wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 02:53 PM JST

PDB ID	:	5XDQ
Title	:	Bovine heart cytochrome c oxidase in the fully oxidized state with pH 7.3 at 1.77 angstrom resolution
Authors	:	Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2017-03-29
Resolution	:	1.77 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

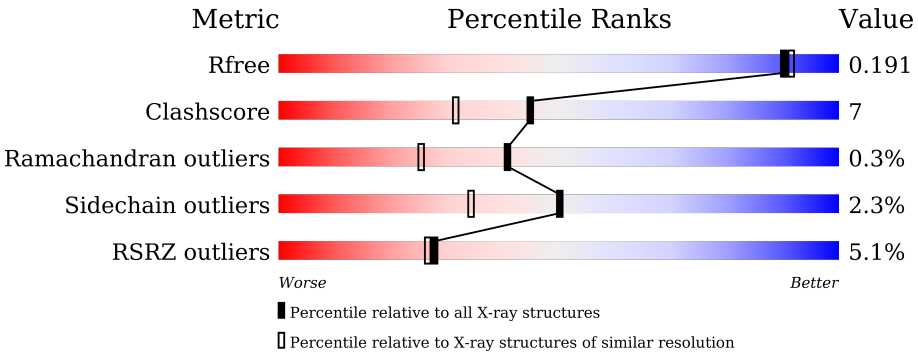
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	85% 15%
1	N	514	89% 11%
2	B	227	88% 11%
2	O	227	87% 13%
3	C	261	85% 14%

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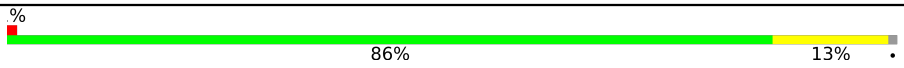
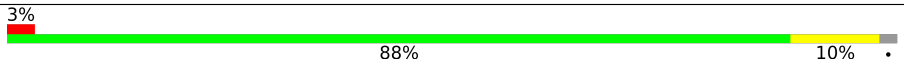
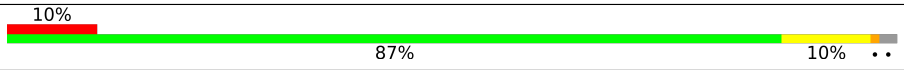
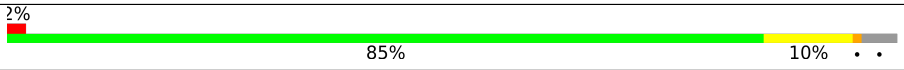
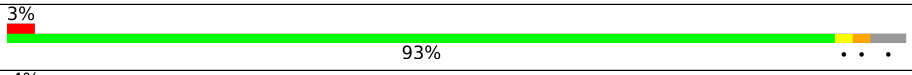
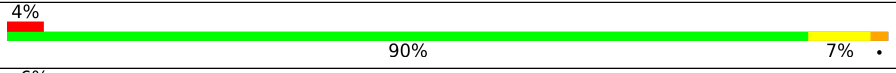
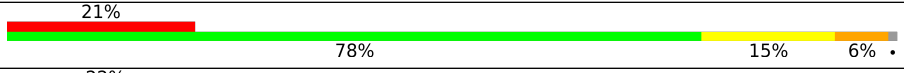
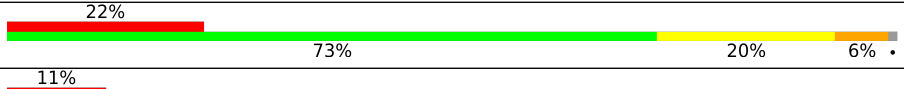
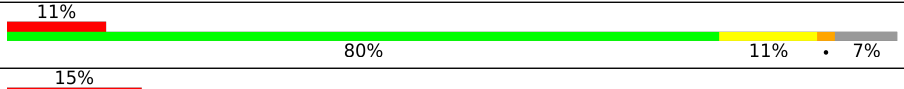
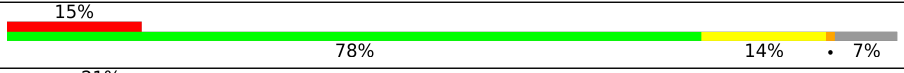
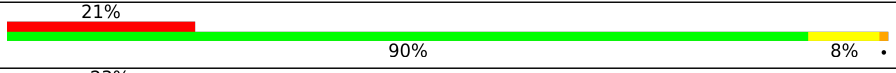
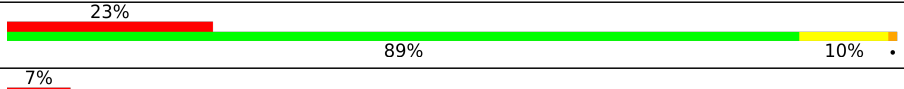
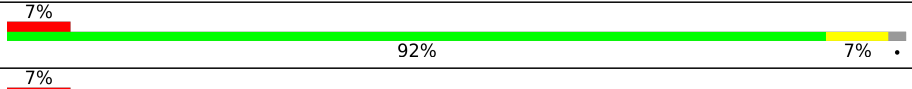
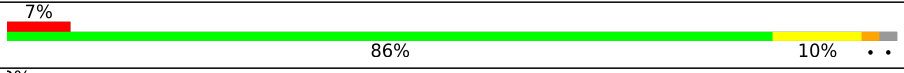
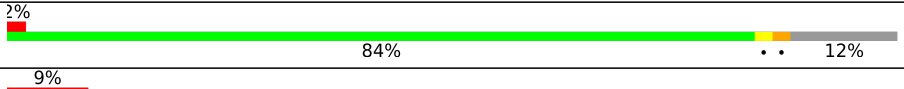
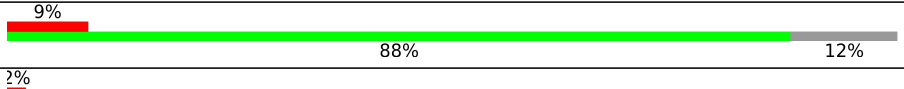
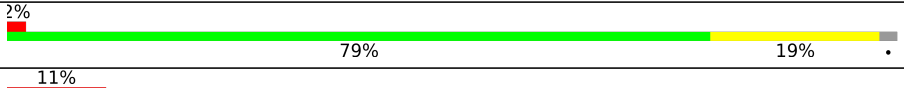
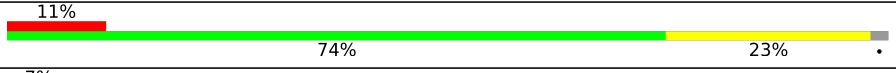
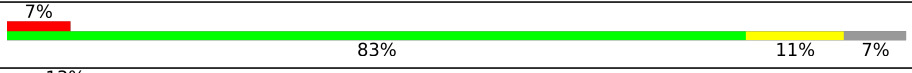
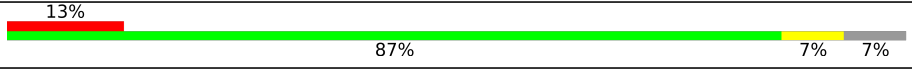
Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	94	
6	S	94	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	619	-	-	X	X
20	EDO	T	105	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	W	102	-	-	-	X
27	DMU	C	313	-	-	-	X
27	DMU	W	104	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 34218 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	33	0
			4118	2757	626	690	45			
1	N	514	Total	C	N	O	S	0	30	0
			4109	2744	627	689	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	11	0
			1859	1207	285	345	22			
2	O	227	Total	C	N	O	S	0	10	0
			1851	1200	284	345	22			

- 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	13	0
			2143	1434	336	357	16			
3	P	259	Total	C	N	O	S	0	12	0
			2140	1430	337	357	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1200	780	198	218	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	2	0
			858	549	144	162	3			
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	94	Total	C	N	O	S	0	1	0
			719	446	127	140	6			
6	S	94	Total	C	N	O	S	0	2	0
			722	449	127	140	6			

- 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
			674	431	129	112	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			674	431	129	112	1	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	2	0
			466	301	78	83	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			462	299	78	81	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			388	254	65	66	3			
11	X	49	Total	C	N	O	S	0	0	0
			383	250	65	66	2			

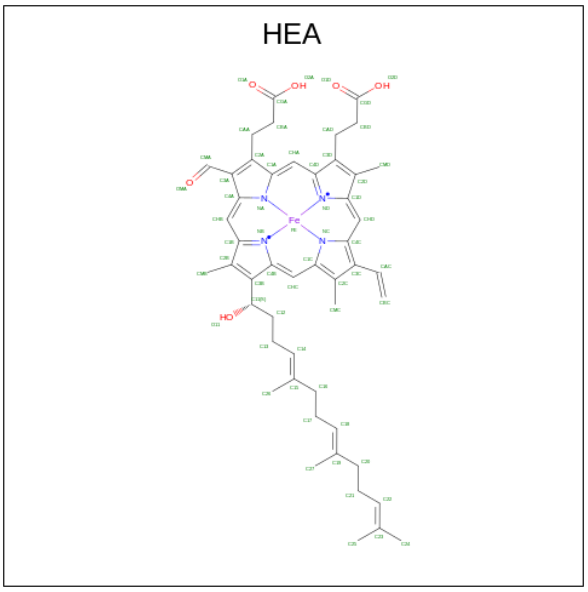
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	4	0
			399	266	66	64	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			339	228	53	58			
13	Z	43	Total	C	N	O	0	0	0
			334	223	53	58			

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



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

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

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

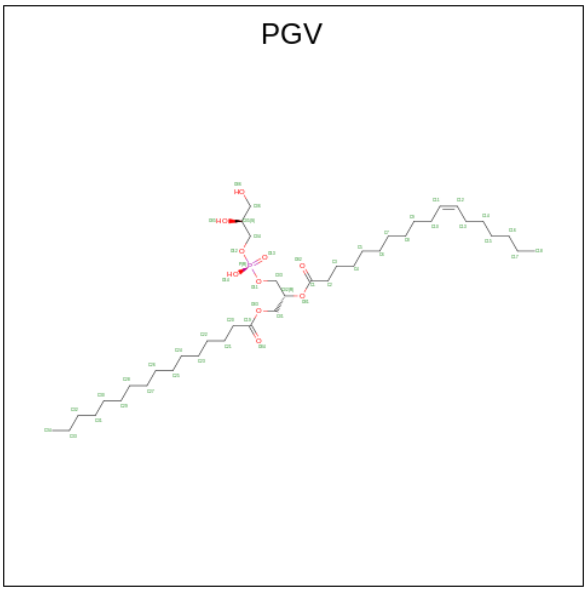
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is (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
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0

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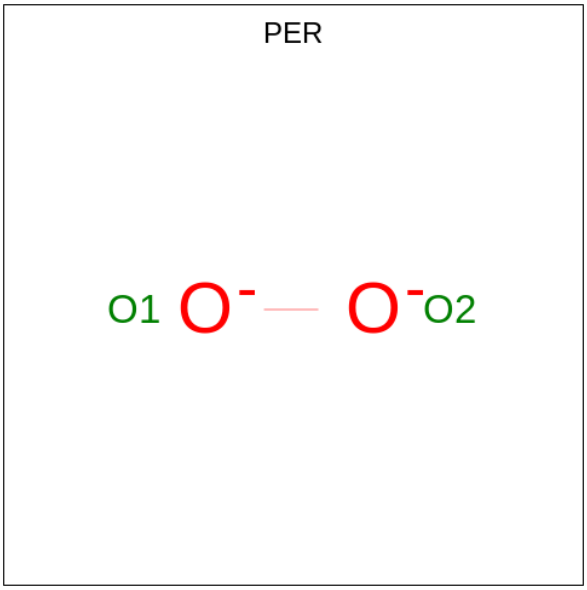
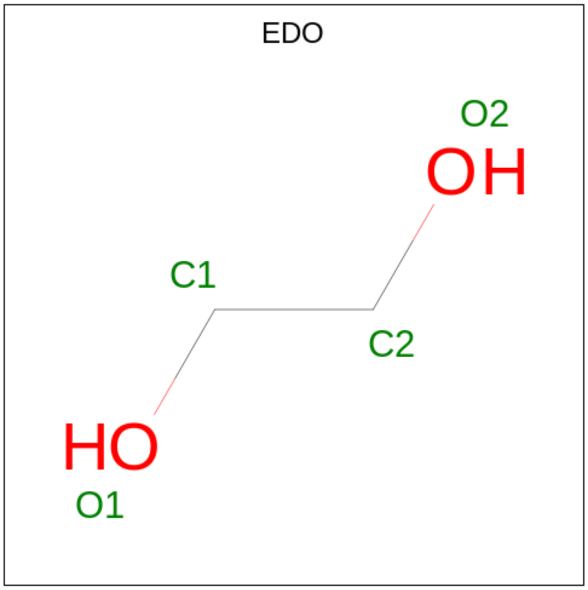
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	U	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	1
			4	4		
19	N	1	Total	O	0	1
			4	4		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	E	1	Total	C	O	0	0
			4	2	2		
20	F	1	Total	C	O	0	0
			4	2	2		
20	F	1	Total	C	O	0	0
			4	2	2		
20	G	1	Total	C	O	0	0
			4	2	2		
20	H	1	Total	C	O	0	0
			4	2	2		
20	J	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		

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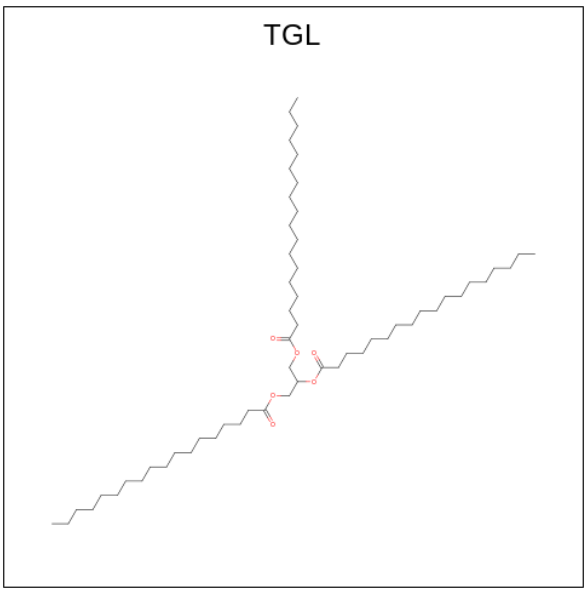
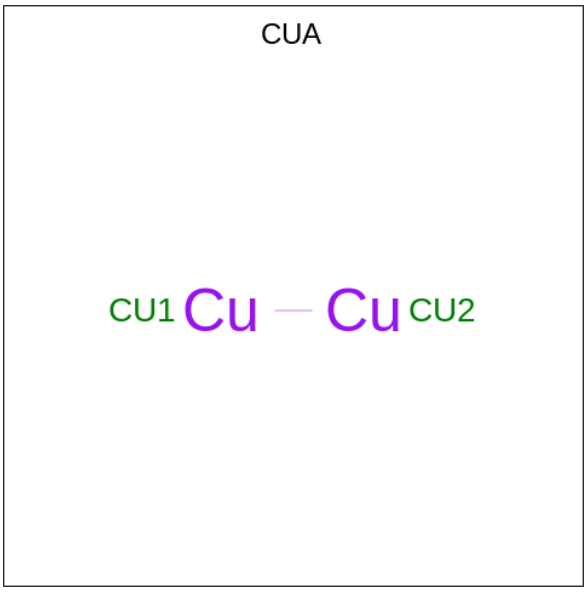
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total	C	O	0	0
			4	2	2		
20	O	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20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

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



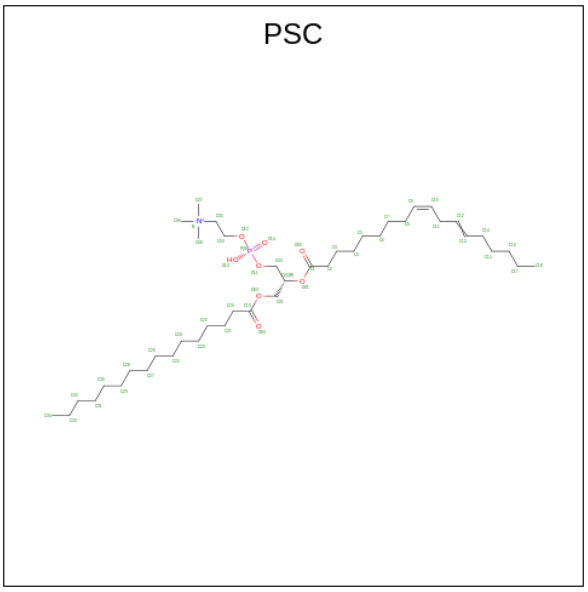
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C O 63 57 6	0	0
21	D	1	Total C O 63 57 6	0	0
21	L	1	Total C O 63 57 6	0	0
21	N	1	Total C O 63 57 6	0	0
21	O	1	Total C O 63 57 6	0	0
21	Q	1	Total C O 63 57 6	0	0

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



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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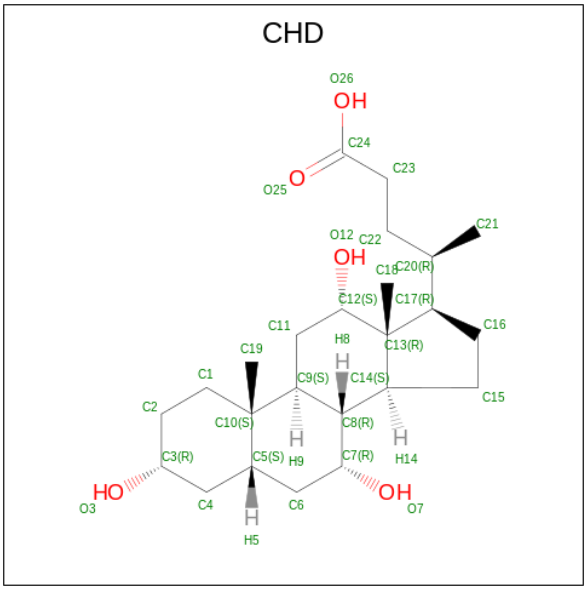
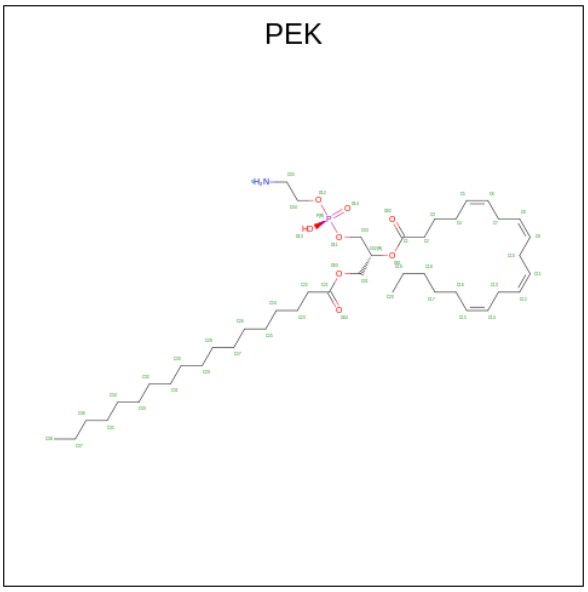
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



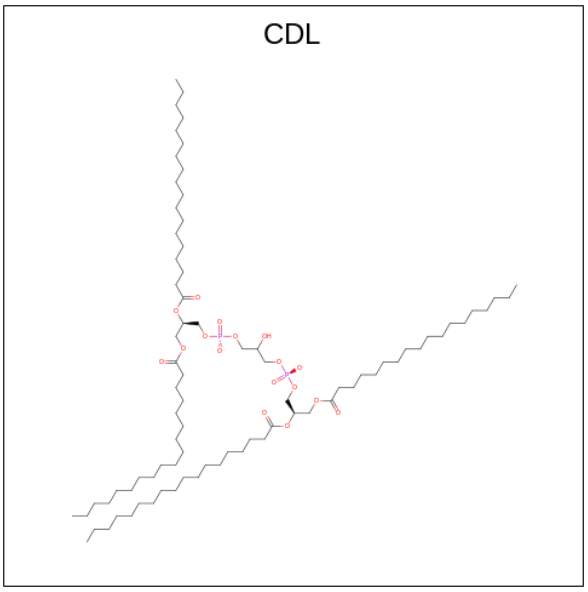
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	B	1	Total	C	O		0	0
			29	24	5			
24	C	1	Total	C	O		0	0
			29	24	5			
24	C	1	Total	C	O		0	0
			29	24	5			
24	G	1	Total	C	O		0	0
			29	24	5			
24	J	1	Total	C	O		0	0
			29	24	5			
24	P	1	Total	C	O		0	0
			29	24	5			
24	P	1	Total	C	O		0	0
			29	24	5			
24	W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

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



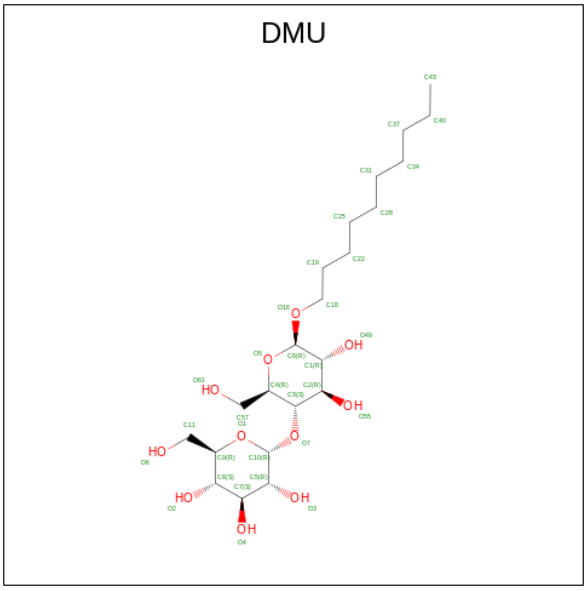
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



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

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



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	257	Total O 257 257	0	0
29	B	229	Total O 230 230	0	1
29	C	164	Total O 164 164	0	0
29	D	214	Total O 214 214	0	0
29	E	154	Total O 154 154	0	0
29	F	162	Total O 162 162	0	0
29	G	95	Total O 95 95	0	0
29	H	84	Total O 84 84	0	0
29	I	78	Total O 78 78	0	0
29	J	44	Total O 44 44	0	0

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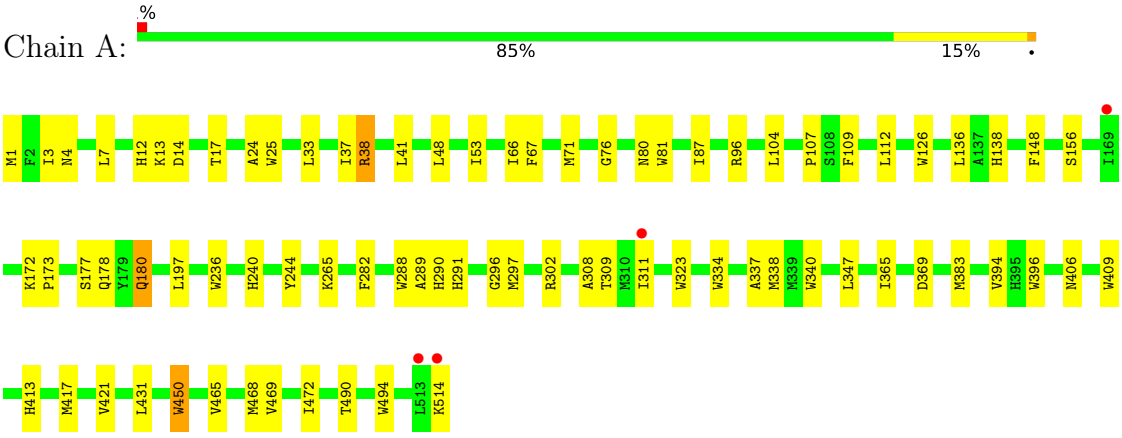
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	42	Total O 42 42	0	0
29	L	57	Total O 57 57	0	0
29	M	29	Total O 29 29	0	0
29	N	267	Total O 267 267	0	0
29	O	186	Total O 186 186	0	0
29	P	151	Total O 151 151	0	0
29	Q	98	Total O 98 98	0	0
29	R	115	Total O 115 115	0	0
29	S	126	Total O 126 126	0	0
29	T	87	Total O 87 87	0	0
29	U	74	Total O 74 74	0	0
29	V	57	Total O 57 57	0	0
29	W	32	Total O 32 32	0	0
29	X	22	Total O 22 22	0	0
29	Y	37	Total O 37 37	0	0
29	Z	21	Total O 21 21	0	0

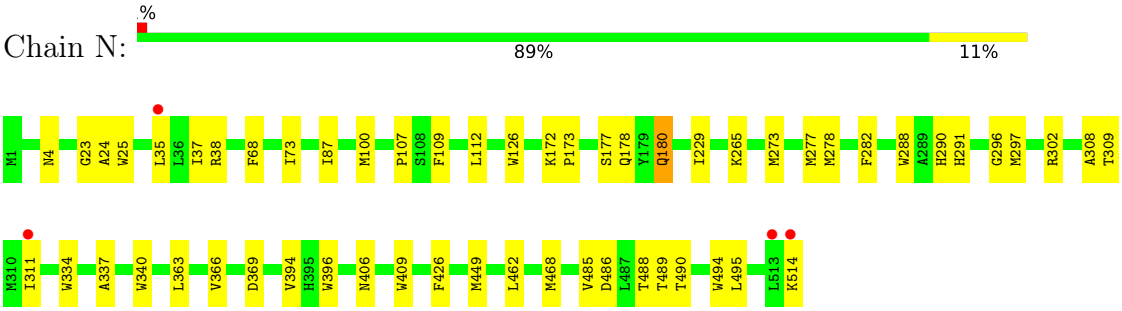
3 Residue-property plots (i)

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.

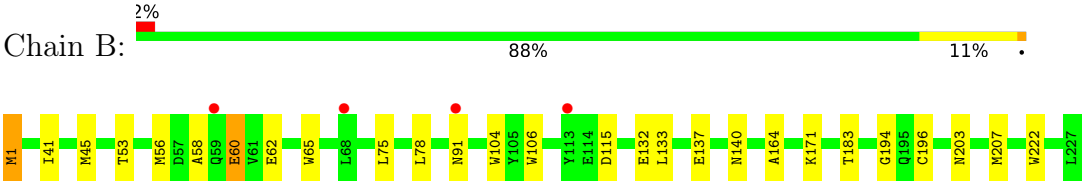
• Molecule 1: Cytochrome c oxidase subunit 1



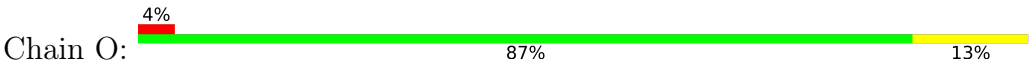
• Molecule 1: Cytochrome c oxidase subunit 1

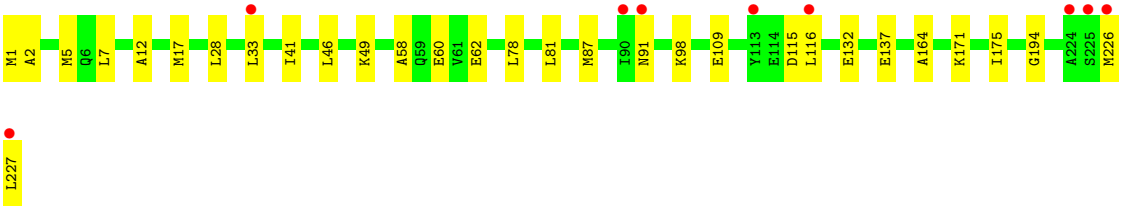


• Molecule 2: Cytochrome c oxidase subunit 2

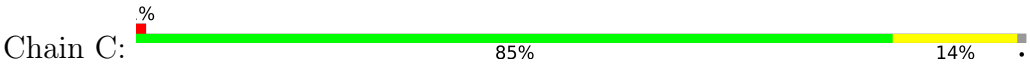


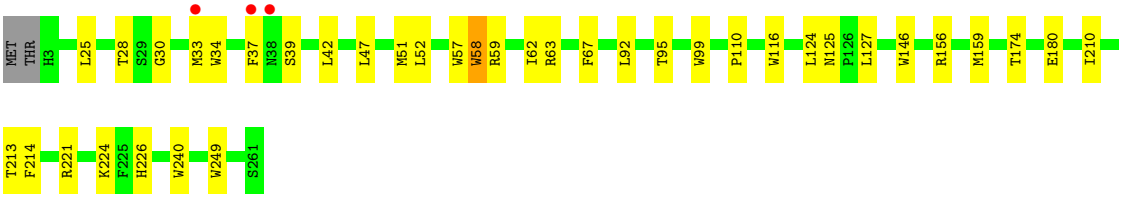
• Molecule 2: Cytochrome c oxidase subunit 2



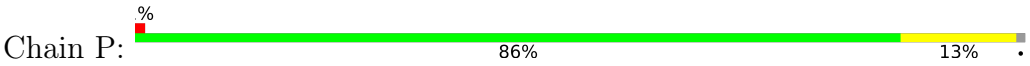


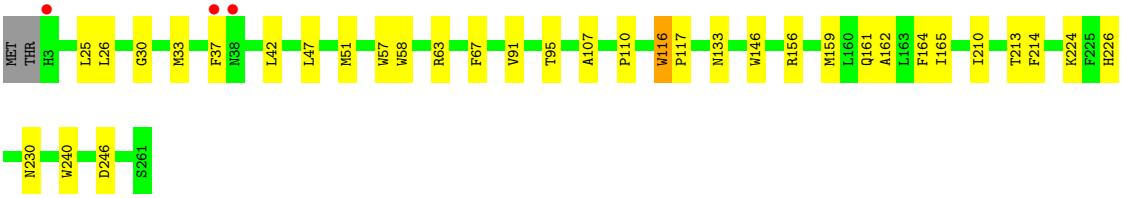
• Molecule 3: Cytochrome c oxidase subunit 3



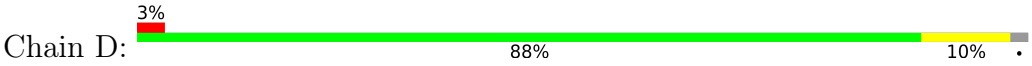


• Molecule 3: Cytochrome c oxidase subunit 3

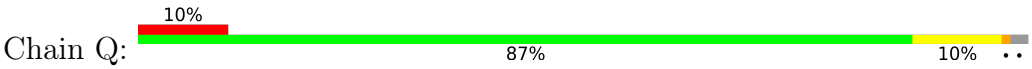


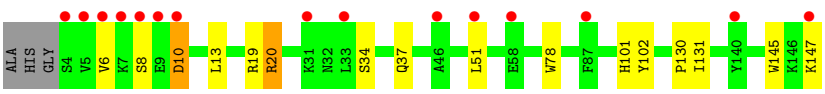


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

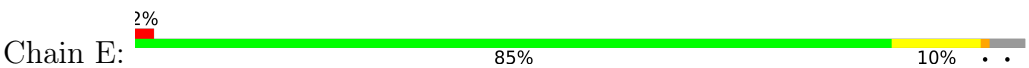


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



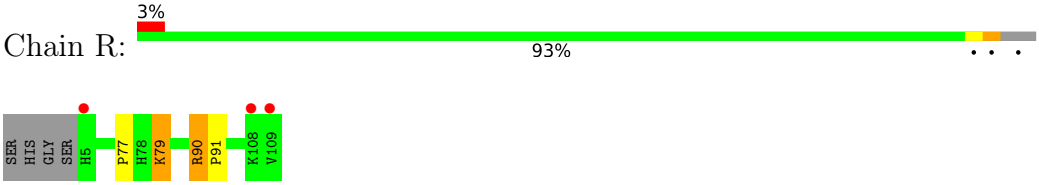


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



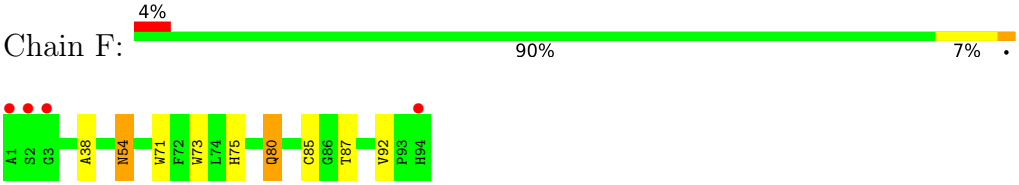
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



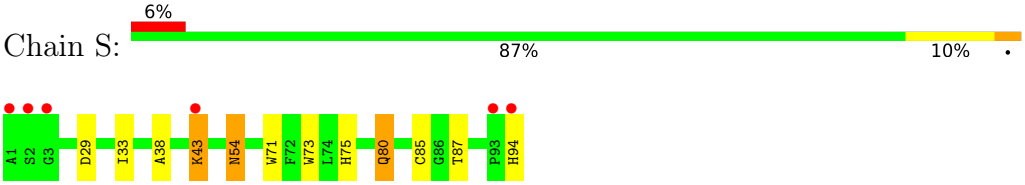
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



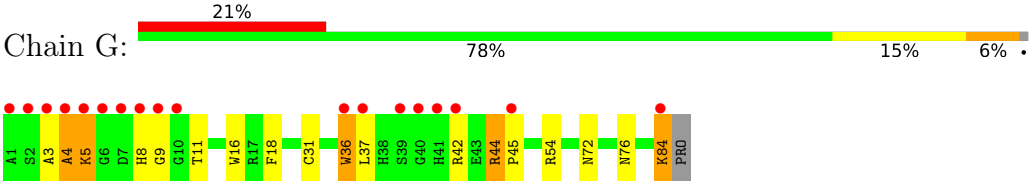
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



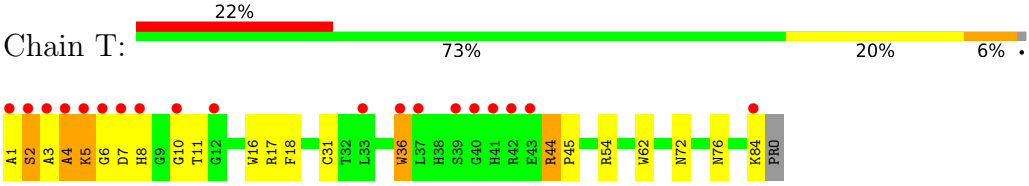
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



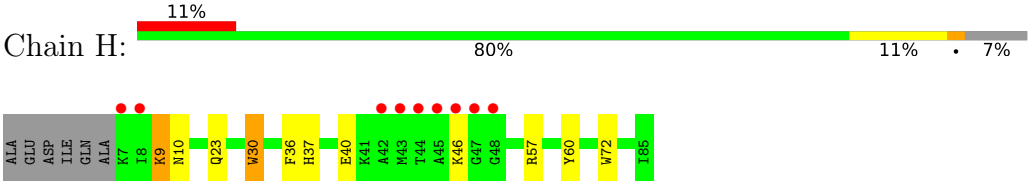
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



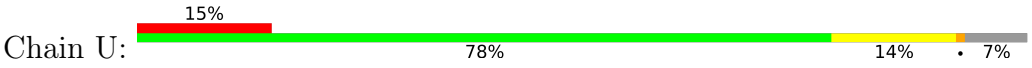
• Molecule 8: Cytochrome c oxidase subunit 6B1

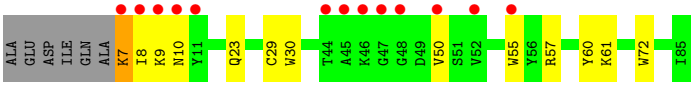
Chain H:



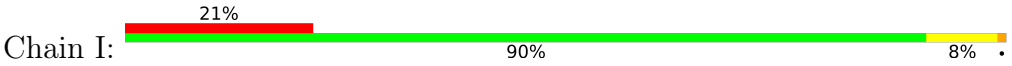
• Molecule 8: Cytochrome c oxidase subunit 6B1

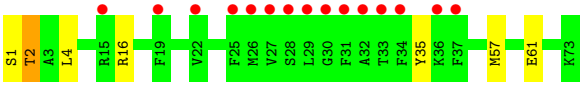
Chain U:



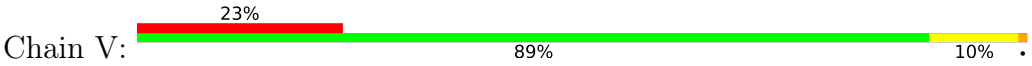


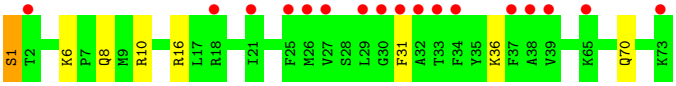
• Molecule 9: Cytochrome c oxidase subunit 6C



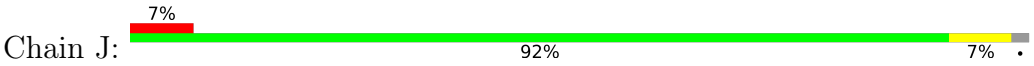


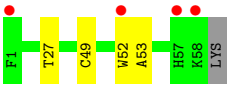
• Molecule 9: Cytochrome c oxidase subunit 6C



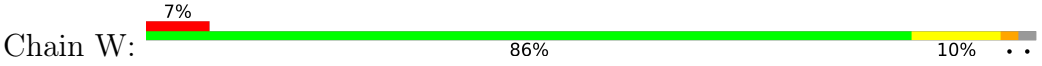


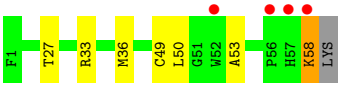
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



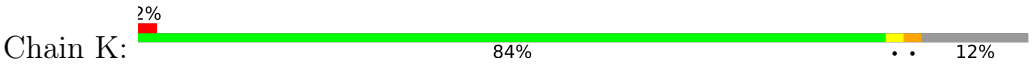


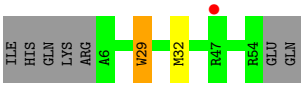
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



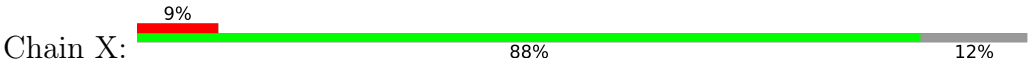


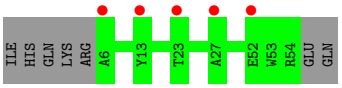
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





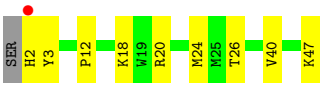
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





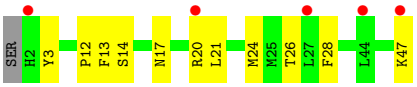
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



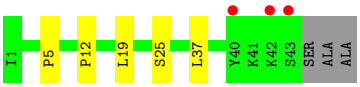
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



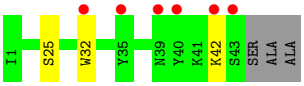
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	183.31Å 205.90Å 177.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.45 – 1.77 134.45 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (134.45-1.77) 99.7 (134.45-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.164 , 0.190 0.166 , 0.191	Depositor DCC
R_{free} test set	32362 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 85.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	34218	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.65	10/4405 (0.2%)	0.58	1/6009 (0.0%)
1	N	0.62	7/4385 (0.2%)	0.57	0/5979
2	B	0.55	3/1946 (0.2%)	0.64	0/2648
2	O	0.51	0/1938	0.57	0/2637
3	C	0.70	7/2298 (0.3%)	0.52	0/3139
3	P	0.69	4/2292 (0.2%)	0.53	0/3131
4	D	0.62	4/1229 (0.3%)	0.53	0/1658
4	Q	0.58	2/1240 (0.2%)	0.51	0/1673
5	E	0.52	0/886	0.53	0/1202
5	R	0.49	0/871	0.53	0/1182
6	F	0.55	2/740 (0.3%)	0.58	0/1003
6	S	0.52	1/748 (0.1%)	0.54	0/1014
7	G	0.68	2/689 (0.3%)	0.60	0/936
7	T	0.67	3/689 (0.4%)	0.59	0/936
8	H	0.62	2/682 (0.3%)	0.54	0/921
8	U	0.62	2/682 (0.3%)	0.52	0/921
9	I	0.40	0/605	0.49	0/802
9	V	0.37	0/605	0.48	0/802
10	J	0.51	0/487	0.49	0/657
10	W	0.51	0/478	0.48	0/645
11	K	0.67	1/405 (0.2%)	0.51	0/555
11	X	0.66	0/397	0.49	0/545
12	L	0.59	0/430	0.51	0/575
12	Y	0.54	0/401	0.49	0/536
13	M	0.54	0/352	0.50	0/480
13	Z	0.52	1/344 (0.3%)	0.47	0/469
All	All	0.60	51/30224 (0.2%)	0.55	1/41055 (0.0%)

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	57	TRP	CD2-CE2	5.75	1.48	1.41
3	C	57	TRP	CD2-CE2	5.73	1.48	1.41
1	A	288	TRP	CD2-CE2	5.54	1.48	1.41
1	A	340	TRP	CD2-CE2	5.49	1.48	1.41
7	G	16	TRP	CD2-CE2	5.46	1.48	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ARG	NE-CZ-NH2	-5.05	117.77	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	4118	0	4147	75	0
1	N	4109	0	4118	57	0
2	B	1859	0	1889	17	0
2	O	1851	0	1866	23	0
3	C	2143	0	2072	40	0
3	P	2140	0	2058	33	0
4	D	1195	0	1183	15	0
4	Q	1200	0	1186	7	0
5	E	858	0	855	21	0
5	R	852	0	845	2	0
6	F	719	0	702	6	0
6	S	722	0	709	10	0
7	G	674	0	644	14	0
7	T	674	0	644	15	0
8	H	662	0	623	7	0
8	U	662	0	623	5	0
9	I	601	0	613	5	0
9	V	601	0	613	7	0
10	J	466	0	466	7	0
10	W	462	0	464	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	388	0	375	1	0
11	X	383	0	366	0	0
12	L	399	0	395	9	0
12	Y	382	0	381	10	0
13	M	339	0	363	6	0
13	Z	334	0	352	2	0
14	A	129	0	88	8	0
14	N	129	0	88	17	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	8	0
18	C	102	0	152	7	0
18	N	102	0	152	3	0
18	P	51	0	76	1	0
18	U	51	0	76	2	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	44	0	66	8	0
20	B	20	0	30	2	0
20	C	12	0	18	0	0
20	E	4	0	6	0	0
20	F	8	0	12	0	0
20	G	4	0	6	0	0
20	H	4	0	6	1	0
20	J	4	0	6	2	0
20	L	16	0	24	2	0
20	M	8	0	12	0	0
20	N	20	0	30	1	0
20	O	4	0	6	0	0
20	P	24	0	36	0	0
20	Q	4	0	6	0	0
20	R	16	0	24	0	0
20	S	12	0	18	0	0
20	T	8	0	12	0	0
20	W	8	0	12	0	0
20	Y	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	63	0	110	3	0
21	D	63	0	110	6	0
21	L	63	0	110	4	0
21	N	63	0	110	4	0
21	O	63	0	110	4	0
21	Q	63	0	110	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	5	0
24	B	29	0	39	1	0
24	C	58	0	78	2	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	5	0
24	W	29	0	39	2	0
25	C	106	0	154	6	0
25	G	53	0	77	1	0
25	P	53	0	77	2	0
25	T	106	0	154	7	0
26	C	100	0	156	16	0
26	G	100	0	156	12	0
26	P	100	0	156	9	0
26	T	100	0	156	7	0
27	C	66	0	84	10	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	W	33	0	42	11	0
27	Z	33	0	42	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	257	0	0	3	0
29	B	230	0	0	4	0
29	C	164	0	0	1	0
29	D	214	0	0	6	0
29	E	154	0	0	3	0
29	F	162	0	0	0	0
29	G	95	0	0	0	0
29	H	84	0	0	1	0
29	I	78	0	0	1	0
29	J	44	0	0	0	0
29	K	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	57	0	0	4	0
29	M	29	0	0	0	0
29	N	267	0	0	3	0
29	O	186	0	0	0	0
29	P	151	0	0	2	0
29	Q	98	0	0	0	0
29	R	115	0	0	0	0
29	S	126	0	0	1	0
29	T	87	0	0	1	0
29	U	74	0	0	0	0
29	V	57	0	0	2	0
29	W	32	0	0	1	0
29	X	22	0	0	0	0
29	Y	37	0	0	0	0
29	Z	21	0	0	0	0
All	All	34218	0	32142	413	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 7.

The worst 5 of 413 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:33[A]:MET:SD	27:C:313:DMU:H11	1.64	1.36
27:C:313:DMU:H8	10:J:53:ALA:HB2	1.25	1.18
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C23	1.77	1.13
3:P:33[A]:MET:SD	27:W:104:DMU:H11	1.88	1.13
1:A:468[B]:MET:HE1	14:A:601[B]:HEA:H212	1.35	1.09

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	545/514 (106%)	532 (98%)	13 (2%)	0	100	100
1	N	542/514 (105%)	528 (97%)	14 (3%)	0	100	100
2	B	236/227 (104%)	230 (98%)	6 (2%)	0	100	100
2	O	235/227 (104%)	231 (98%)	4 (2%)	0	100	100
3	C	270/261 (103%)	266 (98%)	4 (2%)	0	100	100
3	P	269/261 (103%)	265 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	143/147 (97%)	136 (95%)	5 (4%)	2 (1%)	11	2
5	E	105/109 (96%)	105 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	94/94 (100%)	93 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	71 (88%)	8 (10%)	2 (2%)	5	1
7	T	81/85 (95%)	72 (89%)	4 (5%)	5 (6%)	1	0
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	75 (97%)	1 (1%)	1 (1%)	12	3
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	71 (100%)	0	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	47/47 (100%)	44 (94%)	3 (6%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
13	M	42/46 (91%)	42 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3620/3606 (100%)	3528 (98%)	82 (2%)	10 (0%)	41	25

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	4	ALA
7	T	5	LYS

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Mol	Chain	Res	Type
7	G	5	LYS
4	Q	8	SER

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	459/426 (108%)	453 (99%)	6 (1%)	69 59
1	N	456/426 (107%)	450 (99%)	6 (1%)	69 59
2	B	221/210 (105%)	214 (97%)	7 (3%)	39 22
2	O	220/210 (105%)	214 (97%)	6 (3%)	44 28
3	C	237/226 (105%)	234 (99%)	3 (1%)	69 59
3	P	236/226 (104%)	233 (99%)	3 (1%)	69 59
4	D	128/129 (99%)	127 (99%)	1 (1%)	81 76
4	Q	129/129 (100%)	125 (97%)	4 (3%)	40 22
5	E	94/95 (99%)	93 (99%)	1 (1%)	73 65
5	R	92/95 (97%)	90 (98%)	2 (2%)	52 36
6	F	79/78 (101%)	77 (98%)	2 (2%)	47 31
6	S	80/78 (103%)	76 (95%)	4 (5%)	24 9
7	G	67/68 (98%)	60 (90%)	7 (10%)	7 1
7	T	67/68 (98%)	62 (92%)	5 (8%)	13 3
8	H	71/75 (95%)	69 (97%)	2 (3%)	43 27
8	U	71/75 (95%)	67 (94%)	4 (6%)	21 7
9	I	57/57 (100%)	56 (98%)	1 (2%)	59 45
9	V	57/57 (100%)	55 (96%)	2 (4%)	36 19
10	J	51/50 (102%)	51 (100%)	0	100 100
10	W	50/50 (100%)	48 (96%)	2 (4%)	31 14
11	K	40/46 (87%)	40 (100%)	0	100 100
11	X	39/46 (85%)	39 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	43/40 (108%)	42 (98%)	1 (2%)	50 34
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47 31
13	M	38/38 (100%)	38 (100%)	0	100 100
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44 28
All	All	3159/3076 (103%)	3088 (98%)	71 (2%)	50 36

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	18	PHE
7	T	44	ARG
9	V	36	LYS
7	G	44	ARG
7	G	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	68	GLN
6	S	80	GLN
3	P	161	GLN
5	R	5	HIS
9	V	8	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FME	O	1	2	8,9,10	0.60	0	7,9,11	1.17	0
7	TPO	T	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.81	0
9	SAC	I	1	9	7,8,9	2.04	2 (28%)	8,9,11	1.08	0
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.59	2 (28%)
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	0.78	0
2	FME	B	1	2	8,9,10	0.78	0	7,9,11	3.14	2 (28%)
1	FME	N	1	1	8,9,10	0.57	0	7,9,11	1.29	0
9	SAC	V	1	9	7,8,9	2.04	2 (28%)	8,9,11	1.37	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	2/9/11/13	-
9	SAC	I	1	9	-	2/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	5/7/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	4.66	1.33	1.23
9	V	1	SAC	OAC-C1A	4.49	1.33	1.23
7	G	11	TPO	P-O1P	2.81	1.59	1.50
9	V	1	SAC	CA-N	2.80	1.50	1.46
7	T	11	TPO	P-O1P	2.80	1.59	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-6.99	112.07	122.82
1	A	1	FME	C-CA-N	3.05	115.23	109.73
2	B	1	FME	C-CA-N	2.94	115.03	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CB-CA-N	-2.46	105.03	110.55
1	A	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	1	0
2	B	1	FME	1	0
9	V	1	SAC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 118 ligands modelled in this entry, 10 are monoatomic - leaving 108 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	$\#\|Z\| > 2$
22	CUA	O	302	2	0,1,1	-	-	-		
24	CHD	P	301	-	32,32,32	0.60	0	51,51,51	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CDL	P	305	-	99,99,99	1.33	12 (12%)	105,111,111	1.07	5 (4%)
14	HEA	N	602	1,19	57,67,67	1.60	12 (21%)	61,103,103	1.37	8 (13%)
20	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.24	0
20	EDO	A	616	-	3,3,3	0.41	0	2,2,2	0.43	0
20	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.36	0
19	PER	A	607[B]	14,15	0,1,1	-	-	-		
20	EDO	A	618	-	3,3,3	0.47	0	2,2,2	0.28	0
26	CDL	C	307	-	99,99,99	1.33	12 (12%)	105,111,111	1.07	4 (3%)
14	HEA	N	601[B]	-	57,67,67	1.62	13 (22%)	61,103,103	1.34	9 (14%)
20	EDO	E	201	-	3,3,3	0.44	0	2,2,2	0.40	0
20	EDO	N	610	-	3,3,3	0.48	0	2,2,2	0.28	0
20	EDO	M	103	-	3,3,3	0.45	0	2,2,2	0.35	0
14	HEA	N	601[A]	-	57,67,67	1.62	13 (22%)	61,103,103	1.38	10 (16%)
20	EDO	P	311	-	3,3,3	0.54	0	2,2,2	0.20	0
20	EDO	J	102	-	3,3,3	0.42	0	2,2,2	0.46	0
25	PEK	G	103	-	52,52,52	0.91	2 (3%)	55,57,57	0.97	4 (7%)
18	PGV	C	306	-	50,50,50	0.99	2 (4%)	53,56,56	0.99	3 (5%)
20	EDO	R	203	-	3,3,3	0.42	0	2,2,2	0.37	0
14	HEA	A	601[A]	-	57,67,67	1.61	13 (22%)	61,103,103	1.48	12 (19%)
20	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.24	0
19	PER	N	608[B]	14,15	0,1,1	-	-	-		
20	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.28	0
27	DMU	C	312	-	34,34,34	0.49	0	45,45,45	0.87	2 (4%)
20	EDO	T	105	-	3,3,3	0.45	0	2,2,2	0.35	0
19	PER	N	608[A]	14,15	0,1,1	-	-	-		
20	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.33	0
24	CHD	C	301	-	32,32,32	0.64	0	51,51,51	1.05	2 (3%)
25	PEK	T	102	-	52,52,52	0.96	2 (3%)	55,57,57	0.88	3 (5%)
20	EDO	C	309	-	3,3,3	0.39	0	2,2,2	0.58	0
20	EDO	A	612	-	3,3,3	0.39	0	2,2,2	0.24	0
20	EDO	L	105	-	3,3,3	0.43	0	2,2,2	0.33	0
21	TGL	O	301	-	62,62,62	1.25	6 (9%)	65,65,65	1.08	3 (4%)
20	EDO	P	309	-	3,3,3	0.46	0	2,2,2	0.29	0
21	TGL	Q	201	-	62,62,62	1.27	6 (9%)	65,65,65	1.08	4 (6%)
26	CDL	G	101	-	99,99,99	1.31	12 (12%)	105,111,111	1.10	6 (5%)
20	EDO	R	204	-	3,3,3	0.49	0	2,2,2	0.30	0
20	EDO	N	611	-	3,3,3	0.48	0	2,2,2	0.36	0
19	PER	A	607[A]	14,15	0,1,1	-	-	-		
27	DMU	C	313	-	34,34,34	0.53	1 (2%)	45,45,45	0.90	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PEK	T	101	-	52,52,52	0.95	2 (3%)	55,57,57	0.96	3 (5%)
27	DMU	Z	101	-	34,34,34	0.45	0	45,45,45	0.78	0
24	CHD	W	101	-	32,32,32	0.59	0	51,51,51	1.44	7 (13%)
21	TGL	N	606	-	62,62,62	1.26	6 (9%)	65,65,65	1.10	3 (4%)
18	PGV	N	607	-	50,50,50	0.95	2 (4%)	53,56,56	0.97	5 (9%)
27	DMU	W	104	-	34,34,34	0.55	1 (2%)	45,45,45	0.75	1 (2%)
20	EDO	M	102	-	3,3,3	0.42	0	2,2,2	0.37	0
20	EDO	G	104	-	3,3,3	0.48	0	2,2,2	0.23	0
20	EDO	L	103	-	3,3,3	0.47	0	2,2,2	0.26	0
27	DMU	M	101	-	34,34,34	0.44	0	45,45,45	0.88	1 (2%)
20	EDO	W	103	-	3,3,3	0.42	0	2,2,2	0.42	0
20	EDO	N	613	-	3,3,3	0.44	0	2,2,2	0.17	0
20	EDO	L	102	-	3,3,3	0.41	0	2,2,2	0.45	0
20	EDO	R	201	-	3,3,3	0.47	0	2,2,2	0.34	0
23	PSC	O	303	-	51,51,51	1.10	3 (5%)	57,59,59	1.07	3 (5%)
25	PEK	P	303	-	52,52,52	0.90	2 (3%)	55,57,57	0.89	2 (3%)
25	PEK	C	303	-	52,52,52	0.87	2 (3%)	55,57,57	0.80	2 (3%)
20	EDO	F	102	-	3,3,3	0.50	0	2,2,2	0.20	0
20	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.19	0
20	EDO	L	104	-	3,3,3	0.44	0	2,2,2	0.35	0
20	EDO	F	103	-	3,3,3	0.43	0	2,2,2	0.33	0
20	EDO	A	614	-	3,3,3	0.39	0	2,2,2	0.41	0
20	EDO	A	619	-	3,3,3	0.44	0	2,2,2	0.25	0
24	CHD	G	102	-	32,32,32	0.66	0	51,51,51	1.06	3 (5%)
18	PGV	A	606	-	50,50,50	0.97	2 (4%)	53,56,56	1.01	3 (5%)
20	EDO	B	307	-	3,3,3	0.50	0	2,2,2	0.28	0
20	EDO	A	615	-	3,3,3	0.37	0	2,2,2	0.51	0
20	EDO	P	308	-	3,3,3	0.43	0	2,2,2	0.39	0
18	PGV	P	304	-	50,50,50	0.88	2 (4%)	53,56,56	0.78	1 (1%)
18	PGV	N	609	-	50,50,50	0.87	2 (4%)	53,56,56	0.91	2 (3%)
20	EDO	B	309	-	3,3,3	0.56	0	2,2,2	0.22	0
20	EDO	B	305	-	3,3,3	0.49	0	2,2,2	0.21	0
20	EDO	B	308	-	3,3,3	0.42	0	2,2,2	0.41	0
14	HEA	A	602	1,19	57,67,67	1.53	12 (21%)	61,103,103	1.37	10 (16%)
18	PGV	A	608	-	50,50,50	0.95	2 (4%)	53,56,56	0.85	3 (5%)
20	EDO	S	104	-	3,3,3	0.40	0	2,2,2	0.48	0
20	EDO	O	304	-	3,3,3	0.46	0	2,2,2	0.36	0
27	DMU	P	313	-	34,34,34	0.54	0	45,45,45	1.17	5 (11%)
18	PGV	U	101	-	50,50,50	0.96	2 (4%)	53,56,56	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CUA	B	302	2	0,1,1	-	-	-		
20	EDO	T	104	-	3,3,3	0.43	0	2,2,2	0.37	0
20	EDO	C	311	-	3,3,3	0.52	0	2,2,2	0.25	0
24	CHD	J	101	-	32,32,32	0.59	0	51,51,51	1.39	7 (13%)
26	CDL	T	103	-	99,99,99	1.32	12 (12%)	105,111,111	1.09	5 (4%)
20	EDO	B	306	-	3,3,3	0.34	0	2,2,2	0.29	0
20	EDO	P	310	-	3,3,3	0.43	0	2,2,2	0.35	0
25	PEK	C	304	-	52,52,52	0.94	2 (3%)	55,57,57	0.98	2 (3%)
24	CHD	B	304	-	32,32,32	0.65	0	51,51,51	1.01	2 (3%)
24	CHD	P	306	-	32,32,32	0.58	0	51,51,51	1.36	7 (13%)
18	PGV	C	305	-	50,50,50	0.88	2 (4%)	53,56,56	0.81	1 (1%)
14	HEA	A	601[B]	-	57,67,67	1.61	13 (22%)	61,103,103	1.44	11 (18%)
20	EDO	Y	101	-	3,3,3	0.46	0	2,2,2	0.33	0
24	CHD	C	308	-	32,32,32	0.67	0	51,51,51	1.72	10 (19%)
20	EDO	P	312	-	3,3,3	0.49	0	2,2,2	0.28	0
20	EDO	A	613	-	3,3,3	0.58	0	2,2,2	0.50	0
20	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.44	0
20	EDO	S	102	-	3,3,3	0.47	0	2,2,2	0.16	0
20	EDO	W	102	-	3,3,3	0.46	0	2,2,2	0.33	0
21	TGL	L	101	-	62,62,62	1.28	6 (9%)	65,65,65	1.12	3 (4%)
20	EDO	H	101	-	3,3,3	0.41	0	2,2,2	0.41	0
21	TGL	B	301	-	62,62,62	1.21	6 (9%)	65,65,65	1.10	4 (6%)
20	EDO	N	614	-	3,3,3	0.50	0	2,2,2	0.33	0
23	PSC	B	303	-	51,51,51	1.12	3 (5%)	57,59,59	0.96	2 (3%)
20	EDO	R	202	-	3,3,3	0.41	0	2,2,2	0.41	0
21	TGL	D	201	-	62,62,62	1.25	6 (9%)	65,65,65	0.99	4 (6%)
20	EDO	P	307	-	3,3,3	0.43	0	2,2,2	0.43	0
20	EDO	S	103	-	3,3,3	0.50	0	2,2,2	0.28	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
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
26	CDL	P	305	-	-	69/110/110/110	-
14	HEA	N	602	1,19	-	4/32/76/76	-
20	EDO	Q	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
26	CDL	C	307	-	-	66/110/110/110	-
14	HEA	N	601[B]	-	-	7/32/76/76	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	M	103	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	5/32/76/76	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
25	PEK	G	103	-	-	31/56/56/56	-
18	PGV	C	306	-	-	26/55/55/55	-
20	EDO	R	203	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	7/32/76/76	-
20	EDO	C	310	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
27	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	T	105	-	-	1/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
25	PEK	T	102	-	-	31/56/56/56	-
20	EDO	C	309	-	-	0/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
20	EDO	L	105	-	-	1/1/1/1	-
21	TGL	O	301	-	-	34/65/65/65	-
20	EDO	P	309	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	34/65/65/65	-
26	CDL	G	101	-	-	64/110/110/110	-
20	EDO	R	204	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
27	DMU	C	313	-	-	10/19/59/59	0/2/2/2
25	PEK	T	101	-	-	26/56/56/56	-
27	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
24	CHD	W	101	-	-	6/9/74/74	1/4/4/4
21	TGL	N	606	-	-	33/65/65/65	-
18	PGV	N	607	-	-	29/55/55/55	-
27	DMU	W	104	-	-	9/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	M	102	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
27	DMU	M	101	-	-	8/19/59/59	0/2/2/2
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	L	102	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
23	PSC	O	303	-	-	31/55/55/55	-
25	PEK	P	303	-	-	16/56/56/56	-
25	PEK	C	303	-	-	17/56/56/56	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	L	104	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	A	619	-	-	1/1/1/1	-
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4
18	PGV	A	606	-	-	25/55/55/55	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
20	EDO	P	308	-	-	1/1/1/1	-
18	PGV	P	304	-	-	18/55/55/55	-
18	PGV	N	609	-	-	12/55/55/55	-
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	B	308	-	-	1/1/1/1	-
14	HEA	A	602	1,19	-	4/32/76/76	-
18	PGV	A	608	-	-	11/55/55/55	-
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
27	DMU	P	313	-	-	8/19/59/59	0/2/2/2
18	PGV	U	101	-	-	29/55/55/55	-
20	EDO	T	104	-	-	0/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
24	CHD	J	101	-	-	5/9/74/74	0/4/4/4
26	CDL	T	103	-	-	61/110/110/110	-
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	P	310	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	C	304	-	-	26/56/56/56	-
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
24	CHD	P	306	-	-	9/9/74/74	0/4/4/4
18	PGV	C	305	-	-	19/55/55/55	-
14	HEA	A	601[B]	-	-	7/32/76/76	-
20	EDO	Y	101	-	-	0/1/1/1	-
24	CHD	C	308	-	-	8/9/74/74	0/4/4/4
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	W	102	-	-	0/1/1/1	-
21	TGL	L	101	-	-	33/65/65/65	-
20	EDO	H	101	-	-	1/1/1/1	-
21	TGL	B	301	-	-	43/65/65/65	-
20	EDO	N	614	-	-	0/1/1/1	-
23	PSC	B	303	-	-	29/55/55/55	-
20	EDO	R	202	-	-	0/1/1/1	-
21	TGL	D	201	-	-	38/65/65/65	-
20	EDO	P	307	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG2-CB1	4.71	1.47	1.34
26	C	307	CDL	OA8-CA7	4.65	1.46	1.33
21	N	606	TGL	OG2-CB1	4.59	1.47	1.34
26	P	305	CDL	OB8-CB7	4.57	1.46	1.33
26	P	305	CDL	OA8-CA7	4.57	1.46	1.33

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	308	CHD	C17-C13-C12	-4.59	113.47	117.67
21	L	101	TGL	OG2-CB1-CB2	4.59	121.39	111.50
26	G	101	CDL	OA6-CA5-C11	4.58	121.37	111.50
23	O	303	PSC	O01-C1-C2	4.43	121.05	111.50
24	C	308	CHD	C16-C17-C20	4.41	118.97	112.15

There are no chirality outliers.

5 of 991 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	C	305	PGV	C10-C11-C12-C13
18	C	306	PGV	C03-O11-P-O12
18	C	306	PGV	C03-O11-P-O13

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	W	101	CHD	C1-C10-C2-C3-C4-C5

48 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	301	CHD	1	0
26	P	305	CDL	9	0
14	N	602	HEA	3	0
26	C	307	CDL	16	0
14	N	601[B]	HEA	13	0
14	N	601[A]	HEA	1	0
20	J	102	EDO	2	0
25	G	103	PEK	1	0
18	C	306	PGV	1	0
14	A	601[A]	HEA	1	0
25	T	102	PEK	4	0
20	A	612	EDO	1	0
21	O	301	TGL	4	0
21	Q	201	TGL	2	0
26	G	101	CDL	12	0
27	C	313	DMU	10	0
25	T	101	PEK	3	0
27	Z	101	DMU	1	0
24	W	101	CHD	2	0
21	N	606	TGL	4	0
18	N	607	PGV	3	0
27	W	104	DMU	11	0
20	L	103	EDO	2	0
20	N	613	EDO	1	0
23	O	303	PSC	5	0
25	P	303	PEK	2	0

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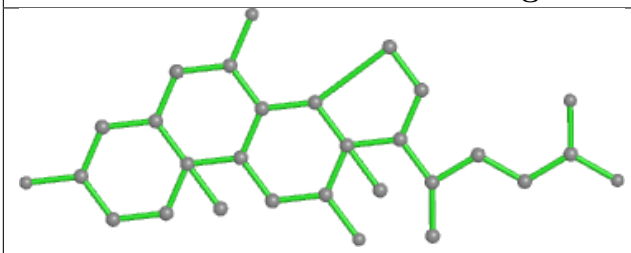
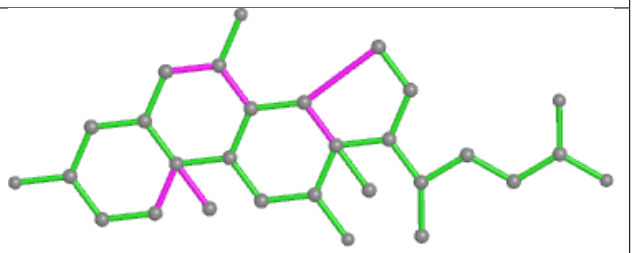
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	303	PEK	3	0
20	A	619	EDO	6	0
18	A	606	PGV	6	0
20	A	615	EDO	1	0
18	P	304	PGV	1	0
14	A	602	HEA	2	0
18	A	608	PGV	2	0
18	U	101	PGV	2	0
24	J	101	CHD	2	0
26	T	103	CDL	7	0
20	B	306	EDO	2	0
25	C	304	PEK	3	0
24	B	304	CHD	1	0
24	P	306	CHD	4	0
18	C	305	PGV	6	0
14	A	601[B]	HEA	5	0
24	C	308	CHD	2	0
21	L	101	TGL	4	0
20	H	101	EDO	1	0
21	B	301	TGL	3	0
23	B	303	PSC	6	0
21	D	201	TGL	6	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.

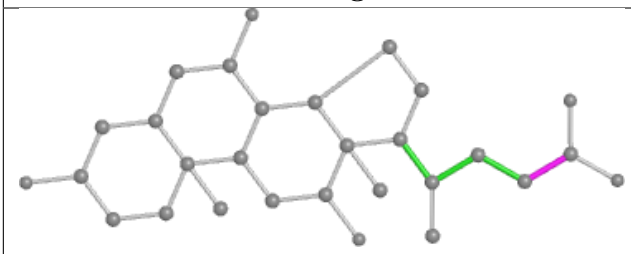
Ligand CHD P 301



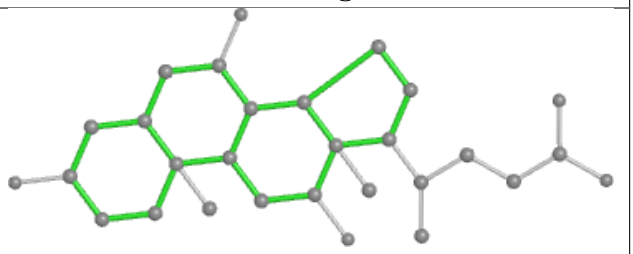
Bond lengths



Bond angles

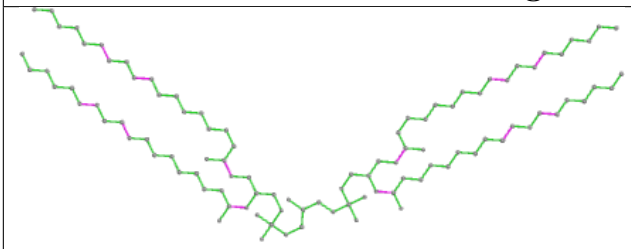


Torsions

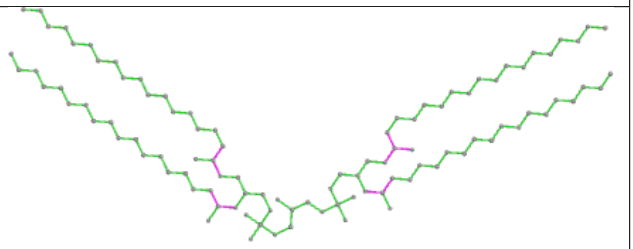


Rings

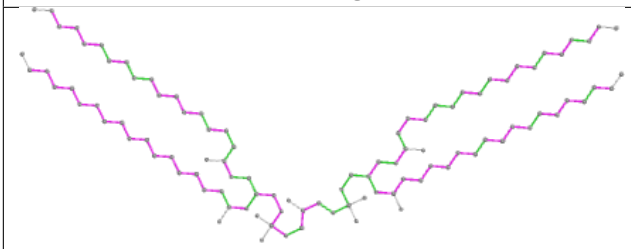
Ligand CDL P 305



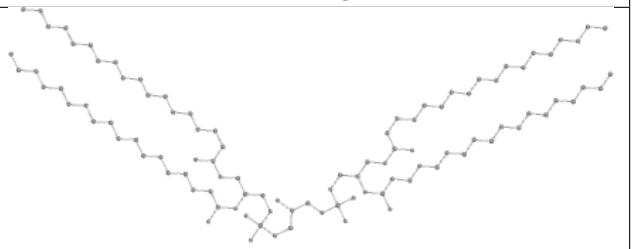
Bond lengths



Bond angles

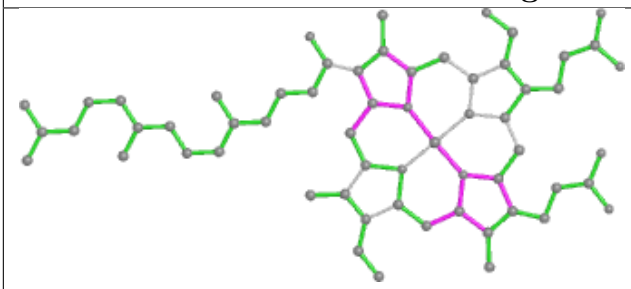


Torsions

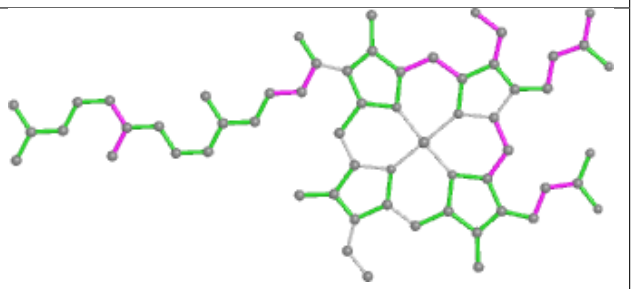


Rings

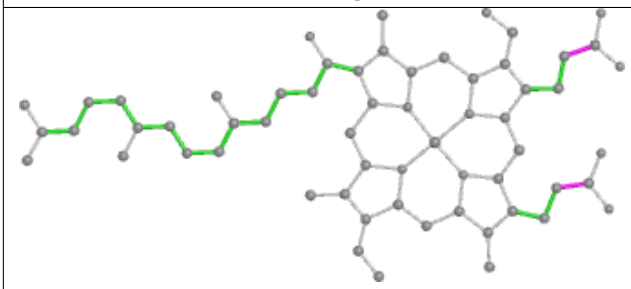
Ligand HEA N 602



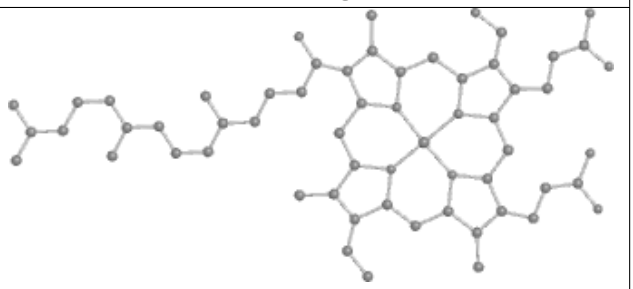
Bond lengths



Bond angles

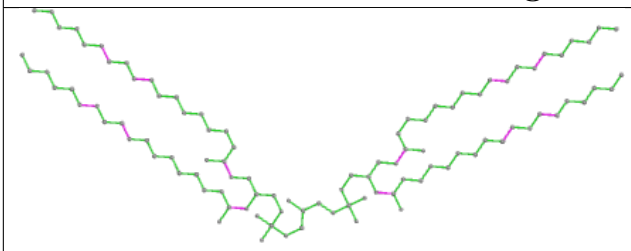


Torsions

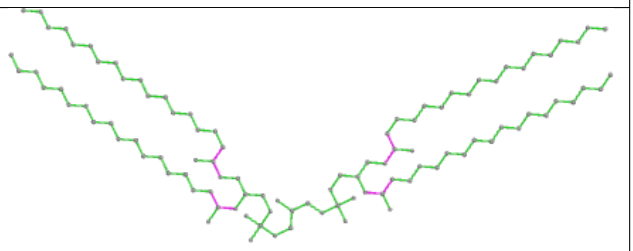


Rings

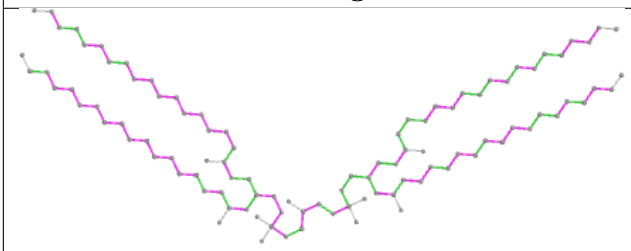
Ligand CDL C 307



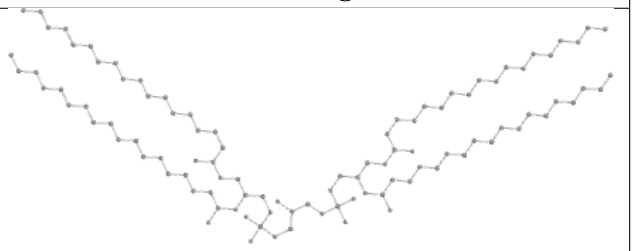
Bond lengths



Bond angles

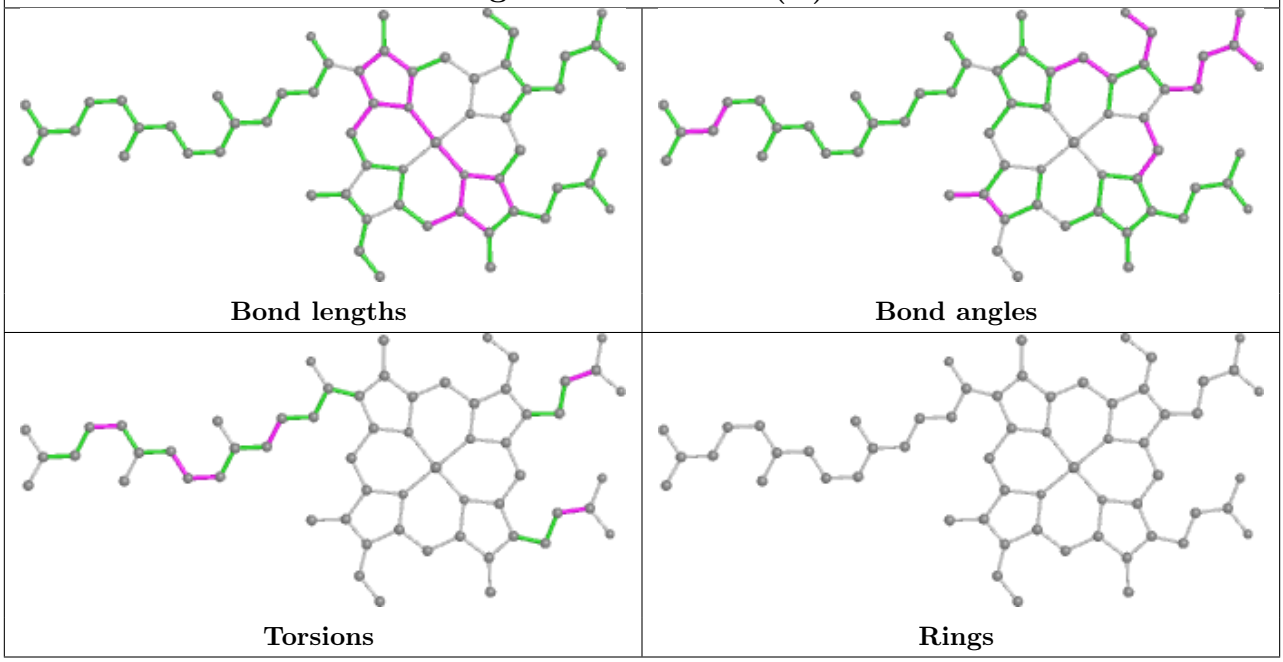


Torsions

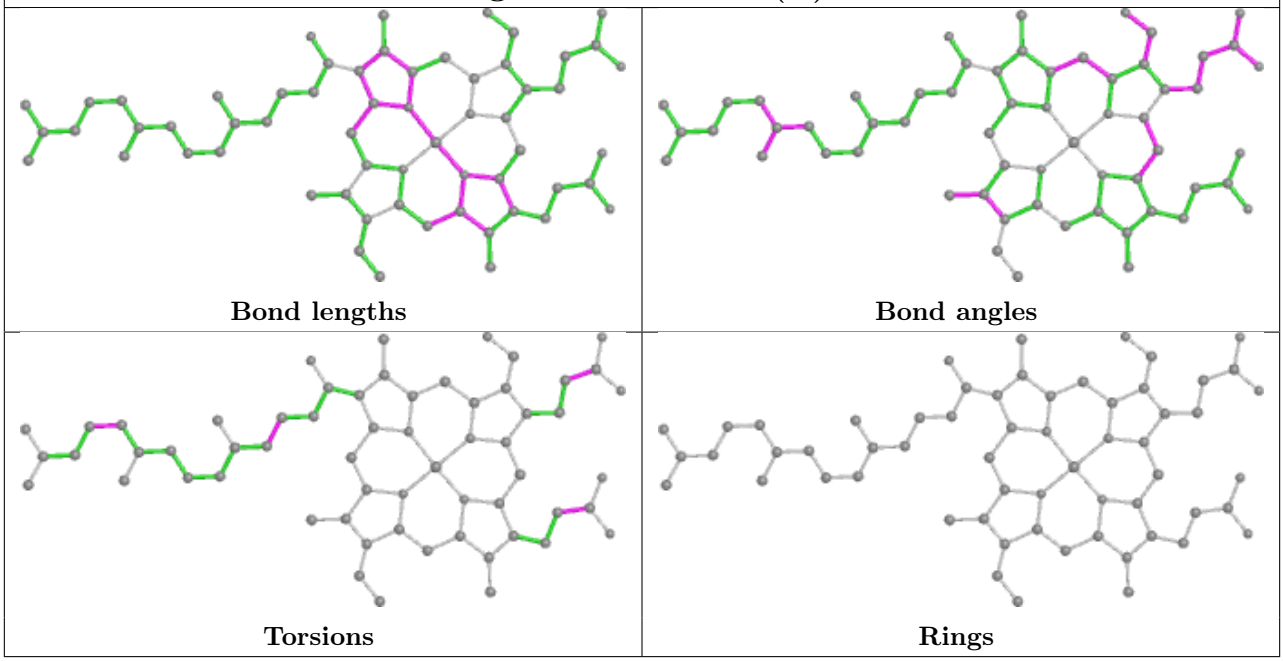


Rings

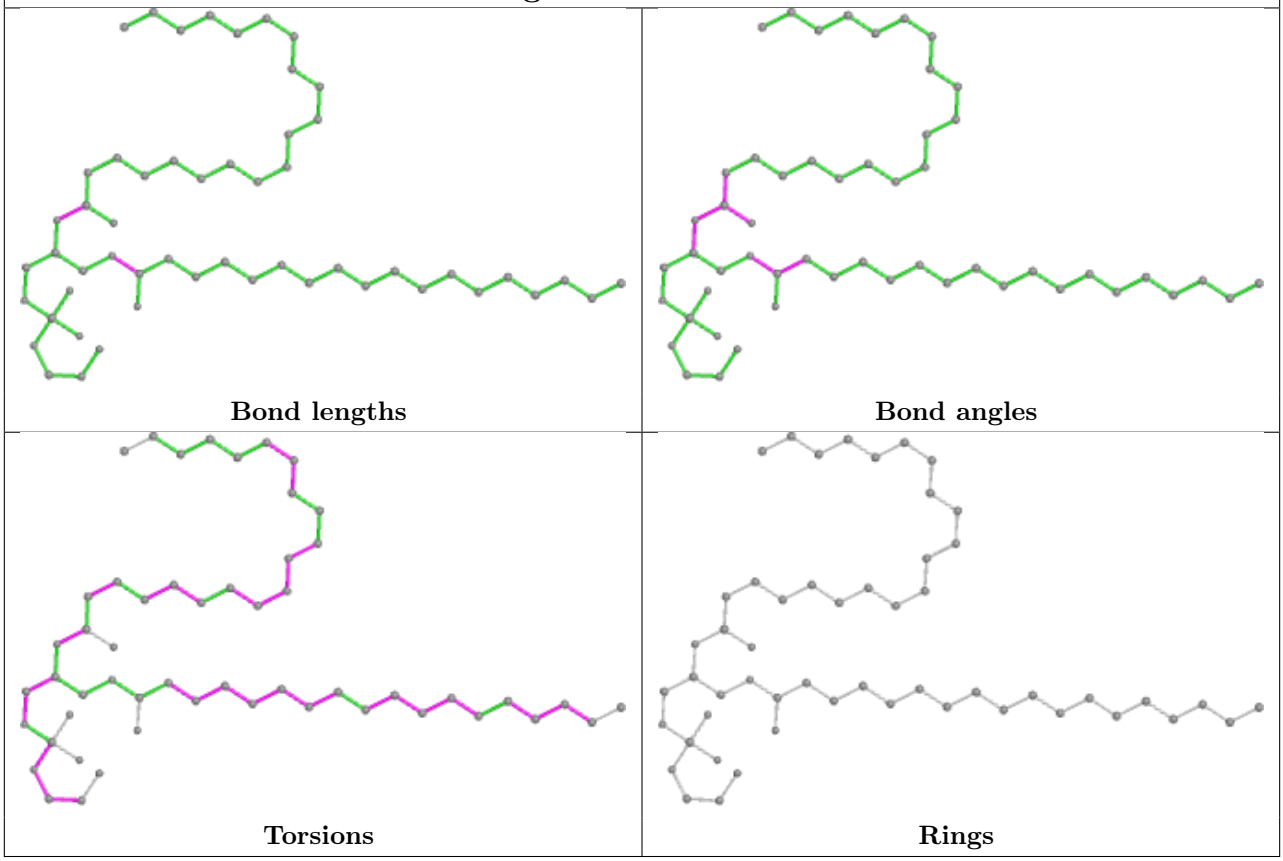
Ligand HEA N 601 (B)



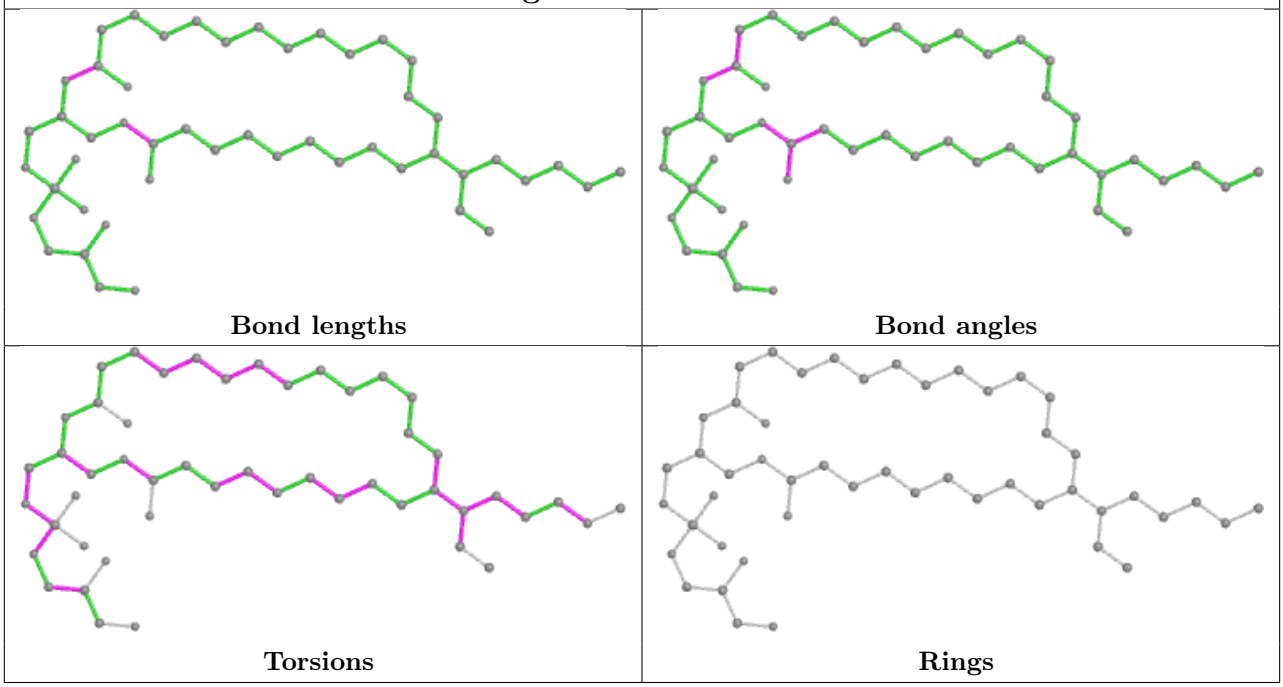
Ligand HEA N 601 (A)



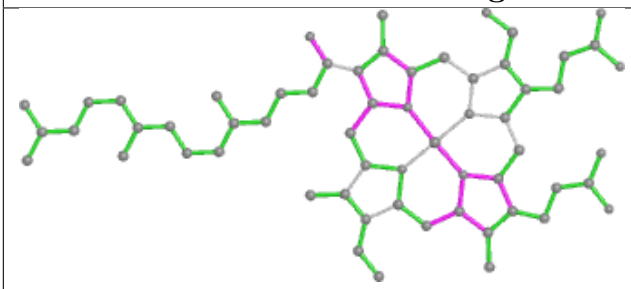
Ligand PEK G 103



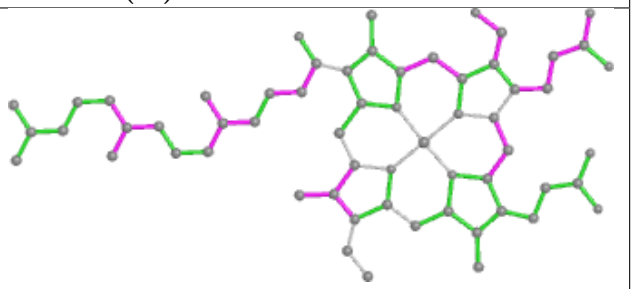
Ligand PGV C 306



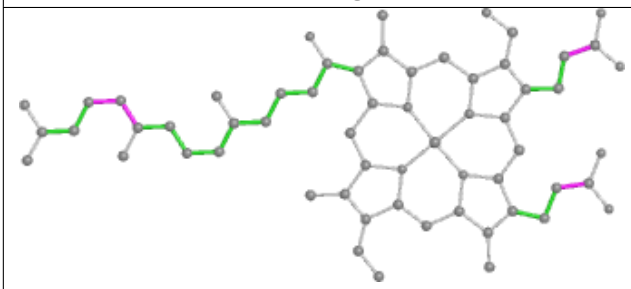
Ligand HEA A 601 (A)



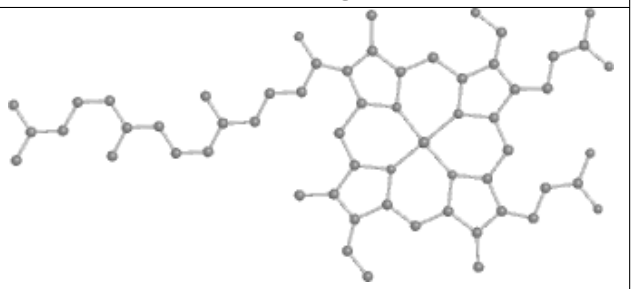
Bond lengths



Bond angles

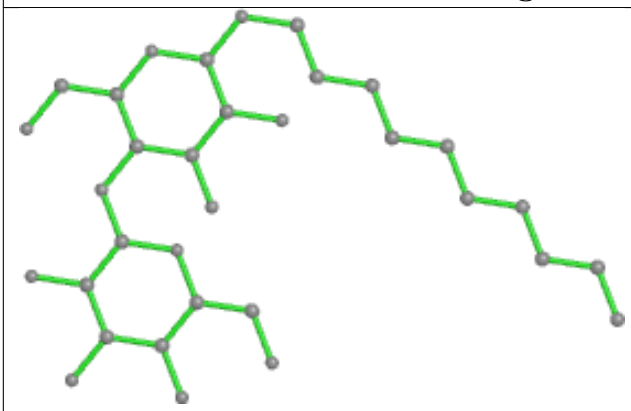


Torsions

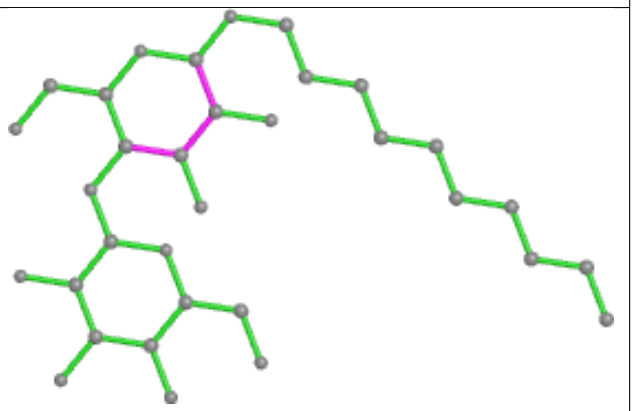


Rings

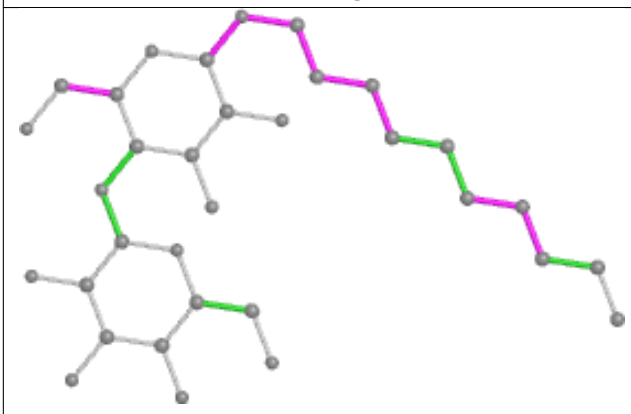
Ligand DMU C 312



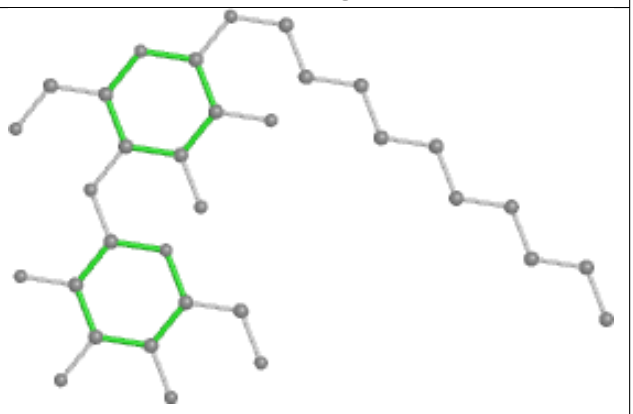
Bond lengths



Bond angles

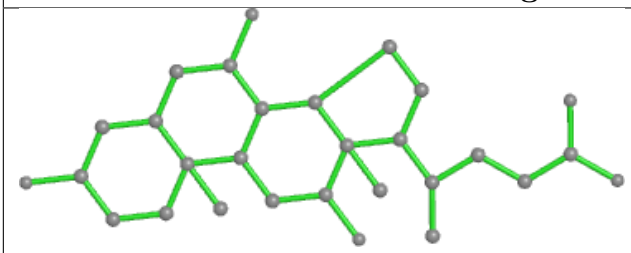


Torsions

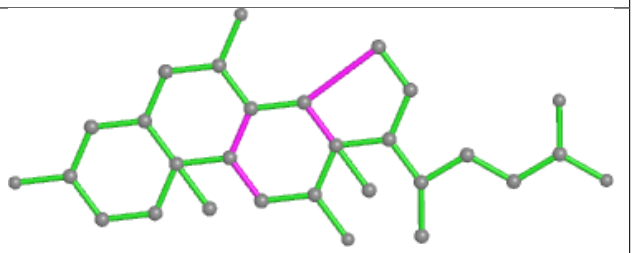


Rings

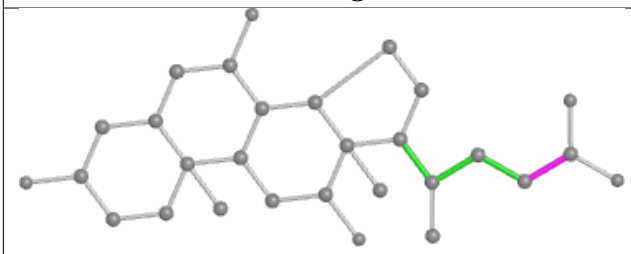
Ligand CHD C 301



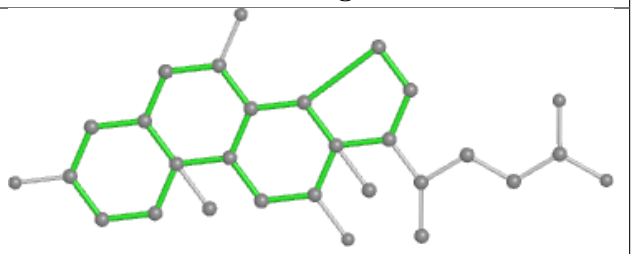
Bond lengths



Bond angles

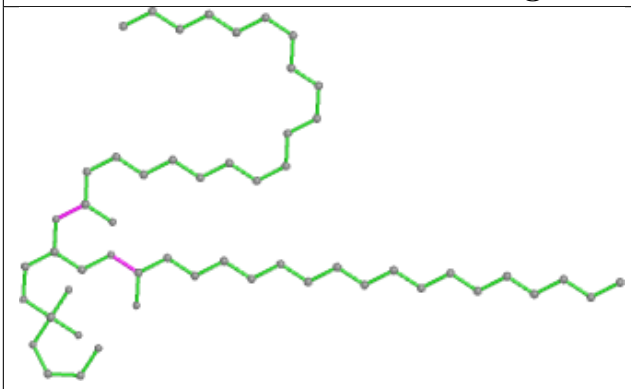


Torsions

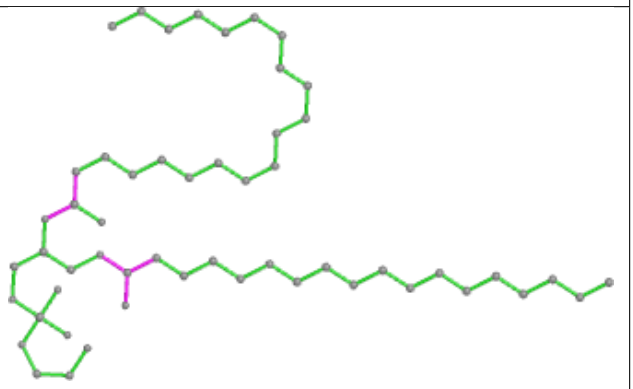


Rings

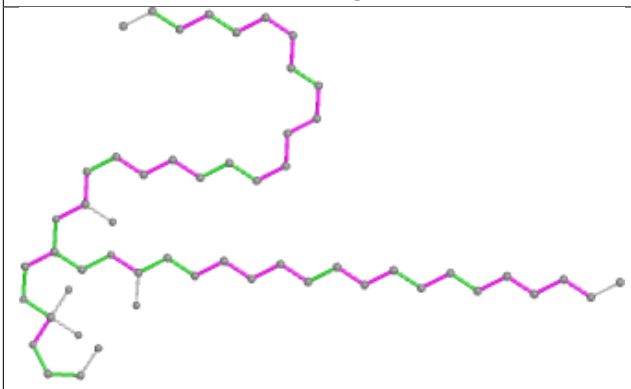
Ligand PEK T 102



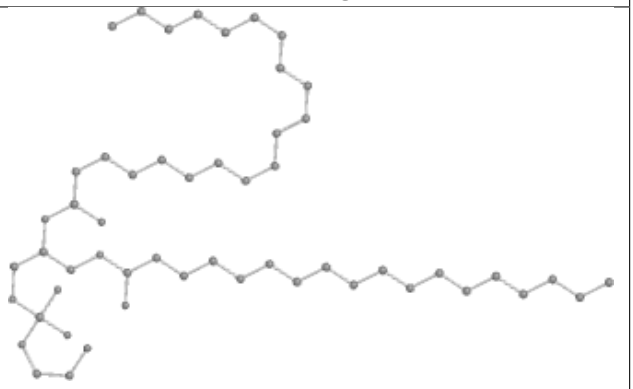
Bond lengths



Bond angles

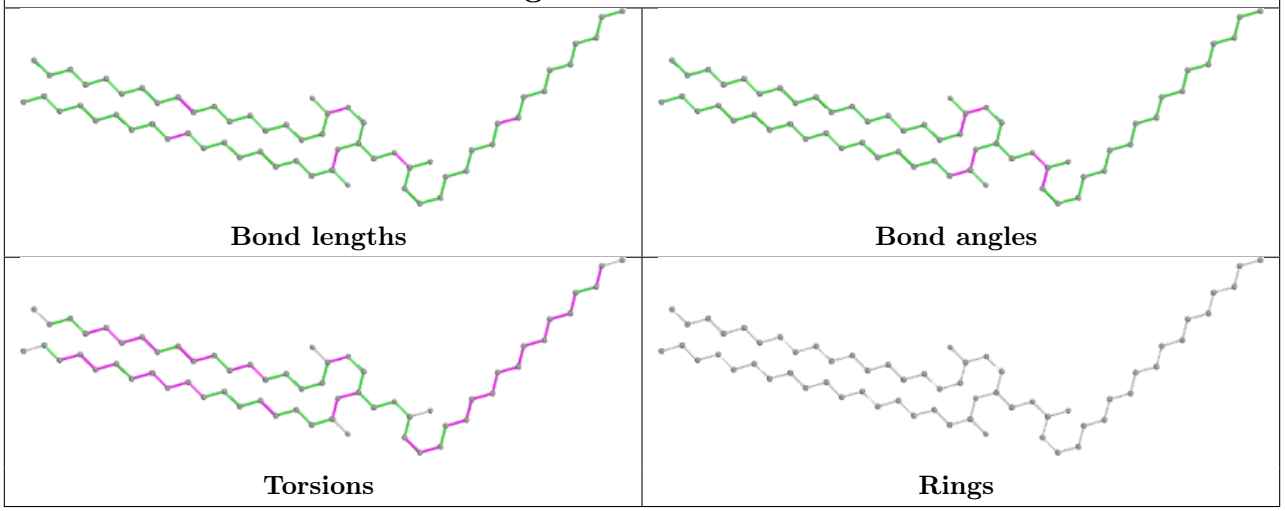


Torsions

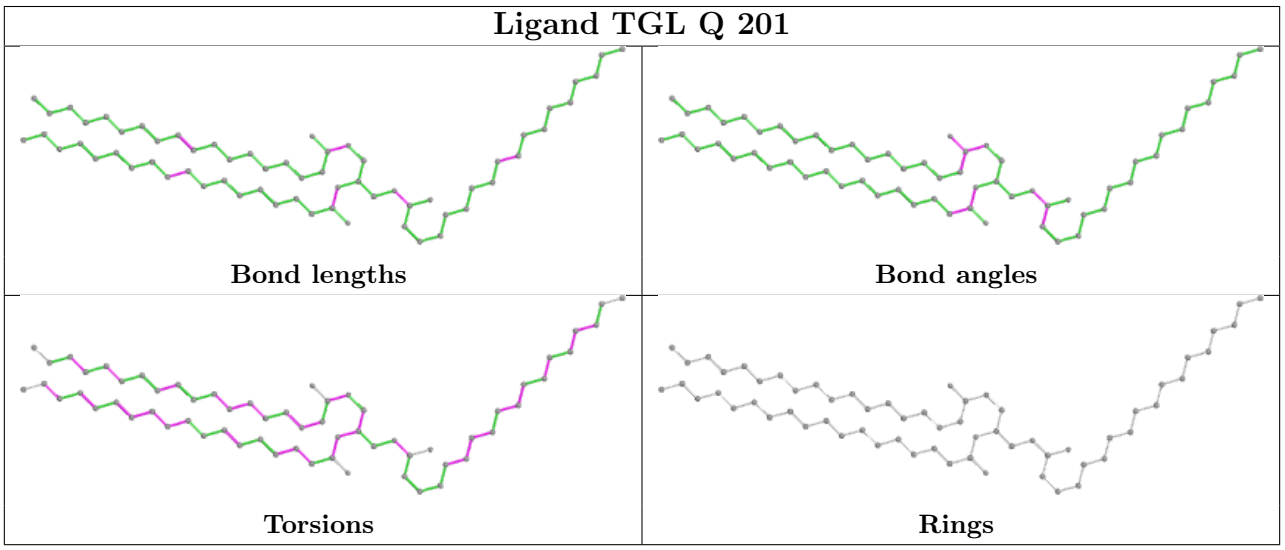


Rings

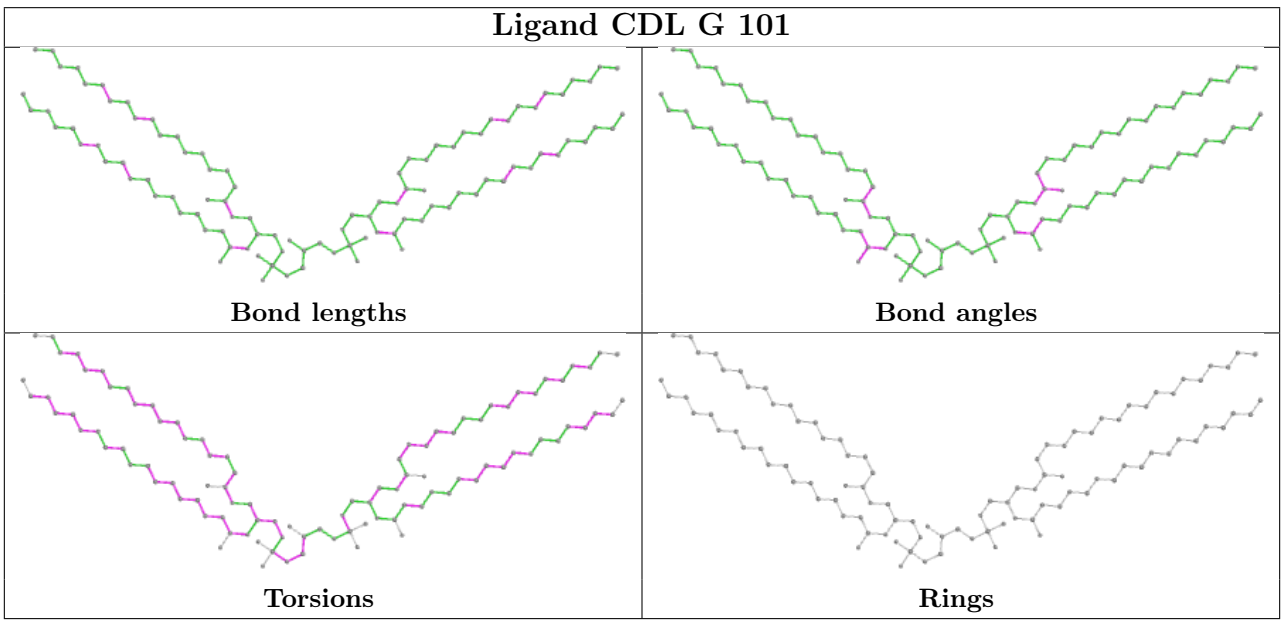
Ligand TGL O 301



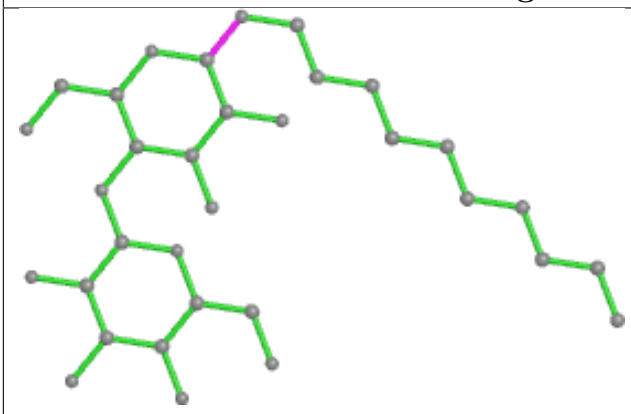
Ligand TGL Q 201



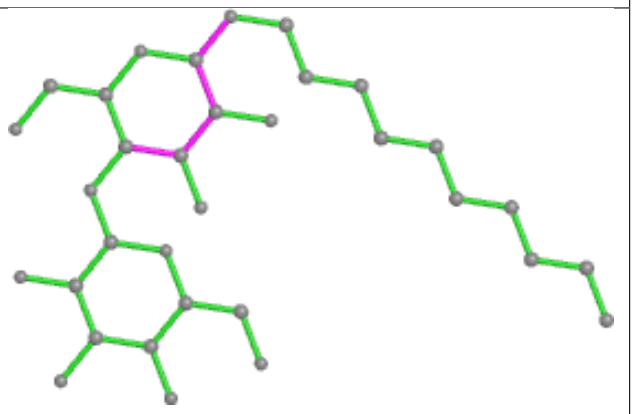
Ligand CDL G 101



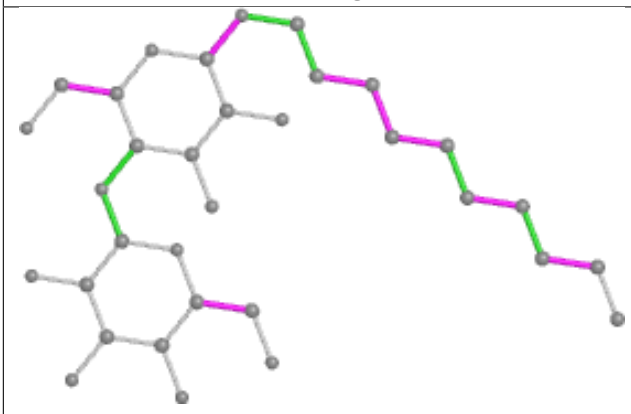
Ligand DMU C 313



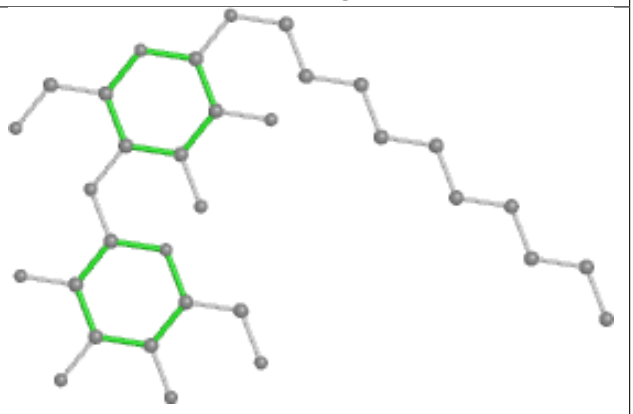
Bond lengths



Bond angles

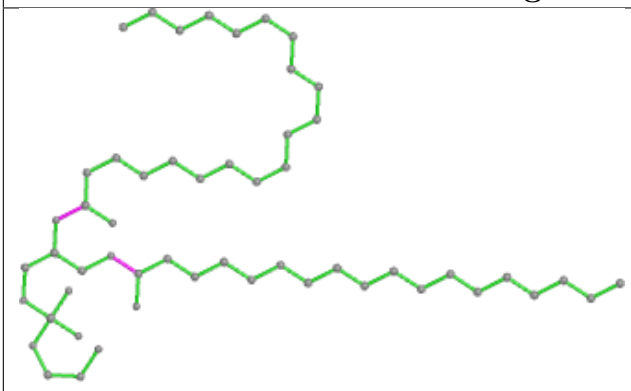


Torsions

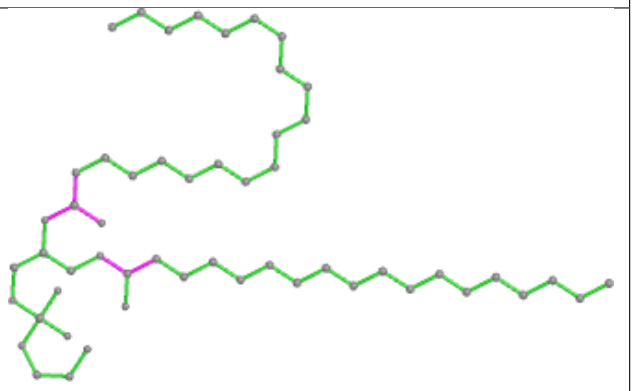


Rings

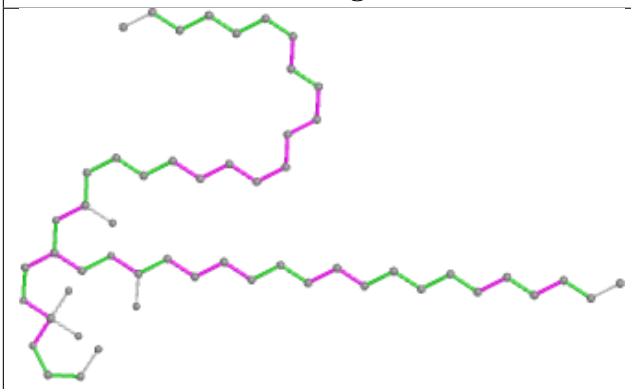
Ligand PEK T 101



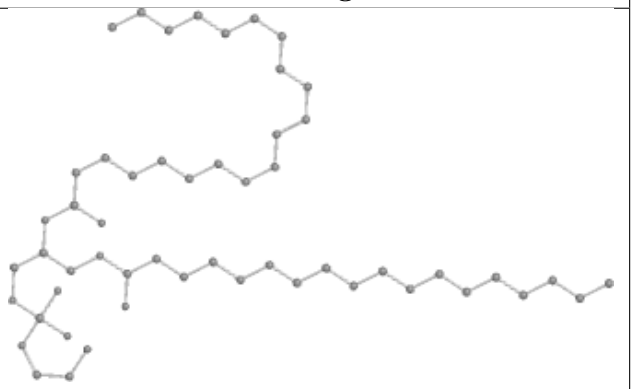
Bond lengths



Bond angles

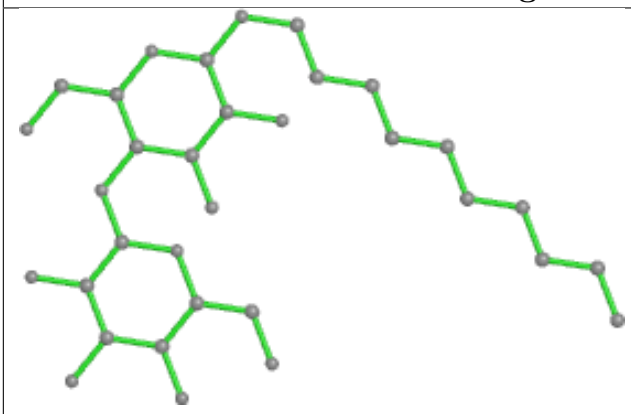


Torsions

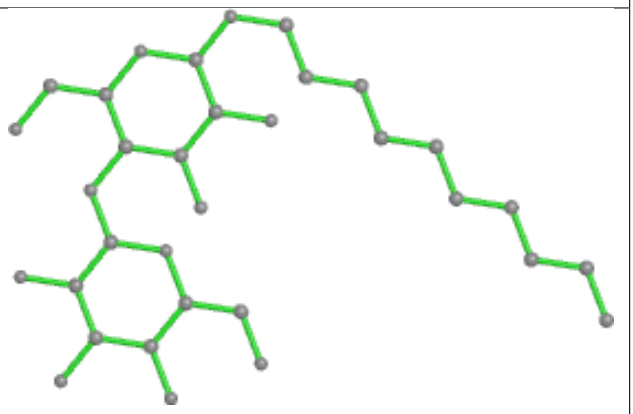


Rings

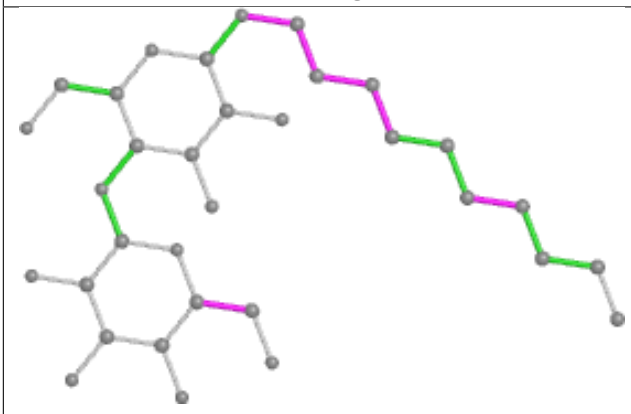
Ligand DMU Z 101



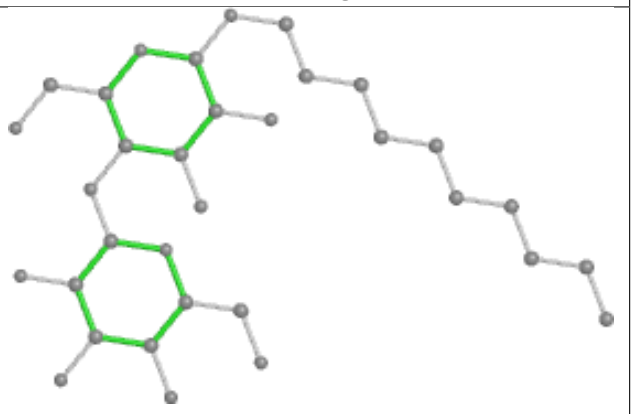
Bond lengths



Bond angles

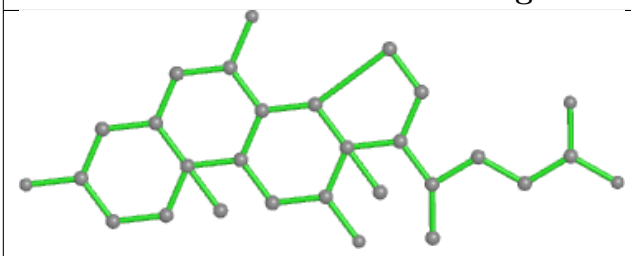


Torsions

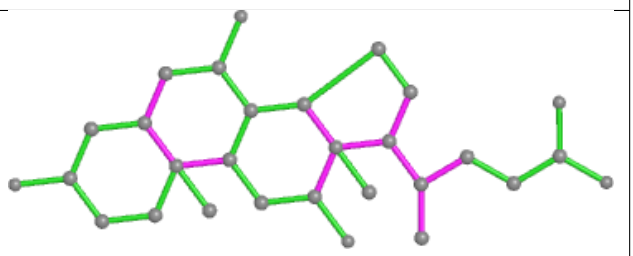


Rings

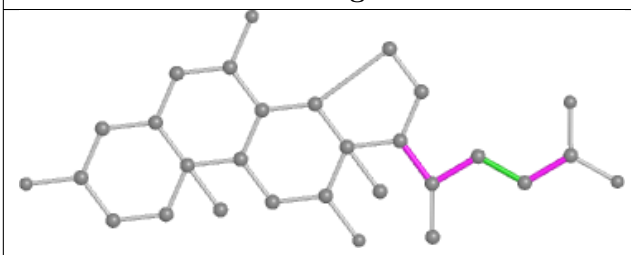
Ligand CHD W 101



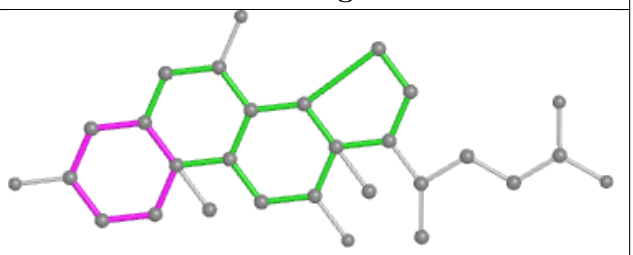
Bond lengths



Bond angles

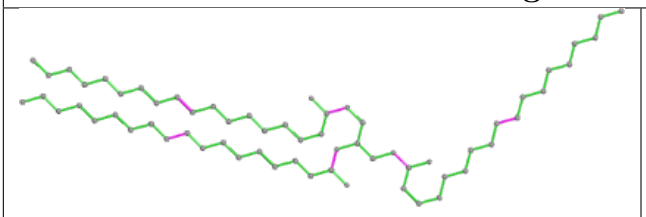


Torsions

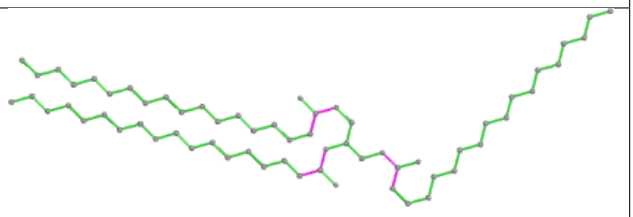


Rings

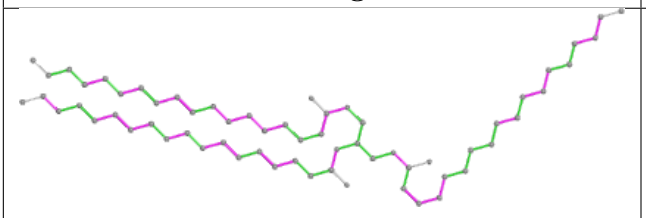
Ligand TGL N 606



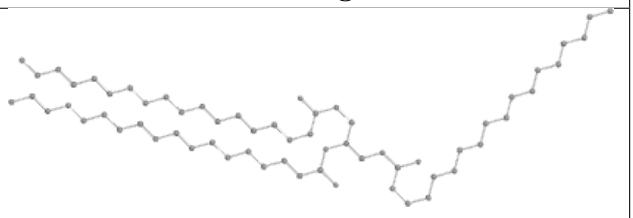
Bond lengths



Bond angles

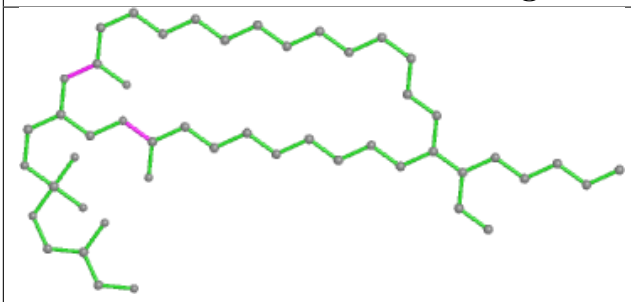


Torsions

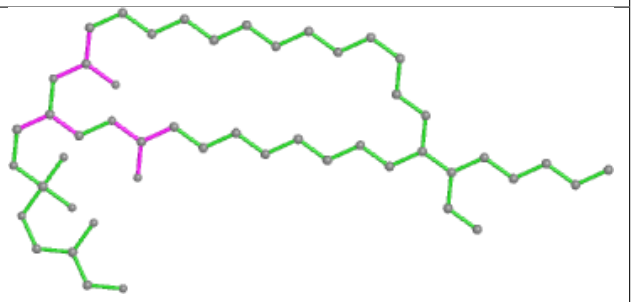


Rings

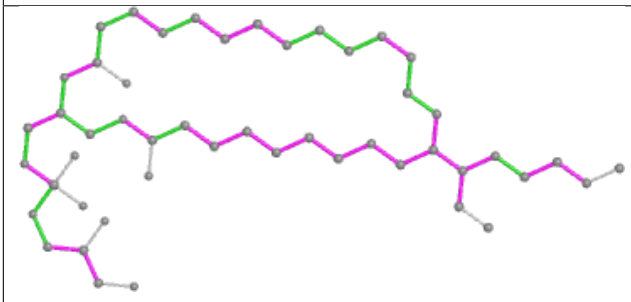
Ligand PGV N 607



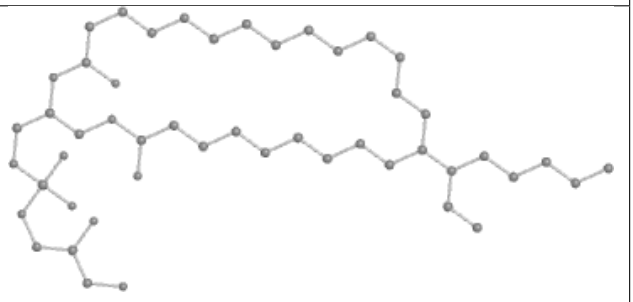
Bond lengths



Bond angles

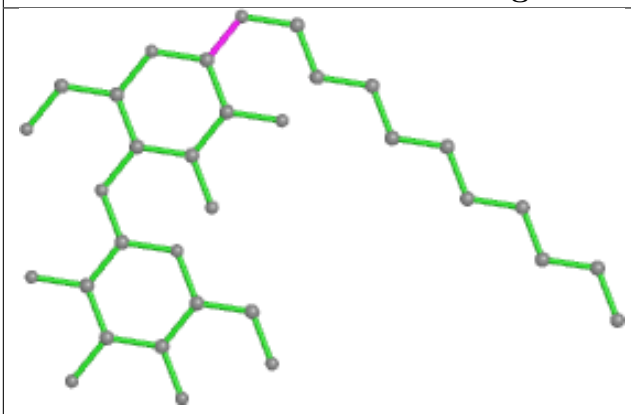


Torsions

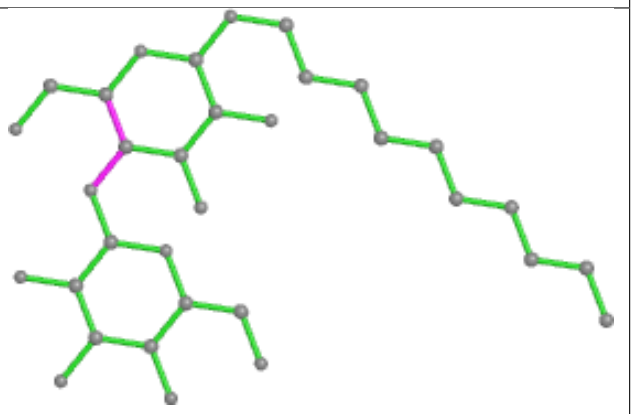


Rings

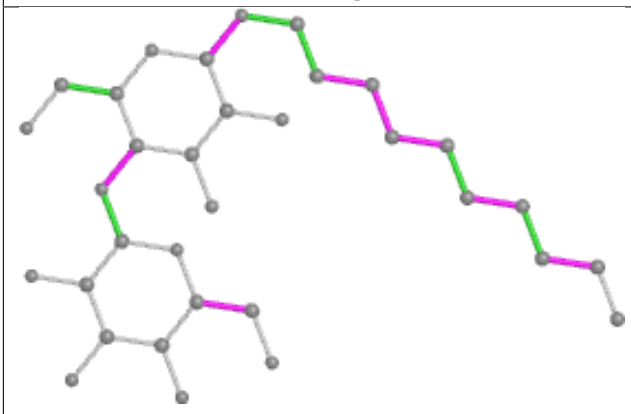
Ligand DMU W 104



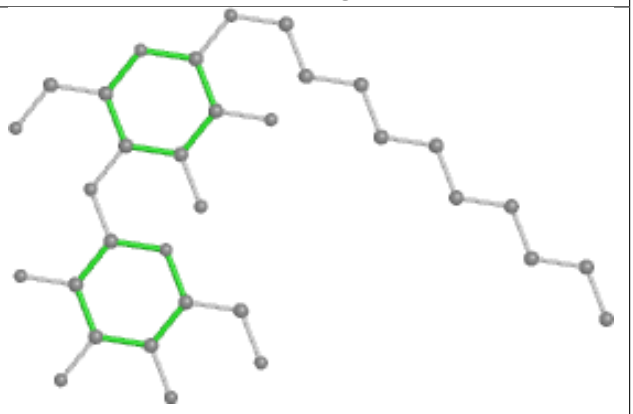
Bond lengths



Bond angles

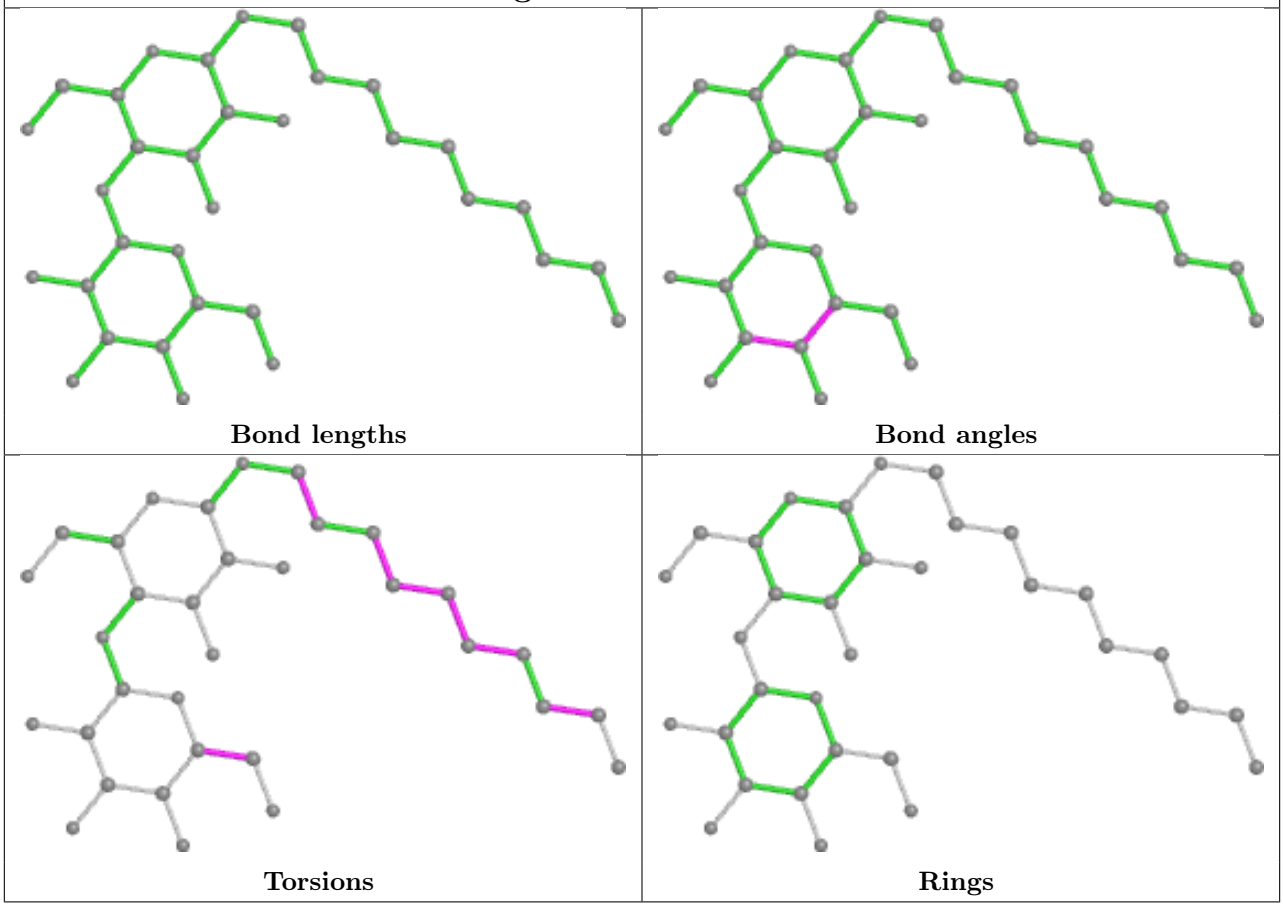


Torsions

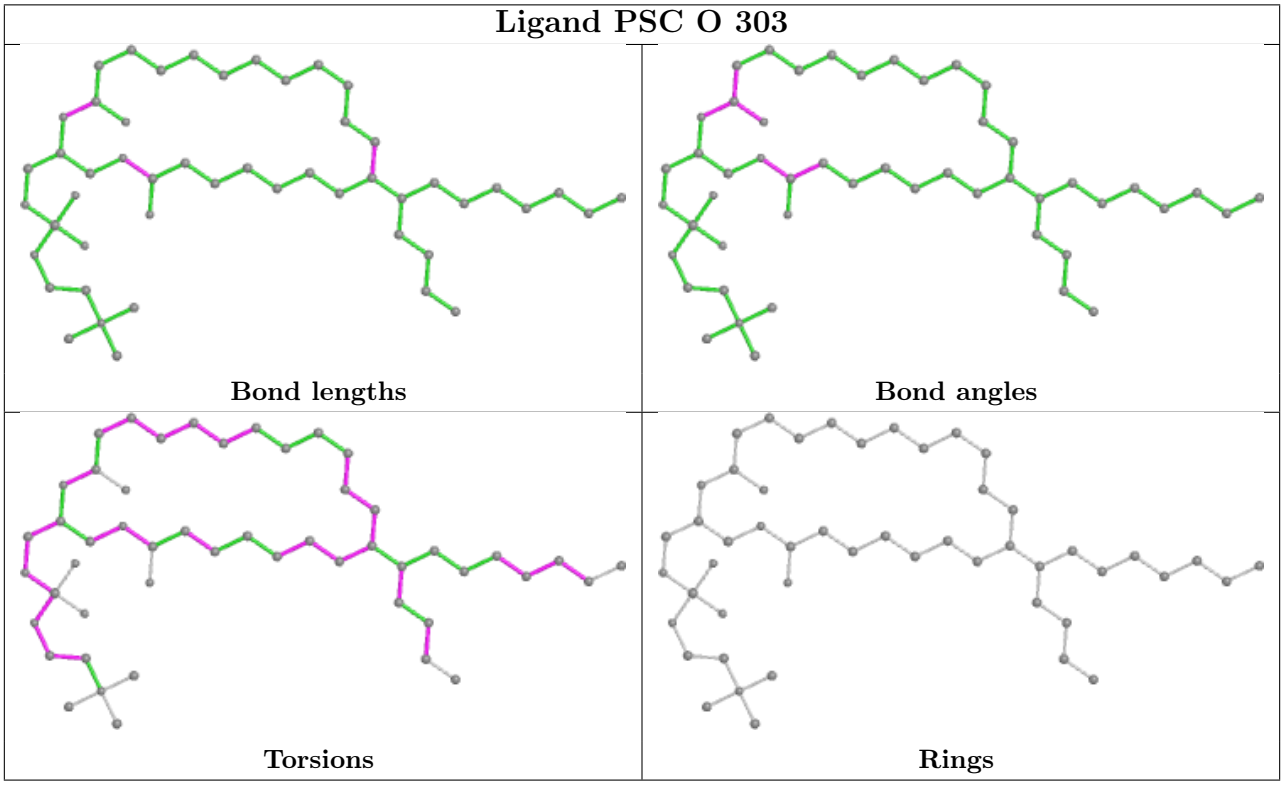


Rings

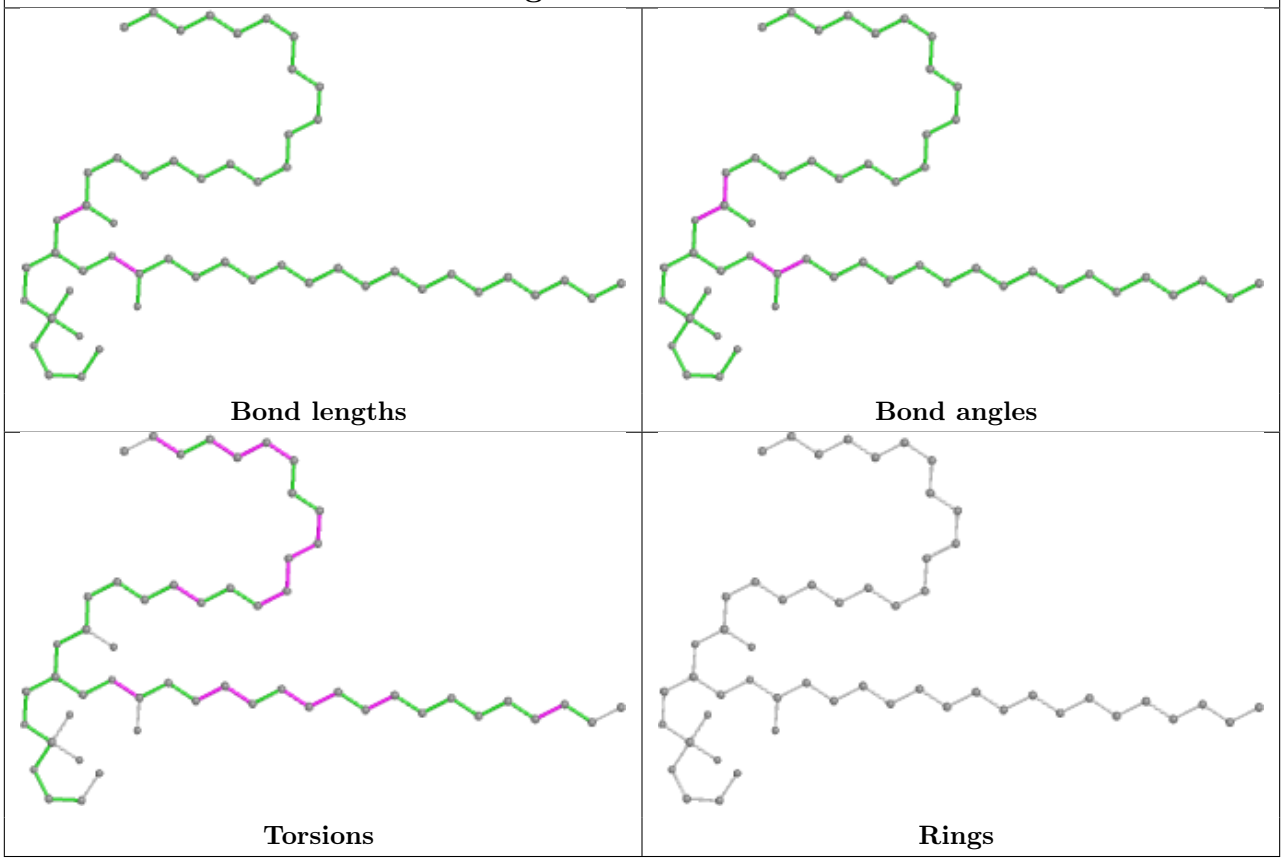
Ligand DMU M 101



Ligand PSC O 303



Ligand PEK P 303



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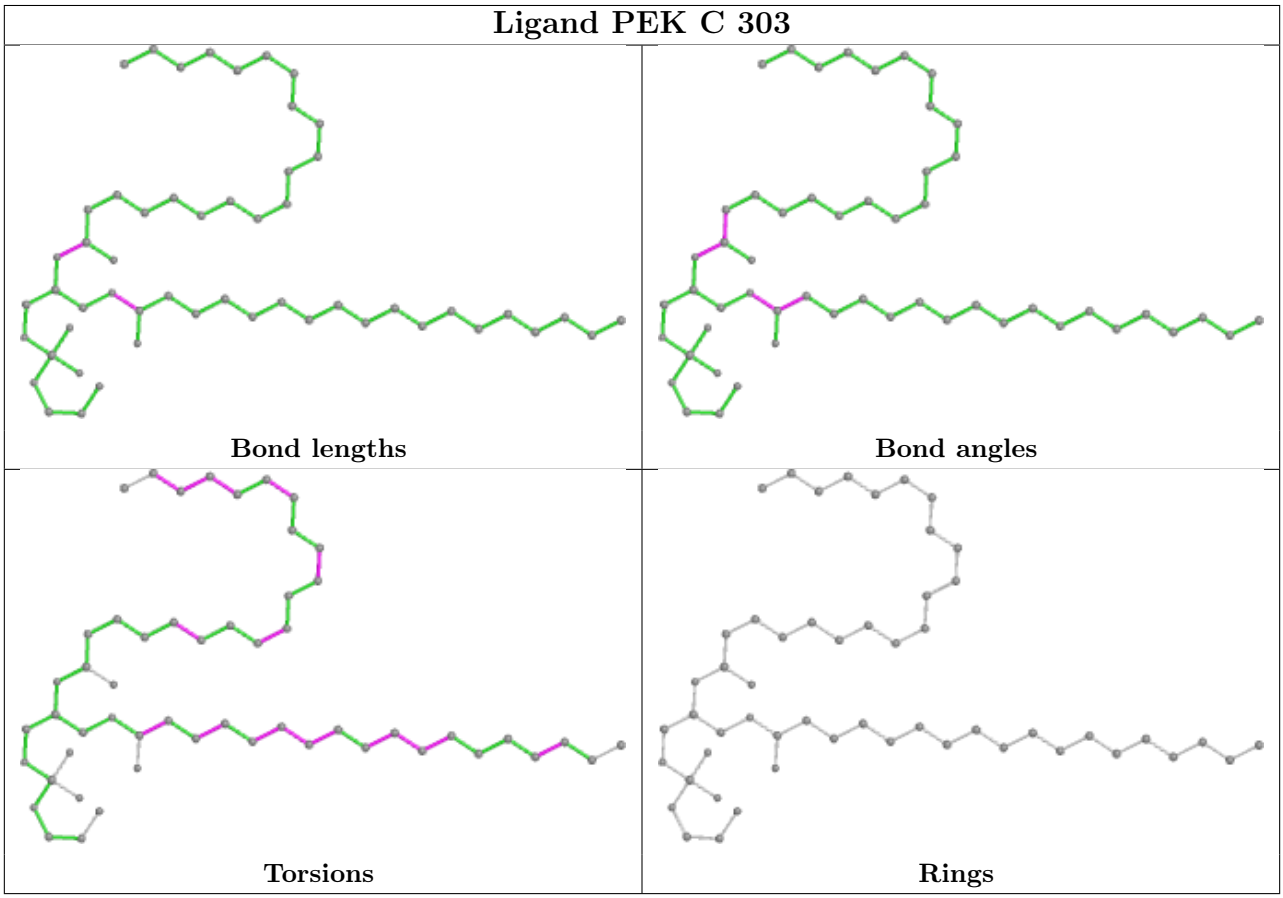
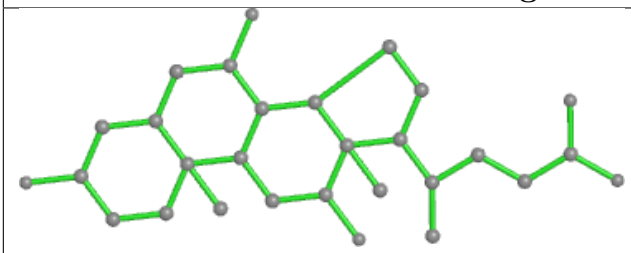
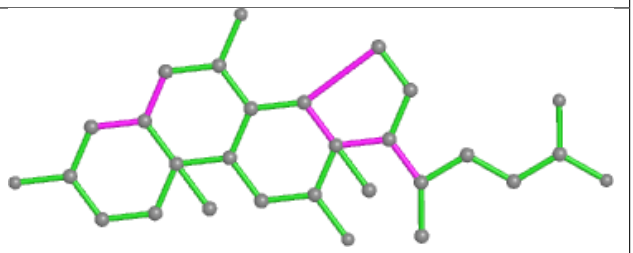


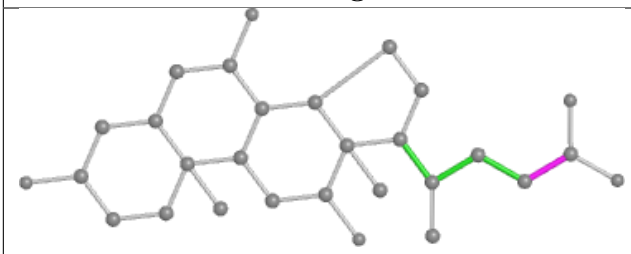
Ligand CHD G 102



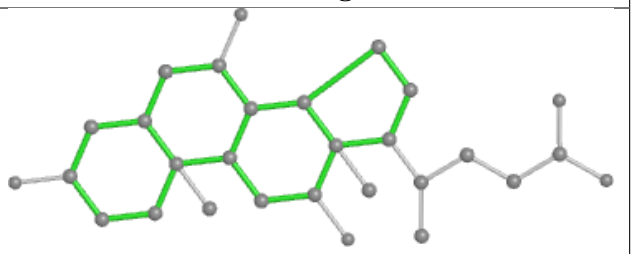
Bond lengths



Bond angles

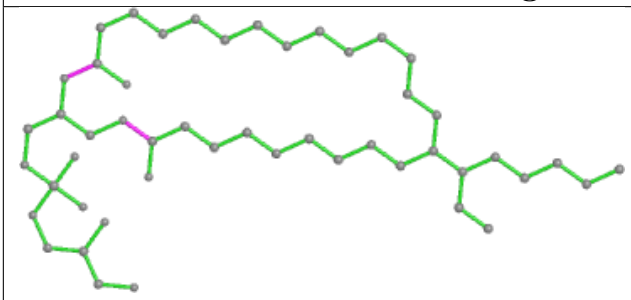


Torsions

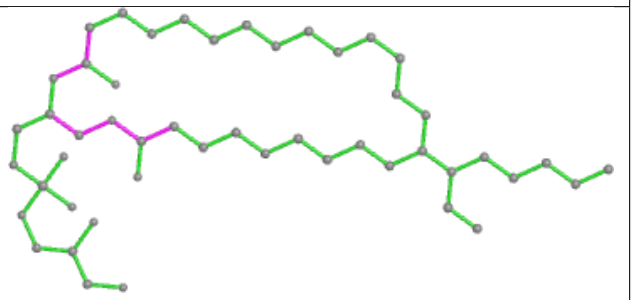


Rings

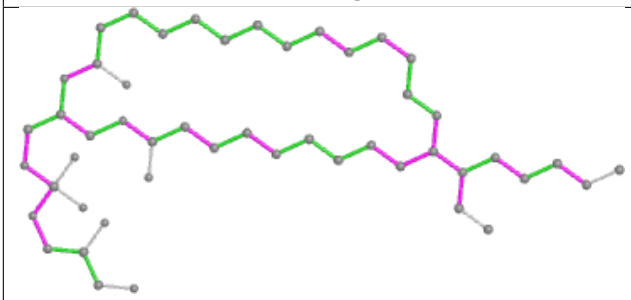
Ligand PGV A 606



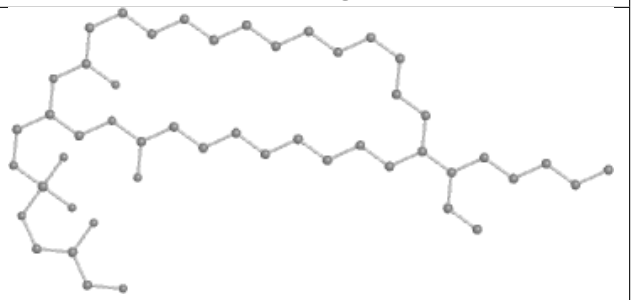
Bond lengths



Bond angles

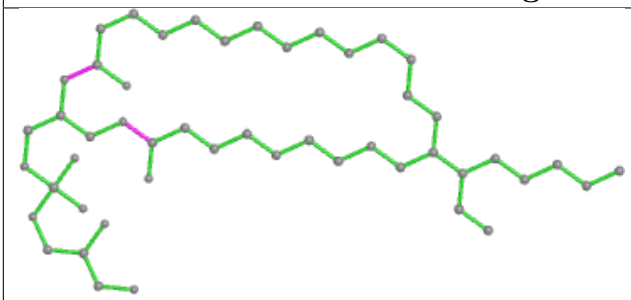


Torsions

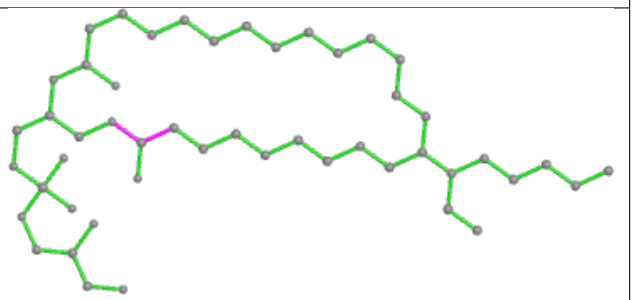


Rings

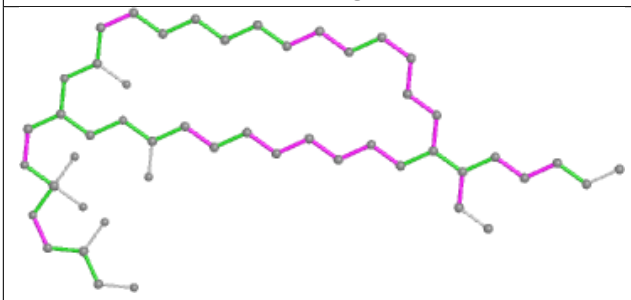
Ligand PGV P 304



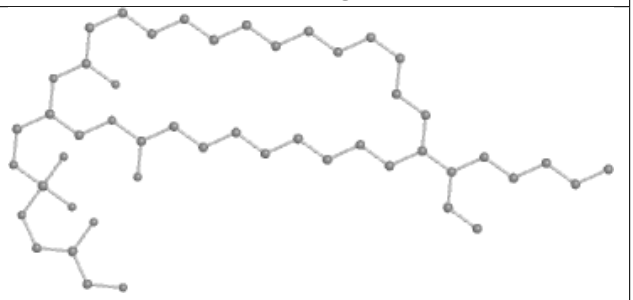
Bond lengths



Bond angles

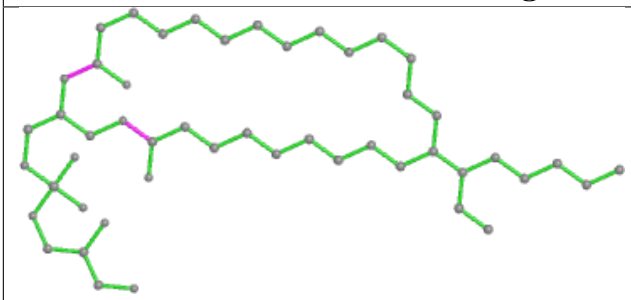


Torsions

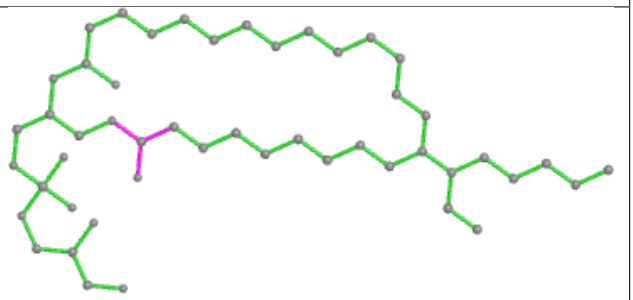


Rings

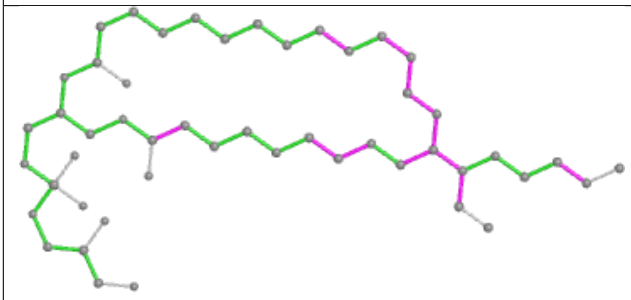
Ligand PGV N 609



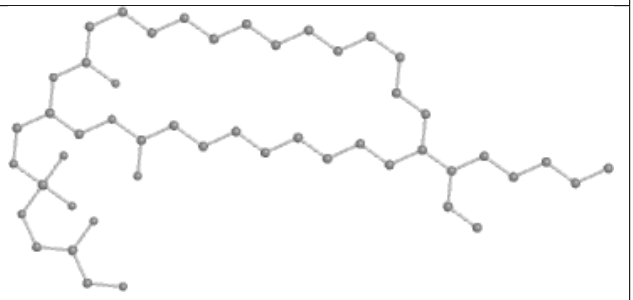
Bond lengths



Bond angles

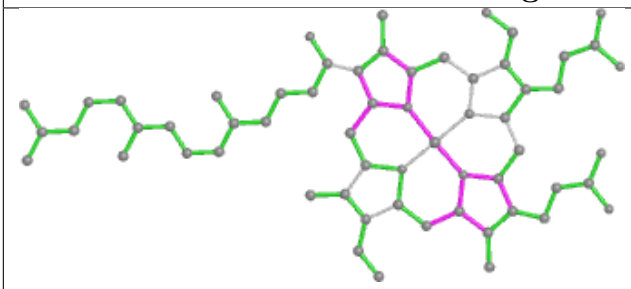


Torsions

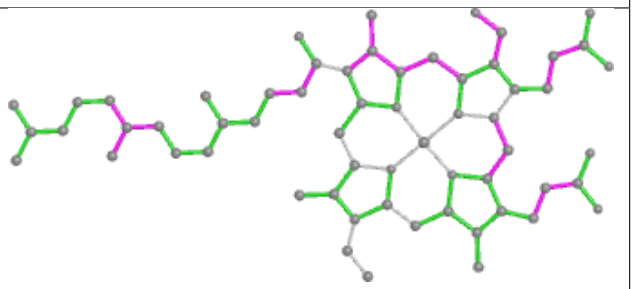


Rings

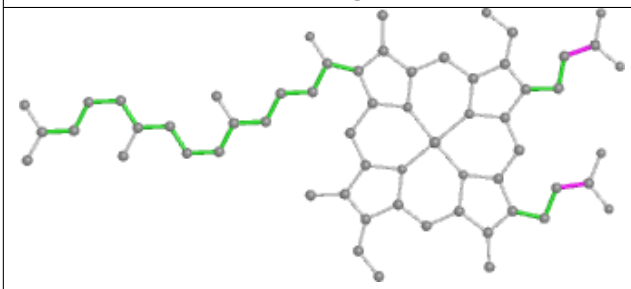
Ligand HEA A 602



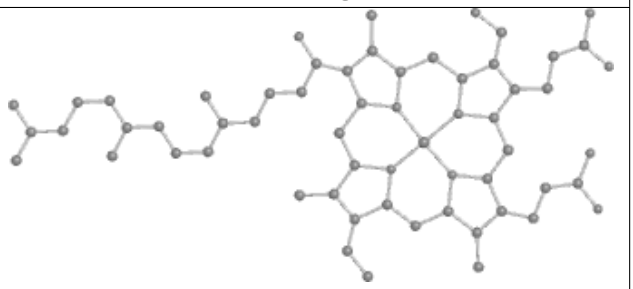
Bond lengths



Bond angles

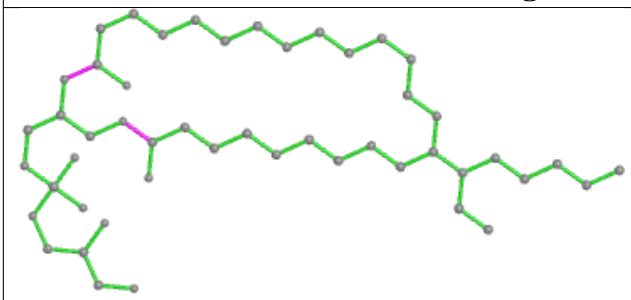


Torsions

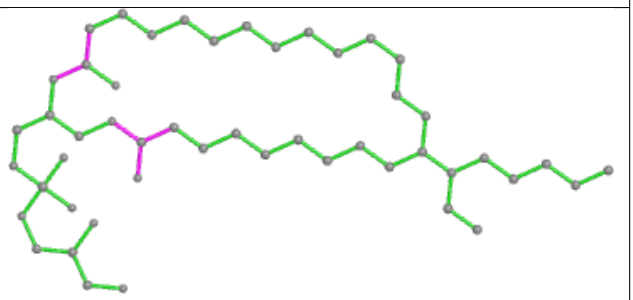


Rings

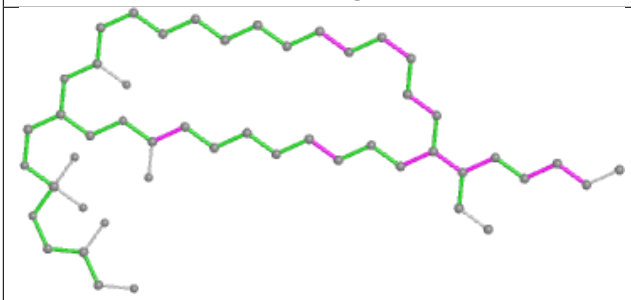
Ligand PGV A 608



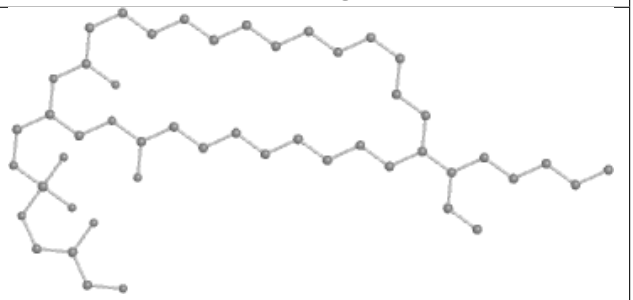
Bond lengths



Bond angles

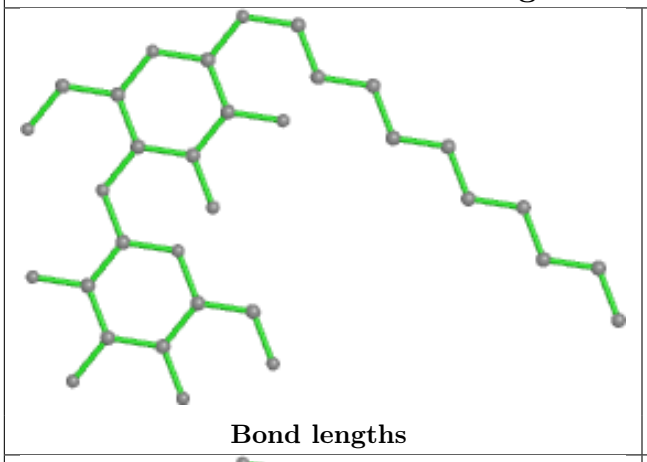


Torsions

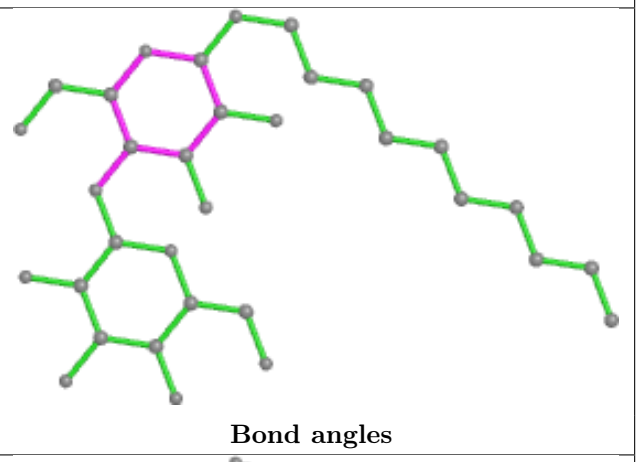


Rings

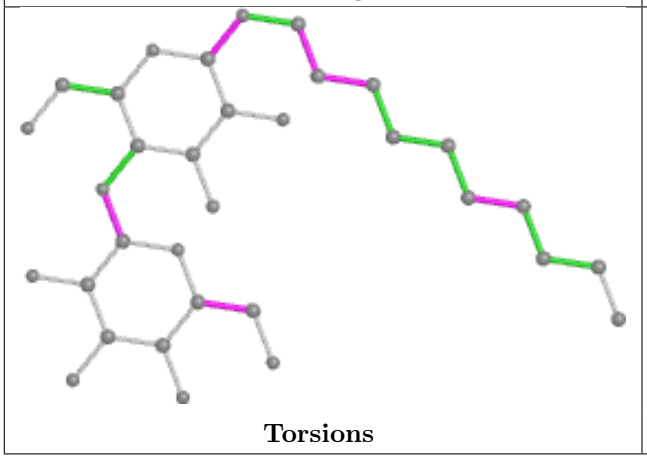
Ligand DMU P 313



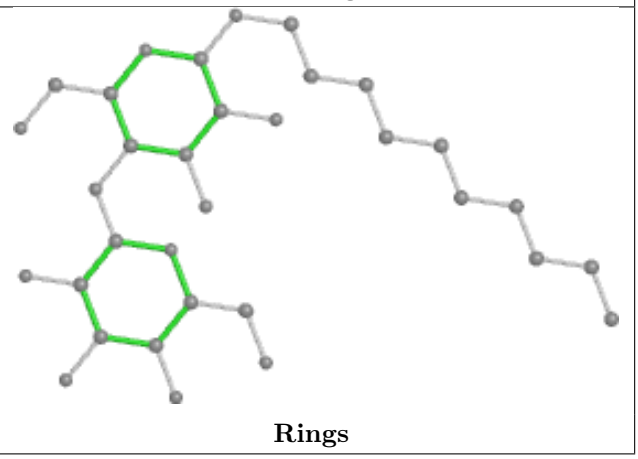
Bond lengths



Bond angles

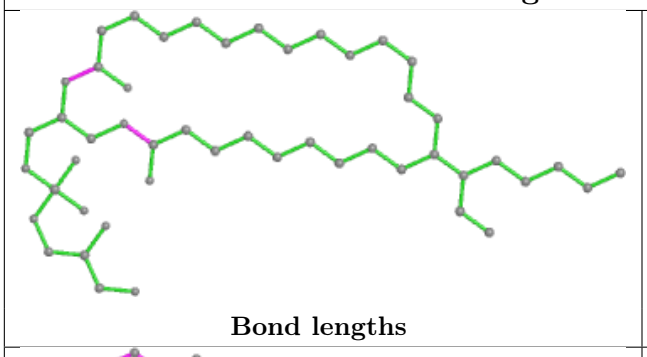


Torsions

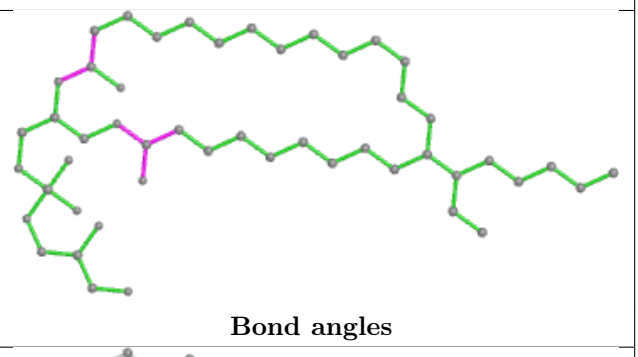


Rings

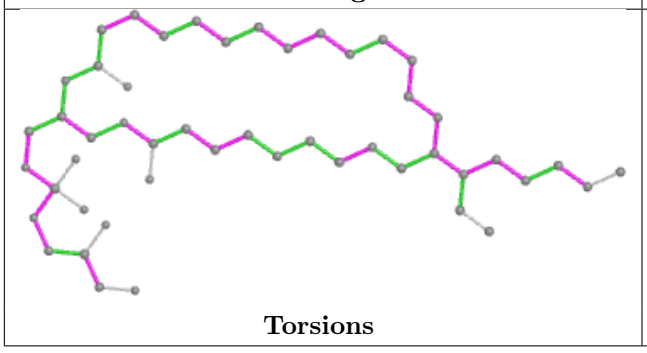
Ligand PGV U 101



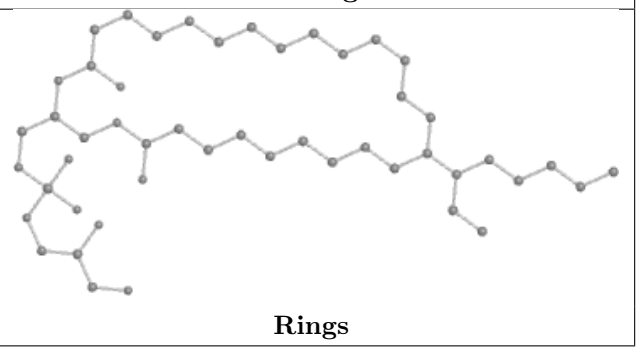
Bond lengths



Bond angles

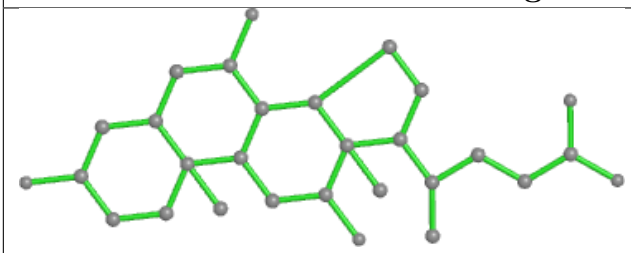


Torsions

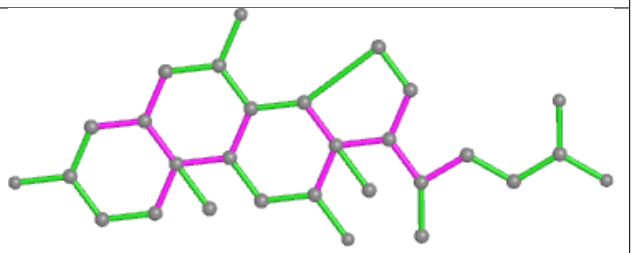


Rings

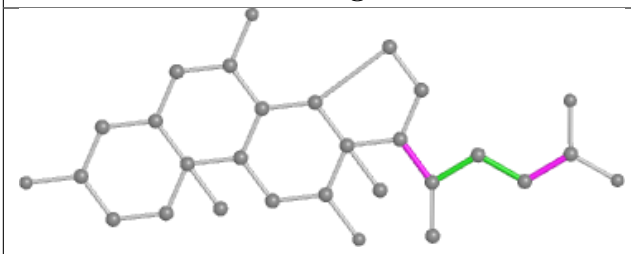
Ligand CHD J 101



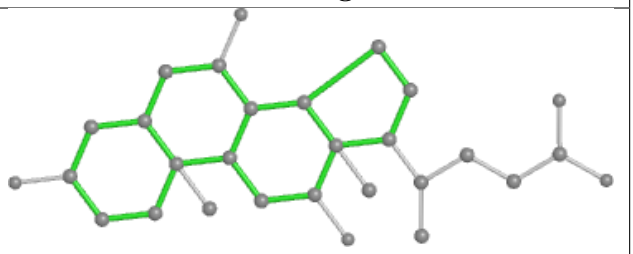
Bond lengths



Bond angles

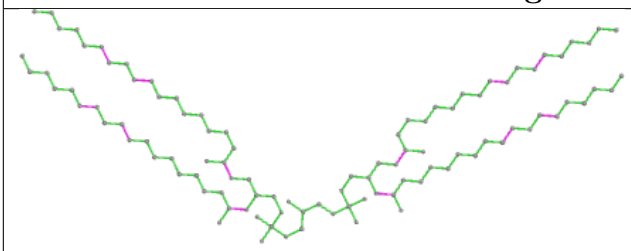


Torsions

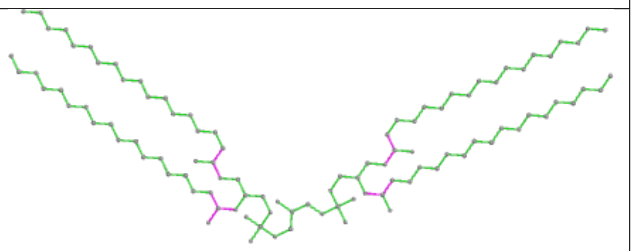


Rings

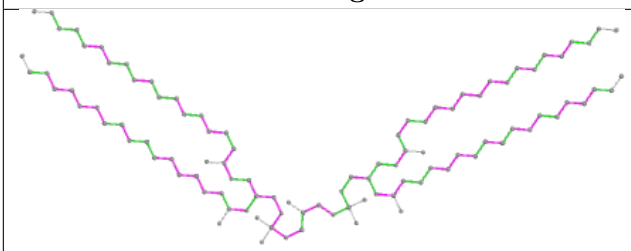
Ligand CDL T 103



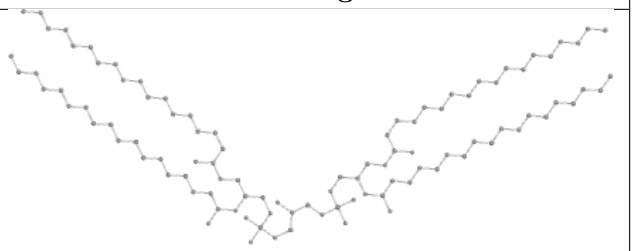
Bond lengths



Bond angles

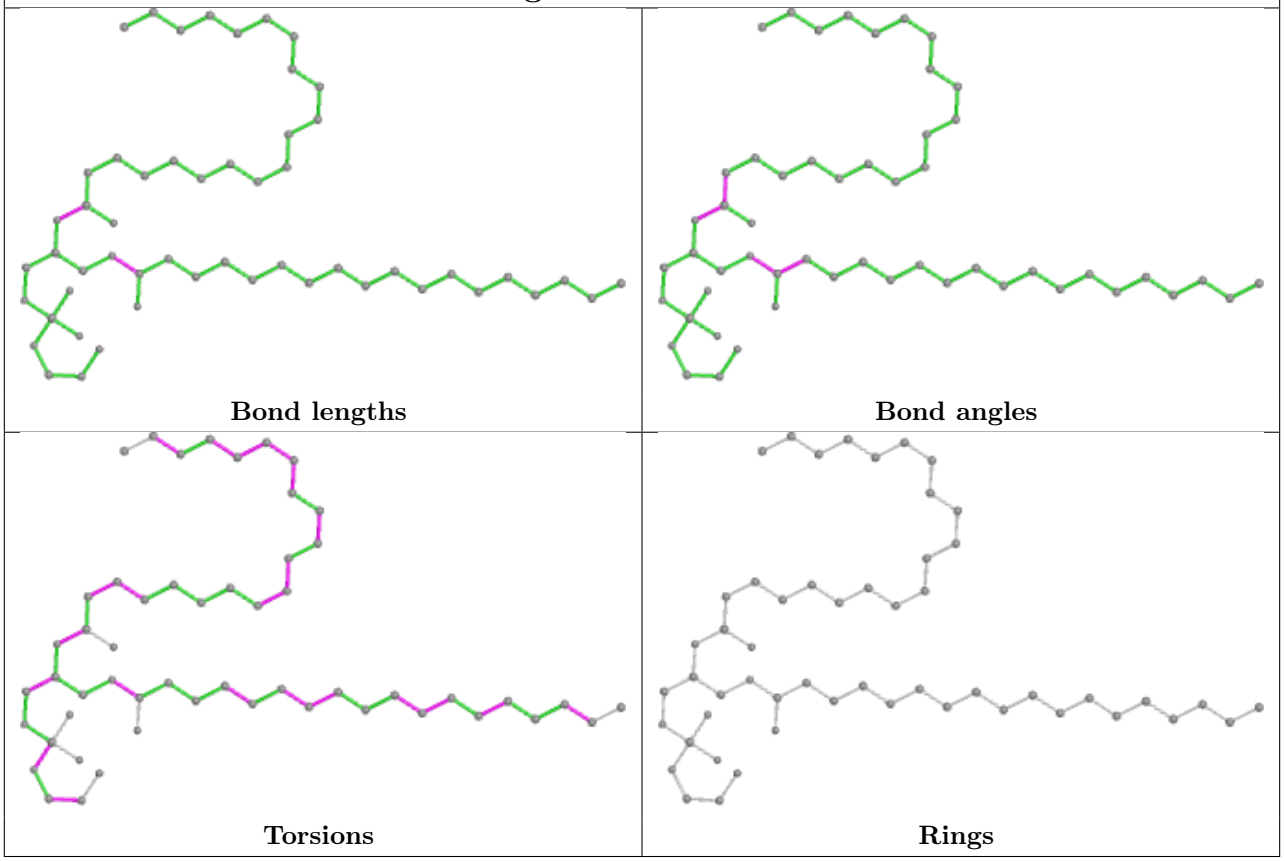


Torsions

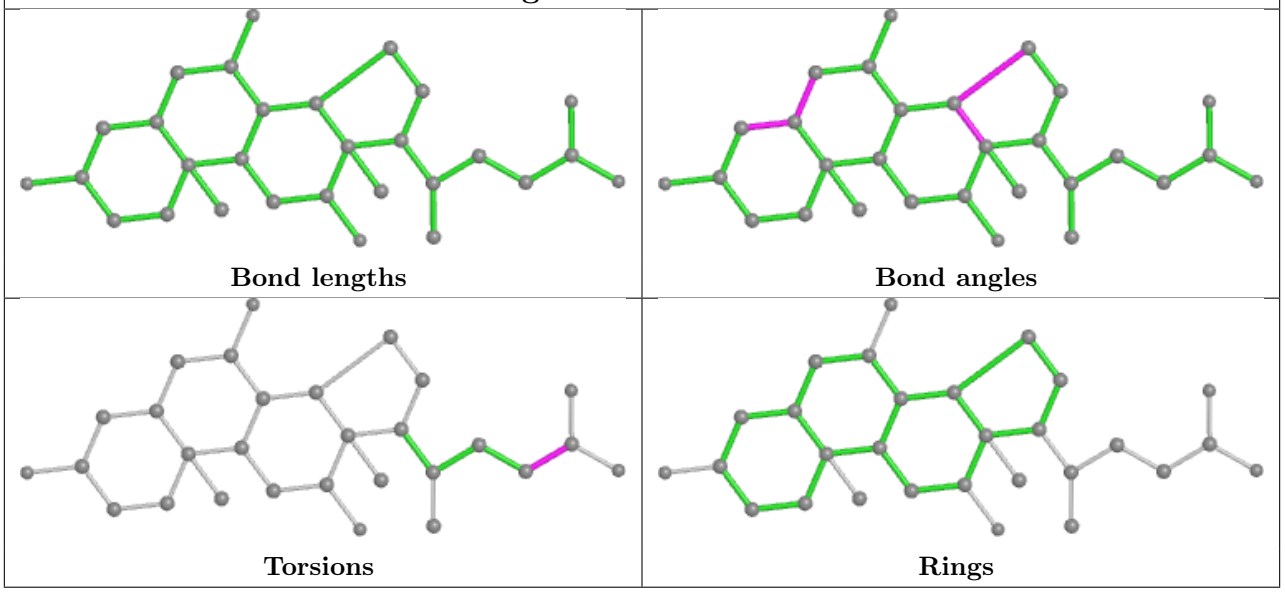


Rings

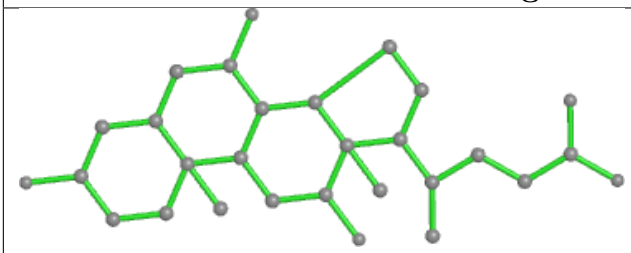
Ligand PEK C 304



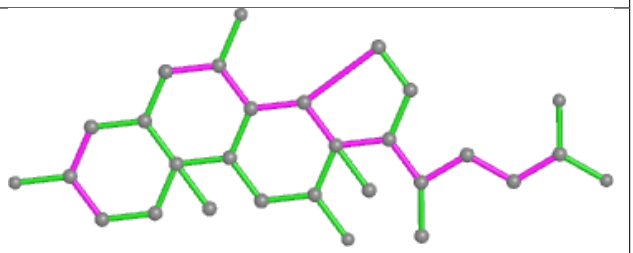
Ligand CHD B 304



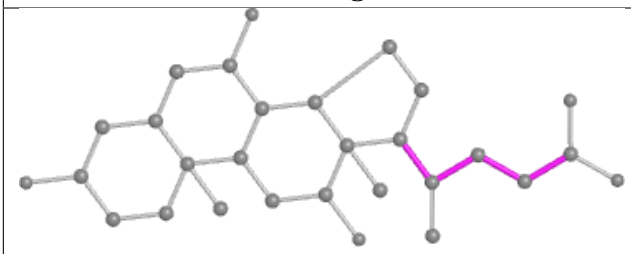
Ligand CHD P 306



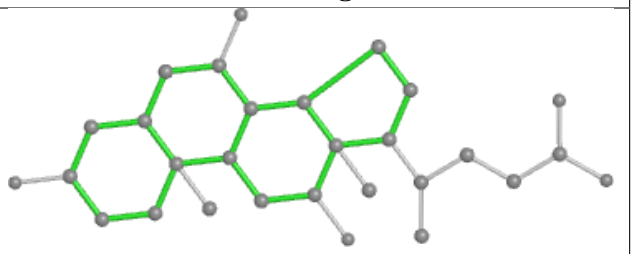
Bond lengths



Bond angles

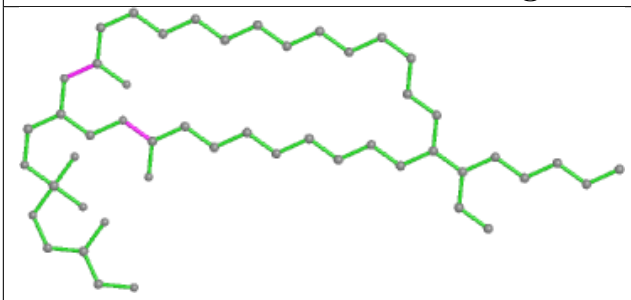


Torsions

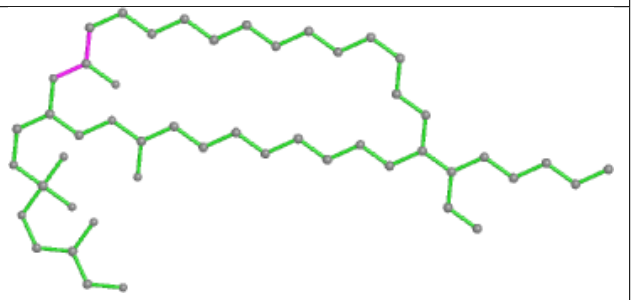


Rings

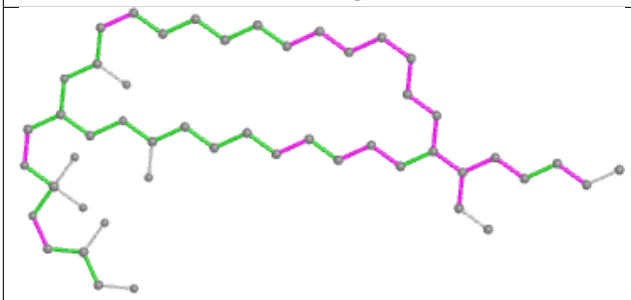
Ligand PGV C 305



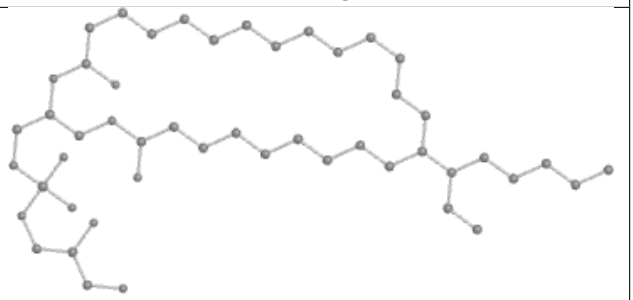
Bond lengths



Bond angles

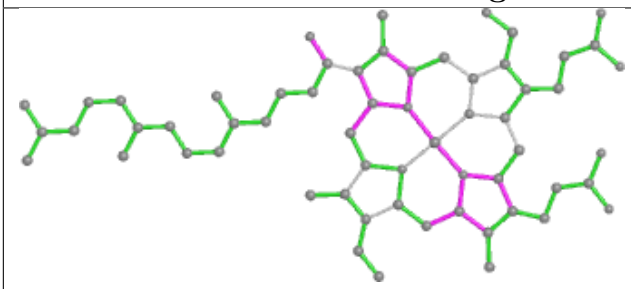


Torsions

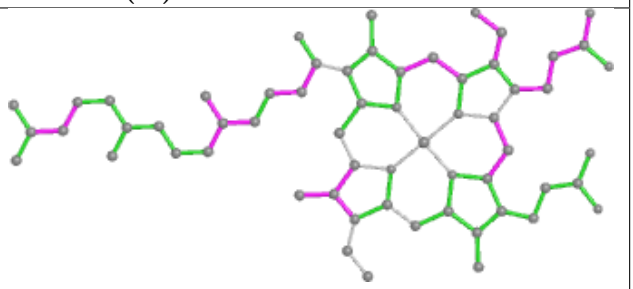


Rings

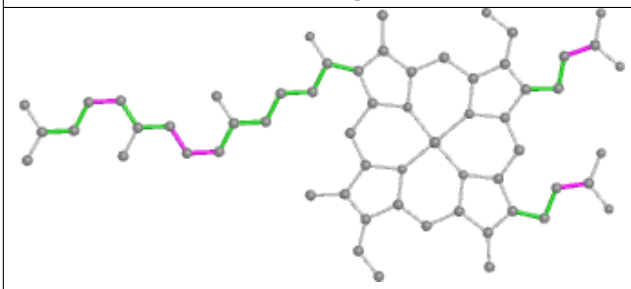
Ligand HEA A 601 (B)



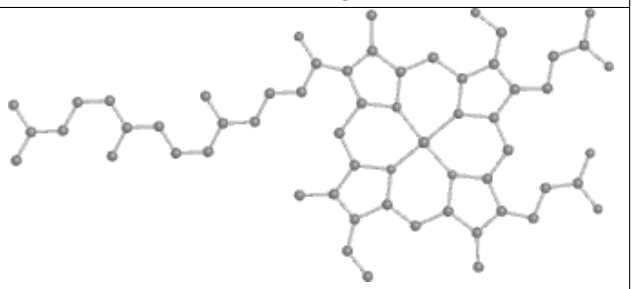
Bond lengths



Bond angles

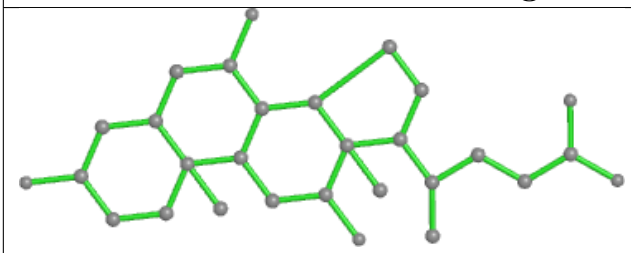


Torsions

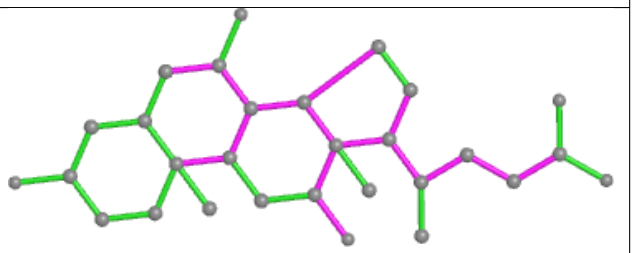


Rings

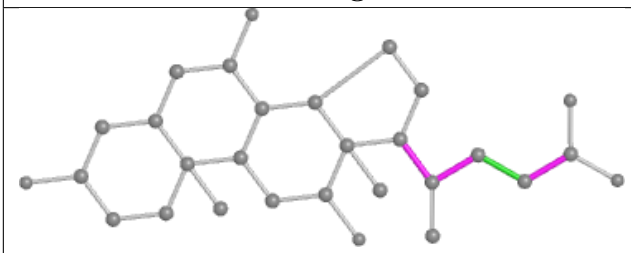
Ligand CHD C 308



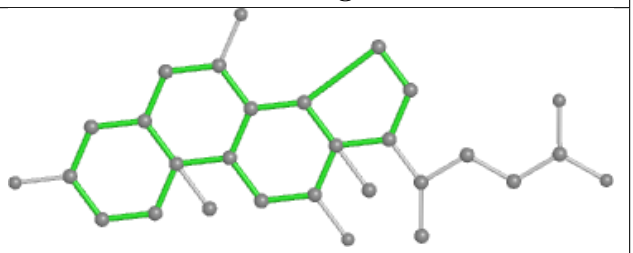
Bond lengths



Bond angles

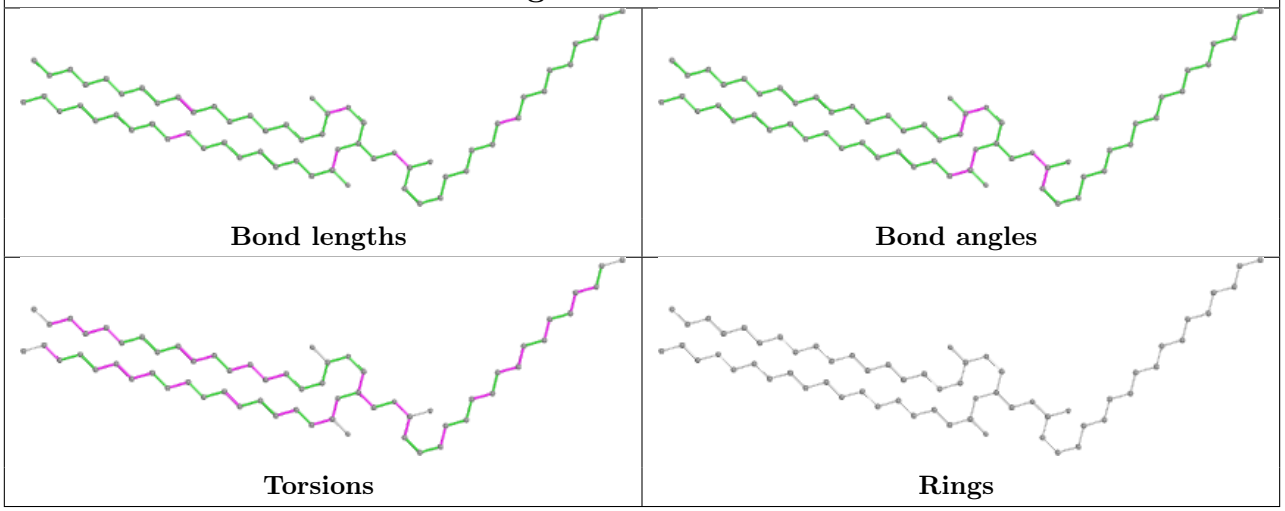


Torsions

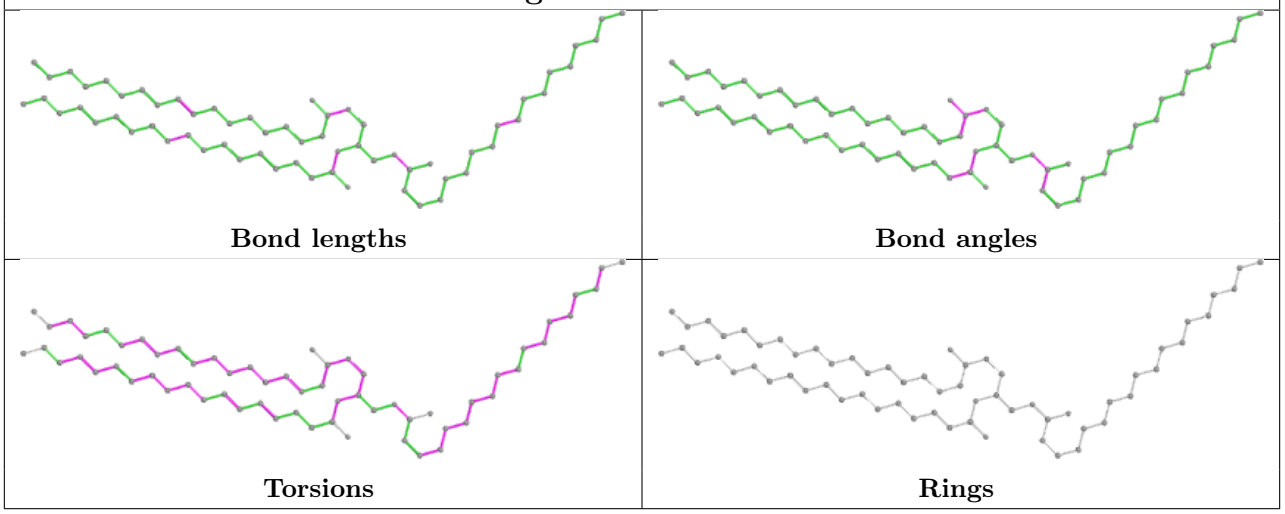


Rings

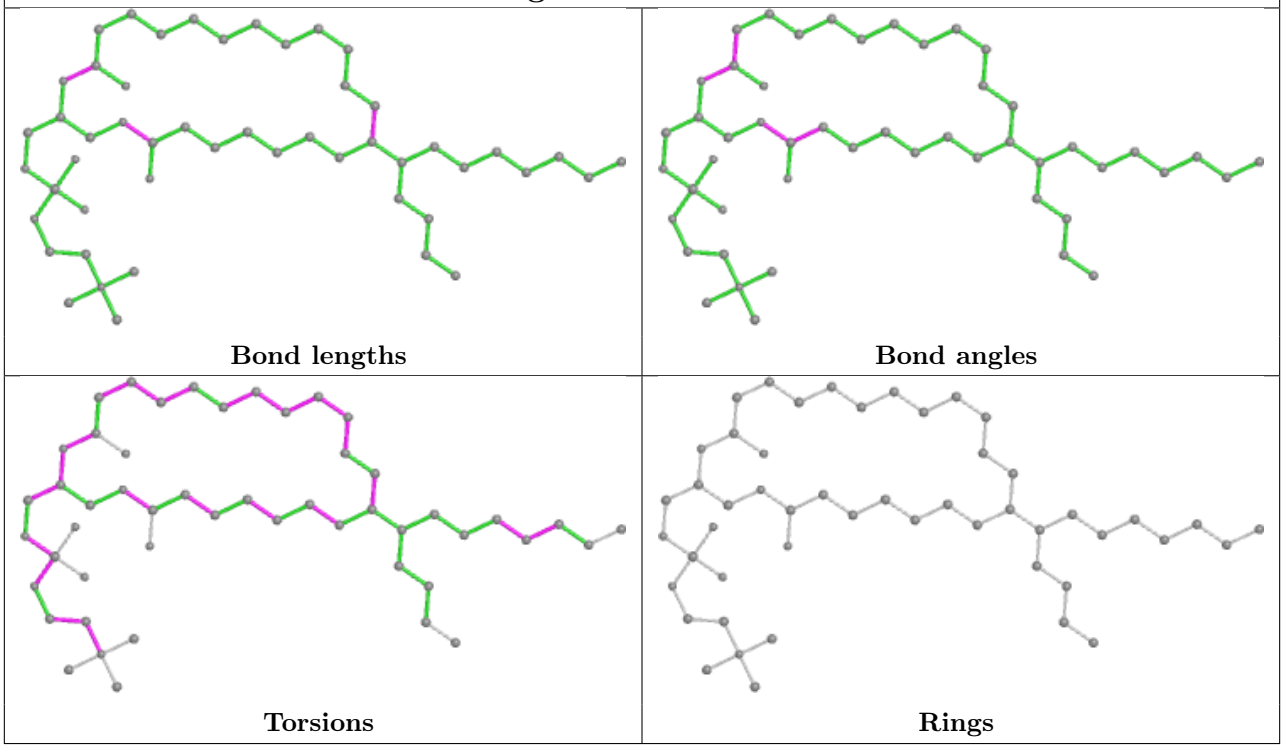
Ligand TGL L 101



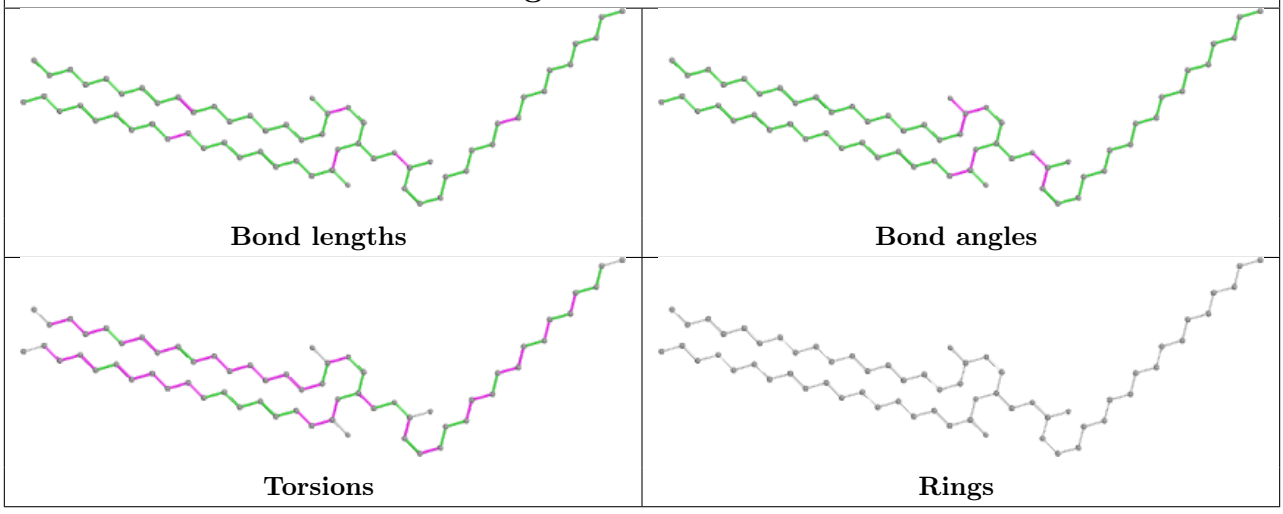
Ligand TGL B 301



Ligand PSC B 303



Ligand TGL D 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	0.24	4 (0%) 86 86	23, 28, 35, 78	0
1	N	513/514 (99%)	0.19	4 (0%) 86 86	26, 33, 44, 76	0
2	B	226/227 (99%)	0.17	4 (1%) 68 68	27, 34, 49, 70	0
2	O	226/227 (99%)	0.40	9 (3%) 38 36	31, 44, 67, 98	0
3	C	259/261 (99%)	0.18	3 (1%) 79 79	26, 31, 42, 77	0
3	P	259/261 (99%)	0.20	3 (1%) 79 79	27, 34, 45, 70	0
4	D	144/147 (97%)	0.08	4 (2%) 53 51	29, 37, 55, 75	0
4	Q	144/147 (97%)	0.96	15 (10%) 6 6	36, 54, 80, 139	0
5	E	105/109 (96%)	0.14	2 (1%) 66 67	29, 35, 56, 108	0
5	R	105/109 (96%)	0.35	3 (2%) 51 50	34, 43, 60, 131	0
6	F	94/94 (100%)	0.42	4 (4%) 35 33	28, 39, 59, 116	0
6	S	94/94 (100%)	0.45	6 (6%) 19 18	29, 40, 71, 116	0
7	G	83/85 (97%)	1.12	18 (21%) 0 0	30, 39, 106, 139	0
7	T	83/85 (97%)	1.44	19 (22%) 0 0	30, 43, 98, 139	0
8	H	79/85 (92%)	0.64	9 (11%) 5 4	32, 42, 87, 103	0
8	U	79/85 (92%)	0.89	13 (16%) 1 1	39, 49, 95, 120	0
9	I	72/73 (98%)	1.15	15 (20%) 1 0	32, 44, 78, 97	0
9	V	72/73 (98%)	1.41	17 (23%) 0 0	33, 59, 86, 93	0
10	J	58/59 (98%)	0.49	4 (6%) 16 16	31, 41, 64, 106	0
10	W	58/59 (98%)	0.67	4 (6%) 16 16	37, 48, 72, 120	0
11	K	49/56 (87%)	0.06	1 (2%) 65 65	35, 42, 55, 61	0
11	X	49/56 (87%)	0.65	5 (10%) 6 6	47, 57, 74, 79	0
12	L	46/47 (97%)	0.27	1 (2%) 62 61	29, 34, 50, 94	0
12	Y	46/47 (97%)	0.55	5 (10%) 5 5	37, 46, 64, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.45	3 (6%) 16 16	31, 35, 72, 105	0
13	Z	43/46 (93%)	0.59	6 (13%) 2 2	42, 49, 81, 124	0
All	All	3542/3606 (98%)	0.40	181 (5%) 28 26	23, 36, 67, 139	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	22.9
4	Q	6	VAL	20.3
2	O	227	LEU	13.1
7	T	10	GLY	12.7
4	Q	4	SER	12.6

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	T	11	11/12	0.51	0.35	107,125,143,144	0
9	SAC	V	1	9/10	0.51	0.38	109,117,122,124	0
7	TPO	G	11	11/12	0.55	0.28	74,90,145,146	0
9	SAC	I	1	9/10	0.84	0.18	62,71,77,78	0
1	FME	A	1	10/11	0.94	0.14	40,47,73,88	0
2	FME	B	1	10/11	0.94	0.14	32,35,51,58	0
1	FME	N	1	10/11	0.96	0.12	47,55,88,93	0
2	FME	O	1	10/11	0.97	0.10	43,46,57,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	DMU	P	313	33/33	0.28	0.32	84,143,147,148	0
20	EDO	M	103	4/4	0.48	0.24	113,116,116,117	0
27	DMU	C	313	33/33	0.55	0.52	76,136,146,147	0
25	PEK	C	304	53/53	0.57	0.24	45,80,138,146	0
27	DMU	W	104	33/33	0.60	0.43	78,131,146,146	0
26	CDL	T	103	100/100	0.65	0.28	56,83,115,139	0
20	EDO	L	102	4/4	0.66	0.30	86,90,91,91	0
20	EDO	T	105	4/4	0.66	0.88	144,145,145,145	4
27	DMU	C	312	33/33	0.66	0.23	83,116,143,145	0
20	EDO	W	102	4/4	0.67	0.42	103,107,108,109	0
26	CDL	G	101	100/100	0.69	0.32	58,89,138,147	0
21	TGL	Q	201	63/63	0.69	0.21	56,76,92,95	0
25	PEK	T	102	53/53	0.70	0.23	39,77,126,137	0
25	PEK	T	101	53/53	0.71	0.27	51,87,142,148	0
23	PSC	B	303	52/52	0.72	0.33	45,83,142,149	0
20	EDO	Y	101	4/4	0.73	0.28	96,97,99,100	0
20	EDO	L	104	4/4	0.73	0.24	97,97,98,99	0
26	CDL	P	305	100/100	0.74	0.28	45,82,111,117	0
25	PEK	G	103	53/53	0.74	0.24	52,87,125,139	0
21	TGL	N	606	63/63	0.74	0.26	49,73,104,120	0
17	NA	C	302	1/1	0.75	0.27	53,53,53,53	0
26	CDL	C	307	100/100	0.75	0.29	41,74,102,117	0
18	PGV	U	101	51/51	0.75	0.24	48,83,126,143	0
24	CHD	W	101	29/29	0.76	0.31	62,72,98,102	0
24	CHD	J	101	29/29	0.78	0.24	53,65,103,108	0
20	EDO	H	101	4/4	0.78	0.21	75,75,77,78	0
20	EDO	C	311	4/4	0.79	0.24	48,56,58,61	0
18	PGV	N	607	51/51	0.79	0.31	49,81,128,140	0
21	TGL	D	201	63/63	0.79	0.17	46,68,87,89	0
20	EDO	P	307	4/4	0.79	0.38	89,96,96,98	0
20	EDO	A	619	4/4	0.79	0.63	81,83,87,89	4
20	EDO	W	103	4/4	0.80	0.17	72,78,78,81	0
20	EDO	L	105	4/4	0.80	0.22	85,86,87,87	0
20	EDO	P	309	4/4	0.80	0.22	88,91,92,95	0
21	TGL	L	101	63/63	0.80	0.23	37,59,92,99	0
20	EDO	P	312	4/4	0.80	0.15	57,65,67,67	0
20	EDO	L	103	4/4	0.80	0.28	45,61,62,66	0
20	EDO	N	613	4/4	0.80	0.36	85,92,94,99	0
18	PGV	C	306	51/51	0.81	0.20	45,73,111,133	0
20	EDO	B	309	4/4	0.81	0.17	42,52,53,55	0
20	EDO	A	611	4/4	0.82	0.22	70,77,78,81	0
23	PSC	O	303	52/52	0.82	0.24	40,76,138,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	A	618	4/4	0.83	0.18	55,58,59,61	0
17	NA	P	302	1/1	0.83	0.19	49,49,49,49	0
18	PGV	A	606	51/51	0.84	0.23	35,74,106,132	0
21	TGL	B	301	63/63	0.84	0.21	36,69,89,100	0
21	TGL	O	301	63/63	0.85	0.21	50,76,98,105	0
20	EDO	R	204	4/4	0.85	0.30	55,63,67,67	0
27	DMU	Z	101	33/33	0.86	0.20	55,66,92,94	0
20	EDO	P	310	4/4	0.87	0.24	86,90,94,97	0
20	EDO	A	609	4/4	0.87	0.23	45,51,52,53	0
20	EDO	R	202	4/4	0.88	0.25	88,90,90,94	0
20	EDO	R	203	4/4	0.88	0.36	90,92,93,95	0
20	EDO	B	308	4/4	0.88	0.22	88,89,93,97	0
20	EDO	B	306	4/4	0.88	0.20	47,52,54,55	0
20	EDO	M	102	4/4	0.88	0.17	83,84,85,85	0
20	EDO	A	615	4/4	0.89	0.35	64,67,70,72	0
20	EDO	P	308	4/4	0.89	0.23	97,100,100,102	0
20	EDO	S	104	4/4	0.89	0.26	74,75,77,80	0
24	CHD	P	306	29/29	0.90	0.16	45,55,61,76	0
20	EDO	Q	202	4/4	0.90	0.22	43,54,59,68	0
27	DMU	M	101	33/33	0.90	0.12	44,51,71,86	0
20	EDO	N	614	4/4	0.90	0.16	52,53,56,57	0
20	EDO	T	104	4/4	0.90	0.23	98,101,103,104	0
20	EDO	A	616	4/4	0.90	0.17	85,86,89,93	0
20	EDO	A	610	4/4	0.92	0.16	36,39,39,40	0
20	EDO	B	307	4/4	0.92	0.15	50,54,56,58	0
16	MG	N	604	1/1	0.93	0.19	39,39,39,39	0
20	EDO	A	617	4/4	0.93	0.15	38,44,48,49	0
24	CHD	C	308	29/29	0.93	0.15	48,54,65,67	0
20	EDO	P	311	4/4	0.93	0.17	48,49,51,52	0
20	EDO	C	309	4/4	0.93	0.18	41,47,51,54	0
20	EDO	N	612	4/4	0.94	0.15	58,62,66,66	0
20	EDO	N	611	4/4	0.95	0.13	34,35,38,39	0
20	EDO	A	612	4/4	0.95	0.32	54,63,64,64	0
20	EDO	S	102	4/4	0.95	0.12	31,33,33,34	0
20	EDO	S	103	4/4	0.95	0.11	44,44,46,46	0
20	EDO	A	614	4/4	0.95	0.22	73,73,76,77	0
20	EDO	J	102	4/4	0.95	0.21	55,65,65,67	0
20	EDO	N	610	4/4	0.96	0.12	40,40,42,42	0
20	EDO	C	310	4/4	0.96	0.09	39,43,43,43	0
20	EDO	R	201	4/4	0.96	0.19	49,49,49,52	0
20	EDO	A	613	4/4	0.96	0.13	28,28,32,32	0
24	CHD	B	304	29/29	0.96	0.11	29,32,35,41	0

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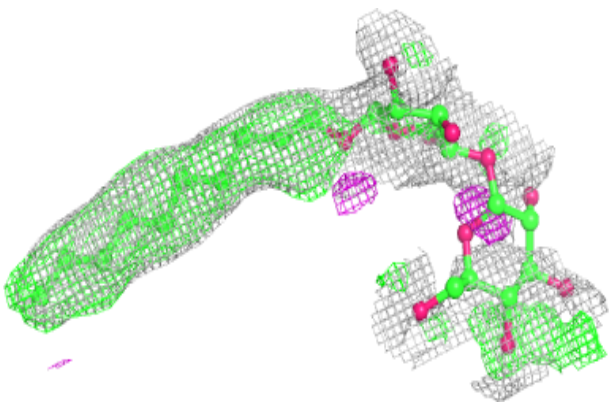
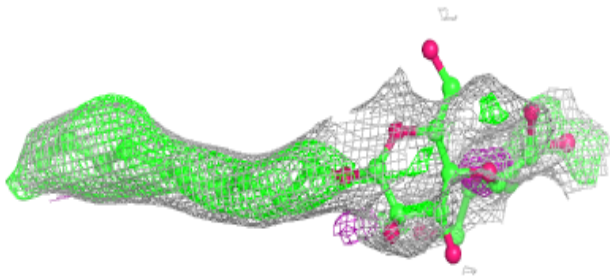
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CHD	C	301	29/29	0.96	0.09	28,31,35,36	0
20	EDO	F	102	4/4	0.96	0.14	29,30,30,32	0
20	EDO	F	103	4/4	0.96	0.14	43,45,45,46	0
20	EDO	E	201	4/4	0.97	0.10	48,49,51,51	0
20	EDO	O	304	4/4	0.97	0.12	44,46,48,48	0
25	PEK	C	303	53/53	0.97	0.15	30,47,86,95	0
20	EDO	G	104	4/4	0.97	0.11	37,39,40,40	0
24	CHD	P	301	29/29	0.97	0.10	30,33,36,39	0
25	PEK	P	303	53/53	0.97	0.15	30,49,94,97	0
18	PGV	N	609	51/51	0.98	0.13	30,43,65,70	0
18	PGV	P	304	51/51	0.98	0.13	31,40,70,78	0
14	HEA	A	601[A]	60/60	0.98	0.12	22,26,38,41	9
14	HEA	A	601[B]	60/60	0.98	0.12	22,26,33,38	9
20	EDO	B	305	4/4	0.98	0.12	34,36,36,37	0
24	CHD	G	102	29/29	0.98	0.11	29,32,34,42	0
14	HEA	N	601[A]	60/60	0.98	0.12	28,34,43,49	9
14	HEA	N	601[B]	60/60	0.98	0.12	28,33,39,41	9
18	PGV	A	608	51/51	0.98	0.13	27,38,61,65	0
18	PGV	C	305	51/51	0.98	0.13	29,34,81,94	0
14	HEA	N	602	60/60	0.98	0.11	25,29,34,37	0
16	MG	A	604	1/1	0.98	0.17	30,30,30,30	0
22	CUA	O	302	2/2	0.98	0.14	39,39,39,39	0
17	NA	N	605	1/1	0.99	0.07	41,41,41,41	0
14	HEA	A	602	60/60	0.99	0.10	21,25,30,34	0
22	CUA	B	302	2/2	0.99	0.16	29,29,29,30	0
19	PER	N	608[B]	2/2	1.00	0.17	15,15,15,16	2
17	NA	A	605	1/1	1.00	0.09	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.17	27,27,27,27	0
15	CU	N	603	1/1	1.00	0.18	31,31,31,31	0
19	PER	A	607[A]	2/2	1.00	0.17	24,24,24,25	0
19	PER	A	607[B]	2/2	1.00	0.17	6,6,6,6	2
19	PER	N	608[A]	2/2	1.00	0.17	28,28,28,31	0
28	ZN	F	101	1/1	1.00	0.15	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.13	37,37,37,37	0

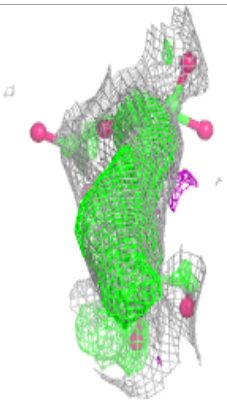
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU P 313:

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

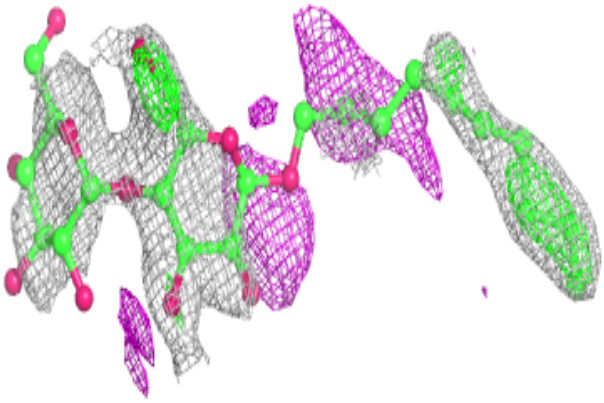


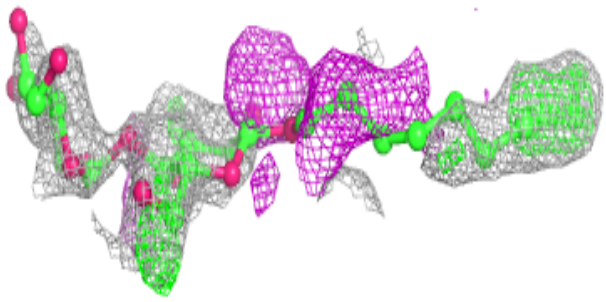


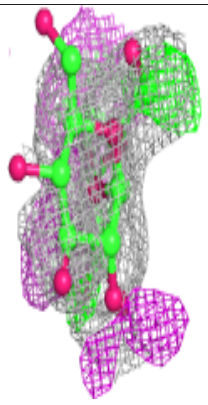


Electron density around DMU C 313:

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

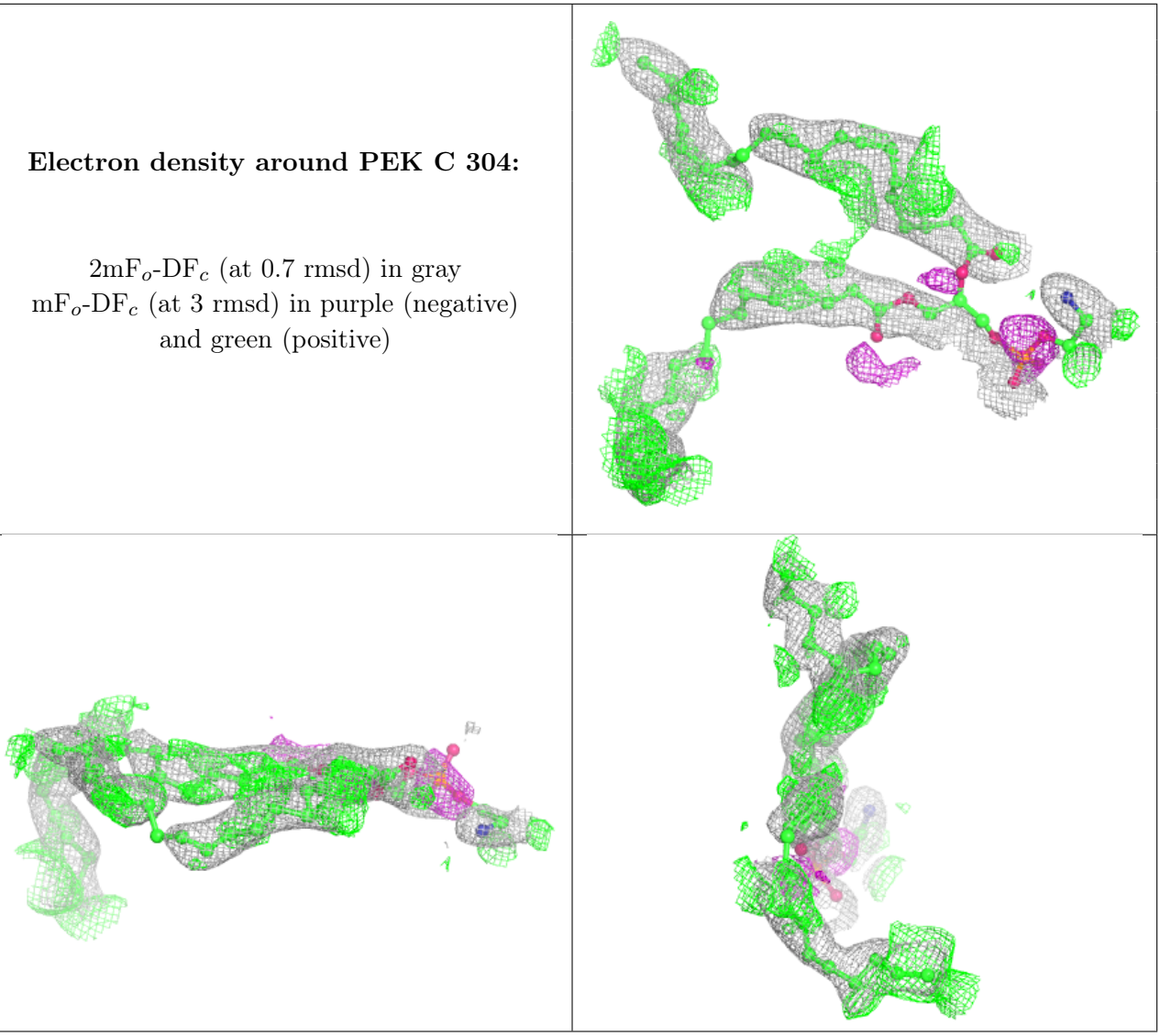






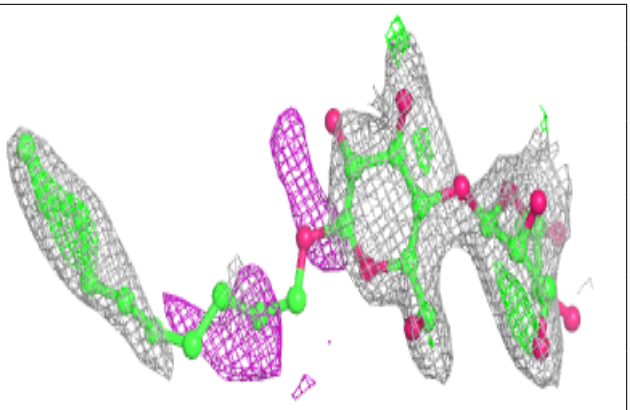
Electron density around PEK C 304:

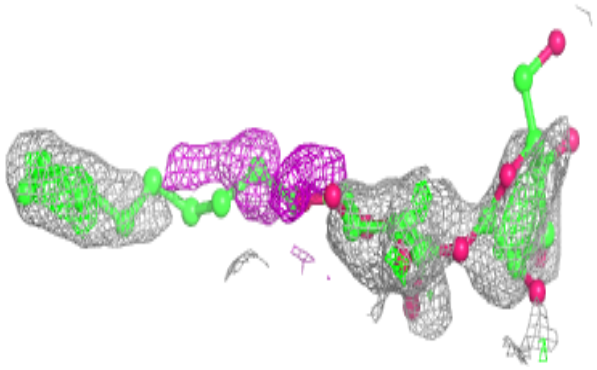
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

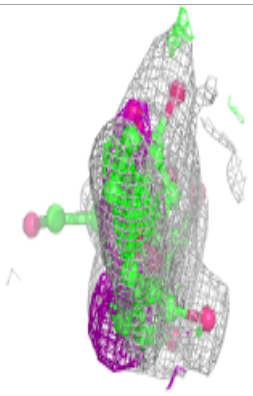


Electron density around DMU W 104:

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

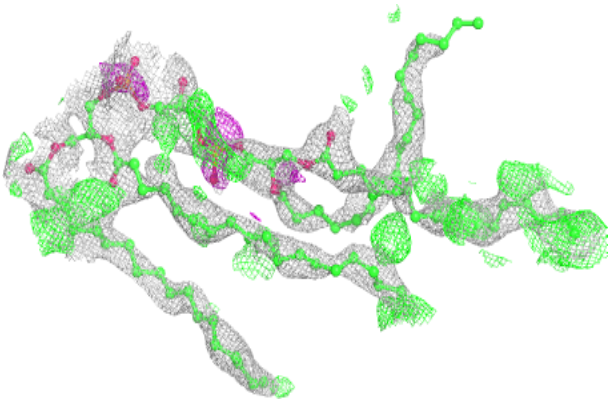


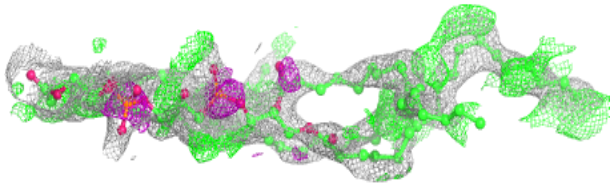


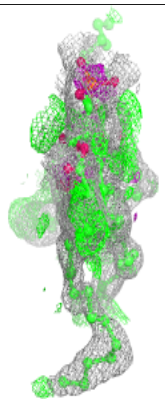


Electron density around CDL T 103:

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

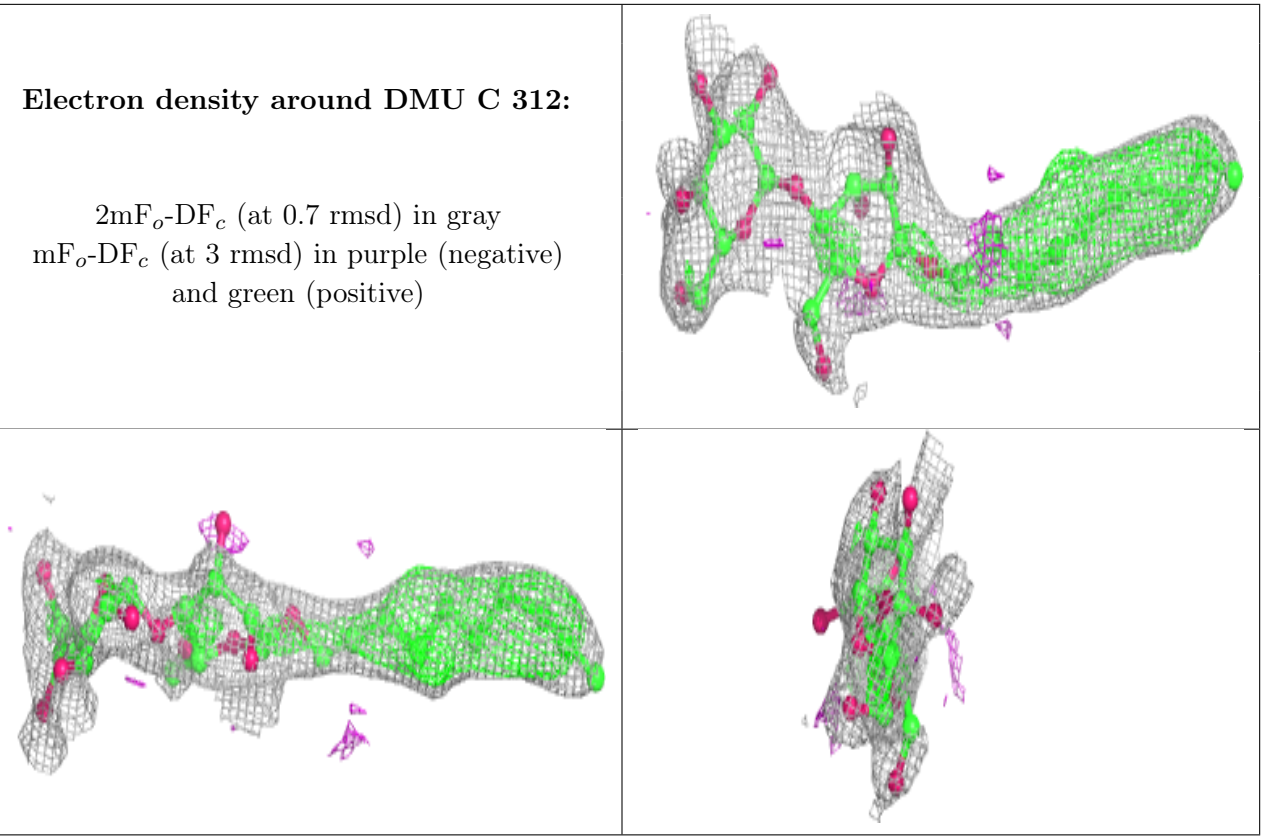






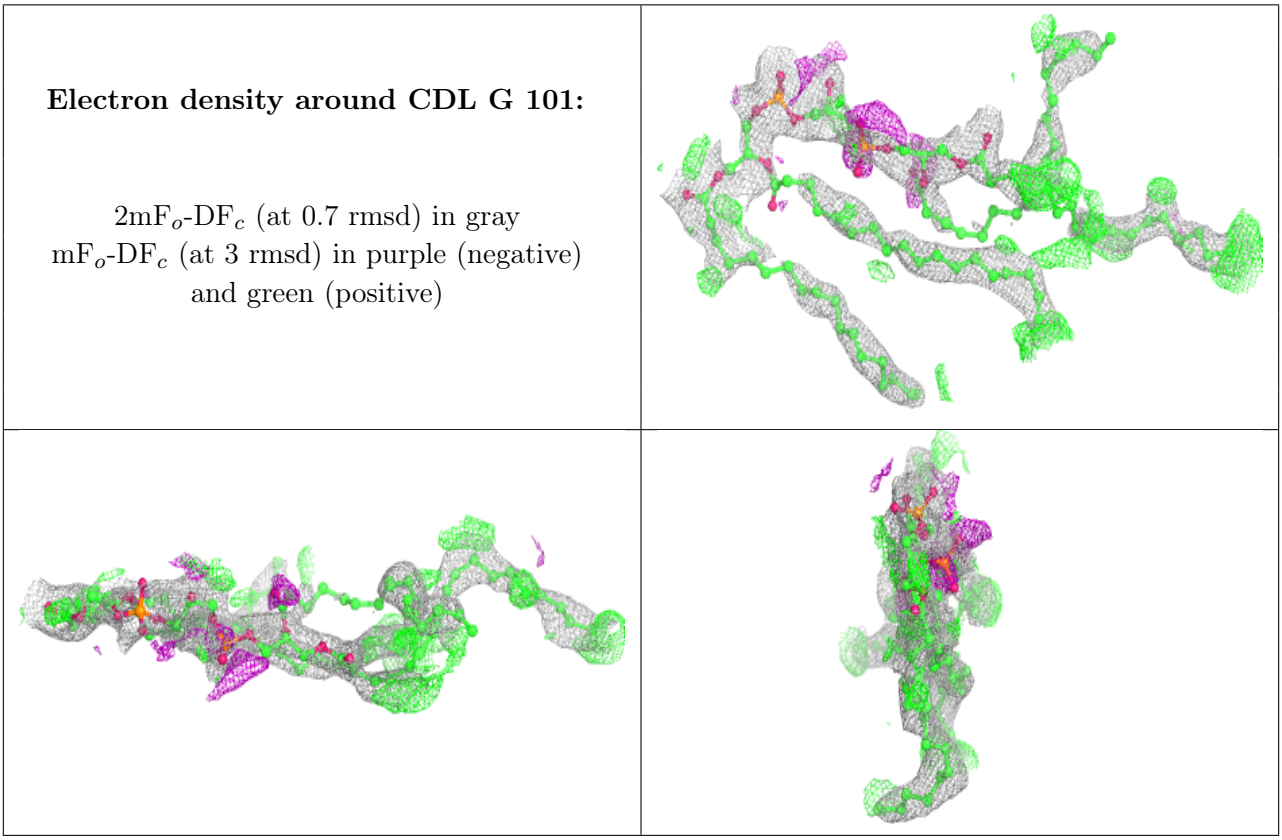
Electron density around DMU C 312:

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



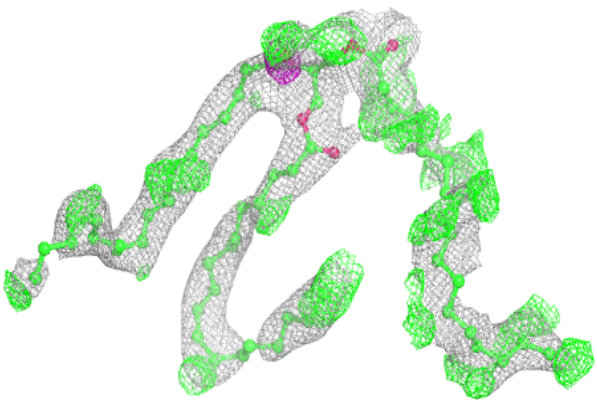
Electron density around CDL G 101:

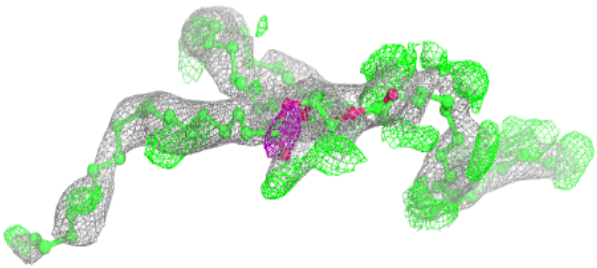
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

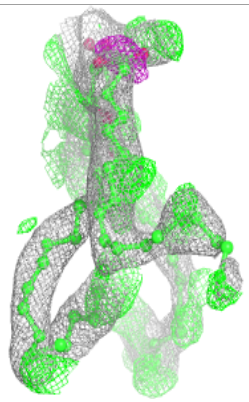


Electron density around TGL Q 201:

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

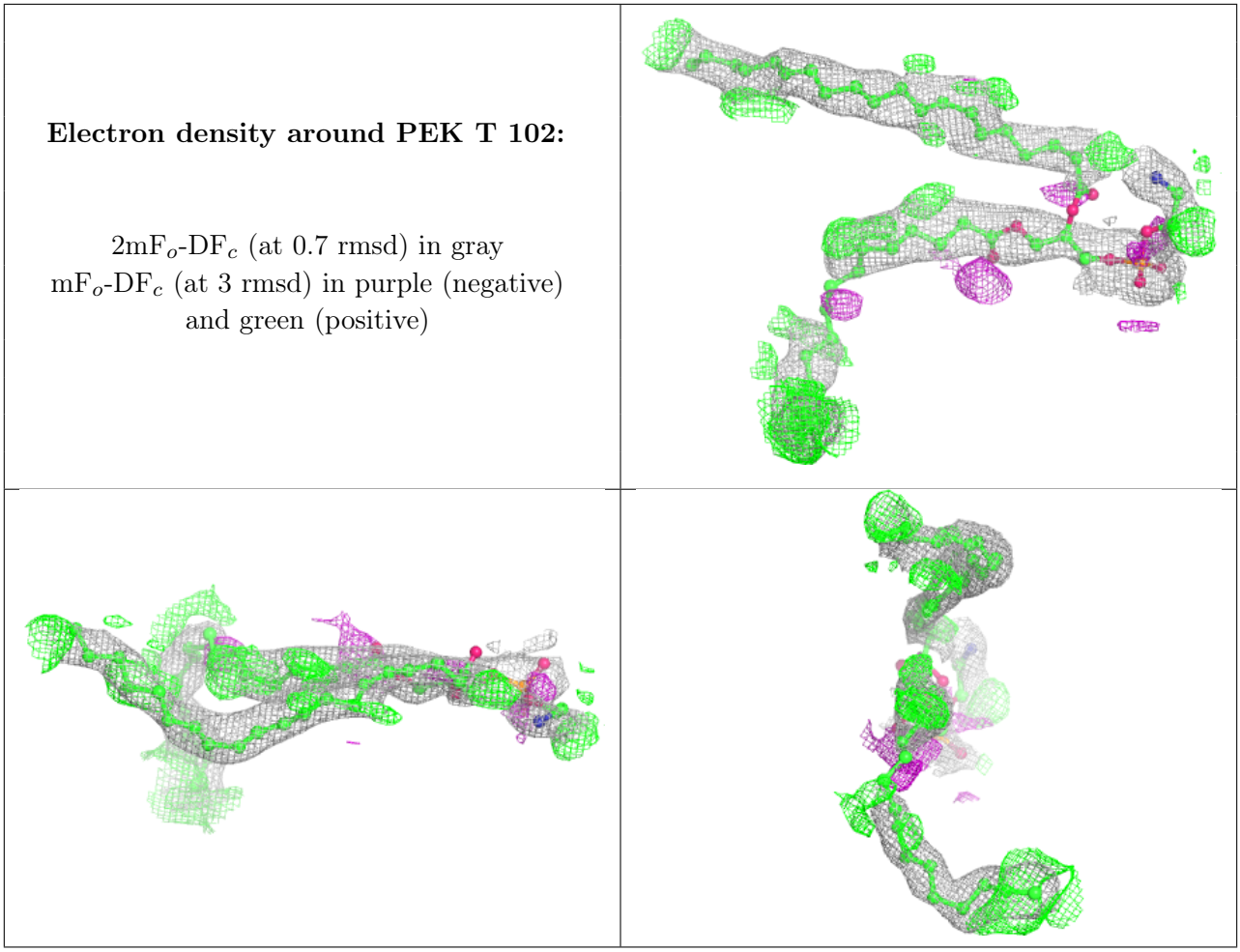






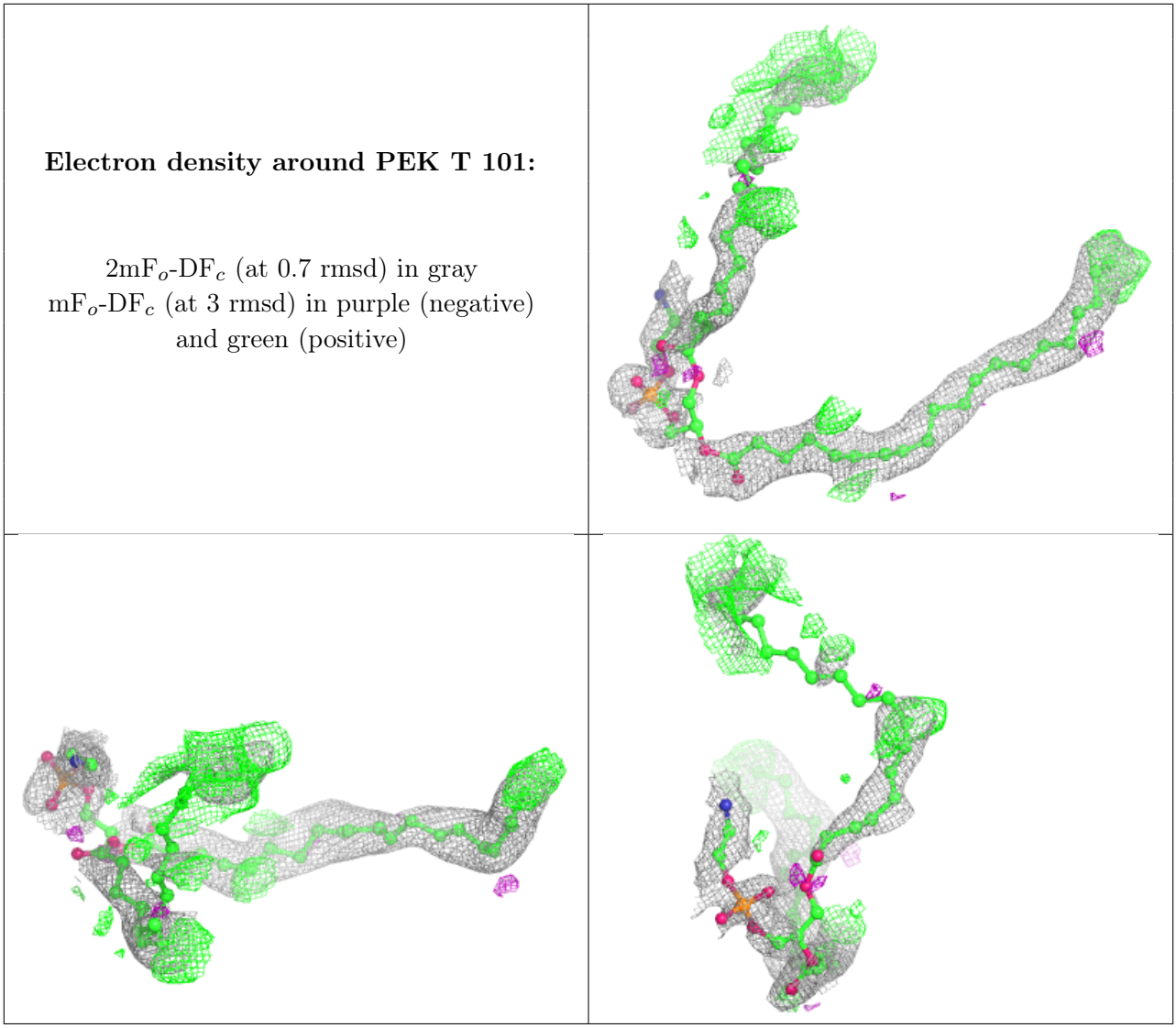
Electron density around PEK T 102:

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



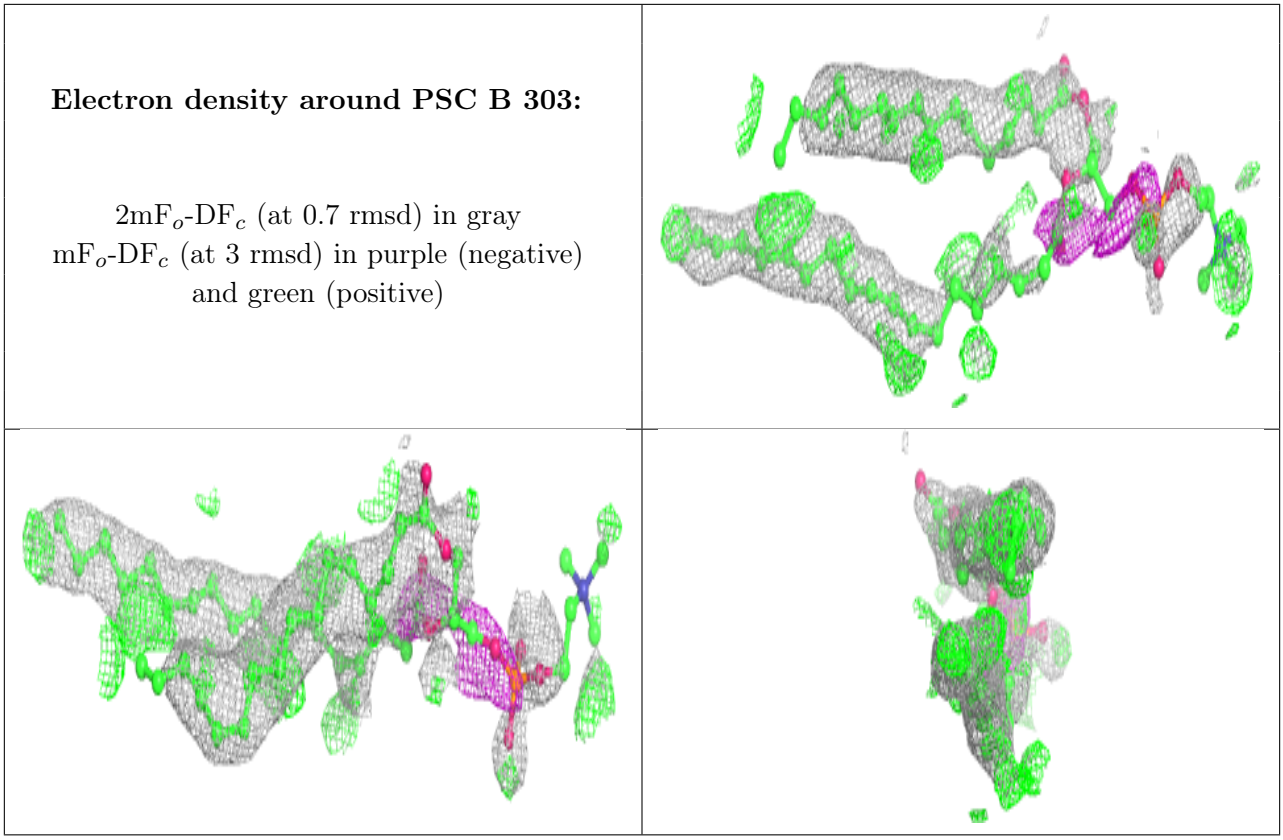
Electron density around PEK T 101:

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



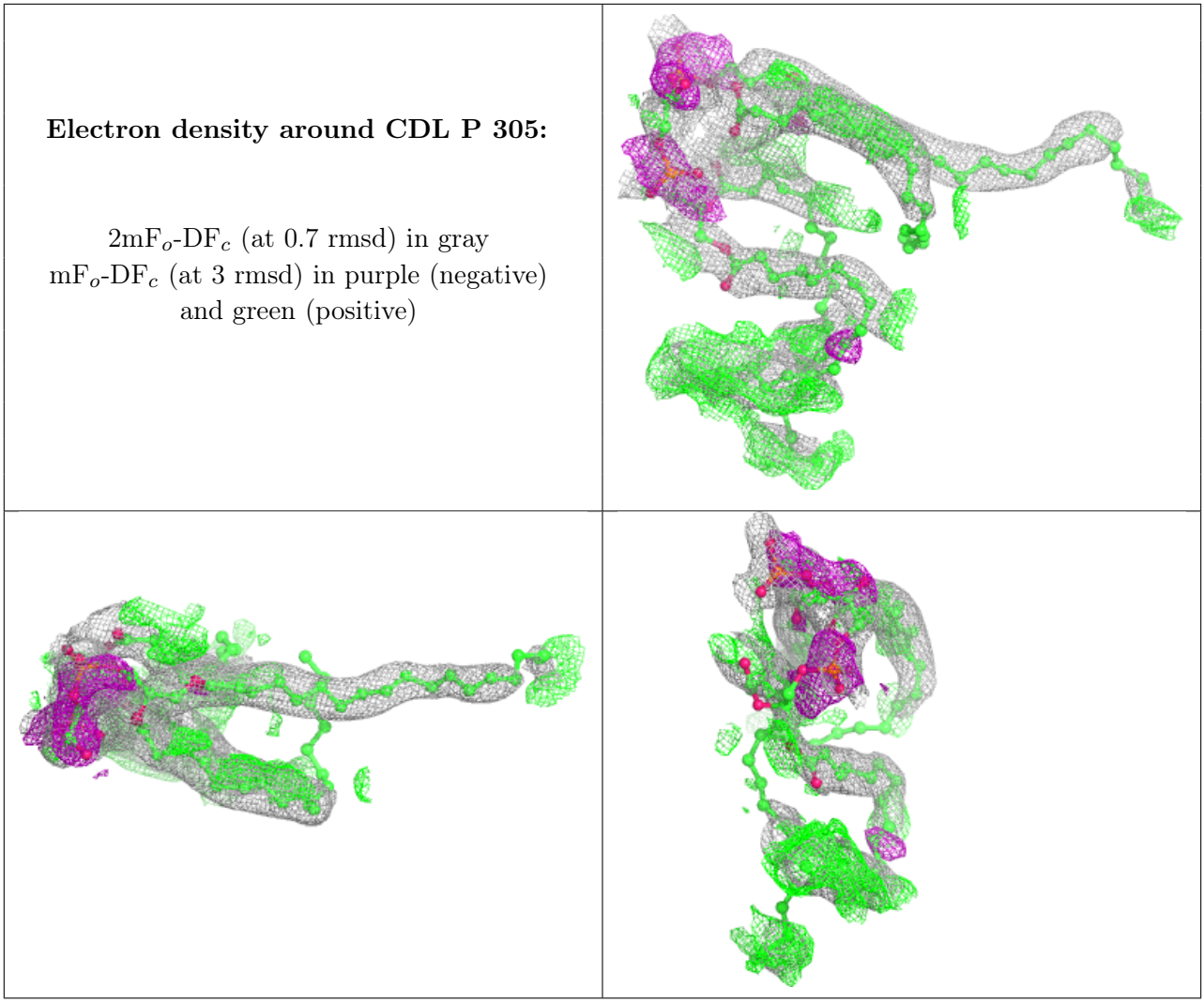
Electron density around PSC B 303:

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



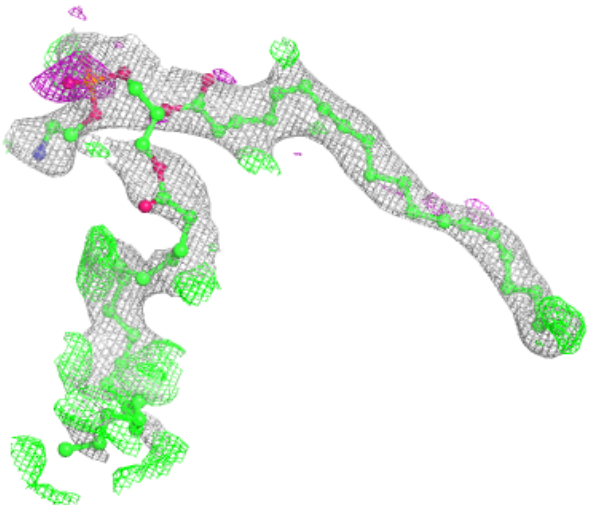
Electron density around CDL P 305:

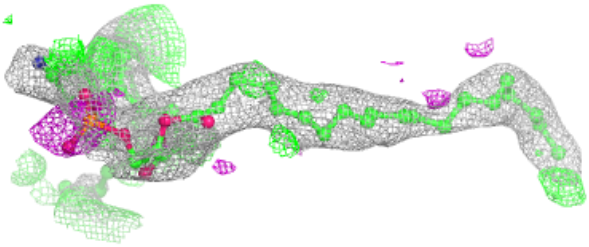
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

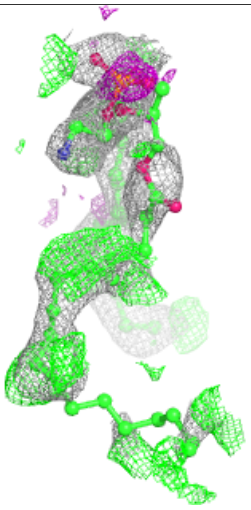


Electron density around PEK G 103:

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

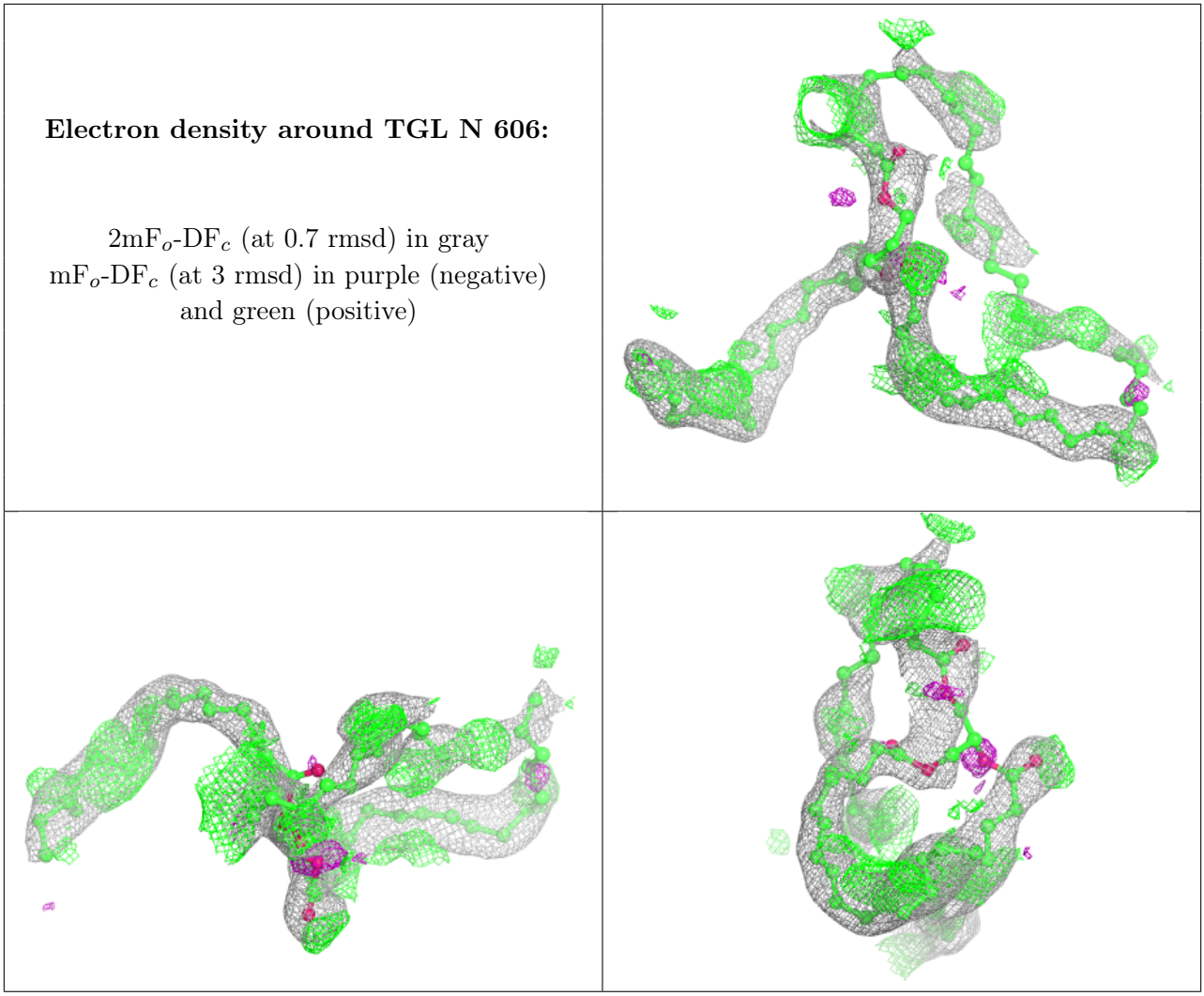






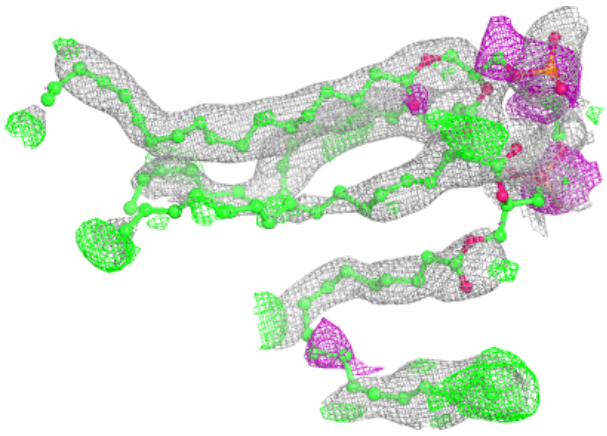
Electron density around TGL N 606:

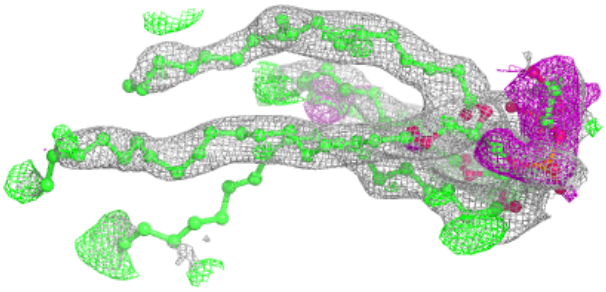
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

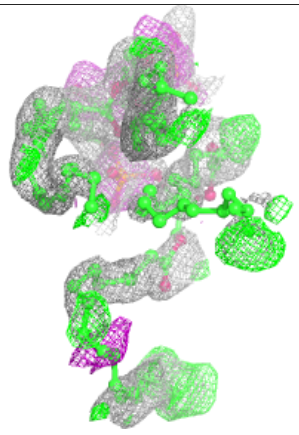


Electron density around CDL C 307:

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

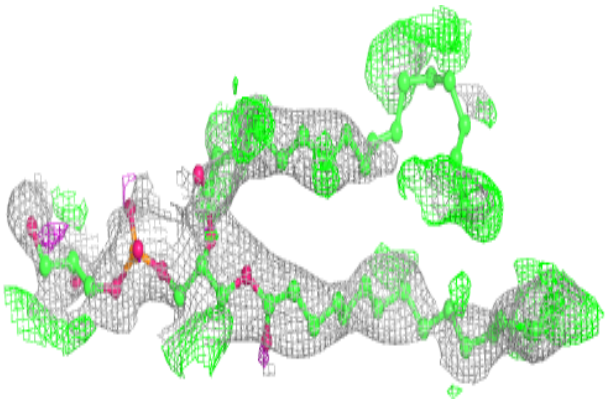


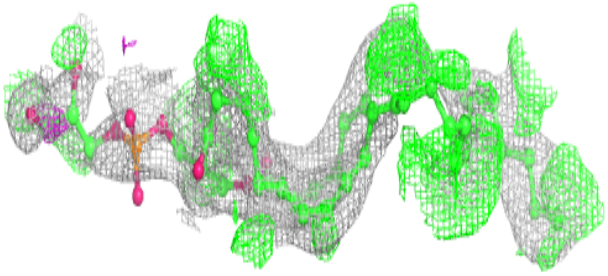


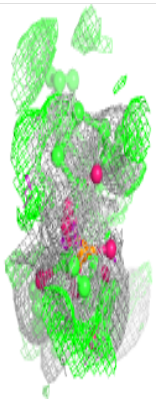


Electron density around PGV U 101:

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

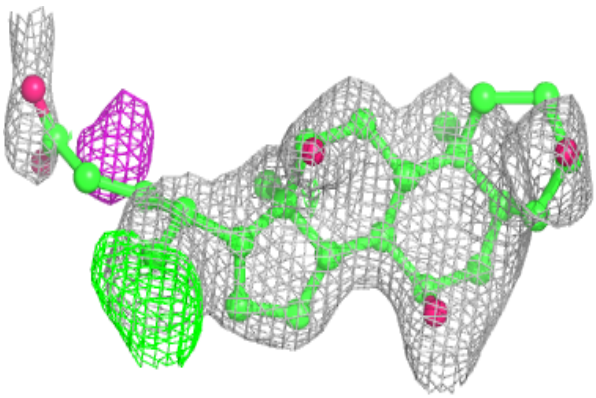


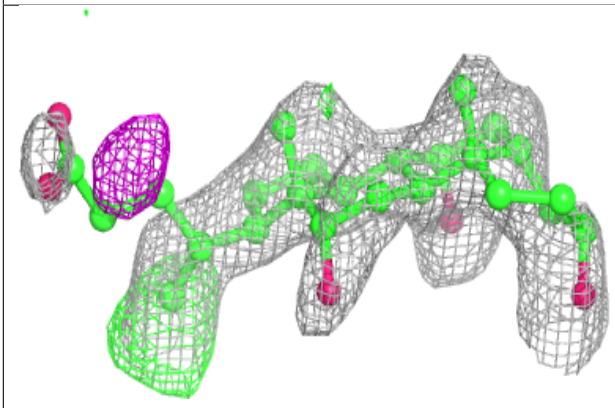


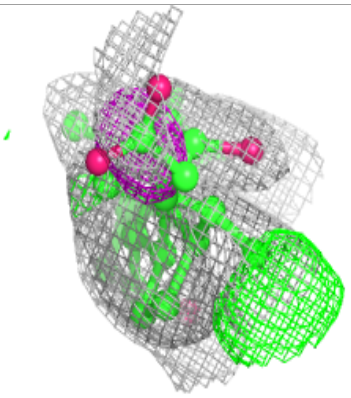


Electron density around CHD W 101:

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

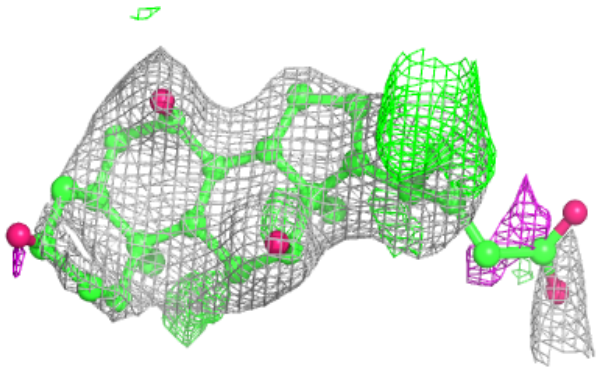


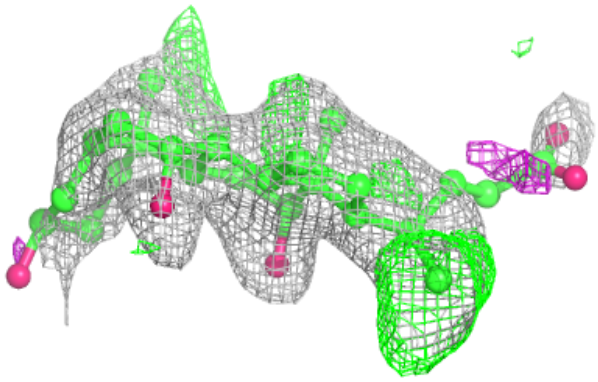


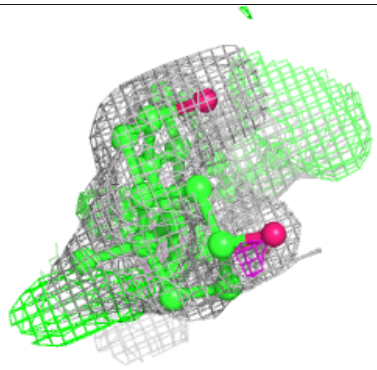


Electron density around CHD J 101:

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

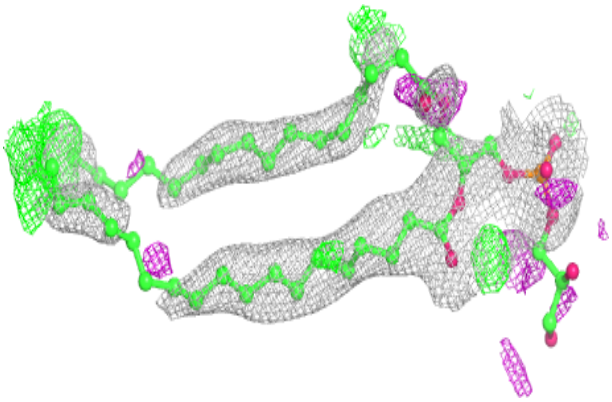


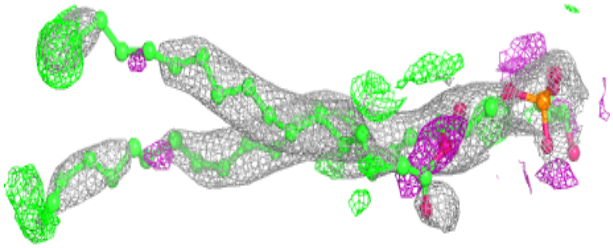


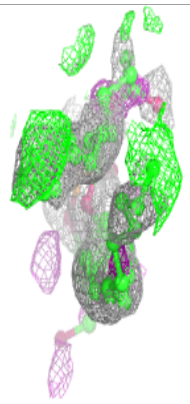


Electron density around PGV N 607:

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

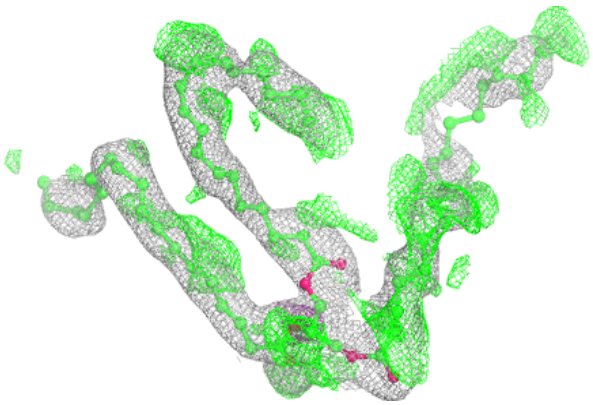


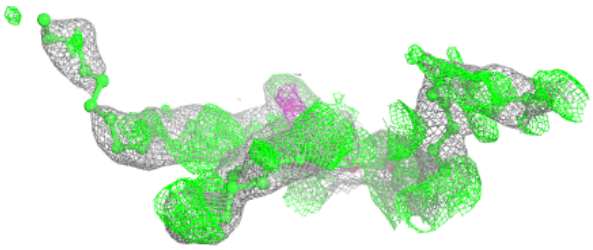




Electron density around TGL D 201:

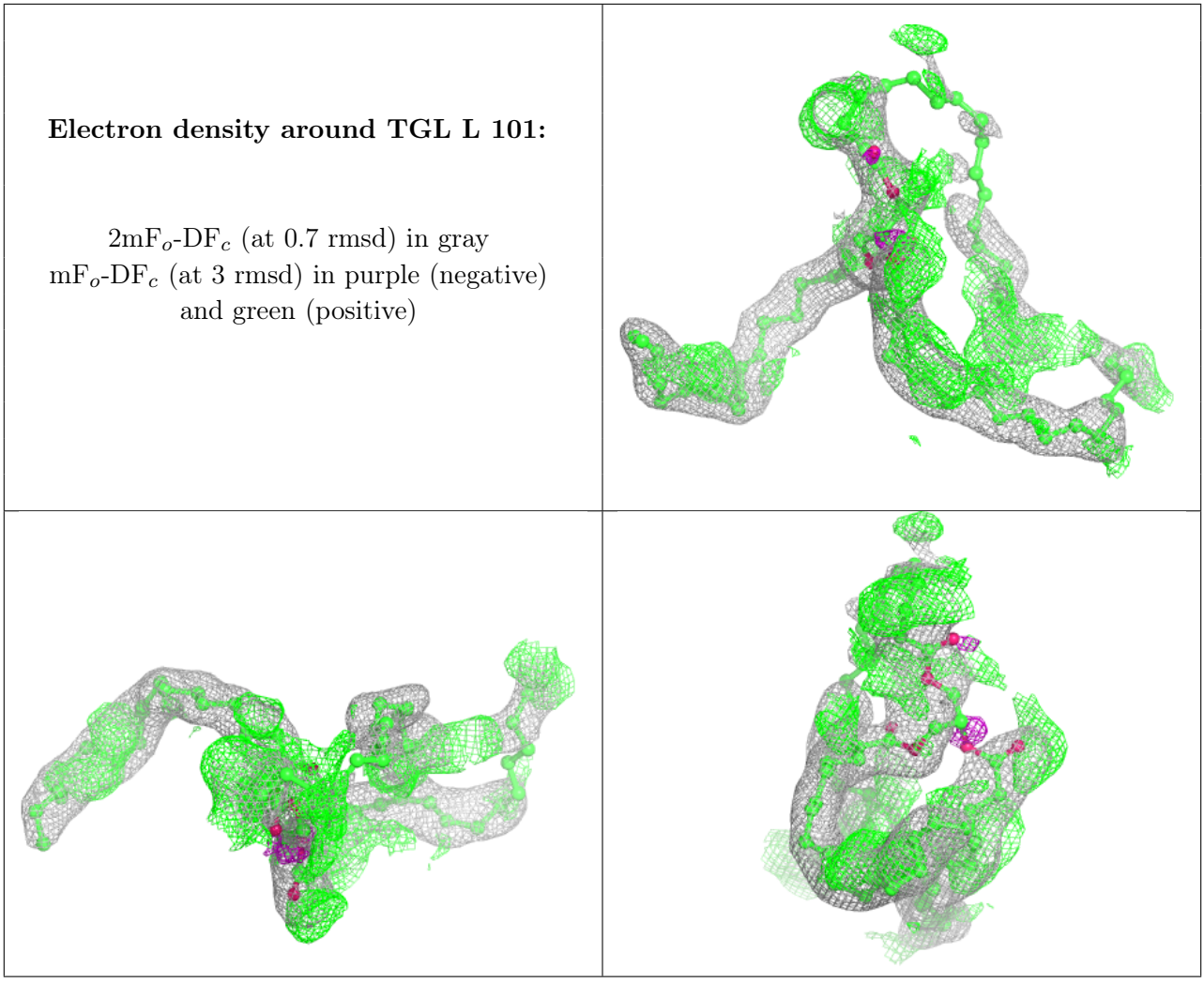
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





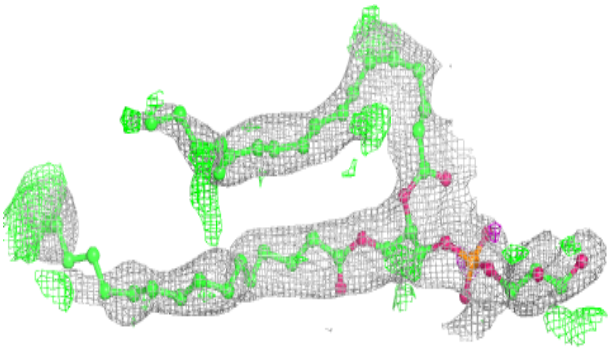
Electron density around TGL L 101:

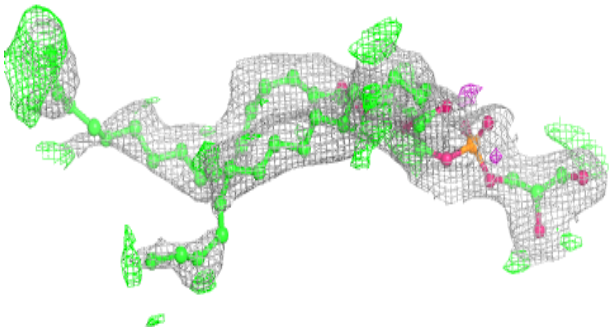
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

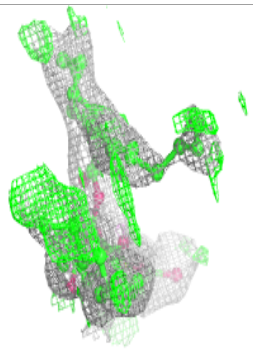


Electron density around PGV C 306:

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

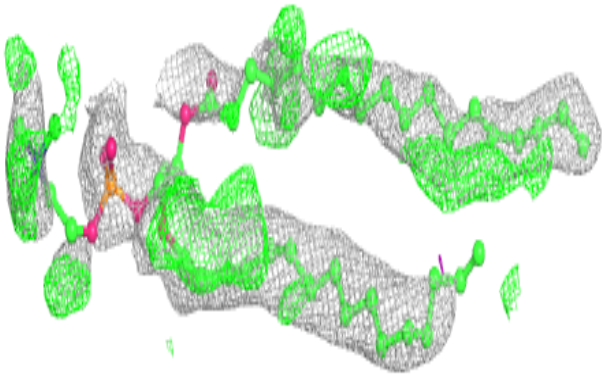


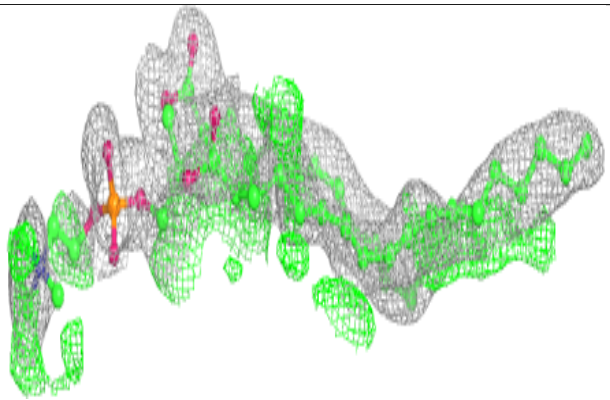


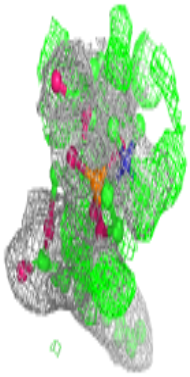


Electron density around PSC O 303:

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

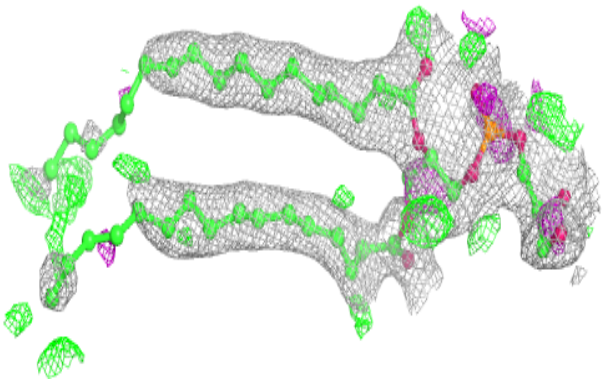


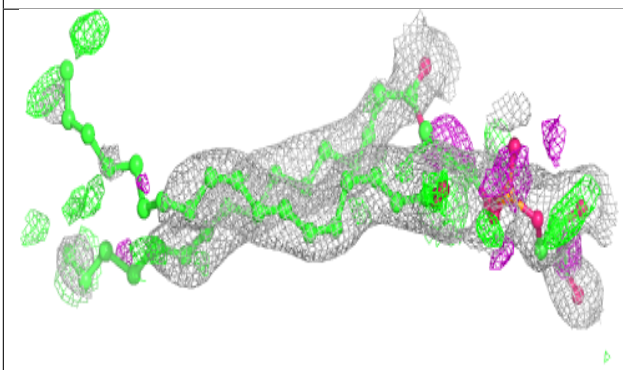


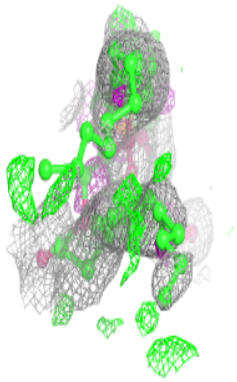


Electron density around PGV A 606:

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

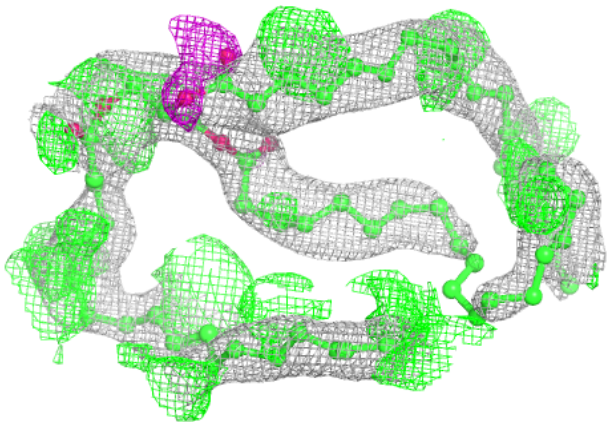


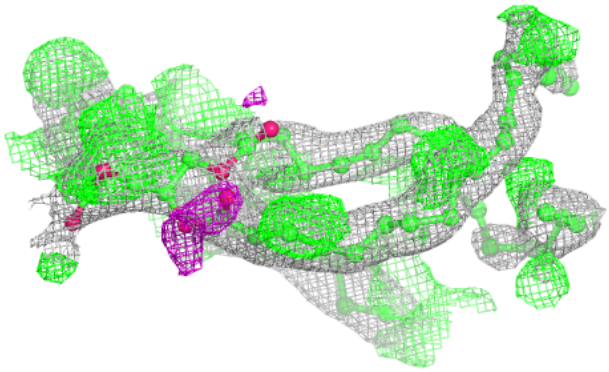


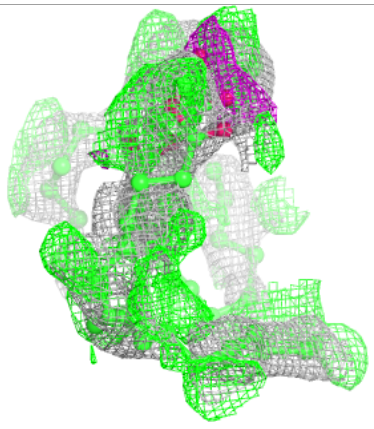


Electron density around TGL B 301:

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

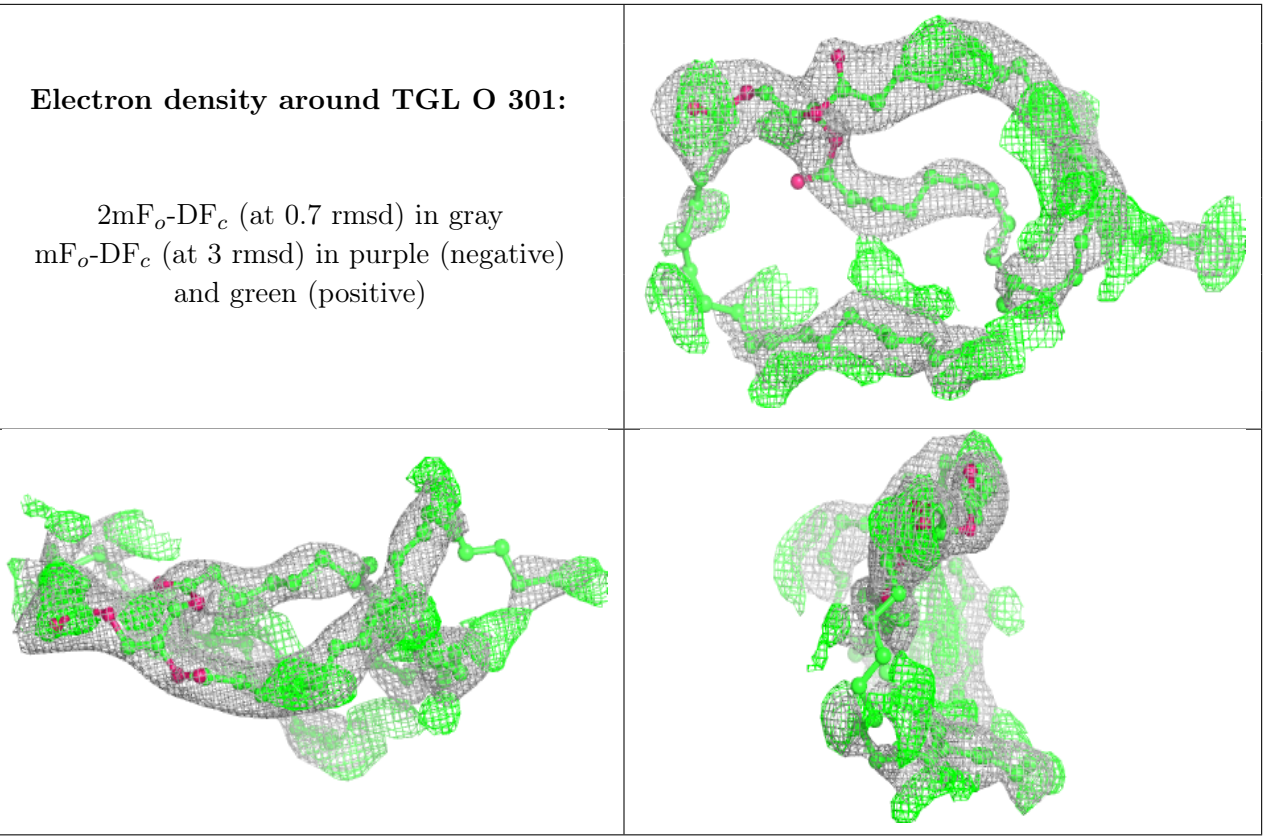






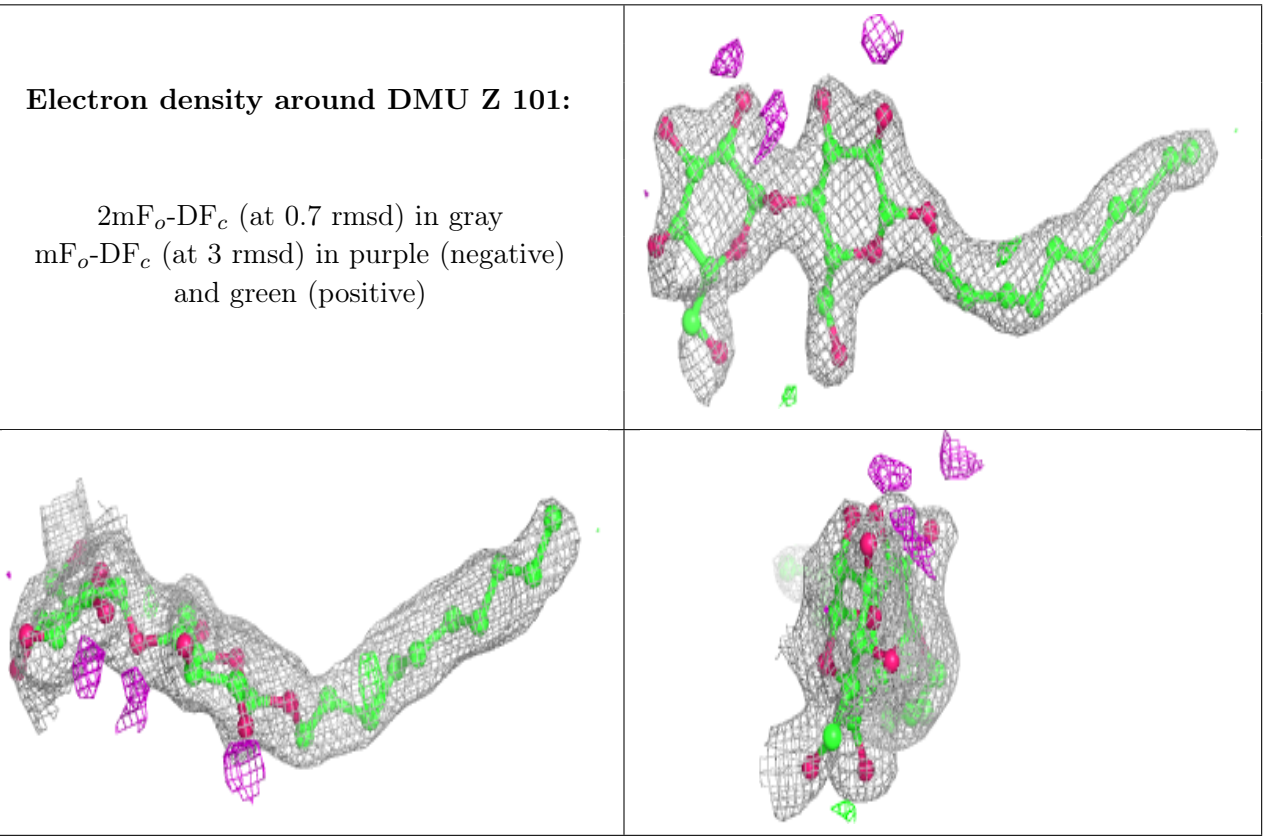
Electron density around TGL O 301:

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



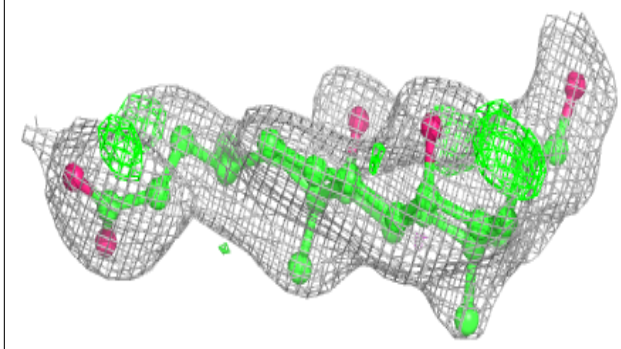
Electron density around DMU Z 101:

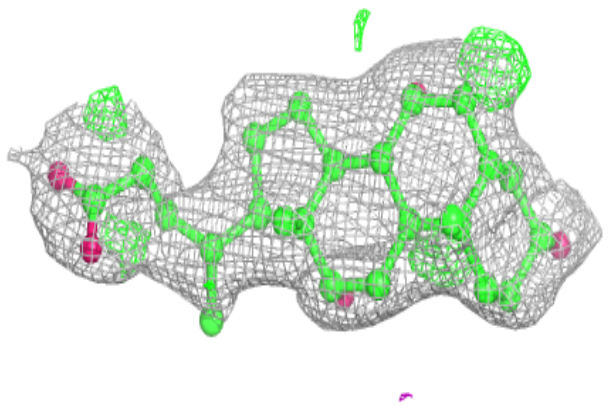
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

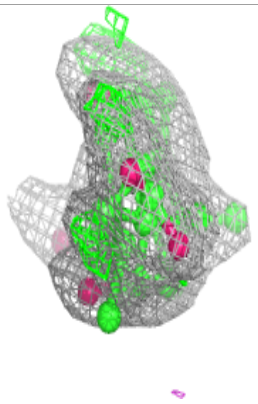


Electron density around CHD P 306:

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

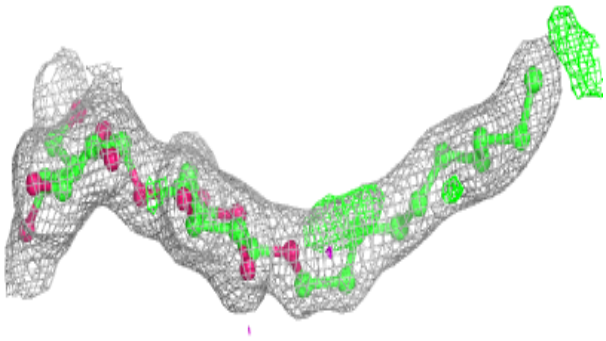


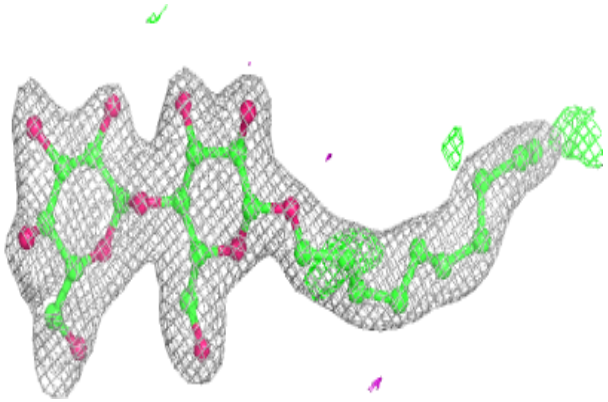


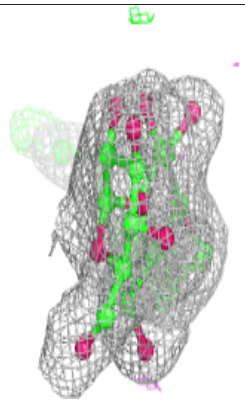


Electron density around DMU M 101:

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

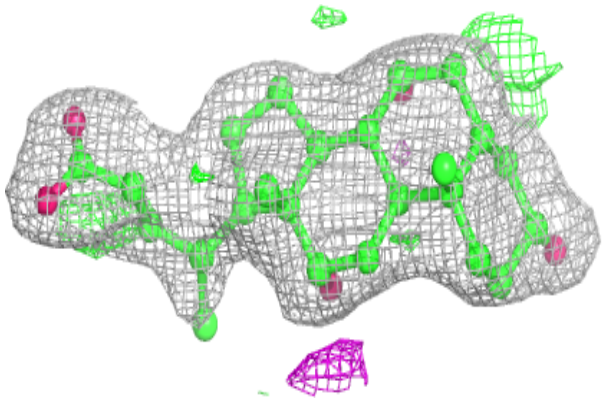


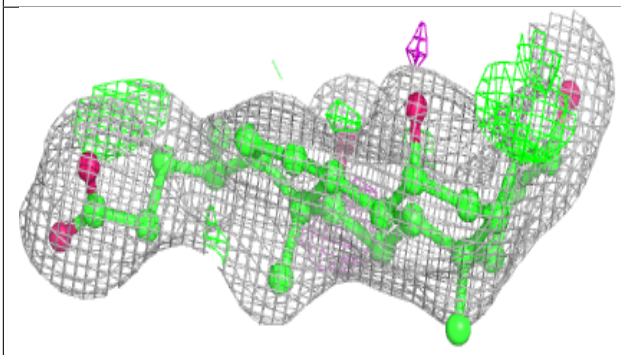


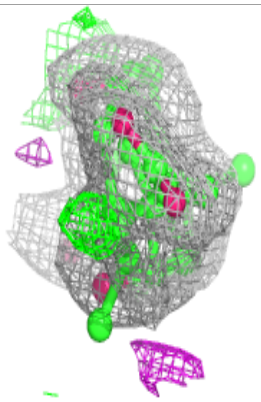


Electron density around CHD C 308:

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

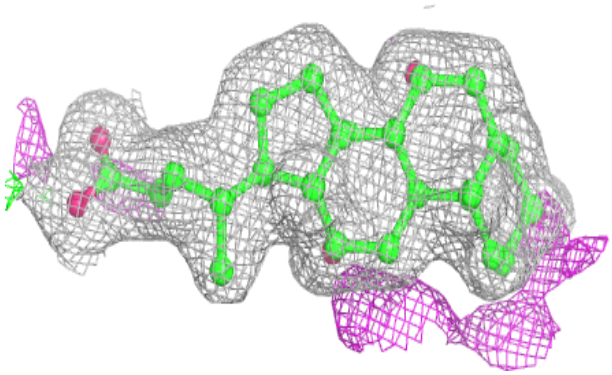


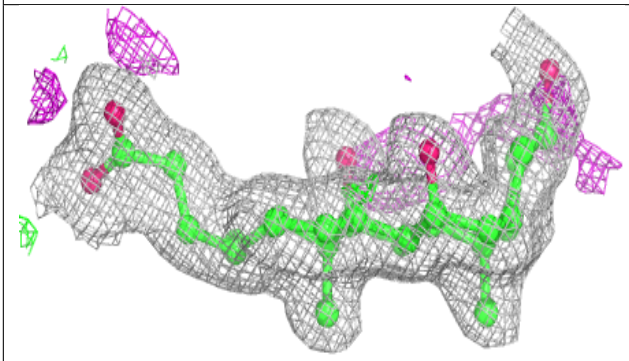


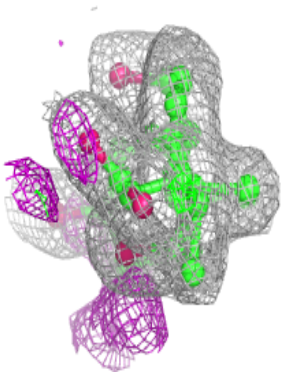


Electron density around CHD B 304:

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

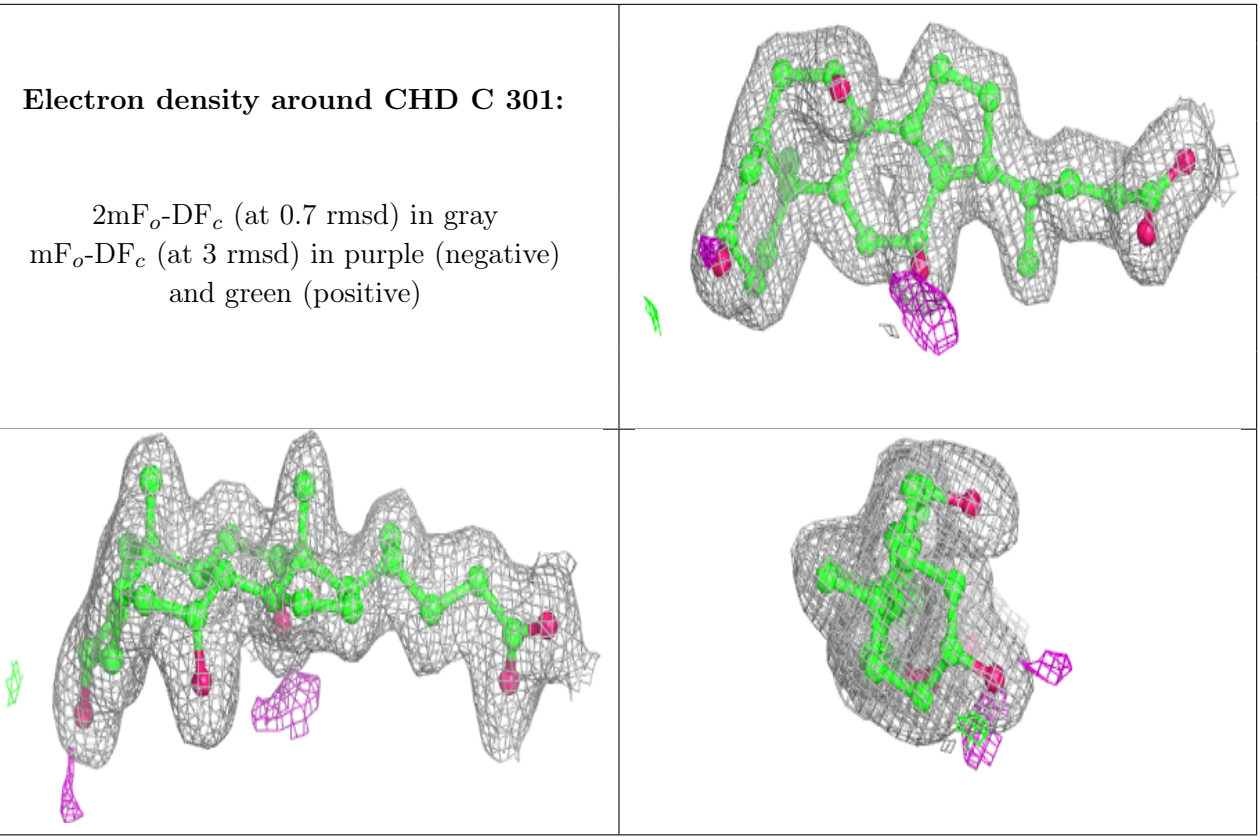






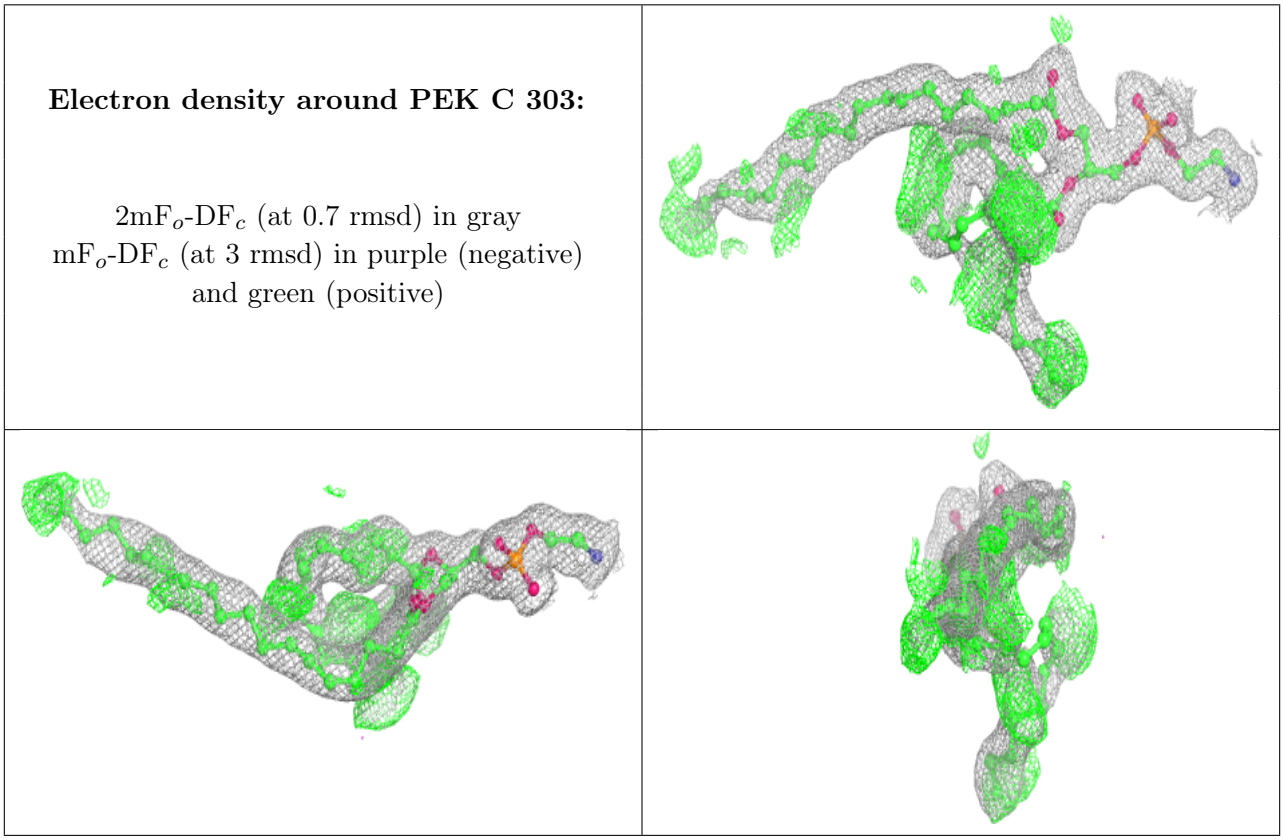
Electron density around CHD C 301:

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



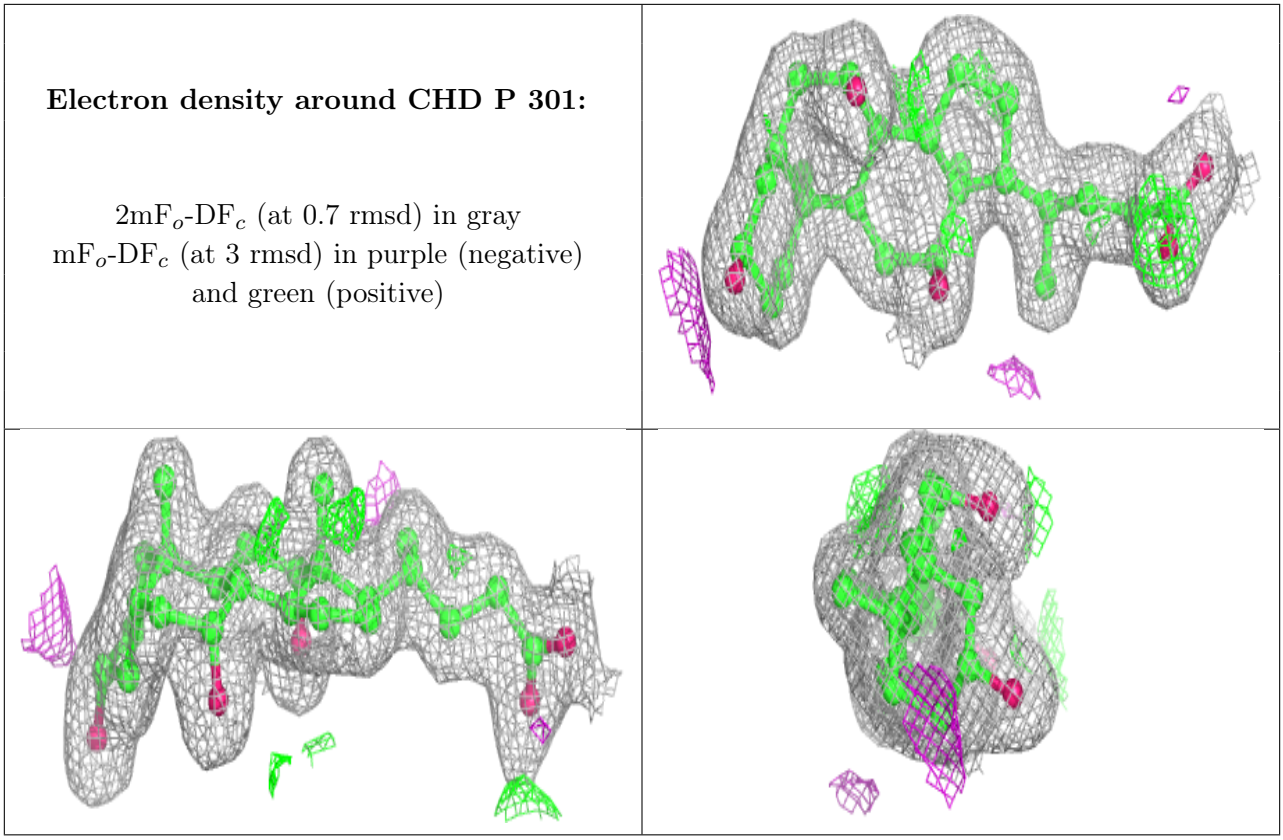
Electron density around PEK C 303:

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



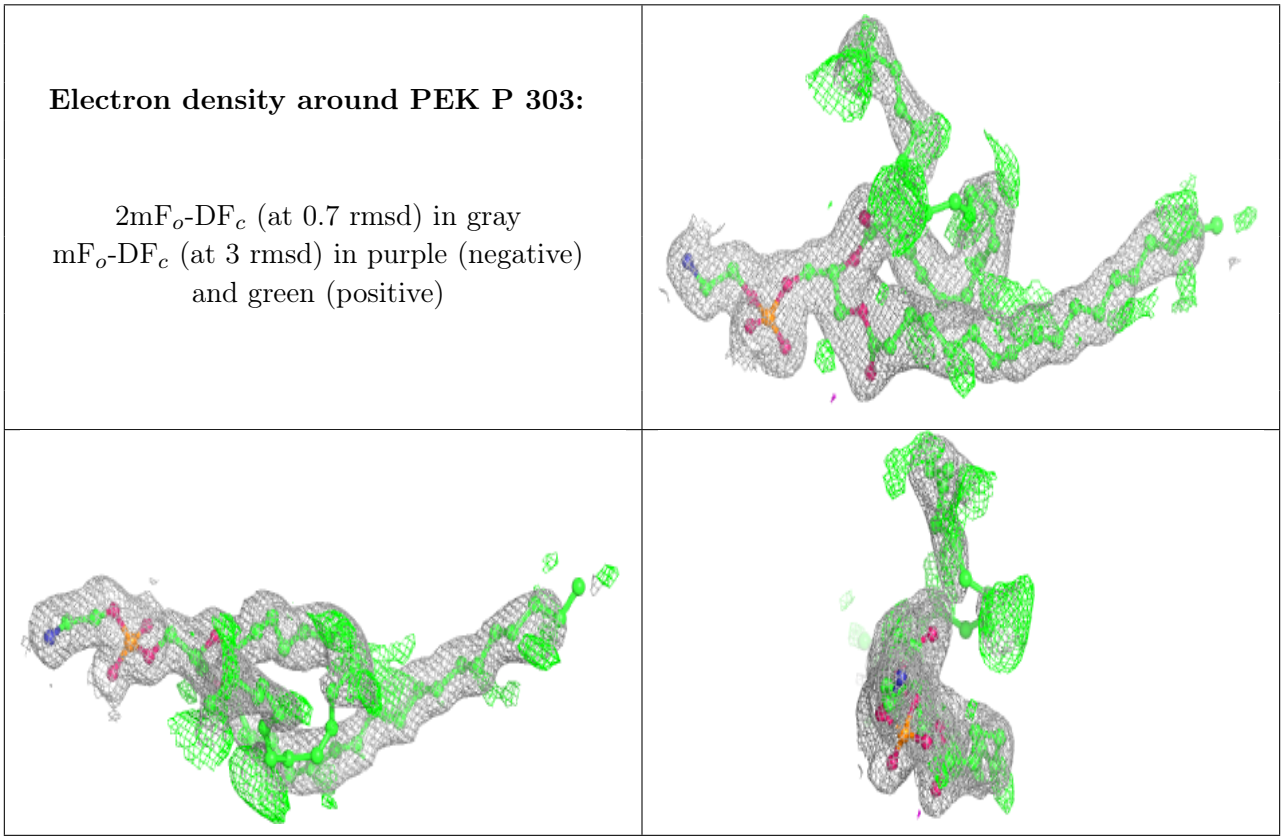
Electron density around CHD P 301:

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



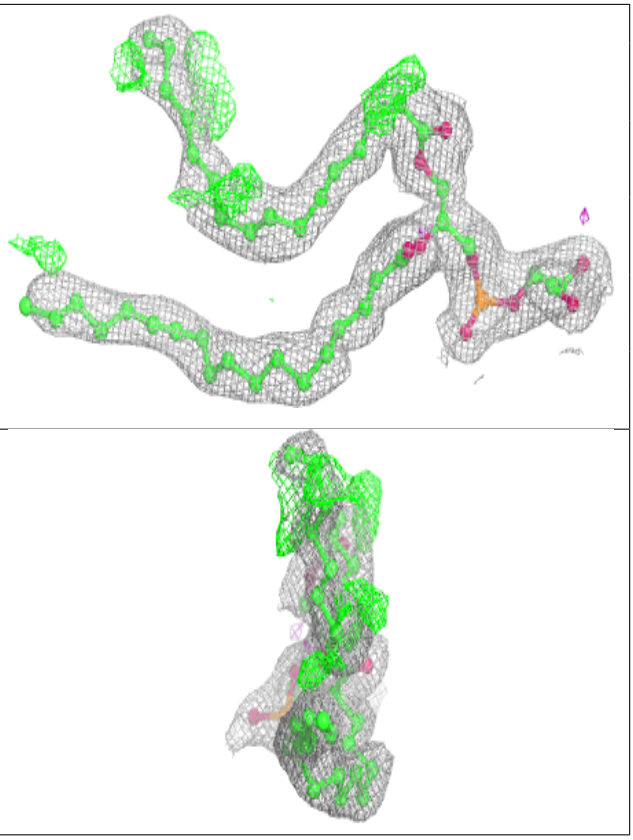
Electron density around PEK P 303:

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



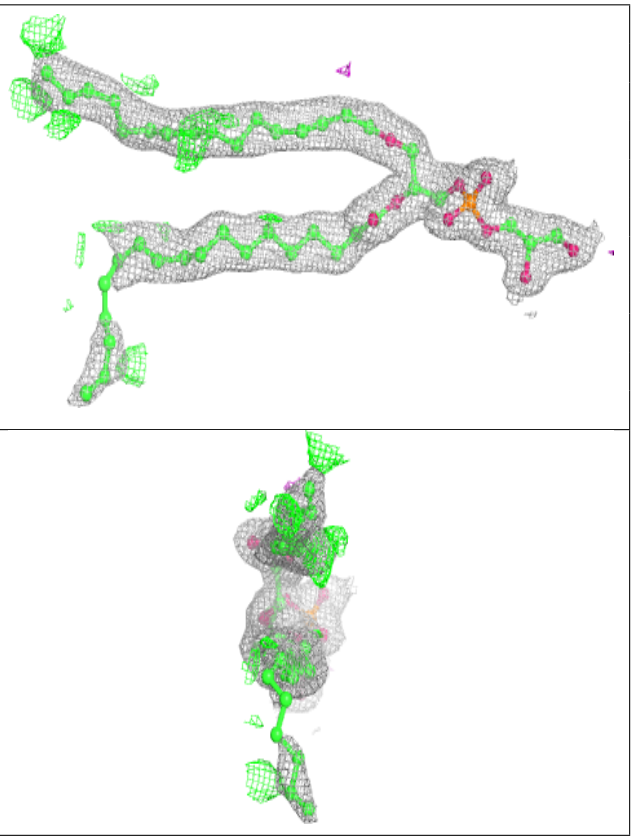
Electron density around PGV N 609:

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



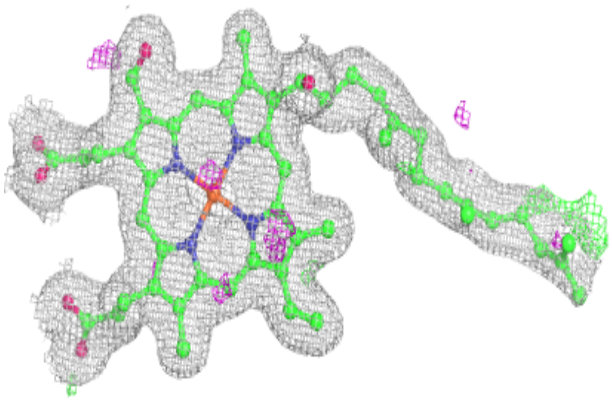
Electron density around PGV P 304:

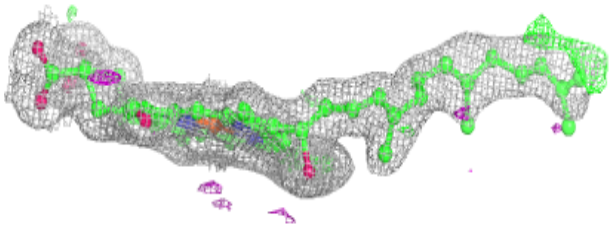
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

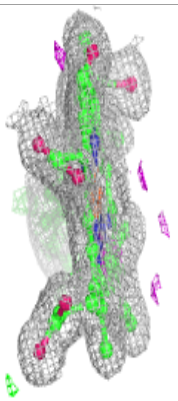


Electron density around HEA A 601 (A):

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

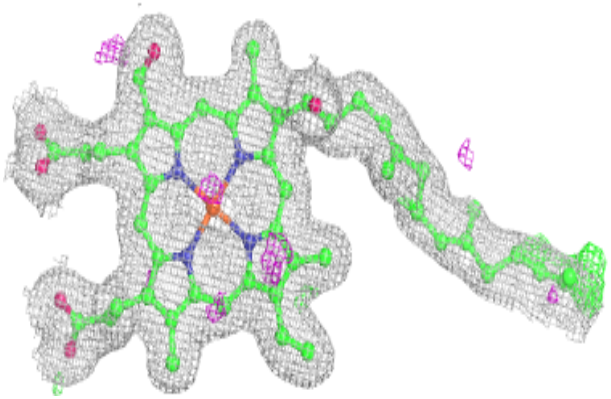


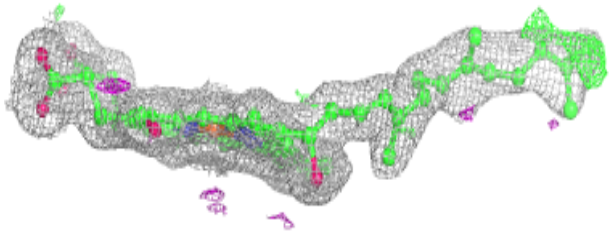


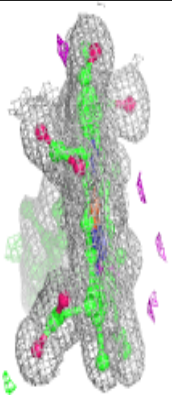


Electron density around HEA A 601 (B):

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

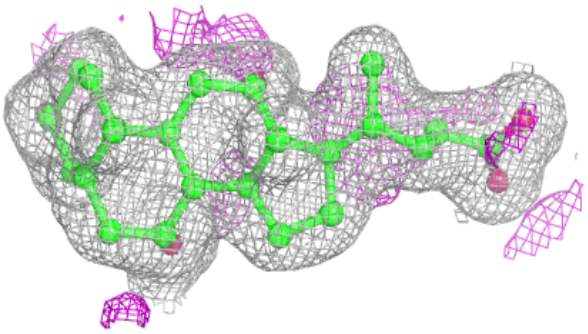


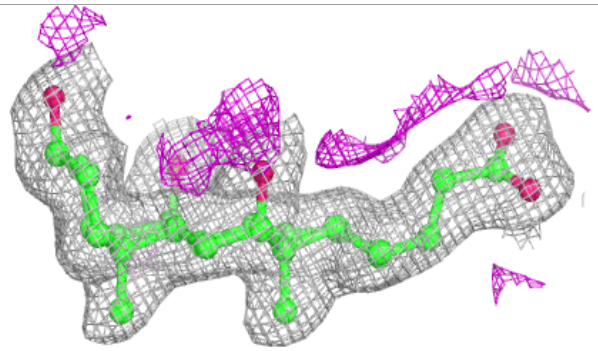


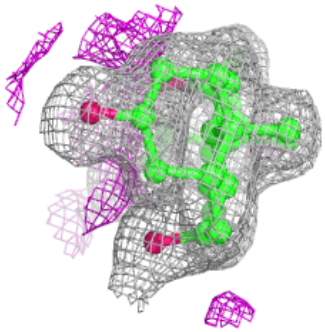


Electron density around CHD G 102:

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

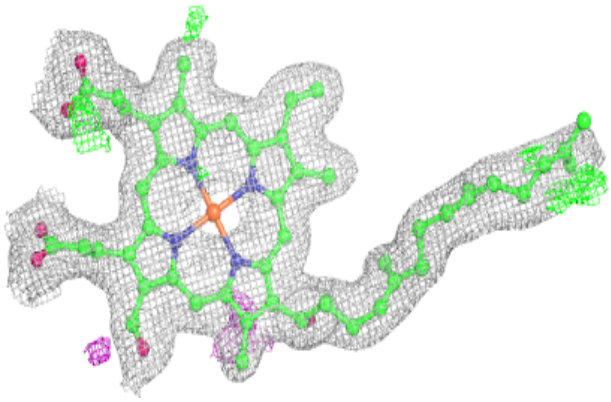


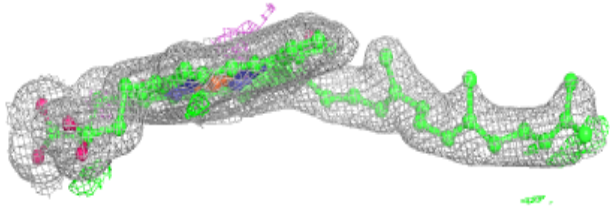


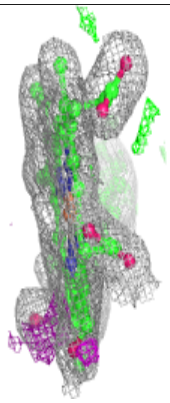


Electron density around HEA N 601 (A):

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

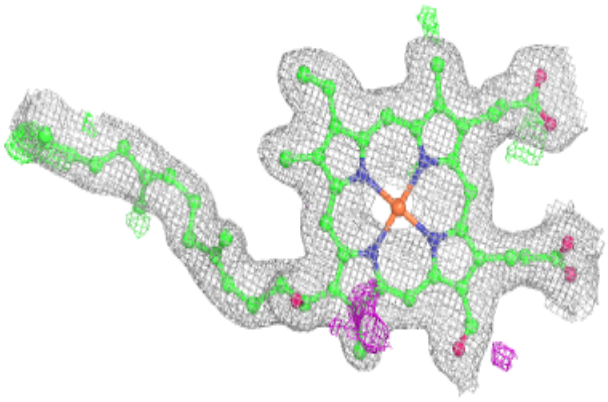


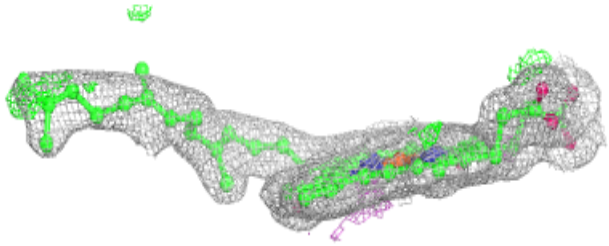


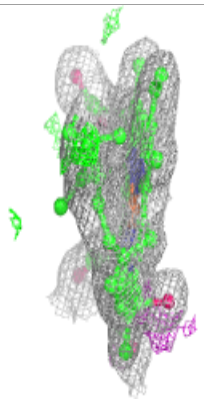


Electron density around HEA N 601 (B):

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

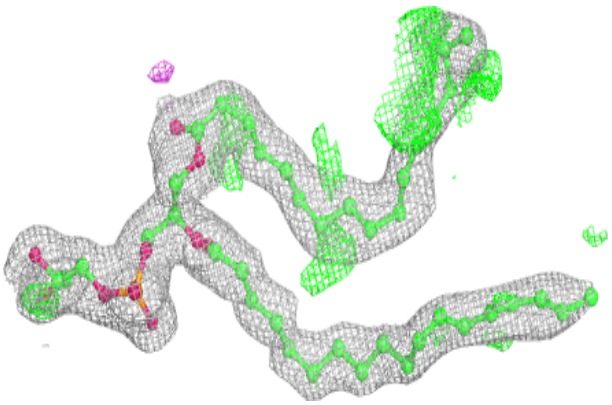


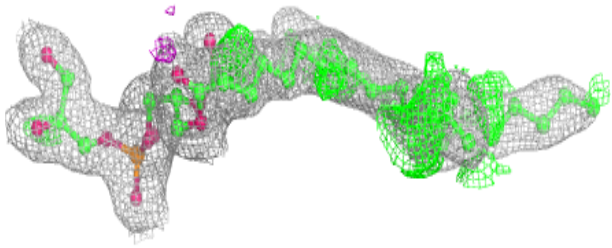


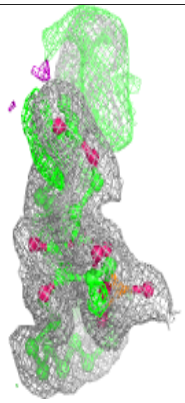


Electron density around PGV A 608:

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

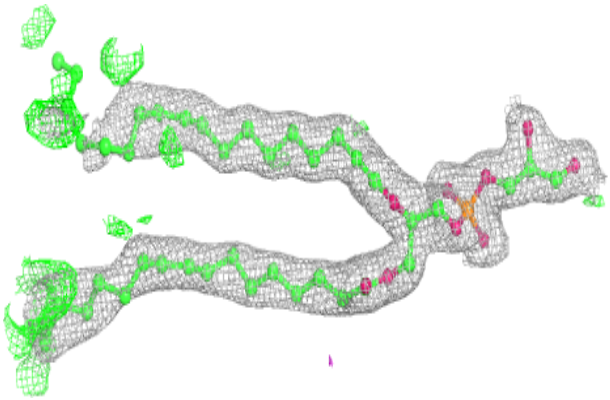


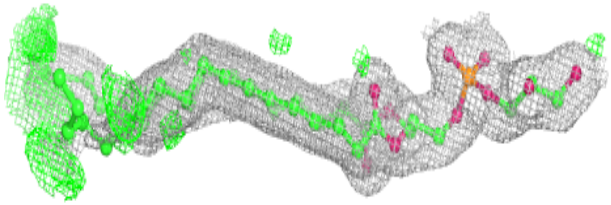


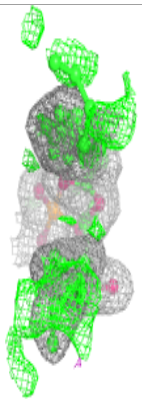


Electron density around PGV C 305:

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

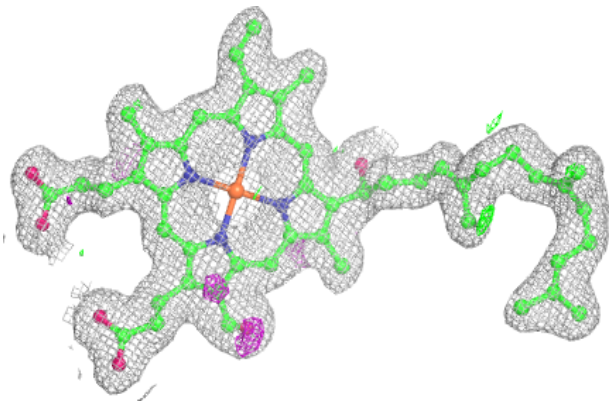


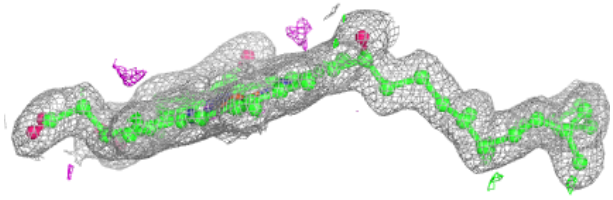


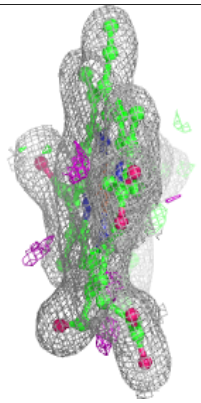


Electron density around HEA N 602:

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

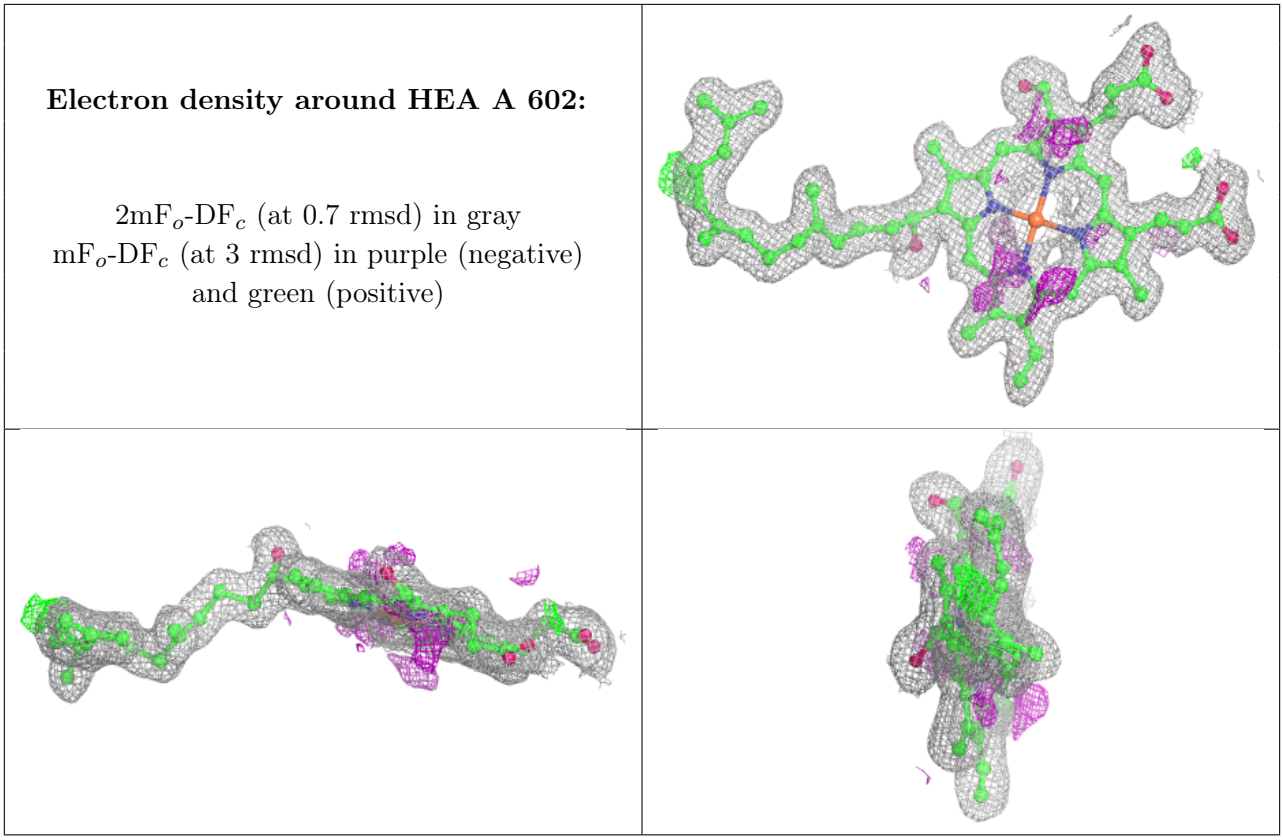






Electron density around HEA A 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.