wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 01:19 PM JST

PDB ID	:	5ZCQ
Title	:	Azide-bound cytochrome c oxidase structure determined using the crystals exposed to 10 mM azide solution for 2 days
Authors	:	Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on	:	2018-02-19
Resolution	:	1.65 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:

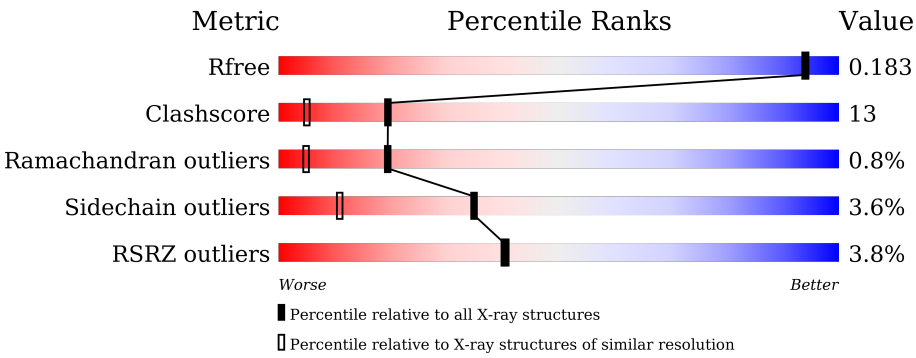
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	77% 20% •
1	N	514	79% 19% •
2	B	227	2% 72% 23% 5%
2	O	227	2% 72% 24% •
3	C	261	80% 18% ••
3	P	261	% 78% 19% • •

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Mol	Chain	Length	Quality of chain
4	D	147	%, 80%, 16%
4	Q	147	6%, 80%, 12%
5	E	109	2%, 81%, 13%
5	R	109	2%, 81%, 15%
6	F	98	8%, 78%, 16%, 5%
6	S	98	9%, 78%, 14%
7	G	85	20%, 65%, 19%, 13%
7	T	85	20%, 66%, 22%, 9%
8	H	85	9%, 64%, 20%, 8%, 7%
8	U	85	11%, 75%, 14%, 7%
9	I	73	11%, 77%, 21%
9	V	73	10%, 74%, 22%
10	J	59	7%, 78%, 17%
10	W	59	8%, 80%, 19%
11	K	56	75%, 12%, 12%
11	X	56	5%, 75%, 11%, 12%
12	L	47	2%, 68%, 23%, 6%
12	Y	47	2%, 79%, 17%
13	M	46	9%, 72%, 20%, 7%
13	Z	46	9%, 83%, 11%, 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	606[B]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	607[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FME	B	1	-	-	X	-
21	EDO	A	611	-	-	X	-
21	EDO	A	621	-	-	X	-
21	EDO	D	202	-	-	X	-
21	EDO	E	202	-	-	X	-
21	EDO	F	103	-	-	-	X
21	EDO	H	101	-	X	X	-
21	EDO	P	312	-	X	-	-
22	CHD	J	101	-	-	-	X
22	CHD	W	101	-	-	-	X
24	PSC	B	303	-	-	X	-
27	CDL	C	305	-	-	X	-
27	CDL	G	102	-	-	X	-
27	CDL	P	305	-	-	X	-
27	CDL	T	103	-	-	X	-
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33657 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
			Total	C	N	O	S			
1	A	514	4193	2793	649	709	42	0	22	0
1	N	514	4179	2786	647	704	42	0	20	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1907	1238	293	356	20	0	10	0
2	O	227	1870	1215	288	347	20	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2168	1447	347	359	15	0	7	0
3	P	259	2185	1457	349	363	16	0	9	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1242	809	206	223	4	0	5	0
4	Q	144	1224	797	202	221	4	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	98	771	477	138	150	6	0	3	0
6	S	98	763	473	136	148	6	0	2	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
7	G	84	686	440	130	114	1	1	0	1	0
7	T	84	686	440	130	114	1	1	0	1	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	W	58	469	302	79	85	3	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	49	384	250	65	67	2	0	0	0
			Total	C	N	O	S			
11	X	49	391	255	66	68	2	0	1	0

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

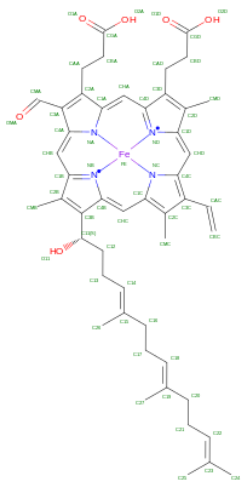
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	388	259	65	61	3	0	1	0

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

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

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

HEA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	A	1	120	98	2	8	12	0	1
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	120	98	2	8	12	0	1

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

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

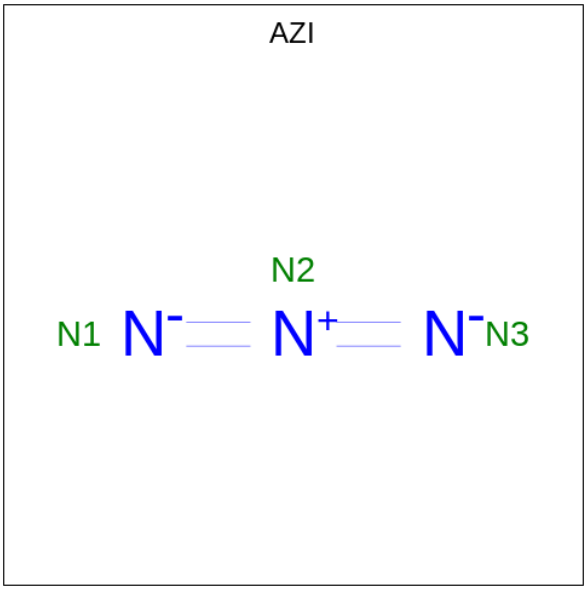
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

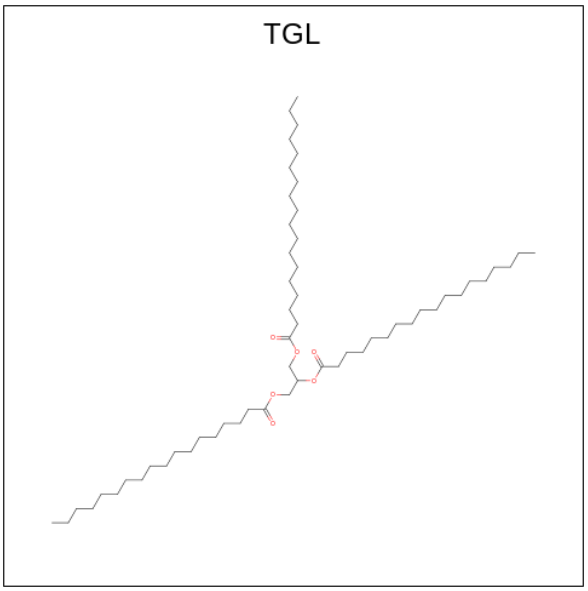
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N_3).



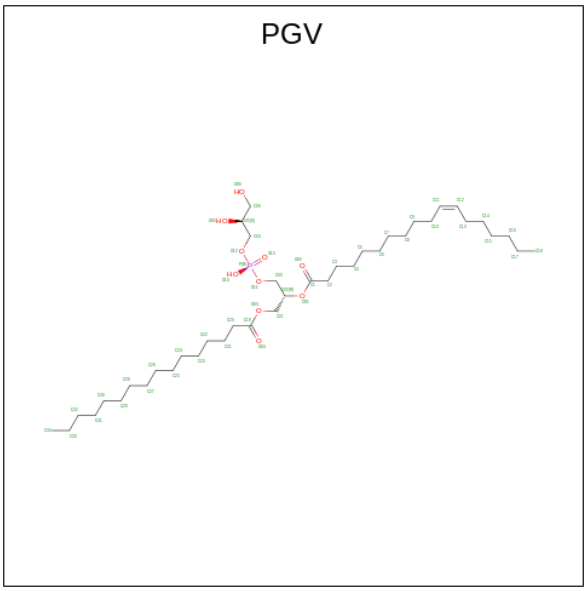
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
18	A	1	3	3	0	1
			Total	N		
18	A	1	6	6	0	1
			Total	N		
18	N	1	3	3	0	1
			Total	N		
18	N	1	6	6	0	1

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



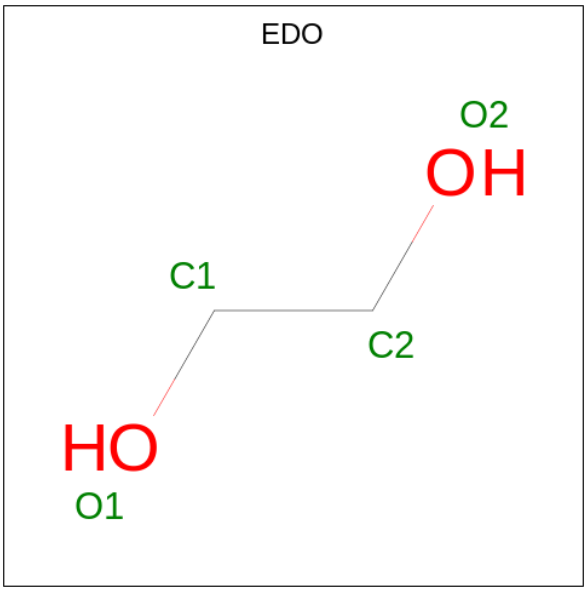
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 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
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	N	1	51	40	10	1	0	0
			Total	C	O	P		
20	P	1	51	40	10	1	0	0
			Total	C	O	P		
20	P	1	51	40	10	1	0	0
			Total	C	O	P		
20	X	1	51	40	10	1	0	0

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	C	1	4	2	2	0	0
21	C	1	4	2	2	0	0
21	C	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	D	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	E	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	F	1	4	2	2	0	0
21	G	1	4	2	2	0	0
21	G	1	4	2	2	0	0
21	H	1	4	2	2	0	0
21	L	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0

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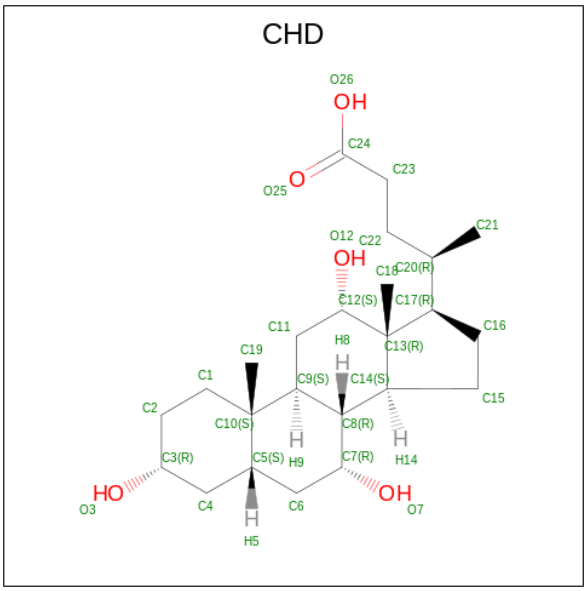
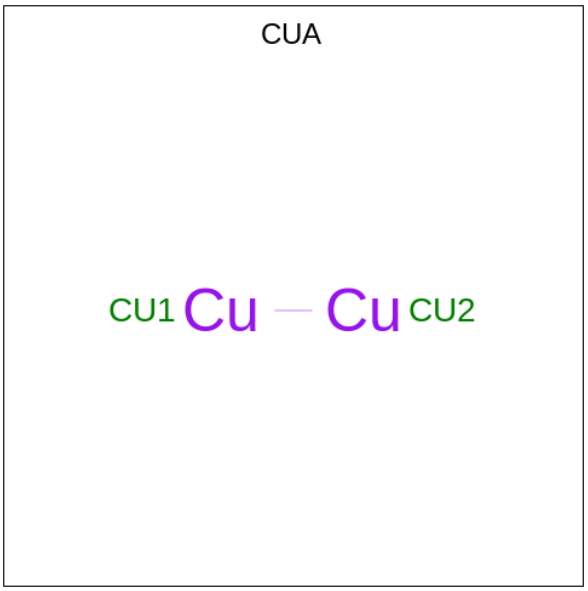
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	T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

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



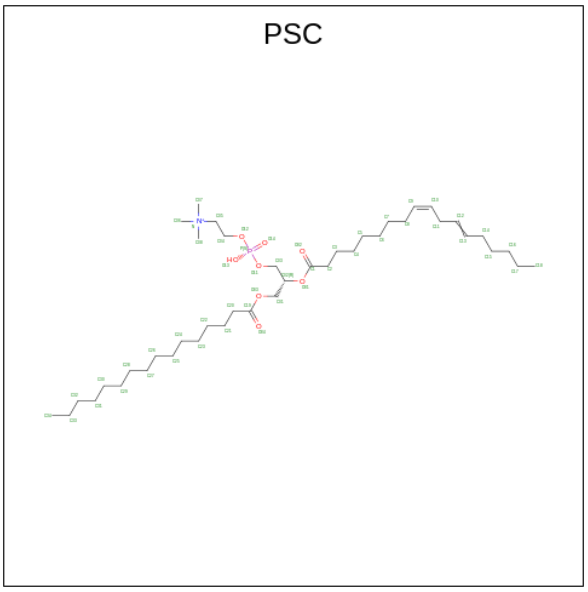
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	B	1	Total	C	O		0	0
			29	24	5			
22	C	1	Total	C	O		0	0
			29	24	5			
22	C	1	Total	C	O		0	0
			29	24	5			
22	G	1	Total	C	O		0	0
			29	24	5			
22	J	1	Total	C	O		0	0
			29	24	5			
22	P	1	Total	C	O		0	0
			29	24	5			
22	P	1	Total	C	O		0	0
			29	24	5			
22	W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

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



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

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



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

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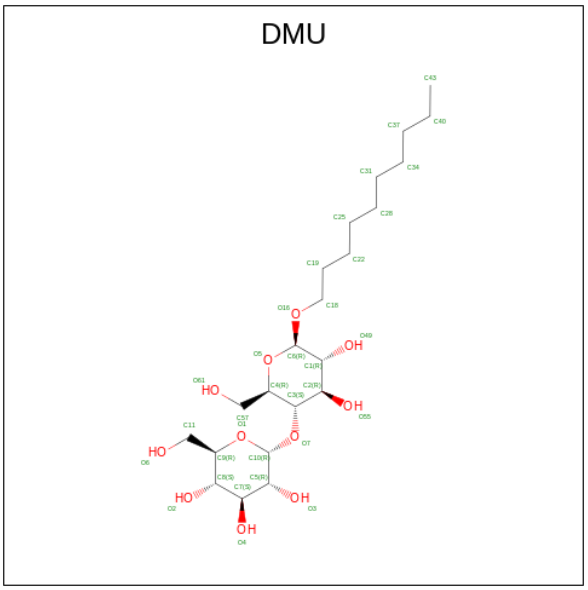
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	O	1	52	42	1	8	1	0	0

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

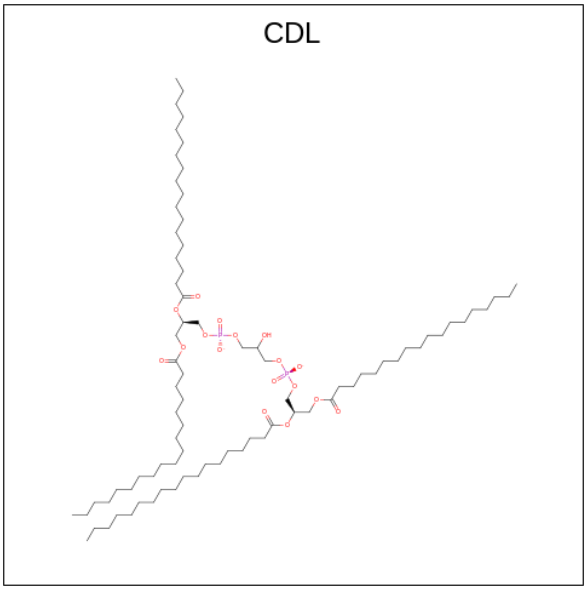


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	C	1	33	22	11	0	0
25	C	1	33	22	11	0	0
25	C	1	33	22	11	0	0
25	L	1	33	22	11	0	0
25	M	1	33	22	11	0	0
25	P	1	33	22	11	0	0
25	P	1	33	22	11	0	0
25	P	1	33	22	11	0	0
25	Z	1	33	22	11	0	0

- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

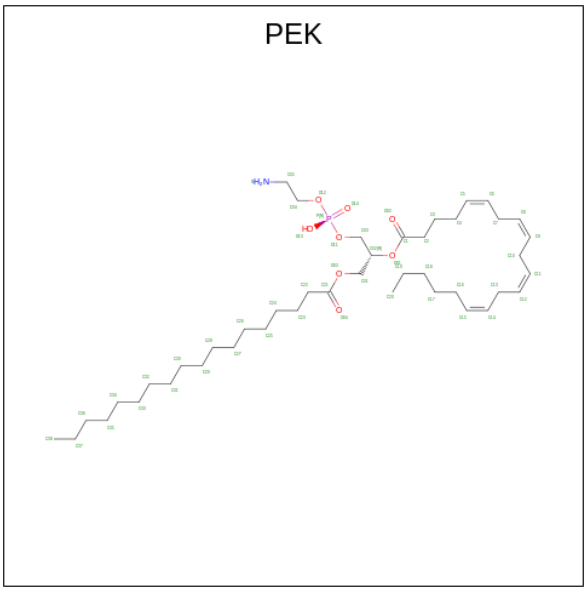
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
26	C	1	1	1	0	0
			Total	X		
26	P	1	1	1	0	0

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 28 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
			Total	C	N	O	P		
28	C	1	53	43	1	8	1	0	0
28	G	1	53	43	1	8	1	0	0
28	G	1	53	43	1	8	1	0	0
28	P	1	53	43	1	8	1	0	0
28	T	1	53	43	1	8	1	0	0
28	T	1	53	43	1	8	1	0	0

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	A	228	228	228	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	B	154	155	155	0	1
			Total	O		
30	C	101	101	101	0	0
			Total	O		
30	D	96	96	96	0	0
			Total	O		
30	E	80	80	80	0	0
			Total	O		
30	F	85	85	85	0	0
			Total	O		
30	G	46	46	46	0	0
			Total	O		
30	H	55	55	55	0	0
			Total	O		
30	I	26	26	26	0	0
			Total	O		
30	J	16	16	16	0	0
			Total	O		
30	K	15	15	15	0	0
			Total	O		
30	L	24	24	24	0	0
			Total	O		
30	M	19	19	19	0	0
			Total	O		
30	N	215	215	215	0	0
			Total	O		
30	O	109	110	110	0	1
			Total	O		
30	P	105	105	105	0	0
			Total	O		
30	Q	37	37	37	0	0
			Total	O		
30	R	49	49	49	0	0
			Total	O		
30	S	79	79	79	0	0
			Total	O		
30	T	36	36	36	0	0
			Total	O		
30	U	38	38	38	0	0
			Total	O		
30	V	14	14	14	0	0

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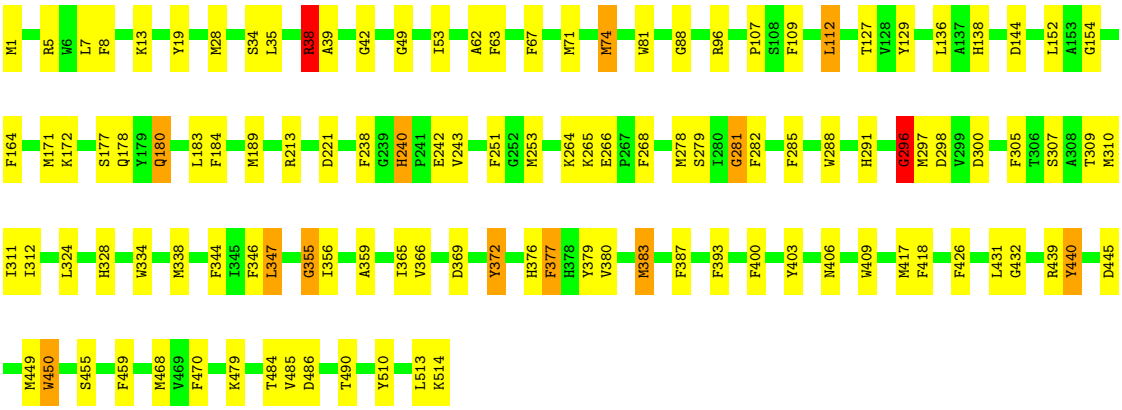
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	W	13	13	13	0	0
			Total	O		
30	X	11	11	11	0	0
			Total	O		
30	Y	13	13	13	0	0
			Total	O		
30	Z	12	12	12	0	0

3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:

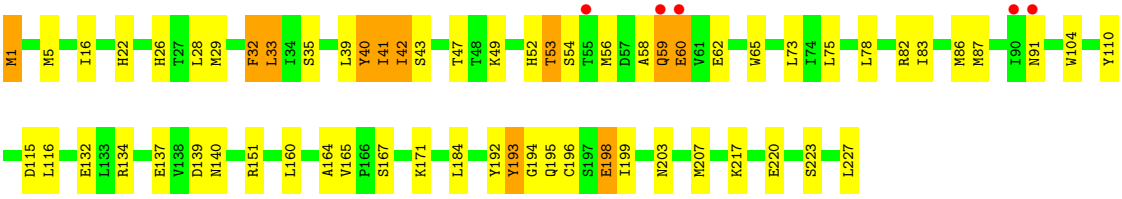


• Molecule 1: Cytochrome c oxidase subunit 1

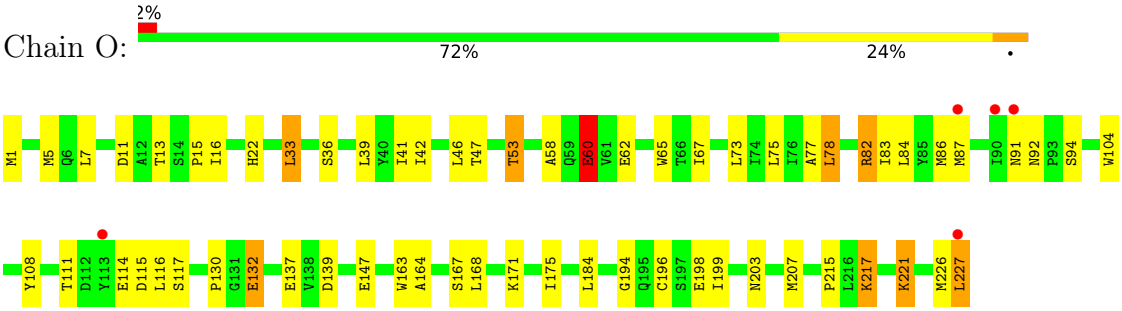
Chain N:

• Molecule 2: Cytochrome c oxidase subunit 2

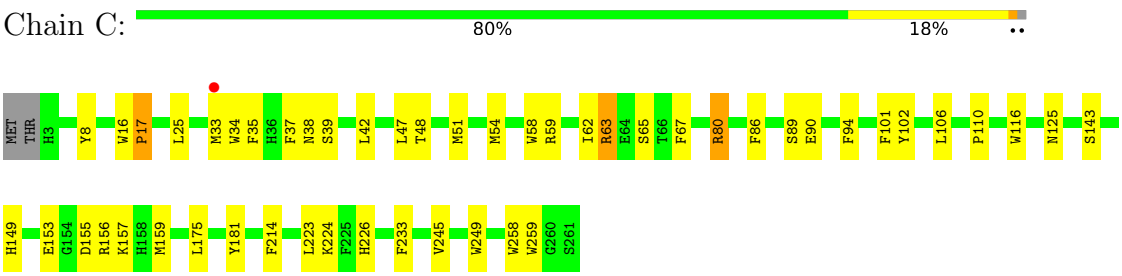
Chain B:



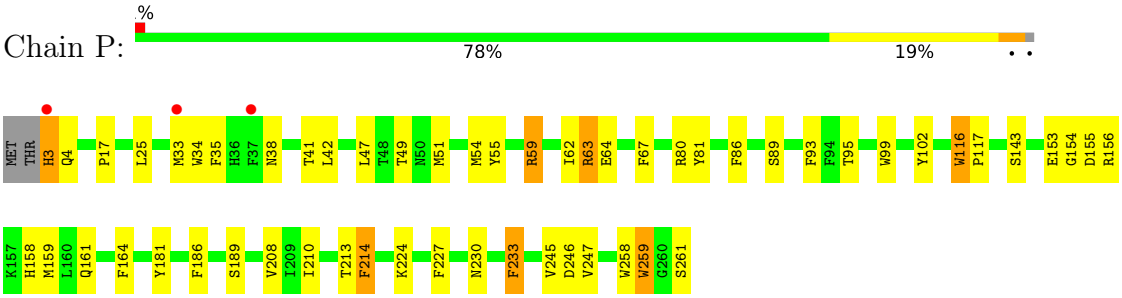
• Molecule 2: Cytochrome c oxidase subunit 2



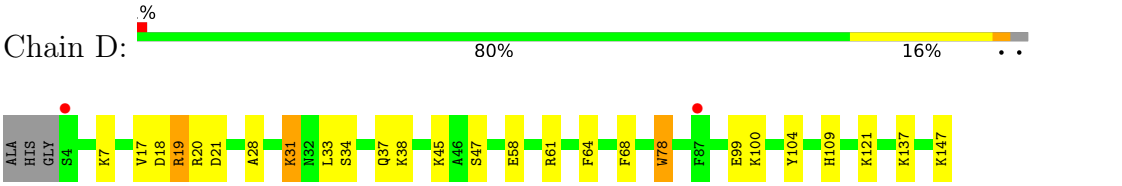
• Molecule 3: Cytochrome c oxidase subunit 3



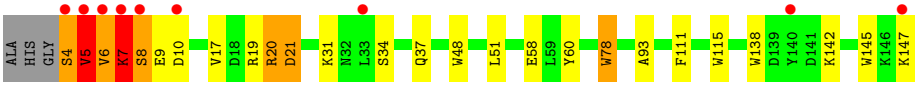
• Molecule 3: Cytochrome c oxidase subunit 3



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



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

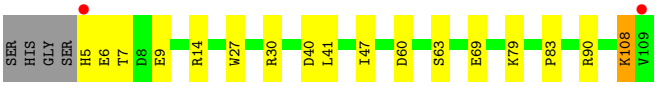


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:

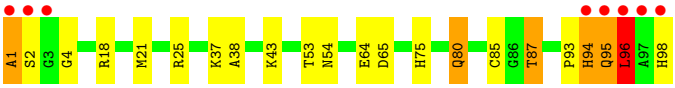
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



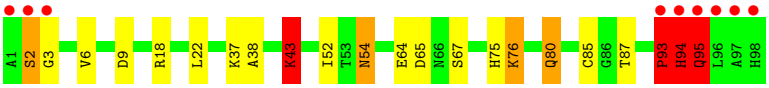
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



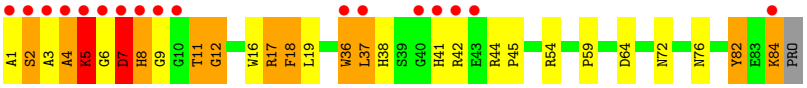
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



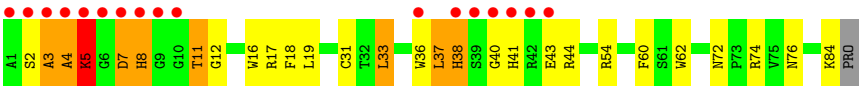
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



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

Chain T:

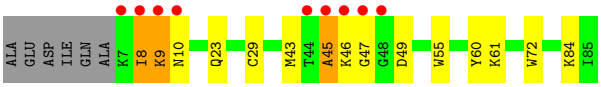


• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

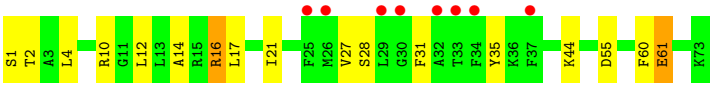
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



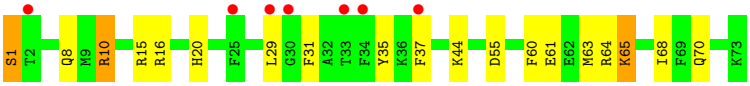
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:

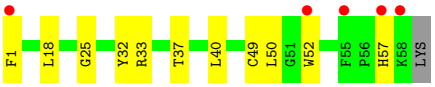


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:

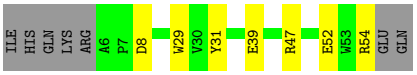
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



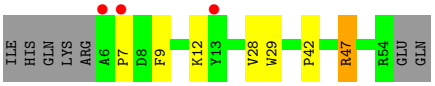
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



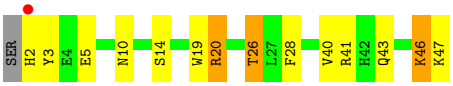
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



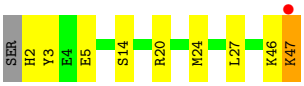
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



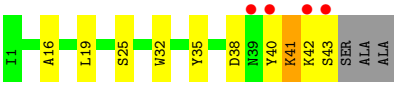
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



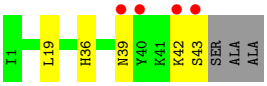
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.33Å 204.83Å 177.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 136.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.65) 99.9 (136.19-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.162 , 0.182 0.164 , 0.183	Depositor DCC
R_{free} test set	39619 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33657	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: DMU, CUA, CDL, PEK, PGV, SAC, PSC, UNX, EDO, FME, NA, CU, TGL, ZN, MG, CHD, AZI, HEA, TPO

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	1.66	30/4322 (0.7%)	1.51	49/5897 (0.8%)
1	N	1.62	33/4308 (0.8%)	1.39	35/5878 (0.6%)
2	B	1.64	17/1945 (0.9%)	1.45	15/2648 (0.6%)
2	O	1.37	12/1908 (0.6%)	1.21	9/2597 (0.3%)
3	C	1.64	17/2255 (0.8%)	1.33	13/3080 (0.4%)
3	P	1.58	17/2272 (0.7%)	1.33	16/3102 (0.5%)
4	D	1.60	9/1277 (0.7%)	1.37	6/1720 (0.3%)
4	Q	1.27	6/1259 (0.5%)	1.37	6/1698 (0.4%)
5	E	1.56	4/871 (0.5%)	1.75	12/1182 (1.0%)
5	R	1.39	6/871 (0.7%)	1.31	7/1182 (0.6%)
6	F	1.51	3/788 (0.4%)	1.37	6/1069 (0.6%)
6	S	1.40	2/780 (0.3%)	1.31	6/1058 (0.6%)
7	G	1.64	5/702 (0.7%)	1.36	8/953 (0.8%)
7	T	1.54	5/702 (0.7%)	1.27	6/953 (0.6%)
8	H	1.55	5/682 (0.7%)	1.23	3/921 (0.3%)
8	U	1.27	2/682 (0.3%)	1.05	0/921
9	I	1.44	4/605 (0.7%)	1.34	4/802 (0.5%)
9	V	1.15	0/605	1.15	2/802 (0.2%)
10	J	1.40	2/471 (0.4%)	1.18	1/636 (0.2%)
10	W	1.34	2/480 (0.4%)	1.22	2/648 (0.3%)
11	K	1.51	3/398 (0.8%)	1.34	5/546 (0.9%)
11	X	1.23	2/405 (0.5%)	0.92	0/556
12	L	1.60	5/393 (1.3%)	1.46	4/526 (0.8%)
12	Y	1.42	1/401 (0.2%)	1.15	0/536
13	M	1.51	2/345 (0.6%)	1.24	1/470 (0.2%)
13	Z	1.37	0/345	0.99	0/470
All	All	1.54	194/30072 (0.6%)	1.36	216/40851 (0.5%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	3
2	B	0	1
5	R	0	1
6	F	0	2
6	S	0	3
7	T	0	1
8	H	0	1
9	V	0	1
All	All	0	17

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	CD-OE2	-10.57	1.14	1.25
2	B	198	GLU	CD-OE1	-10.16	1.14	1.25
4	D	58	GLU	CD-OE1	10.12	1.36	1.25
12	Y	5	GLU	CD-OE2	-9.64	1.15	1.25
2	O	198	GLU	CD-OE2	-9.48	1.15	1.25

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	20	ARG	NE-CZ-NH2	-24.32	108.14	120.30
5	E	90	ARG	NE-CZ-NH1	23.80	132.20	120.30
4	Q	20	ARG	NE-CZ-NH1	22.14	131.37	120.30
5	E	90	ARG	NE-CZ-NH2	-21.09	109.75	120.30
1	A	71	MET	CG-SD-CE	-18.87	70.01	100.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	38	ARG	Sidechain
2	B	40	TYR	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	94	0
1	N	4179	0	4154	107	0
2	B	1907	0	1901	55	0
2	O	1870	0	1868	46	0
3	C	2168	0	2084	53	0
3	P	2185	0	2097	48	0
4	D	1242	0	1235	38	1
4	Q	1224	0	1211	19	0
5	E	852	0	845	16	0
5	R	852	0	845	2	0
6	F	771	0	748	23	0
6	S	763	0	742	32	0
7	G	686	0	650	48	0
7	T	686	0	651	25	0
8	H	662	0	623	24	0
8	U	662	0	623	10	0
9	I	601	0	613	19	0
9	V	601	0	613	15	0
10	J	460	0	459	9	0
10	W	469	0	464	6	0
11	K	384	0	366	1	0
11	X	391	0	374	10	0
12	L	380	0	380	18	0
12	Y	388	0	388	20	0
13	M	335	0	352	5	0
13	Z	335	0	352	4	0
14	A	180	0	162	23	0
14	N	180	0	162	22	0
15	A	1	0	0	1	0
15	N	1	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	9	0	0	8	0
18	N	9	0	0	6	0
19	A	63	0	110	1	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	11	0
19	N	63	0	110	5	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	11	0
20	C	102	0	152	7	0
20	N	51	0	76	1	0
20	P	102	0	152	14	0
20	X	51	0	76	10	0
21	A	44	0	66	16	0
21	B	12	0	18	0	0
21	C	12	0	18	0	0
21	D	16	0	24	15	0
21	E	12	0	18	9	0
21	F	16	0	24	0	0
21	G	8	0	12	1	0
21	H	4	0	6	5	0
21	L	4	0	6	0	0
21	N	28	0	42	2	0
21	O	8	0	12	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	20	0	30	0	0
21	T	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	4	0
22	P	58	0	77	4	0
22	W	29	0	39	5	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	21	0
24	O	52	0	80	11	0
25	C	99	0	126	13	0
25	L	33	0	42	4	0
25	M	33	0	42	0	0
25	P	99	0	126	16	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	1	0	0	0	0
27	C	100	0	156	26	0
27	G	100	0	156	24	0
27	P	100	0	156	28	0
27	T	100	0	156	24	0
28	C	53	0	77	14	0
28	G	106	0	154	26	0
28	P	53	0	77	5	0
28	T	106	0	154	2	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	228	0	0	23	0
30	B	155	0	0	9	2
30	C	101	0	0	1	0
30	D	96	0	0	11	0
30	E	80	0	0	8	0
30	F	85	0	0	3	0
30	G	46	0	0	5	0
30	H	55	0	0	1	0
30	I	26	0	0	6	0
30	J	16	0	0	1	0
30	K	15	0	0	0	0
30	L	24	0	0	7	1
30	M	19	0	0	1	0
30	N	215	0	0	16	0
30	O	110	0	0	2	0
30	P	105	0	0	6	0
30	Q	37	0	0	1	0
30	R	49	0	0	0	0
30	S	79	0	0	3	0
30	T	36	0	0	0	0
30	U	38	0	0	0	0
30	V	14	0	0	1	0
30	W	13	0	0	0	0
30	X	11	0	0	3	0
30	Y	13	0	0	0	0
30	Z	12	0	0	0	0
All	All	33657	0	32632	830	2

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 13.

The worst 5 of 830 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)
1:A:74:MET:CG	1:A:74:MET:CB	1.77	1.58
2:B:1:FME:CN	2:B:1:FME:N	1.71	1.50
4:D:38:LYS:HE2	30:D:303:HOH:O	1.16	1.31
24:B:303:PSC:O02	9:I:14:ALA:CB	1.80	1.28
2:B:1:FME:N	2:B:1:FME:O1	1.65	1.26

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:541:HOH:O	30:L:219:HOH:O[2_584]	2.09	0.11
4:D:7:LYS:CD	30:B:405:HOH:O[2_585]	2.11	0.09

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	534/514 (104%)	518 (97%)	16 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
3	C	264/261 (101%)	259 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	137 (94%)	4 (3%)	4 (3%)	5	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	3
6	F	99/98 (101%)	93 (94%)	3 (3%)	3 (3%)	4	0
6	S	98/98 (100%)	93 (95%)	3 (3%)	2 (2%)	7	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	82/85 (96%)	69 (84%)	9 (11%)	4 (5%)	2	0
7	T	82/85 (96%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	2	0
8	U	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	45 (100%)	0	0	100	100
13	M	41/46 (89%)	38 (93%)	1 (2%)	2 (5%)	2	0
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3595/3614 (100%)	3465 (96%)	103 (3%)	27 (1%)	19	5

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS

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	447/426 (105%)	441 (99%)	6 (1%)	69	50
1	N	445/426 (104%)	438 (98%)	7 (2%)	62	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	220/210 (105%)	210 (96%)	10 (4%)	27	7
2	O	215/210 (102%)	205 (95%)	10 (5%)	26	6
3	C	231/226 (102%)	228 (99%)	3 (1%)	69	50
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	29
4	D	133/129 (103%)	128 (96%)	5 (4%)	33	10
4	Q	131/129 (102%)	122 (93%)	9 (7%)	15	2
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	12
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	7
6	F	84/81 (104%)	81 (96%)	3 (4%)	35	11
6	S	83/81 (102%)	76 (92%)	7 (8%)	11	1
7	G	68/68 (100%)	60 (88%)	8 (12%)	5	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	2
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	2
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	36
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	32
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	9
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	22
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	21
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	22
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	19
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	4
All	All	3129/3082 (102%)	3017 (96%)	112 (4%)	35	11

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	78	LEU
13	Z	42	LYS
4	Q	7	LYS
12	Y	47	LYS
8	U	29	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	195	GLN
5	R	94	ASN
3	P	3	HIS
3	P	76	GLN
6	S	80	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	$\#\|Z\| > 2$
7	TPO	T	11	7	8,10,11	2.06	2 (25%)	10,14,16	1.88	4 (40%)
1	FME	A	1	1	8,9,10	0.94	1 (12%)	7,9,11	2.16	5 (71%)
2	FME	B	1	2	8,9,10	5.13	6 (75%)	7,9,11	9.46	3 (42%)
9	SAC	I	1	9	7,8,9	1.11	1 (14%)	8,9,11	2.33	1 (12%)
2	FME	O	1	2	8,9,10	1.45	2 (25%)	7,9,11	1.59	1 (14%)
7	TPO	G	11	7	8,10,11	1.98	2 (25%)	10,14,16	1.70	2 (20%)
9	SAC	V	1	9	7,8,9	2.00	1 (14%)	8,9,11	2.36	3 (37%)
1	FME	N	1	1	8,9,10	1.22	1 (12%)	7,9,11	1.27	1 (14%)

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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	11.20	1.71	1.33
2	B	1	FME	CA-N	5.36	1.53	1.46
9	V	1	SAC	CA-N	5.06	1.53	1.46
2	B	1	FME	CB-CG	4.89	1.70	1.51
2	B	1	FME	CG-SD	-3.59	1.62	1.81

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	O1-CN-N	-22.22	66.76	125.27
2	B	1	FME	CA-N-CN	-10.90	106.06	122.82
9	I	1	SAC	OG-CB-CA	-5.84	96.06	110.97
9	V	1	SAC	CA-N-C1A	4.86	132.10	123.15
7	T	11	TPO	CG2-CB-CA	3.82	120.71	113.16

There are no chirality outliers.

5 of 27 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-OG1
7	G	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
2	B	1	FME	6	0
7	G	11	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 118 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - 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	$\#\|Z\| > 2$
28	PEK	T	102	-	52,52,52	0.95	3 (5%)	55,57,57	1.27	5 (9%)
21	EDO	A	616	-	3,3,3	1.06	0	2,2,2	2.70	2 (100%)
21	EDO	F	104	-	3,3,3	1.59	0	2,2,2	0.63	0
21	EDO	B	306	-	3,3,3	0.56	0	2,2,2	0.03	0
21	EDO	A	618	-	3,3,3	1.10	0	2,2,2	1.10	0
21	EDO	S	102	-	3,3,3	0.86	0	2,2,2	0.43	0
14	HEA	N	601	1	57,67,67	1.64	15 (26%)	61,103,103	2.71	22 (36%)
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	T	104	-	3,3,3	1.14	0	2,2,2	0.72	0
21	EDO	D	204	-	3,3,3	0.58	0	2,2,2	0.60	0
21	EDO	F	103	-	3,3,3	0.79	0	2,2,2	0.19	0
20	PGV	A	609	-	50,50,50	1.11	4 (8%)	53,56,56	1.28	5 (9%)
21	EDO	D	202	-	3,3,3	0.76	0	2,2,2	1.03	0
20	PGV	N	608	-	50,50,50	1.15	5 (10%)	53,56,56	1.53	8 (15%)
20	PGV	C	308	-	50,50,50	1.40	3 (6%)	53,56,56	1.62	7 (13%)
21	EDO	D	205	-	3,3,3	0.26	0	2,2,2	1.60	1 (50%)
25	DMU	C	302	-	34,34,34	0.98	1 (2%)	45,45,45	1.57	5 (11%)
21	EDO	G	105	-	3,3,3	0.97	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	CDL	P	305	-	99,99,99	1.73	21 (21%)	105,111,111	1.57	18 (17%)
21	EDO	H	101	-	3,3,3	0.30	0	2,2,2	2.28	2 (100%)
21	EDO	B	305	-	3,3,3	0.55	0	2,2,2	0.77	0
14	HEA	A	602[A]	18,1	57,67,67	1.56	9 (15%)	61,103,103	2.04	17 (27%)
21	EDO	A	617	-	3,3,3	1.23	0	2,2,2	0.34	0
28	PEK	G	104	-	52,52,52	1.32	3 (5%)	55,57,57	1.47	8 (14%)
22	CHD	P	306	-	32,32,32	1.63	7 (21%)	51,51,51	2.88	20 (39%)
21	EDO	A	620	-	3,3,3	0.62	0	2,2,2	0.41	0
21	EDO	C	312	-	3,3,3	0.44	0	2,2,2	0.79	0
24	PSC	B	303	-	51,51,51	1.54	7 (13%)	57,59,59	2.16	12 (21%)
21	EDO	S	103	-	3,3,3	0.47	0	2,2,2	0.27	0
21	EDO	B	304	-	3,3,3	0.88	0	2,2,2	0.78	0
22	CHD	G	103	-	32,32,32	2.05	13 (40%)	51,51,51	2.38	22 (43%)
21	EDO	C	313	-	3,3,3	1.05	0	2,2,2	0.80	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.59	0
27	CDL	T	103	-	99,99,99	1.58	15 (15%)	105,111,111	1.62	17 (16%)
21	EDO	A	612	-	3,3,3	1.74	1 (33%)	2,2,2	0.97	0
20	PGV	C	304	-	50,50,50	0.82	0	53,56,56	1.31	6 (11%)
21	EDO	N	612	-	3,3,3	0.68	0	2,2,2	0.77	0
21	EDO	P	311	-	3,3,3	0.99	0	2,2,2	0.39	0
14	HEA	A	602[B]	18,1	57,67,67	1.49	9 (15%)	61,103,103	2.34	23 (37%)
21	EDO	P	312	-	3,3,3	1.12	0	2,2,2	2.42	2 (100%)
25	DMU	C	310	-	34,34,34	1.76	8 (23%)	45,45,45	3.10	18 (40%)
19	TGL	L	101	-	62,62,62	1.61	7 (11%)	65,65,65	2.71	21 (32%)
21	EDO	A	619	-	3,3,3	0.39	0	2,2,2	0.70	0
25	DMU	Z	101	-	34,34,34	0.85	3 (8%)	45,45,45	1.43	5 (11%)
20	PGV	P	304	-	50,50,50	0.93	1 (2%)	53,56,56	1.32	5 (9%)
21	EDO	L	103	-	3,3,3	0.59	0	2,2,2	0.29	0
21	EDO	O	304	-	3,3,3	0.82	0	2,2,2	0.54	0
27	CDL	C	305	-	99,99,99	1.64	18 (18%)	105,111,111	1.64	21 (20%)
21	EDO	S	105	-	3,3,3	1.04	0	2,2,2	1.61	1 (50%)
22	CHD	J	101	-	32,32,32	1.23	3 (9%)	51,51,51	3.23	24 (47%)
21	EDO	A	615	-	3,3,3	0.93	0	2,2,2	0.72	0
22	CHD	W	101	-	32,32,32	1.18	2 (6%)	51,51,51	3.62	24 (47%)
21	EDO	A	611	-	3,3,3	0.47	0	2,2,2	0.21	0
25	DMU	C	309	-	34,34,34	0.80	1 (2%)	45,45,45	2.56	12 (26%)
25	DMU	P	307	-	34,34,34	1.20	1 (2%)	45,45,45	1.38	6 (13%)
23	CUA	B	302	2	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	EDO	N	615	-	3,3,3	0.45	0	2,2,2	1.04	0
18	AZI	A	607[A]	14,15	0,2,2	-	-	0,1,1	-	-
25	DMU	P	309	-	34,34,34	0.84	2 (5%)	45,45,45	2.27	12 (26%)
25	DMU	L	102	-	34,34,34	1.11	4 (11%)	45,45,45	1.75	12 (26%)
28	PEK	P	308	-	52,52,52	1.31	3 (5%)	55,57,57	1.42	8 (14%)
14	HEA	N	602[A]	18,1	57,67,67	1.67	12 (21%)	61,103,103	2.00	16 (26%)
21	EDO	C	311	-	3,3,3	1.03	0	2,2,2	0.27	0
14	HEA	A	601	1	57,67,67	1.78	17 (29%)	61,103,103	2.86	29 (47%)
19	TGL	Y	101	-	62,62,62	1.64	7 (11%)	65,65,65	2.16	19 (29%)
20	PGV	P	302	-	50,50,50	1.22	2 (4%)	53,56,56	1.34	4 (7%)
21	EDO	Y	102	-	3,3,3	0.63	0	2,2,2	0.15	0
22	CHD	P	301	-	32,32,32	1.76	9 (28%)	51,51,51	2.35	16 (31%)
27	CDL	G	102	-	99,99,99	1.57	16 (16%)	105,111,111	1.72	22 (20%)
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.56	9 (15%)
22	CHD	C	306	-	32,32,32	1.26	4 (12%)	51,51,51	3.31	21 (41%)
21	EDO	F	102	-	3,3,3	0.99	0	2,2,2	0.31	0
18	AZI	N	606[B]	14	0,2,2	-	-	0,1,1	-	-
19	TGL	A	608	-	62,62,62	1.36	5 (8%)	65,65,65	1.87	11 (16%)
18	AZI	N	607[A]	14,15	0,2,2	-	-	0,1,1	-	-
21	EDO	N	616	-	3,3,3	1.35	1 (33%)	2,2,2	1.66	0
21	EDO	G	106	-	3,3,3	0.53	0	2,2,2	0.94	0
21	EDO	N	611	-	3,3,3	0.70	0	2,2,2	1.02	0
25	DMU	M	101	-	34,34,34	0.97	2 (5%)	45,45,45	1.36	7 (15%)
19	TGL	Q	201	-	62,62,62	1.60	4 (6%)	65,65,65	1.44	9 (13%)
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	E	203	-	3,3,3	0.50	0	2,2,2	0.93	0
21	EDO	A	613	-	3,3,3	0.80	0	2,2,2	0.71	0
21	EDO	N	614	-	3,3,3	1.34	0	2,2,2	0.57	0
21	EDO	R	201	-	3,3,3	0.66	0	2,2,2	0.81	0
21	EDO	A	614	-	3,3,3	1.10	0	2,2,2	0.75	0
14	HEA	N	602[B]	18,1	57,67,67	1.57	11 (19%)	61,103,103	1.94	18 (29%)
21	EDO	N	610	-	3,3,3	1.33	1 (33%)	2,2,2	0.34	0
21	EDO	N	613	-	3,3,3	0.73	0	2,2,2	0.24	0
19	TGL	N	609	-	62,62,62	1.10	4 (6%)	65,65,65	1.91	10 (15%)
20	PGV	X	101	-	50,50,50	1.35	3 (6%)	53,56,56	1.59	8 (15%)
28	PEK	C	307	-	52,52,52	1.37	5 (9%)	55,57,57	1.54	7 (12%)
21	EDO	F	105	-	3,3,3	1.15	0	2,2,2	0.70	0
22	CHD	C	301	-	32,32,32	1.88	8 (25%)	51,51,51	2.37	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	PEK	T	101	-	52,52,52	1.34	2 (3%)	55,57,57	1.62	9 (16%)
20	PGV	A	610	-	50,50,50	1.86	4 (8%)	53,56,56	2.74	10 (18%)
22	CHD	B	301	-	32,32,32	1.98	14 (43%)	51,51,51	2.64	26 (50%)
28	PEK	G	101	-	52,52,52	1.02	3 (5%)	55,57,57	1.34	8 (14%)
21	EDO	D	203	-	3,3,3	0.41	0	2,2,2	0.88	0
18	AZI	N	607[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.60	0
25	DMU	P	310	-	34,34,34	1.06	1 (2%)	45,45,45	1.49	5 (11%)
21	EDO	S	104	-	3,3,3	1.36	0	2,2,2	0.40	0
19	TGL	D	201	-	62,62,62	2.27	6 (9%)	65,65,65	2.97	16 (24%)
21	EDO	A	621	-	3,3,3	0.38	0	2,2,2	1.22	0
23	CUA	O	301	2	0,1,1	-	-	-		
21	EDO	E	202	-	3,3,3	0.91	0	2,2,2	0.57	0
21	EDO	S	106	-	3,3,3	1.15	0	2,2,2	0.83	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
28	PEK	T	102	-	-	16/56/56/56	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
14	HEA	N	601	1	-	4/32/76/76	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
21	EDO	F	103	-	-	1/1/1/1	-
20	PGV	A	609	-	-	7/55/55/55	-
21	EDO	D	202	-	-	0/1/1/1	-
20	PGV	N	608	-	-	7/55/55/55	-
20	PGV	C	308	-	-	37/55/55/55	-
21	EDO	D	205	-	-	1/1/1/1	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
21	EDO	G	105	-	-	0/1/1/1	-
27	CDL	P	305	-	-	59/110/110/110	-
21	EDO	H	101	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	B	305	-	-	0/1/1/1	-
14	HEA	A	602[A]	18,1	-	4/32/76/76	-
21	EDO	A	617	-	-	1/1/1/1	-
28	PEK	G	104	-	-	27/56/56/56	-
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
21	EDO	A	620	-	-	1/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
24	PSC	B	303	-	-	21/55/55/55	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
21	EDO	C	313	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
27	CDL	T	103	-	-	51/110/110/110	-
21	EDO	A	612	-	-	0/1/1/1	-
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
14	HEA	A	602[B]	18,1	-	5/32/76/76	-
21	EDO	P	312	-	-	1/1/1/1	-
25	DMU	C	310	-	-	11/19/59/59	0/2/2/2
19	TGL	L	101	-	-	39/65/65/65	-
21	EDO	A	619	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
20	PGV	P	304	-	-	11/55/55/55	-
21	EDO	L	103	-	-	0/1/1/1	-
21	EDO	O	304	-	-	0/1/1/1	-
27	CDL	C	305	-	-	58/110/110/110	-
21	EDO	S	105	-	-	0/1/1/1	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
21	EDO	A	615	-	-	1/1/1/1	-
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
21	EDO	A	611	-	-	0/1/1/1	-
25	DMU	C	309	-	-	6/19/59/59	0/2/2/2
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
21	EDO	N	615	-	-	1/1/1/1	-
25	DMU	P	309	-	-	6/19/59/59	0/2/2/2
25	DMU	L	102	-	-	14/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEK	P	308	-	-	32/56/56/56	-
14	HEA	N	602[A]	18,1	-	4/32/76/76	-
21	EDO	C	311	-	-	0/1/1/1	-
14	HEA	A	601	1	-	5/32/76/76	-
19	TGL	Y	101	-	-	40/65/65/65	-
20	PGV	P	302	-	-	27/55/55/55	-
21	EDO	Y	102	-	-	1/1/1/1	-
22	CHD	P	301	-	-	3/9/74/74	0/4/4/4
27	CDL	G	102	-	-	71/110/110/110	-
24	PSC	O	302	-	-	28/55/55/55	-
22	CHD	C	306	-	-	7/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	N	616	-	-	1/1/1/1	-
21	EDO	G	106	-	-	1/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
25	DMU	M	101	-	-	2/19/59/59	0/2/2/2
19	TGL	Q	201	-	-	34/65/65/65	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
14	HEA	N	602[B]	18,1	-	5/32/76/76	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	613	-	-	1/1/1/1	-
19	TGL	N	609	-	-	33/65/65/65	-
20	PGV	X	101	-	-	31/55/55/55	-
28	PEK	C	307	-	-	23/56/56/56	-
21	EDO	F	105	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
28	PEK	T	101	-	-	31/56/56/56	-
20	PGV	A	610	-	-	26/55/55/55	-
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
28	PEK	G	101	-	-	17/56/56/56	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	P	310	-	-	7/19/59/59	0/2/2/2
21	EDO	S	104	-	-	0/1/1/1	-
19	TGL	D	201	-	-	39/65/65/65	-
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	S	106	-	-	0/1/1/1	-

The worst 5 of 313 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	11.00	1.55	1.22
19	D	201	TGL	OG2-CB1	8.23	1.57	1.34
20	A	610	PGV	O02-C1	8.05	1.46	1.22
19	L	101	TGL	OG2-CB1	7.02	1.54	1.34
20	A	610	PGV	O01-C1	6.83	1.53	1.34

The worst 5 of 668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	201	TGL	OG2-CB1-CB2	-13.46	82.48	111.50
19	D	201	TGL	OG2-CB1-OB1	12.52	153.95	123.70
22	C	306	CHD	C23-C22-C20	-12.09	92.43	114.52
22	W	101	CHD	C17-C13-C12	11.12	127.81	117.67
20	A	610	PGV	O01-C1-O02	10.68	149.52	123.70

There are no chirality outliers.

5 of 957 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	602[B]	HEA	C2D-C3D-CAD-CBD
19	D	201	TGL	CG2-CG1-OG1-CA1
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2

There are no ring outliers.

61 monomers are involved in 418 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	T	102	PEK	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	616	EDO	3	0
14	N	601	HEA	7	0
18	A	606[B]	AZI	3	0
20	A	609	PGV	6	0
21	D	202	EDO	11	0
20	N	608	PGV	1	0
20	C	308	PGV	6	0
21	D	205	EDO	2	0
25	C	302	DMU	10	0
27	P	305	CDL	28	0
21	H	101	EDO	5	0
14	A	602[A]	HEA	4	0
28	G	104	PEK	19	0
22	P	306	CHD	2	0
24	B	303	PSC	21	0
22	G	103	CHD	1	0
27	T	103	CDL	24	0
20	C	304	PGV	1	0
14	A	602[B]	HEA	10	0
25	C	310	DMU	3	0
19	L	101	TGL	11	0
21	A	619	EDO	2	0
20	P	304	PGV	10	0
27	C	305	CDL	26	0
22	J	101	CHD	4	0
22	W	101	CHD	5	0
21	A	611	EDO	5	0
25	C	309	DMU	1	0
25	P	307	DMU	13	0
25	P	309	DMU	2	0
25	L	102	DMU	4	0
28	P	308	PEK	5	0
14	N	602[A]	HEA	3	0
14	A	601	HEA	9	0
19	Y	101	TGL	20	0
20	P	302	PGV	4	0
22	P	301	CHD	2	0
27	G	102	CDL	24	0
24	O	302	PSC	11	0
22	C	306	CHD	5	0
19	A	608	TGL	1	0
18	N	607[A]	AZI	1	0

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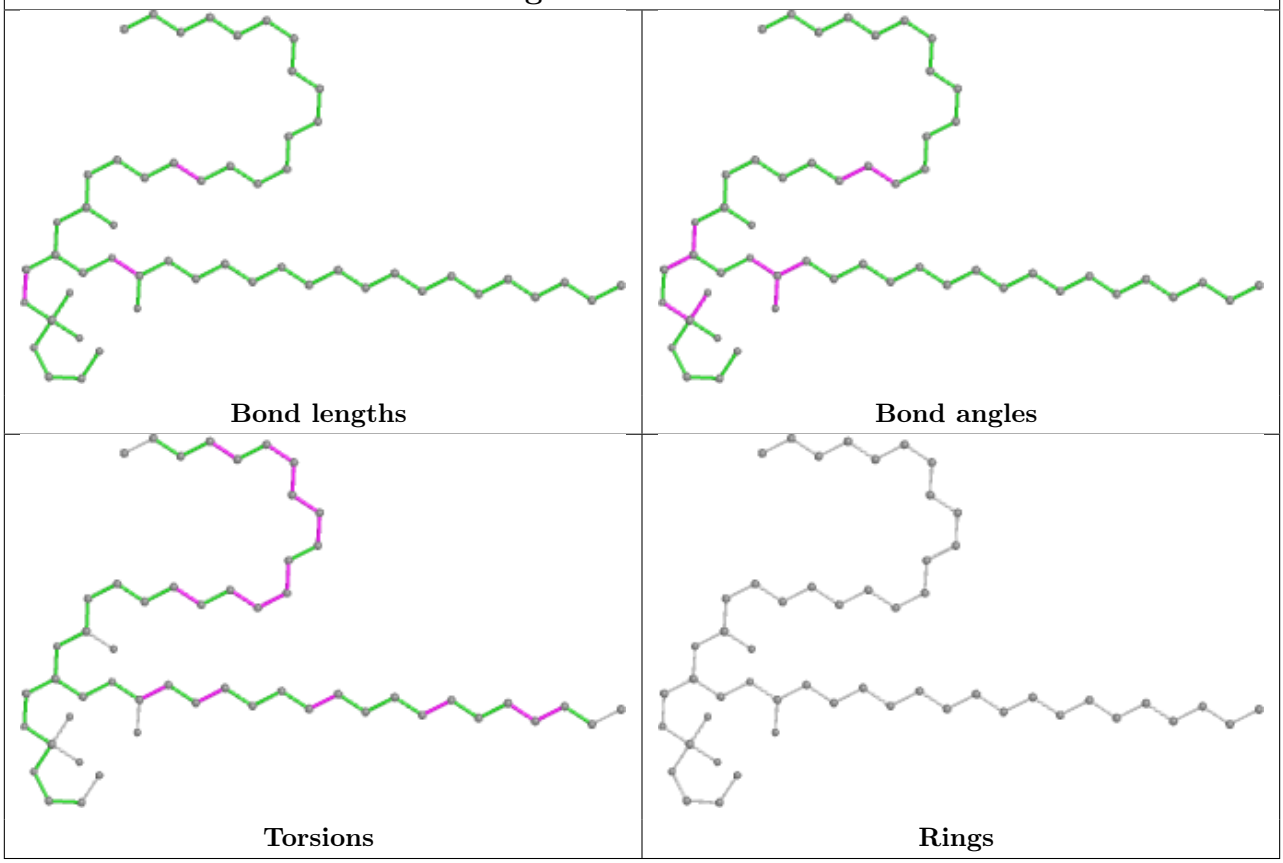
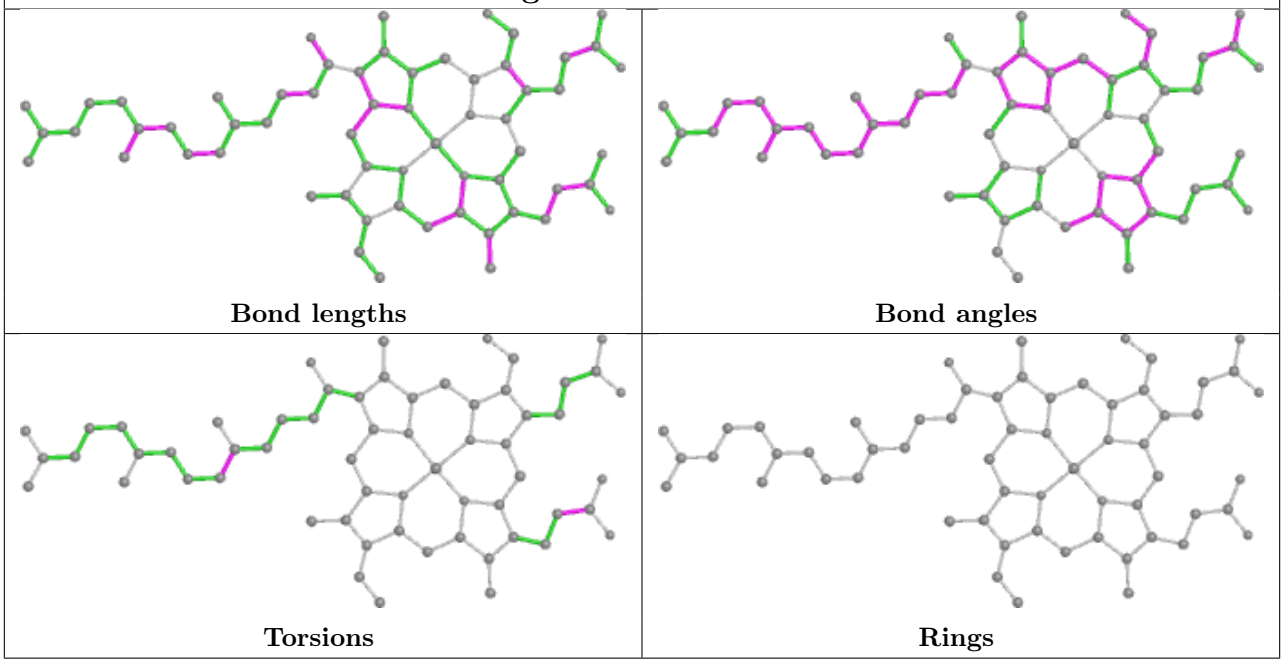
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	616	EDO	2	0
21	G	106	EDO	1	0
19	Q	201	TGL	12	0
18	A	607[B]	AZI	6	0
21	A	614	EDO	2	0
14	N	602[B]	HEA	12	0
19	N	609	TGL	5	0
20	X	101	PGV	10	0
28	C	307	PEK	14	0
22	C	301	CHD	1	0
20	A	610	PGV	5	0
28	G	101	PEK	7	0
21	D	203	EDO	2	0
18	N	607[B]	AZI	5	0
25	P	310	DMU	1	0
19	D	201	TGL	12	0
21	A	621	EDO	9	0
21	E	202	EDO	9	0

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

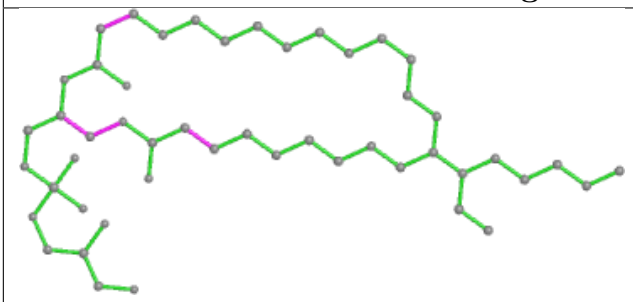
Ligand PEK T 102



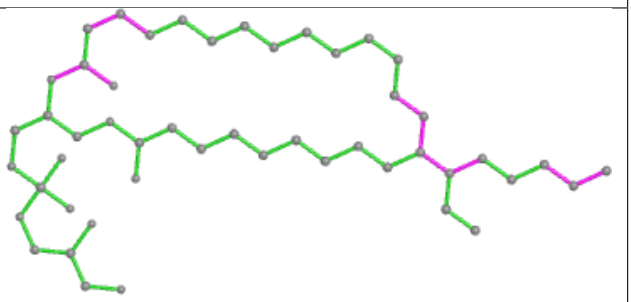
Ligand HEA N 601



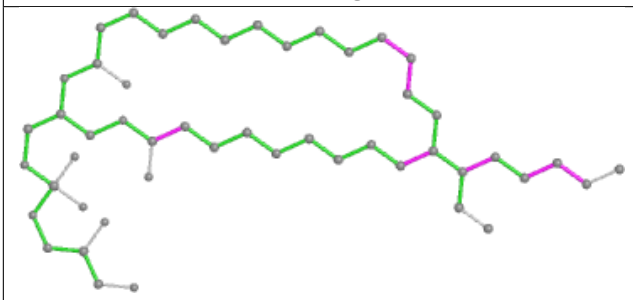
Ligand PGV A 609



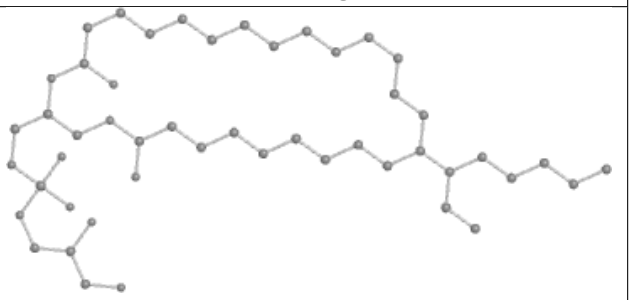
Bond lengths



Bond angles

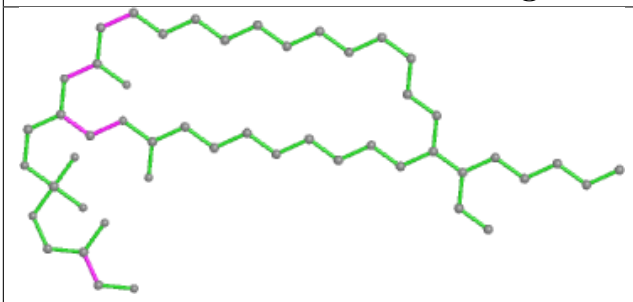


Torsions

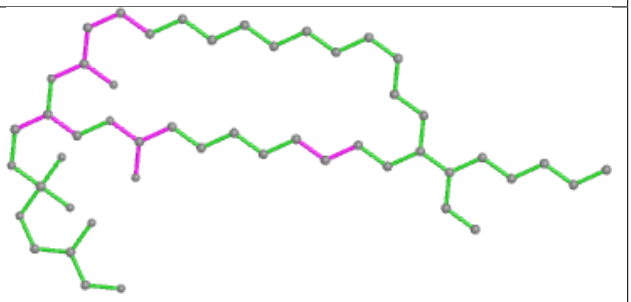


Rings

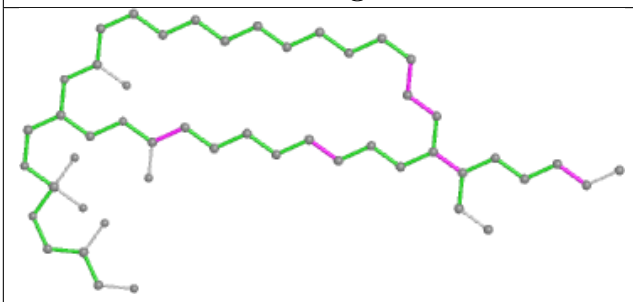
Ligand PGV N 608



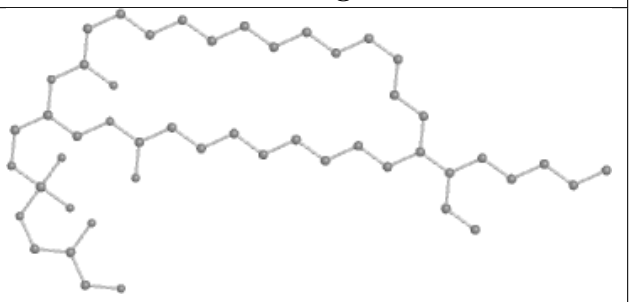
Bond lengths



Bond angles

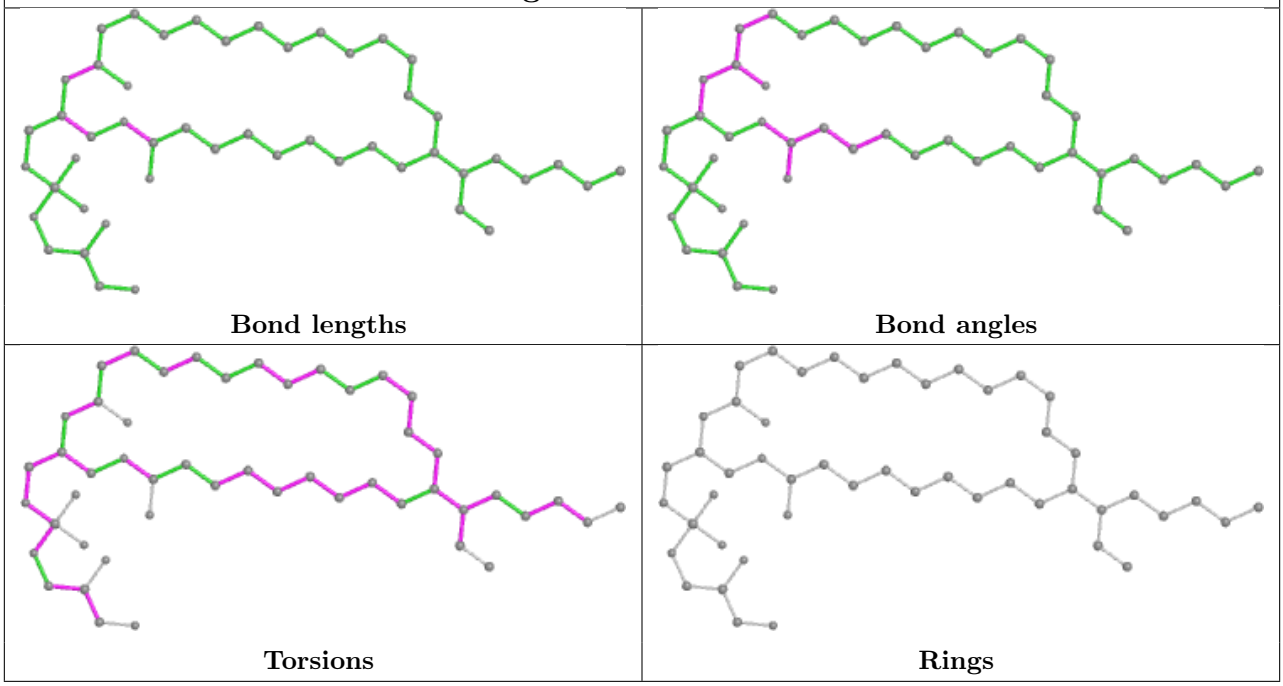


Torsions

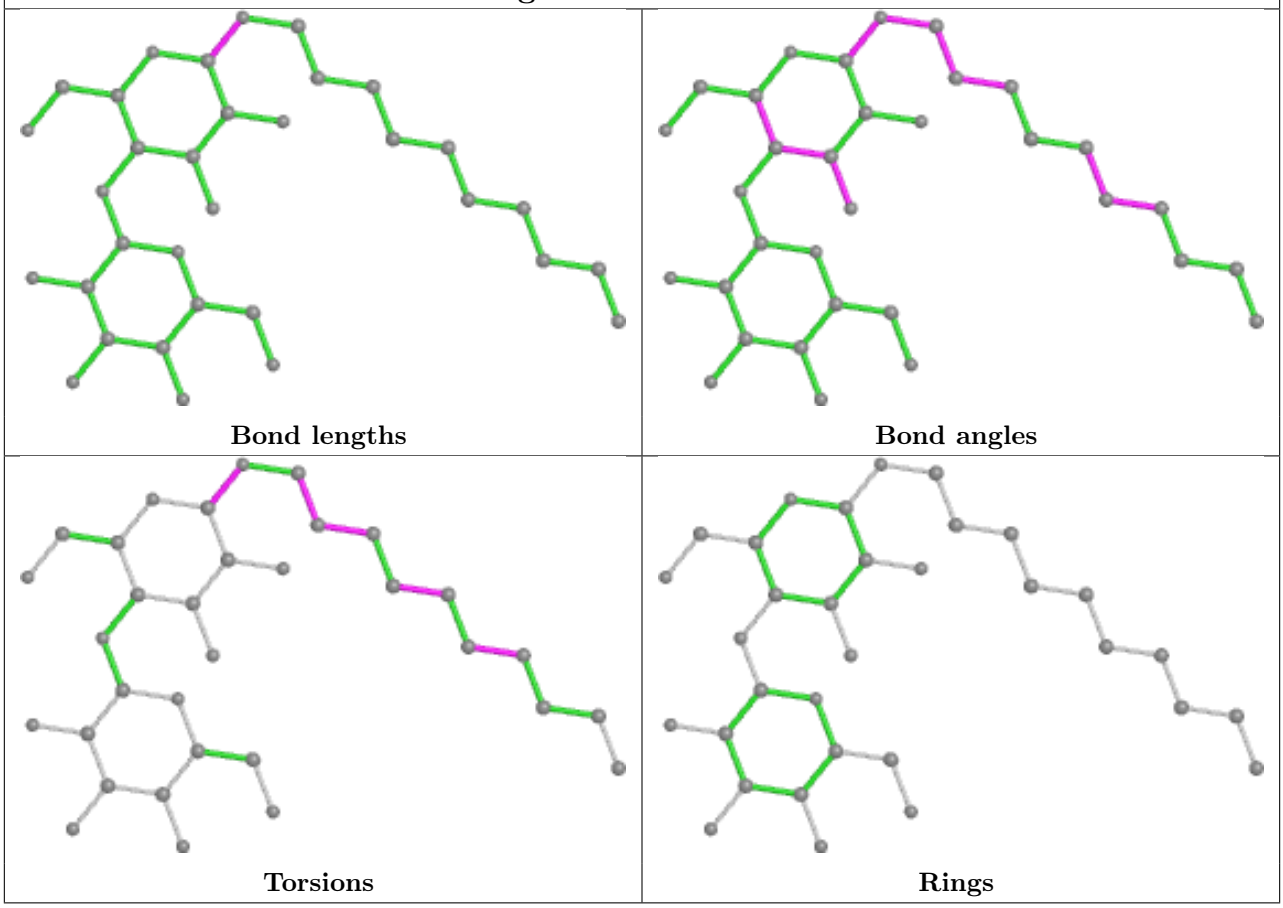


Rings

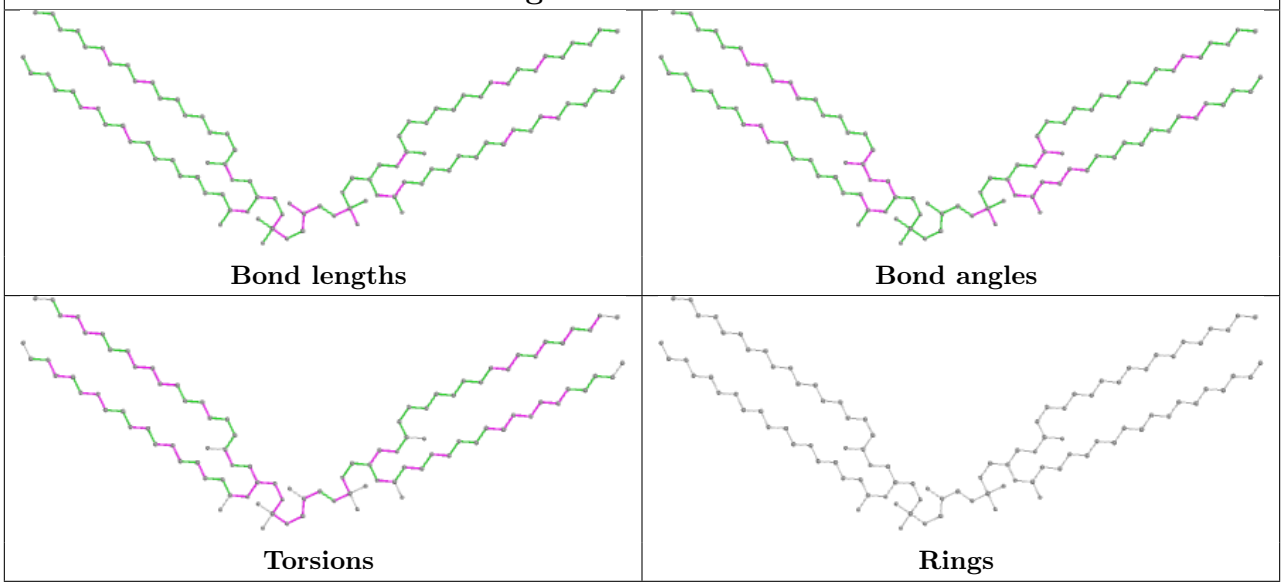
Ligand PGV C 308



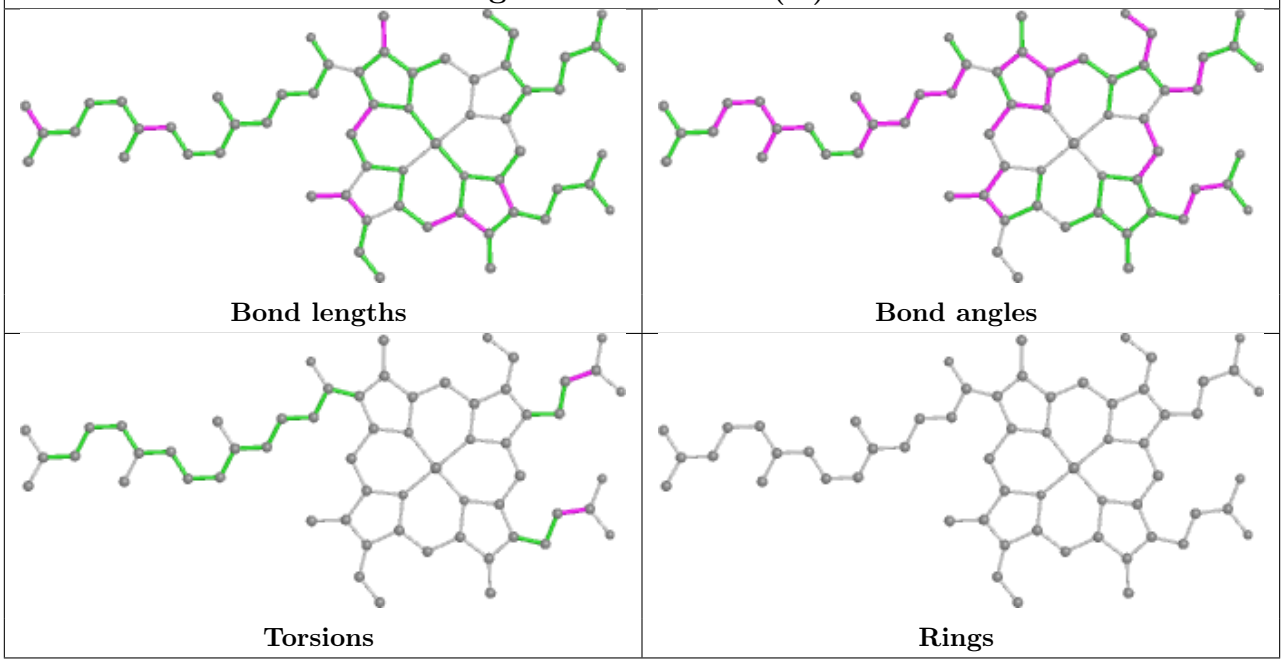
Ligand DMU C 302



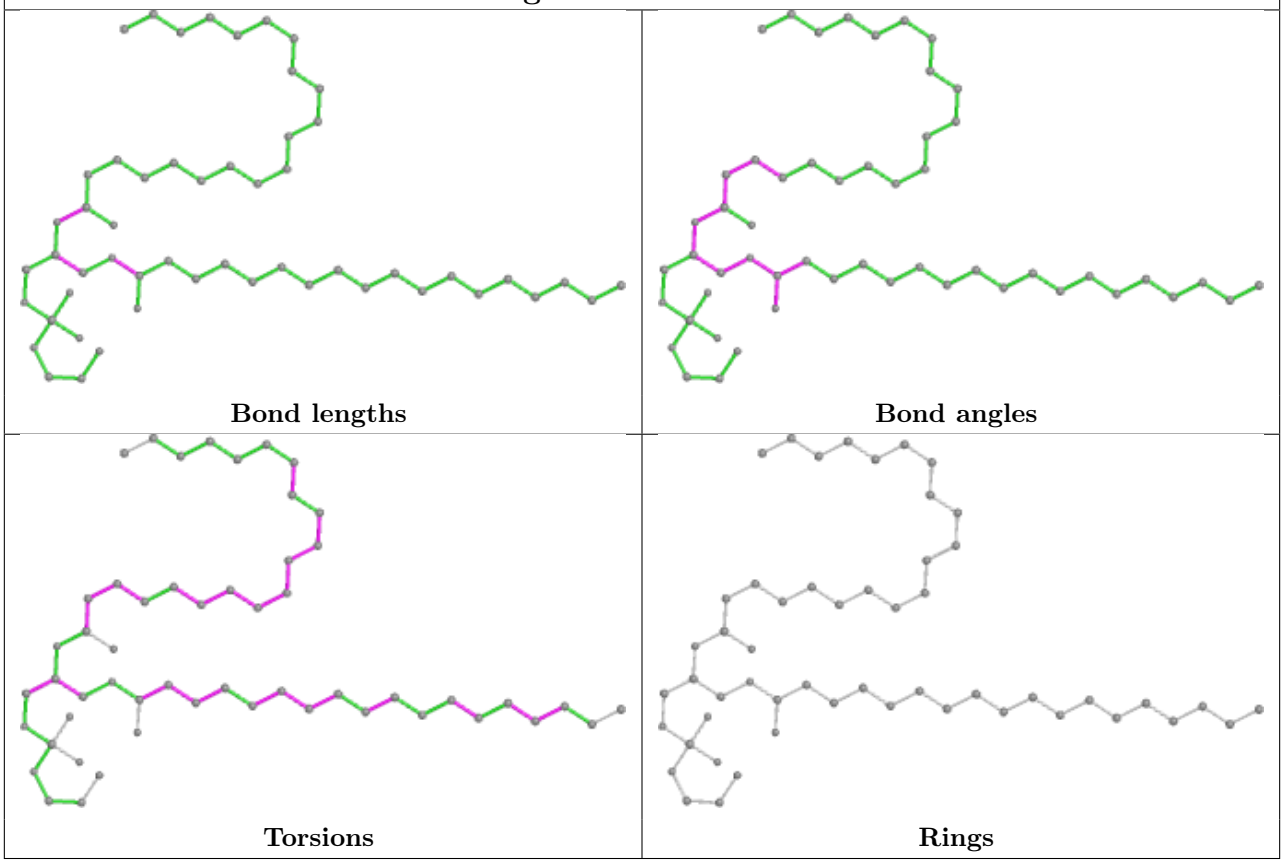
Ligand CDL P 305



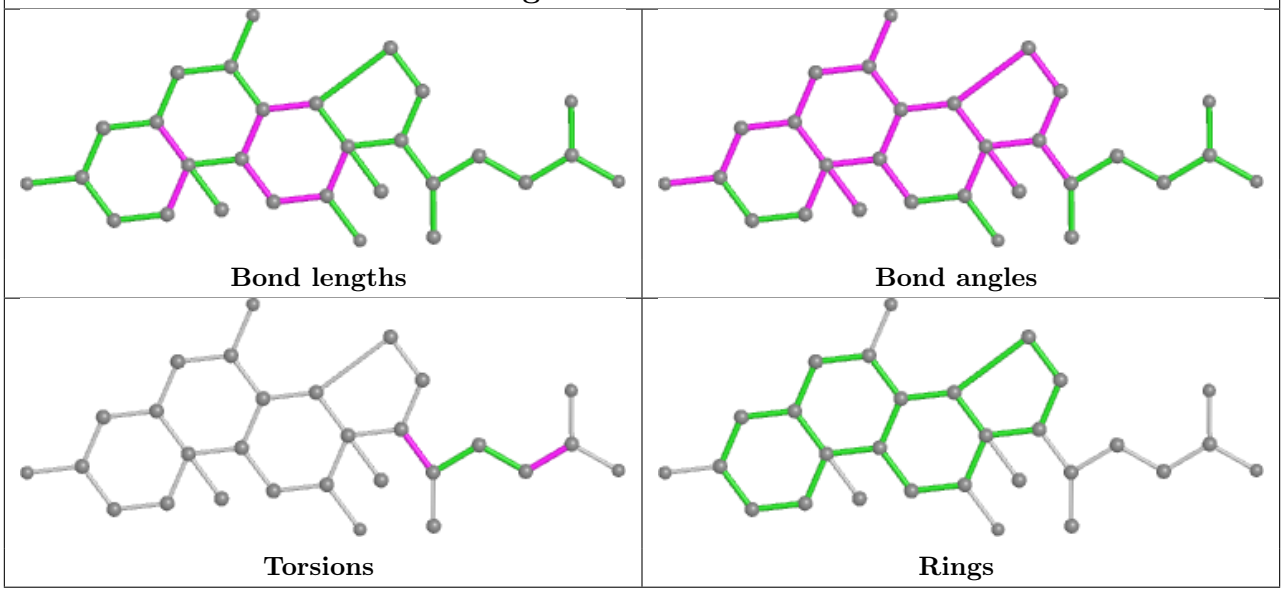
Ligand HEA A 602 (A)



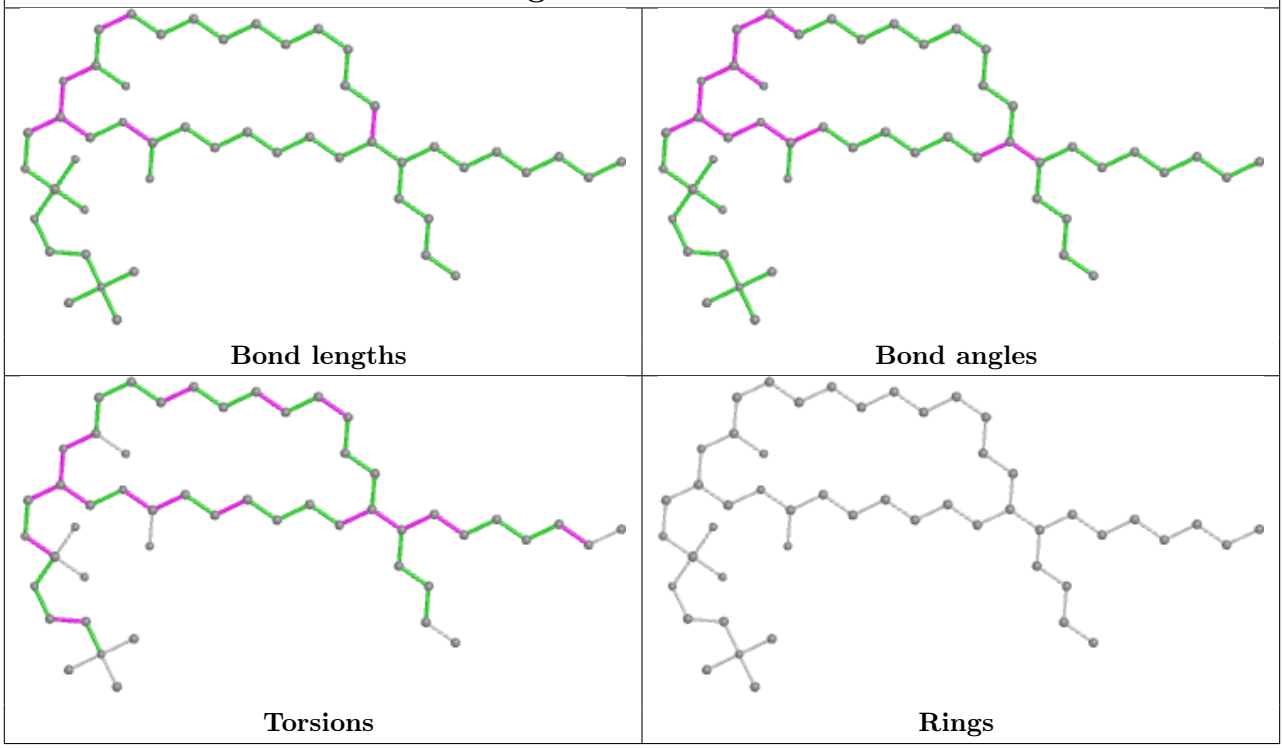
Ligand PEK G 104



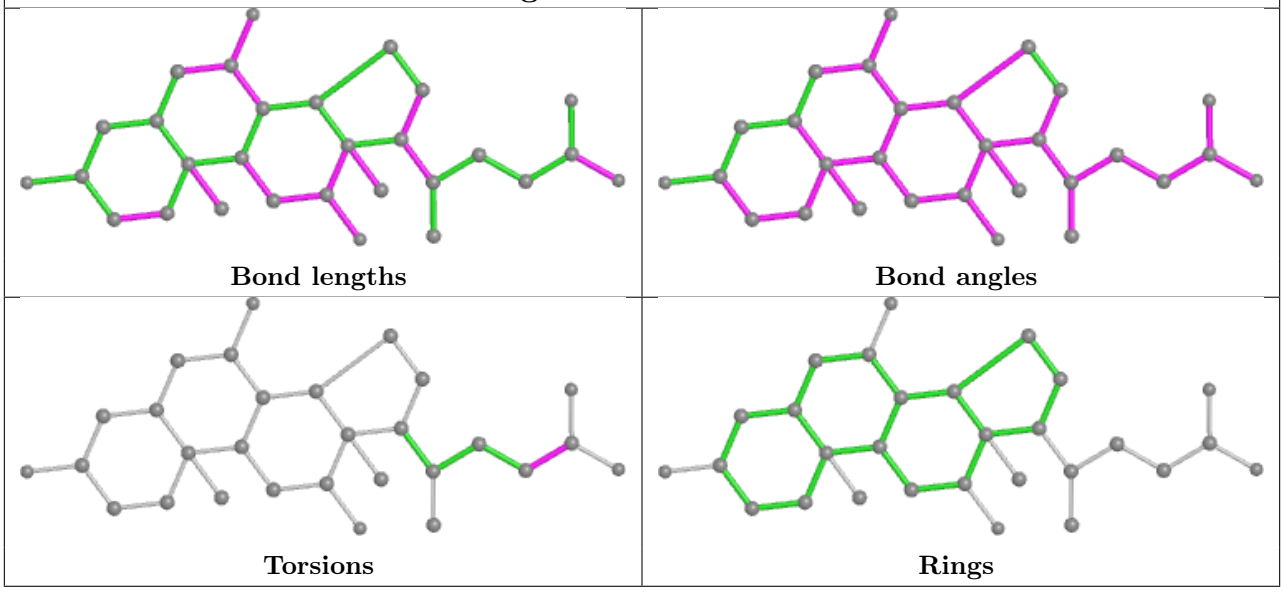
Ligand CHD P 306



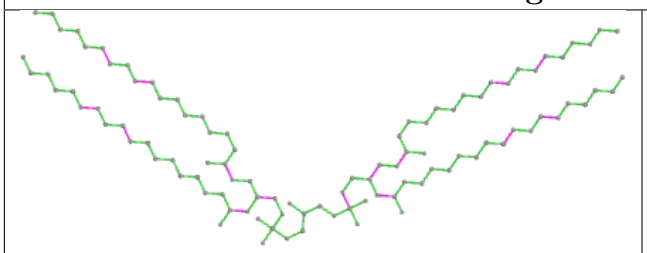
Ligand PSC B 303



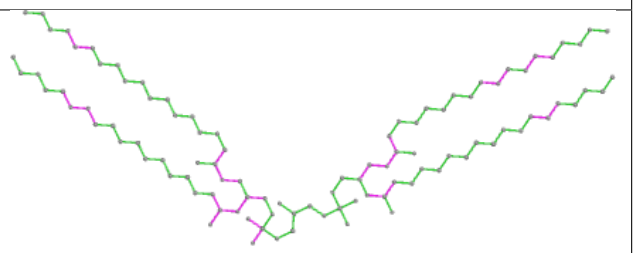
Ligand CHD G 103



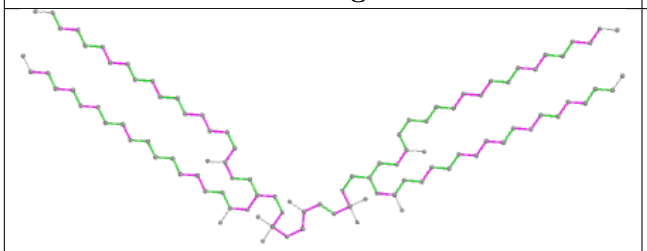
Ligand CDL T 103



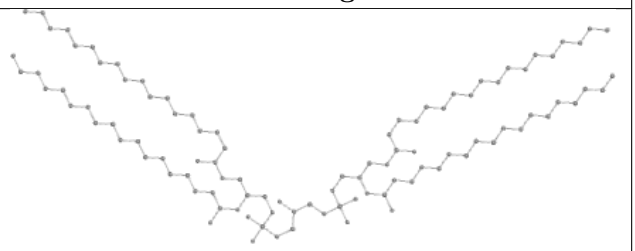
Bond lengths



Bond angles

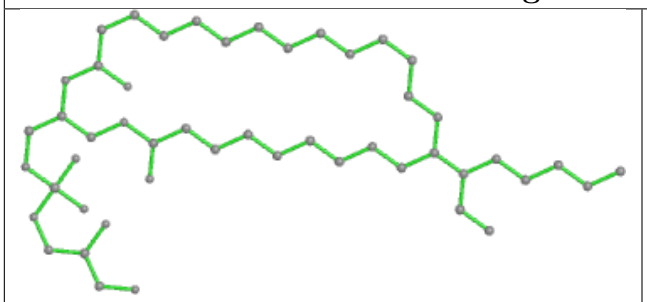


Torsions

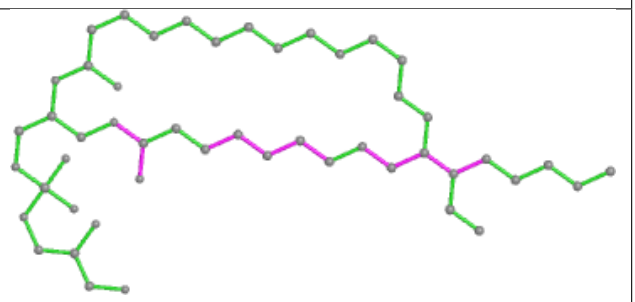


Rings

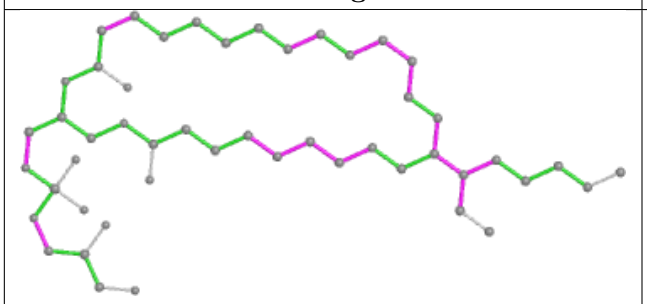
Ligand PGV C 304



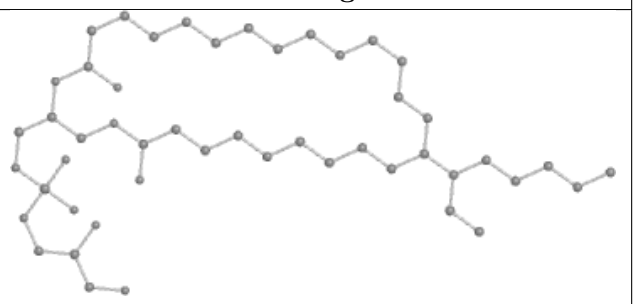
Bond lengths



Bond angles

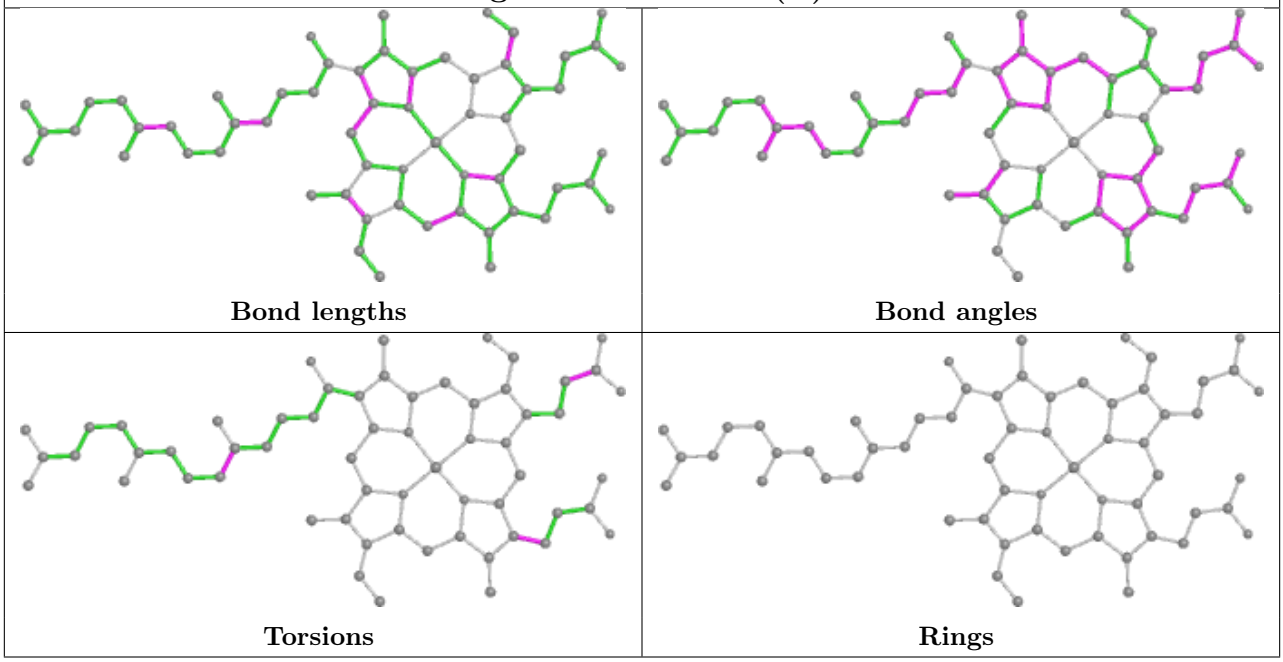


Torsions

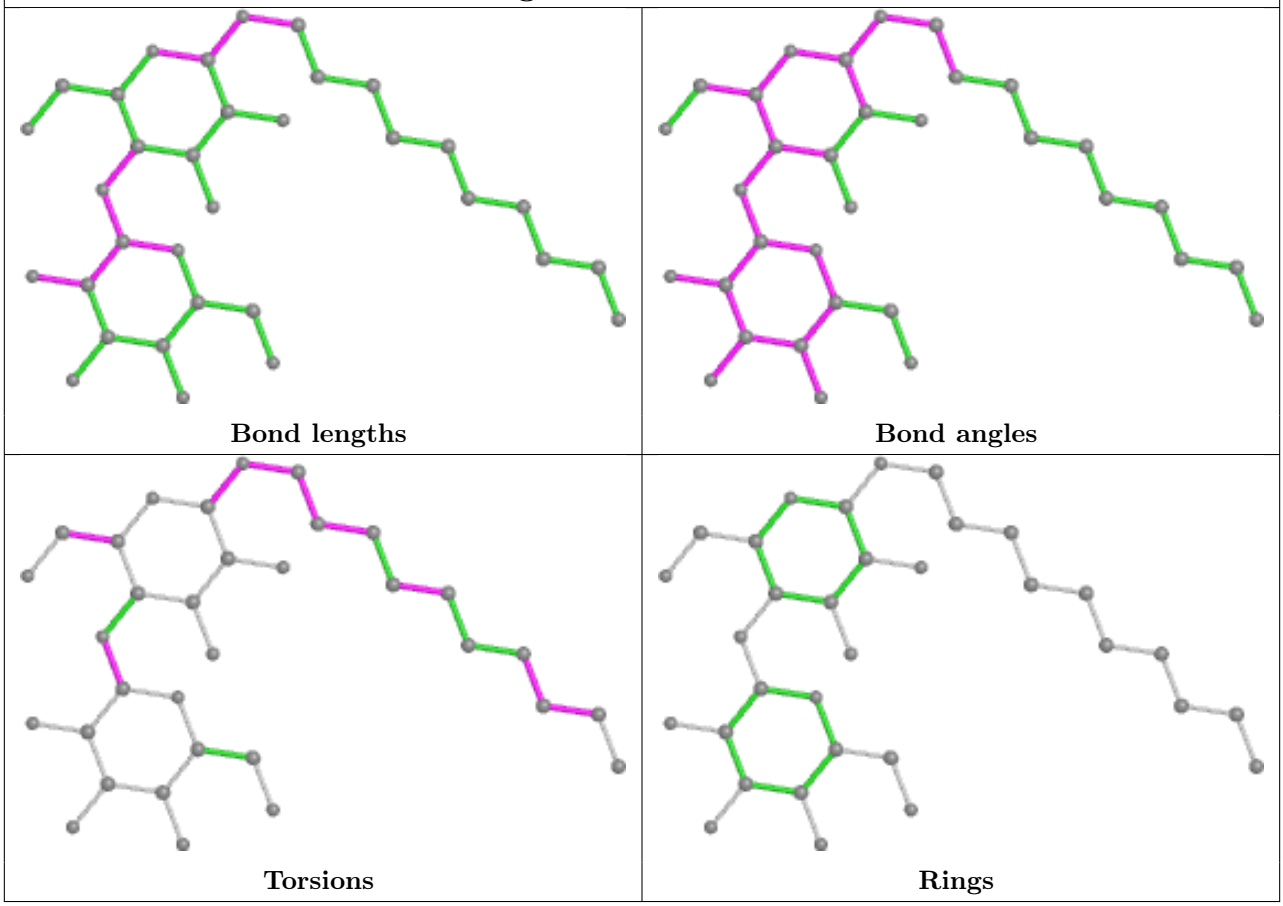


Rings

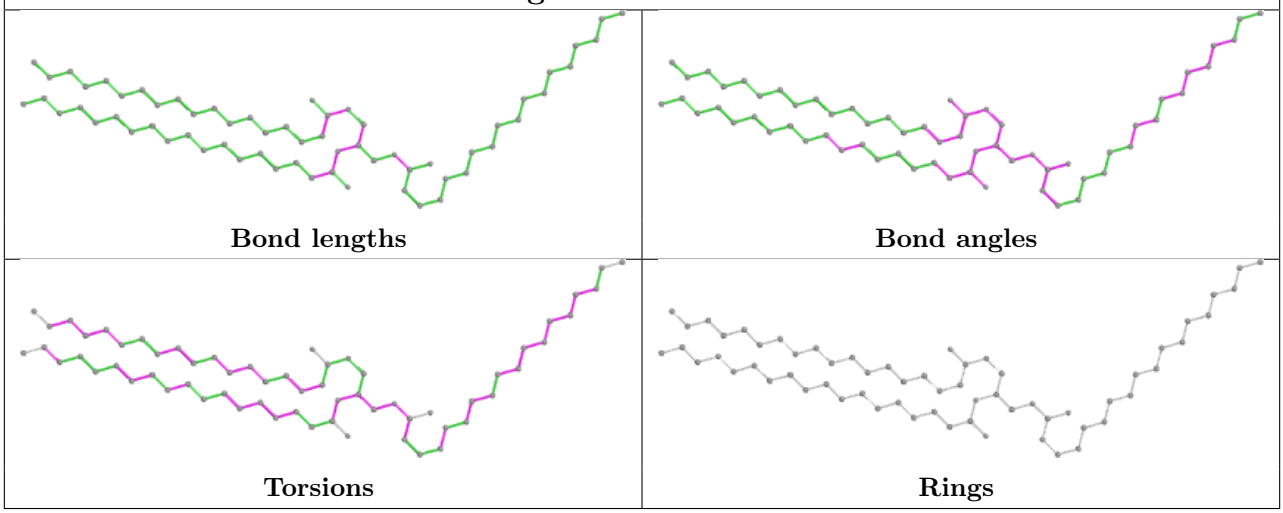
Ligand HEA A 602 (B)



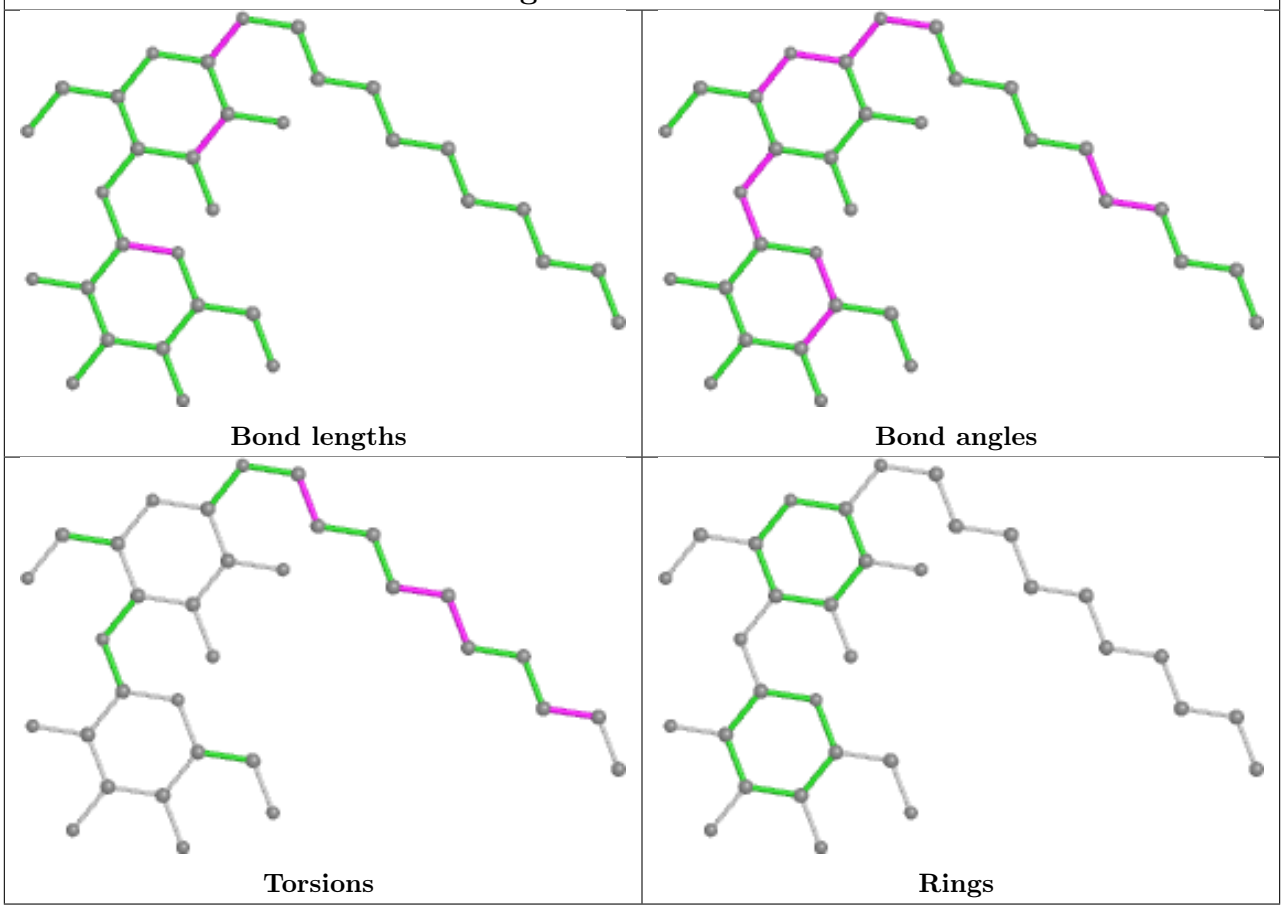
Ligand DMU C 310



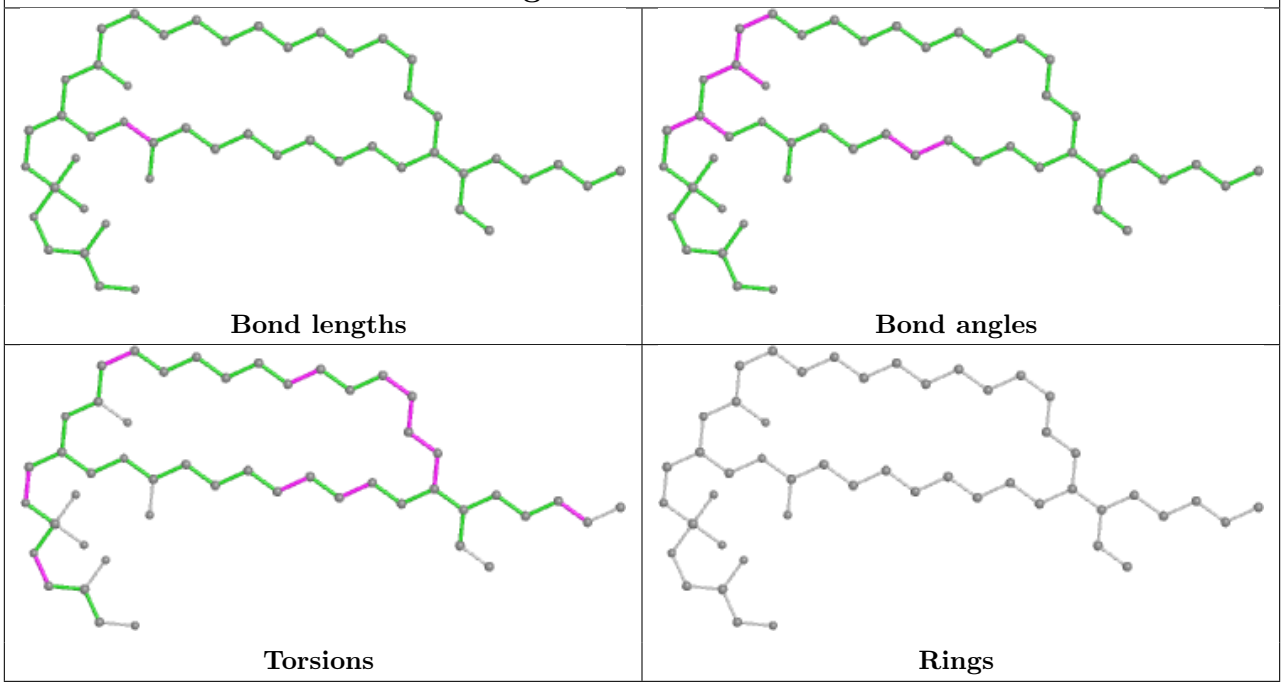
Ligand TGL L 101



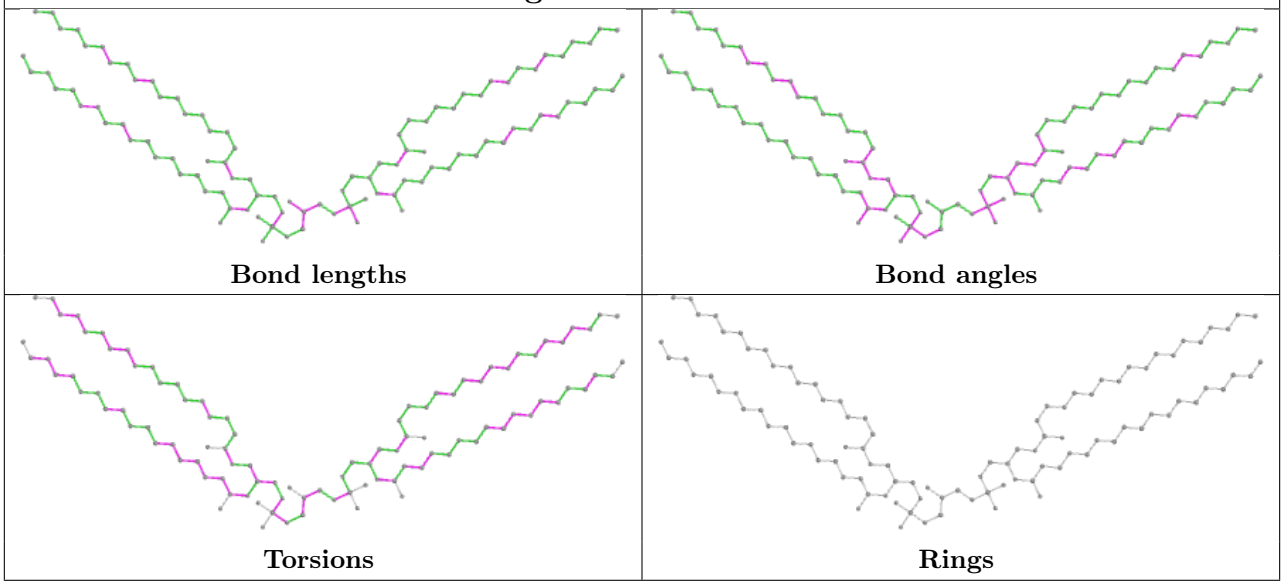
Ligand DMU Z 101



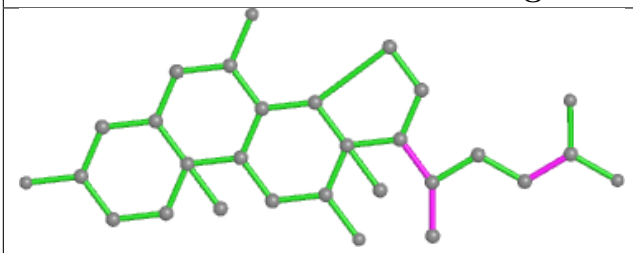
Ligand PGV P 304



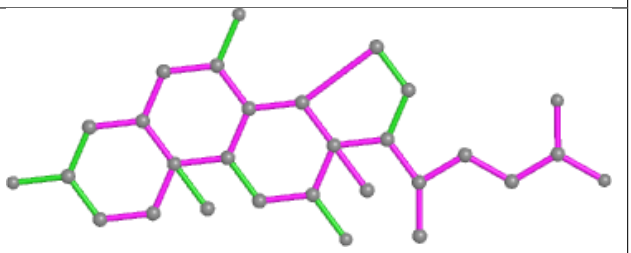
Ligand CDL C 305



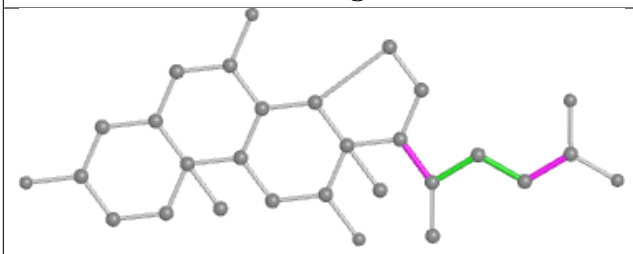
Ligand CHD J 101



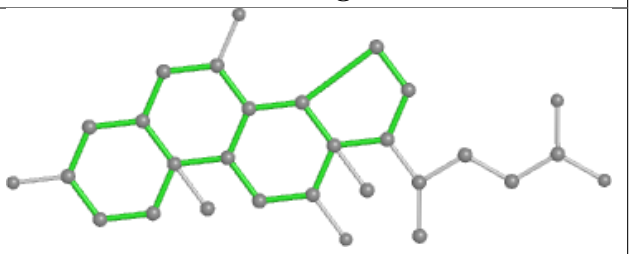
Bond lengths



Bond angles

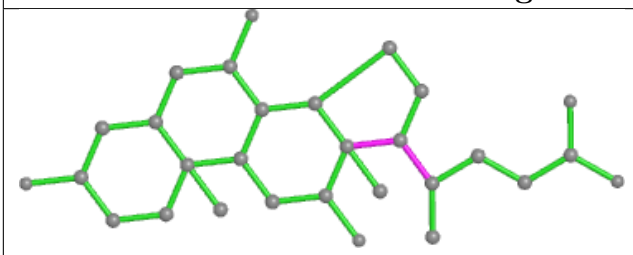


Torsions

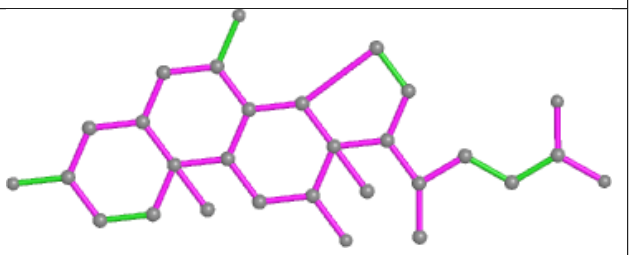


Rings

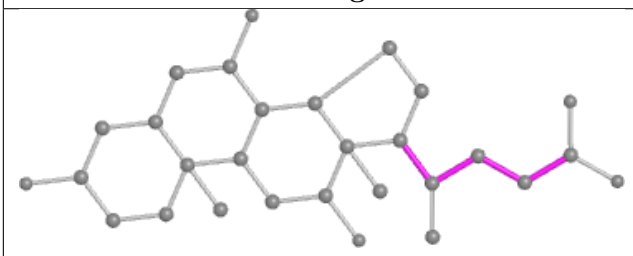
Ligand CHD W 101



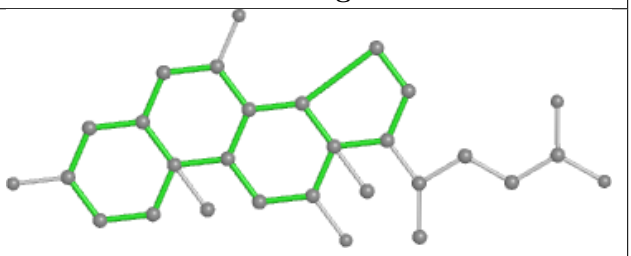
Bond lengths



Bond angles

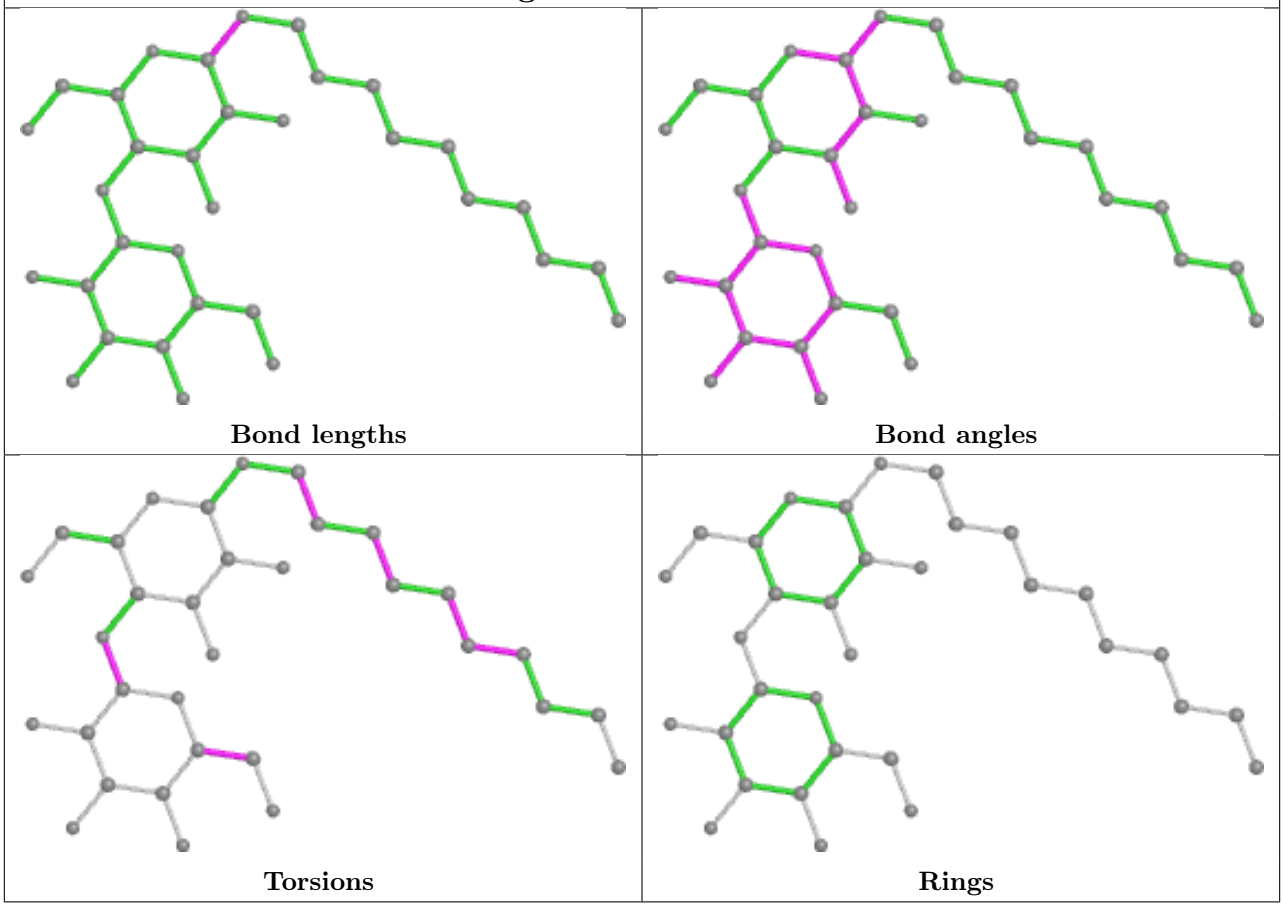


Torsions

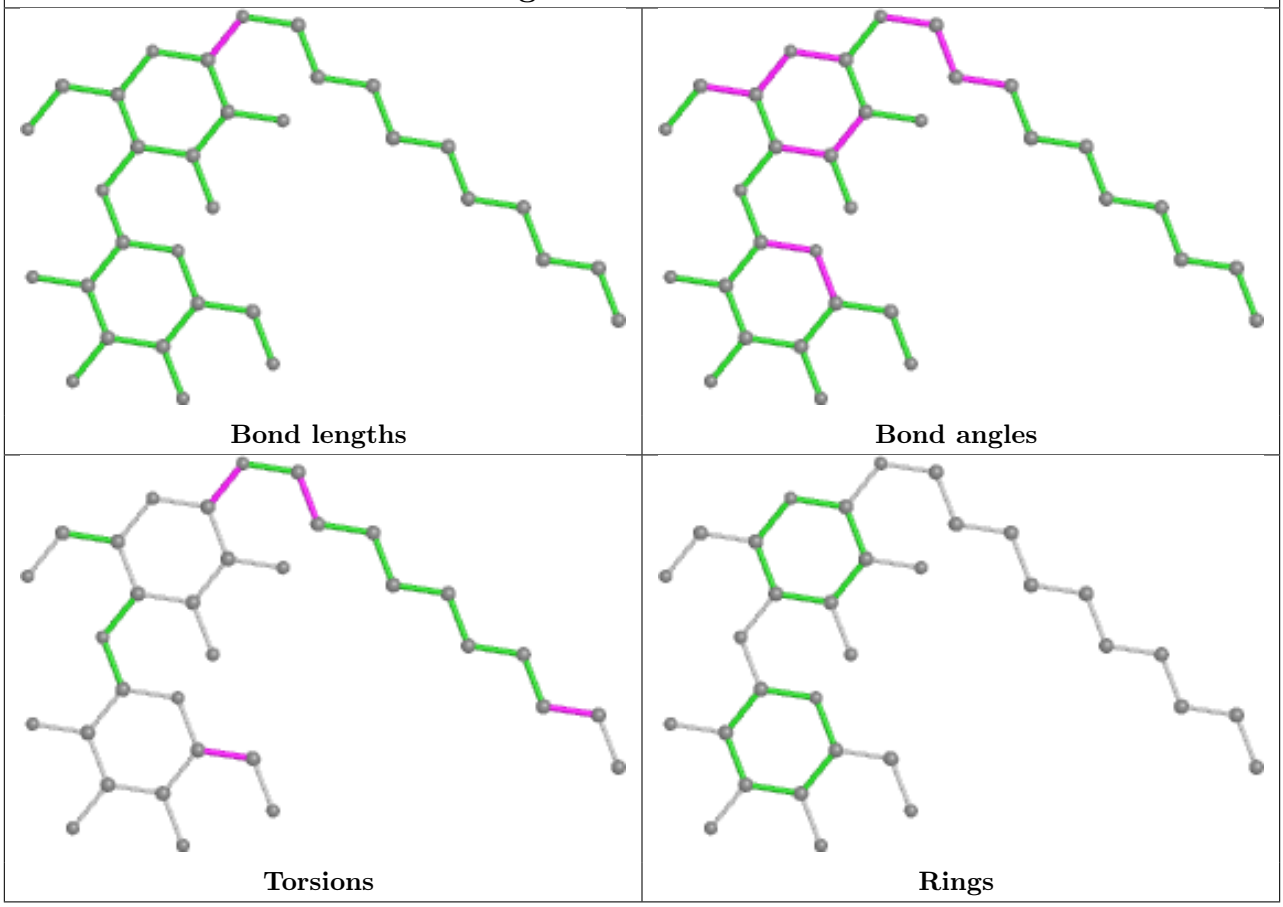


Rings

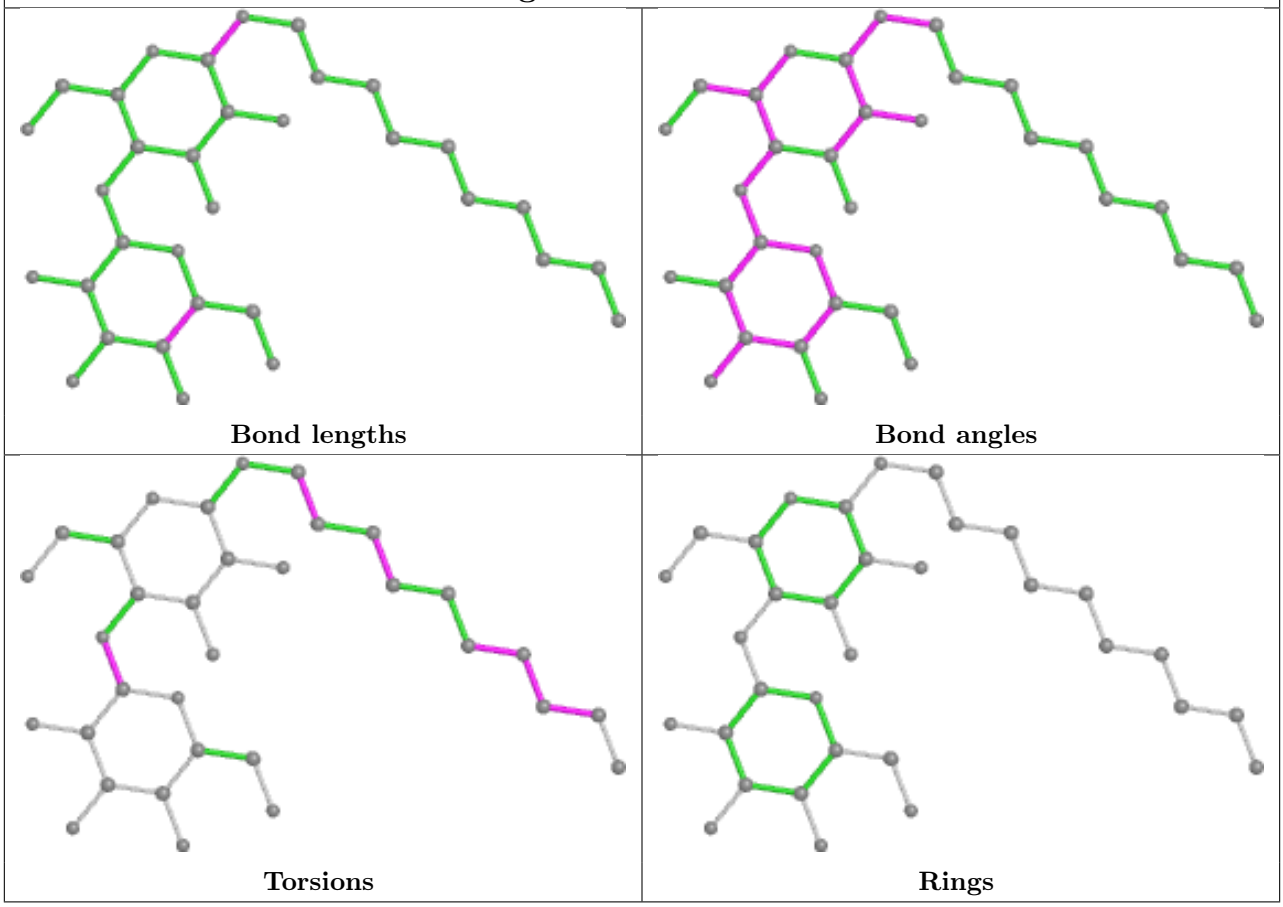
Ligand DMU C 309



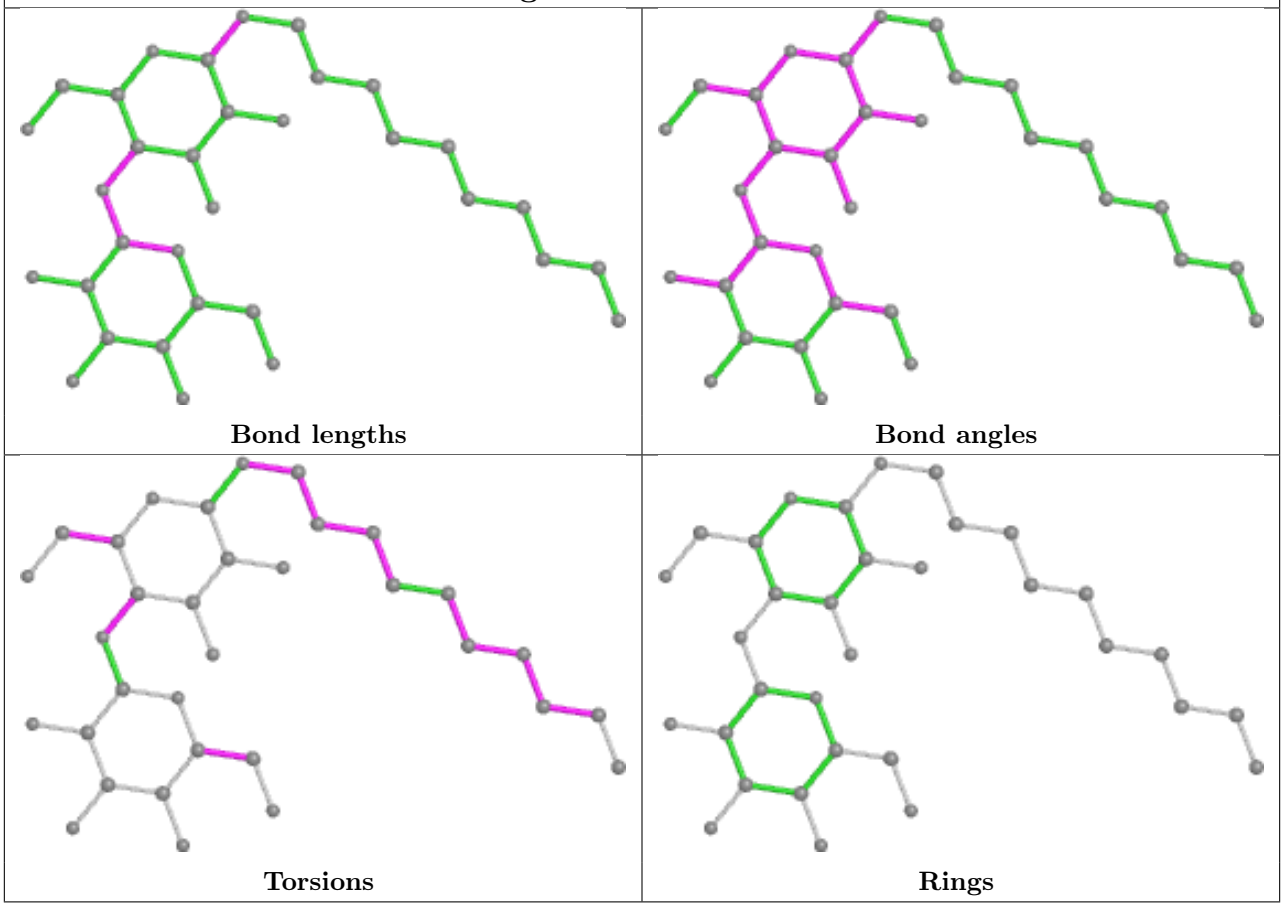
Ligand DMU P 307



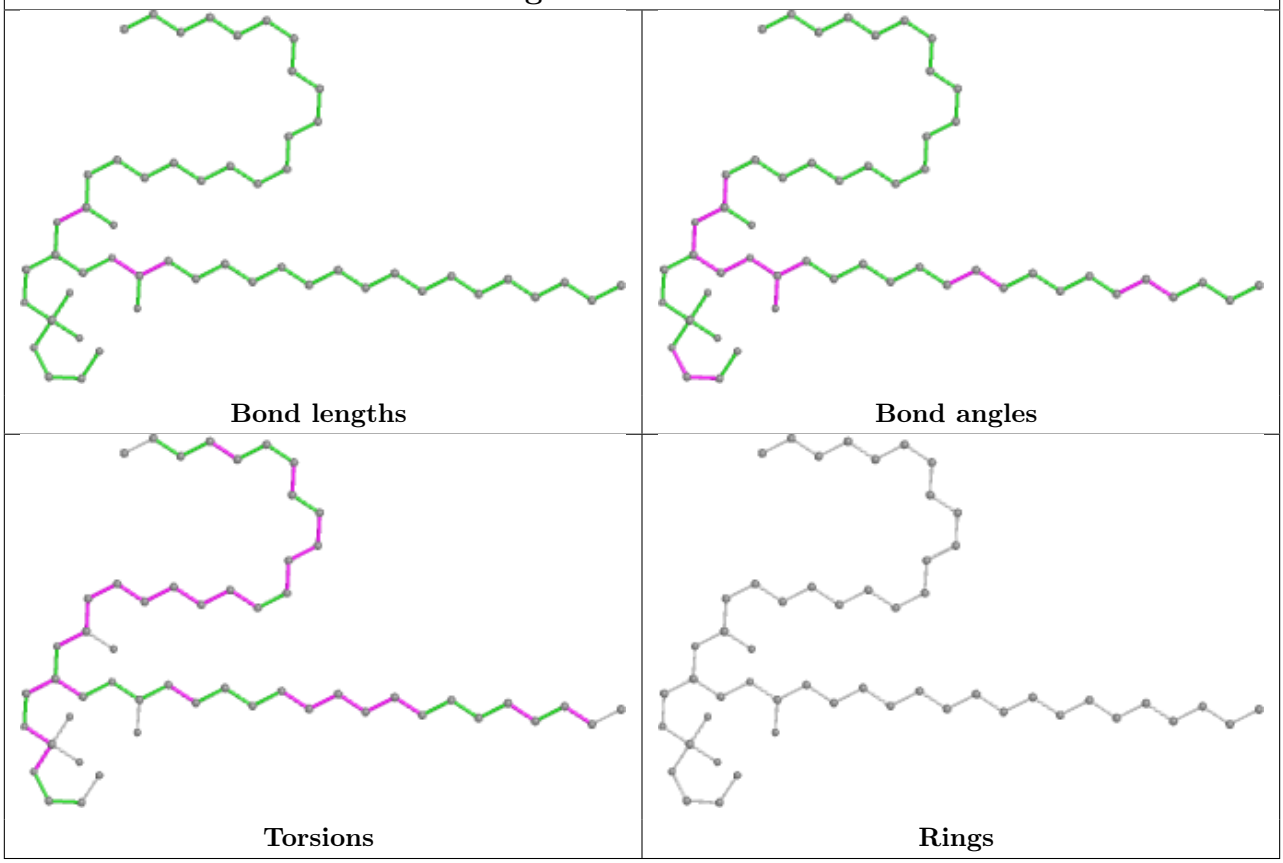
Ligand DMU P 309



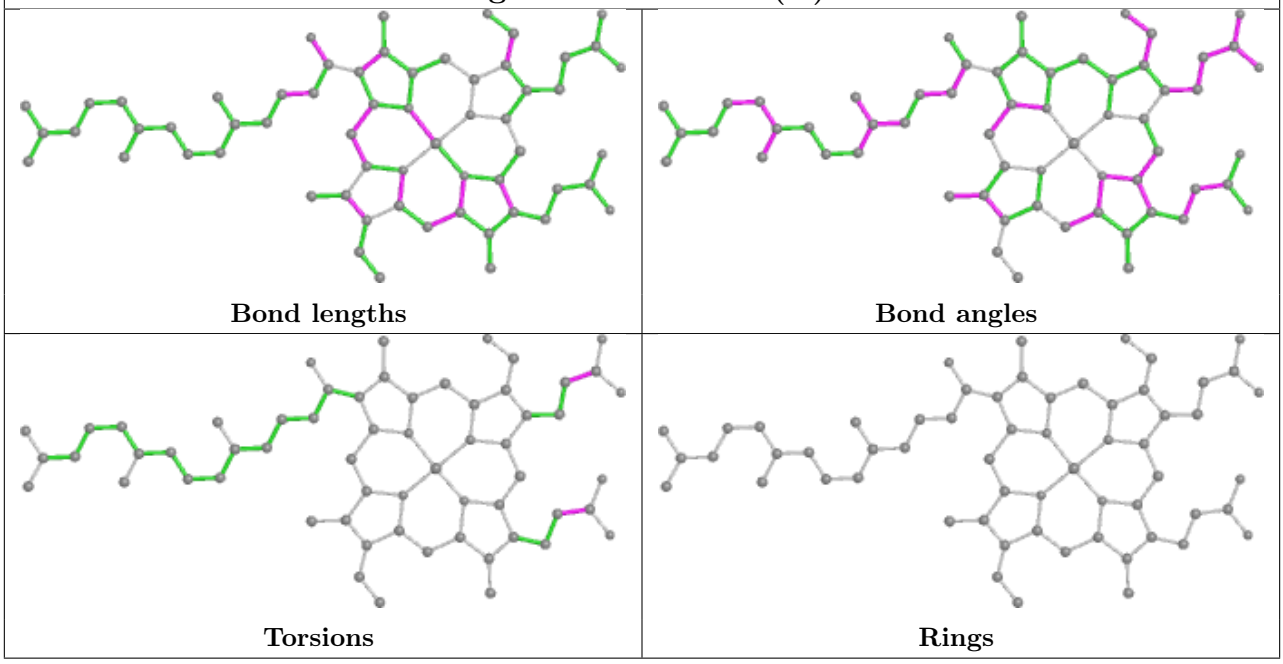
Ligand DMU L 102



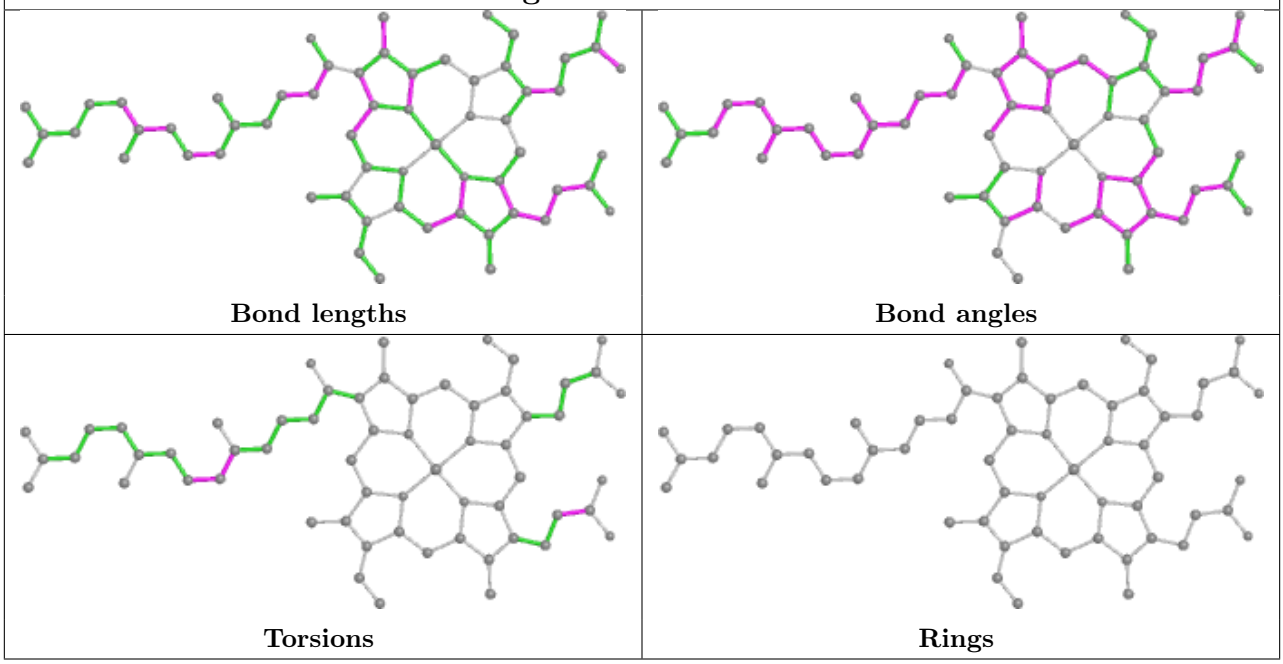
Ligand PEK P 308



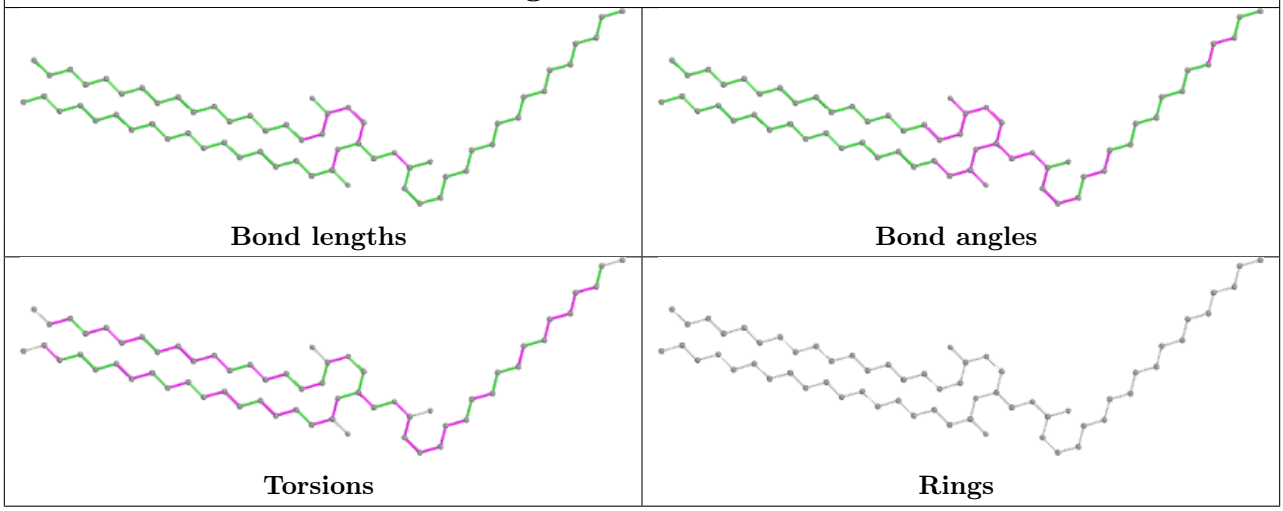
Ligand HEA N 602 (A)



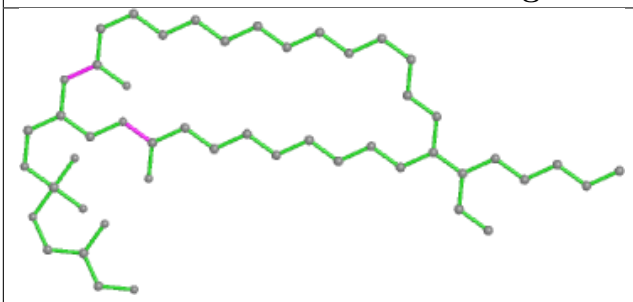
Ligand HEA A 601



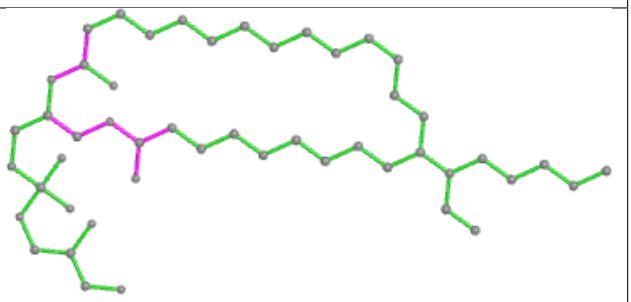
Ligand TGL Y 101



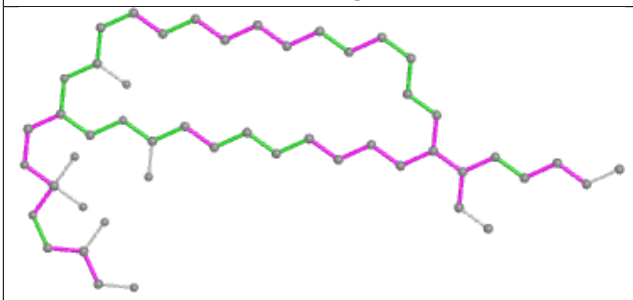
Ligand PGV P 302



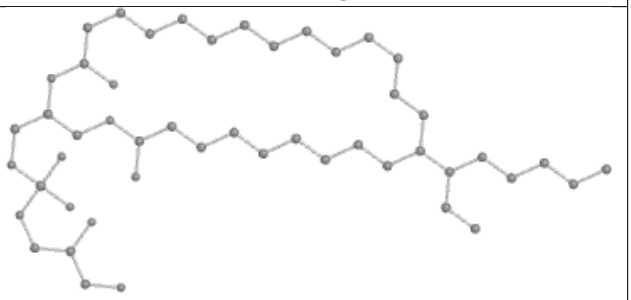
Bond lengths



Bond angles

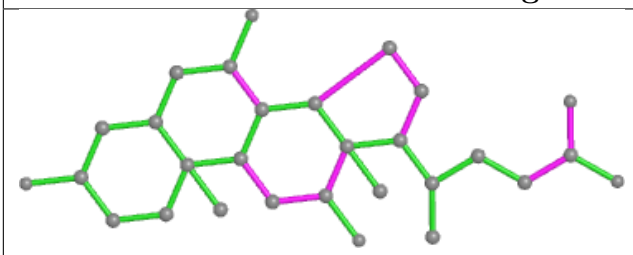


Torsions

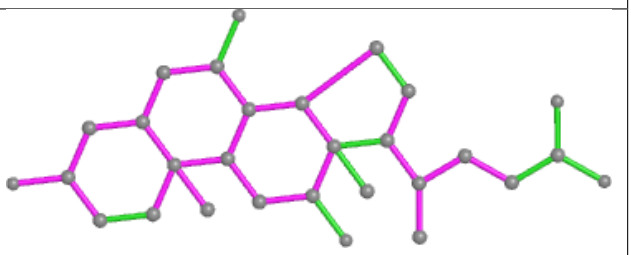


Rings

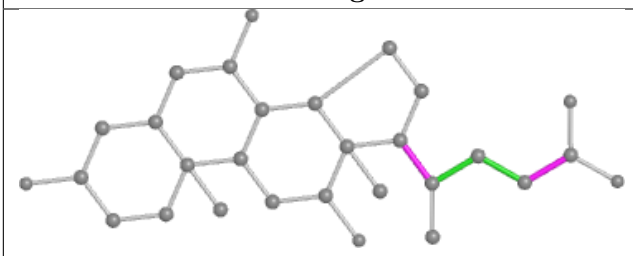
Ligand CHD P 301



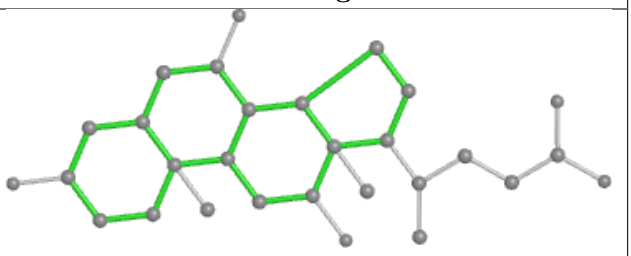
Bond lengths



Bond angles

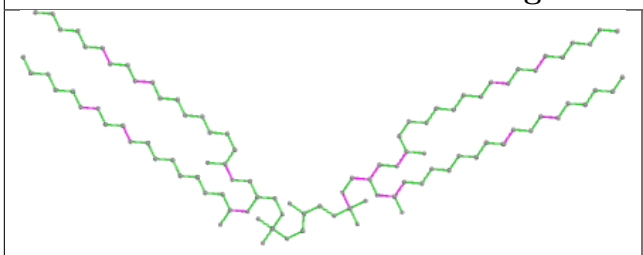


Torsions

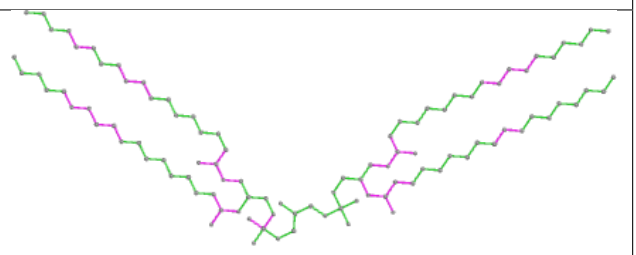


Rings

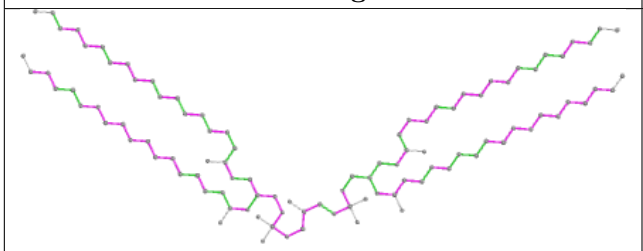
Ligand CDL G 102



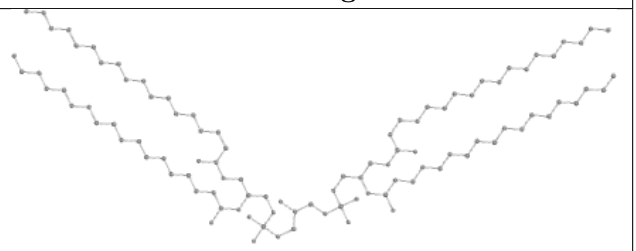
Bond lengths



Bond angles

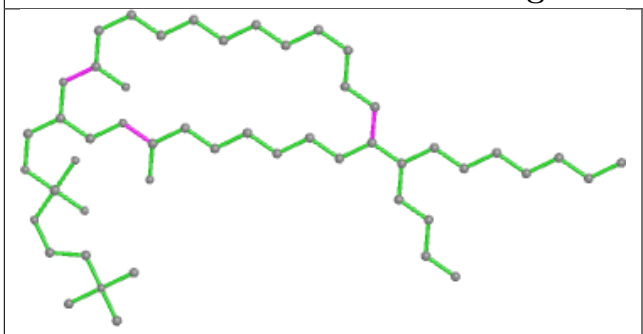


Torsions

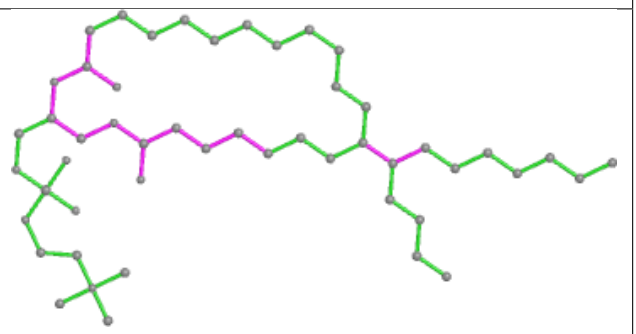


Rings

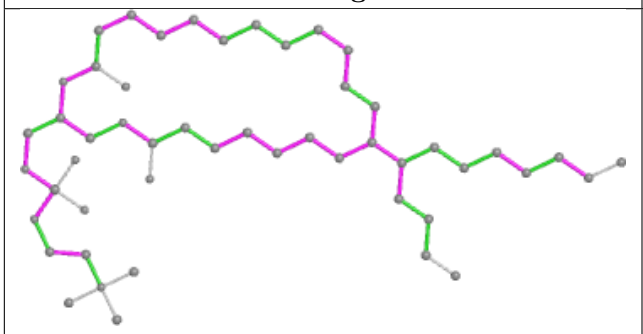
Ligand PSC O 302



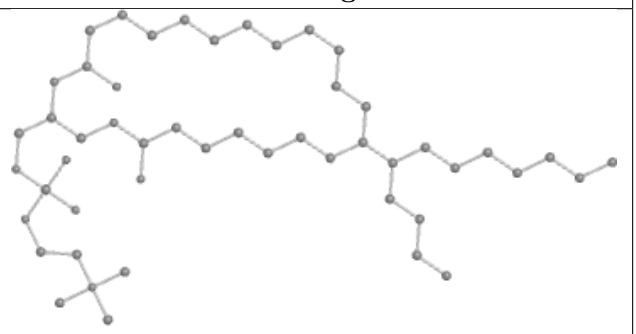
Bond lengths



Bond angles

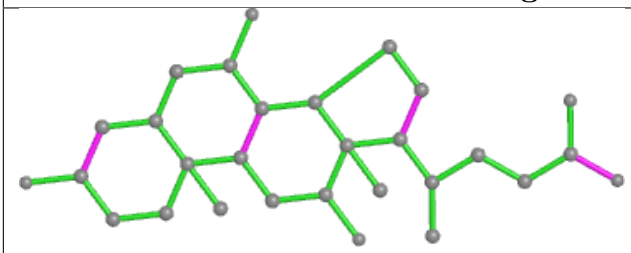


Torsions

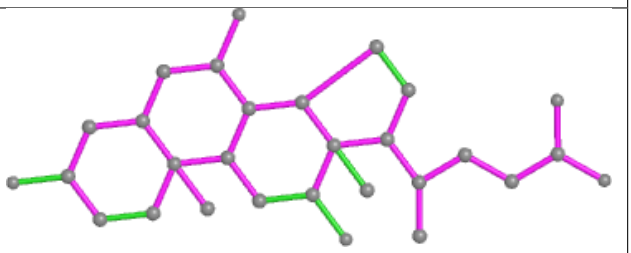


Rings

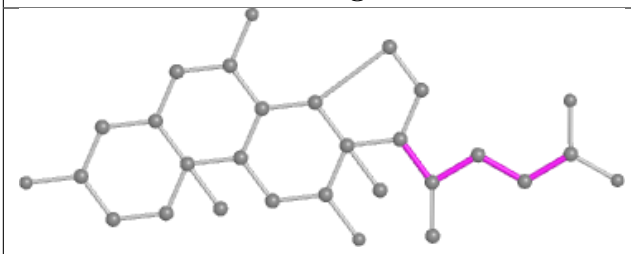
Ligand CHD C 306



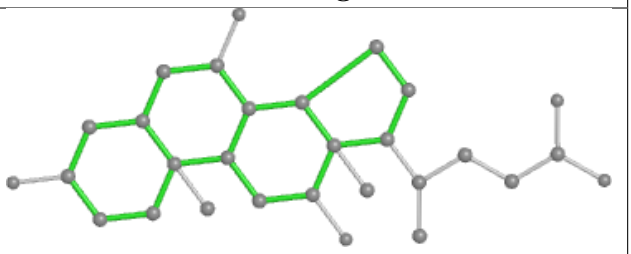
Bond lengths



Bond angles

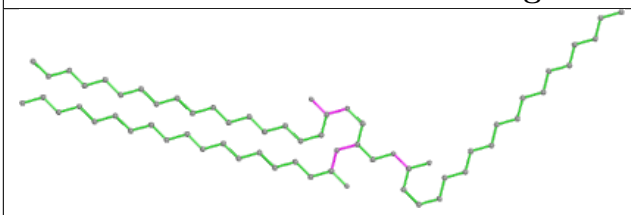


Torsions

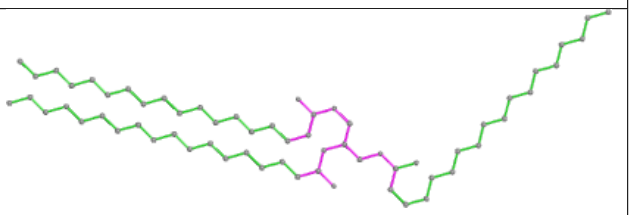


Rings

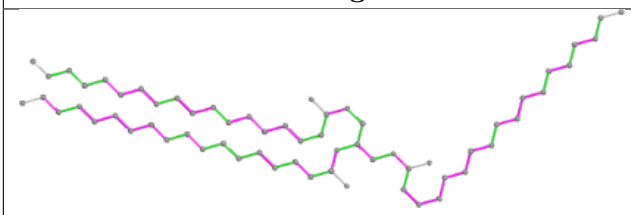
Ligand TGL A 608



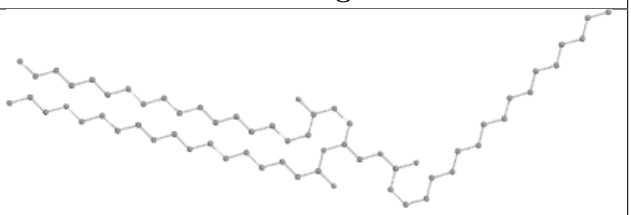
Bond lengths



Bond angles

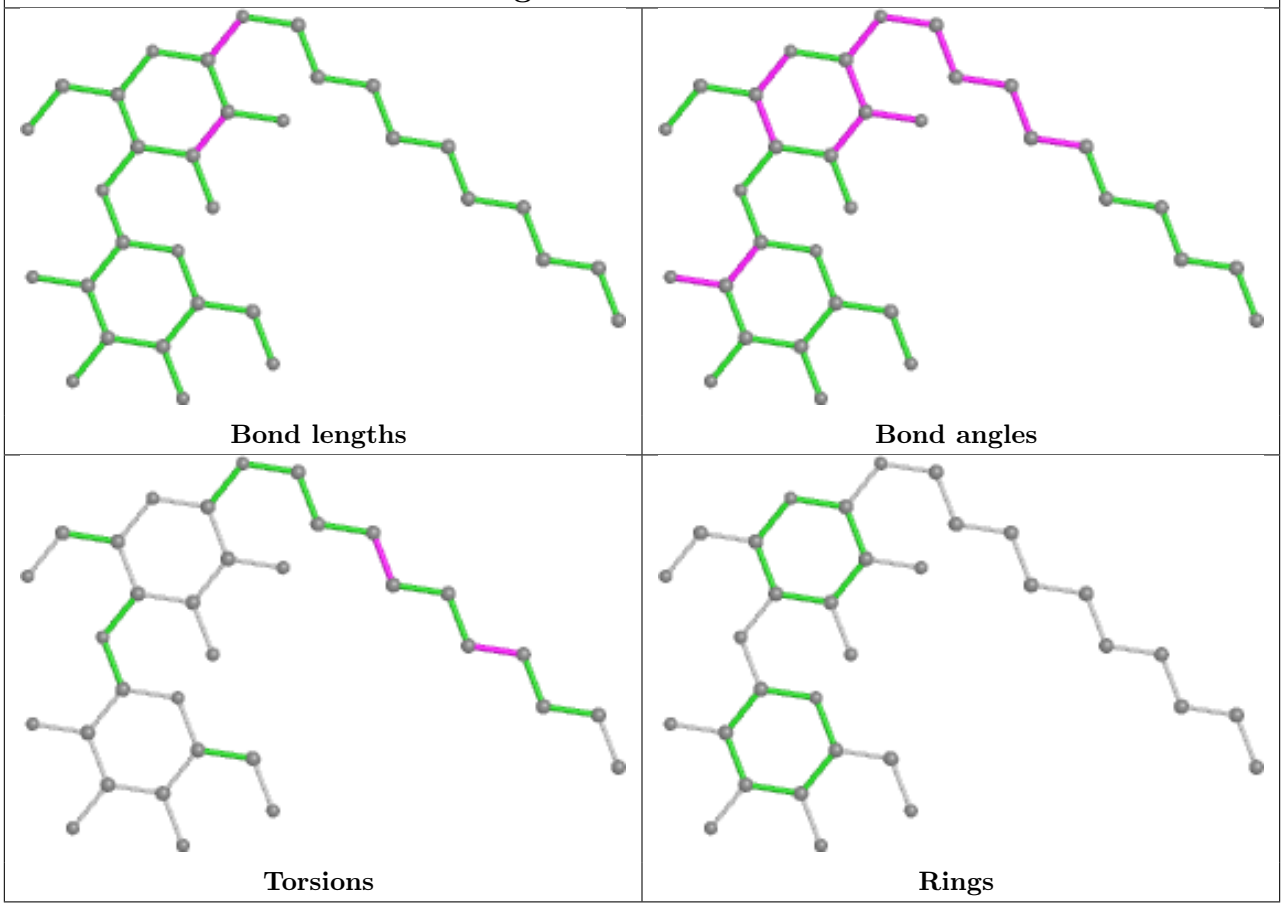


Torsions

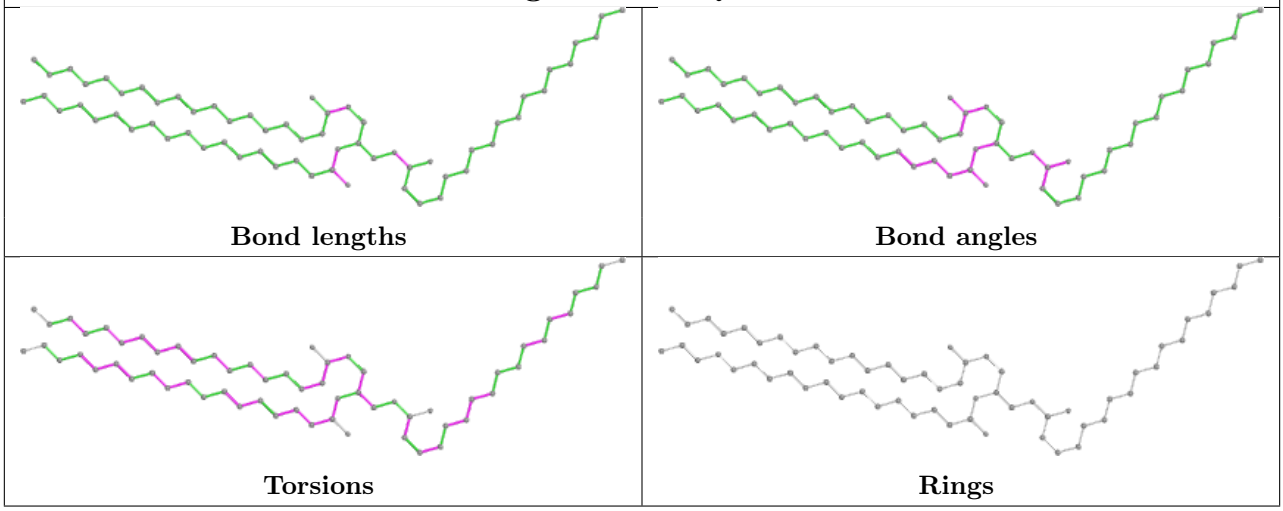


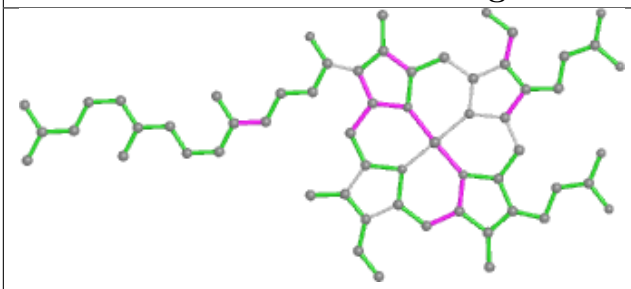
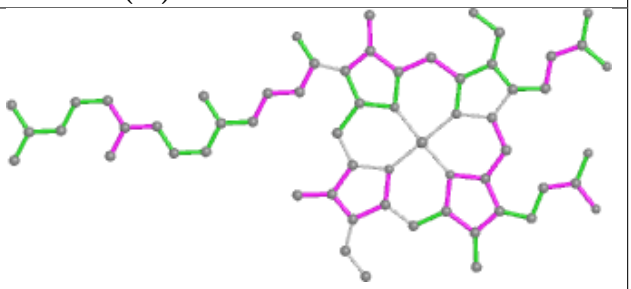
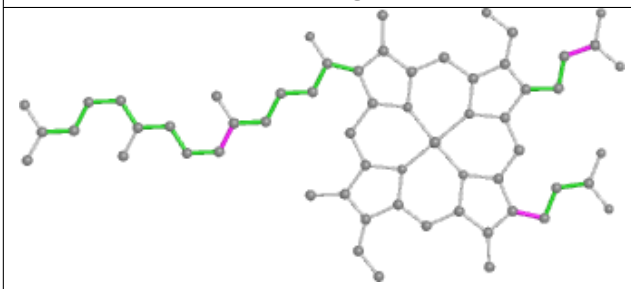
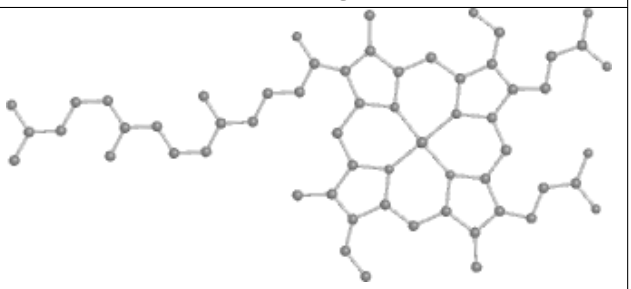
Rings

Ligand DMU M 101



Ligand TGL Q 201



Ligand HEA N 602 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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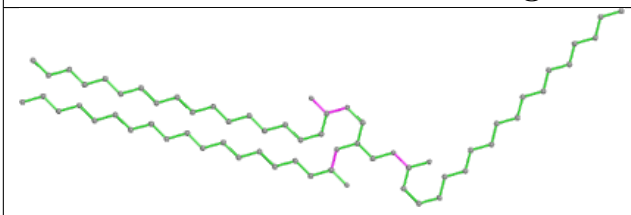
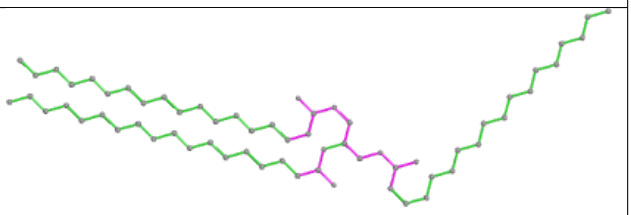
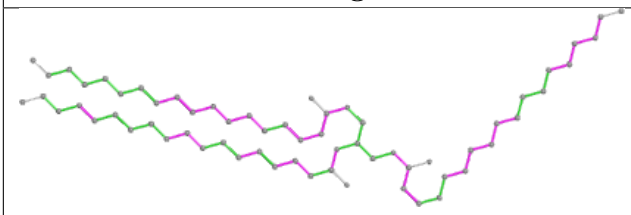
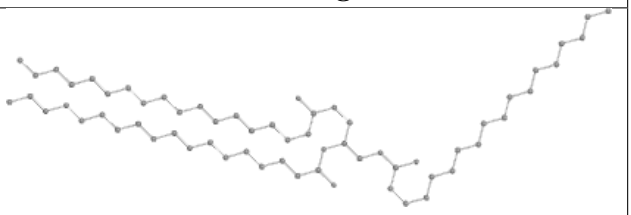
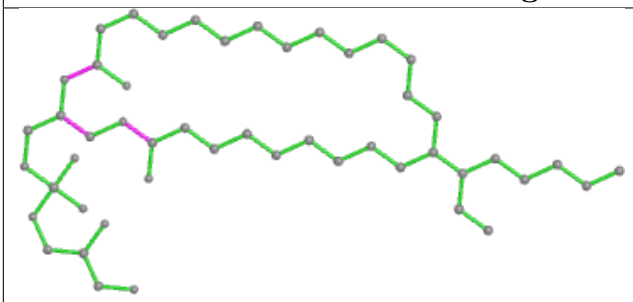
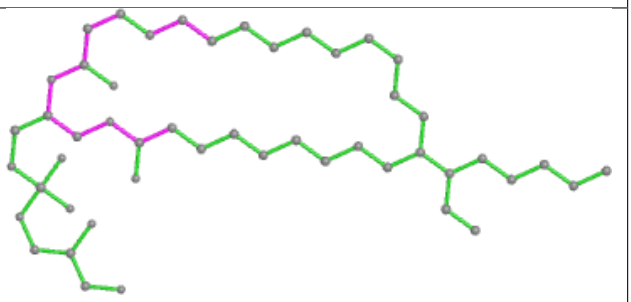
 Bond lengths	 Bond angles
 Torsions	 Rings

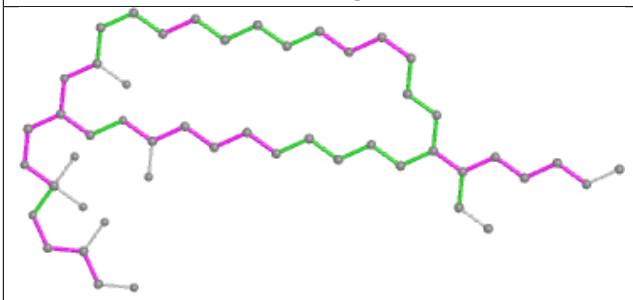
Ligand PGV X 101



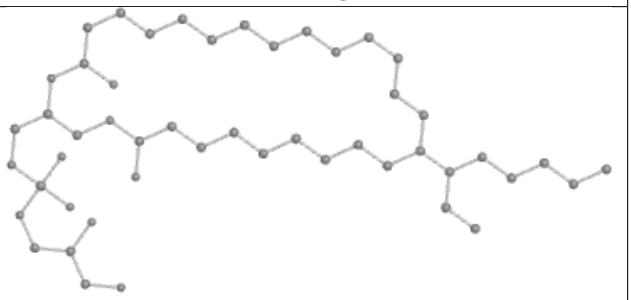
Bond lengths



Bond angles

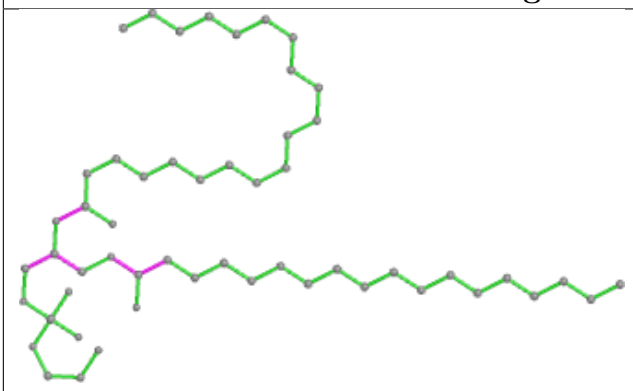


Torsions

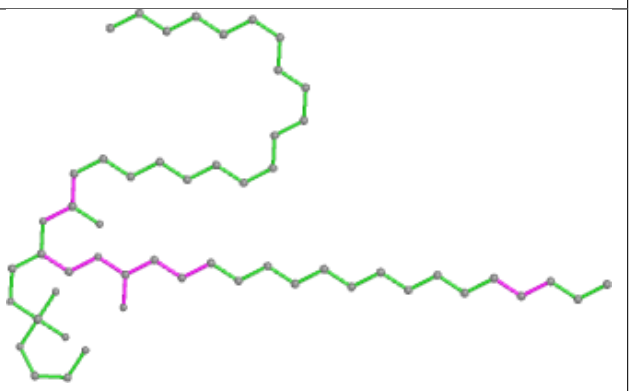


Rings

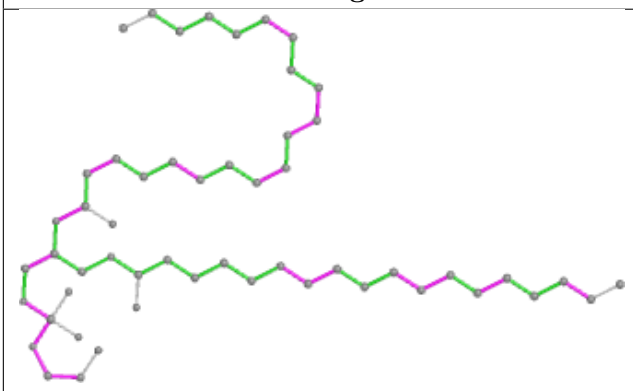
Ligand PEK C 307



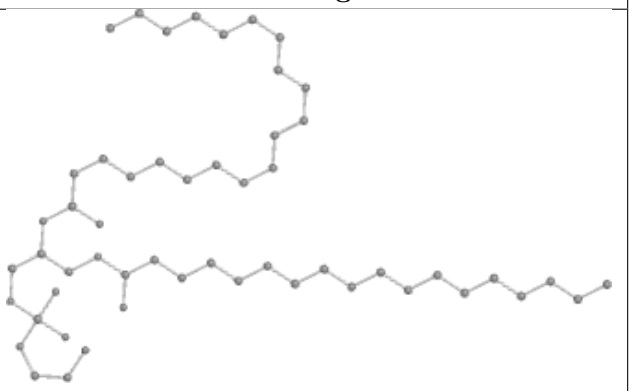
Bond lengths



Bond angles

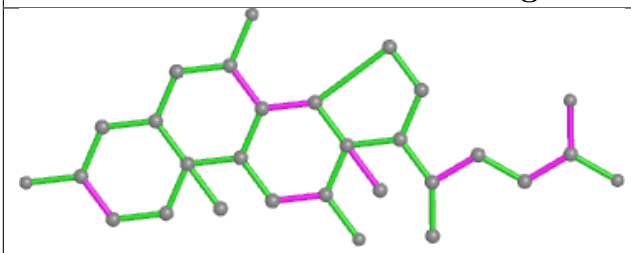


Torsions



Rings

Ligand CHD C 301



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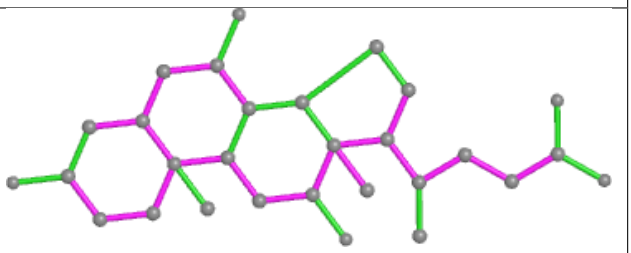
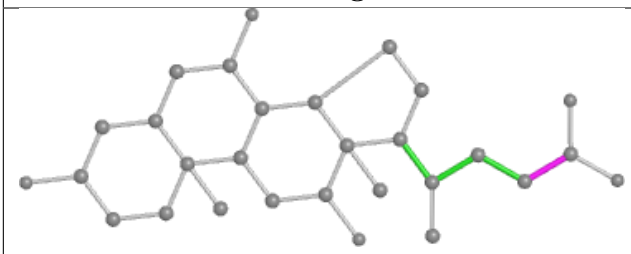


Bond angles



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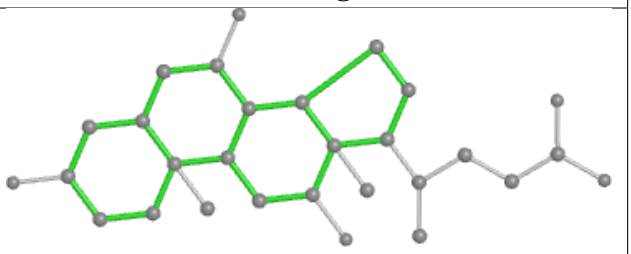
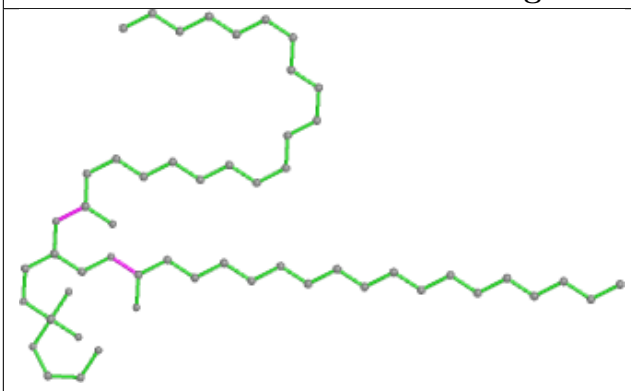


Rings

Ligand PEK T 101



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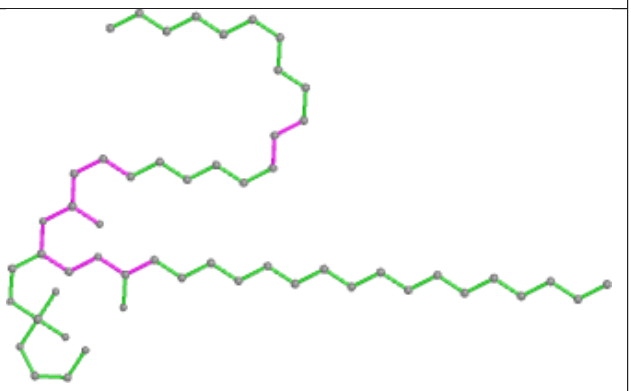
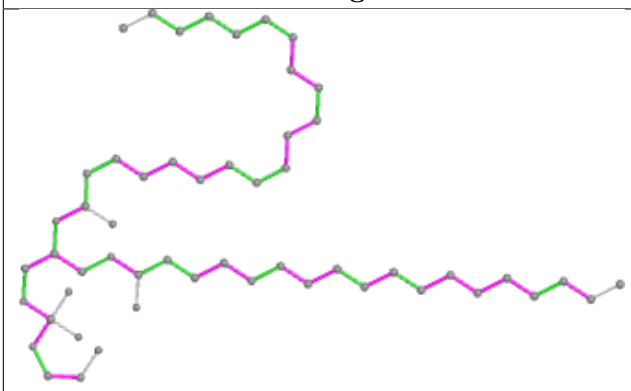


Bond angles



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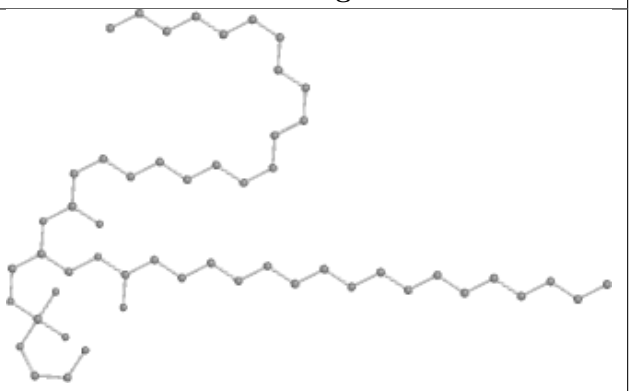
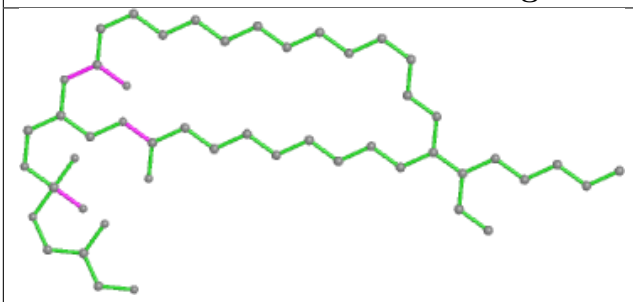


Rings

Ligand PGV A 610



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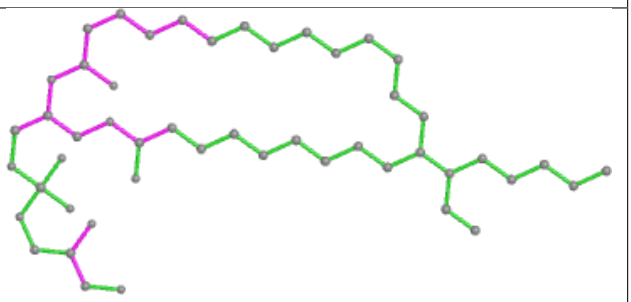
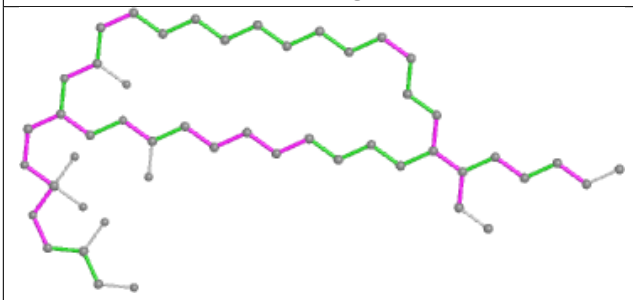


Bond angles



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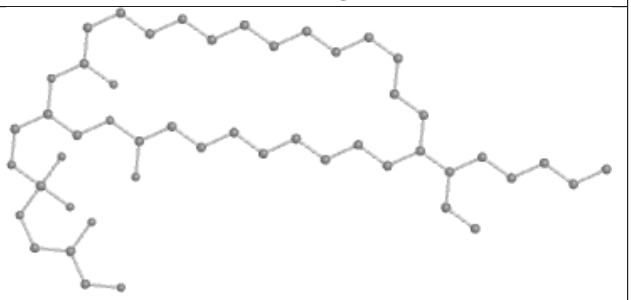
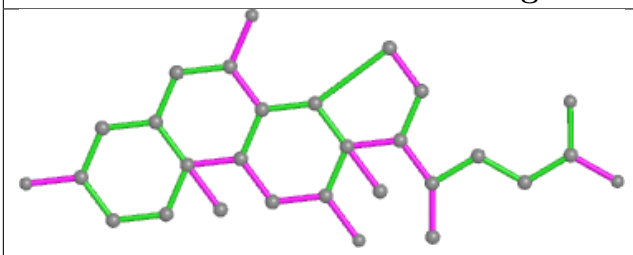
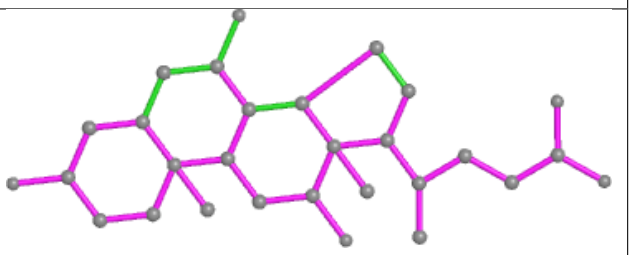


Rings

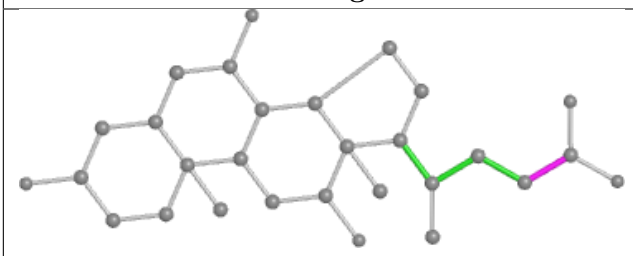
Ligand CHD B 301



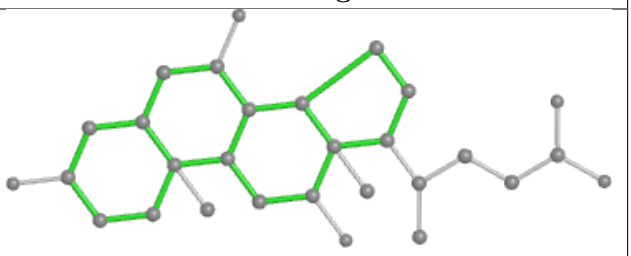
Bond lengths



Bond angles

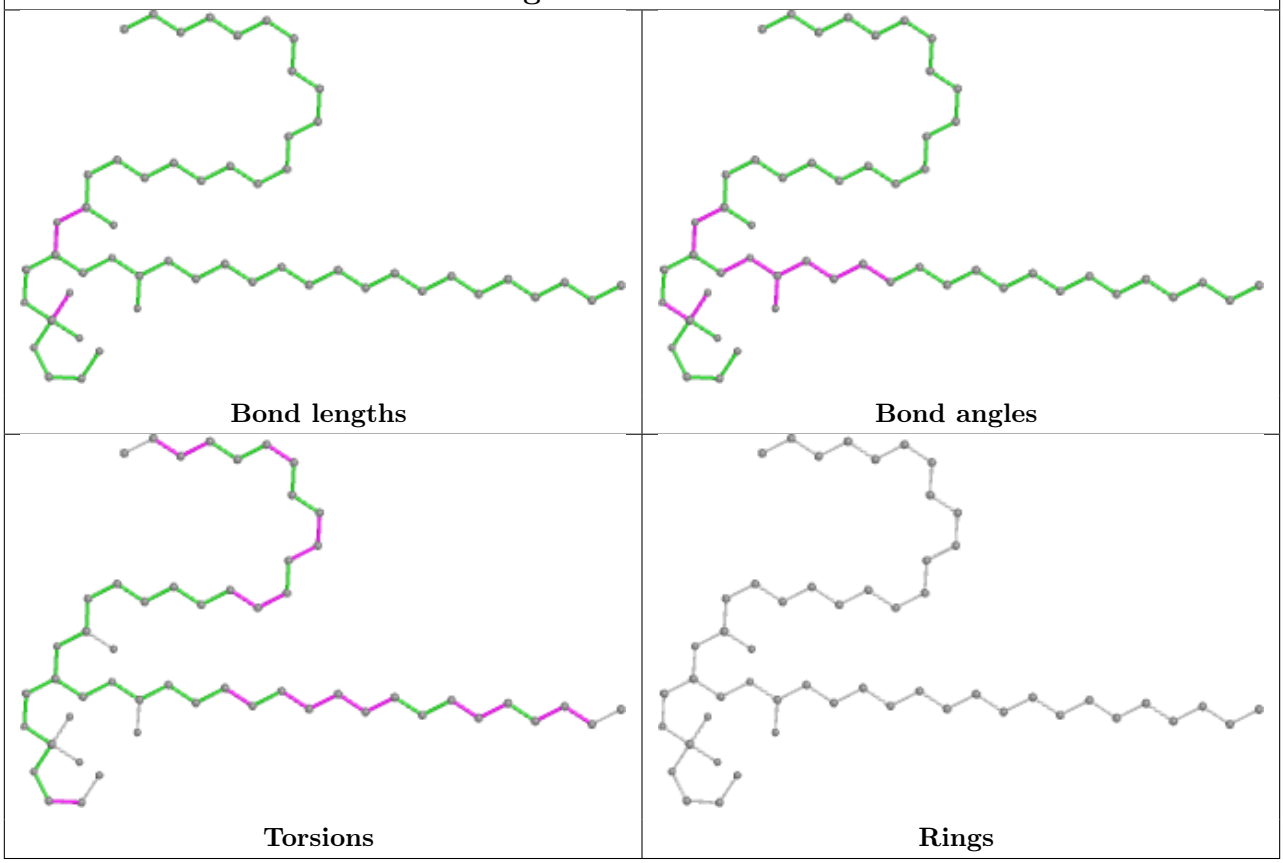


Torsions

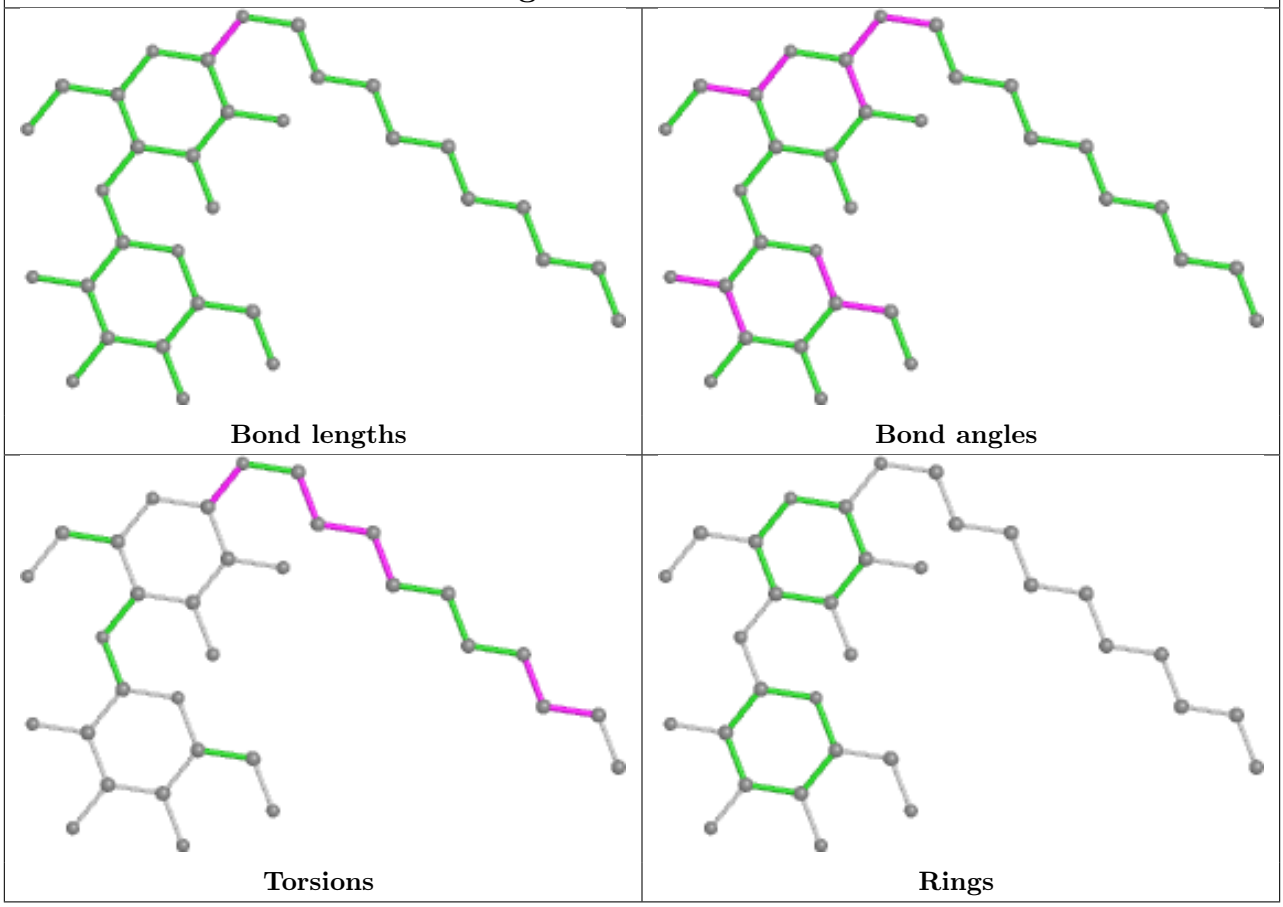


Rings

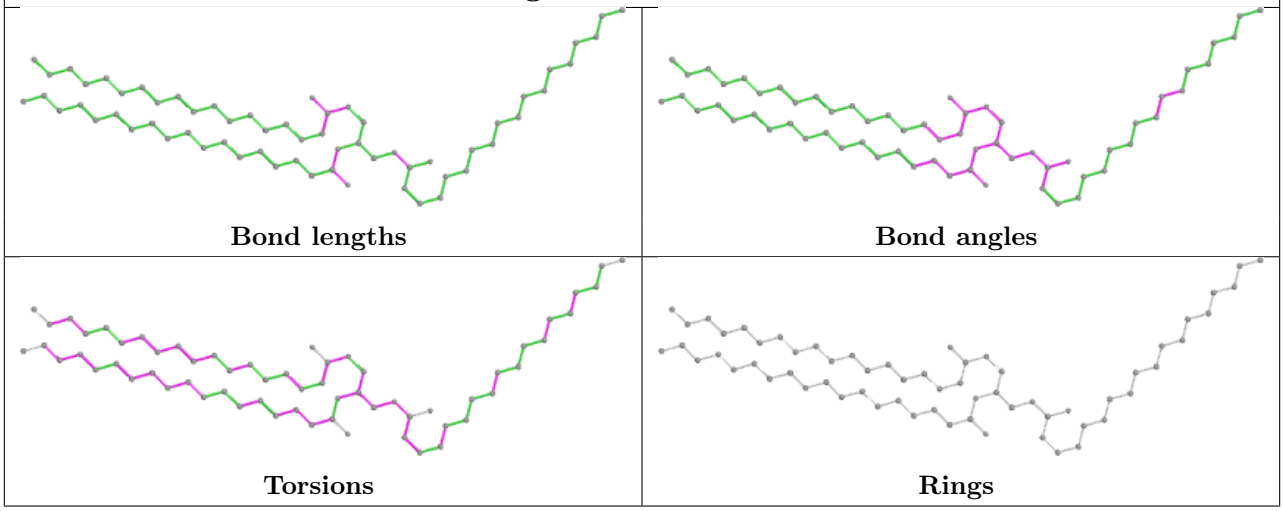
Ligand PEK G 101



Ligand DMU P 310



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.16	0	100	100	19, 23, 31, 69	0
1	N	513/514 (99%)	-0.24	0	100	100	21, 27, 36, 68	0
2	B	226/227 (99%)	-0.13	5 (2%)	62	63	22, 30, 48, 64	0
2	O	226/227 (99%)	-0.15	5 (2%)	62	63	28, 37, 59, 78	0
3	C	259/261 (99%)	-0.23	1 (0%)	92	93	21, 27, 38, 74	0
3	P	259/261 (99%)	-0.25	3 (1%)	79	81	22, 28, 39, 57	0
4	D	144/147 (97%)	-0.32	2 (1%)	75	79	25, 31, 46, 73	0
4	Q	144/147 (97%)	0.49	9 (6%)	20	19	32, 44, 69, 141	0
5	E	105/109 (96%)	-0.29	2 (1%)	66	69	24, 31, 53, 103	0
5	R	105/109 (96%)	-0.24	2 (1%)	66	69	28, 38, 57, 103	0
6	F	98/98 (100%)	0.34	8 (8%)	11	11	23, 33, 88, 139	0
6	S	98/98 (100%)	0.33	9 (9%)	9	8	23, 33, 84, 114	0
7	G	83/85 (97%)	0.81	17 (20%)	1	1	26, 34, 100, 127	0
7	T	83/85 (97%)	0.78	17 (20%)	1	1	25, 37, 93, 135	0
8	H	79/85 (92%)	0.22	8 (10%)	7	6	27, 37, 83, 101	0
8	U	79/85 (92%)	0.33	9 (11%)	5	4	34, 42, 93, 103	0
9	I	72/73 (98%)	0.45	8 (11%)	5	4	28, 40, 75, 85	0
9	V	72/73 (98%)	0.46	7 (9%)	7	6	28, 51, 74, 90	0
10	J	58/59 (98%)	0.15	4 (6%)	16	15	26, 36, 63, 99	0
10	W	58/59 (98%)	0.32	5 (8%)	10	10	29, 39, 68, 115	0
11	K	49/56 (87%)	-0.25	0	100	100	30, 37, 50, 57	0
11	X	49/56 (87%)	0.28	3 (6%)	21	19	39, 46, 65, 76	0
12	L	46/47 (97%)	-0.05	1 (2%)	62	63	24, 29, 47, 83	0
12	Y	46/47 (97%)	-0.03	1 (2%)	62	63	30, 37, 55, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.18	4 (9%)	8	7	26, 29, 61, 107	0
13	Z	43/46 (93%)	0.27	4 (9%)	8	7	33, 40, 75, 116	0
All	All	3550/3614 (98%)	-0.02	134 (3%)	40	40	19, 31, 61, 141	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	26.0
4	Q	6	VAL	16.1
4	Q	8	SER	14.9
6	S	97	ALA	14.5
6	F	97	ALA	11.5

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	0.45	0.41	76,101,117,121	0
7	TPO	G	11	11/12	0.56	0.44	84,110,125,127	0
9	SAC	V	1	9/10	0.63	0.64	107,118,124,126	0
9	SAC	I	1	9/10	0.85	0.25	59,70,74,74	0
1	FME	A	1	10/11	0.95	0.11	33,43,67,83	0
2	FME	B	1	10/11	0.95	0.12	20,28,45,61	0
1	FME	N	1	10/11	0.97	0.11	36,44,71,76	0
2	FME	O	1	10/11	0.98	0.09	36,36,43,57	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
22	CHD	W	101	29/29	0.49	0.43	58,114,135,143	0
24	PSC	B	303	52/52	0.57	0.30	31,74,150,157	0
25	DMU	C	310	33/33	0.59	0.26	46,72,105,111	0
25	DMU	L	102	33/33	0.63	0.23	47,83,107,120	0
27	CDL	G	102	100/100	0.64	0.22	49,86,117,152	0
21	EDO	F	103	4/4	0.65	0.49	52,76,77,81	0
22	CHD	J	101	29/29	0.67	0.43	50,112,133,141	0
20	PGV	C	308	51/51	0.69	0.22	42,72,109,132	0
27	CDL	T	103	100/100	0.69	0.22	51,84,123,146	0
21	EDO	N	615	4/4	0.70	0.17	66,67,67,72	0
28	PEK	G	104	53/53	0.70	0.29	44,88,153,155	0
19	TGL	Q	201	63/63	0.71	0.19	47,72,92,103	0
28	PEK	P	308	53/53	0.71	0.25	37,69,131,149	0
28	PEK	T	101	53/53	0.71	0.26	43,93,153,154	0
28	PEK	C	307	53/53	0.72	0.23	39,79,139,146	0
25	DMU	P	309	33/33	0.73	0.20	53,72,93,94	0
25	DMU	C	302	33/33	0.73	0.35	30,61,103,109	0
27	CDL	P	305	100/100	0.73	0.25	35,80,118,122	0
25	DMU	P	307	33/33	0.73	0.30	38,61,96,102	0
27	CDL	C	305	100/100	0.75	0.21	30,70,103,110	0
25	DMU	P	310	33/33	0.75	0.23	61,74,92,94	0
20	PGV	X	101	51/51	0.76	0.24	42,70,129,151	0
24	PSC	O	302	52/52	0.76	0.25	39,78,148,161	0
22	CHD	P	306	29/29	0.78	0.24	48,58,64,66	0
25	DMU	C	309	33/33	0.78	0.24	51,70,95,98	0
21	EDO	D	203	4/4	0.78	0.35	45,50,64,66	0
20	PGV	P	302	51/51	0.79	0.19	50,77,127,132	0
20	PGV	A	610	51/51	0.80	0.20	30,59,101,112	0
19	TGL	Y	101	63/63	0.81	0.23	39,66,108,129	0
21	EDO	A	618	4/4	0.82	0.17	41,47,51,58	0
22	CHD	C	306	29/29	0.82	0.23	50,61,66,68	0
21	EDO	A	620	4/4	0.83	0.16	54,57,62,64	0
21	EDO	C	313	4/4	0.83	0.24	46,58,62,63	0
19	TGL	N	609	63/63	0.83	0.15	44,70,96,112	0
26	UNX	C	303	1/1	0.83	0.14	24,24,24,24	0
19	TGL	L	101	63/63	0.84	0.17	30,58,91,103	0
21	EDO	E	202	4/4	0.84	0.34	39,41,54,60	0
19	TGL	D	201	63/63	0.85	0.15	27,58,80,93	0
25	DMU	Z	101	33/33	0.86	0.16	44,50,65,65	0
21	EDO	Y	102	4/4	0.86	0.26	59,62,66,70	0
21	EDO	H	101	4/4	0.87	0.14	54,54,59,66	0
21	EDO	S	105	4/4	0.87	0.16	41,47,48,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	O	303	4/4	0.88	0.18	49,51,51,57	0
21	EDO	B	305	4/4	0.89	0.16	45,50,51,54	0
21	EDO	G	106	4/4	0.89	0.14	47,58,62,69	0
25	DMU	M	101	33/33	0.89	0.10	36,40,53,57	0
21	EDO	A	615	4/4	0.89	0.14	43,43,47,61	0
19	TGL	A	608	63/63	0.90	0.15	33,66,93,101	0
21	EDO	A	614	4/4	0.90	0.15	45,49,54,83	0
21	EDO	L	103	4/4	0.91	0.19	43,56,67,73	0
21	EDO	N	612	4/4	0.91	0.17	51,51,59,60	0
21	EDO	D	205	4/4	0.91	0.13	44,47,49,58	0
21	EDO	N	616	4/4	0.92	0.23	26,33,42,59	0
21	EDO	A	617	4/4	0.92	0.11	39,42,42,45	0
21	EDO	F	104	4/4	0.93	0.09	35,39,40,45	0
21	EDO	D	202	4/4	0.93	0.53	31,40,46,85	0
21	EDO	T	104	4/4	0.94	0.10	33,33,41,43	0
21	EDO	C	312	4/4	0.94	0.11	54,56,58,68	0
22	CHD	C	301	29/29	0.94	0.08	24,29,33,35	0
21	EDO	A	619	4/4	0.95	0.31	34,48,49,55	0
21	EDO	O	304	4/4	0.95	0.09	34,35,35,35	0
21	EDO	P	312	4/4	0.95	0.10	29,34,43,47	0
26	UNX	P	303	1/1	0.95	0.15	24,24,24,24	0
21	EDO	A	612	4/4	0.95	0.14	28,28,30,35	0
21	EDO	B	304	4/4	0.95	0.11	36,42,48,49	0
28	PEK	T	102	53/53	0.95	0.12	27,43,78,91	0
21	EDO	F	105	4/4	0.96	0.09	32,33,36,36	0
21	EDO	N	613	4/4	0.96	0.13	34,42,44,45	0
21	EDO	N	614	4/4	0.96	0.11	36,37,42,45	0
28	PEK	G	101	53/53	0.96	0.12	25,43,71,86	0
21	EDO	S	103	4/4	0.96	0.14	35,58,59,60	0
21	EDO	S	104	4/4	0.96	0.10	35,38,42,44	0
21	EDO	A	621	4/4	0.96	0.24	41,45,46,59	0
21	EDO	N	610	4/4	0.96	0.10	29,30,32,38	0
21	EDO	A	611	4/4	0.97	0.12	31,40,44,46	0
20	PGV	P	304	51/51	0.97	0.10	24,33,75,82	0
22	CHD	B	301	29/29	0.97	0.07	23,26,30,37	0
21	EDO	N	611	4/4	0.97	0.09	24,27,31,32	0
21	EDO	B	306	4/4	0.97	0.09	25,26,31,31	0
22	CHD	G	103	29/29	0.97	0.08	24,27,30,34	0
21	EDO	G	105	4/4	0.97	0.08	29,30,37,39	0
22	CHD	P	301	29/29	0.97	0.07	26,30,34,38	0
21	EDO	C	311	4/4	0.97	0.08	34,35,36,37	0
20	PGV	C	304	51/51	0.97	0.10	24,32,80,88	0

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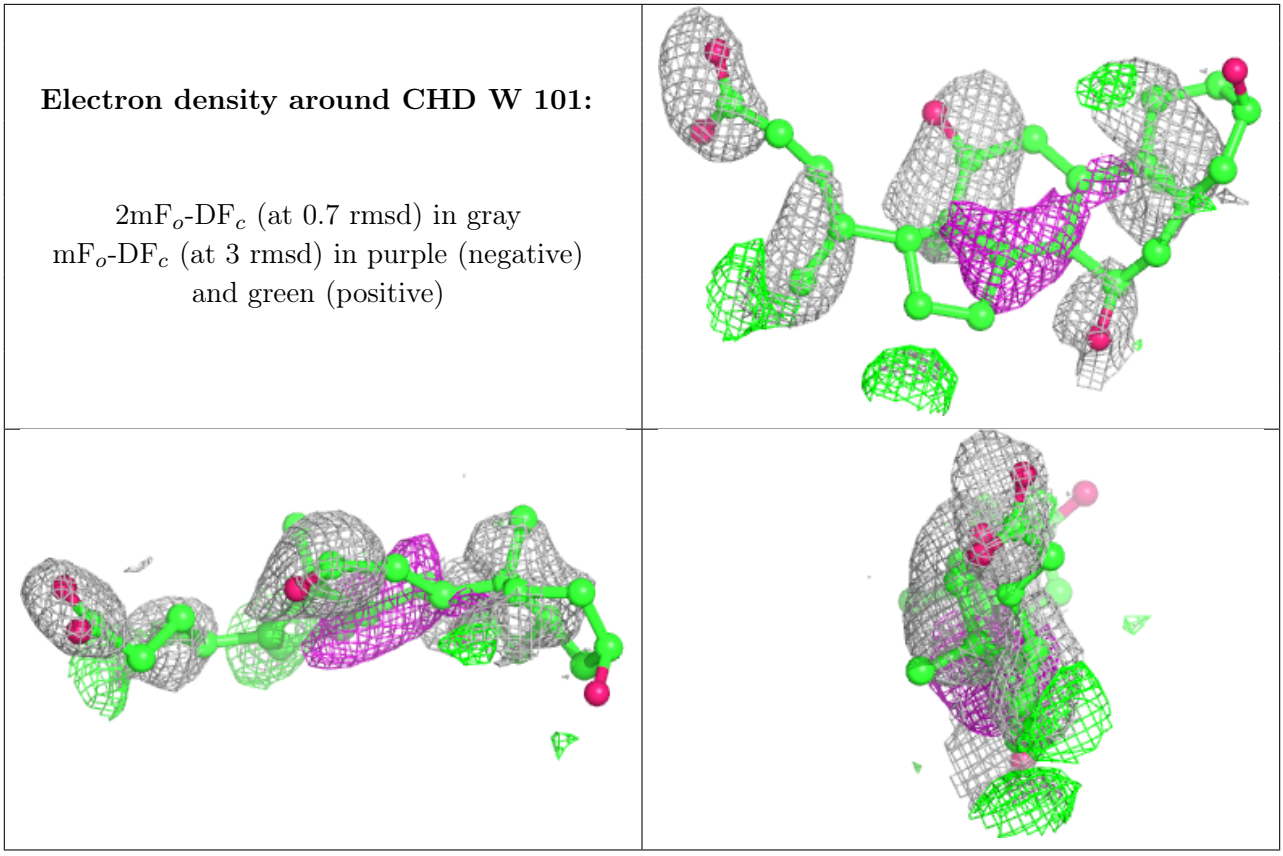
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	S	106	4/4	0.97	0.07	32,33,33,34	0
14	HEA	N	602[A]	60/60	0.98	0.11	19,23,26,27	60
14	HEA	N	602[B]	60/60	0.98	0.11	22,25,38,39	60
21	EDO	A	613	4/4	0.98	0.12	23,24,25,26	0
20	PGV	A	609	51/51	0.98	0.10	21,29,60,64	0
16	MG	N	604	1/1	0.98	0.07	28,28,28,28	0
21	EDO	A	616	4/4	0.98	0.09	32,36,40,45	0
18	AZI	N	606[B]	3/3	0.98	0.15	21,21,23,24	3
21	EDO	D	204	4/4	0.98	0.13	35,35,50,57	0
14	HEA	A	601	60/60	0.98	0.09	19,21,43,47	0
21	EDO	E	201	4/4	0.98	0.08	36,37,39,41	0
20	PGV	N	608	51/51	0.98	0.09	23,32,61,63	0
21	EDO	E	203	4/4	0.98	0.06	34,37,43,45	0
14	HEA	A	602[A]	60/60	0.98	0.11	17,20,25,28	60
21	EDO	P	311	4/4	0.98	0.16	39,40,40,43	0
14	HEA	A	602[B]	60/60	0.98	0.11	17,21,28,31	60
21	EDO	R	201	4/4	0.98	0.10	38,40,42,43	0
21	EDO	S	102	4/4	0.98	0.08	25,25,25,26	0
14	HEA	N	601	60/60	0.98	0.09	23,26,45,50	0
16	MG	A	604	1/1	0.99	0.07	23,23,23,23	0
18	AZI	N	607[A]	3/3	0.99	0.14	25,25,26,29	3
18	AZI	N	607[B]	3/3	0.99	0.14	19,19,20,27	3
18	AZI	A	606[B]	3/3	0.99	0.18	20,20,20,21	3
18	AZI	A	607[A]	3/3	0.99	0.12	20,20,21,24	3
21	EDO	F	102	4/4	0.99	0.08	23,24,26,26	0
18	AZI	A	607[B]	3/3	0.99	0.12	16,16,17,26	3
23	CUA	O	301	2/2	1.00	0.12	29,29,29,30	0
17	NA	N	605	1/1	1.00	0.06	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.13	23,23,23,23	0
15	CU	N	603	1/1	1.00	0.14	26,26,26,26	0
17	NA	A	605	1/1	1.00	0.07	25,25,25,25	0
23	CUA	B	302	2/2	1.00	0.14	23,23,23,23	0
29	ZN	F	101	1/1	1.00	0.12	28,28,28,28	0
29	ZN	S	101	1/1	1.00	0.11	29,29,29,29	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.

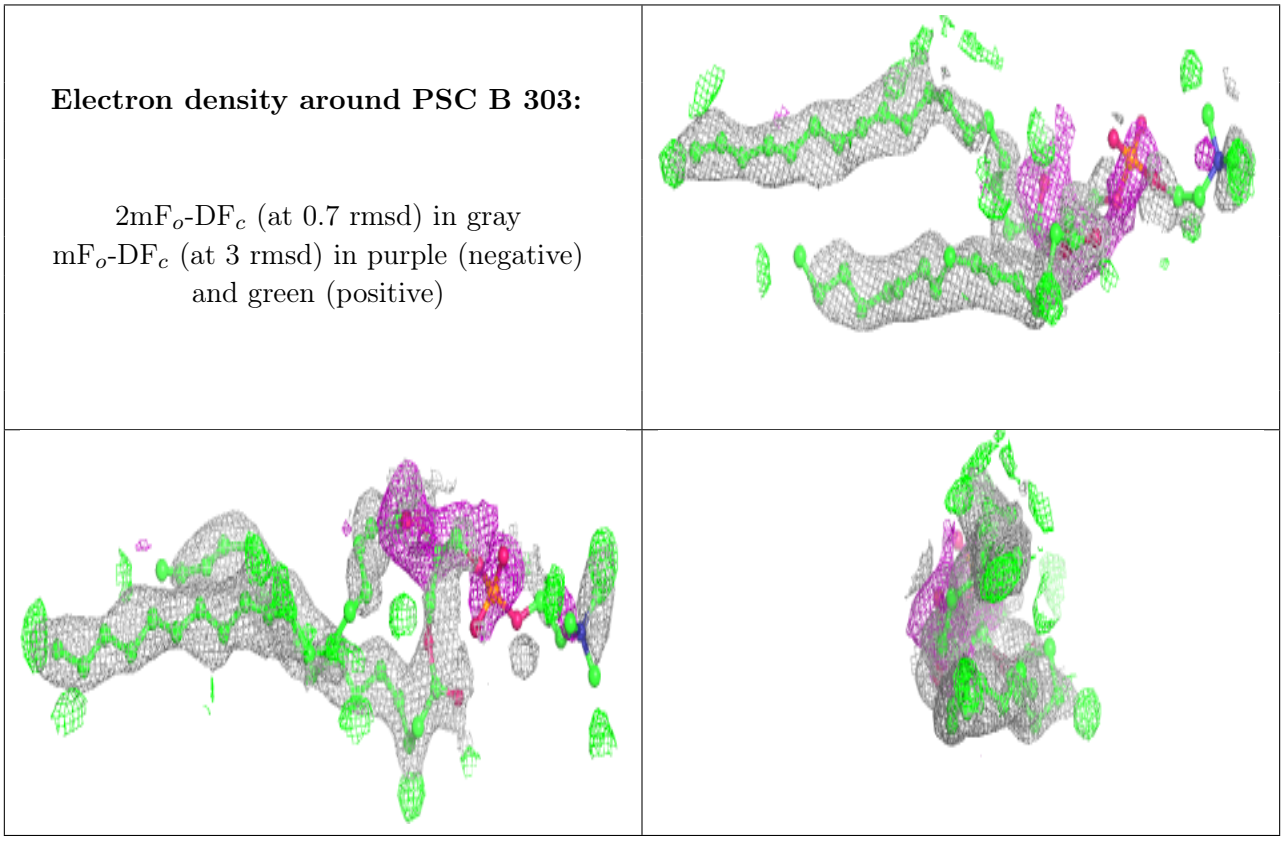
Electron density around CHD W 101:

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



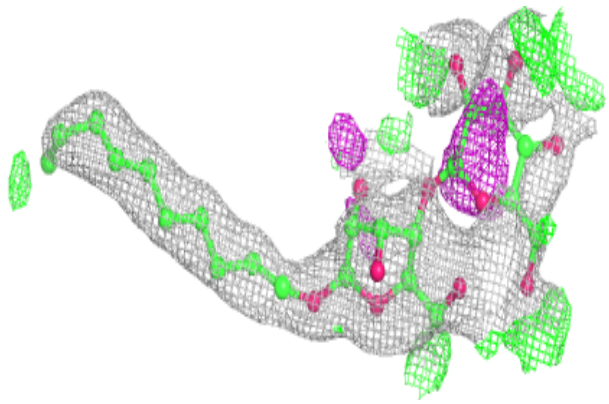
Electron density around PSC B 303:

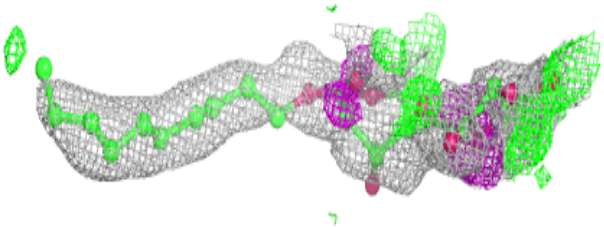
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

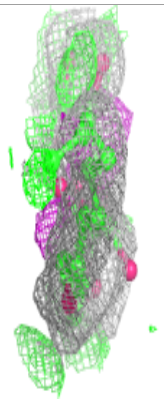


Electron density around DMU C 310:

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

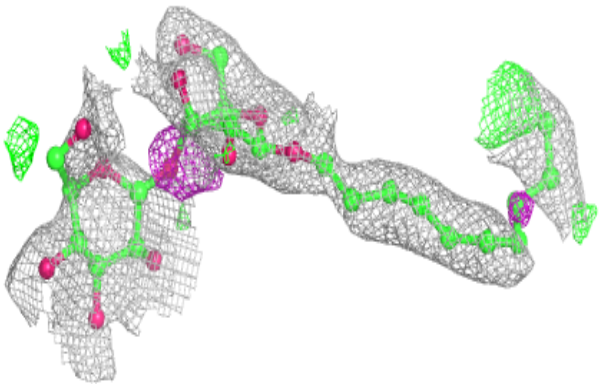


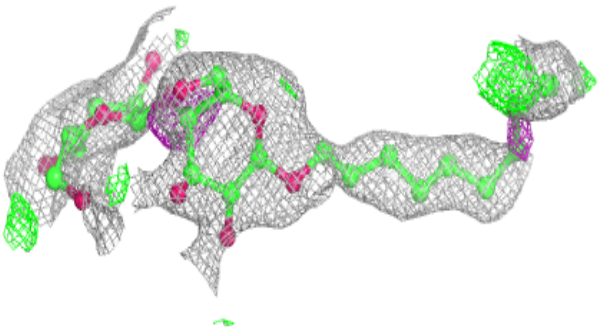


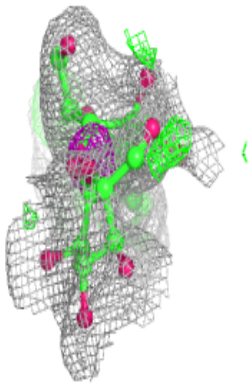


Electron density around DMU L 102:

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

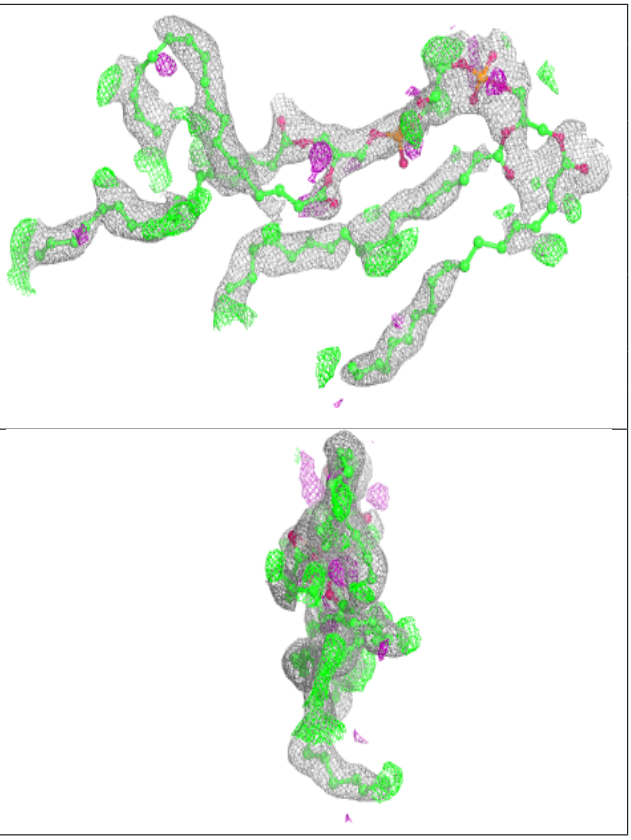


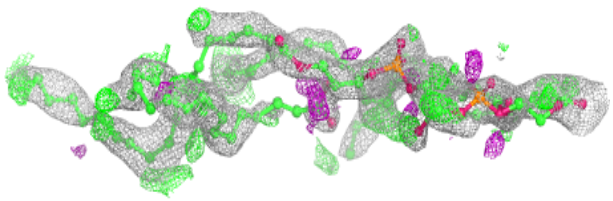




Electron density around CDL G 102:

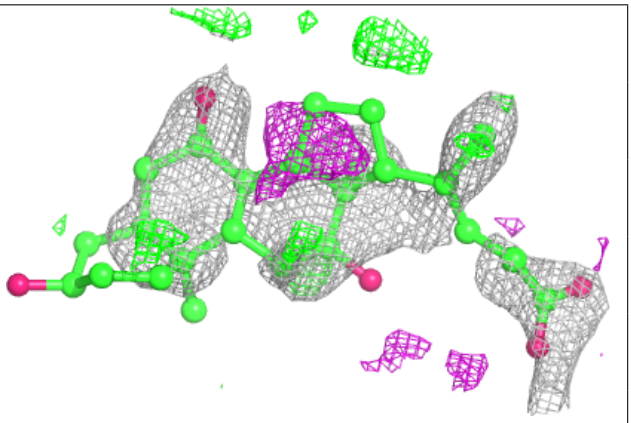
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

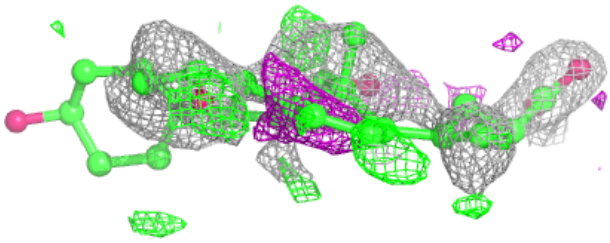


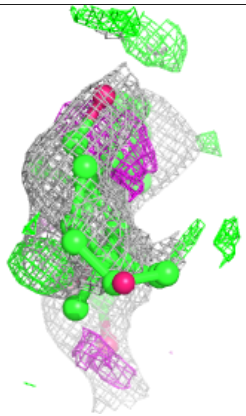


Electron density around CHD J 101:

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

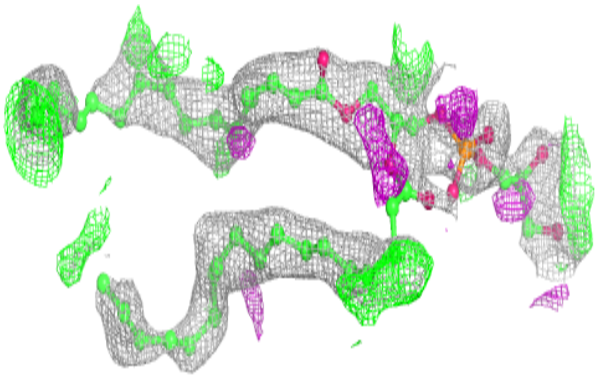


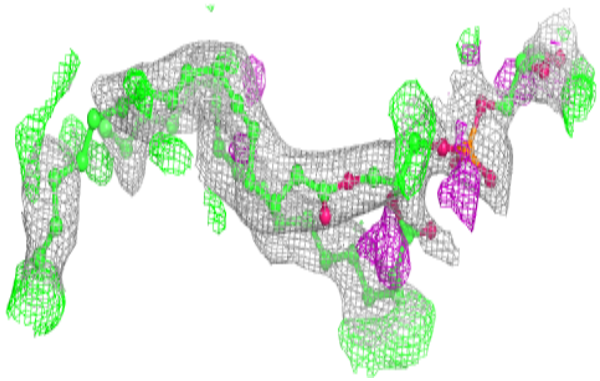


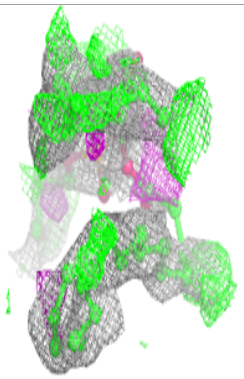


Electron density around PGV C 308:

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

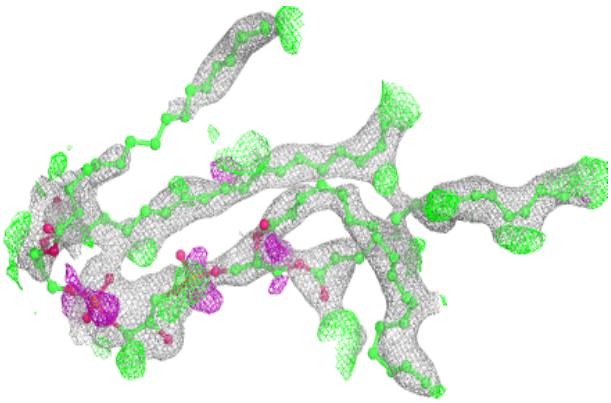


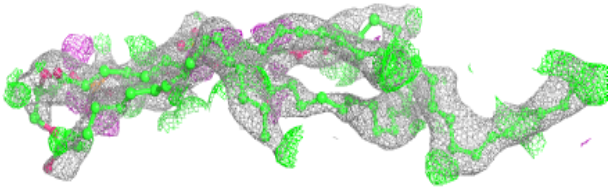


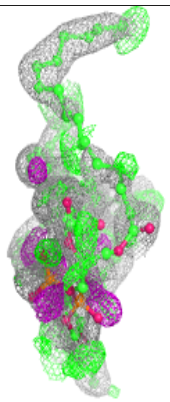


Electron density around CDL T 103:

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

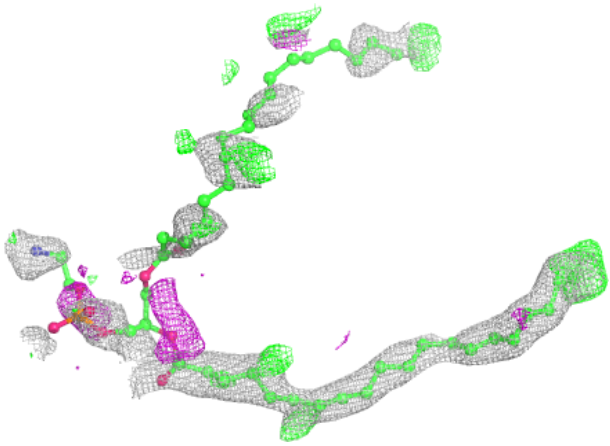


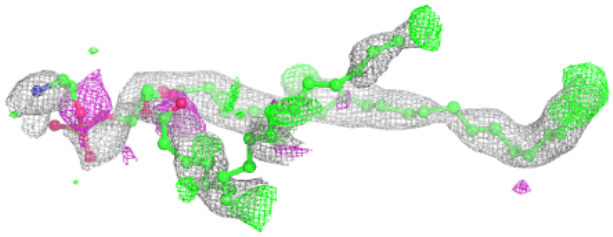


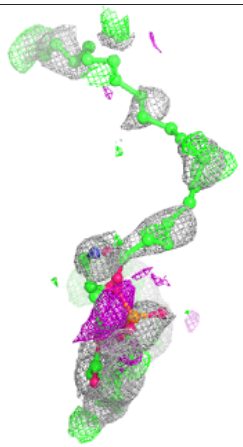


Electron density around PEK G 104:

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

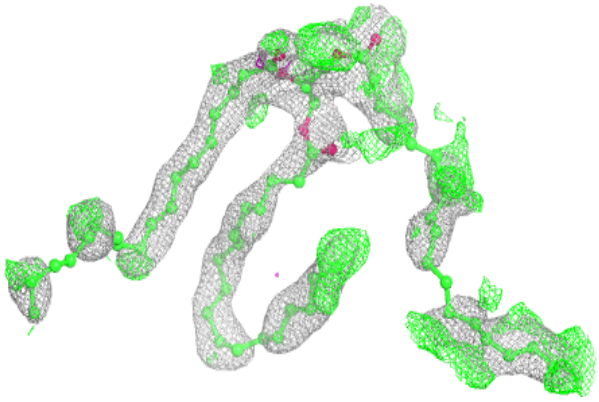


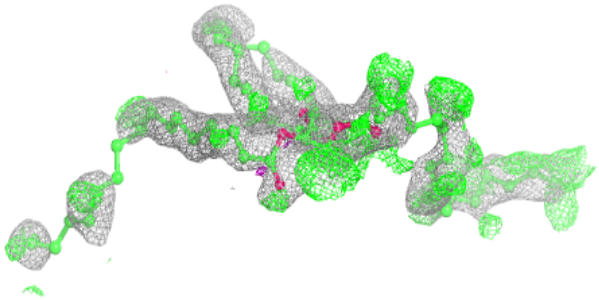


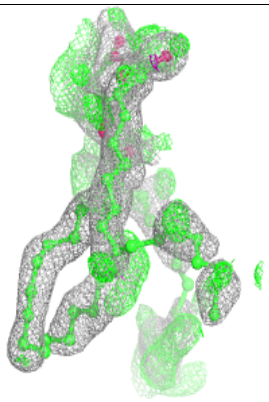


Electron density around TGL Q 201:

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

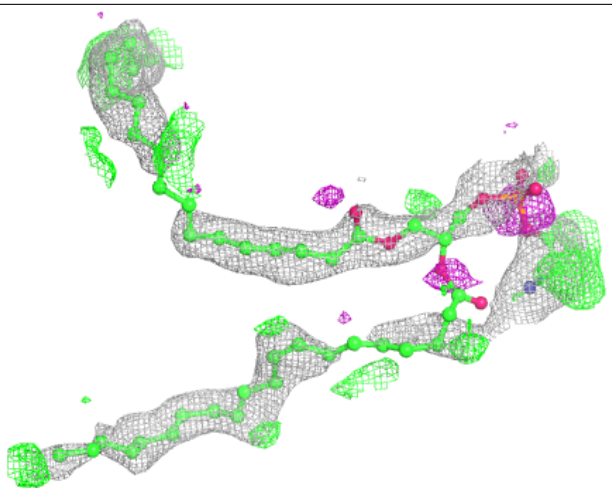


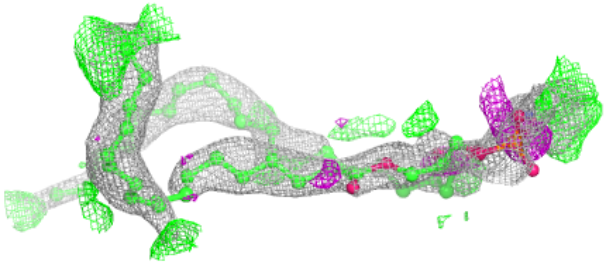


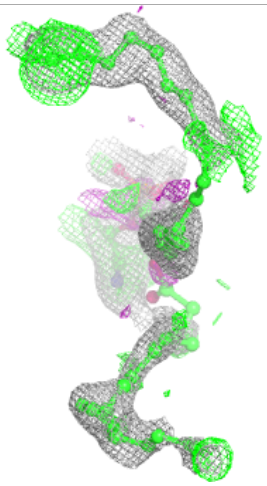


Electron density around PEK P 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

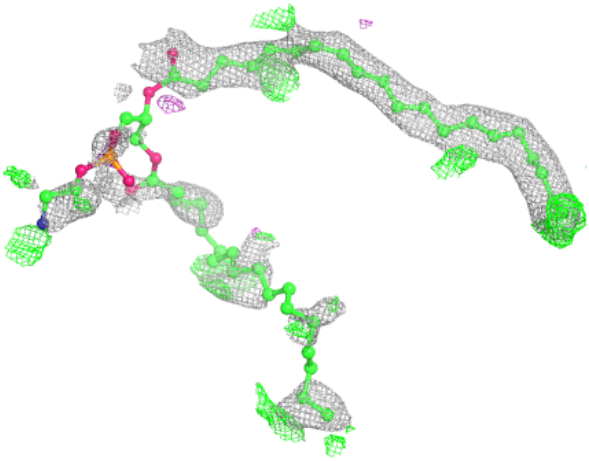


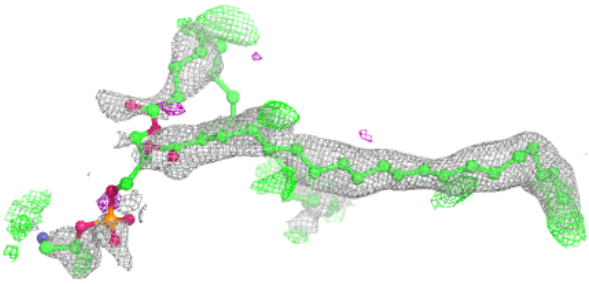


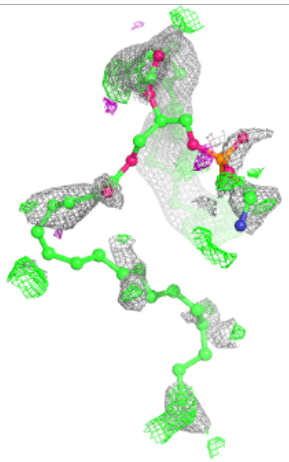


Electron density around PEK T 101:

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

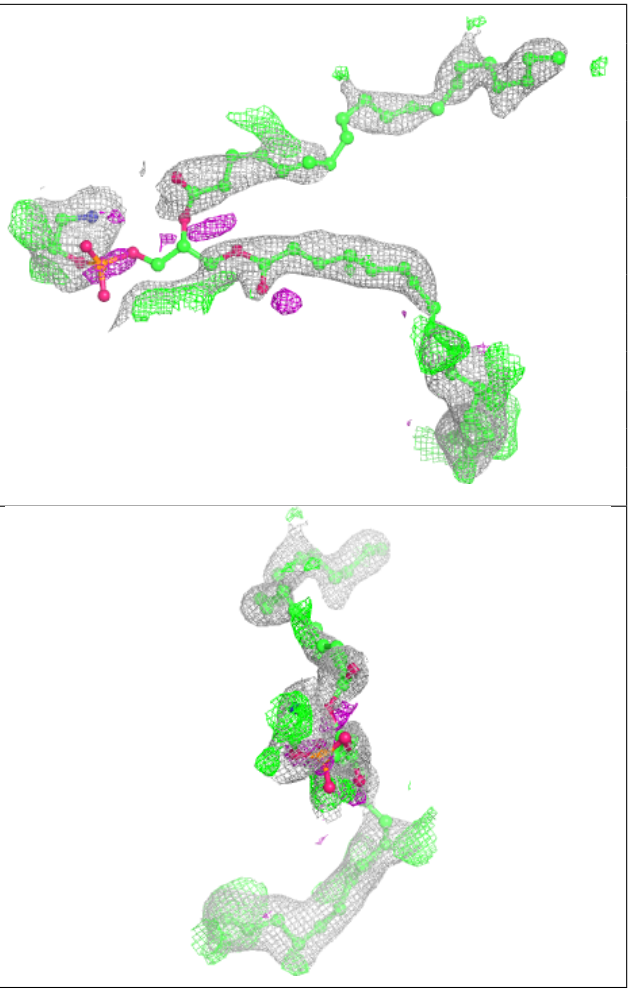






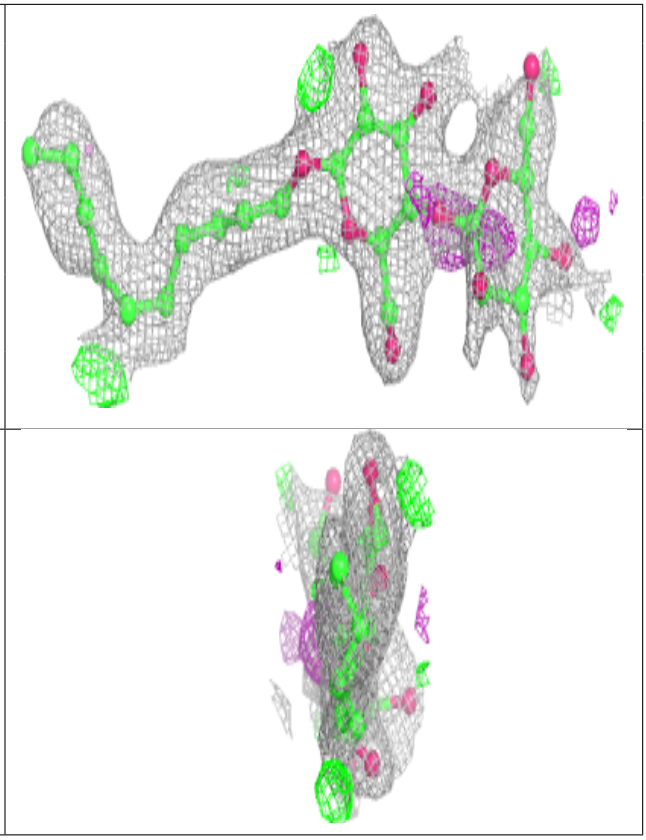
Electron density around PEK C 307:

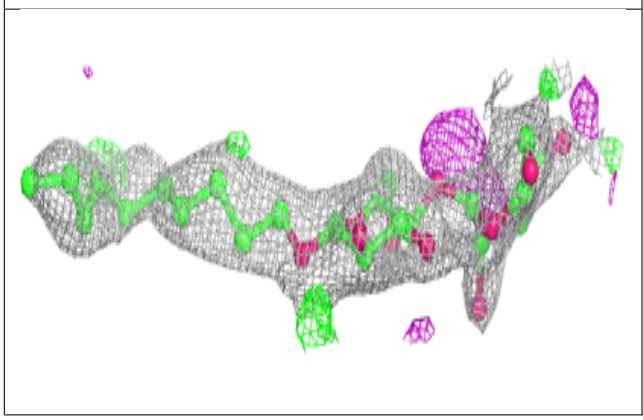
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU P 309:

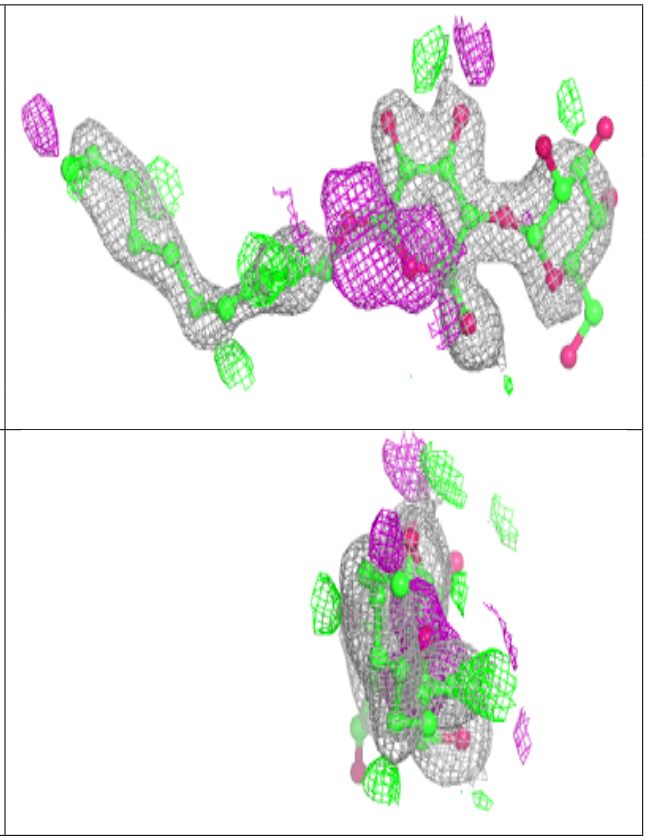
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

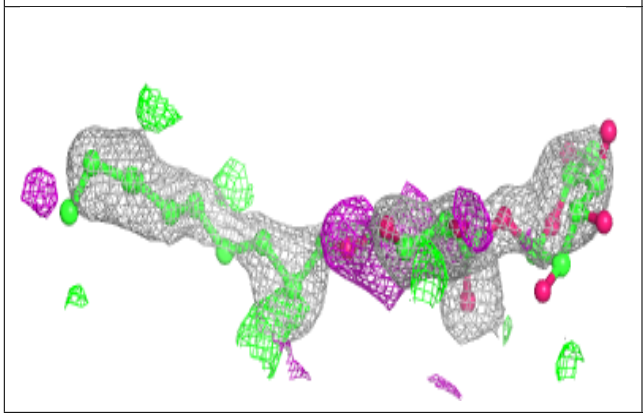




Electron density around DMU C 302:

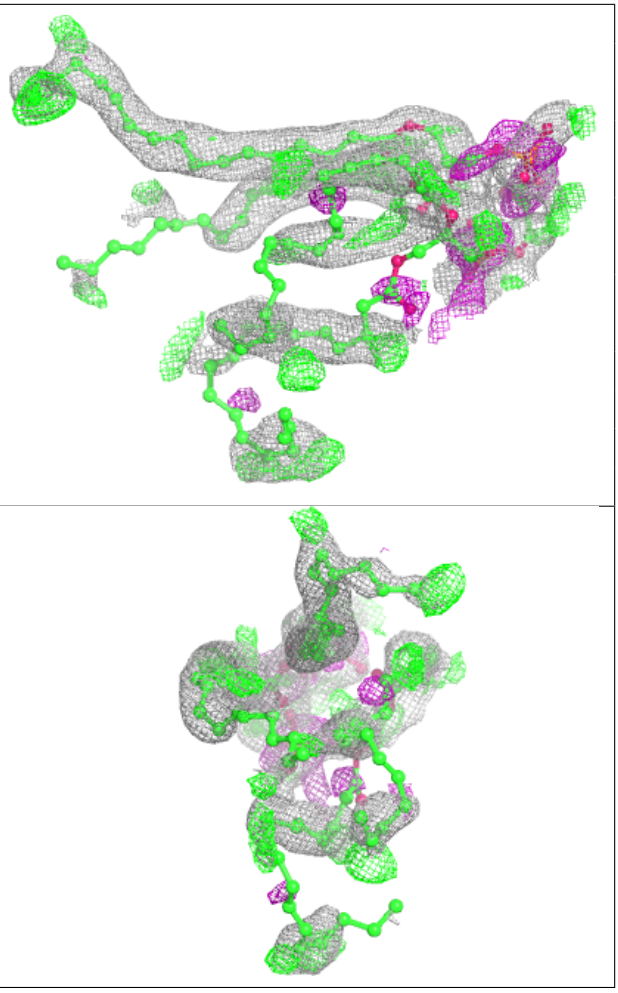
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





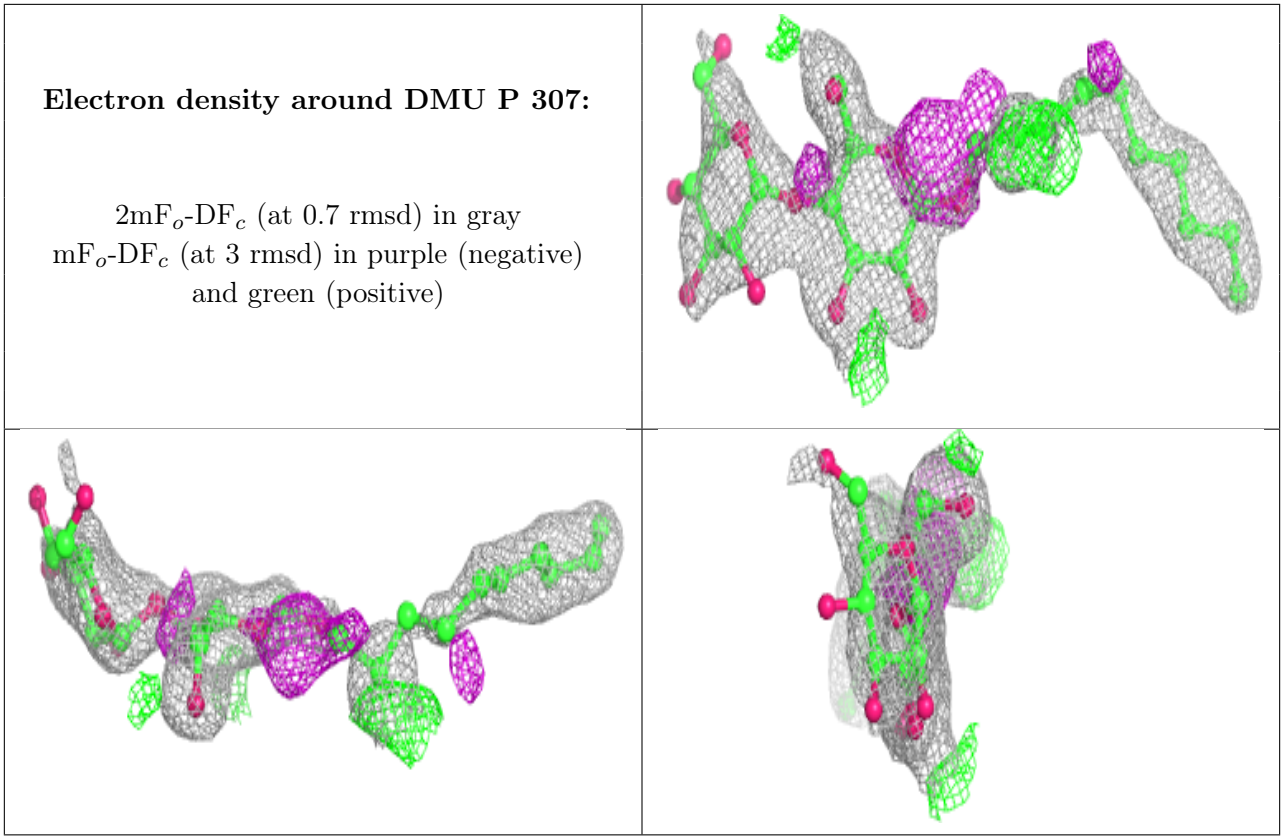
Electron density around CDL P 305:

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



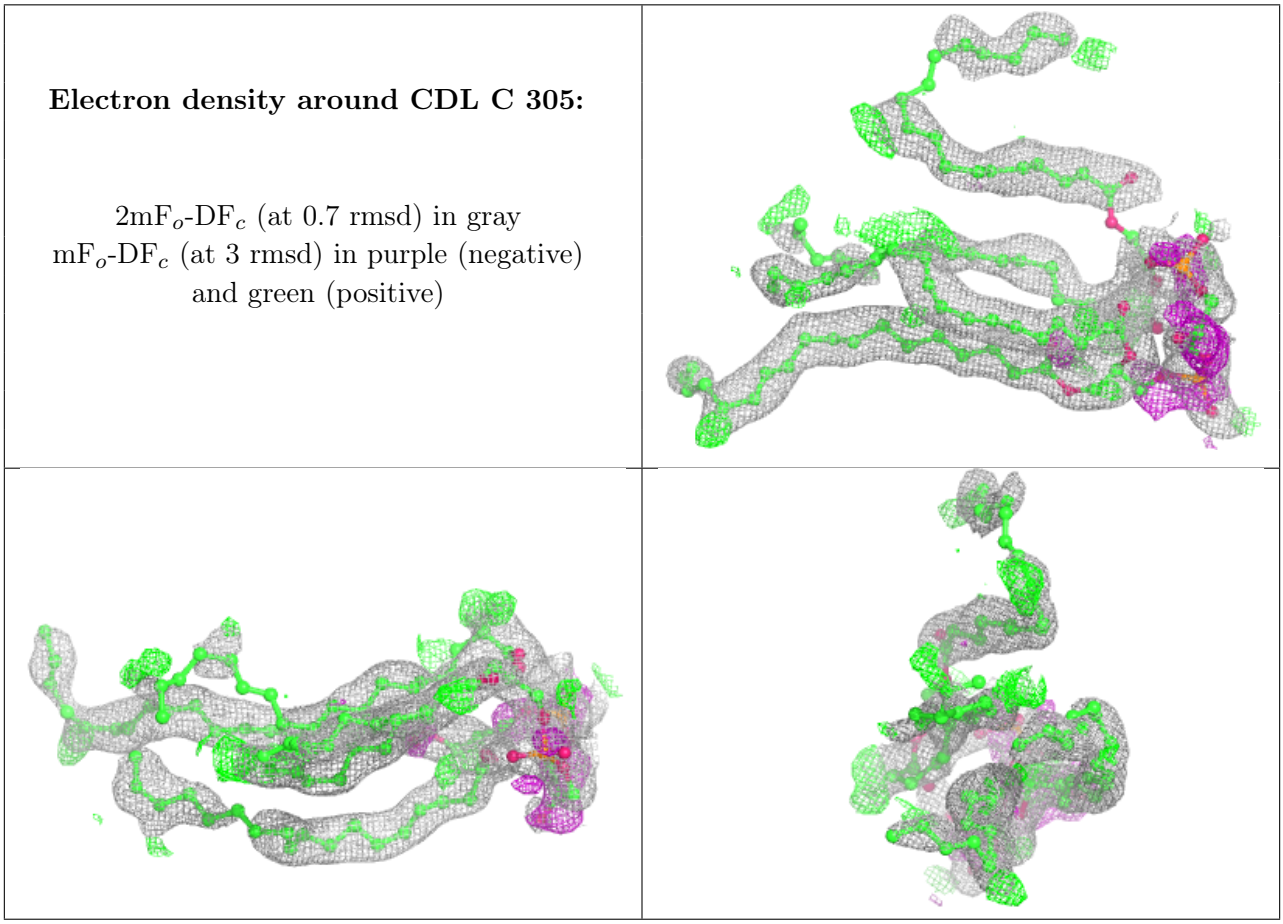
Electron density around DMU P 307:

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



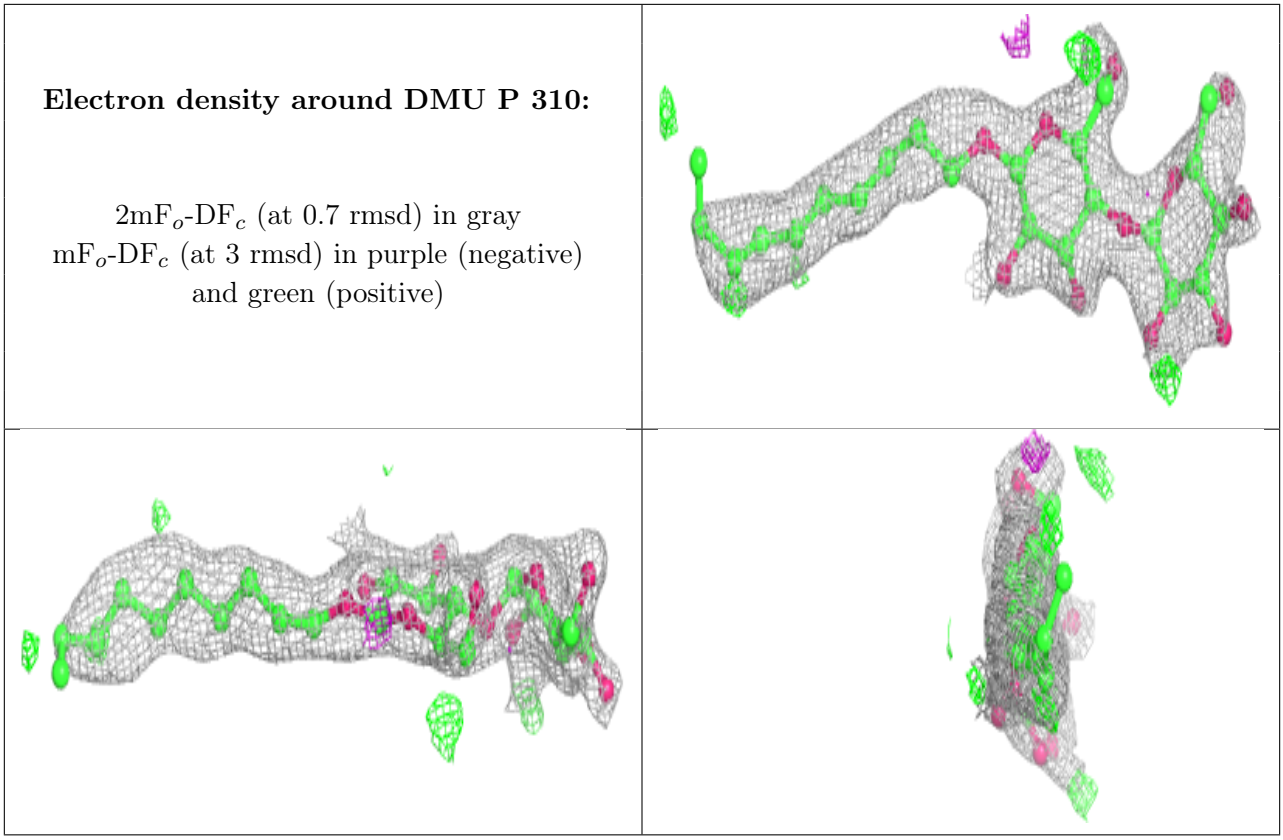
Electron density around CDL C 305:

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



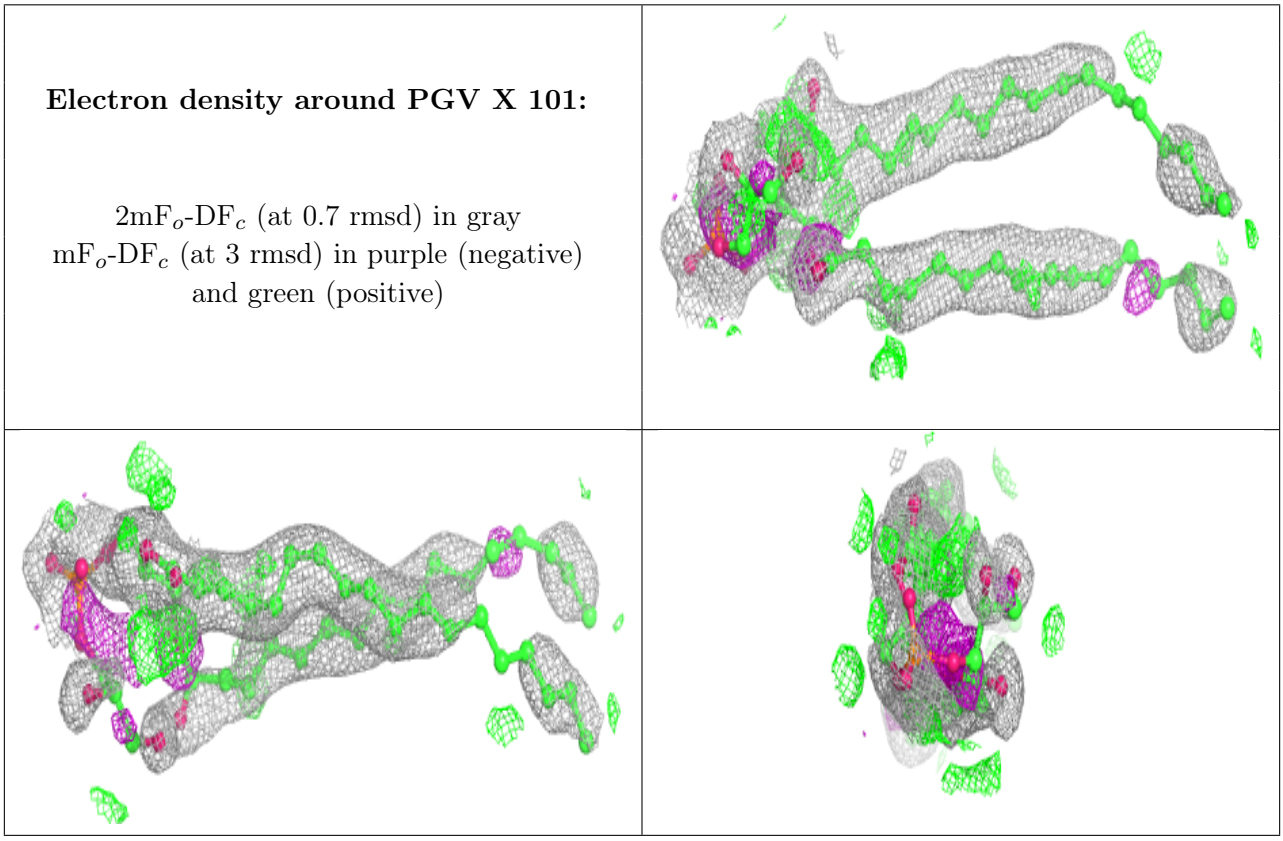
Electron density around DMU P 310:

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



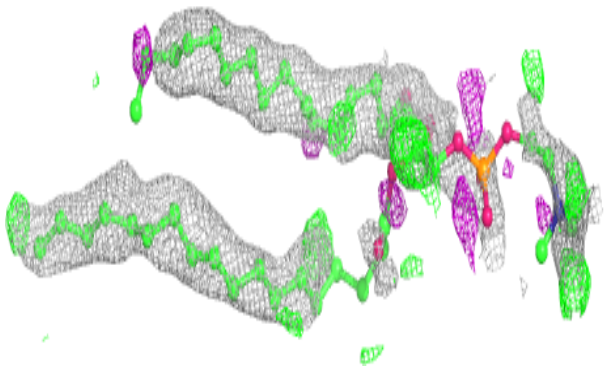
Electron density around PGV X 101:

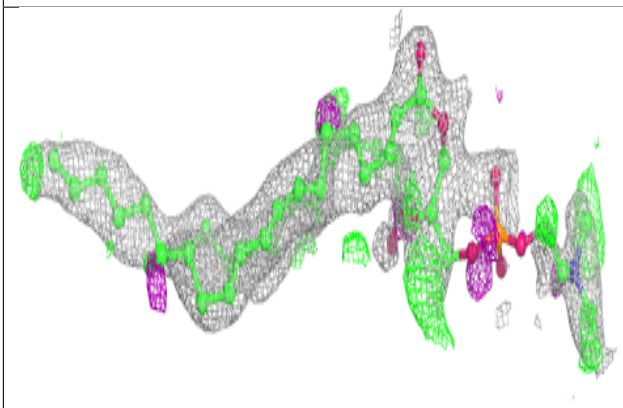
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

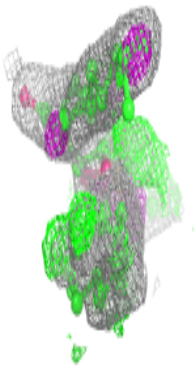


Electron density around PSC O 302:

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

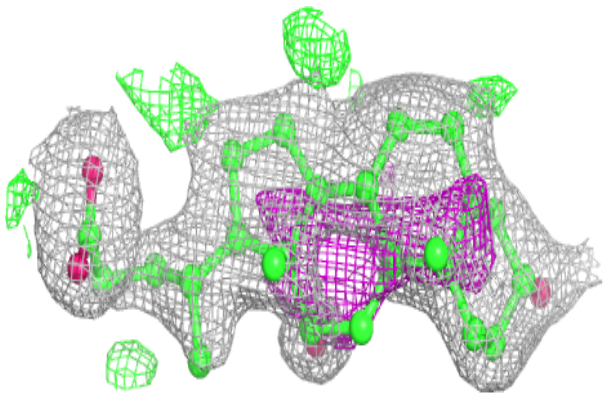


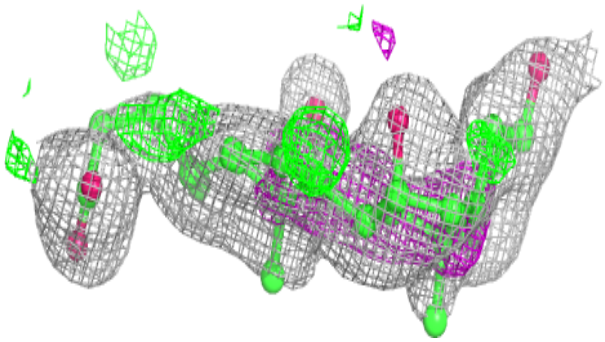


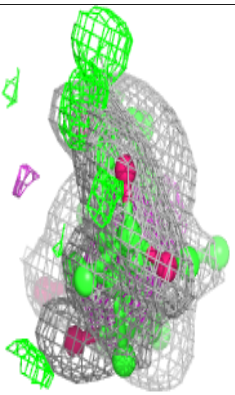


Electron density around CHD P 306:

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

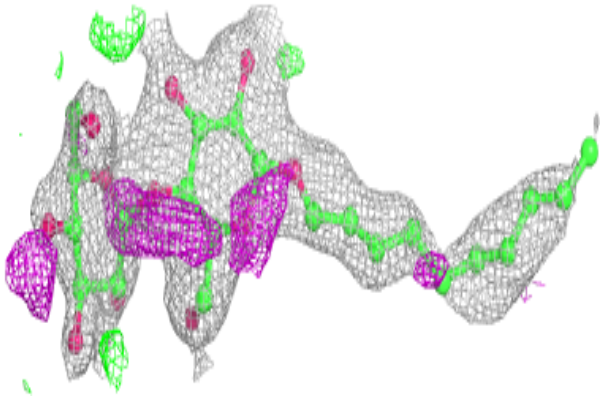


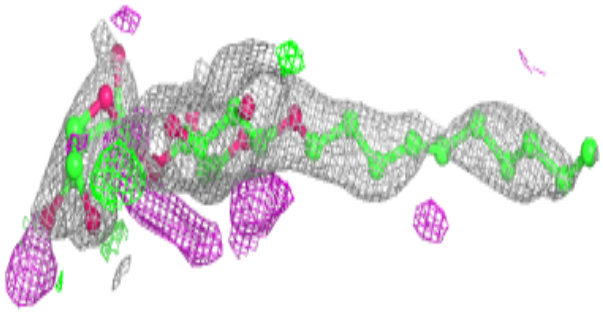


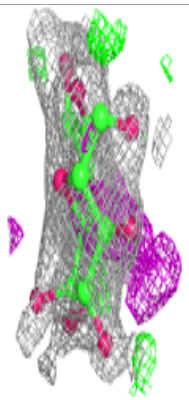


Electron density around DMU C 309:

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

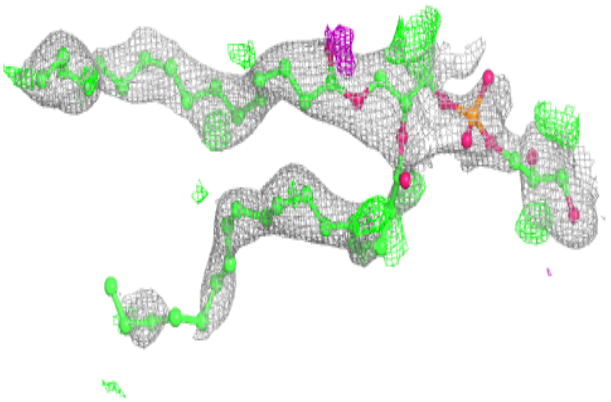


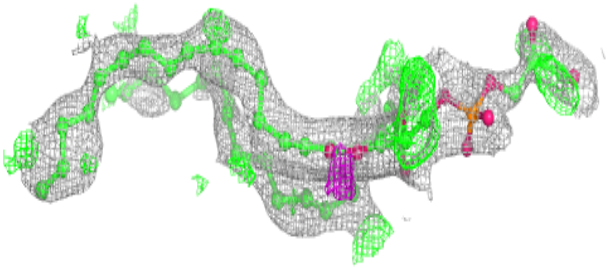


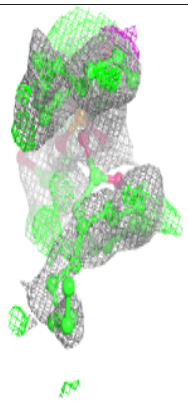


Electron density around PGV P 302:

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

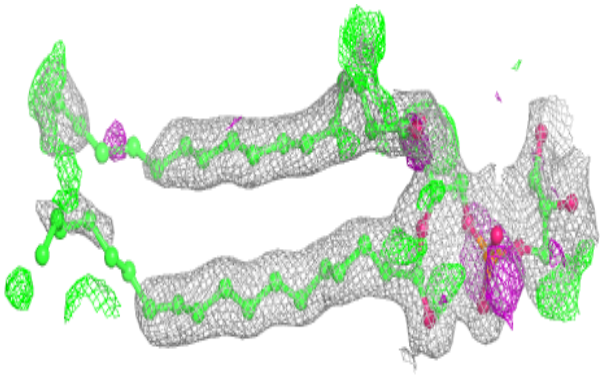


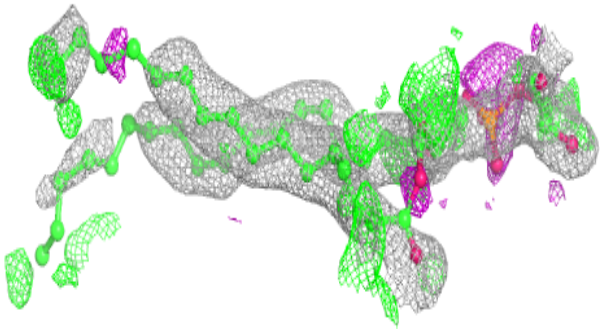


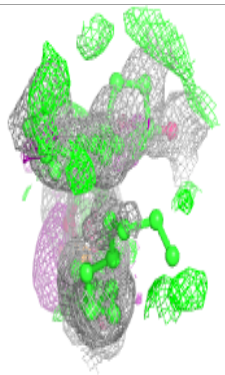


Electron density around PGV A 610:

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

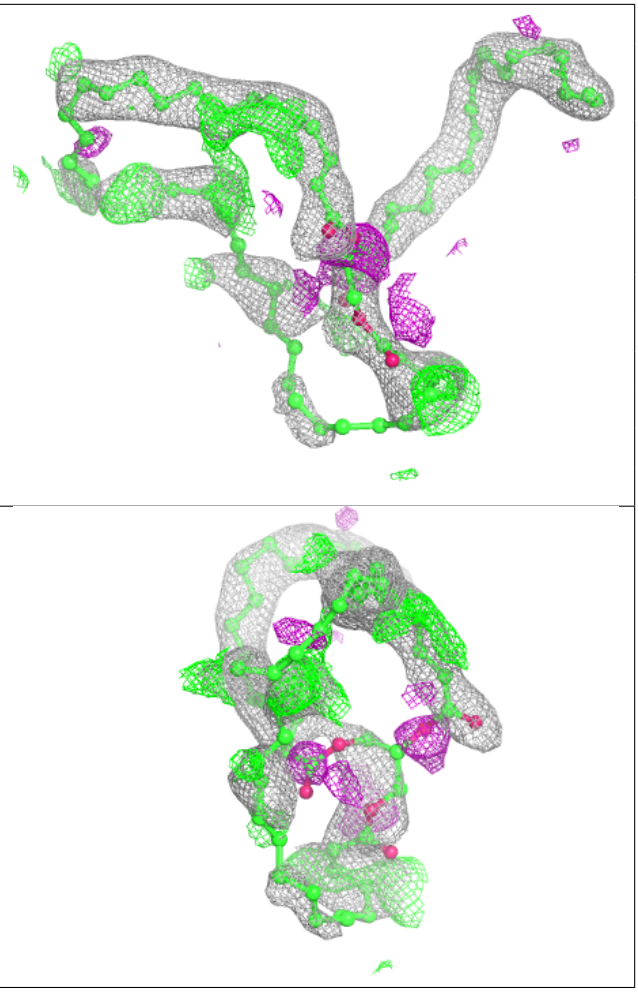






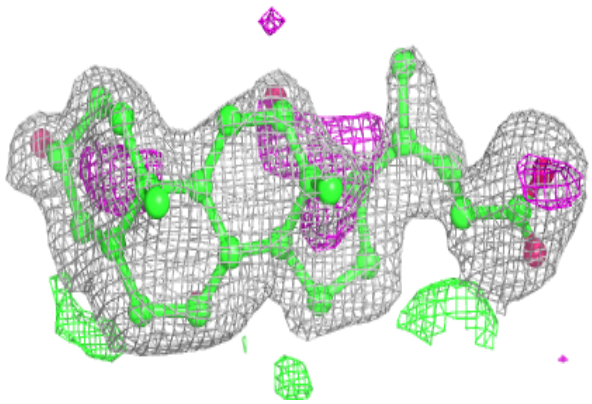
Electron density around TGL Y 101:

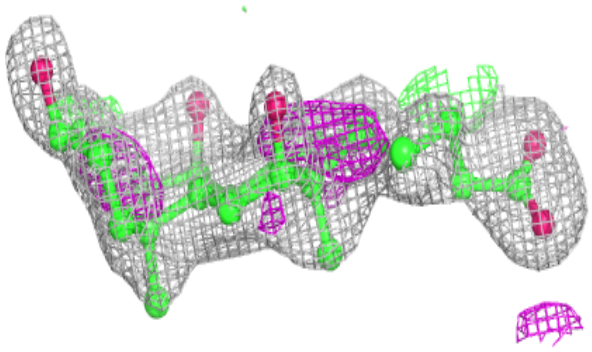
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

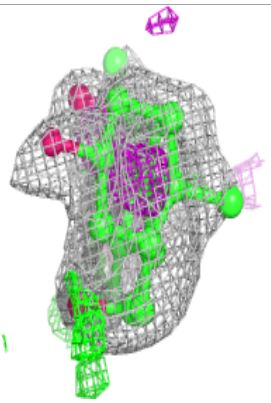


Electron density around CHD C 306:

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

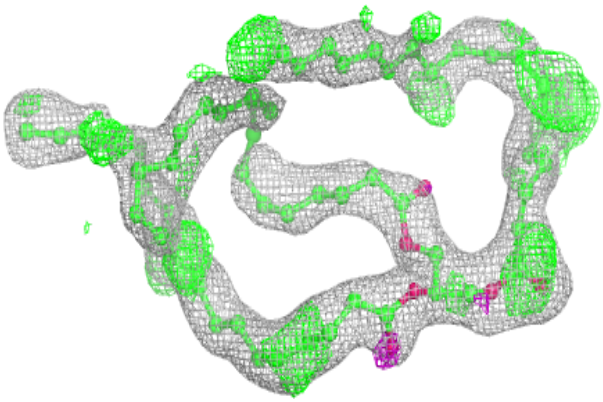


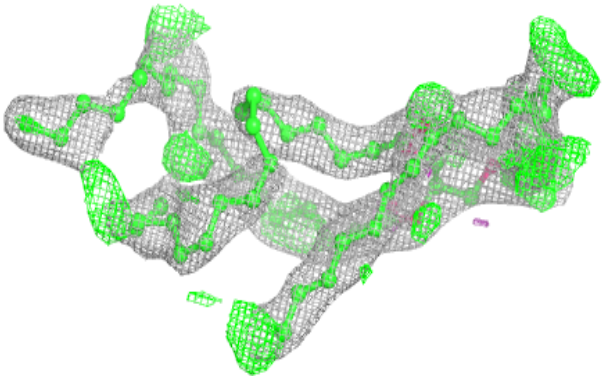


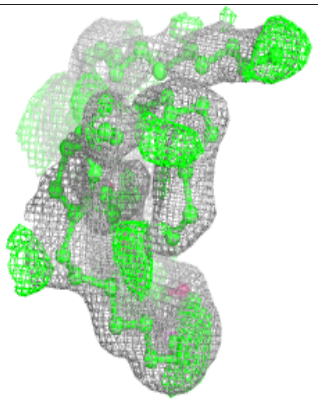


Electron density around TGL N 609:

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

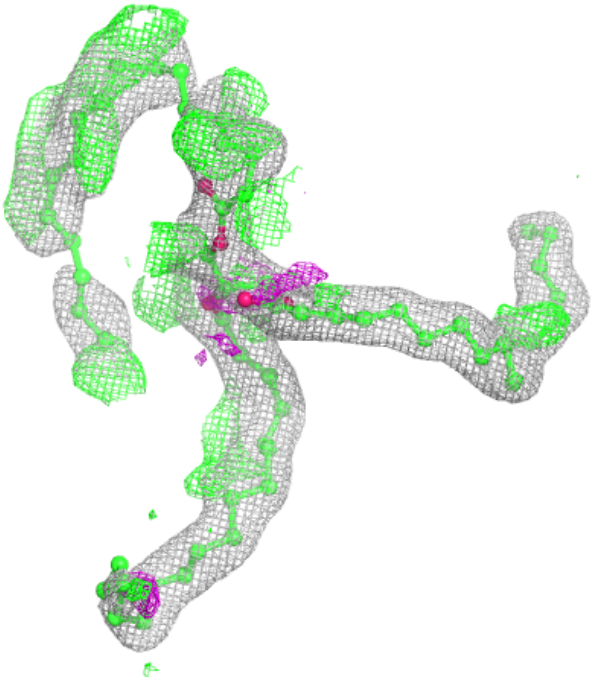


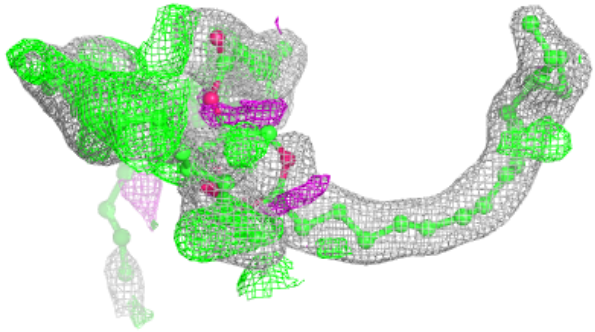


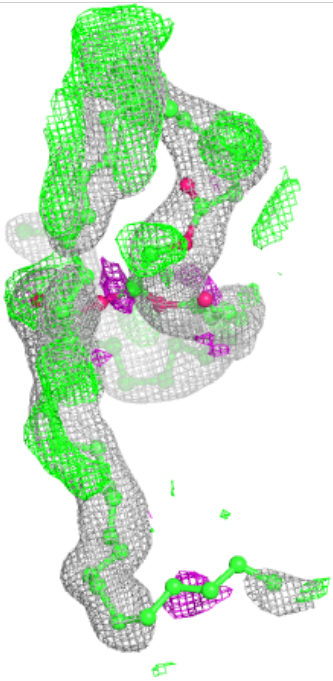


Electron density around TGL L 101:

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

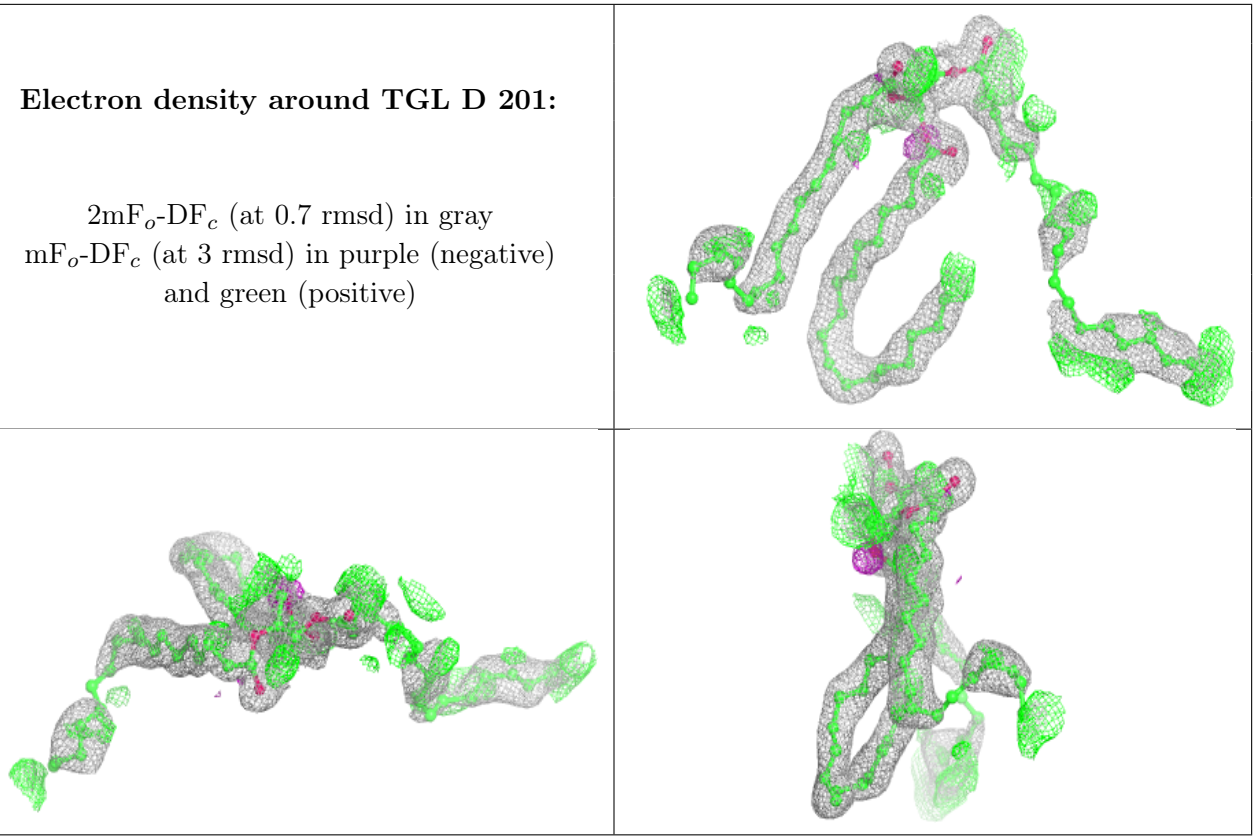






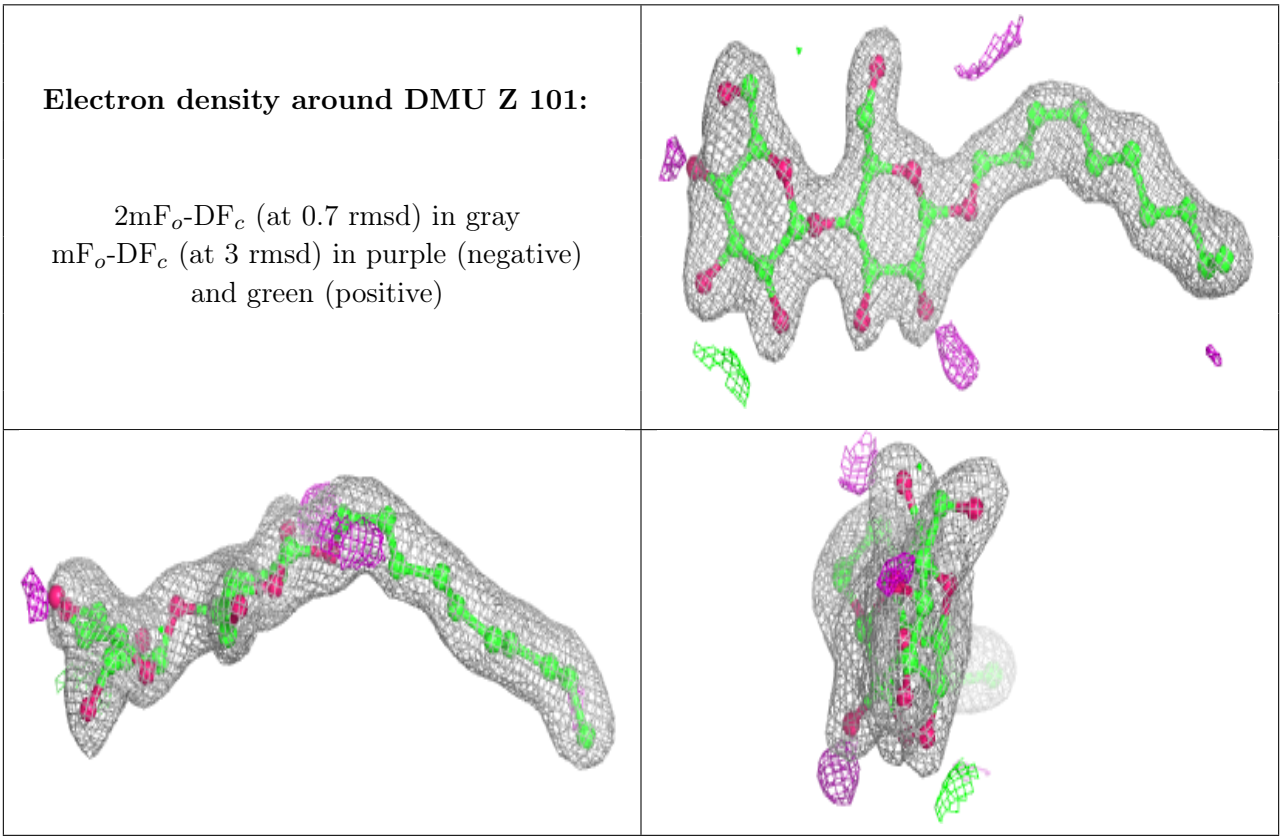
Electron density around TGL D 201:

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



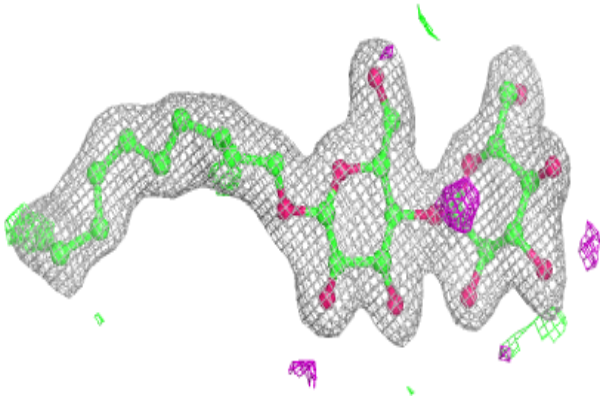
Electron density around DMU Z 101:

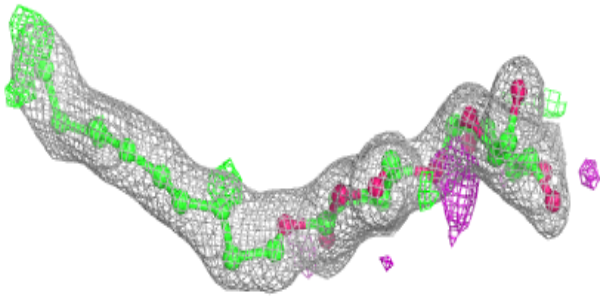
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

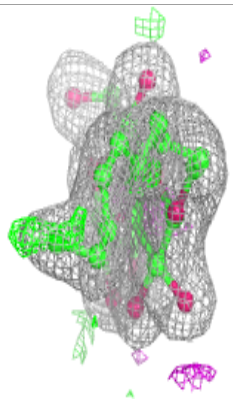


Electron density around DMU M 101:

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

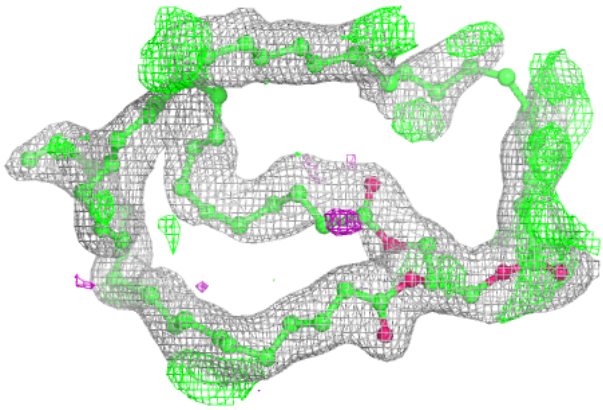


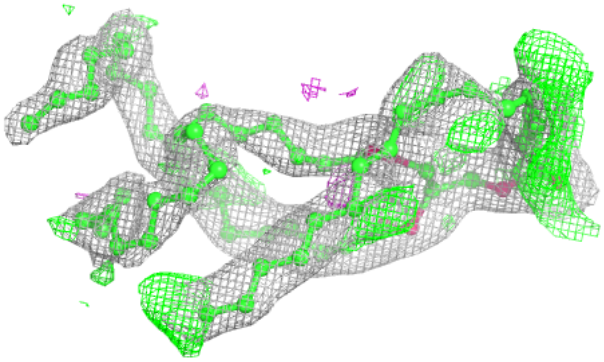


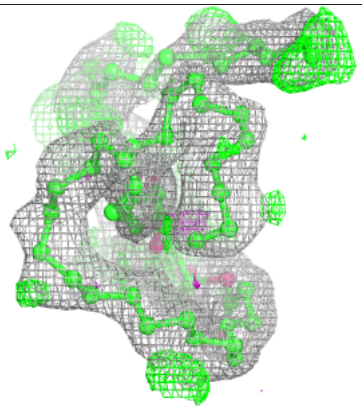


Electron density around TGL A 608:

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

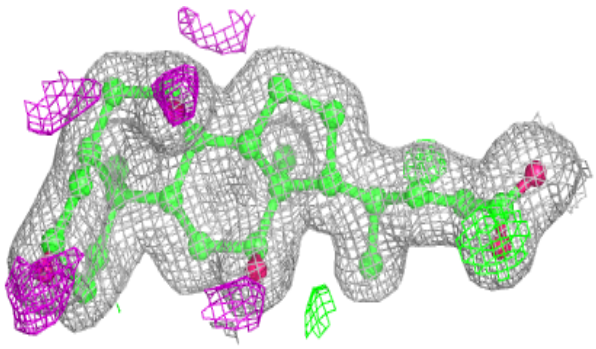


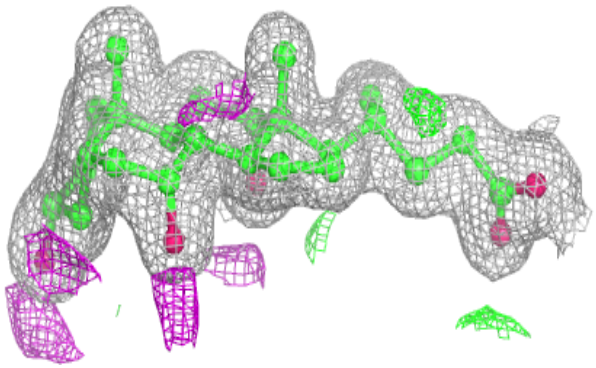


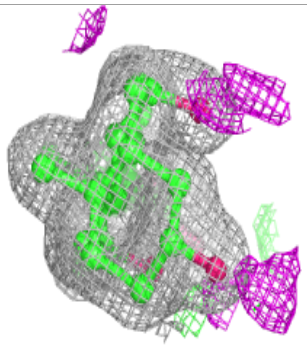


Electron density around CHD C 301:

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

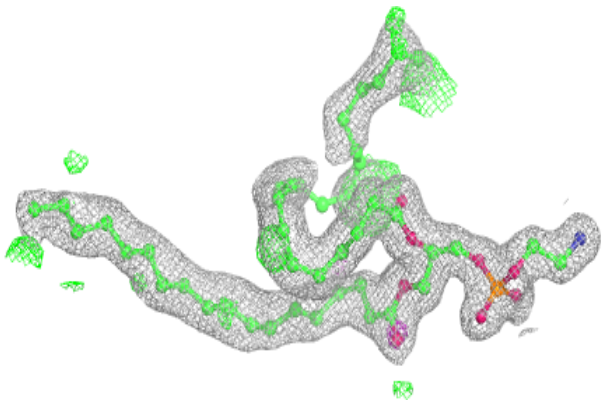


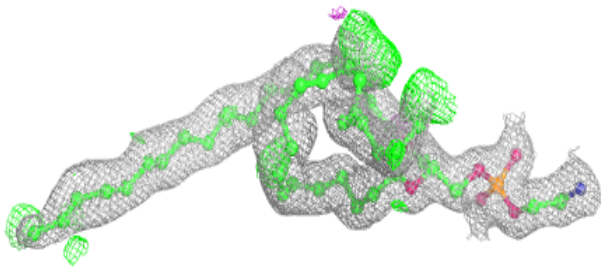


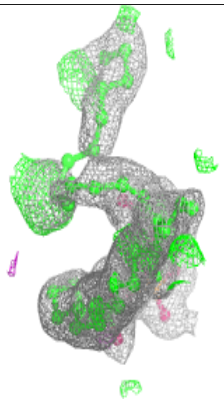


Electron density around PEK T 102:

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

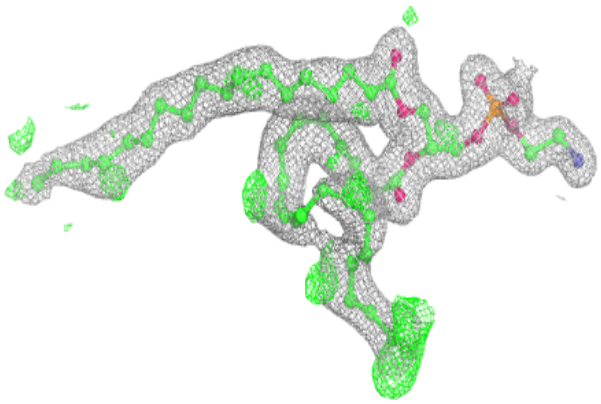


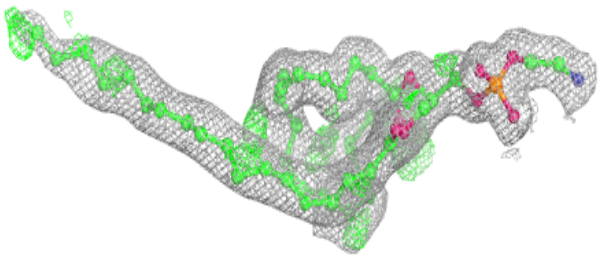


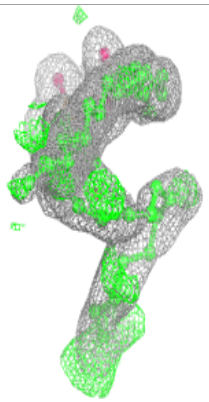


Electron density around PEK G 101:

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

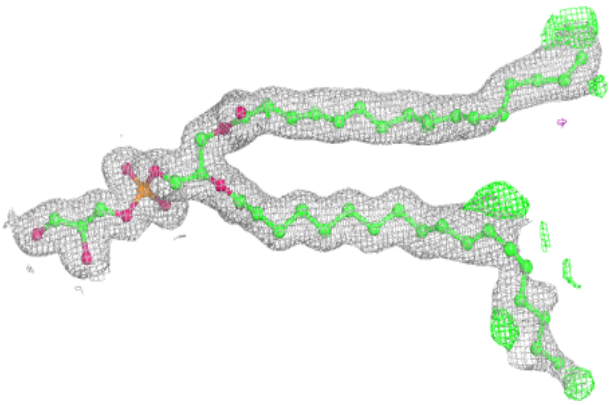


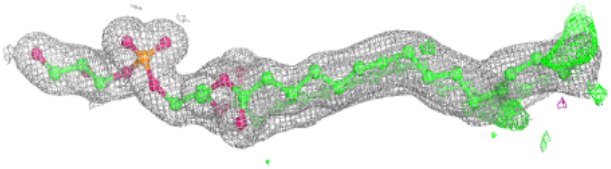


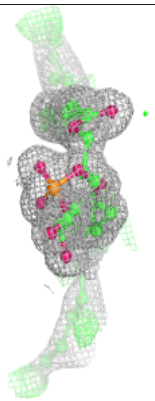


Electron density around PGV P 304:

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

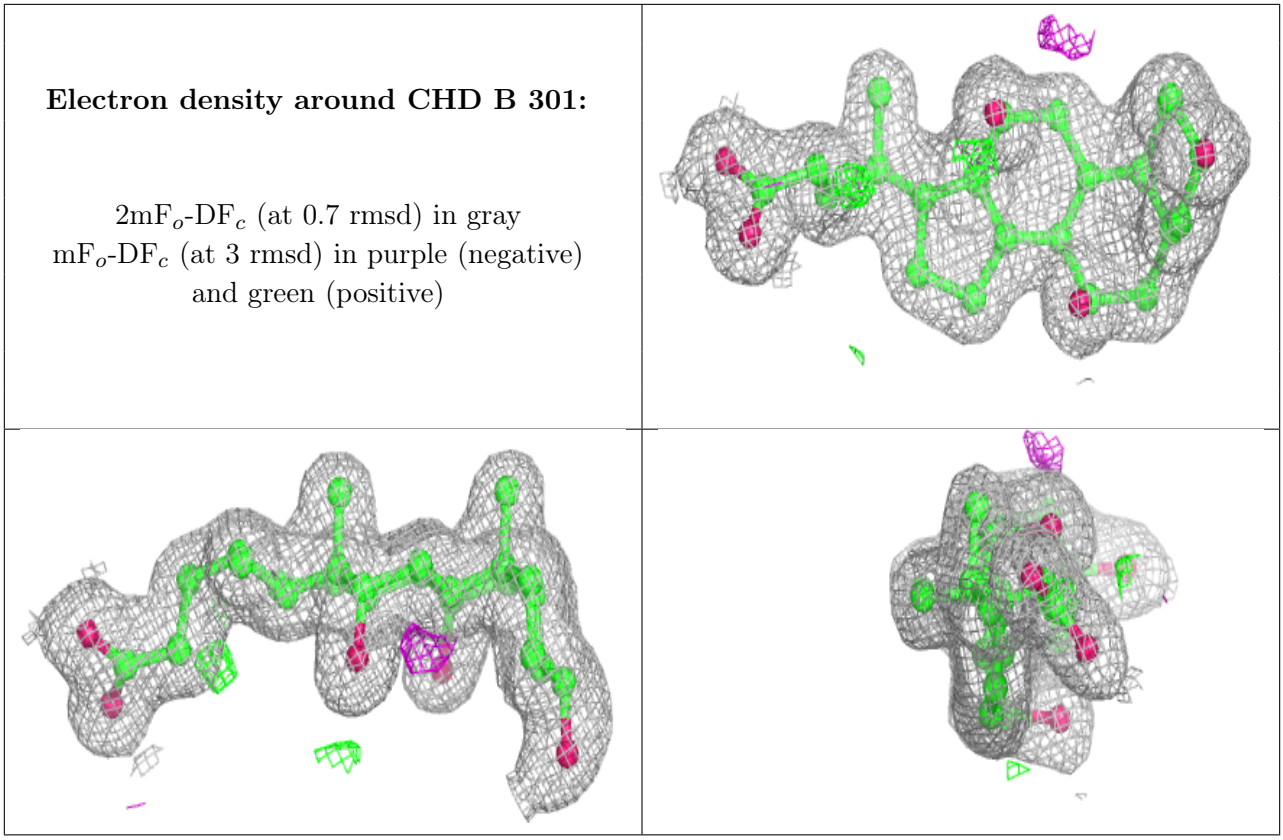






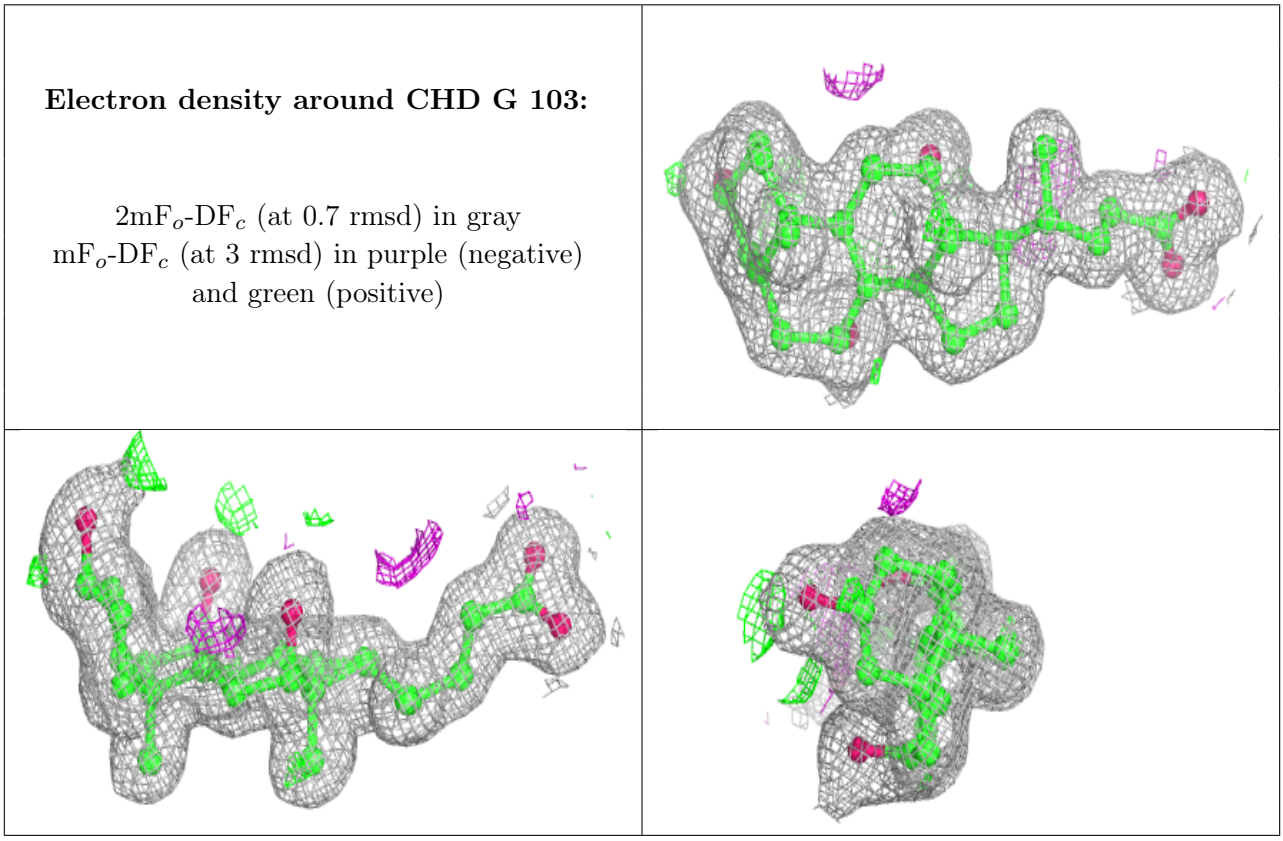
Electron density around CHD B 301:

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



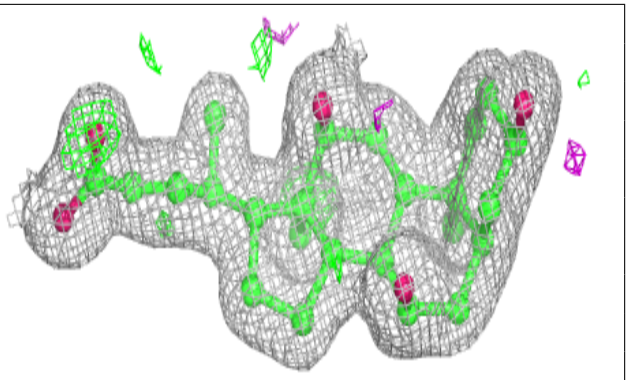
Electron density around CHD G 103:

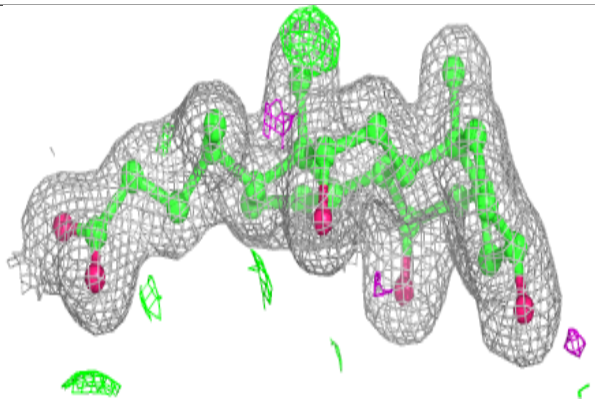
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

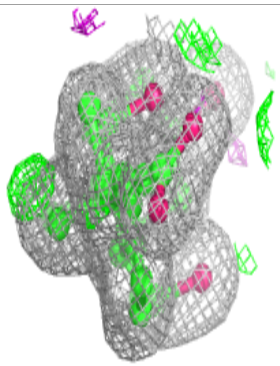


Electron density around CHD P 301:

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

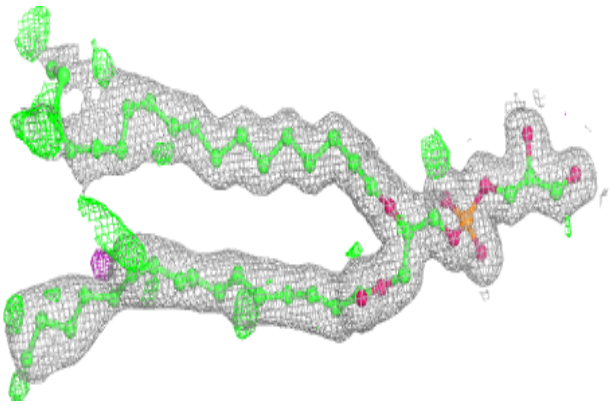


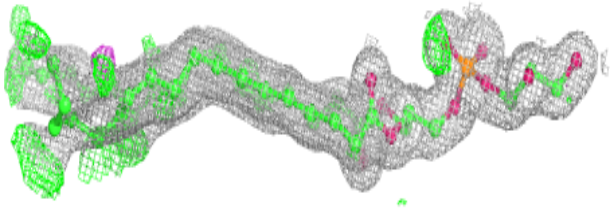


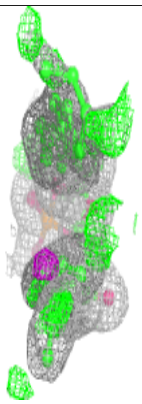


Electron density around PGV C 304:

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

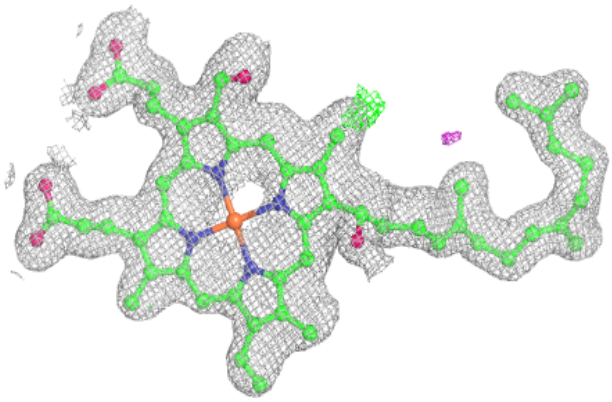


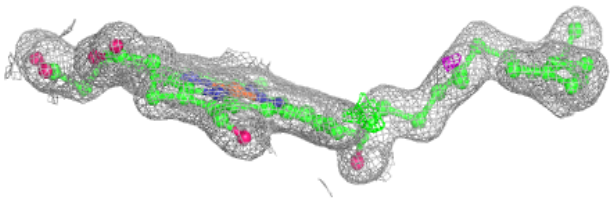


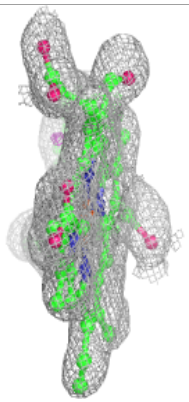


Electron density around HEA N 602 (A):

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

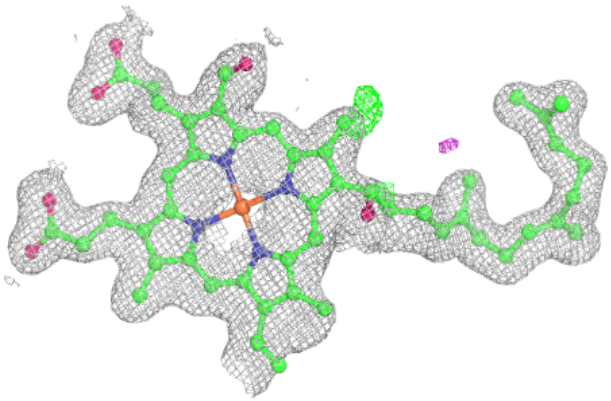


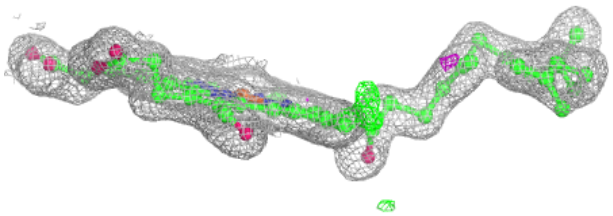


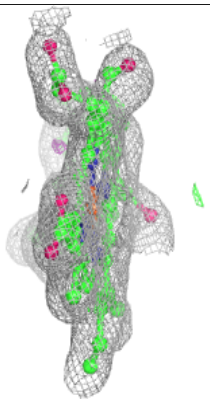


Electron density around HEA N 602 (B):

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

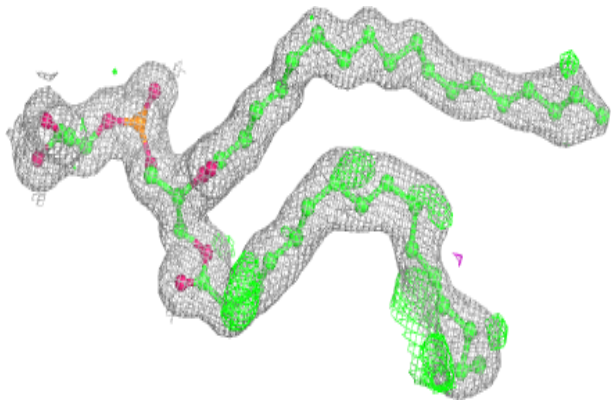


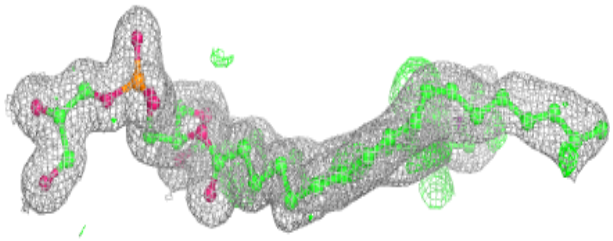


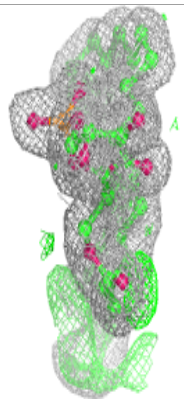


Electron density around PGV A 609:

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

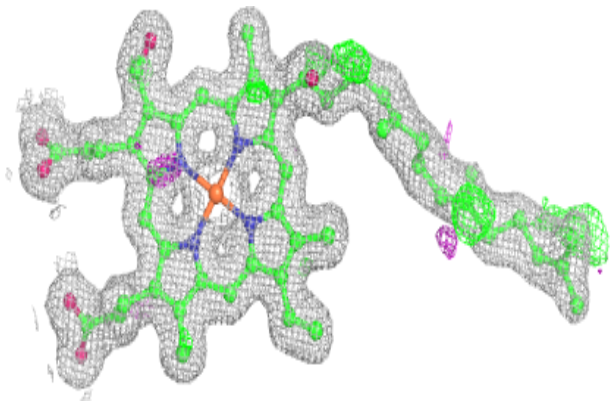


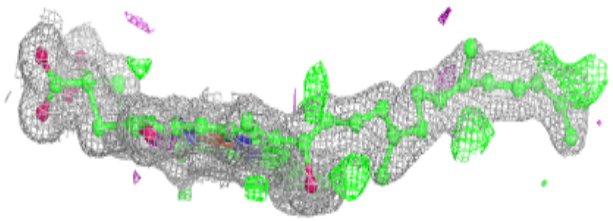


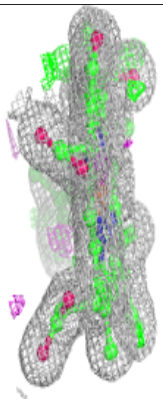


Electron density around HEA A 601:

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

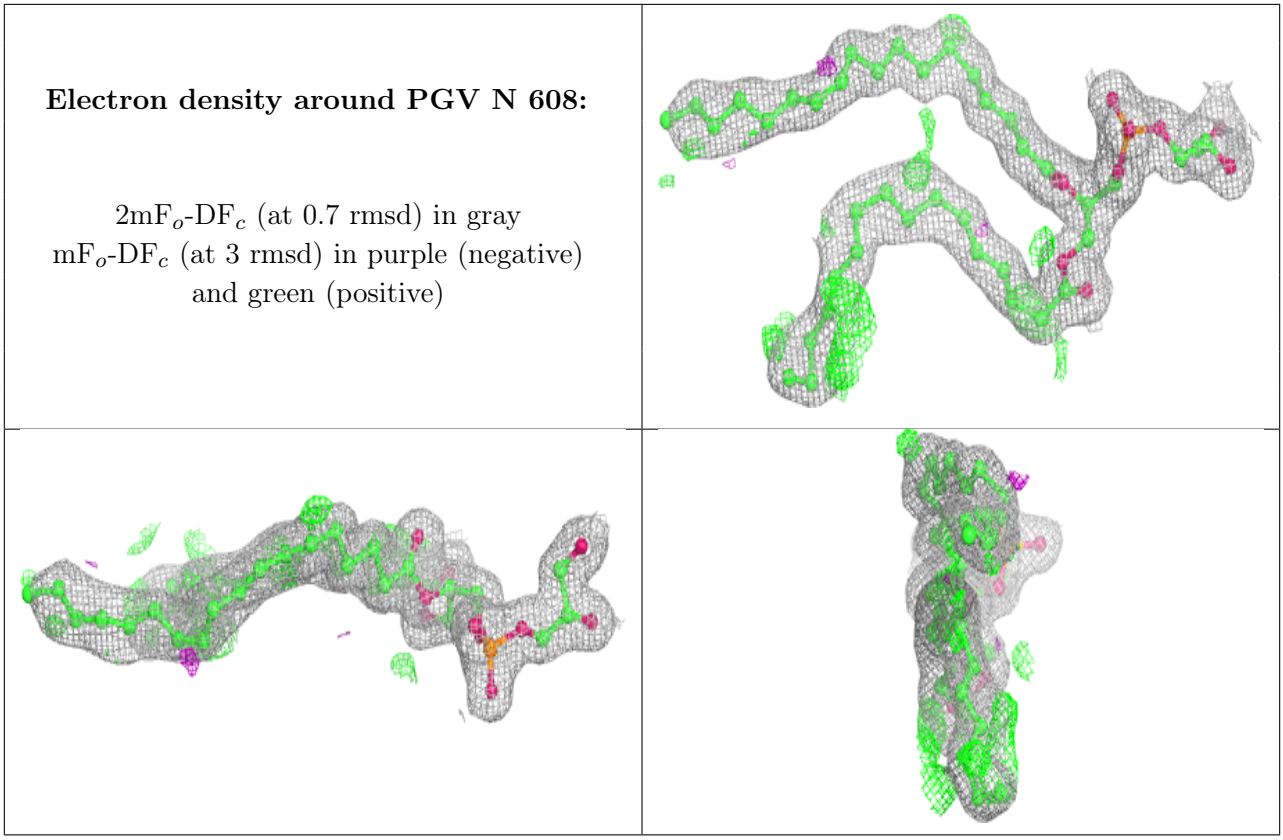






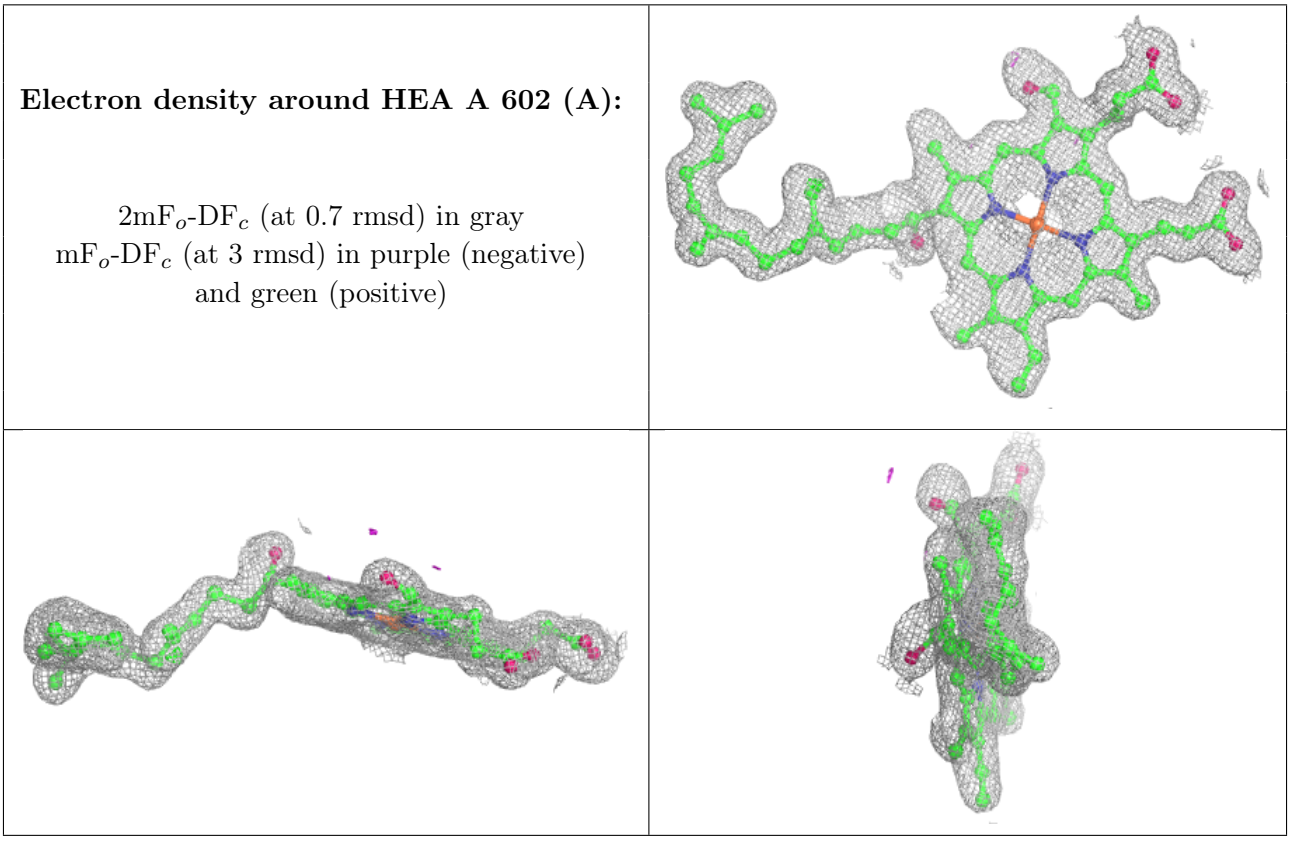
Electron density around PGV N 608:

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



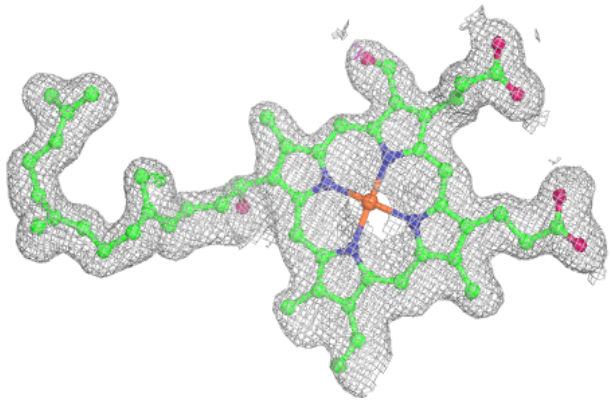
Electron density around HEA A 602 (A):

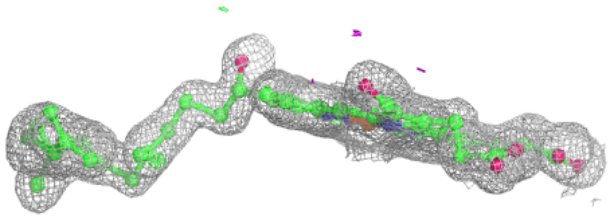
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

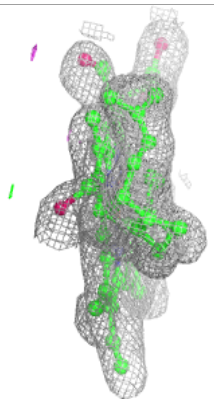


Electron density around HEA A 602 (B):

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

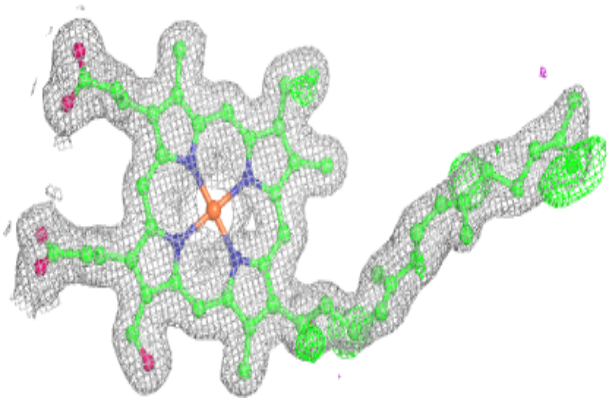


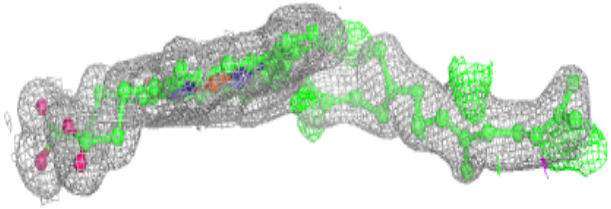


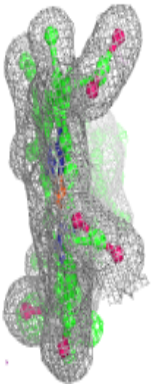


Electron density around HEA N 601:

$2mF_o$-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.