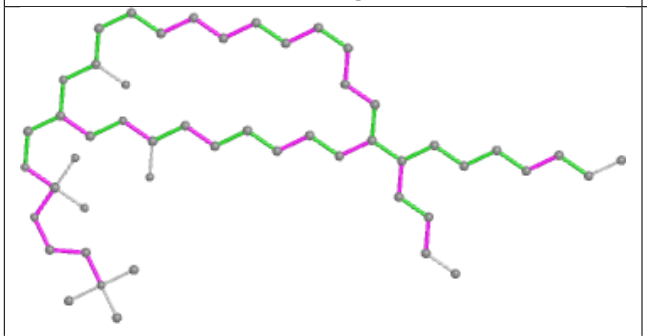
Ligand PSC E 201



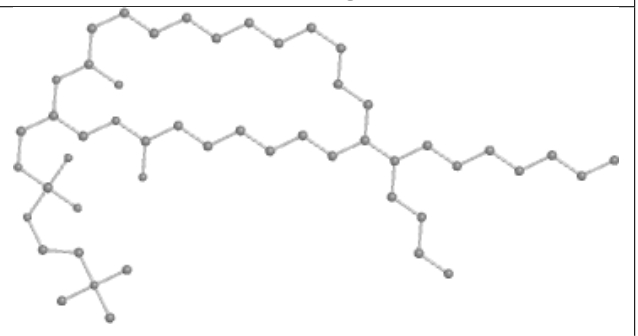
Bond lengths



Bond angles

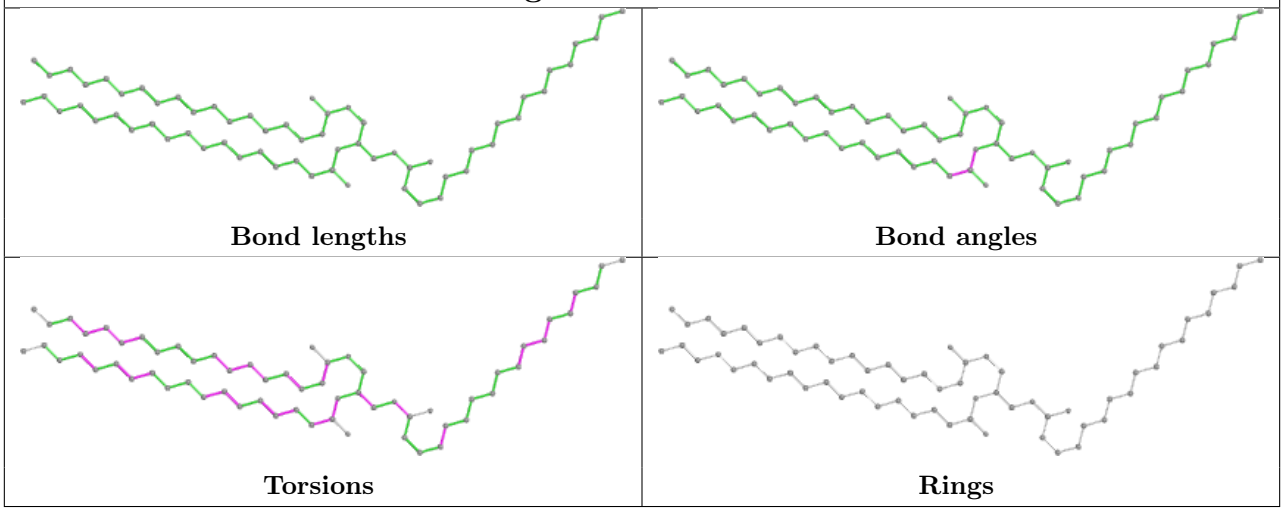


Torsions

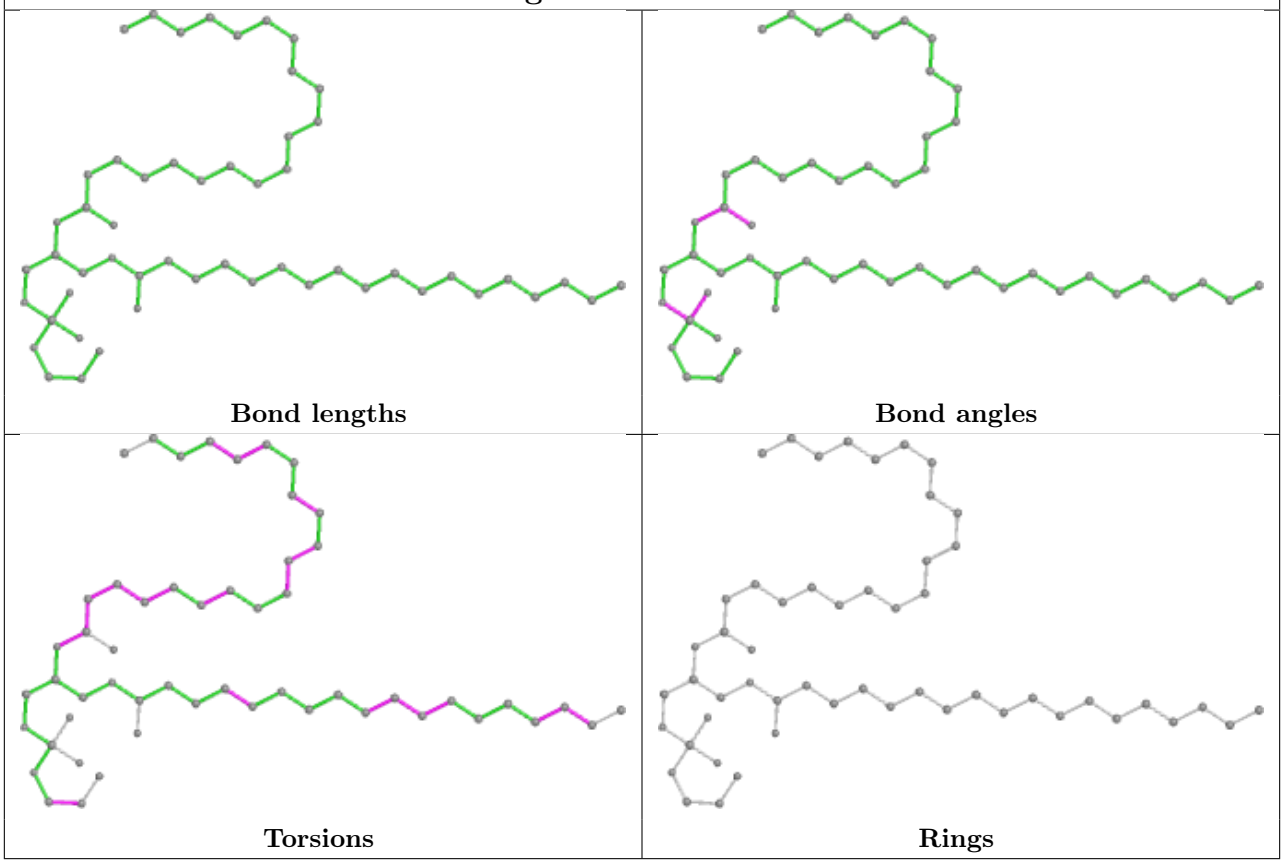


Rings

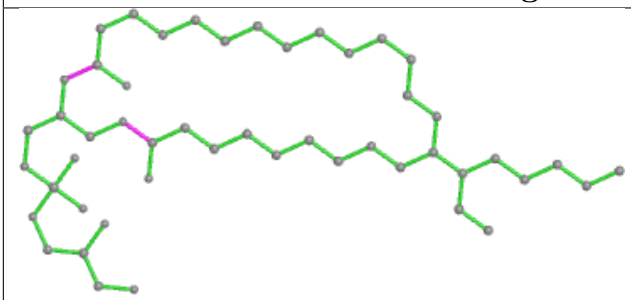
Ligand TGL Y 101



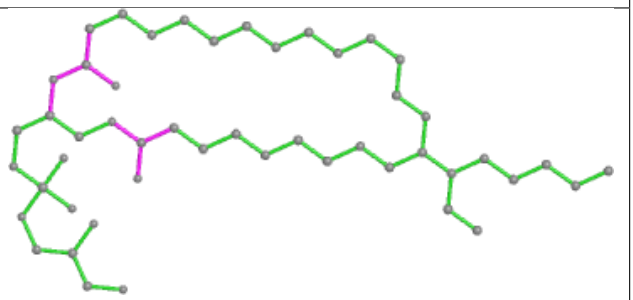
Ligand PEK P 304



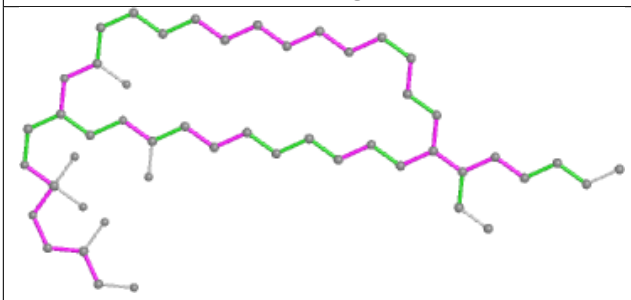
Ligand PGV A 604



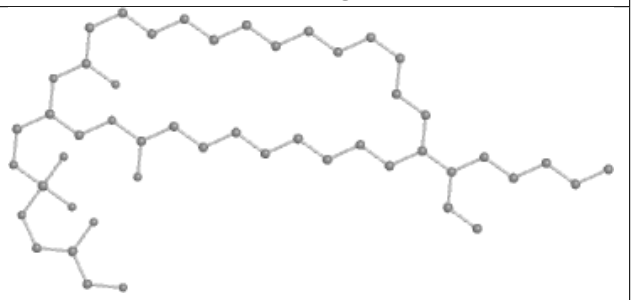
Bond lengths



Bond angles

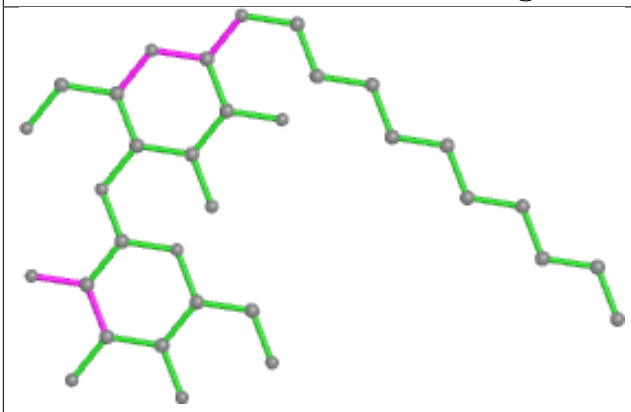


Torsions

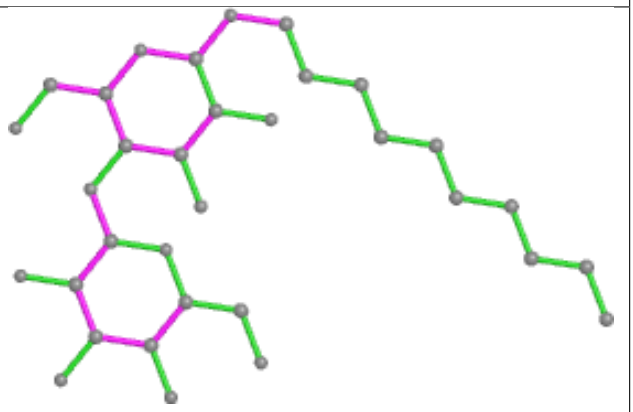


Rings

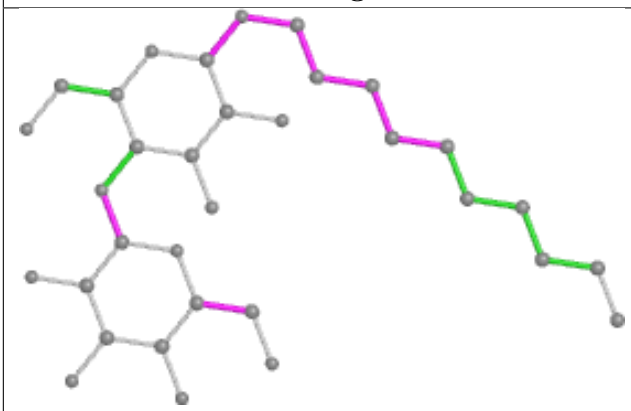
Ligand DMU C 301



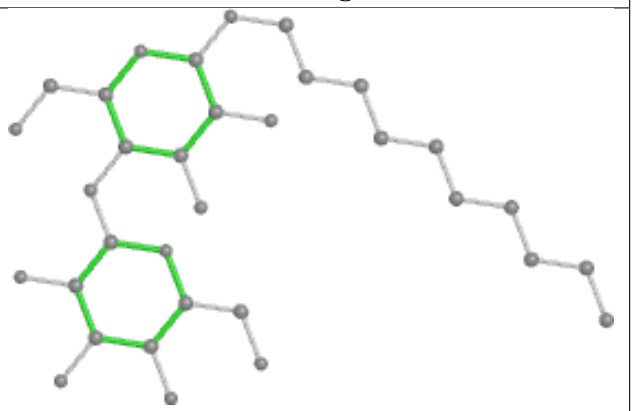
Bond lengths



Bond angles

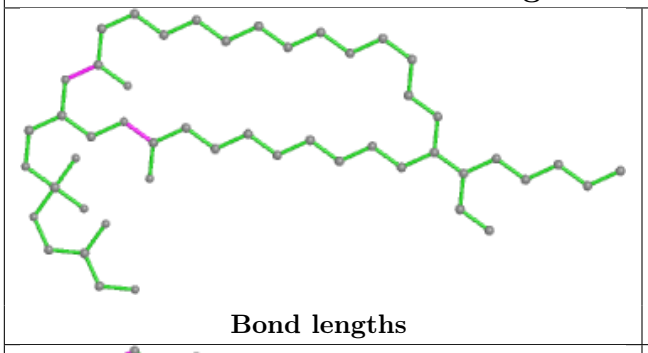


Torsions

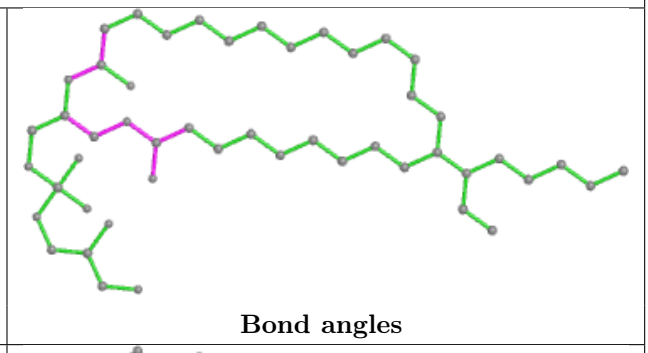


Rings

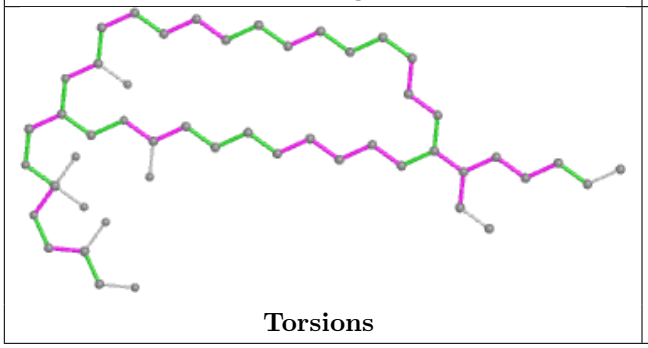
Ligand PGV T 101



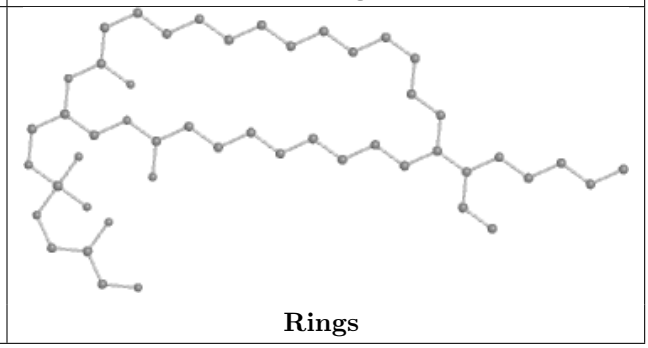
Bond lengths



Bond angles

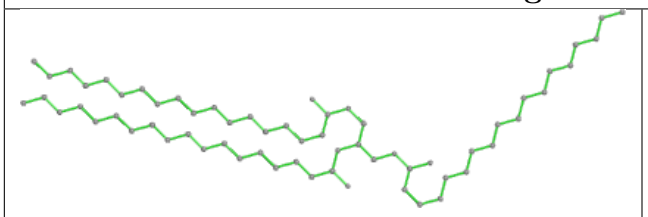


Torsions

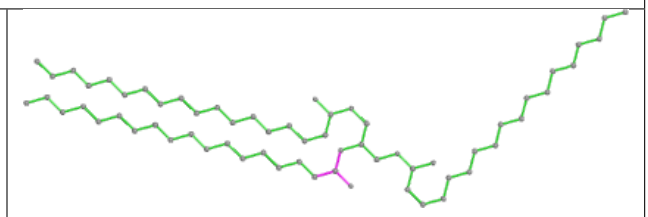


Rings

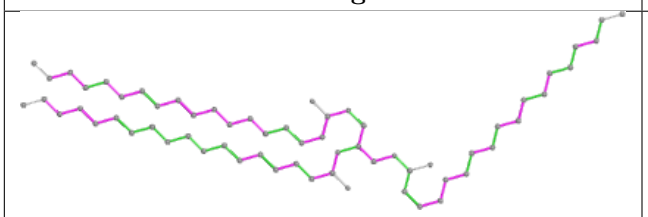
Ligand TGL D 201



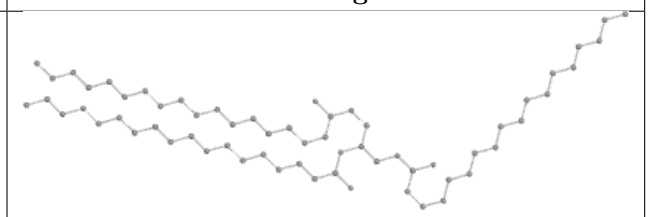
Bond lengths



Bond angles

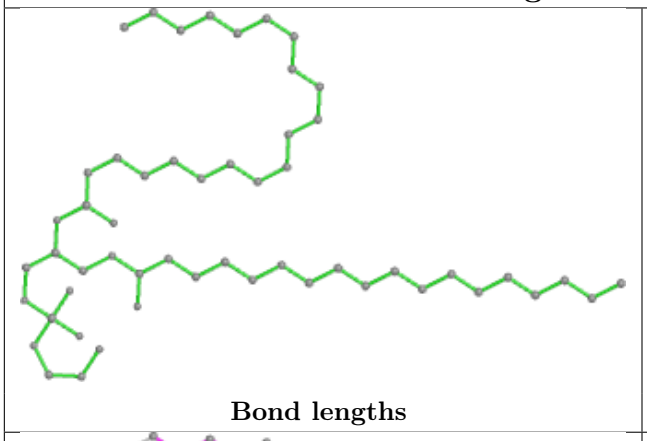


Torsions

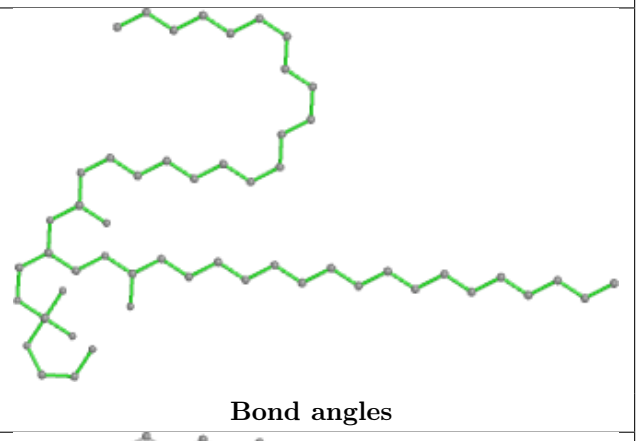


Rings

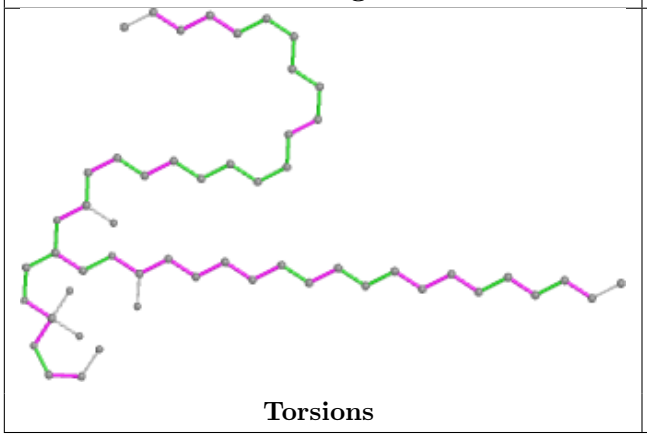
Ligand PEK C 304



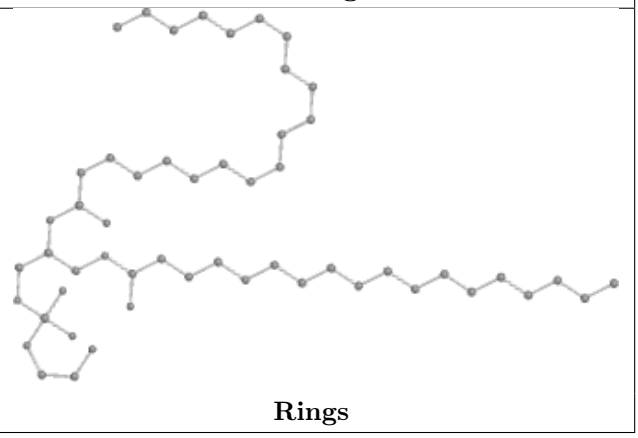
Bond lengths



Bond angles

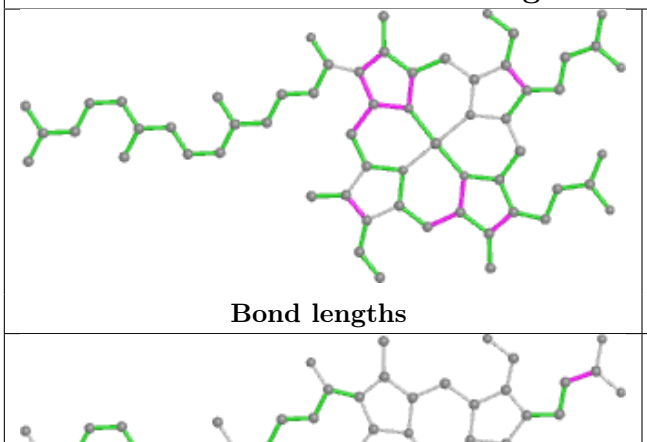


Torsions



Rings

Ligand HEA A 606



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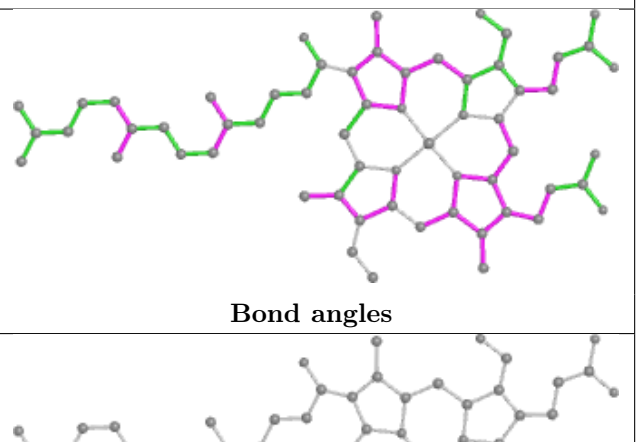
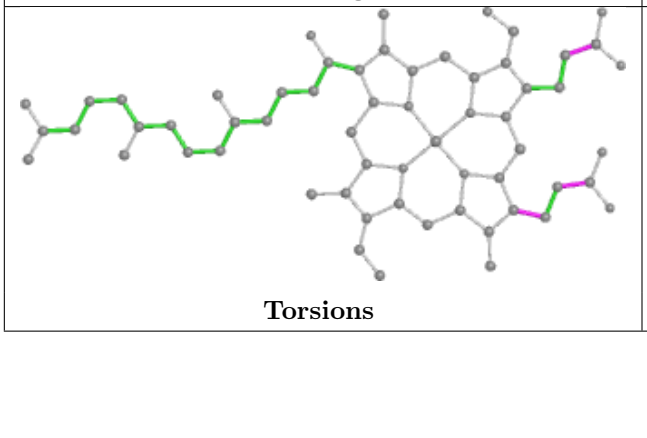
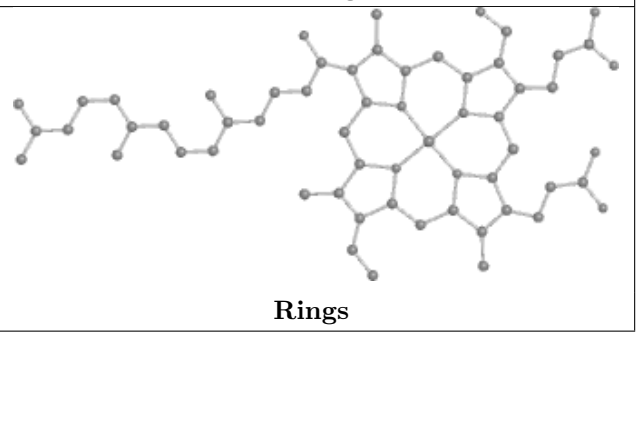


Bond angles

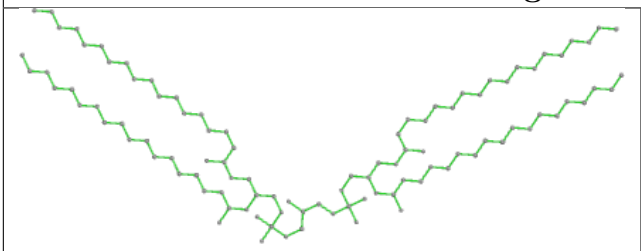


Torsions



Rings

Ligand CDL C 306



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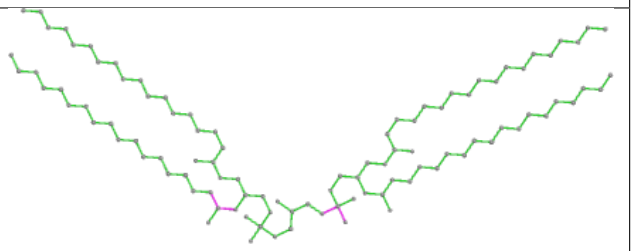
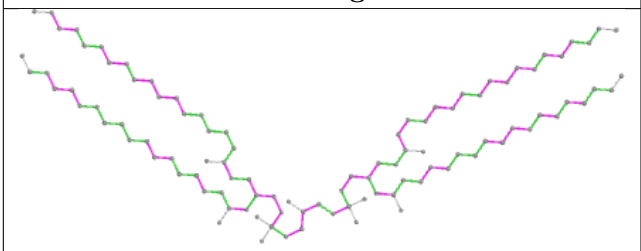
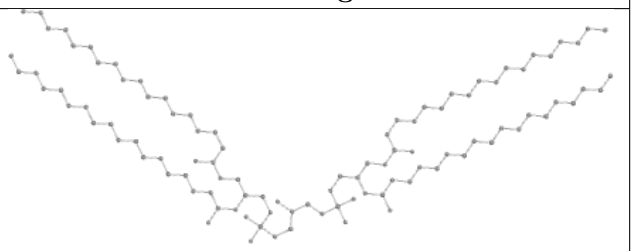


Bond angles

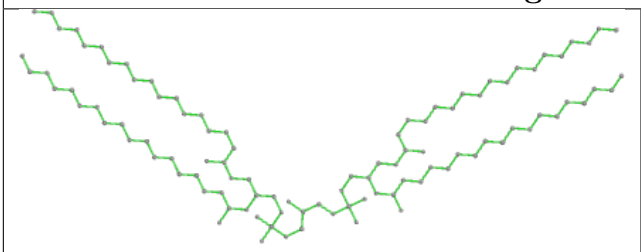


Torsions

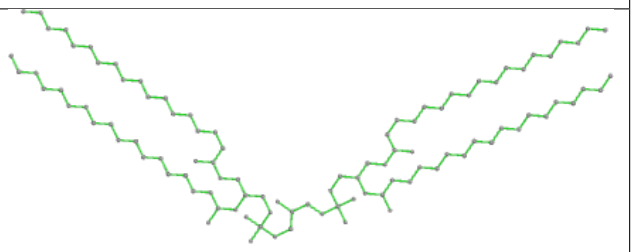


Rings

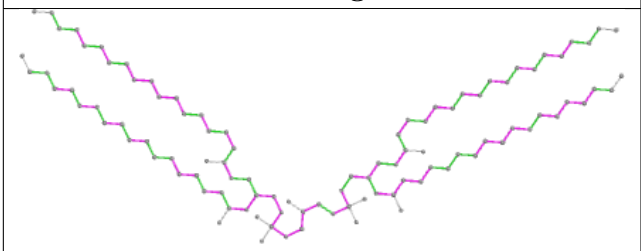
Ligand CDL T 102



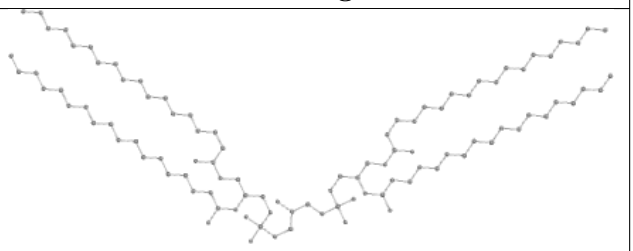
Bond lengths



Bond angles

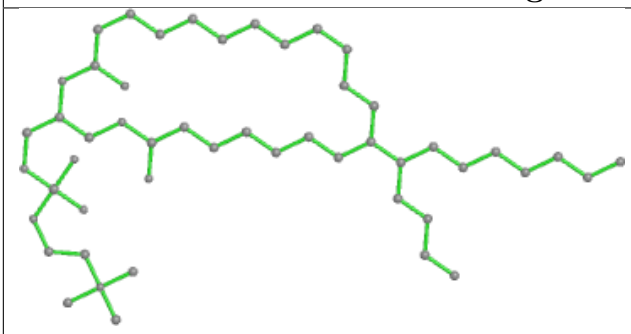


Torsions

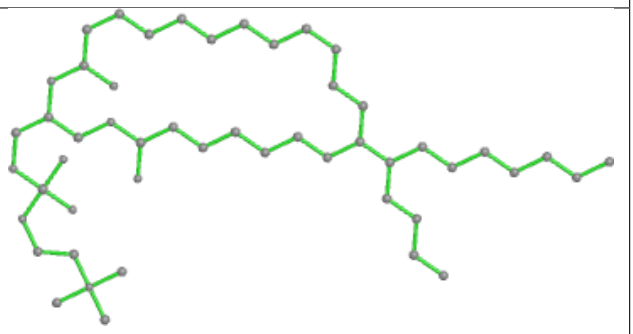


Rings

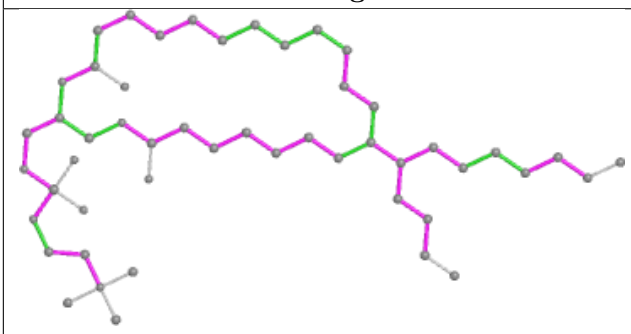
Ligand PSC O 302



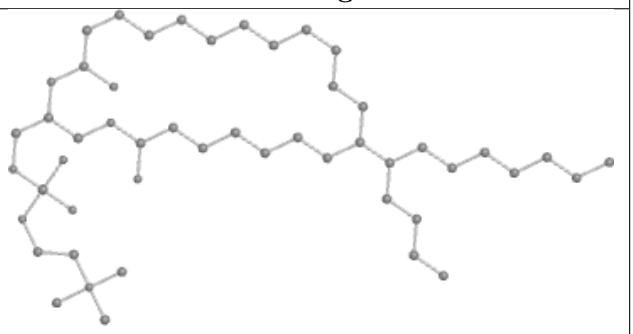
Bond lengths



Bond angles

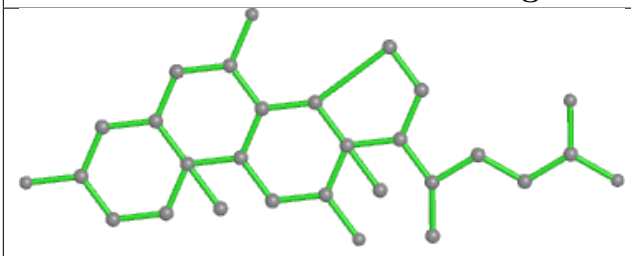


Torsions

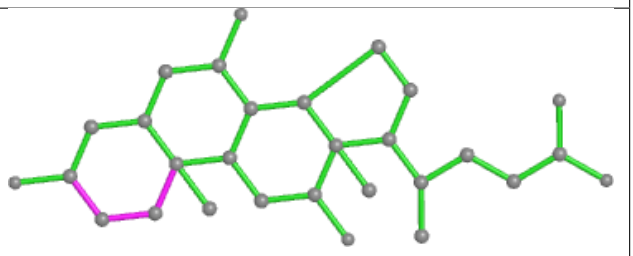


Rings

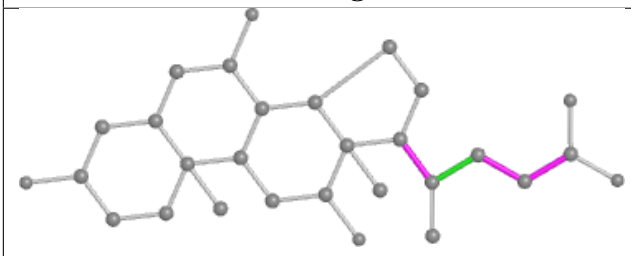
Ligand CHD P 308



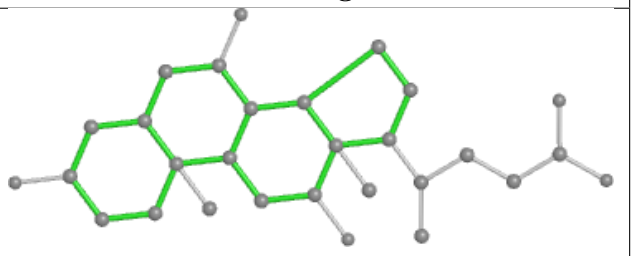
Bond lengths



Bond angles

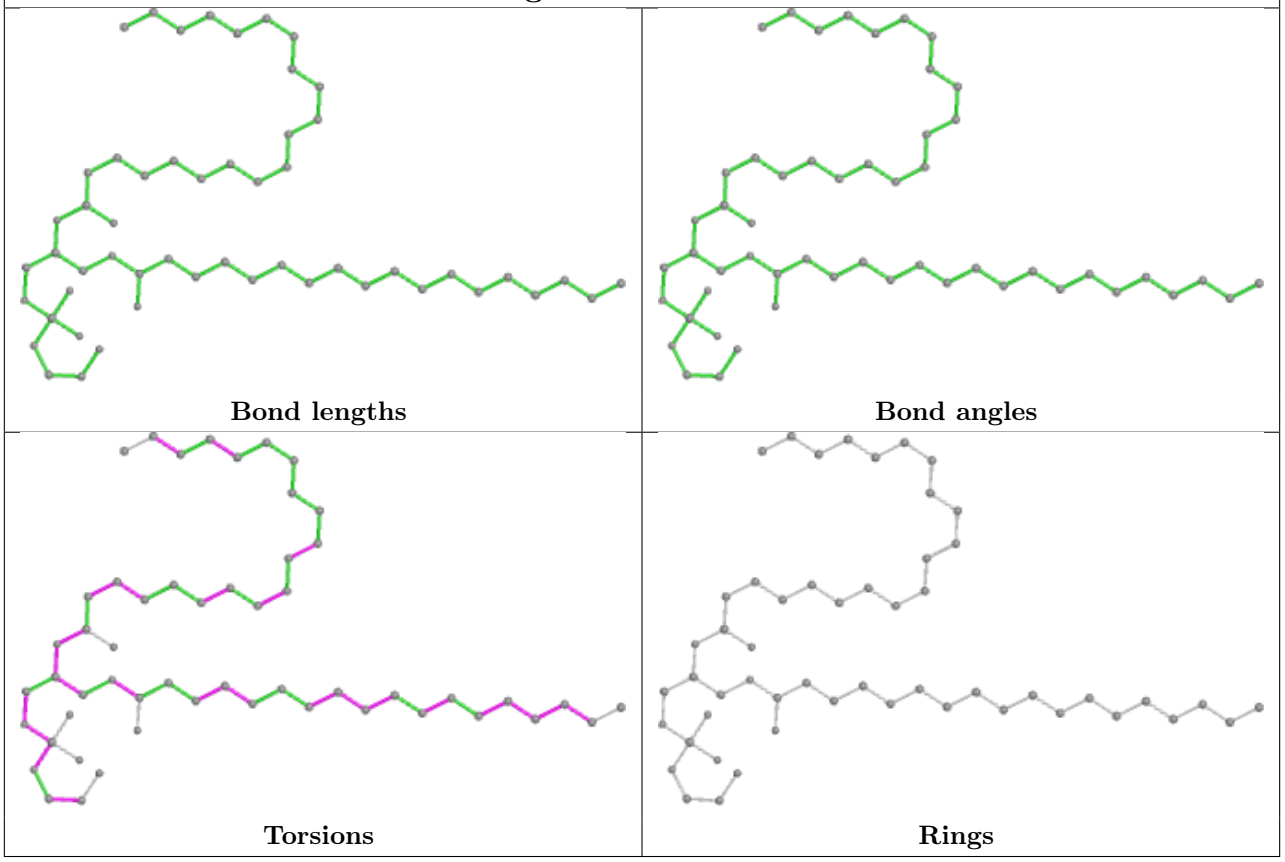


Torsions

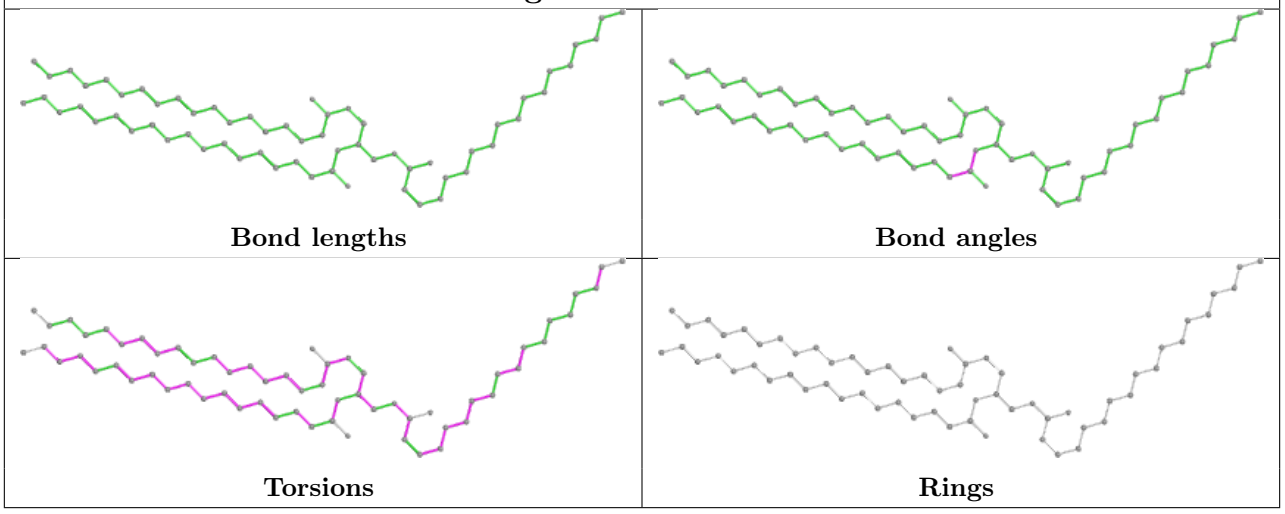


Rings

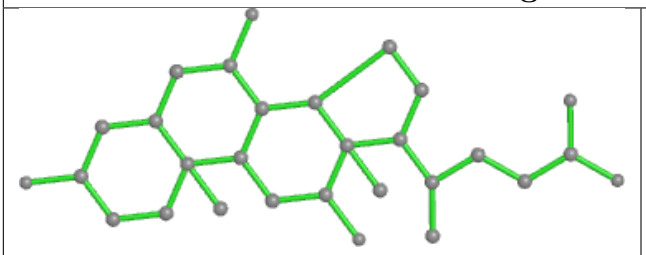
Ligand PEK P 305



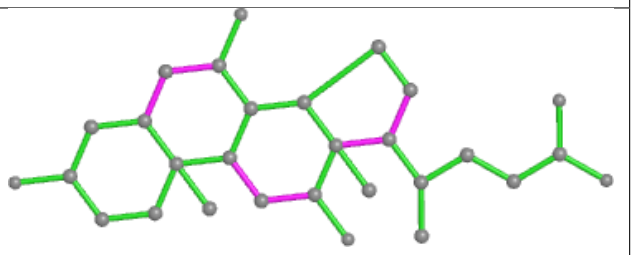
Ligand TGL A 615



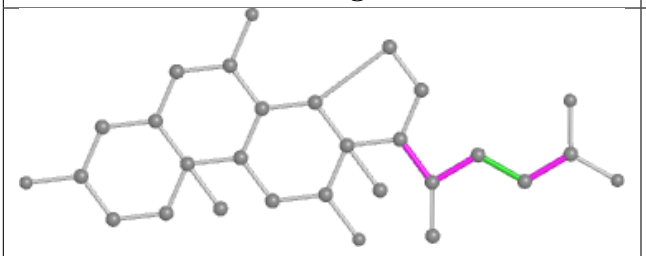
Ligand CHD Y 102



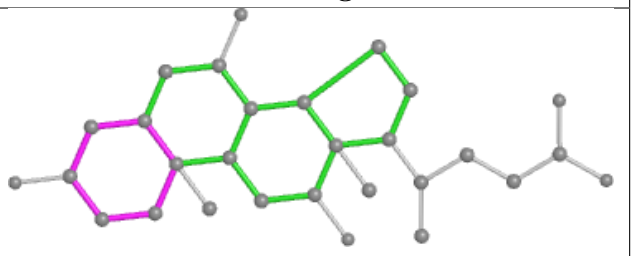
Bond lengths



Bond angles

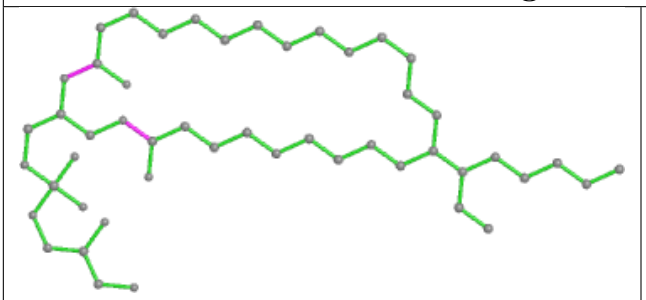


Torsions

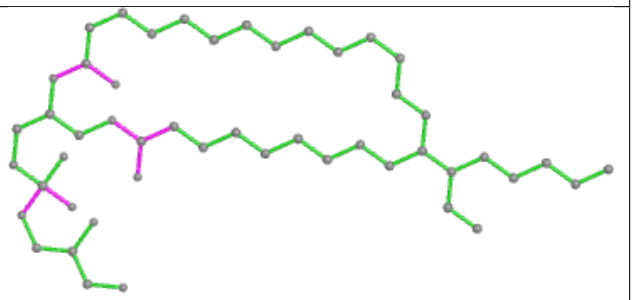


Rings

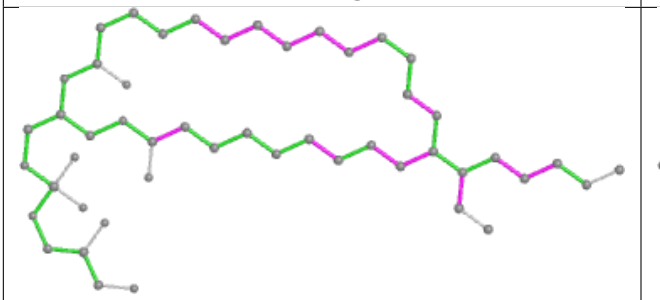
Ligand PGV N 605



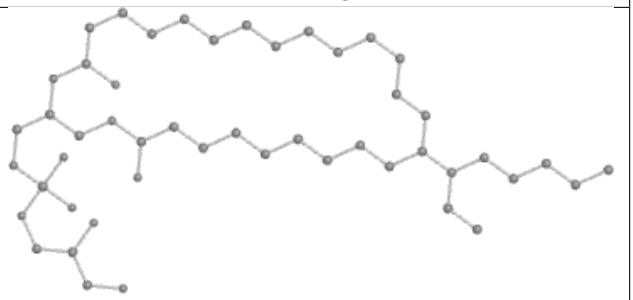
Bond lengths



Bond angles

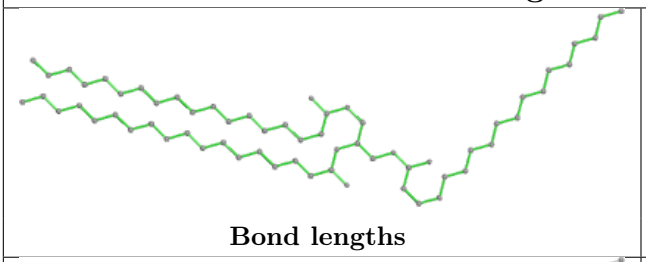


Torsions

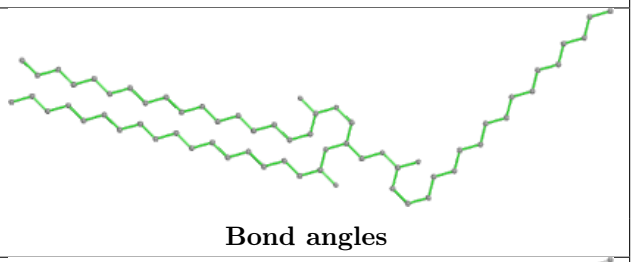


Rings

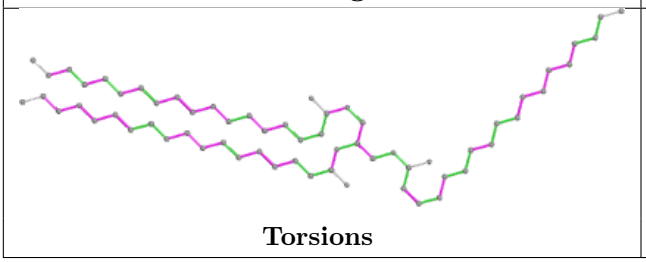
Ligand TGL L 101



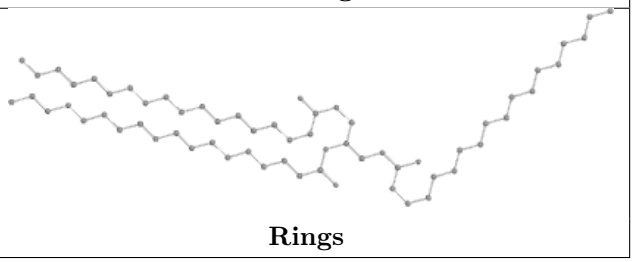
Bond lengths



Bond angles

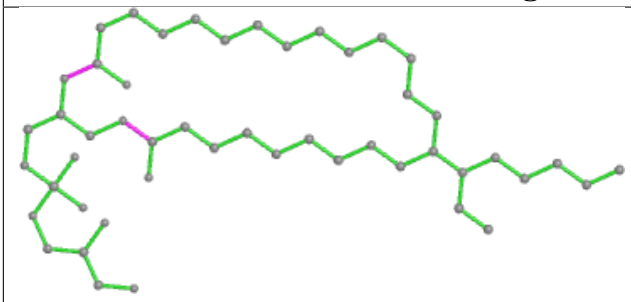


Torsions

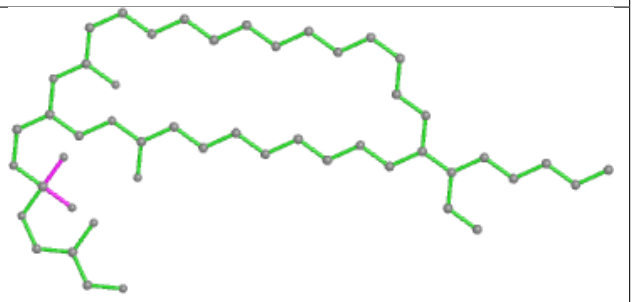


Rings

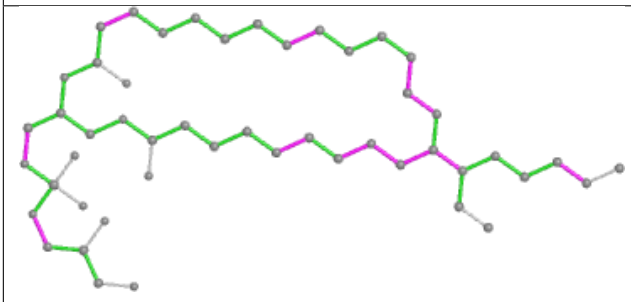
Ligand PGV C 305



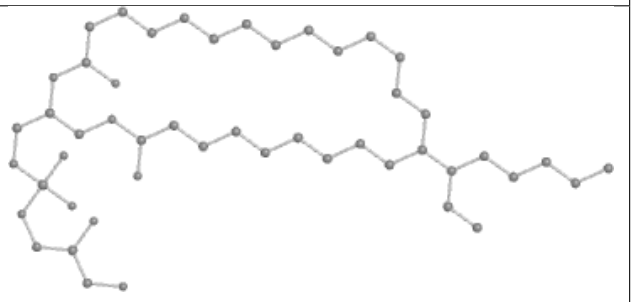
Bond lengths



Bond angles

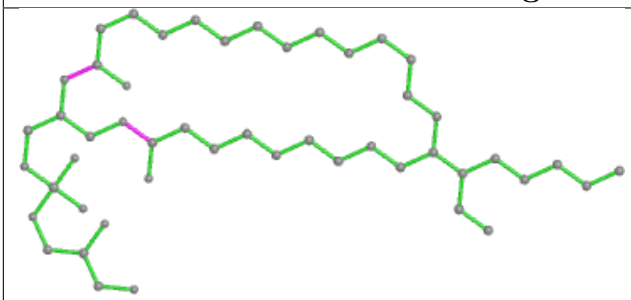


Torsions

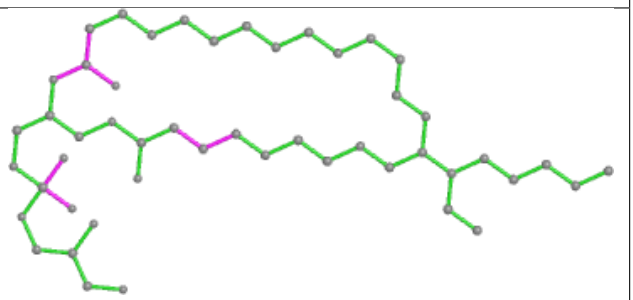


Rings

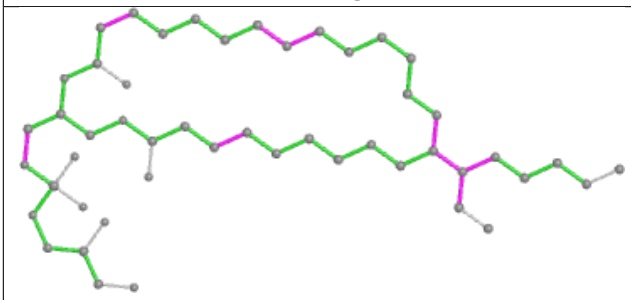
Ligand PGV P 306



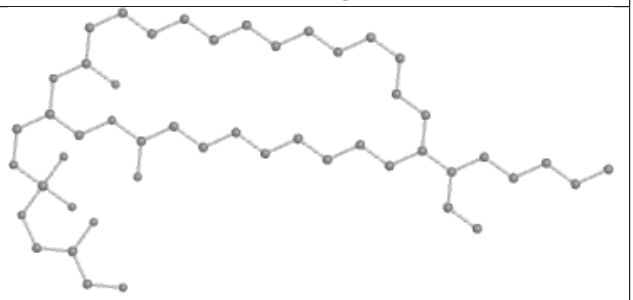
Bond lengths



Bond angles

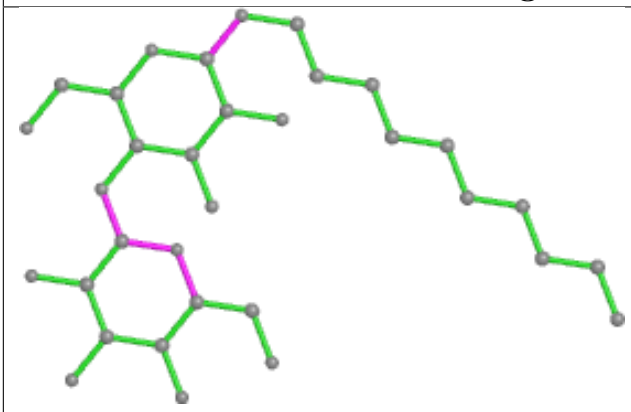


Torsions

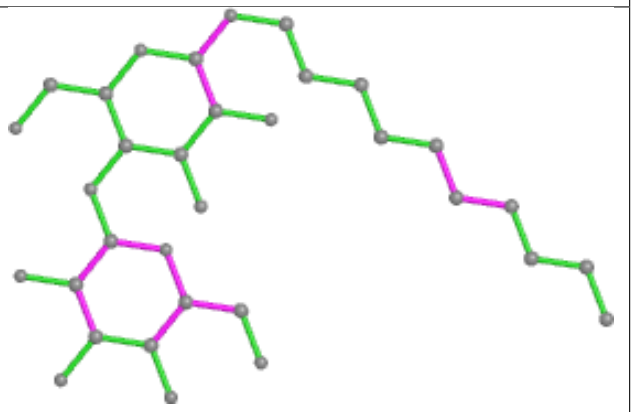


Rings

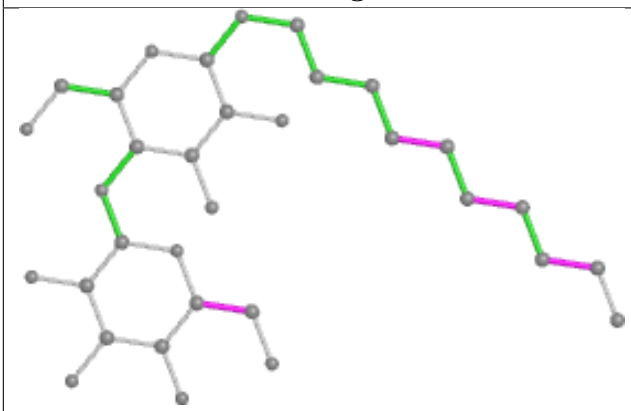
Ligand DMU Z 101



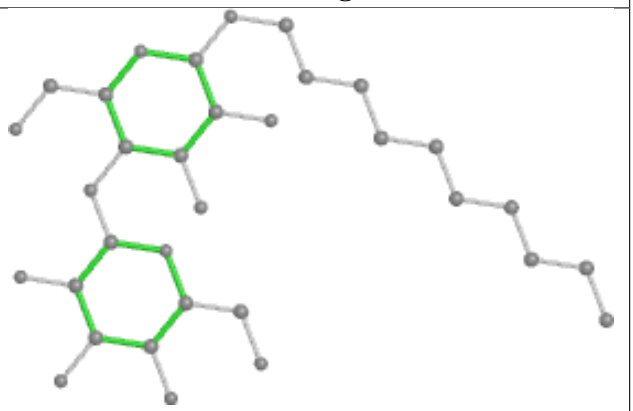
Bond lengths



Bond angles

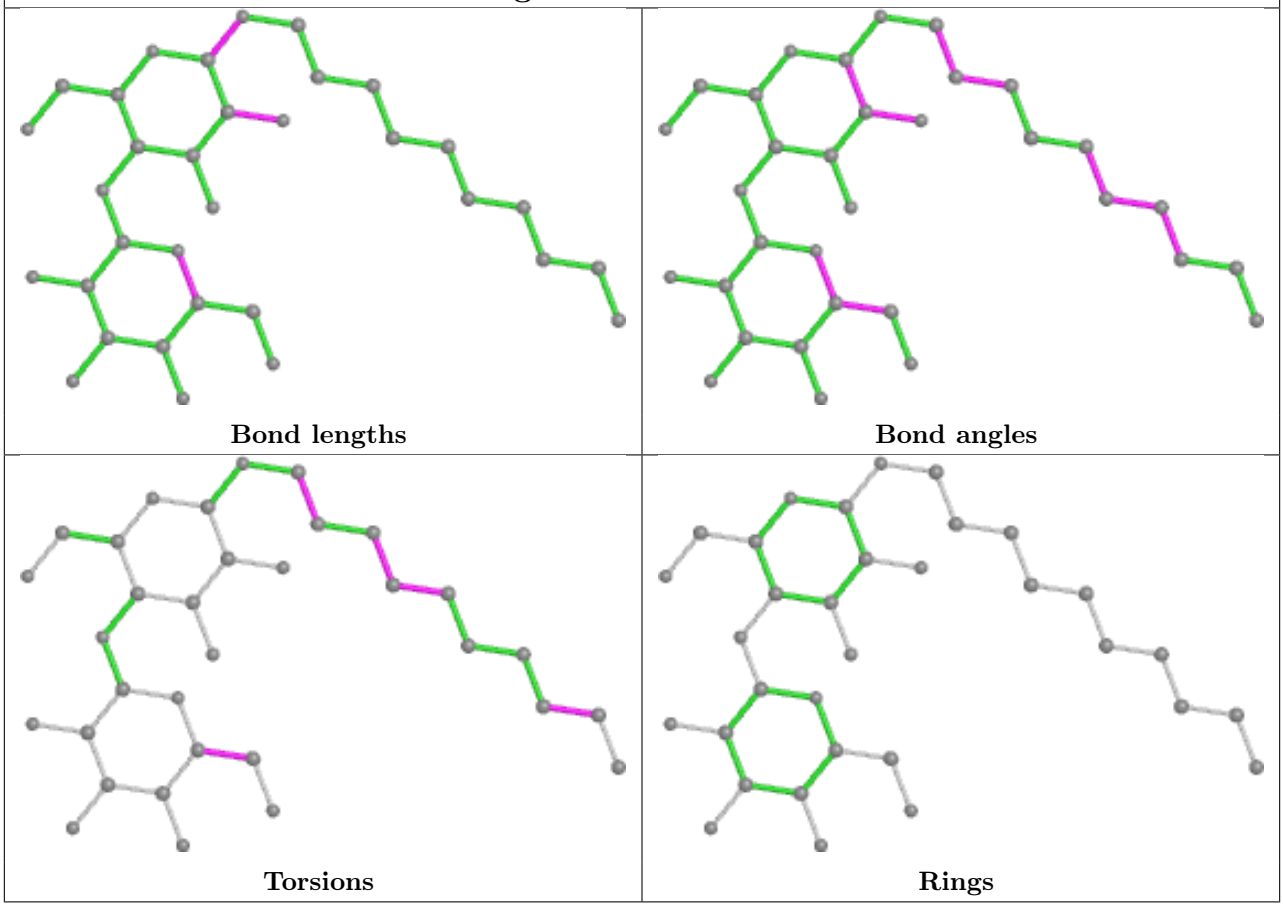


Torsions

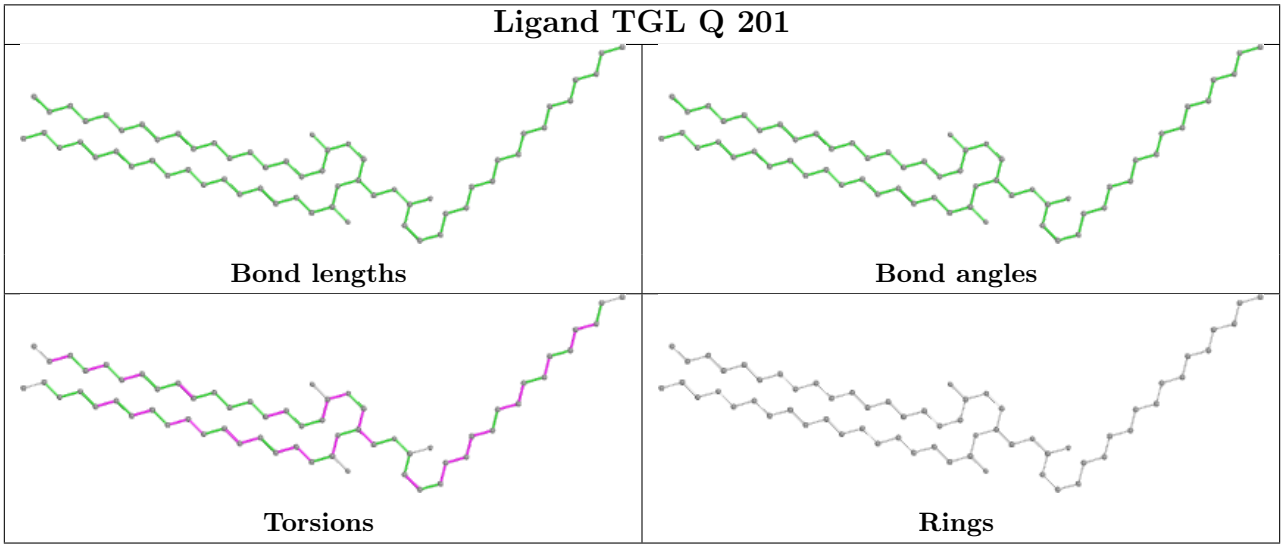


Rings

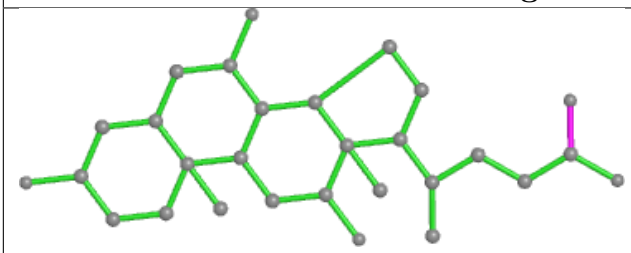
Ligand DMU M 101



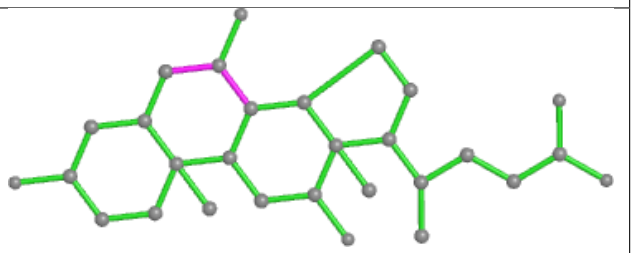
Ligand TGL Q 201



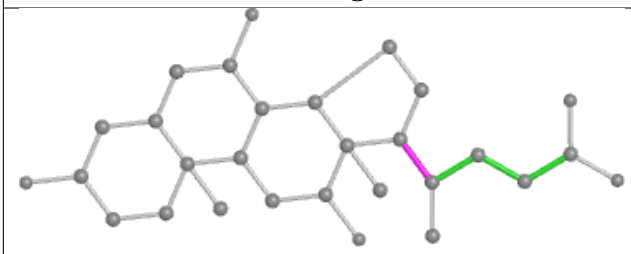
Ligand CHD C 302



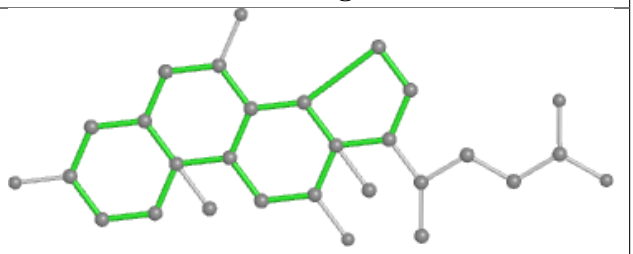
Bond lengths



Bond angles

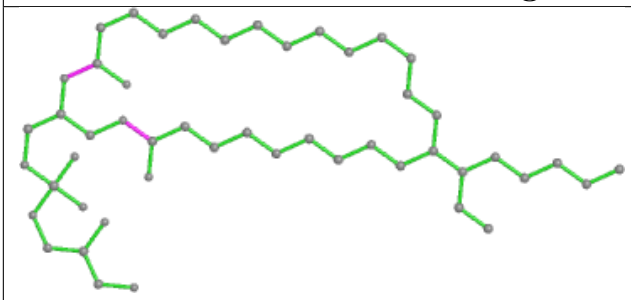


Torsions

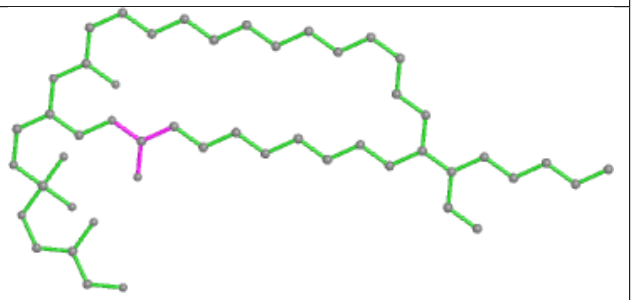


Rings

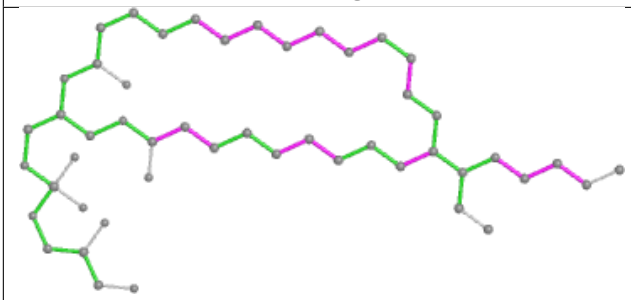
Ligand PGV A 605



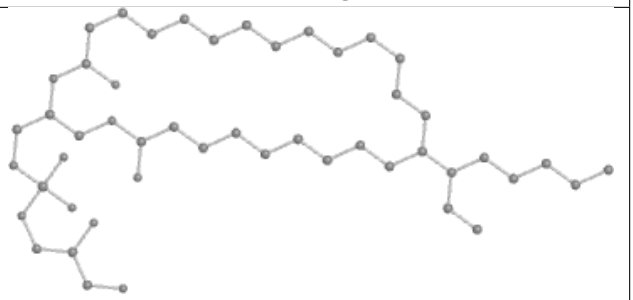
Bond lengths



Bond angles

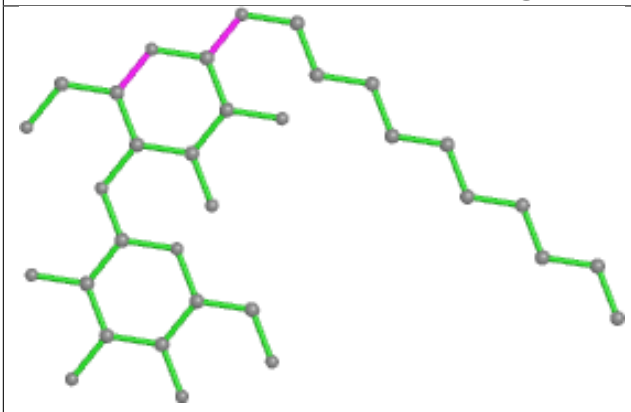


Torsions

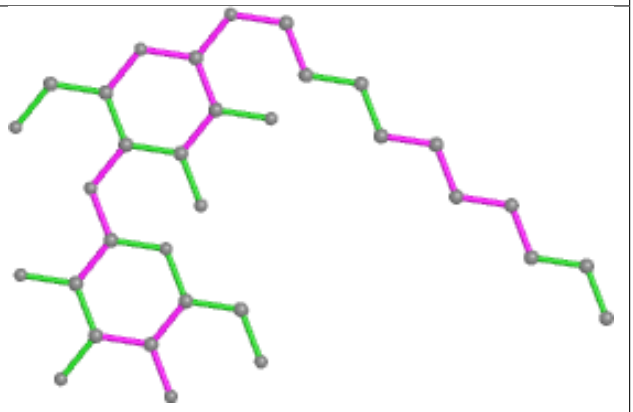


Rings

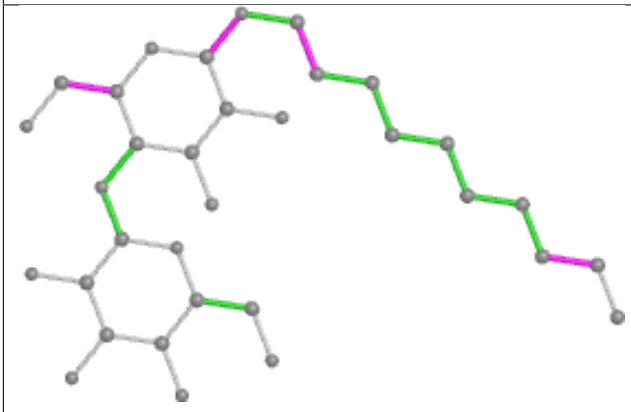
Ligand DMU P 302



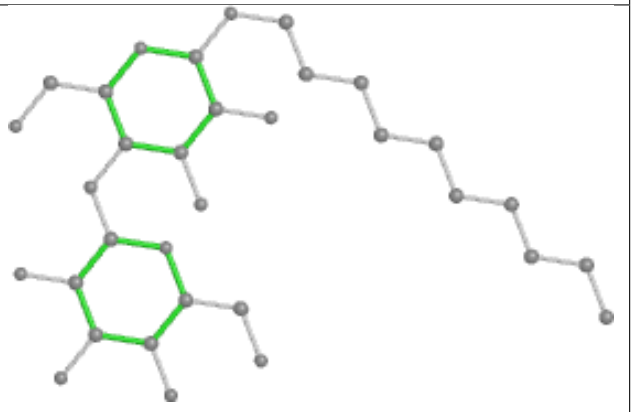
Bond lengths



Bond angles

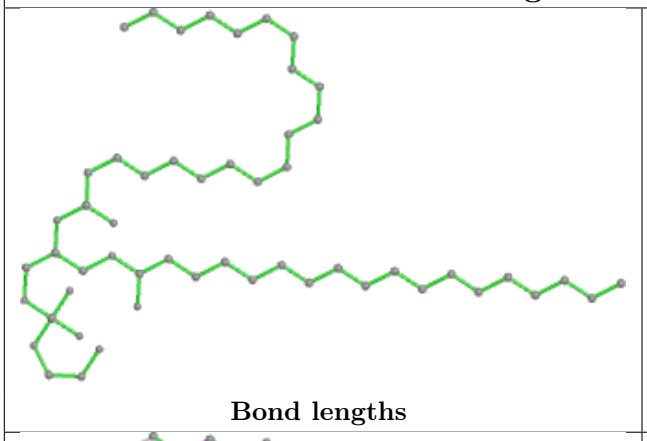


Torsions

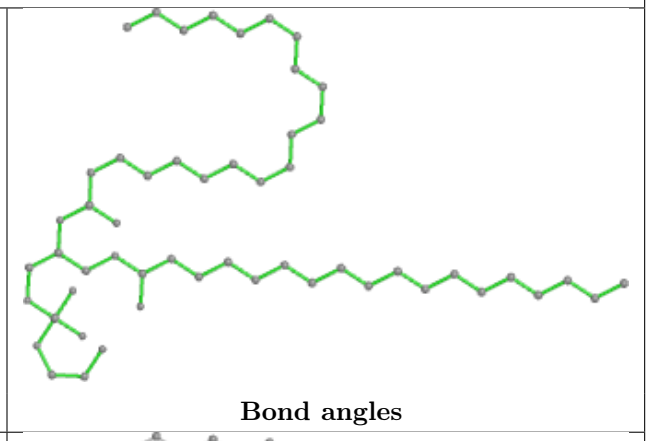


Rings

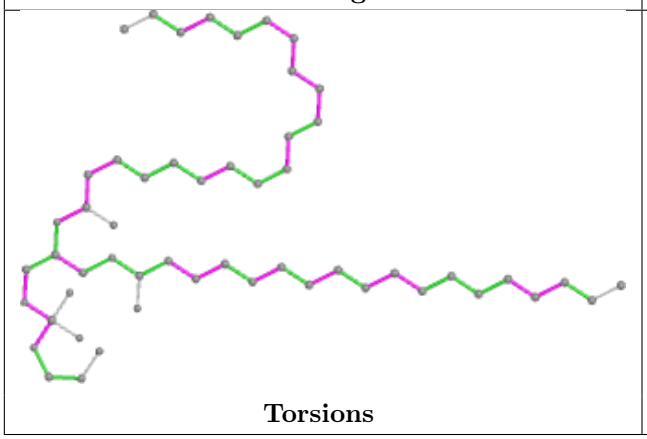
Ligand PEK C 315



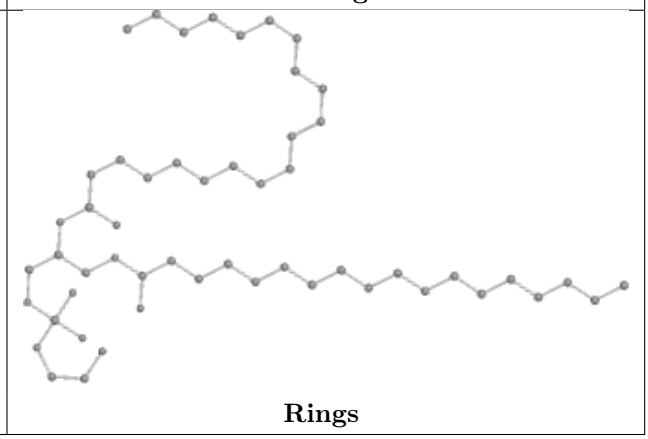
Bond lengths



Bond angles

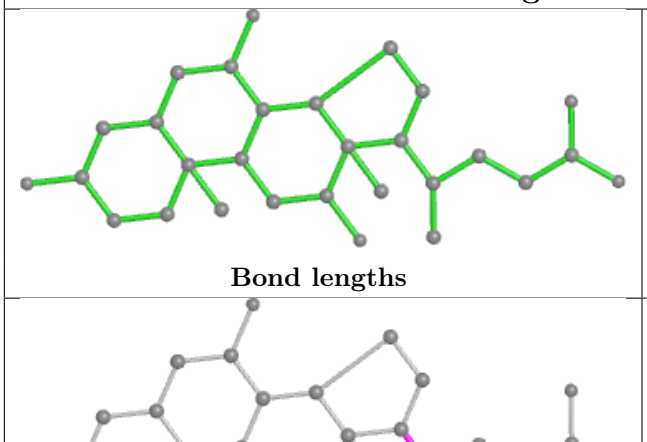


Torsions

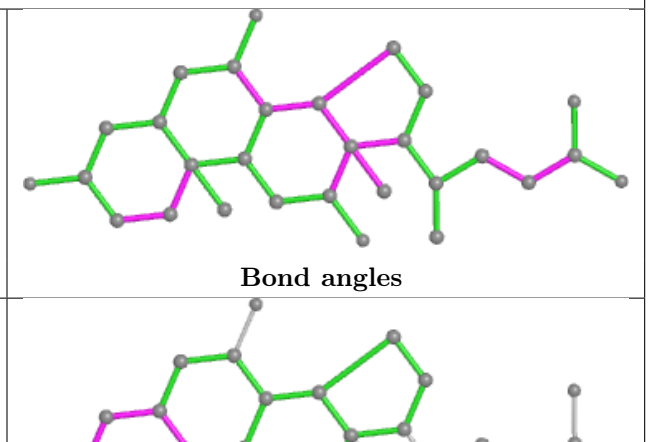


Rings

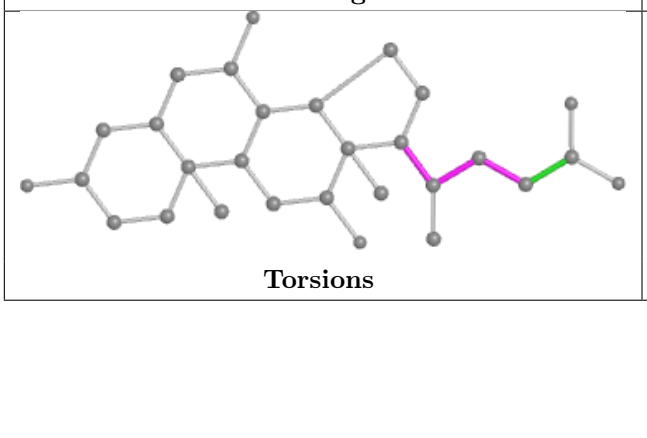
Ligand CHD T 104



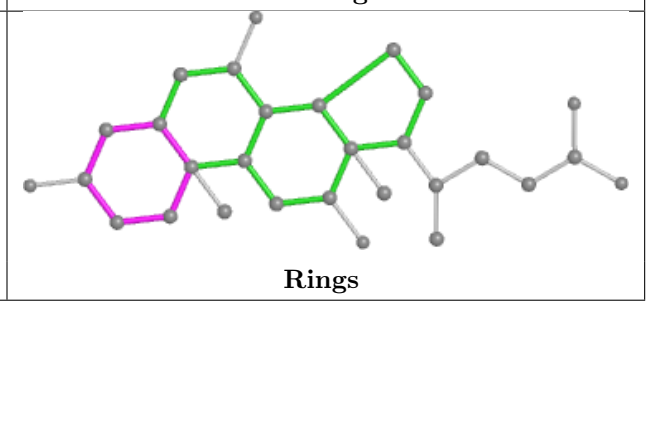
Bond lengths



Bond angles

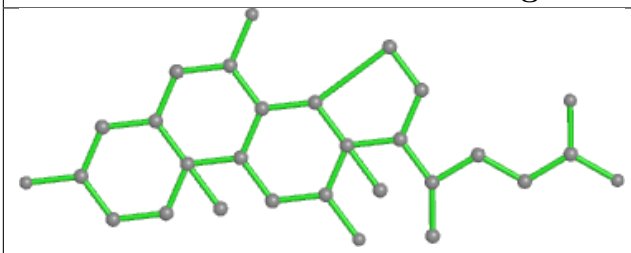


Torsions

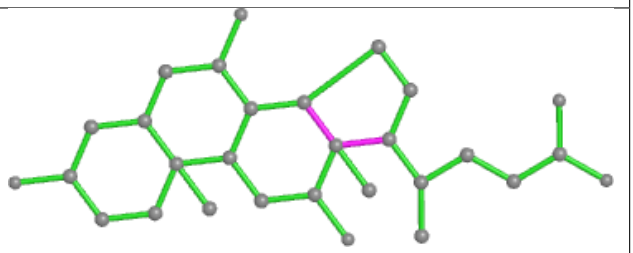


Rings

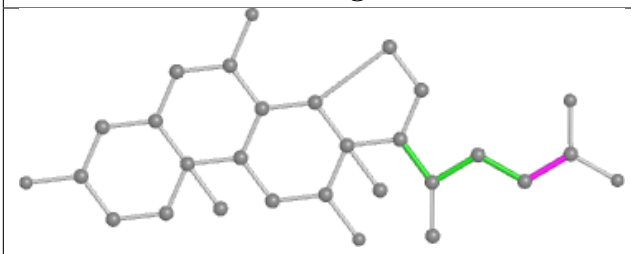
Ligand CHD B 302



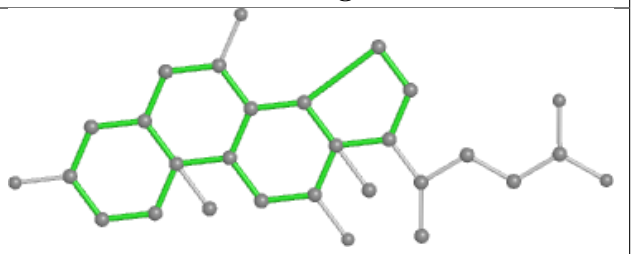
Bond lengths



Bond angles

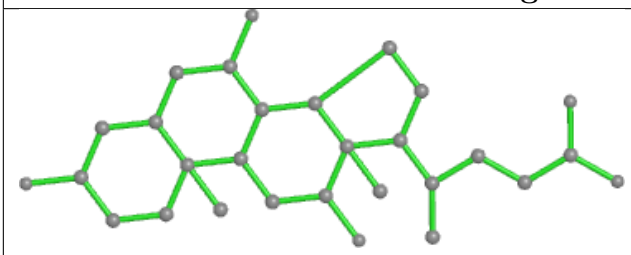


Torsions

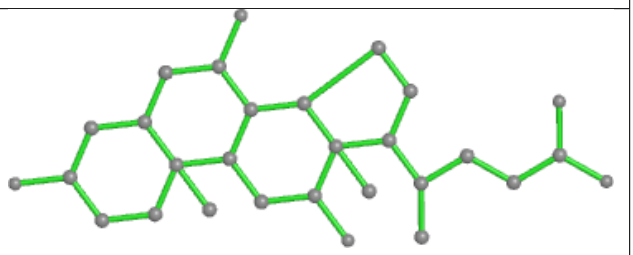


Rings

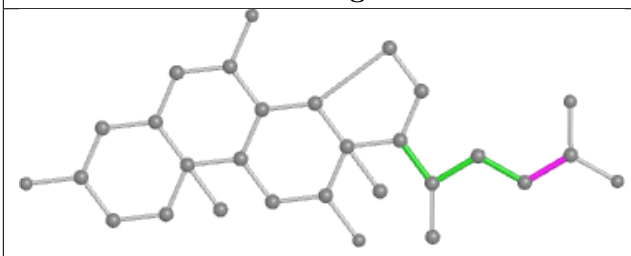
Ligand CHD C 307



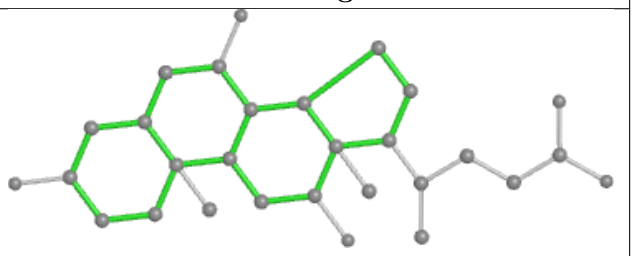
Bond lengths



Bond angles

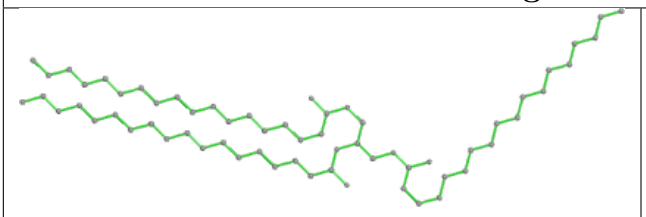


Torsions

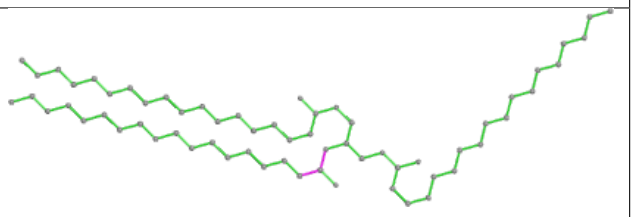


Rings

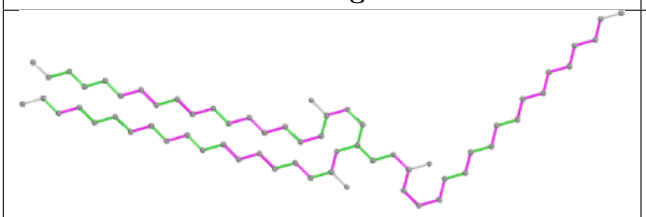
Ligand TGL N 604



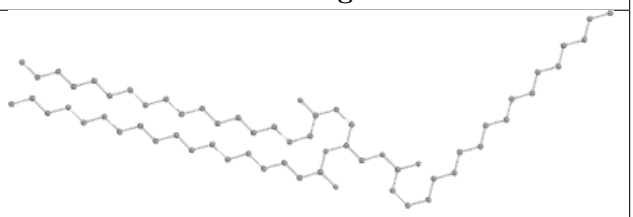
Bond lengths



Bond angles

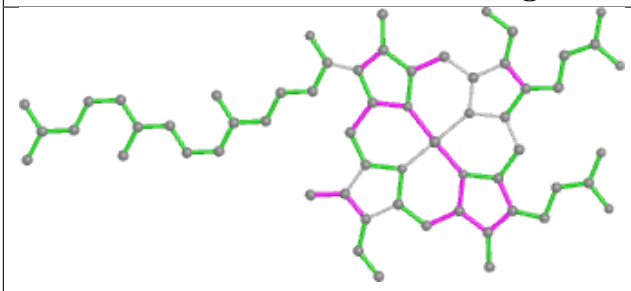


Torsions

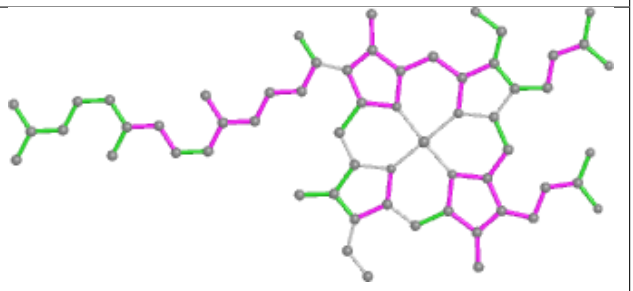


Rings

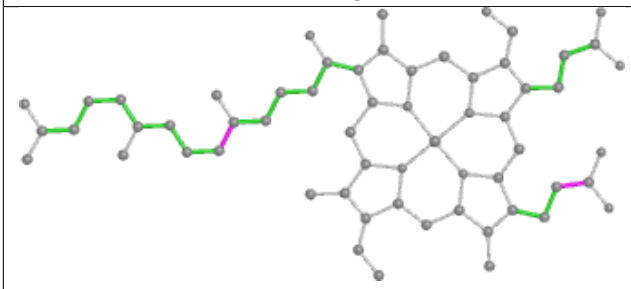
Ligand HEA N 607



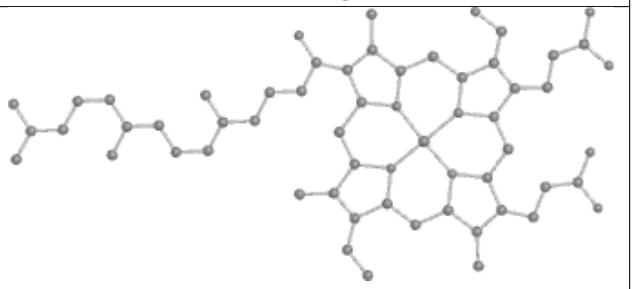
Bond lengths



Bond angles

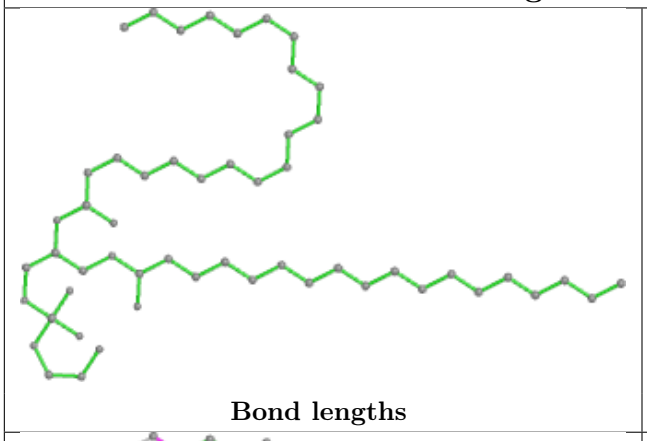


Torsions

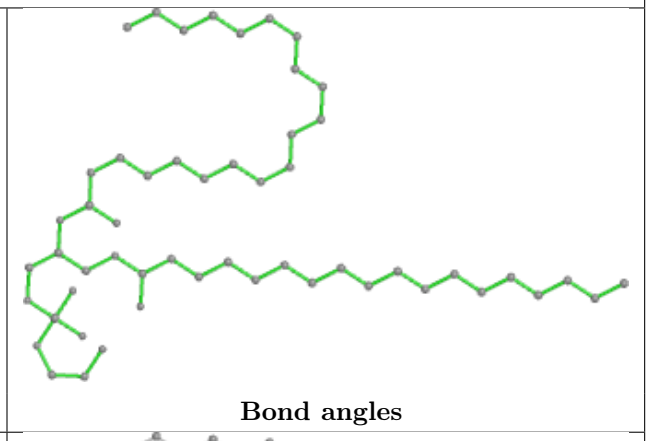


Rings

Ligand PEK P 301

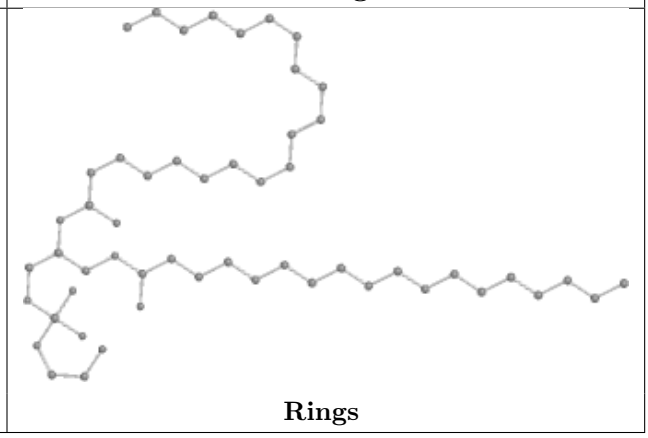


Bond lengths



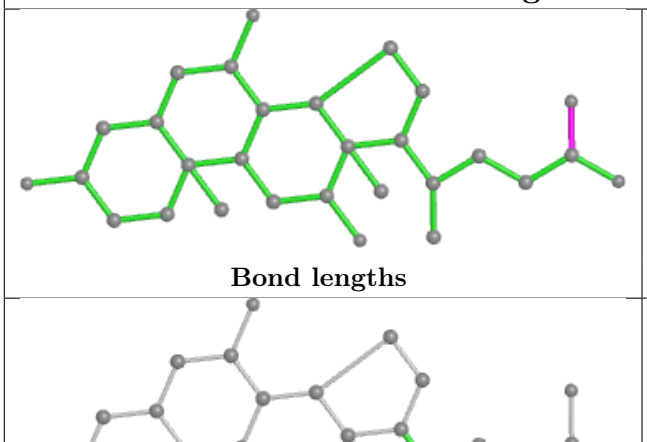
Bond angles

Torsions

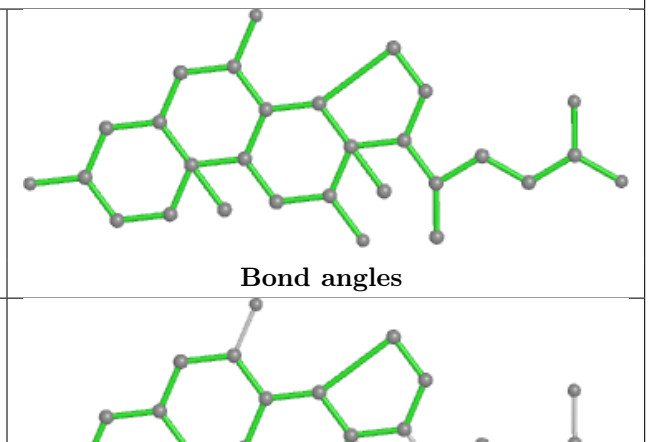


Rings

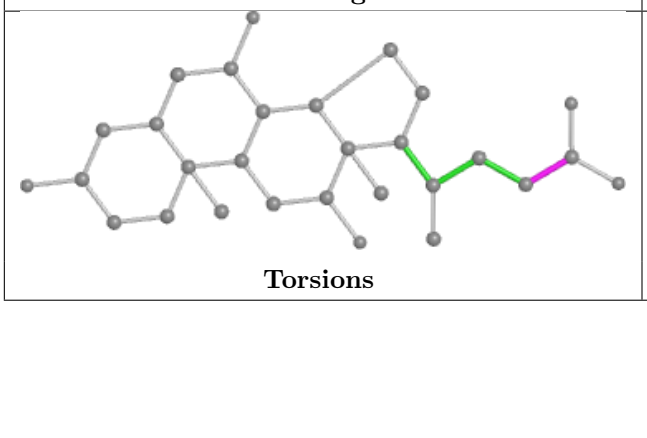
Ligand CHD P 303



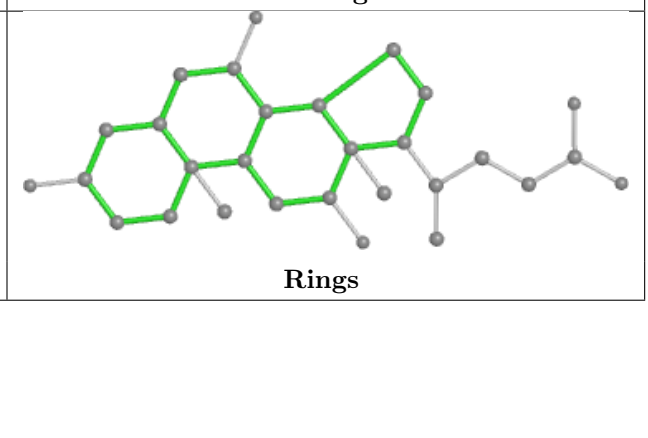
Bond lengths



Bond angles

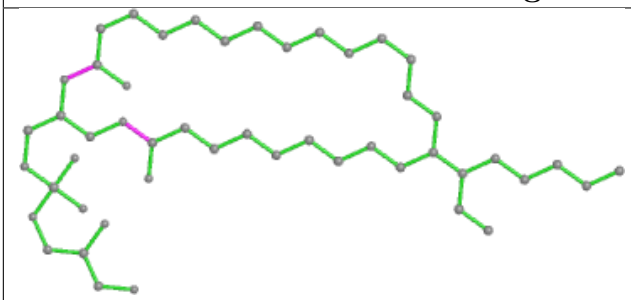


Torsions

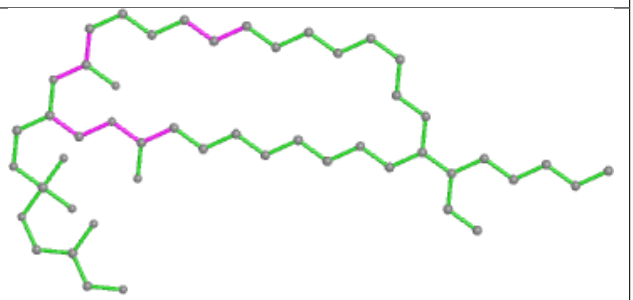


Rings

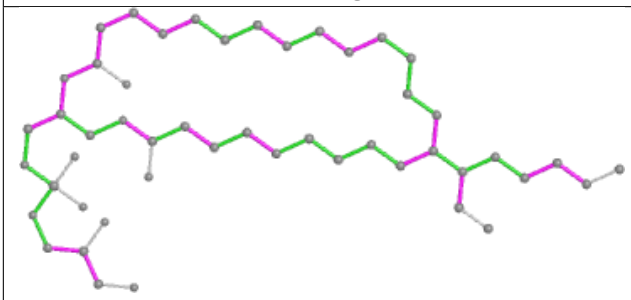
Ligand PGV Z 102



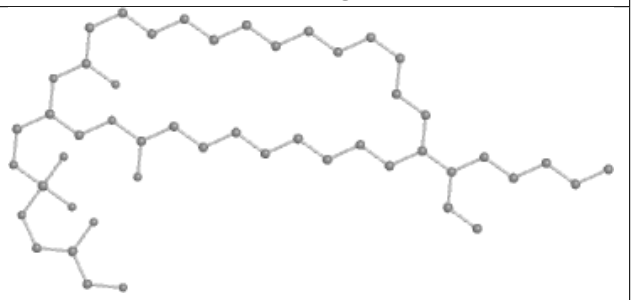
Bond lengths



Bond angles

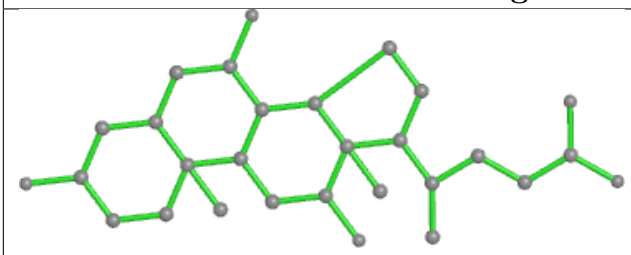


Torsions

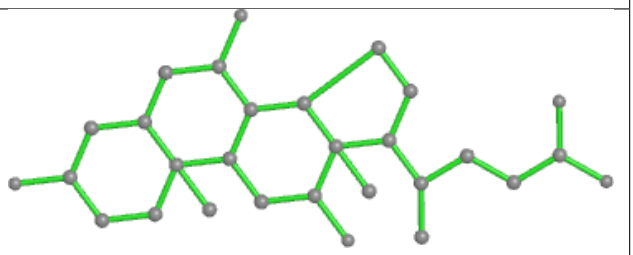


Rings

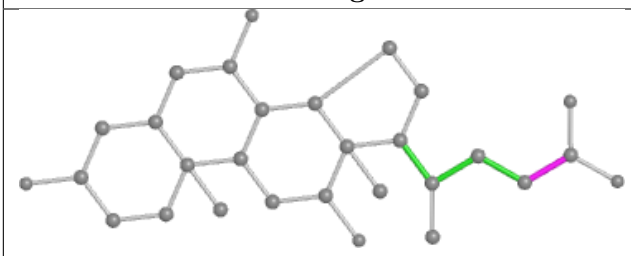
Ligand CHD G 1305



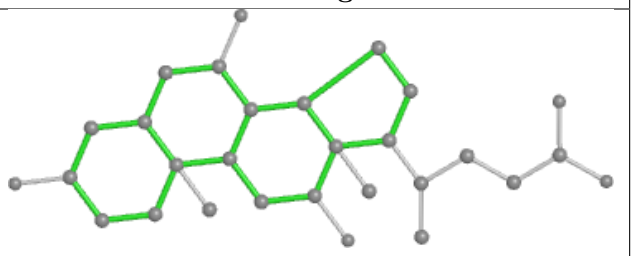
Bond lengths



Bond angles

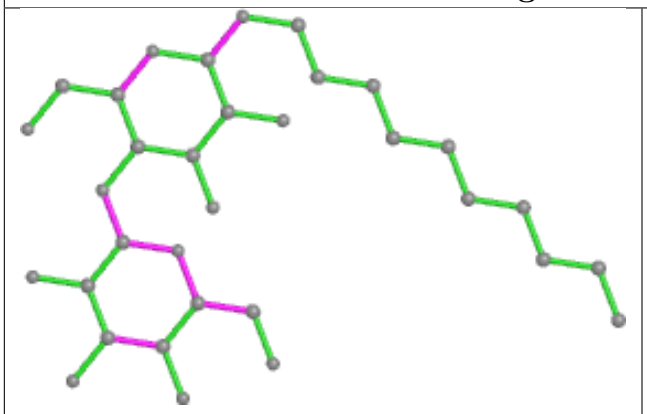


Torsions

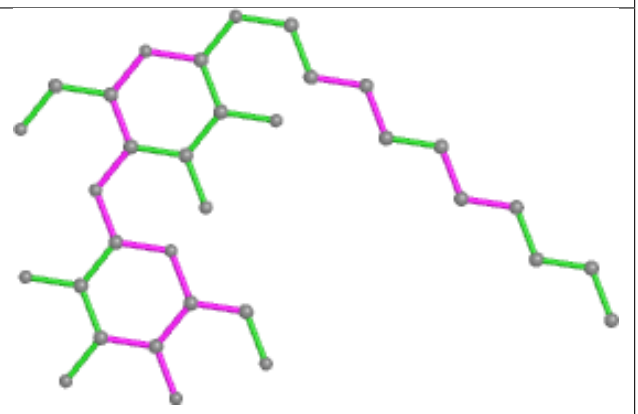


Rings

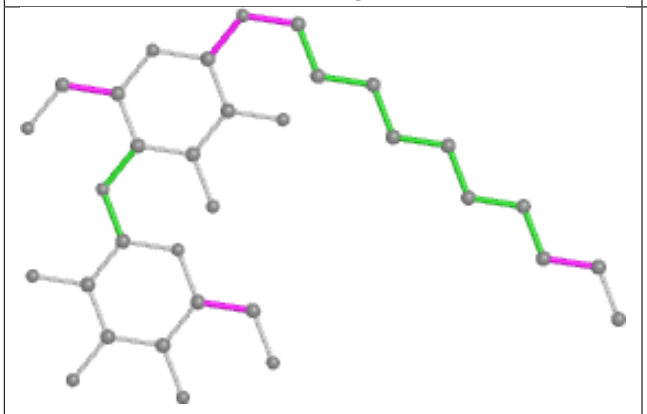
Ligand DMU C 313



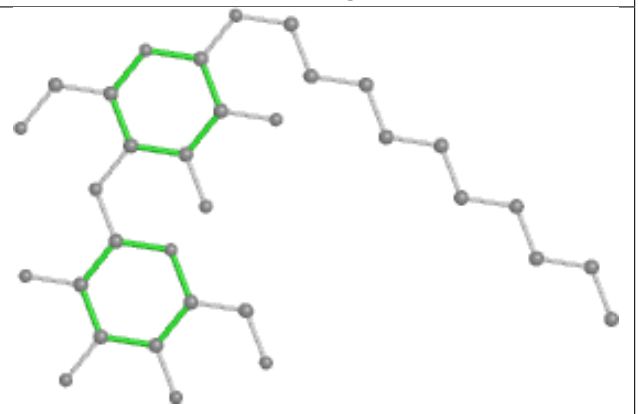
Bond lengths



Bond angles

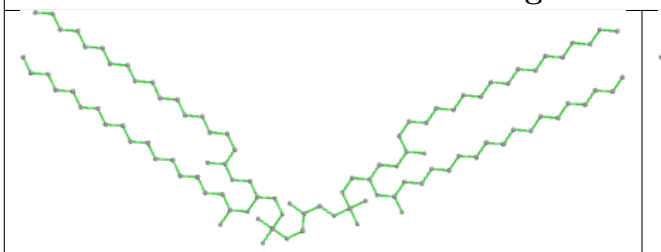


Torsions

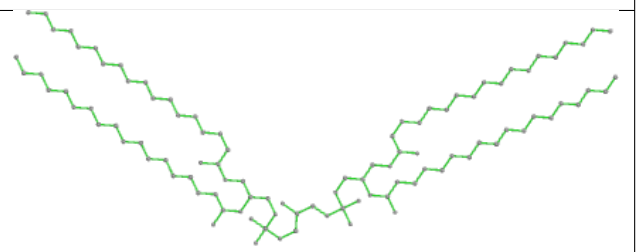


Rings

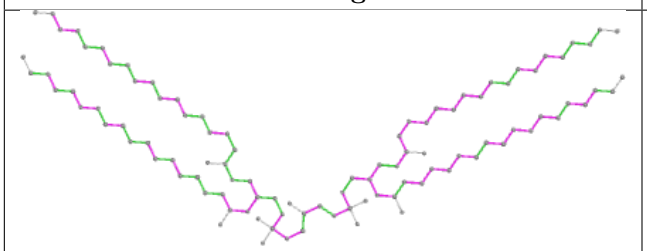
Ligand CDL C 312



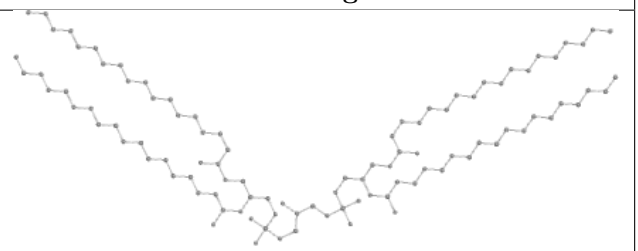
Bond lengths



Bond angles

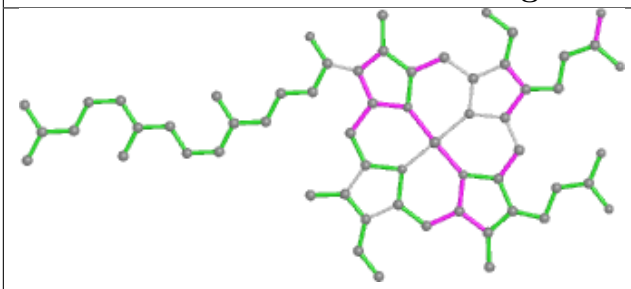


Torsions

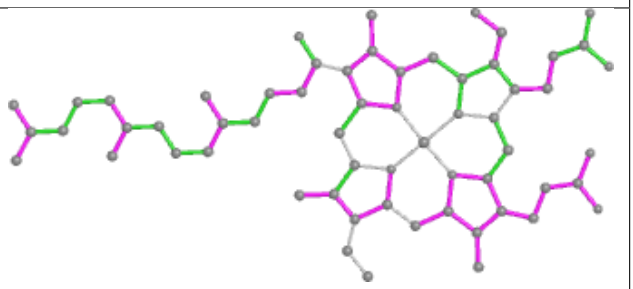


Rings

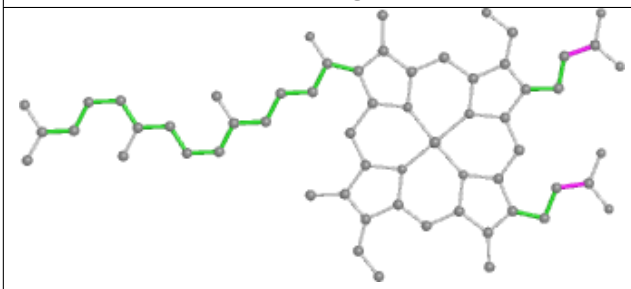
Ligand HEA N 606



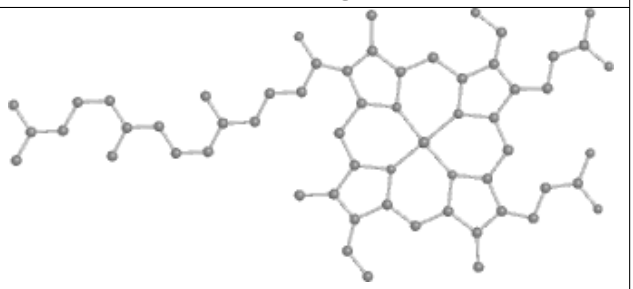
Bond lengths



Bond angles

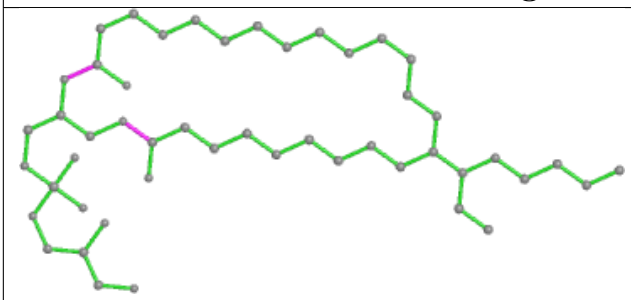


Torsions

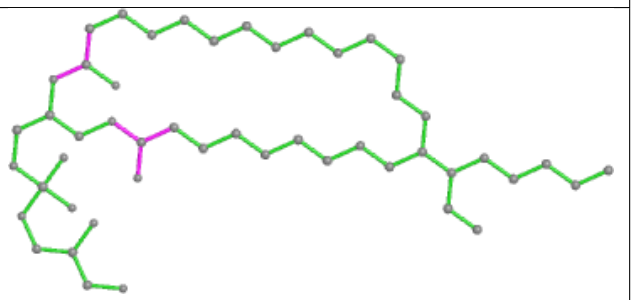


Rings

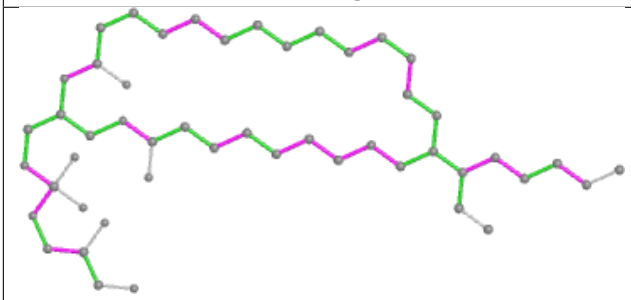
Ligand PGV N 616



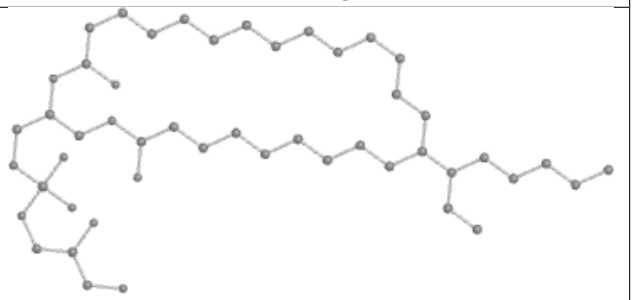
Bond lengths



Bond angles

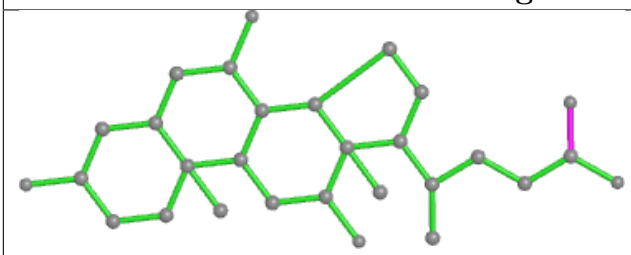


Torsions

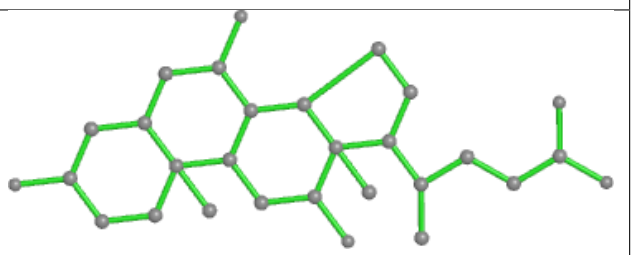


Rings

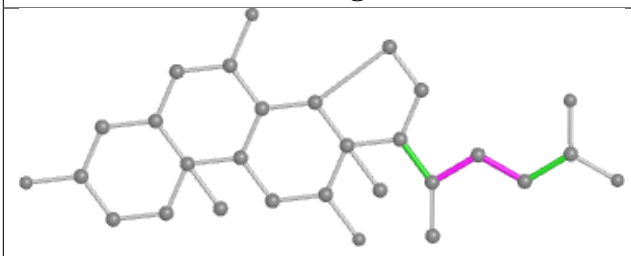
Ligand CHD J 1102



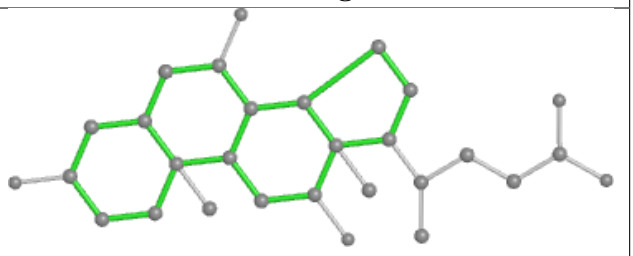
Bond lengths



Bond angles

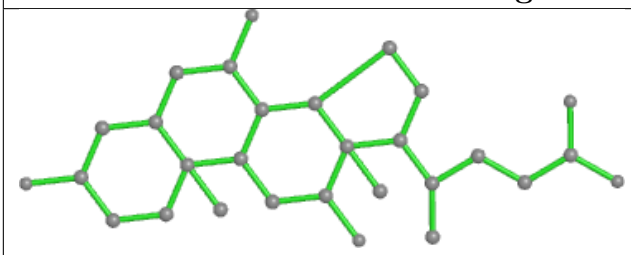


Torsions

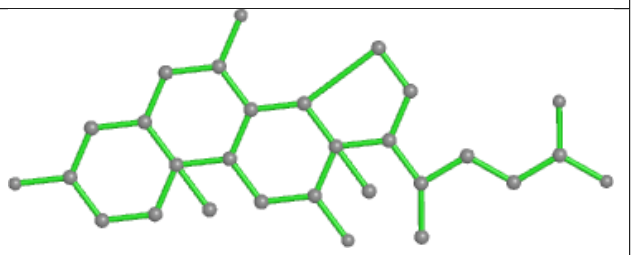


Rings

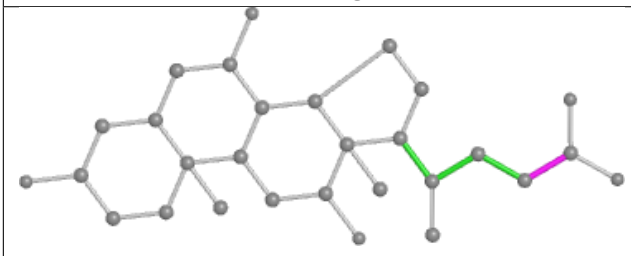
Ligand CHD W 302



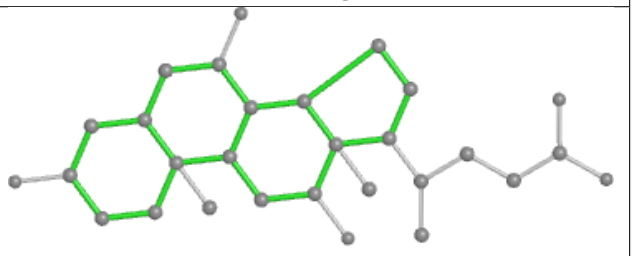
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	0.31	26 (5%) 28 35	27, 33, 42, 79	0
1	N	513/514 (99%)	0.29	20 (3%) 39 47	32, 39, 51, 84	0
2	B	226/227 (99%)	-0.13	4 (1%) 68 74	28, 38, 61, 99	0
2	O	226/227 (99%)	-0.03	10 (4%) 34 41	36, 46, 73, 103	0
3	C	259/261 (99%)	-0.29	0 100 100	30, 37, 49, 83	0
3	P	259/261 (99%)	-0.34	4 (1%) 73 79	32, 41, 55, 87	0
4	D	147/147 (100%)	-0.24	2 (1%) 75 80	35, 43, 59, 90	0
4	Q	147/147 (100%)	0.96	24 (16%) 1 2	41, 57, 98, 154	0
5	E	105/109 (96%)	-0.10	5 (4%) 30 38	37, 45, 69, 123	0
5	R	105/109 (96%)	0.30	8 (7%) 13 19	42, 53, 75, 124	0
6	F	98/98 (100%)	0.61	13 (13%) 3 4	32, 43, 85, 138	0
6	S	98/98 (100%)	0.24	8 (8%) 11 17	37, 48, 82, 117	0
7	G	83/85 (97%)	0.79	21 (25%) 0 0	34, 44, 108, 122	0
7	T	83/85 (97%)	1.31	24 (28%) 0 0	36, 50, 104, 130	0
8	H	79/85 (92%)	0.73	15 (18%) 1 1	35, 48, 97, 110	0
8	U	79/85 (92%)	1.06	14 (17%) 1 1	42, 53, 114, 127	0
9	I	72/73 (98%)	0.50	9 (12%) 3 5	36, 51, 67, 86	0
9	V	72/73 (98%)	0.83	17 (23%) 0 0	40, 57, 80, 99	0
10	J	58/59 (98%)	0.33	8 (13%) 2 4	36, 47, 72, 122	0
10	W	58/59 (98%)	0.46	6 (10%) 6 10	41, 53, 84, 123	0
11	K	52/56 (92%)	0.25	3 (5%) 23 29	37, 46, 65, 111	0
11	X	52/56 (92%)	1.14	9 (17%) 1 2	50, 59, 104, 120	0
12	L	46/47 (97%)	-0.22	2 (4%) 35 42	33, 39, 62, 93	0
12	Y	46/47 (97%)	0.11	2 (4%) 35 42	42, 49, 73, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.23	4 (9%) 8 13	36, 40, 71, 105	0
13	Z	43/46 (93%)	1.18	8 (18%) 1 1	45, 53, 84, 143	0
All	All	3562/3614 (98%)	0.25	266 (7%) 14 20	27, 42, 76, 154	0

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	15.7
4	Q	4	SER	13.9
4	Q	6	VAL	13.6
5	R	109	VAL	13.0
4	Q	5	VAL	13.0

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
7	TPO	G	11	11/12	0.72	0.24	47,87,130,139	0
7	TPO	T	11	11/12	0.84	0.32	54,119,161,165	0
2	FME	O	1	10/11	0.96	0.13	40,48,59,62	0
1	FME	A	1	10/11	0.97	0.17	45,53,79,101	0
2	FME	B	1	10/11	0.98	0.12	36,41,50,58	0
1	FME	N	1	10/11	0.98	0.21	51,59,89,92	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
19	EDO	P	309	4/4	0.05	0.38	81,82,85,87	0
28	SAC	V	101	9/10	0.21	0.75	129,139,152,154	0
23	DMU	C	301	33/33	0.40	0.44	87,130,143,153	0
19	EDO	Z	103	4/4	0.43	0.24	86,94,94,96	0
19	EDO	L	102	4/4	0.51	0.30	68,69,72,75	0
19	EDO	V	103	4/4	0.55	0.21	81,81,90,95	0
19	EDO	K	101	4/4	0.58	0.23	74,75,76,77	0
22	CHD	T	104	29/29	0.60	0.34	81,147,172,175	0
24	PEK	C	315	53/53	0.61	0.26	60,85,124,172	0
19	EDO	G	1306	4/4	0.61	0.15	90,90,93,95	0
20	TGL	Y	101	63/63	0.62	0.28	55,79,120,132	0
24	PEK	P	301	53/53	0.64	0.26	64,88,161,171	0
26	PSC	E	201	52/52	0.64	0.31	46,92,184,199	0
19	EDO	D	206	4/4	0.64	0.27	74,79,83,88	0
20	TGL	Q	201	63/63	0.66	0.21	67,91,111,119	0
25	CDL	C	312	100/100	0.66	0.29	68,105,138,150	0
24	PEK	P	305	53/53	0.67	0.26	59,92,159,171	0
20	TGL	N	604	63/63	0.67	0.29	65,97,118,130	0
22	CHD	Y	102	29/29	0.68	0.34	96,138,156,166	0
28	SAC	I	101	9/10	0.68	0.34	83,101,110,116	0
19	EDO	K	102	4/4	0.68	0.17	66,68,74,75	0
26	PSC	O	302	52/52	0.69	0.31	47,95,173,185	0
25	CDL	T	102	100/100	0.69	0.28	67,112,154,170	0
19	EDO	W	303	4/4	0.69	0.21	60,74,75,76	0
20	TGL	L	101	63/63	0.70	0.24	47,77,104,109	0
19	EDO	P	310	4/4	0.70	0.38	61,83,84,90	0
17	PGV	Z	102	51/51	0.71	0.36	50,90,154,168	0
25	CDL	P	307	100/100	0.72	0.23	52,96,128,136	0
24	PEK	C	304	53/53	0.72	0.25	64,89,138,146	0
19	EDO	I	102	4/4	0.73	0.15	88,88,94,94	0
17	PGV	T	101	51/51	0.74	0.24	56,90,115,134	0
20	TGL	A	615	63/63	0.74	0.26	59,87,139,151	0
23	DMU	G	1302	33/33	0.75	0.18	62,110,125,125	0
20	TGL	D	201	63/63	0.75	0.19	55,86,101,108	0
19	EDO	G	1304	4/4	0.75	0.19	75,79,80,80	0
19	EDO	C	309	4/4	0.76	0.16	75,80,83,84	0
25	CDL	C	306	100/100	0.76	0.24	48,89,122,127	0
19	EDO	S	2207	4/4	0.76	0.19	75,81,84,85	0
17	PGV	A	604	51/51	0.77	0.25	51,83,114,126	0
19	EDO	J	1103	4/4	0.78	0.12	77,77,78,85	0
19	EDO	V	102	4/4	0.78	0.17	78,79,80,83	0
19	EDO	B	304	4/4	0.78	0.21	51,59,64,72	0
19	EDO	N	613	4/4	0.79	0.22	61,65,69,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	C	310	4/4	0.81	0.15	80,89,92,100	0
17	PGV	N	616	51/51	0.81	0.21	66,87,140,156	0
23	DMU	Z	101	33/33	0.81	0.25	54,72,82,84	0
19	EDO	S	2201	4/4	0.81	0.33	58,63,63,78	0
19	EDO	O	303	4/4	0.81	0.20	53,74,76,77	0
19	EDO	F	702	4/4	0.82	0.32	70,84,89,96	0
19	EDO	N	617	4/4	0.82	0.27	87,88,92,93	0
19	EDO	B	306	4/4	0.83	0.19	70,76,78,81	0
19	EDO	G	1303	4/4	0.83	0.20	71,83,83,89	0
19	EDO	A	611	4/4	0.83	0.21	63,81,82,84	0
22	CHD	W	302	29/29	0.83	0.38	78,88,98,106	0
19	EDO	W	304	4/4	0.84	0.21	88,88,91,100	0
23	DMU	P	302	33/33	0.84	0.35	73,106,128,133	0
19	EDO	N	620	4/4	0.84	0.31	65,66,69,79	0
23	DMU	C	313	33/33	0.85	0.27	57,89,100,105	0
19	EDO	R	202	4/4	0.85	0.41	78,85,89,96	0
19	EDO	A	619	4/4	0.85	0.23	66,67,70,78	0
19	EDO	N	612	4/4	0.85	0.33	67,73,74,82	0
19	EDO	A	614	4/4	0.86	0.24	41,44,46,52	0
22	CHD	J	1102	29/29	0.86	0.34	59,74,86,97	0
19	EDO	M	102	4/4	0.87	0.41	72,75,80,83	0
19	EDO	J	1105	4/4	0.87	0.36	56,73,74,88	0
19	EDO	S	2206	4/4	0.87	0.34	55,60,63,70	0
19	EDO	A	610	4/4	0.88	0.26	38,43,46,50	0
19	EDO	S	2205	4/4	0.88	0.24	56,59,69,70	0
19	EDO	E	205	4/4	0.88	0.20	81,82,82,86	0
19	EDO	C	311	4/4	0.88	0.15	83,85,90,99	0
19	EDO	V	104	4/4	0.89	0.17	50,74,76,77	0
19	EDO	A	612	4/4	0.90	0.14	55,56,56,62	0
19	EDO	C	314	4/4	0.90	0.25	62,70,71,79	0
19	EDO	T	103	4/4	0.90	0.31	57,66,69,71	0
19	EDO	D	205	4/4	0.90	0.20	64,77,78,81	0
19	EDO	B	309	4/4	0.90	0.23	75,91,97,105	0
19	EDO	N	611	4/4	0.90	0.13	67,71,73,81	0
19	EDO	I	103	4/4	0.91	0.10	58,63,64,67	0
19	EDO	D	204	4/4	0.91	0.34	60,76,76,78	0
19	EDO	E	204	4/4	0.92	0.28	73,75,75,78	0
19	EDO	W	301	4/4	0.92	0.18	62,74,75,76	0
19	EDO	A	608	4/4	0.92	0.21	50,56,63,68	0
19	EDO	Q	203	4/4	0.92	0.12	73,77,82,86	0
19	EDO	R	201	4/4	0.92	0.16	54,54,55,56	0
19	EDO	U	1501	4/4	0.92	0.24	55,66,68,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	B	308	4/4	0.92	0.21	59,62,69,85	0
19	EDO	D	207	4/4	0.92	0.21	60,63,63,70	0
19	EDO	D	208	4/4	0.93	0.18	62,64,70,74	0
24	PEK	P	304	53/53	0.93	0.18	41,64,101,108	0
19	EDO	J	1104	4/4	0.93	0.12	55,55,58,62	0
19	EDO	P	311	4/4	0.93	0.12	42,51,51,60	0
19	EDO	Q	202	4/4	0.93	0.18	44,56,58,60	0
19	EDO	A	618	4/4	0.93	0.09	56,62,64,73	0
23	DMU	M	101	33/33	0.93	0.20	46,54,68,74	0
22	CHD	C	307	29/29	0.93	0.21	53,60,67,73	0
19	EDO	N	610	4/4	0.93	0.13	52,55,58,59	0
22	CHD	P	308	29/29	0.93	0.19	57,64,73,78	0
19	EDO	B	307	4/4	0.93	0.14	65,67,68,84	0
19	EDO	S	2204	4/4	0.94	0.17	50,66,66,68	0
15	MG	N	602	1/1	0.94	0.11	39,39,39,39	0
19	EDO	B	305	4/4	0.94	0.15	44,54,60,62	0
19	EDO	N	609	4/4	0.94	0.28	50,53,54,55	0
19	EDO	J	1101	4/4	0.95	0.23	52,61,64,68	0
19	EDO	N	615	4/4	0.95	0.14	55,68,73,83	0
24	PEK	C	303	53/53	0.95	0.22	37,62,93,113	0
19	EDO	F	704	4/4	0.95	0.18	61,61,69,71	0
19	EDO	N	618	4/4	0.96	0.16	54,56,62,64	0
17	PGV	A	605	51/51	0.96	0.20	28,48,85,90	0
17	PGV	C	305	51/51	0.96	0.20	32,43,94,101	0
19	EDO	A	620	4/4	0.96	0.18	45,47,52,52	0
17	PGV	N	605	51/51	0.96	0.21	34,49,85,93	0
19	EDO	D	202	4/4	0.96	0.28	62,72,77,81	0
16	NA	N	603	1/1	0.96	0.05	49,49,49,49	0
17	PGV	P	306	51/51	0.96	0.16	35,49,96,106	0
19	EDO	A	613	4/4	0.96	0.13	45,52,57,59	0
16	NA	A	603	1/1	0.96	0.09	35,35,35,35	0
19	EDO	A	616	4/4	0.96	0.12	54,66,68,68	0
19	EDO	N	614	4/4	0.96	0.28	41,45,46,47	0
19	EDO	E	202	4/4	0.96	0.17	51,52,52,54	0
19	EDO	E	203	4/4	0.96	0.20	51,52,57,59	0
15	MG	A	602	1/1	0.97	0.13	32,32,32,32	0
22	CHD	G	1305	29/29	0.97	0.07	35,39,43,46	0
19	EDO	F	705	4/4	0.97	0.21	34,36,37,37	0
22	CHD	P	303	29/29	0.97	0.08	35,40,44,46	0
19	EDO	D	203	4/4	0.97	0.18	61,66,75,83	0
19	EDO	N	619	4/4	0.97	0.12	51,60,68,77	0
19	EDO	Q	204	4/4	0.97	0.15	73,73,75,75	0

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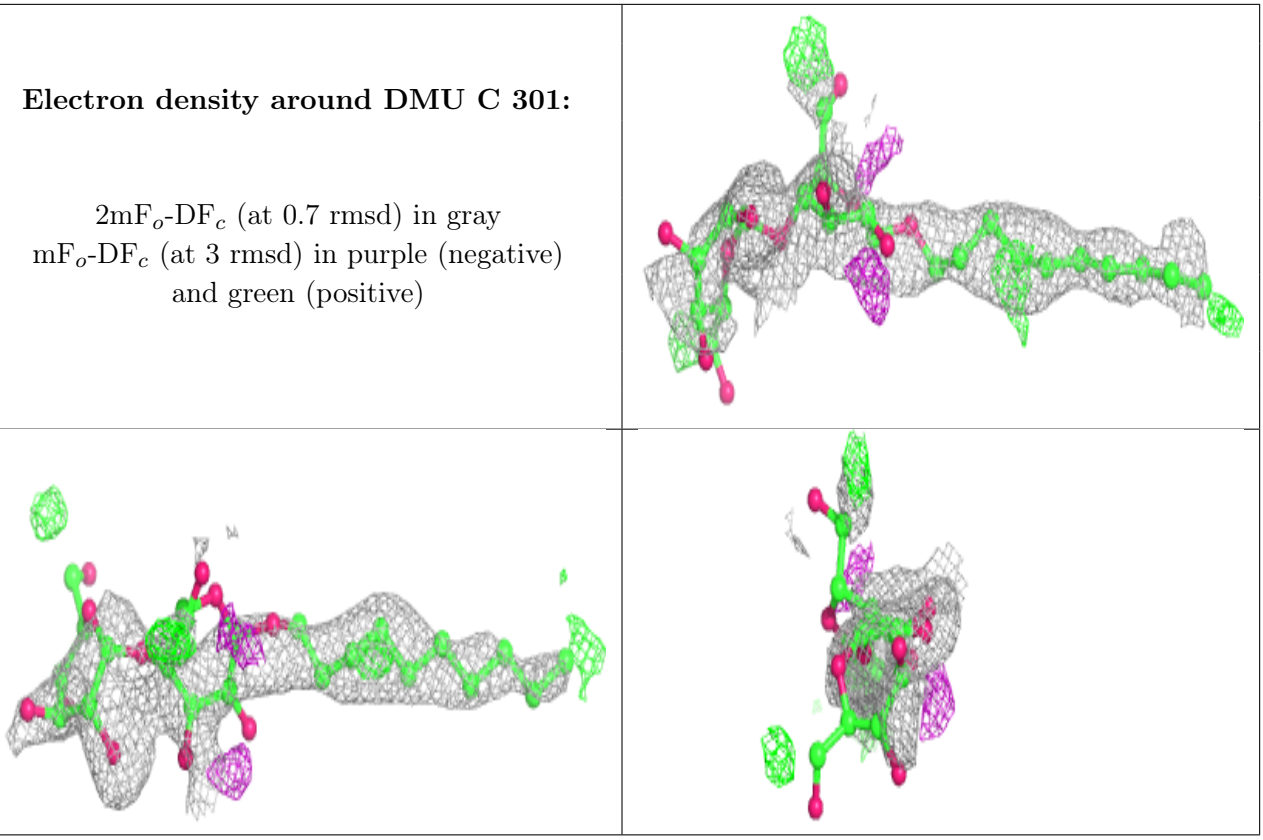
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	T	105	4/4	0.97	0.27	44,46,47,49	0
19	EDO	C	308	4/4	0.97	0.13	43,49,53,61	0
19	EDO	A	609	4/4	0.97	0.17	33,34,35,36	0
19	EDO	N	608	4/4	0.97	0.15	42,42,45,50	0
19	EDO	S	2203	4/4	0.97	0.12	35,36,37,40	0
22	CHD	B	302	29/29	0.97	0.07	33,37,43,46	0
22	CHD	C	302	29/29	0.97	0.08	35,38,41,42	0
19	EDO	F	701	4/4	0.98	0.18	46,48,50,55	0
18	HEA	A	606	60/60	0.98	0.15	24,29,37,43	0
18	HEA	N	606	60/60	0.98	0.15	27,34,43,49	0
19	EDO	O	304	4/4	0.98	0.11	44,45,48,50	0
19	EDO	B	303	4/4	0.98	0.11	32,33,34,37	0
19	EDO	G	1301	4/4	0.98	0.15	39,40,49,51	0
19	EDO	A	617	4/4	0.98	0.26	56,61,62,69	0
18	HEA	N	607	60/60	0.98	0.16	31,36,53,61	0
27	ZN	F	703	1/1	0.99	0.06	38,38,38,38	0
27	ZN	S	2202	1/1	0.99	0.06	42,42,42,42	0
18	HEA	A	607	60/60	0.99	0.15	24,29,48,55	0
21	CUA	O	301	2/2	0.99	0.06	37,37,37,38	0
14	CU	N	601	1/1	1.00	0.13	35,35,35,35	0
14	CU	A	601	1/1	1.00	0.12	29,29,29,29	0
21	CUA	B	301	2/2	1.00	0.08	30,30,30,30	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.

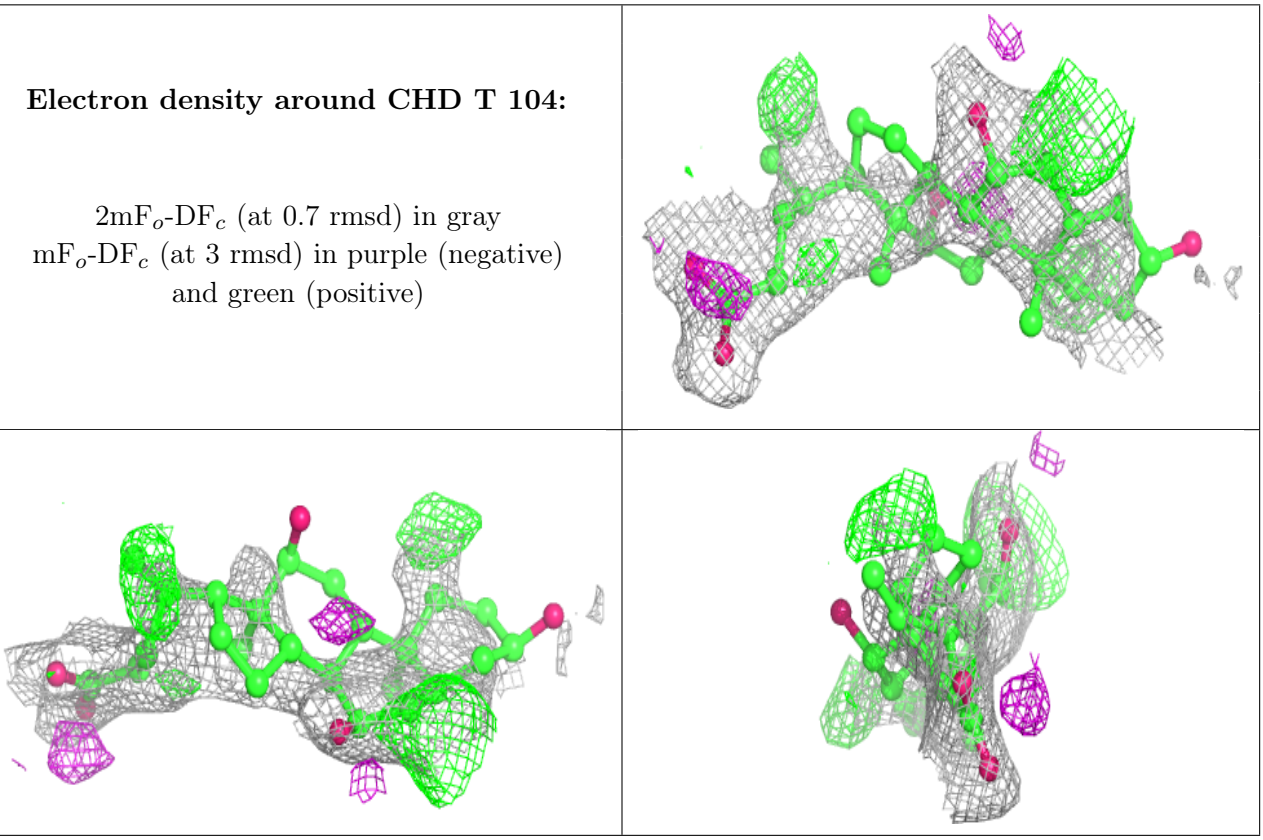
Electron density around DMU C 301:

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



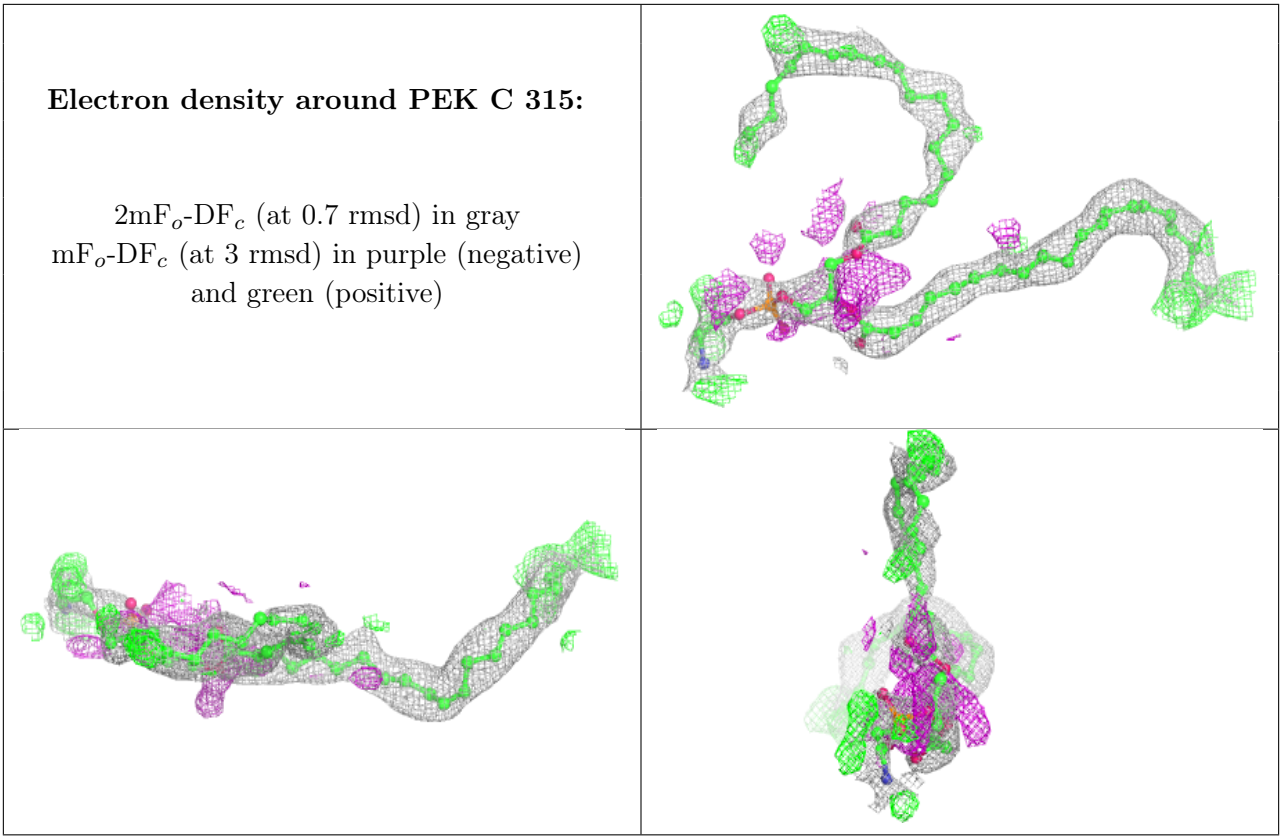
Electron density around CHD T 104:

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



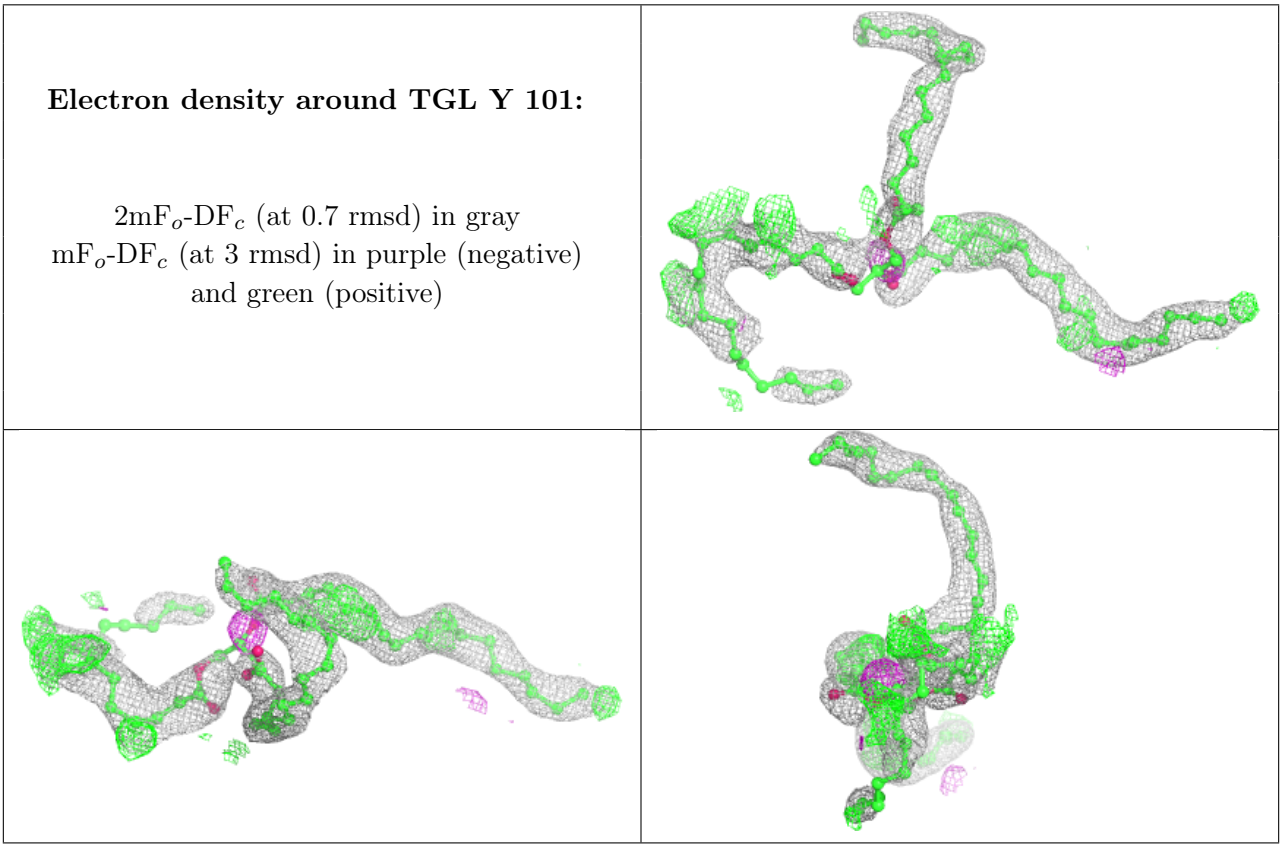
Electron density around PEK C 315:

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



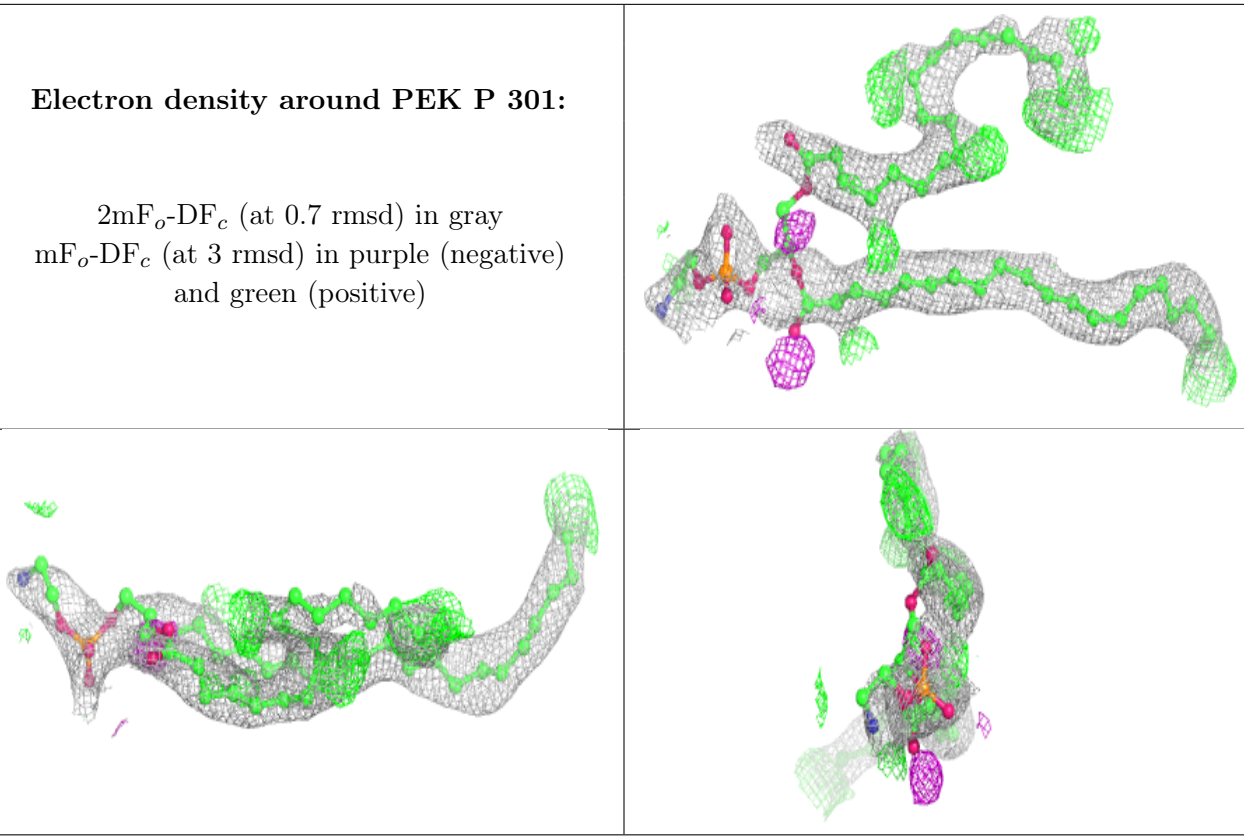
Electron density around TGL Y 101:

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



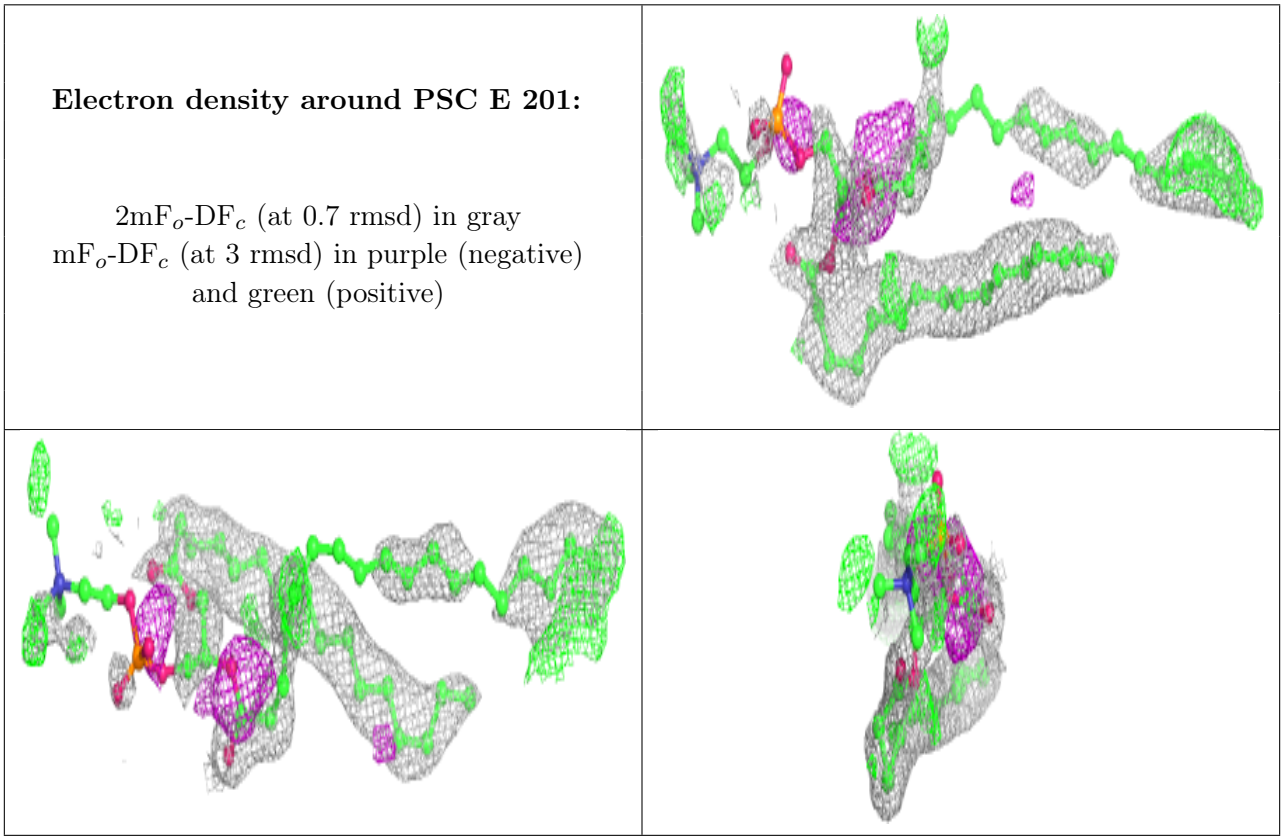
Electron density around PEK P 301:

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



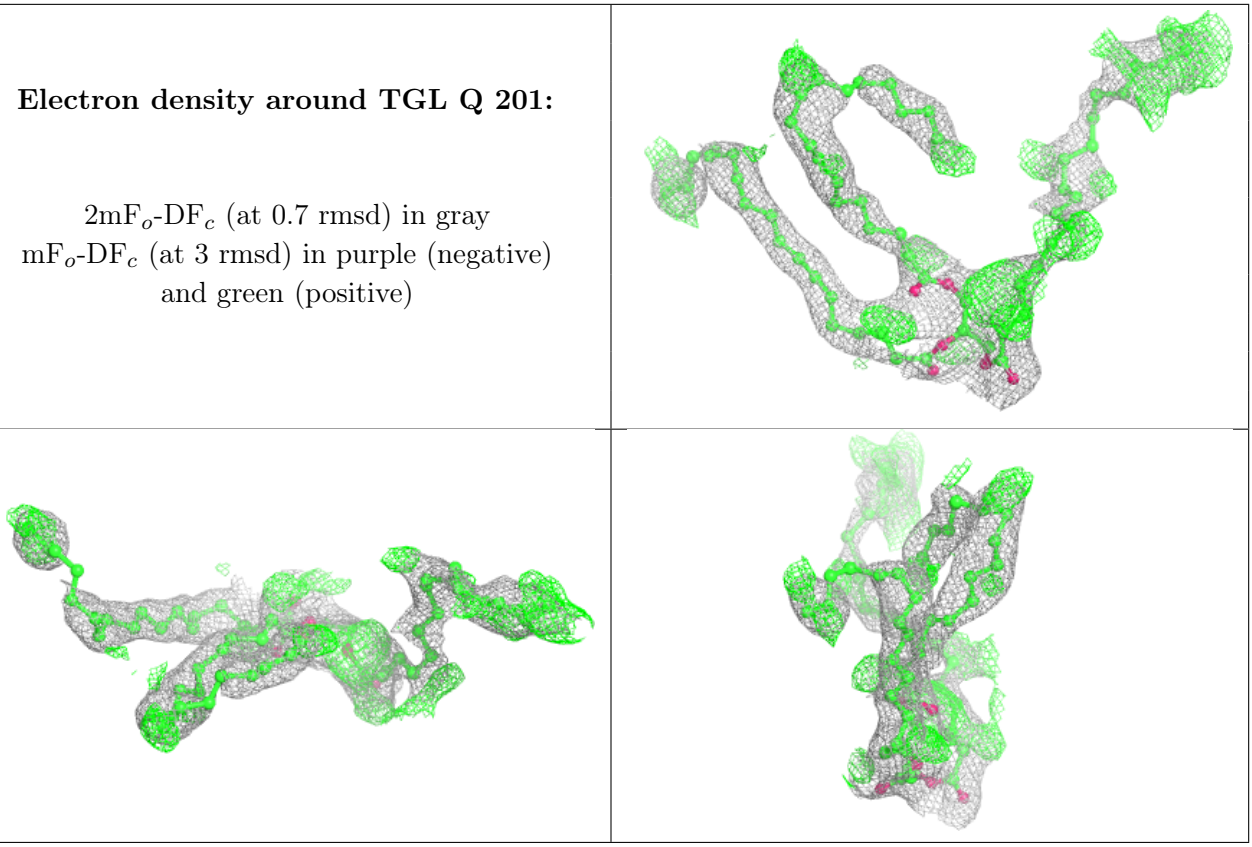
Electron density around PSC E 201:

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



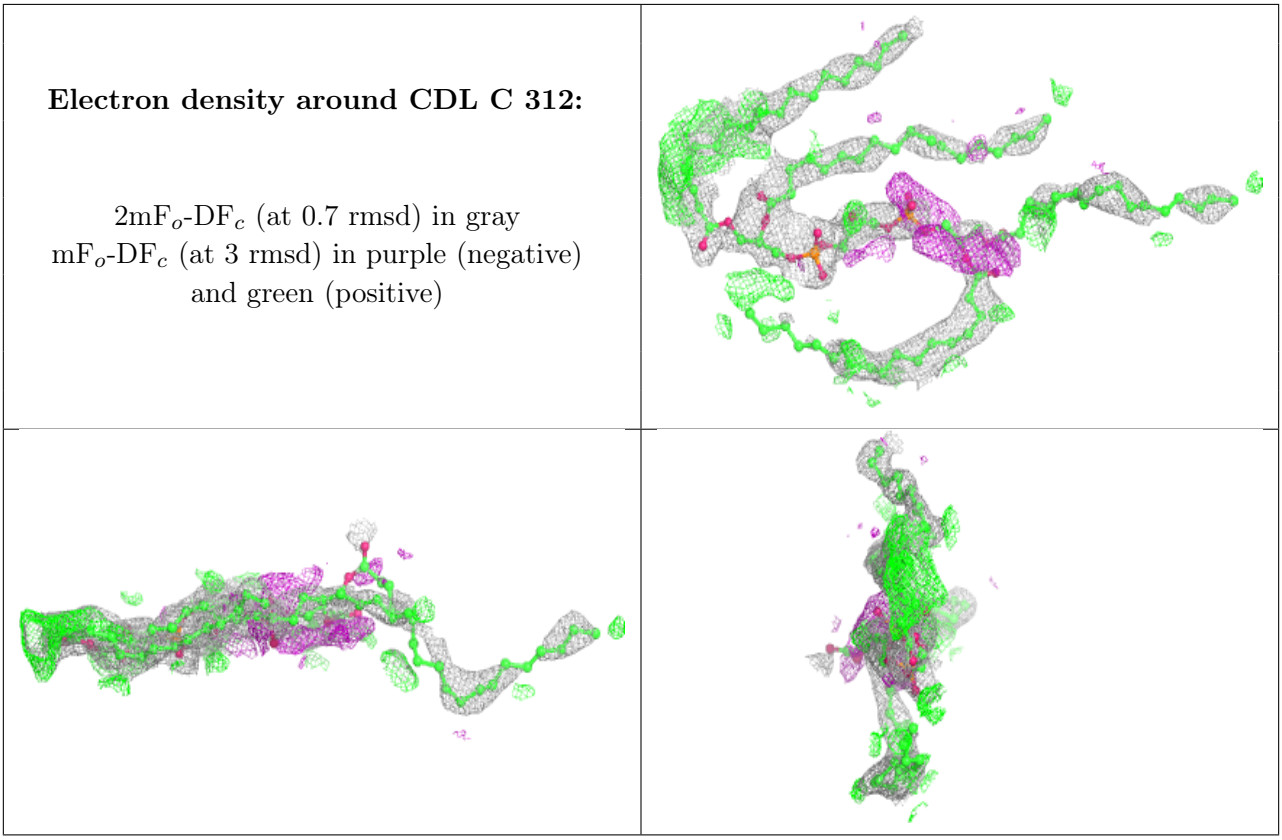
Electron density around TGL Q 201:

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



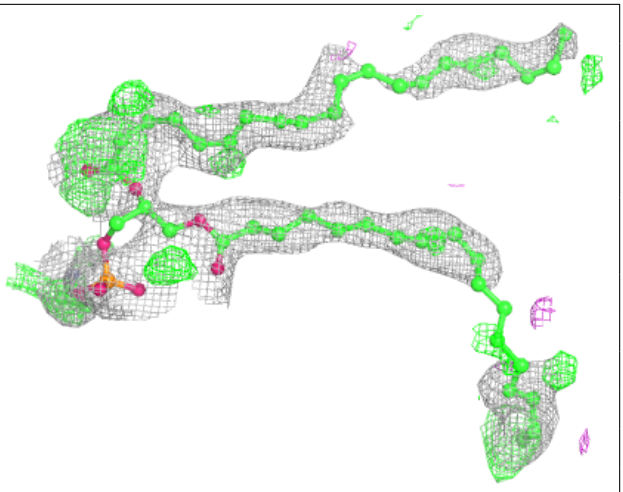
Electron density around CDL C 312:

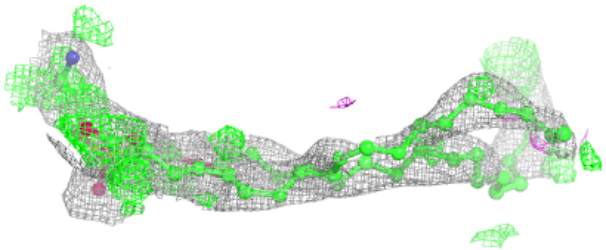
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

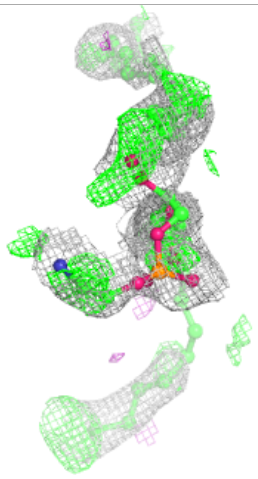


Electron density around PEK P 305:

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

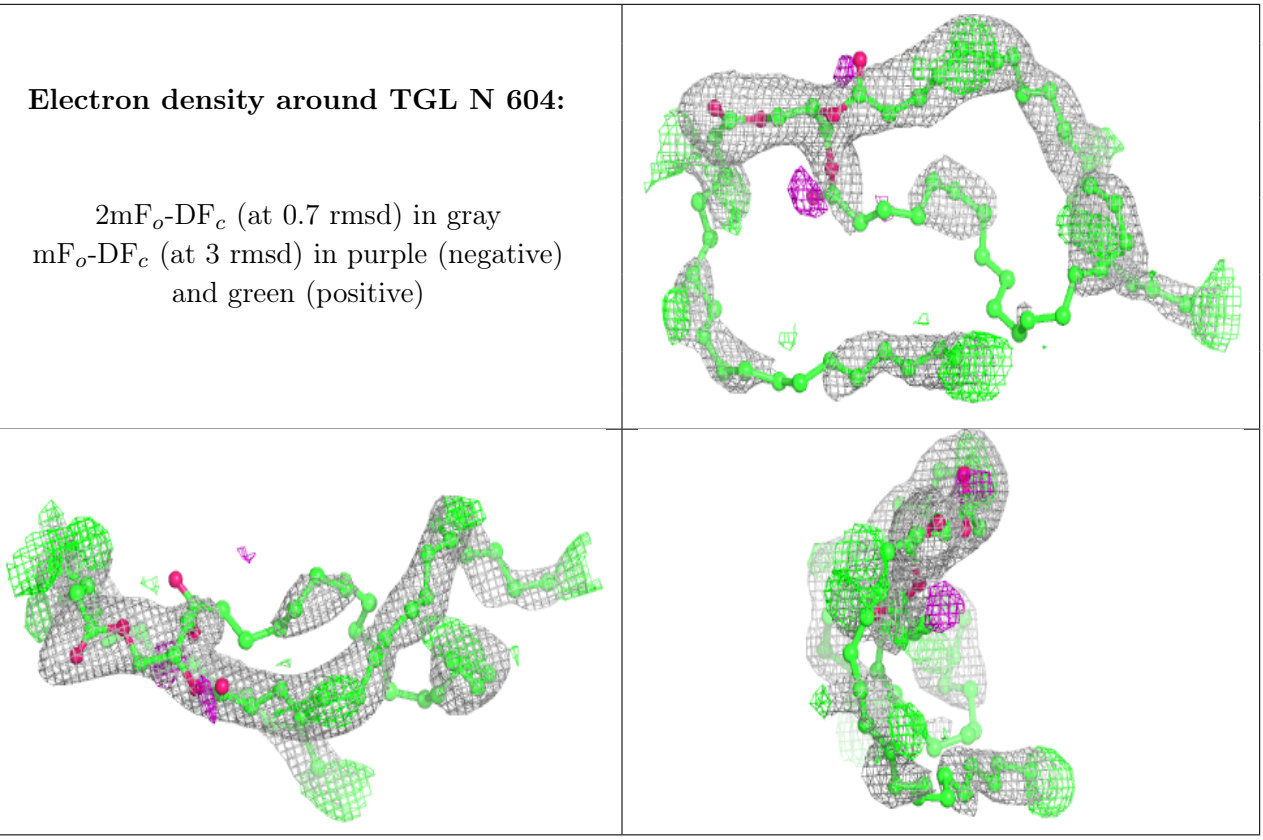






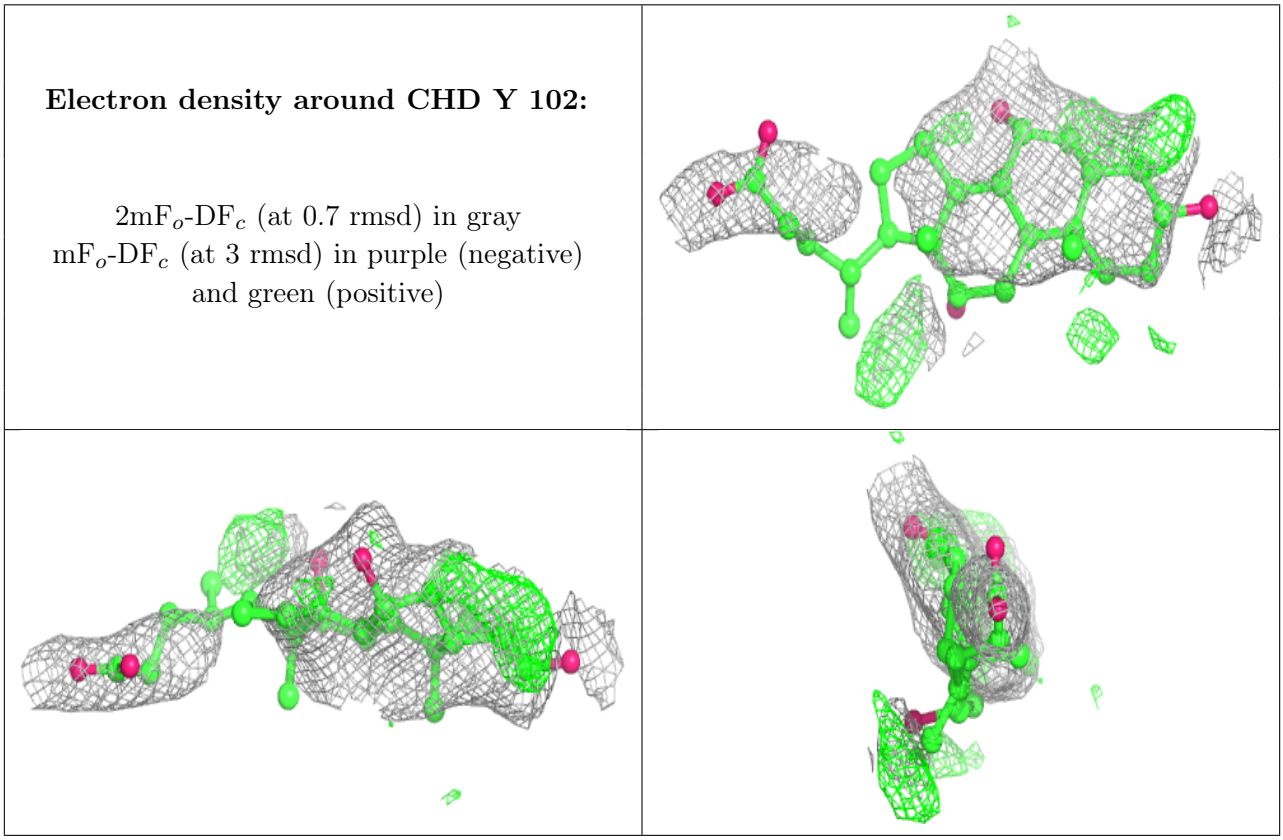
Electron density around TGL N 604:

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



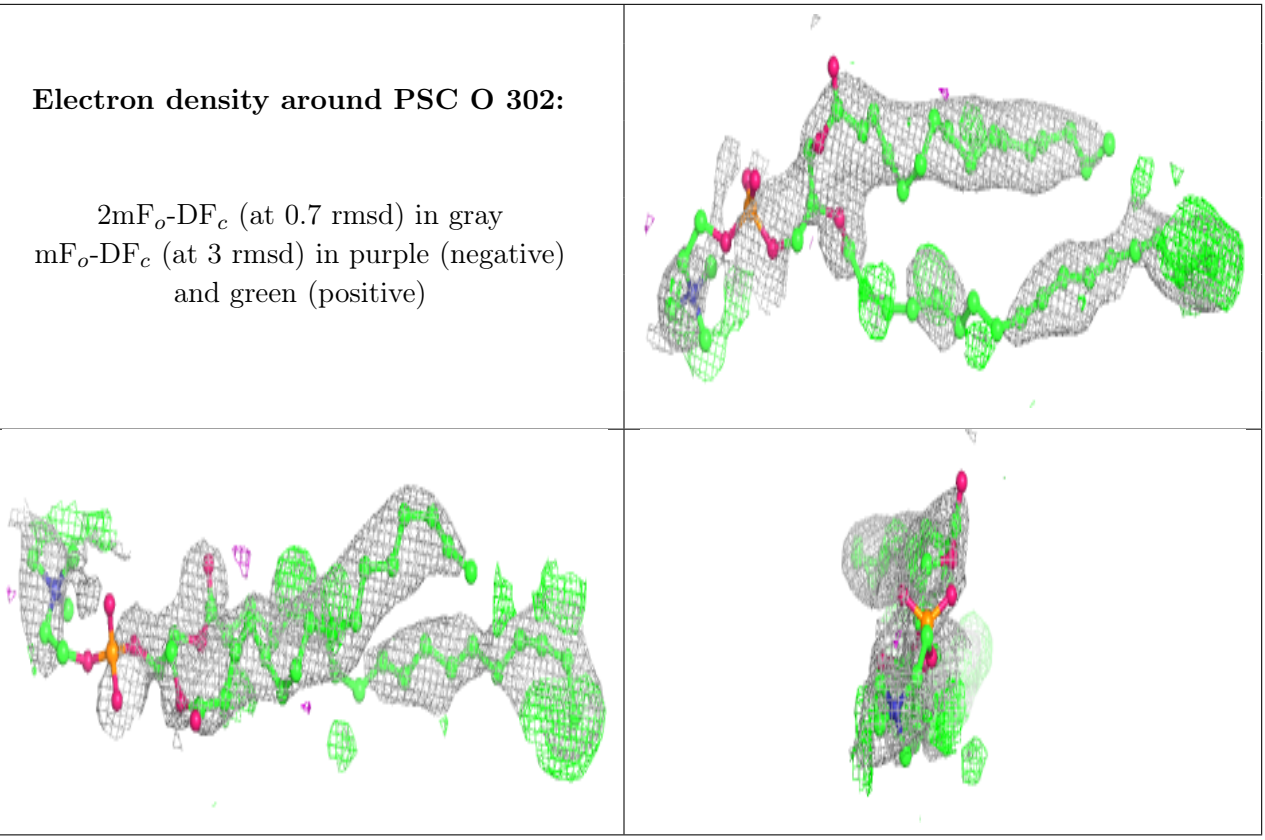
Electron density around CHD Y 102:

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



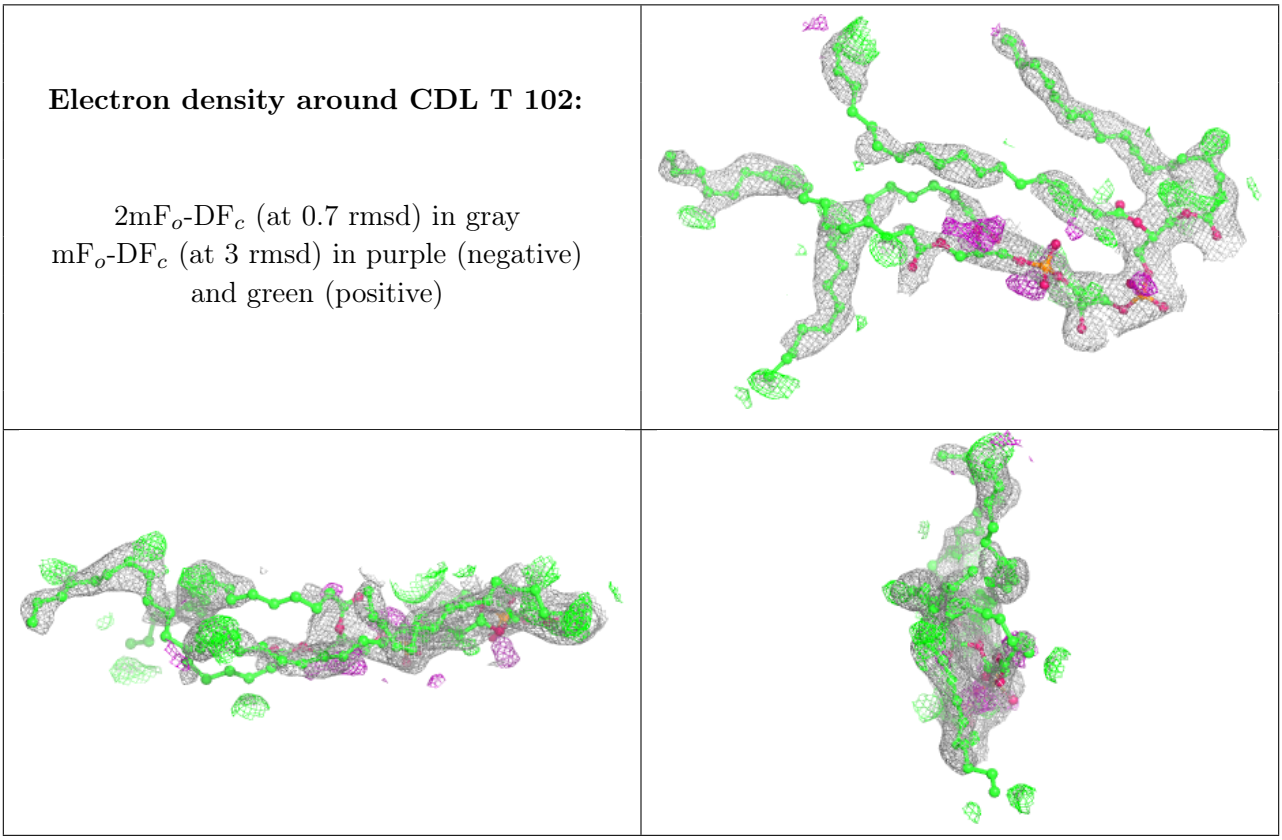
Electron density around PSC O 302:

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



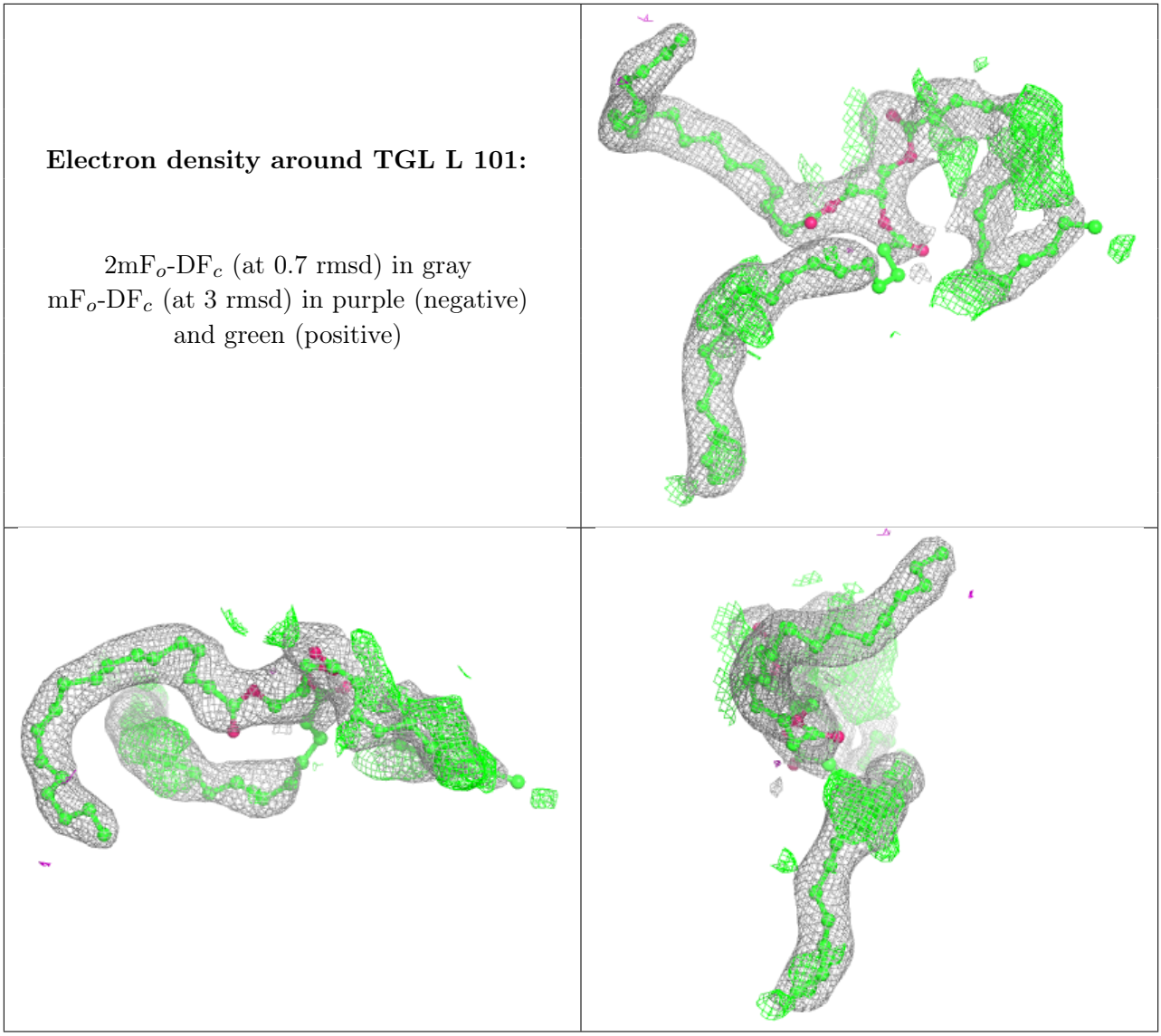
Electron density around CDL T 102:

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



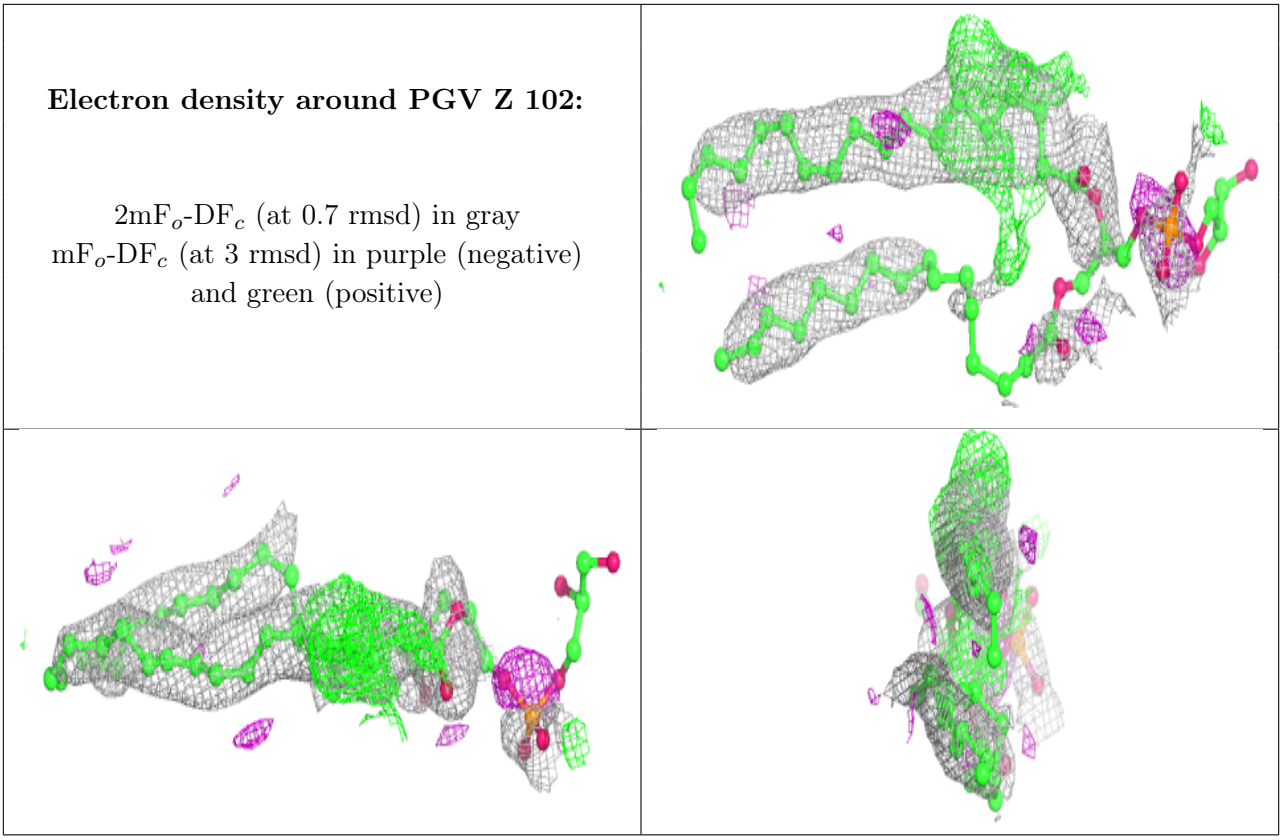
Electron density around TGL L 101:

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



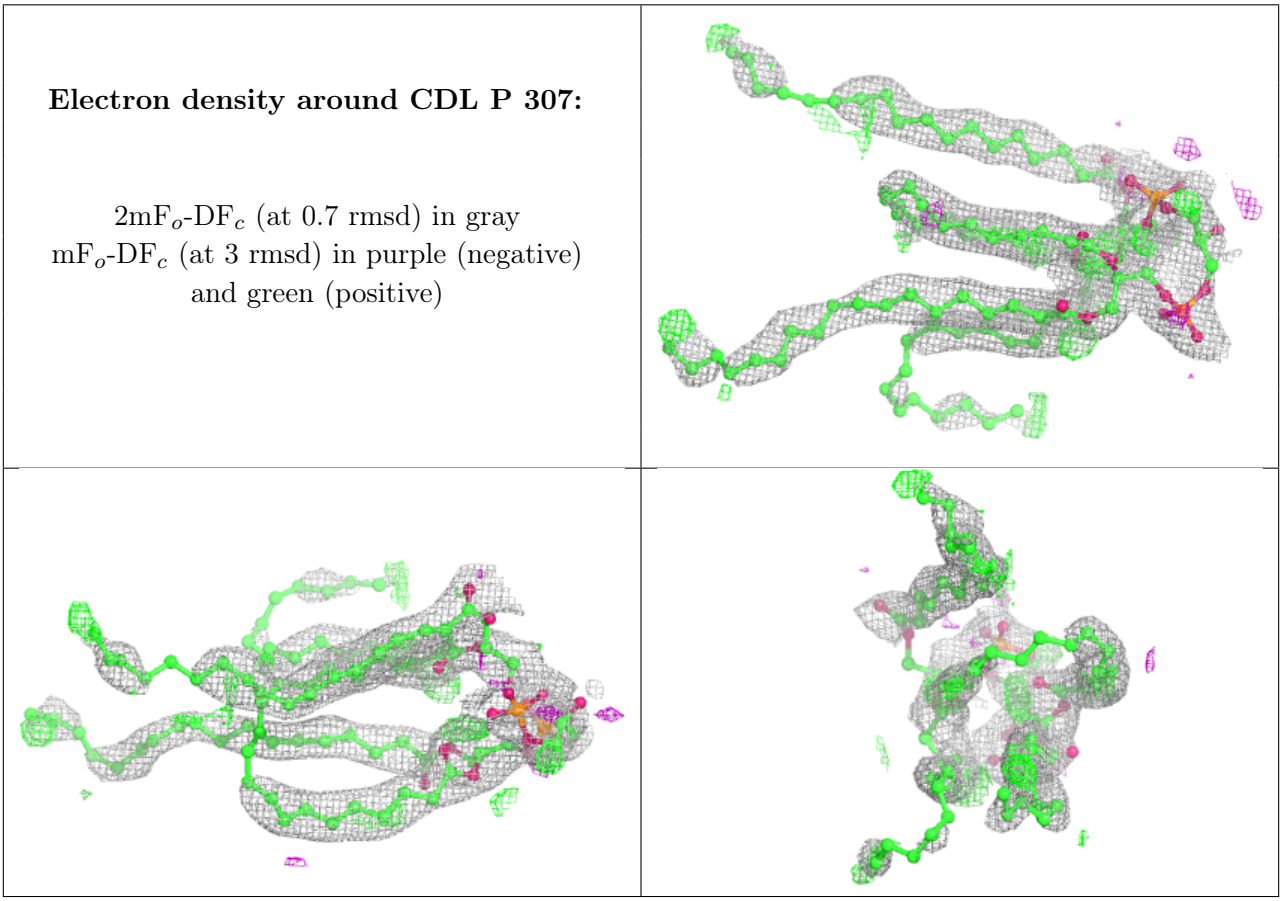
Electron density around PGV Z 102:

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



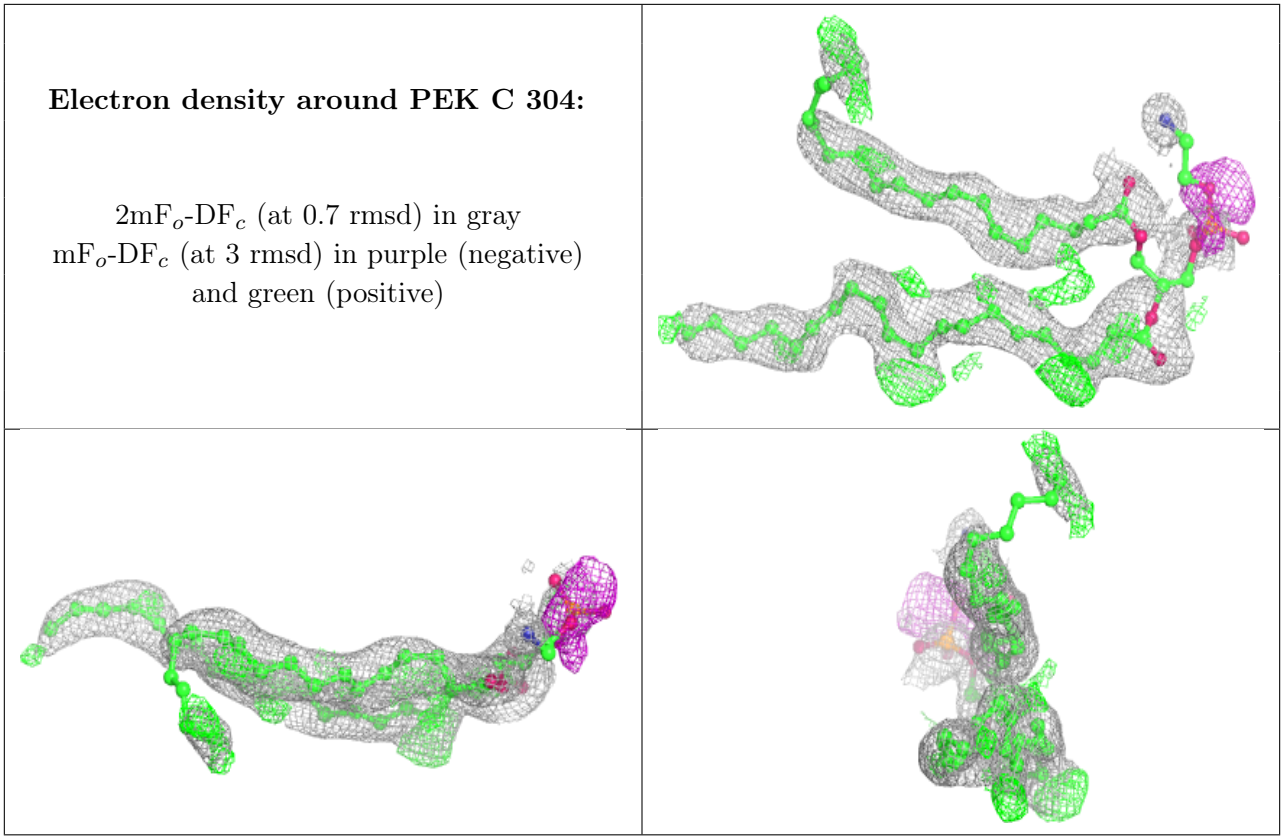
Electron density around CDL P 307:

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



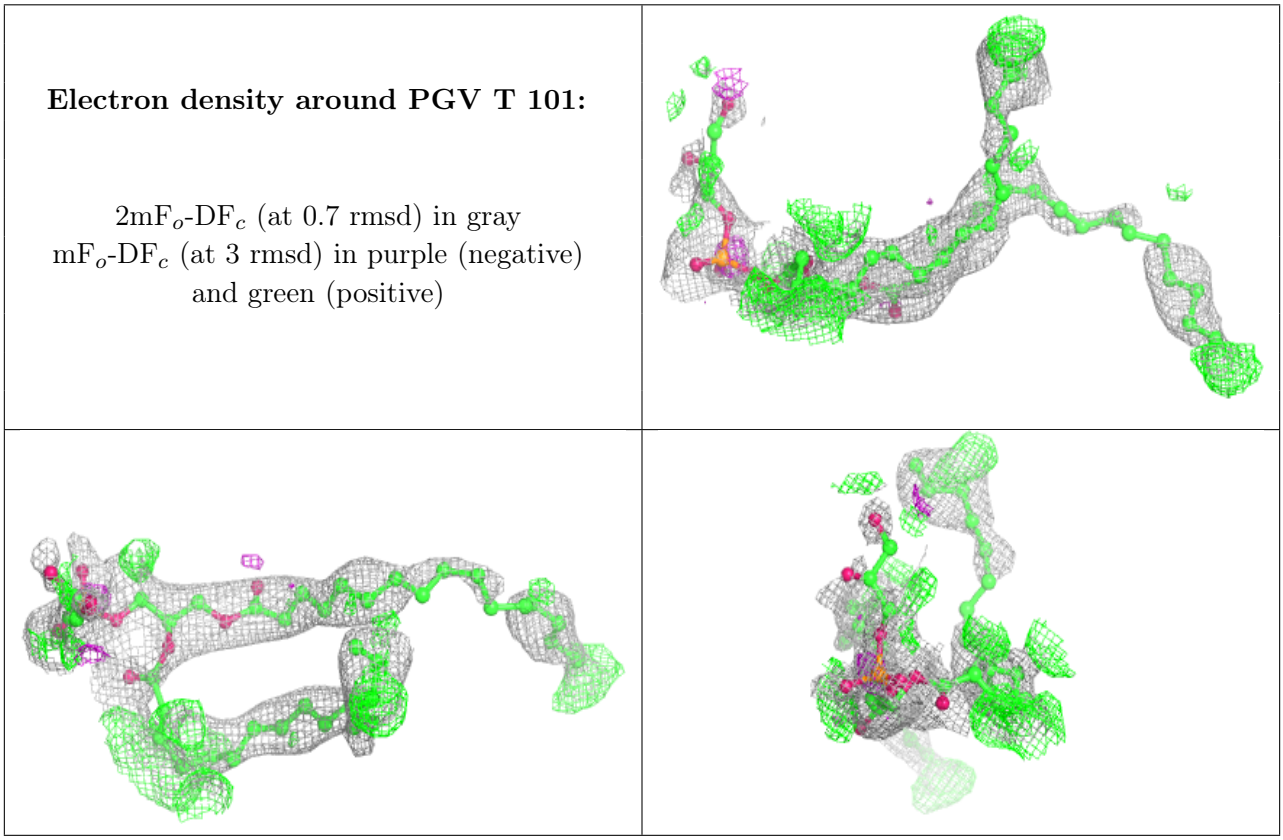
Electron density around PEK C 304:

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



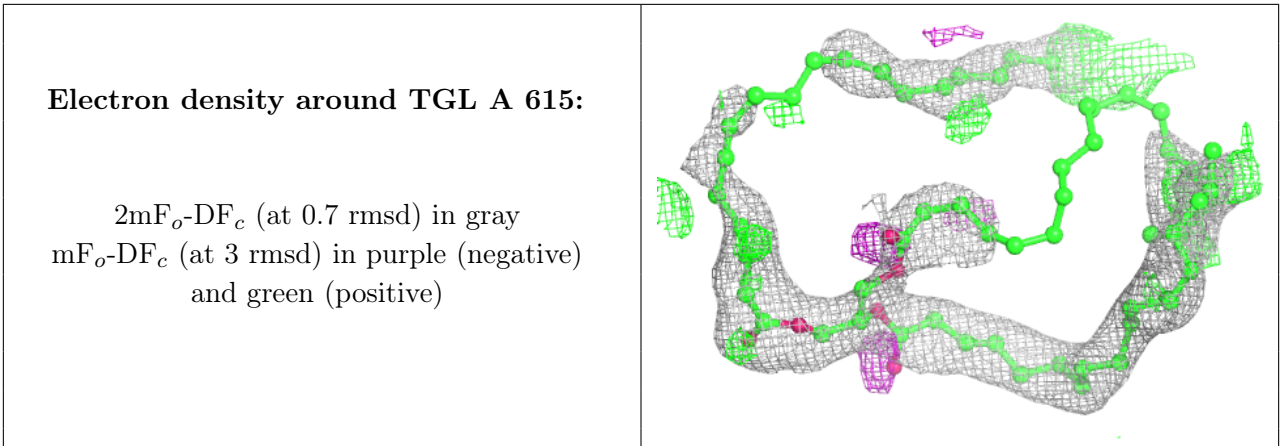
Electron density around PGV T 101:

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



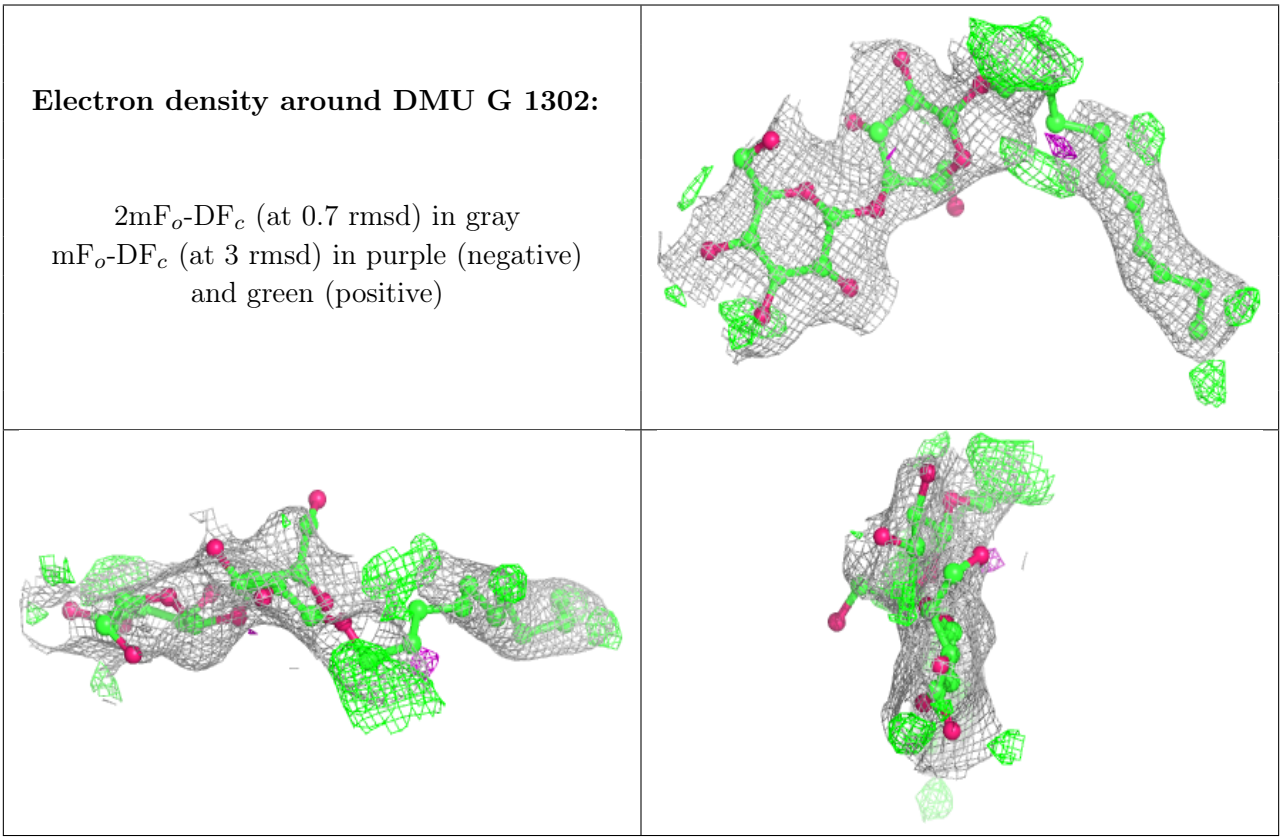
Electron density around TGL A 615:

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



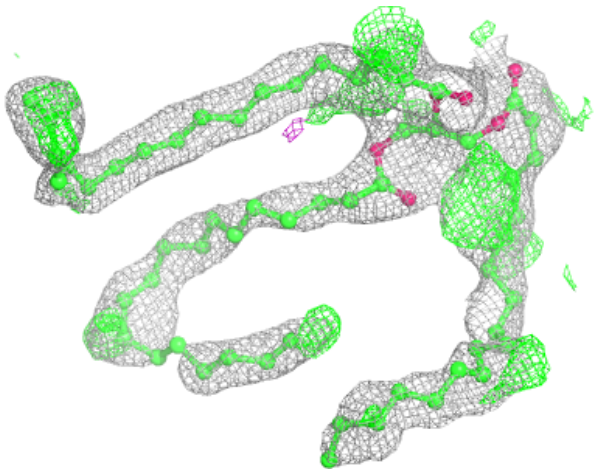
Electron density around DMU G 1302:

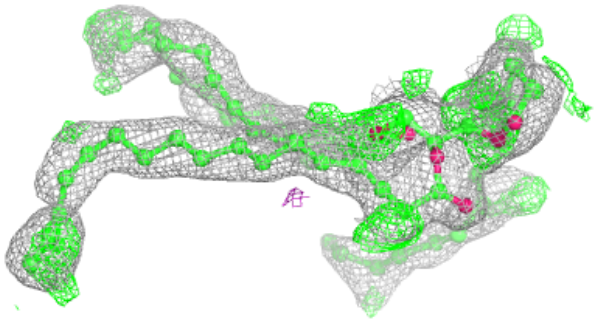
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

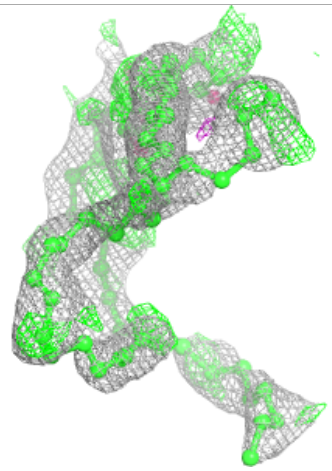


Electron density around TGL D 201:

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

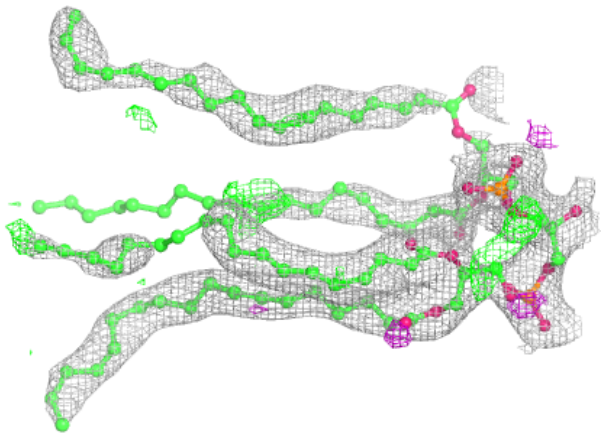


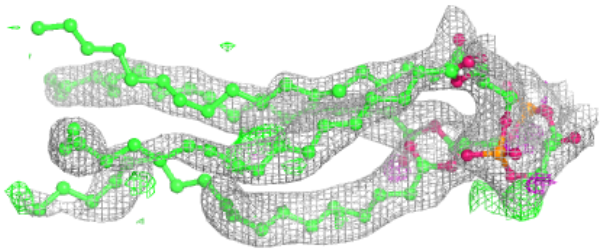


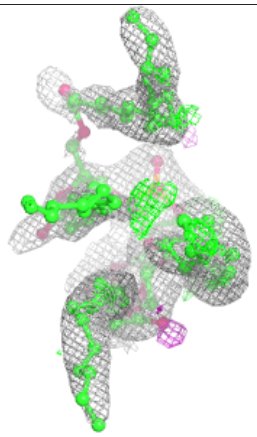


Electron density around CDL C 306:

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

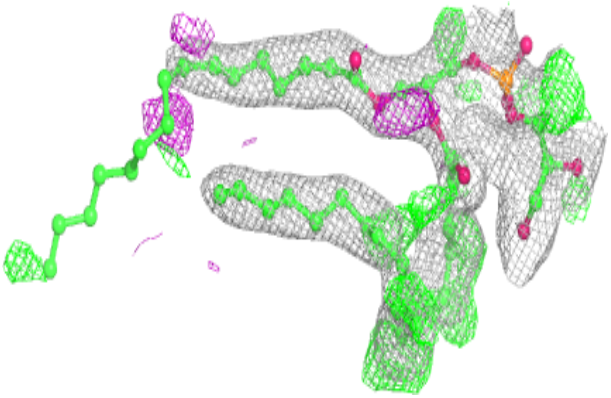


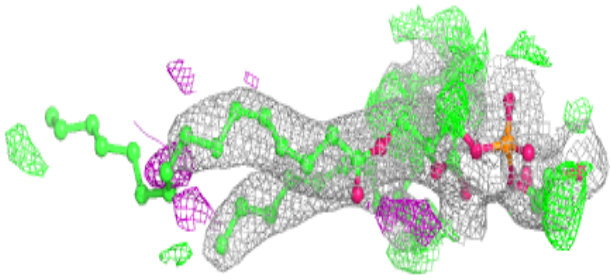


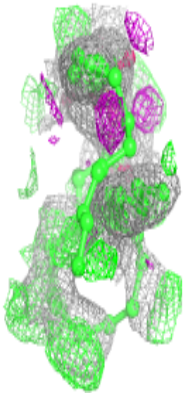


Electron density around PGV A 604:

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

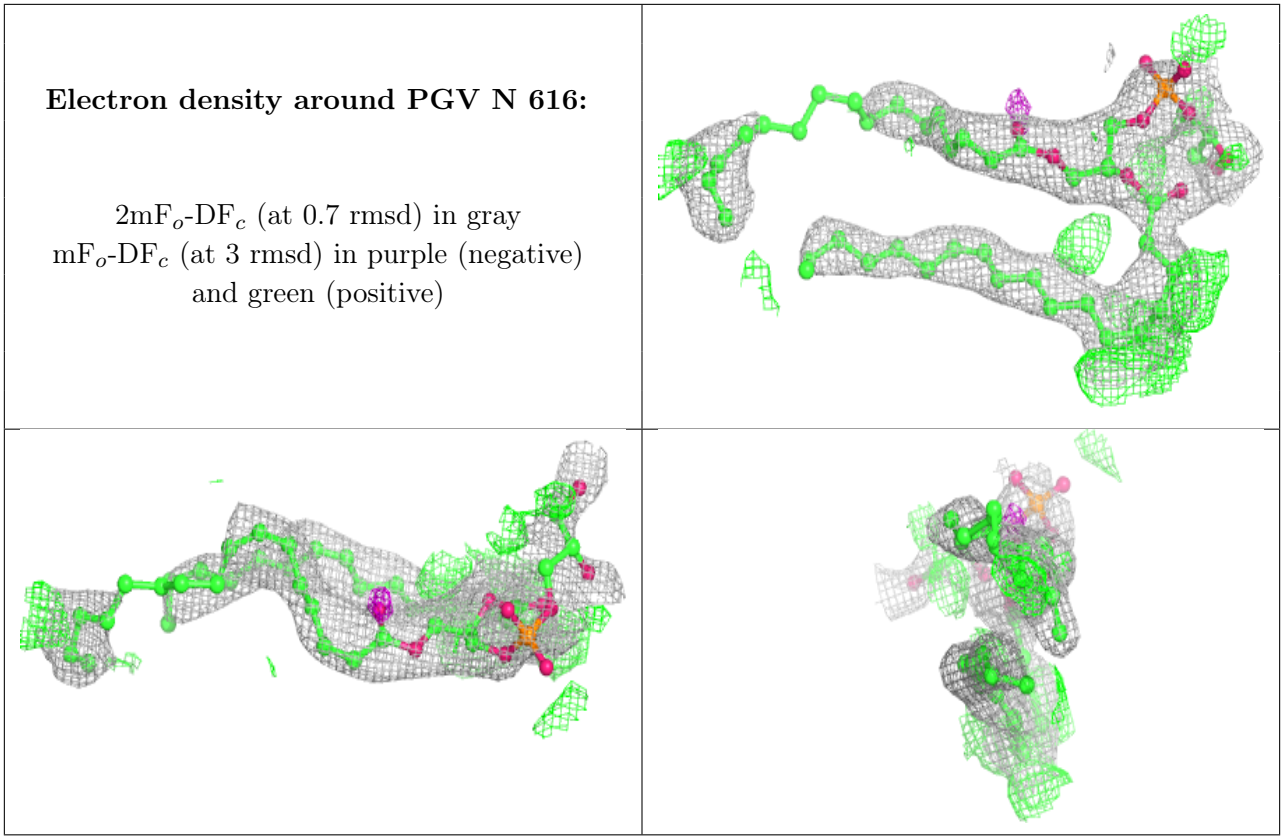






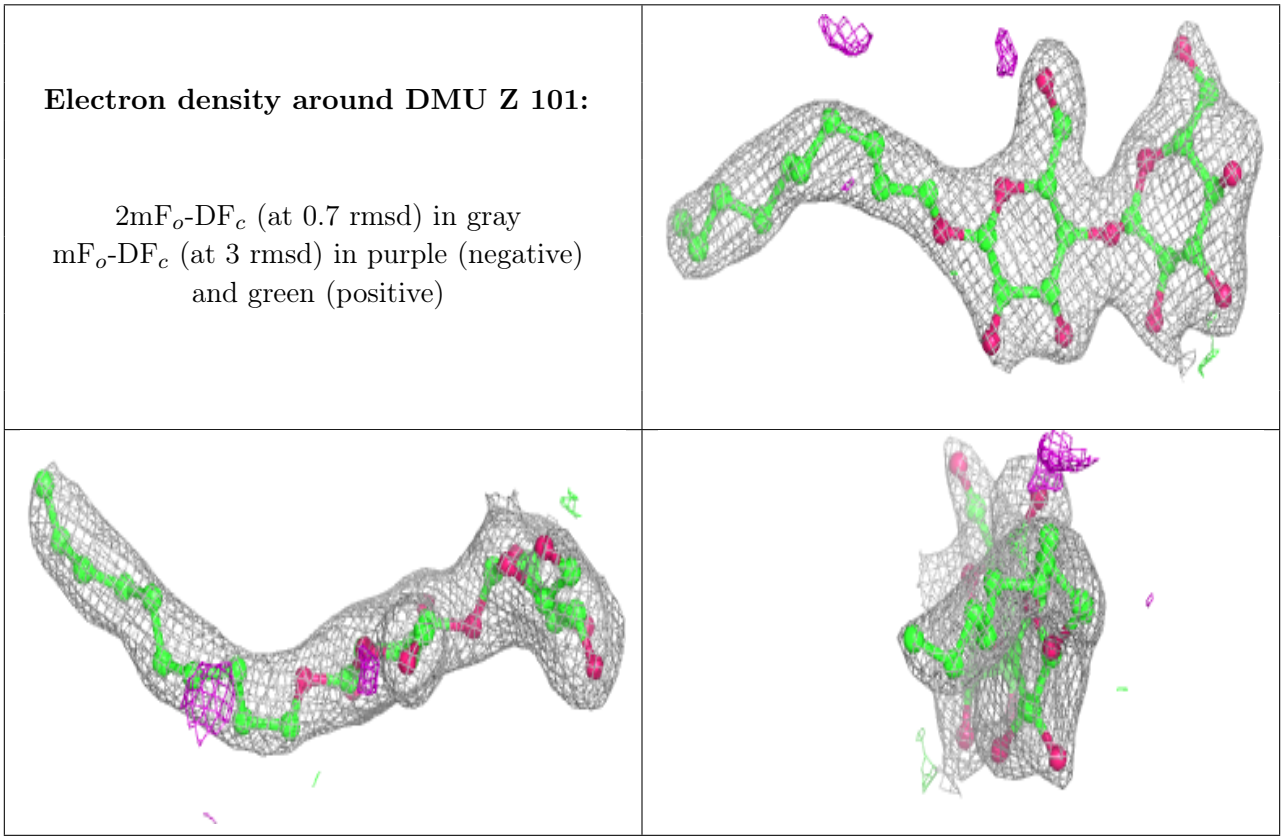
Electron density around PGV N 616:

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



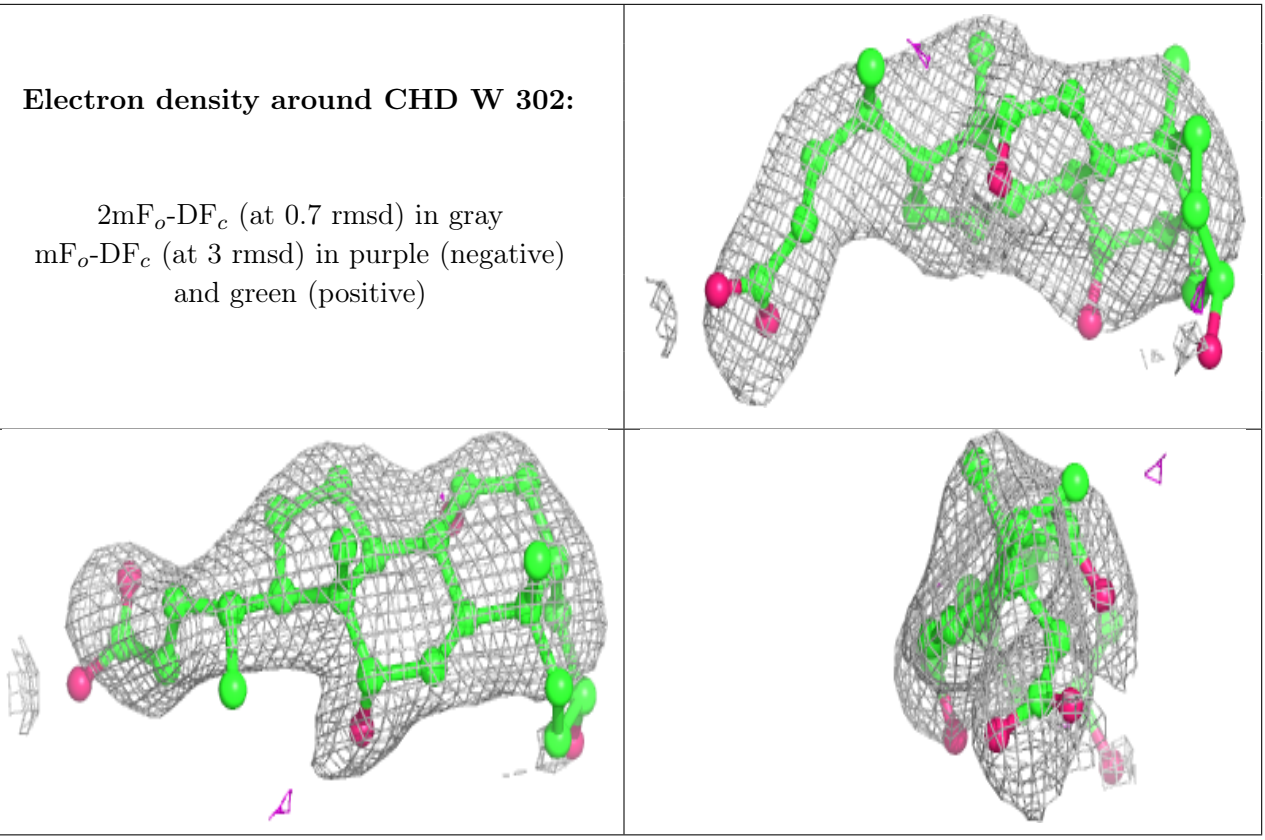
Electron density around DMU Z 101:

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



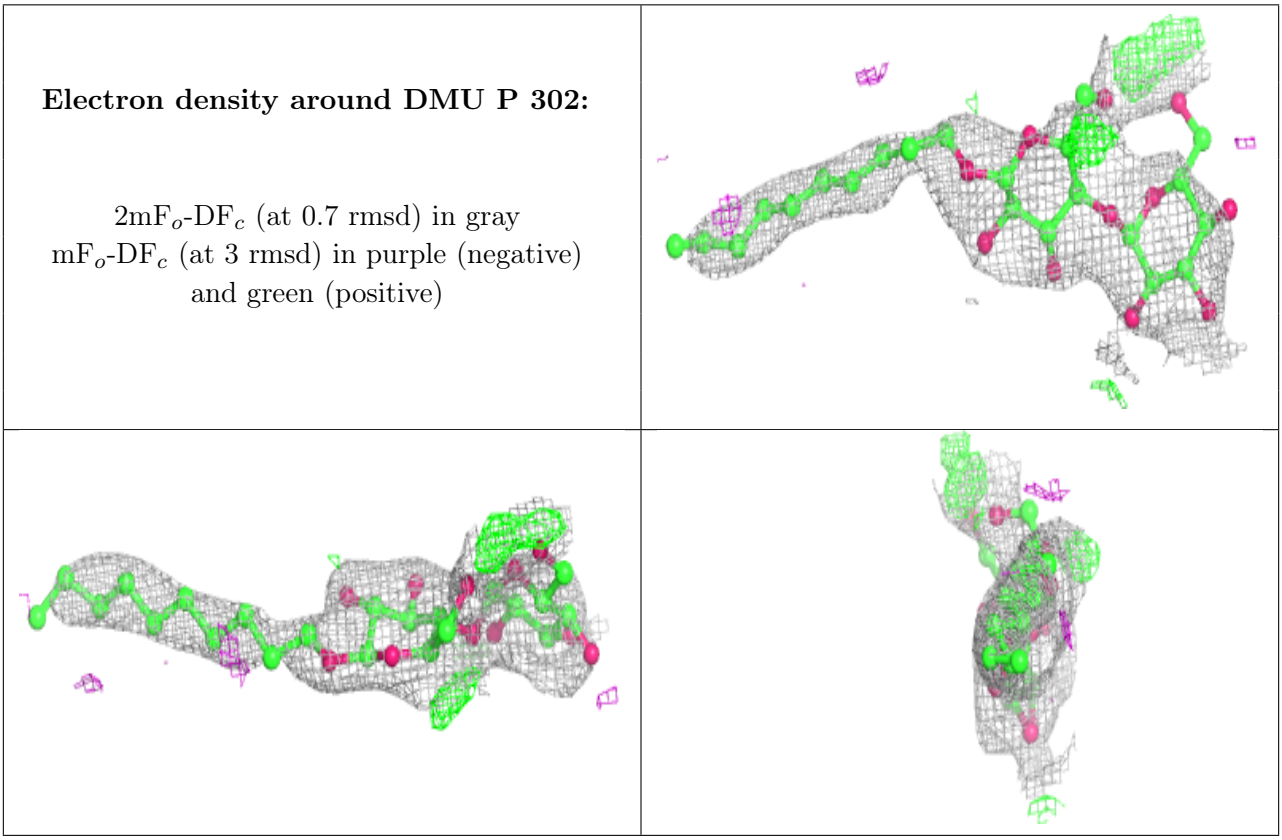
Electron density around CHD W 302:

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



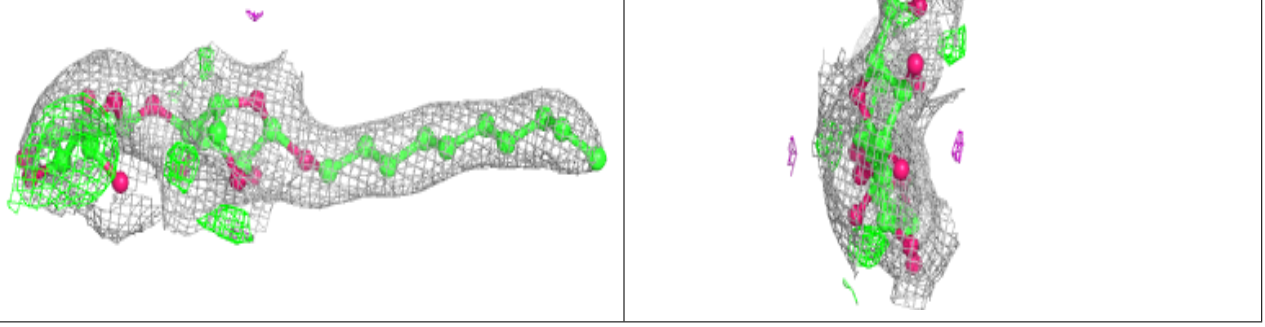
Electron density around DMU P 302:

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



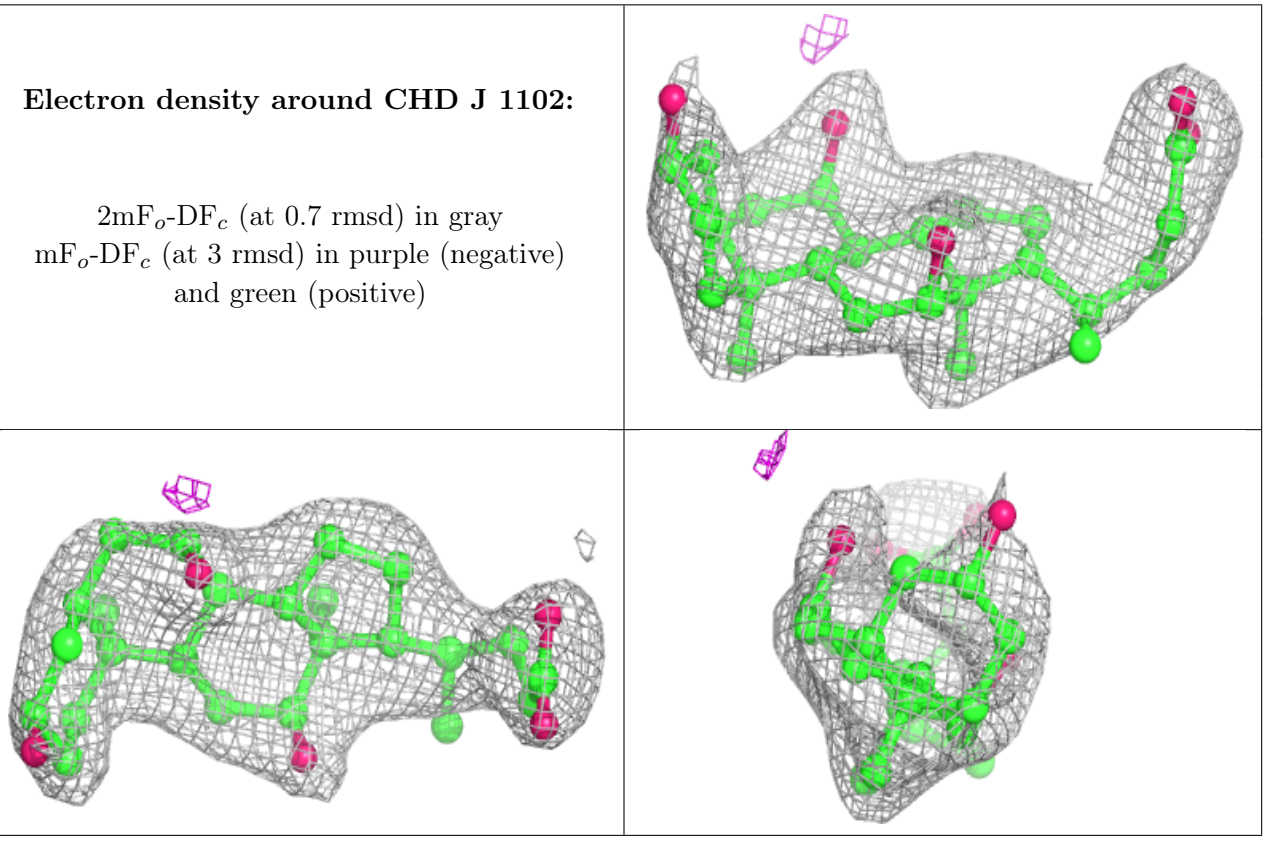
Electron density around DMU C 313:

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



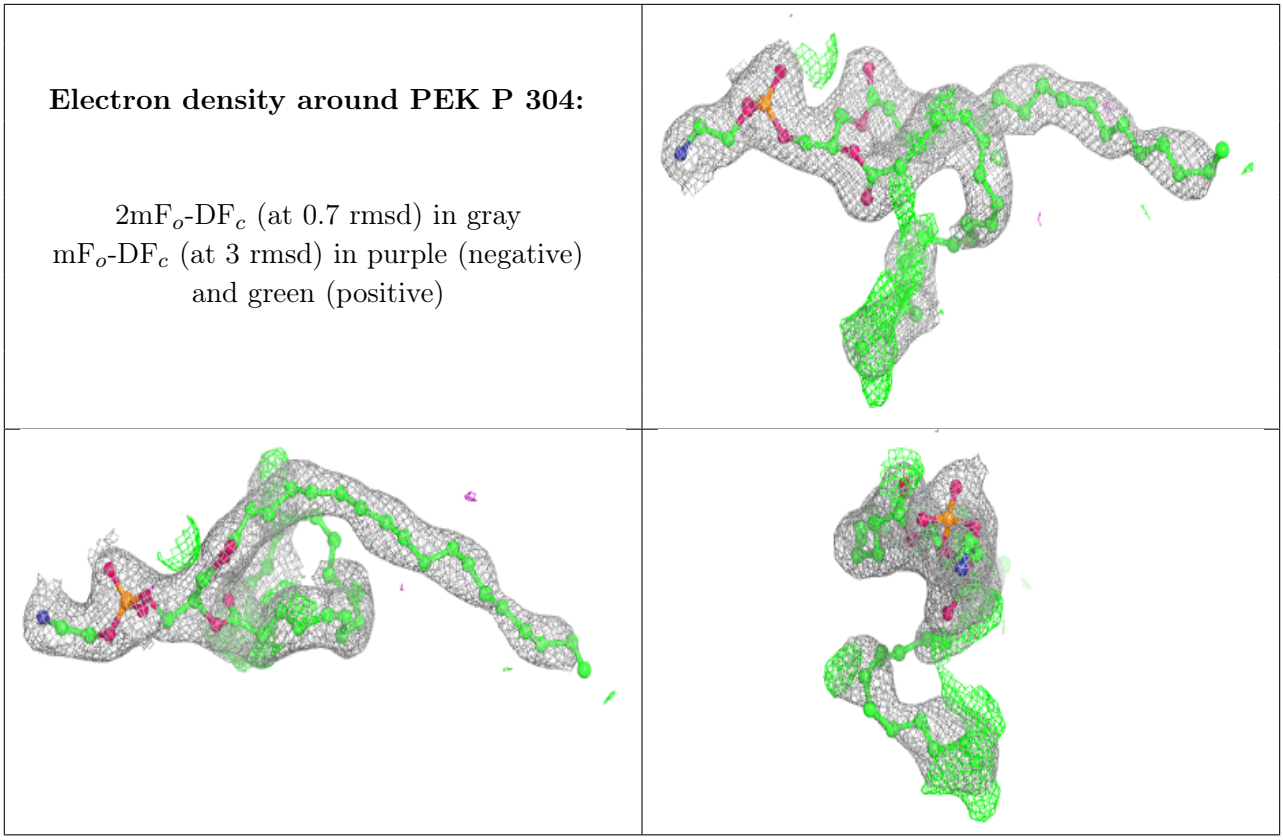
Electron density around CHD J 1102:

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



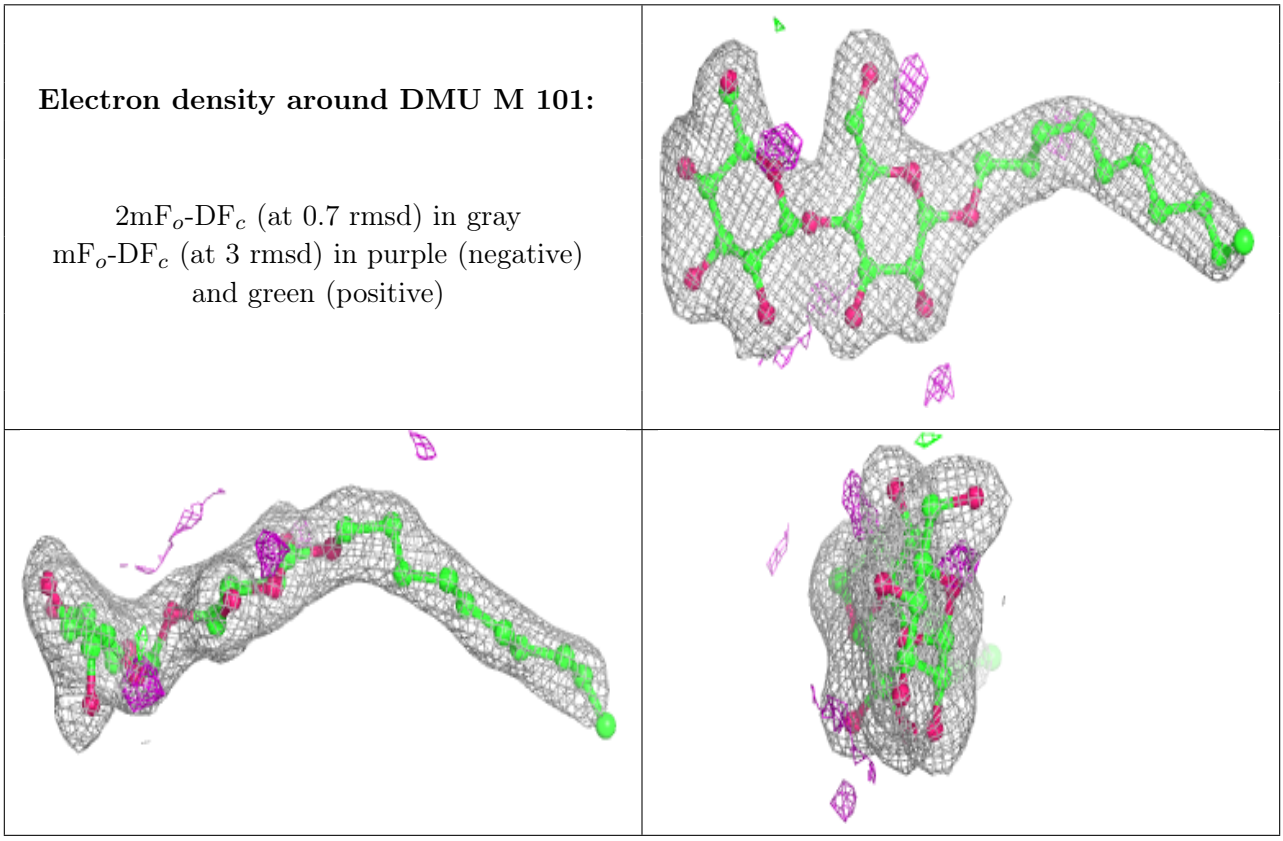
Electron density around PEK P 304:

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



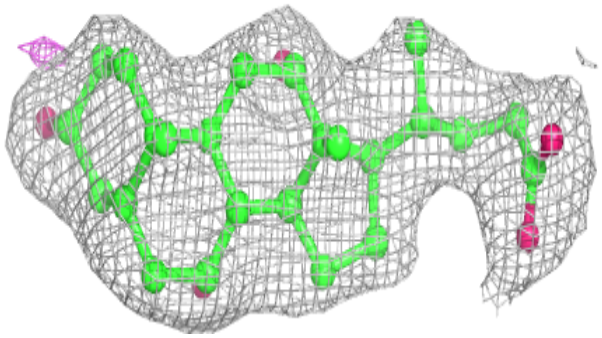
Electron density around DMU M 101:

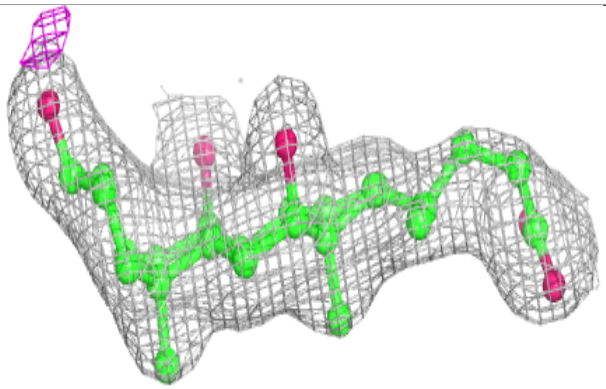
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

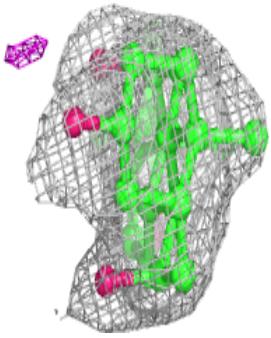


Electron density around CHD C 307:

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

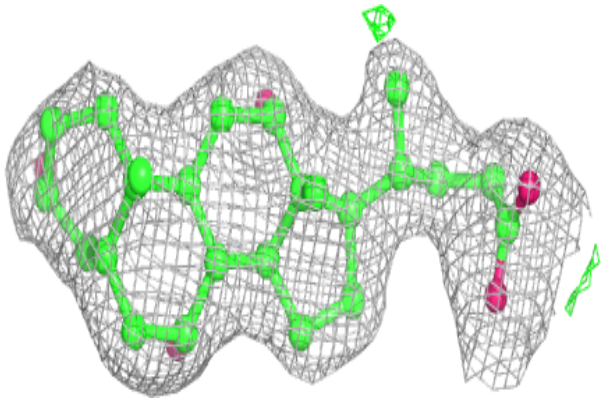


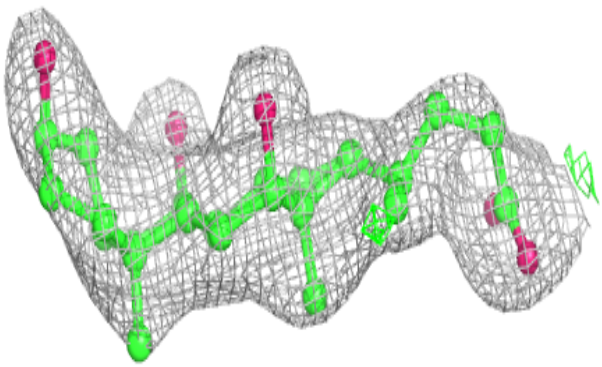


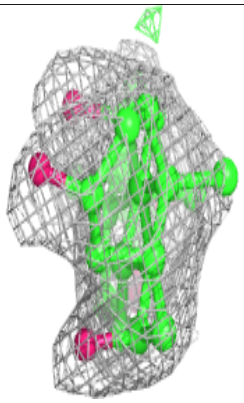


Electron density around CHD P 308:

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

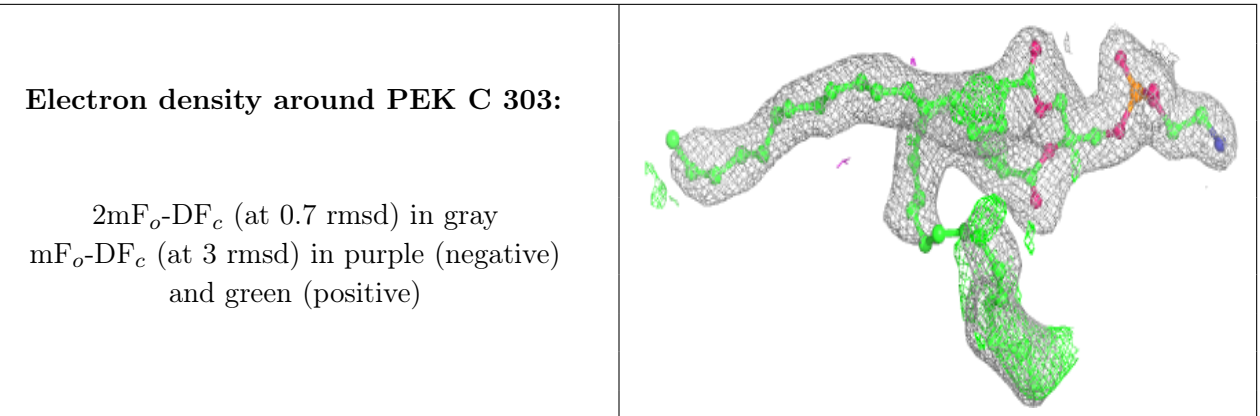


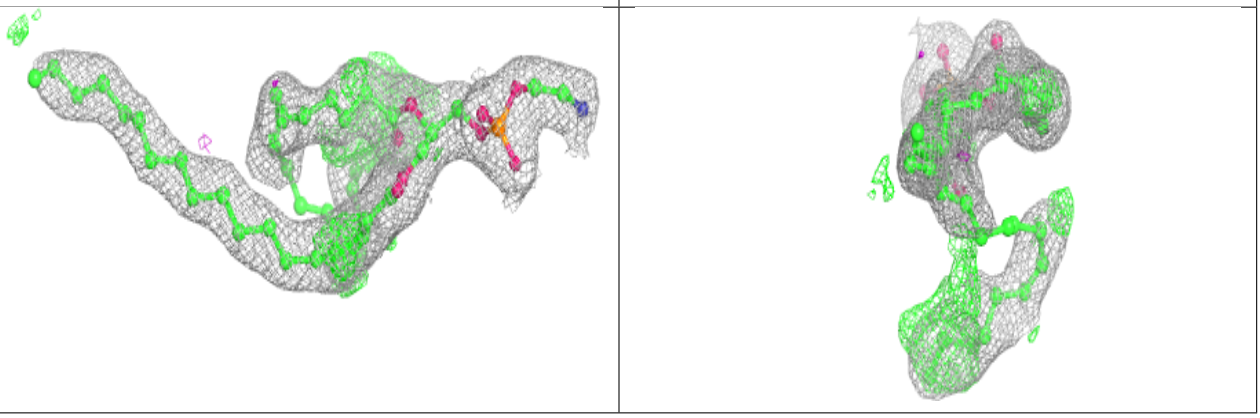




Electron density around PEK C 303:

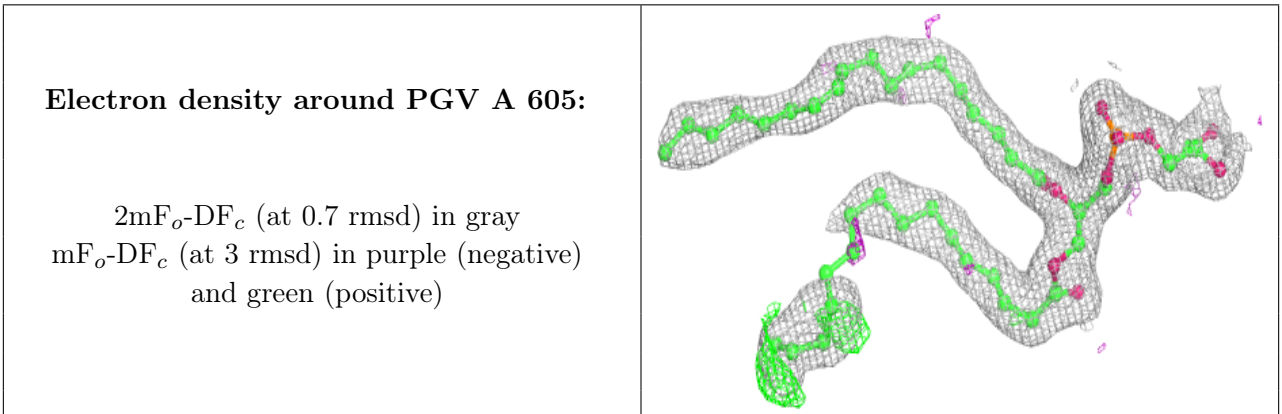
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

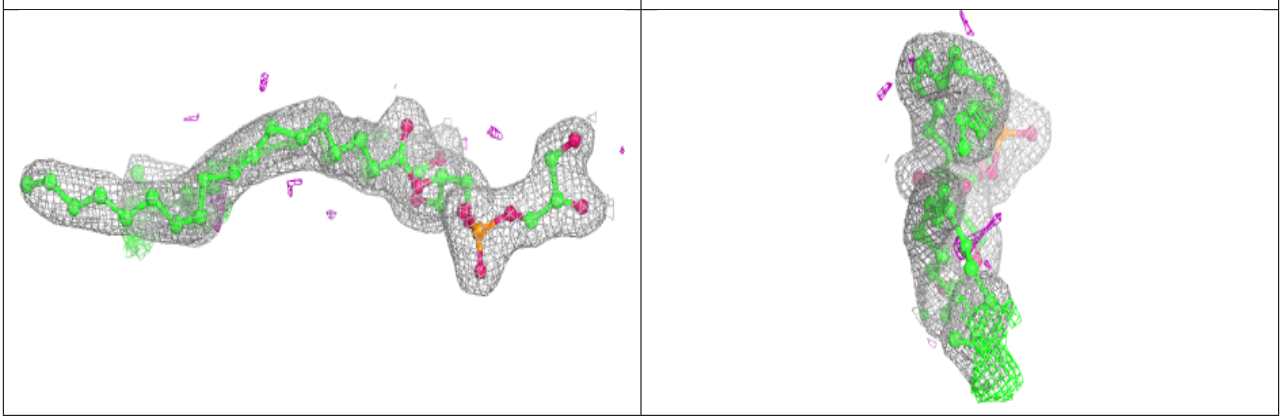




Electron density around PGV A 605:

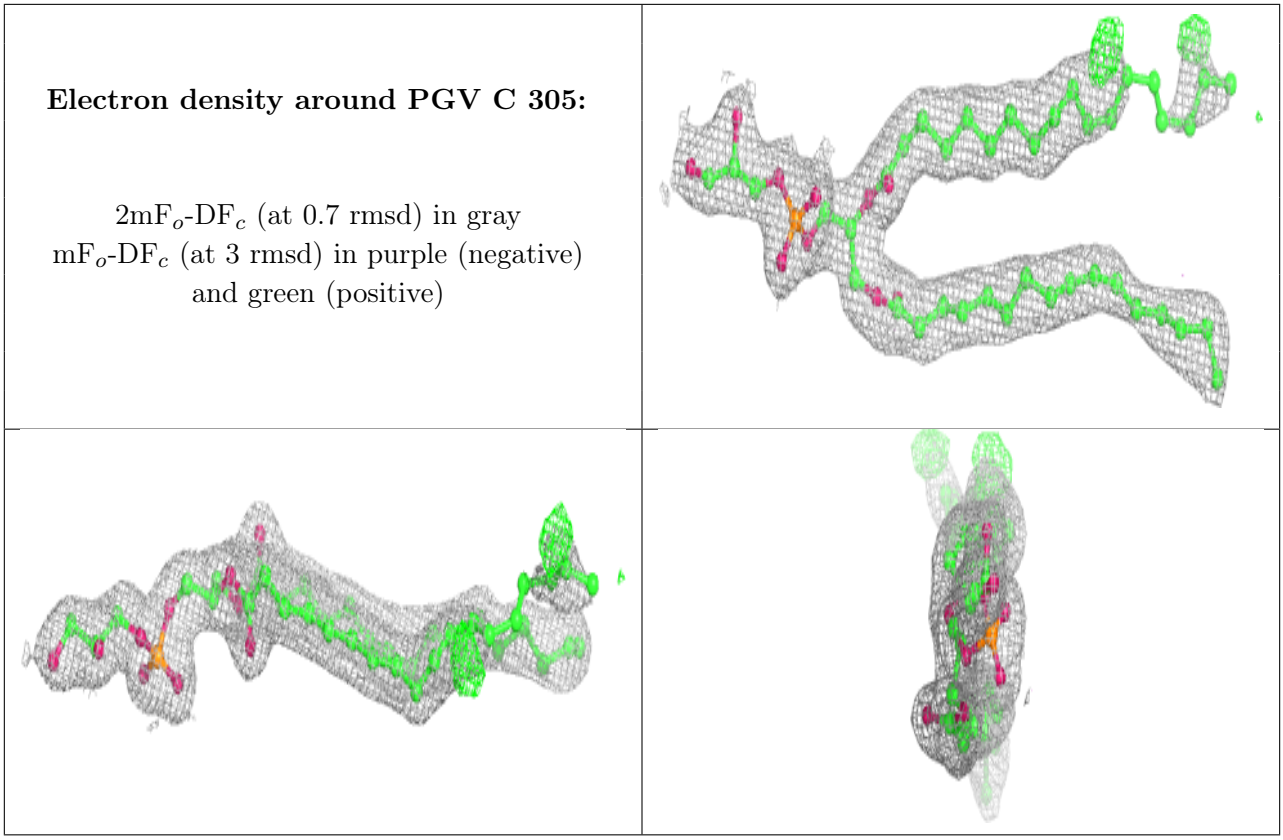
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





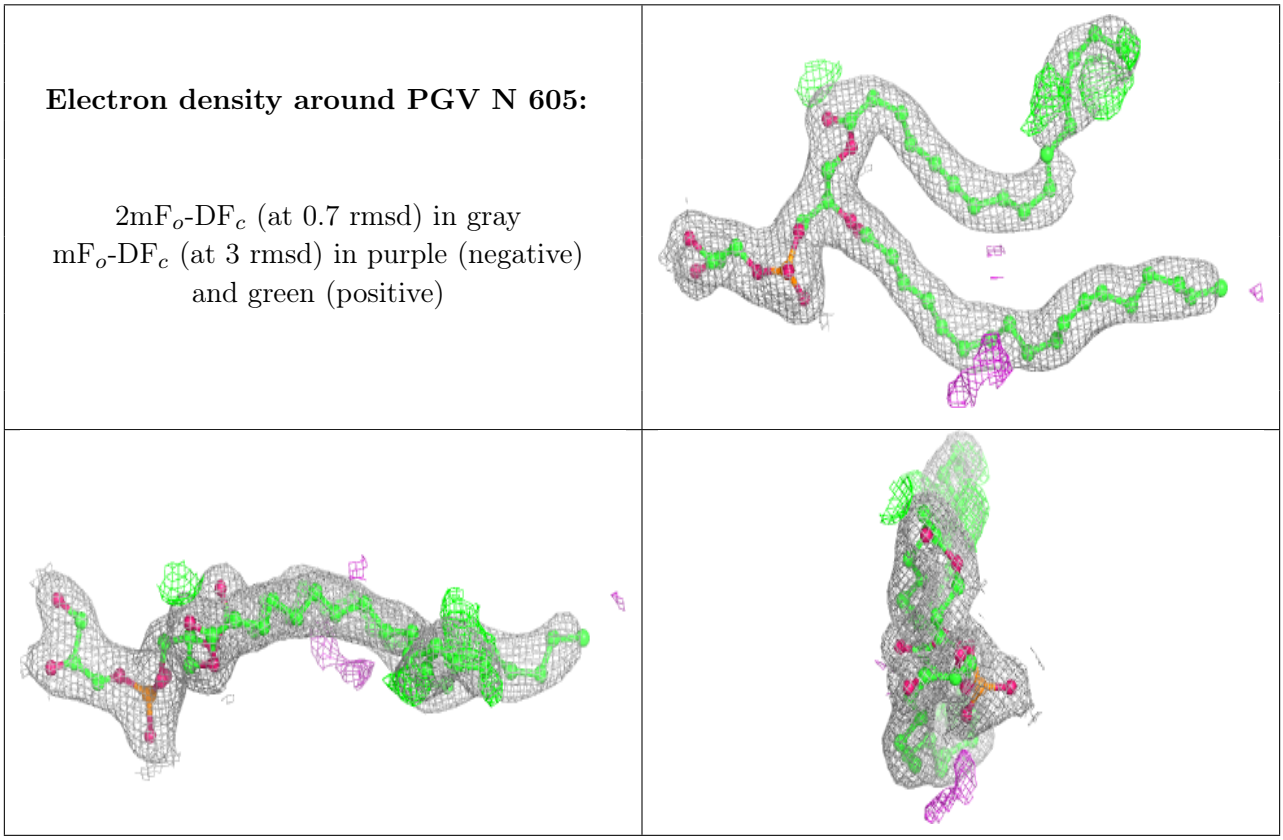
Electron density around PGV C 305:

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



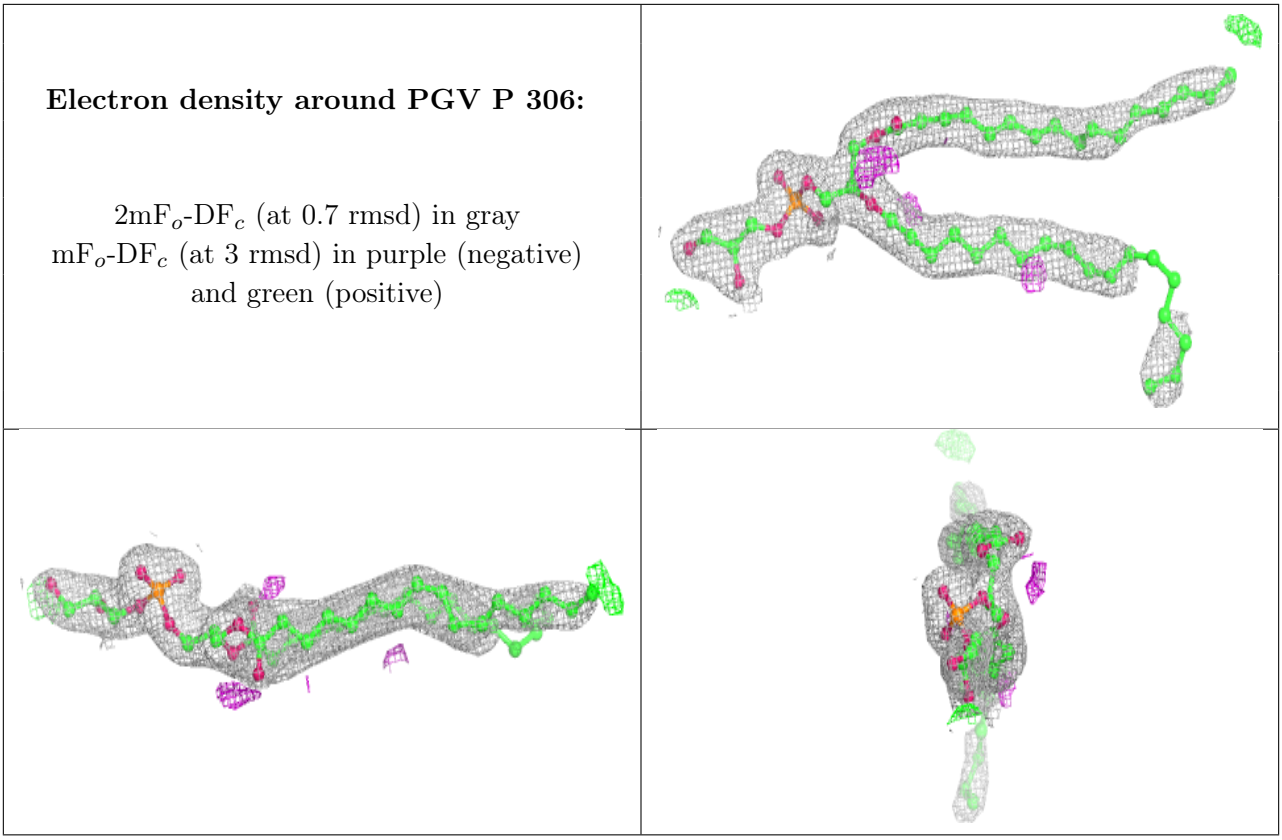
Electron density around PGV N 605:

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



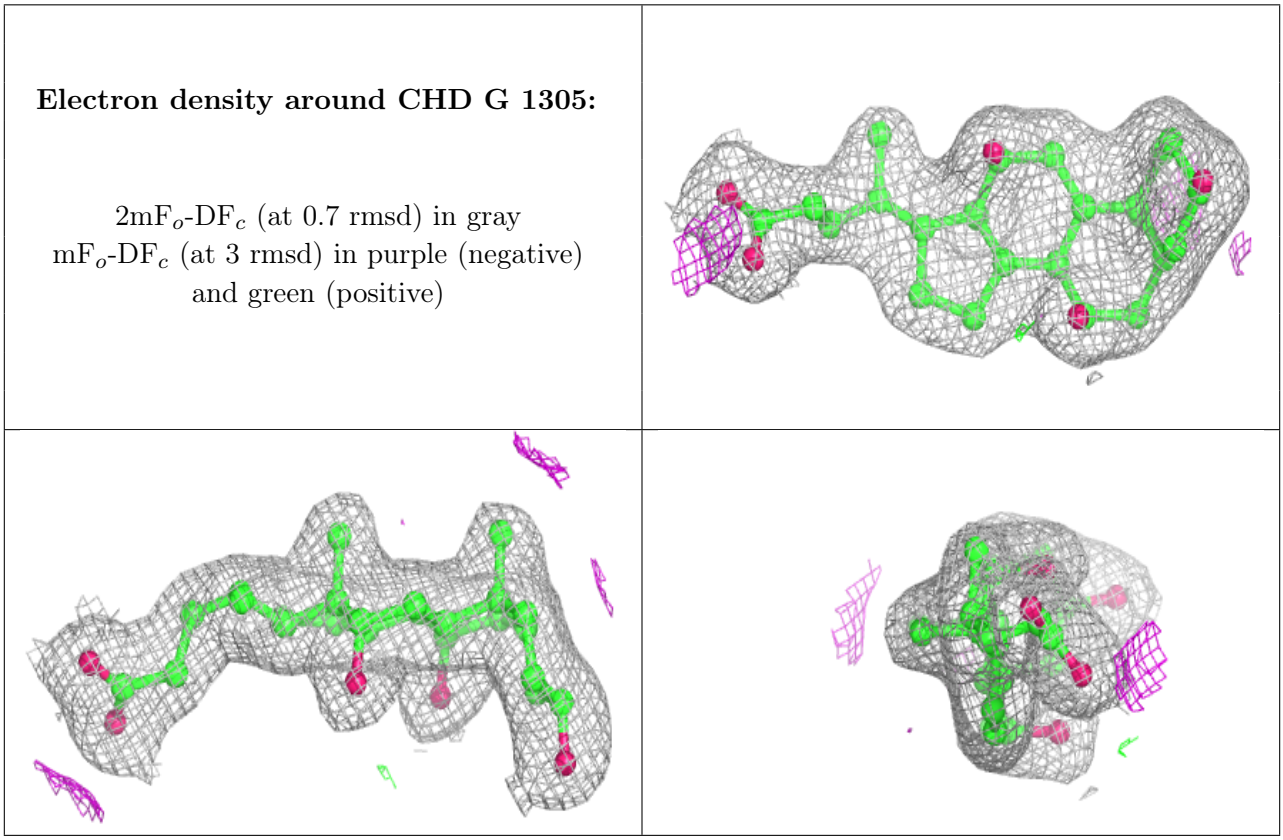
Electron density around PGV P 306:

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



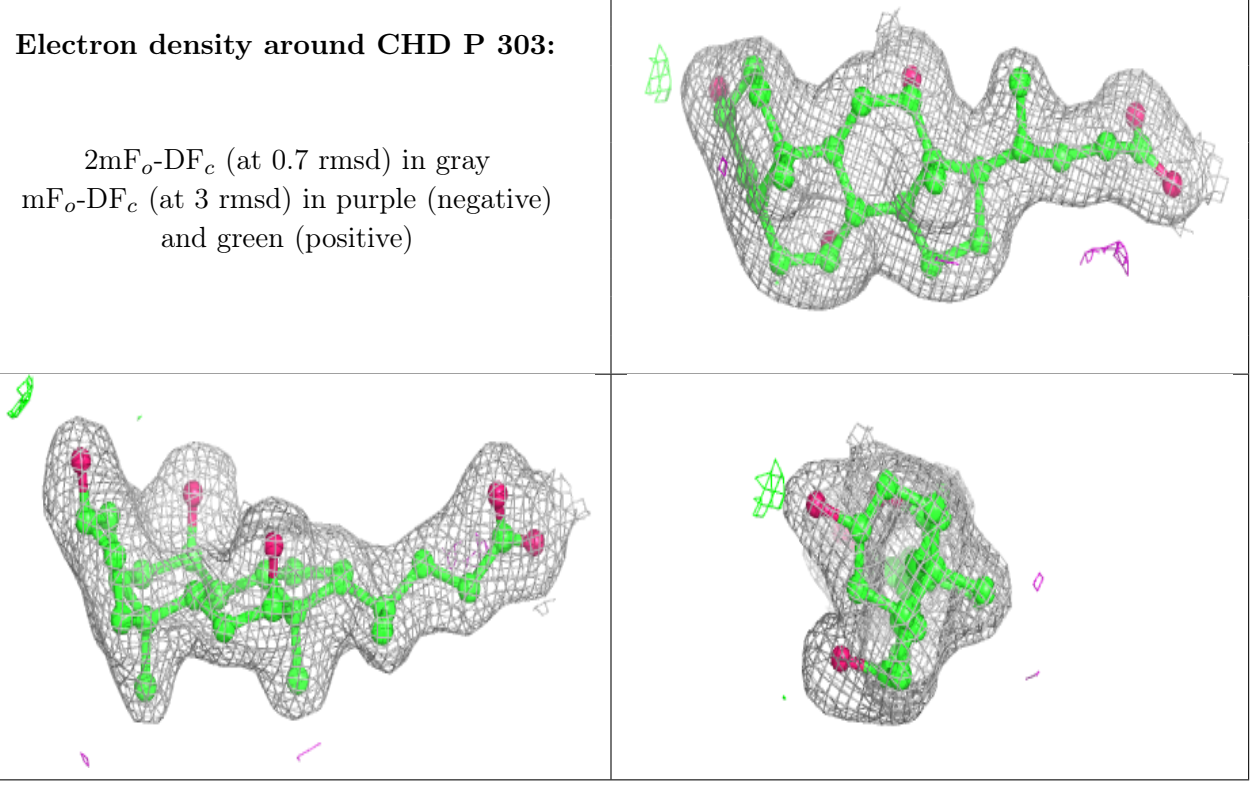
Electron density around CHD G 1305:

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



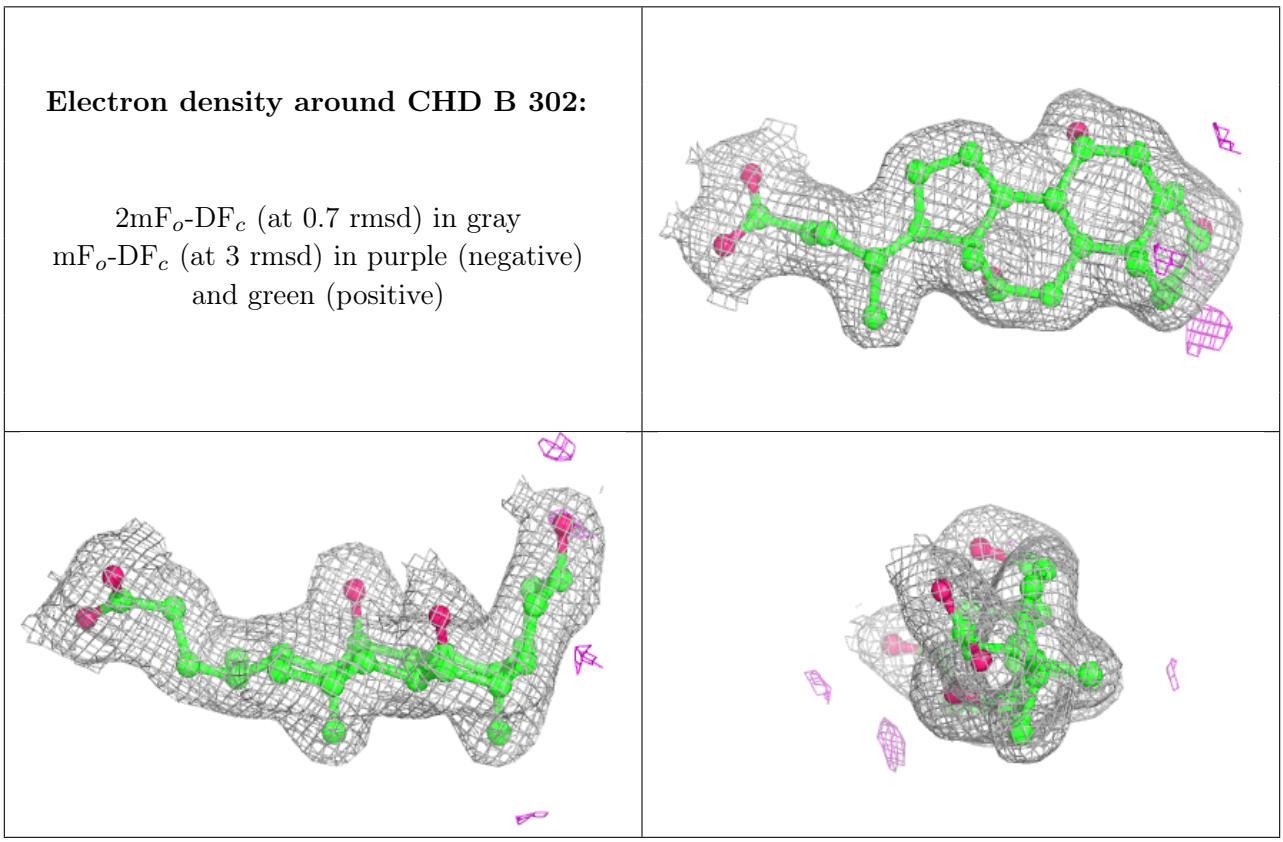
Electron density around CHD P 303:

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



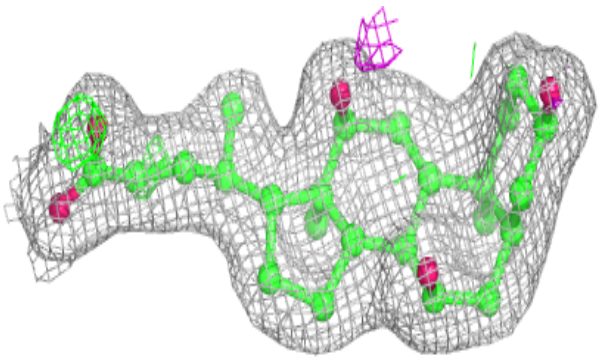
Electron density around CHD B 302:

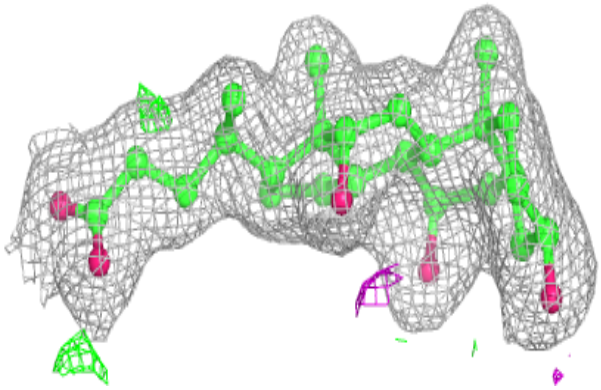
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

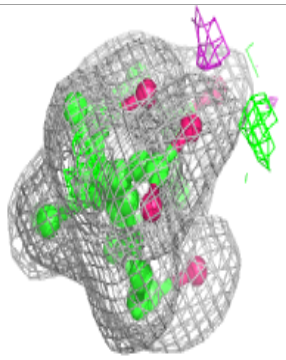


Electron density around CHD C 302:

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

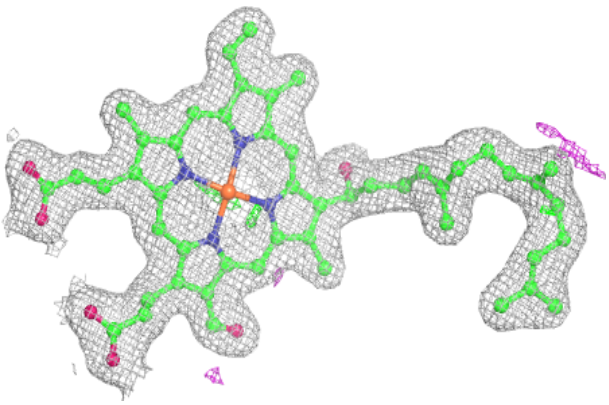


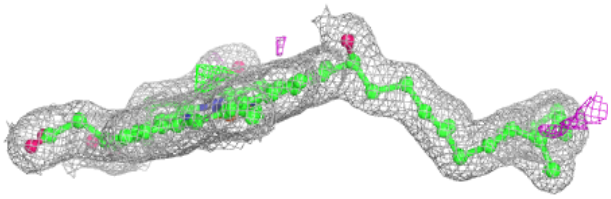


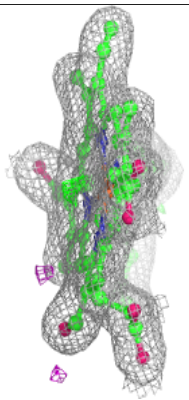


Electron density around HEA A 606:

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

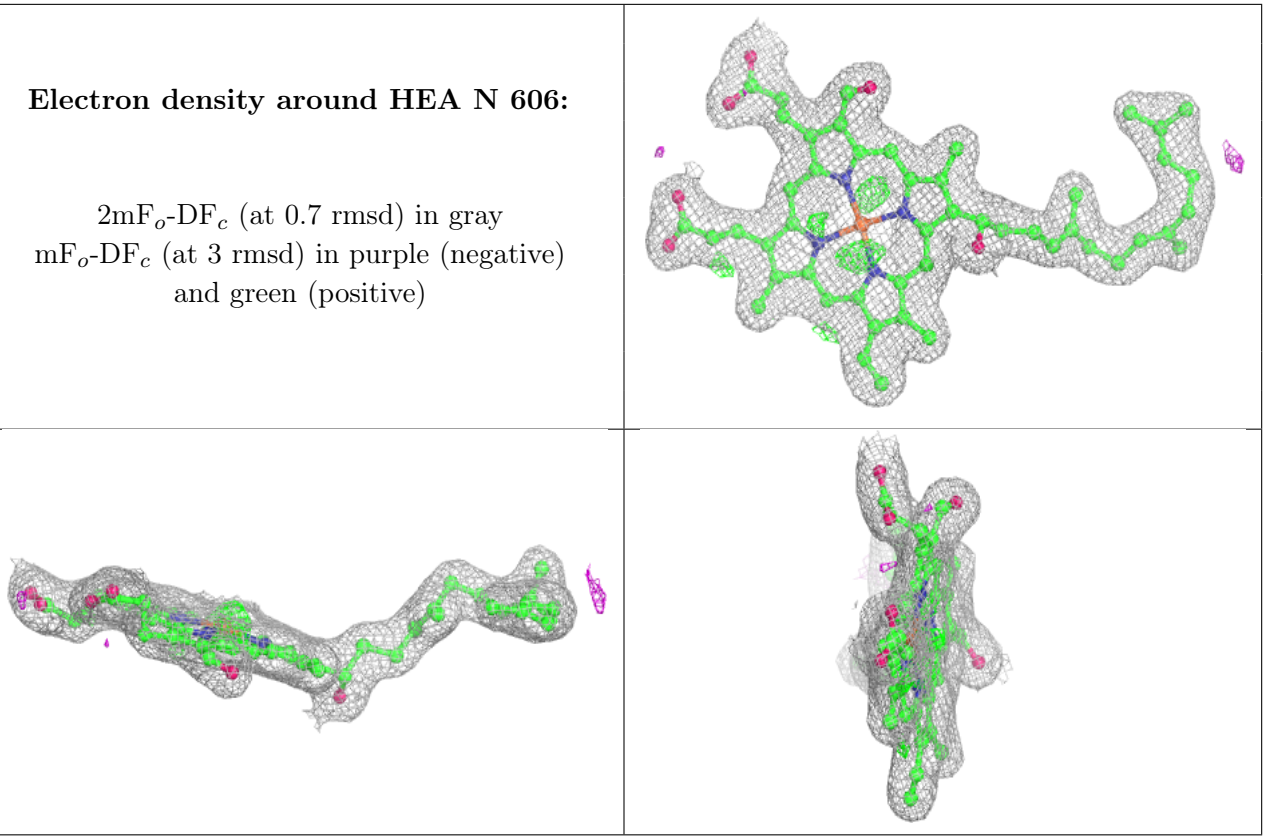






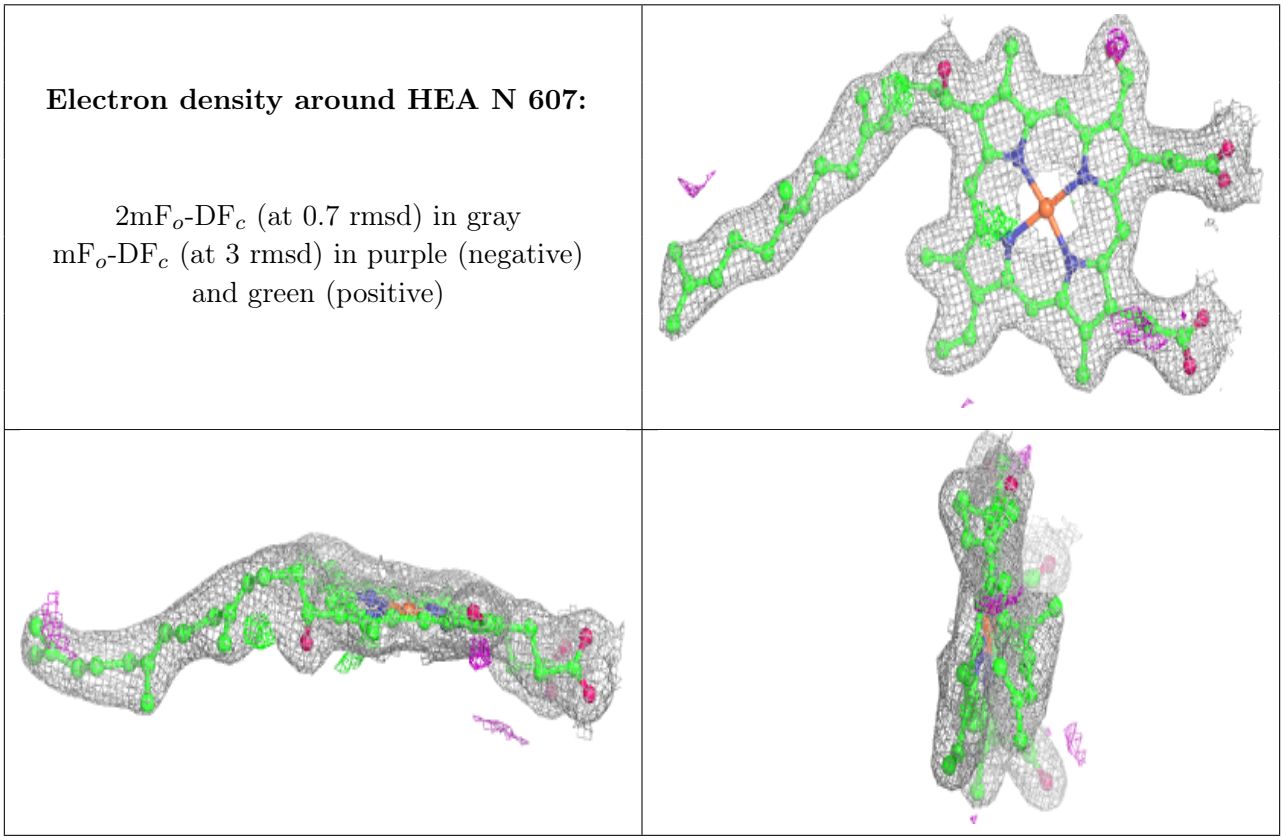
Electron density around HEA N 606:

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



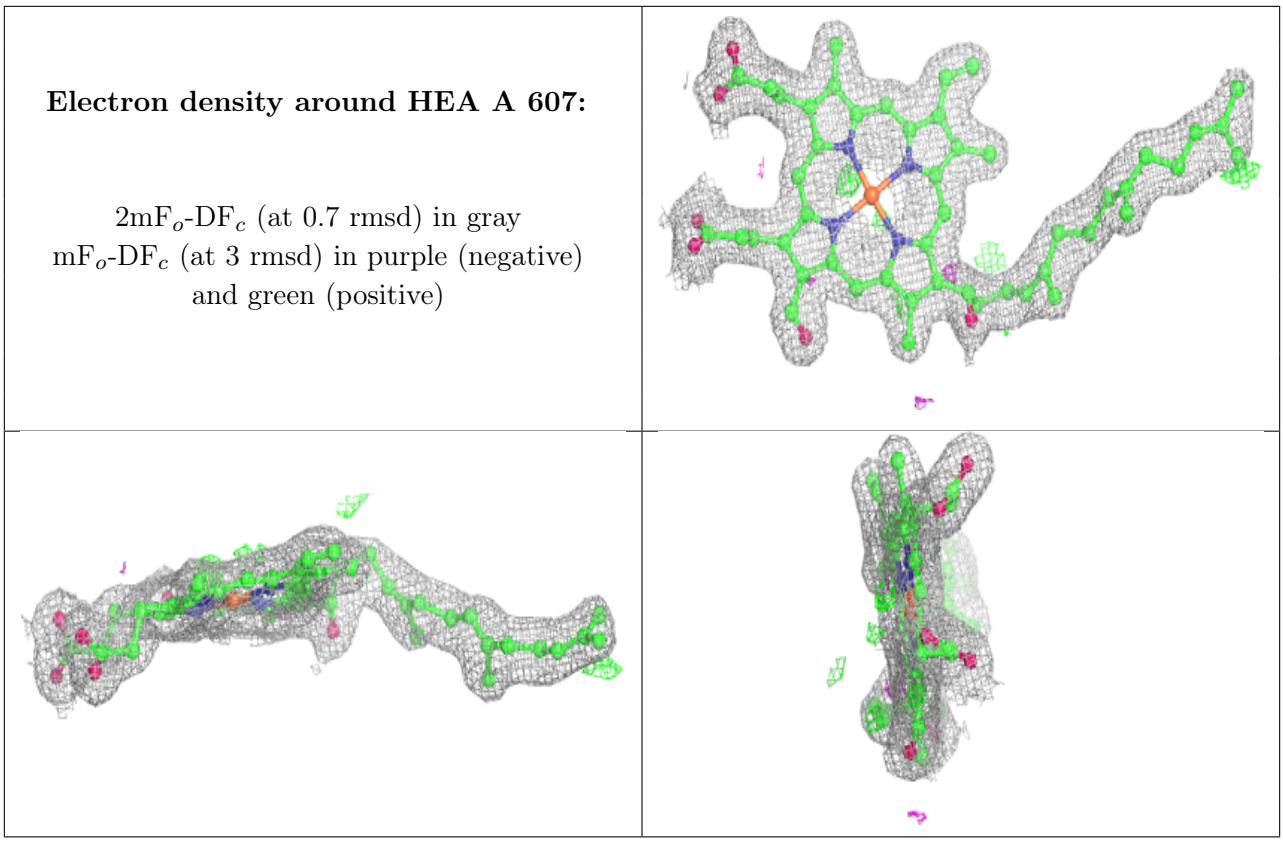
Electron density around HEA N 607:

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



Electron density around HEA A 607:

$2mF_o$-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.