wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 02:58 PM JST

PDB ID	:	5Z84 / pdb_00005z84
Title	:	The structure of azide-bound cytochrome c oxidase determined using the crystals exposed to 20 mM azide solution for 4 days
Authors	:	Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on	:	2018-01-31
Resolution	:	1.85 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:

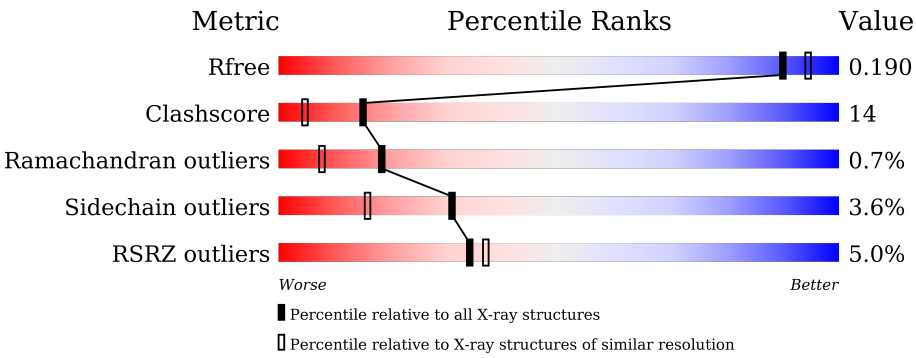
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	.% 72% 24% • •
1	N	514	.% 77% 20% •
2	B	227	7% 69% 24% 7%
2	O	227	5% 75% 22% •
3	C	261	.% 73% 25% • •
3	P	261	2% 73% 25% • •

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Mol	Chain	Length	Quality of chain
4	D	147	3% 72% 22%
4	Q	147	5% 79% 16%
5	E	109	3% 72% 24%
5	R	109	2% 80% 13%
6	F	98	7% 67% 29%
6	S	98	10% 76% 14% 6%
7	G	85	22% 61% 21% 12% 5%
7	T	85	22% 59% 28% 8%
8	H	85	8% 69% 20% 7%
8	U	85	12% 74% 16% 7%
9	I	73	15% 74% 23%
9	V	73	11% 73% 25%
10	J	59	8% 78% 20%
10	W	59	8% 78% 20%
11	K	56	5% 71% 16% 12%
11	X	56	7% 70% 16% 12%
12	L	47	4% 79% 15%
12	Y	47	4% 79% 13%
13	M	46	7% 70% 22% 7%
13	Z	46	4% 72% 17% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	606	-	-	X	-
18	AZI	A	607	-	-	X	-
18	AZI	N	608	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	TGL	D	201	-	-	X	-
21	EDO	A	615	-	X	X	-
21	EDO	A	621	-	-	X	-
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	-
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	N	622	-	-	X	-
24	PSC	B	303	-	-	X	-
28	CDL	C	306	-	-	X	-
28	CDL	P	304	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33735 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	1904	1239	292	353	20	0	10	0
2	O	227	1859	1206	287	346	20	0	4	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	2185	1457	349	363	16	0	9	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	1231	800	205	222	4	0	4	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	778	481	139	152	6	0	4	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	675	431	129	113	1	1	0	0	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 11, 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.

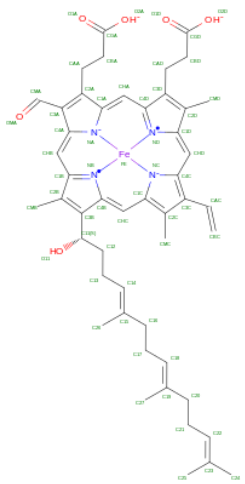
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	385	258	64	60	3	0	1	0
			Total	C	N	O	S			
12	Y	46	388	259	65	61	3	0	1	0

- 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 (CCD ID: 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 (CCD ID: 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

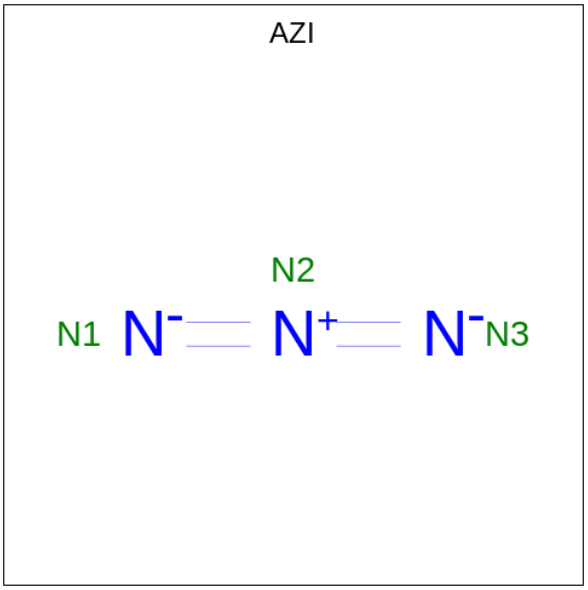
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: NA) (formula: Na).

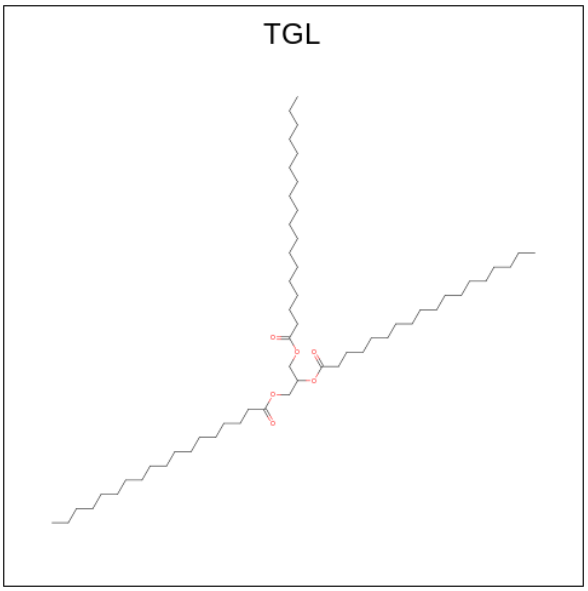
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

- Molecule 18 is AZIDE ION (CCD ID: AZI) (formula: N_3).



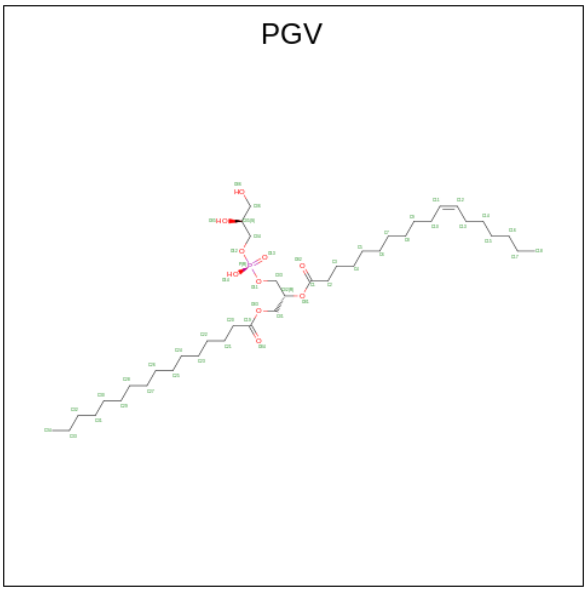
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
18	A	1	3	3	0	0
			Total	N		
18	A	1	3	3	0	0
			Total	N		
18	N	1	3	3	0	0
			Total	N		
18	N	1	3	3	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



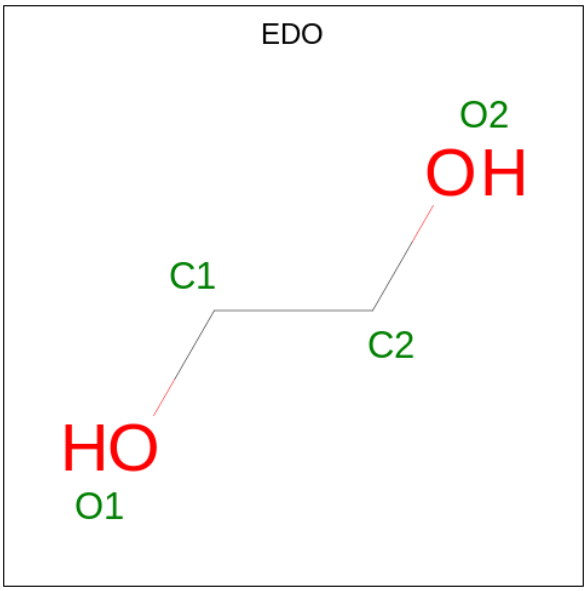
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: 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	G	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	Z	1	51	40	10	1	0	0

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

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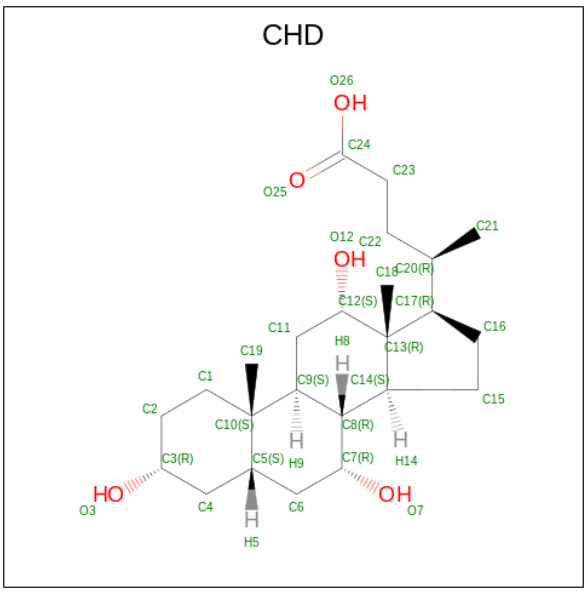
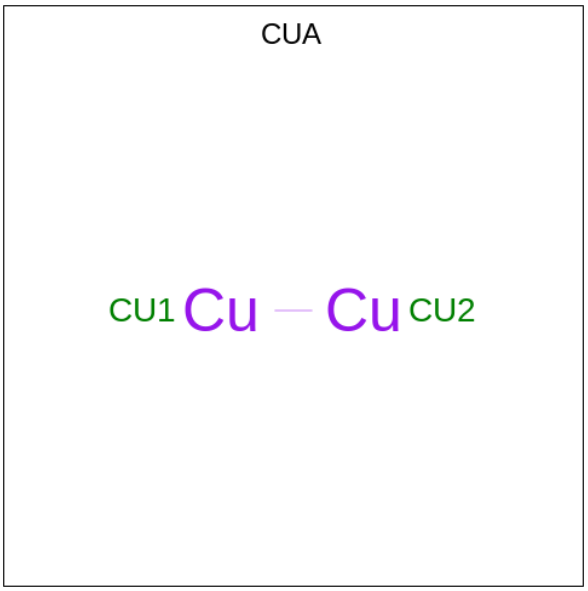
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	N	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	R	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	T	1	4	2	2	0	0
21	U	1	4	2	2	0	0
21	V	1	4	2	2	0	0

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



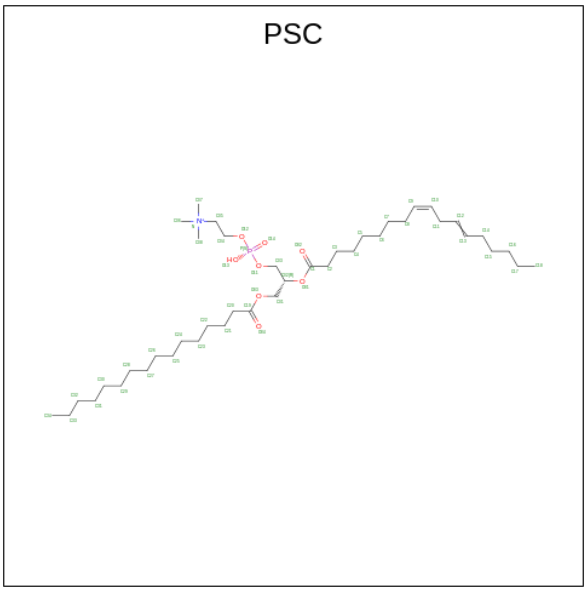
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
22	B	1	29	24	5	0	0
			Total	C	O		
22	C	1	29	24	5	0	0
			Total	C	O		
22	C	1	29	24	5	0	0
			Total	C	O		
22	G	1	29	24	5	0	0
			Total	C	O		
22	J	1	29	24	5	0	0
			Total	C	O		
22	P	1	29	24	5	0	0
			Total	C	O		
22	P	1	29	24	5	0	0
			Total	C	O		
22	W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

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: 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 (CCD ID: 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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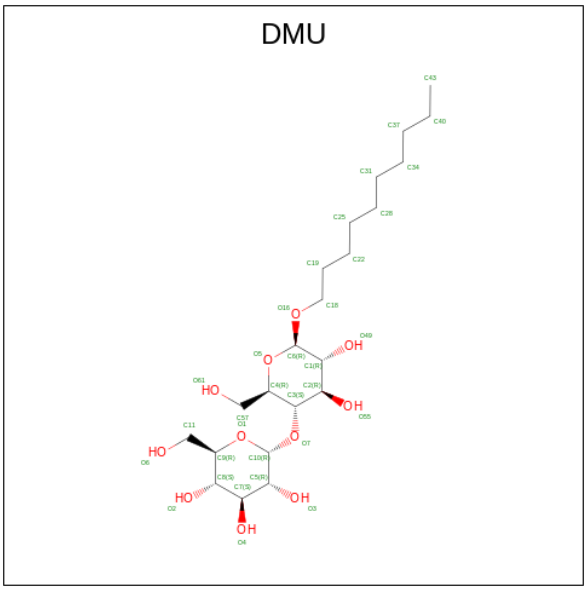
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	O	1	52	42	1	8	1	0	0

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

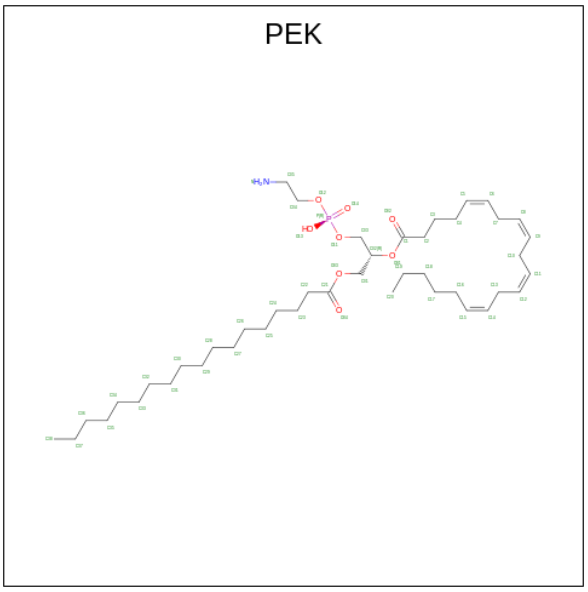


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	L	1	33	22	11	0	0
			Total	C	O		
25	M	1	33	22	11	0	0
			Total	C	O		
25	P	1	33	22	11	0	0
			Total	C	O		
25	P	1	33	22	11	0	0
			Total	C	O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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

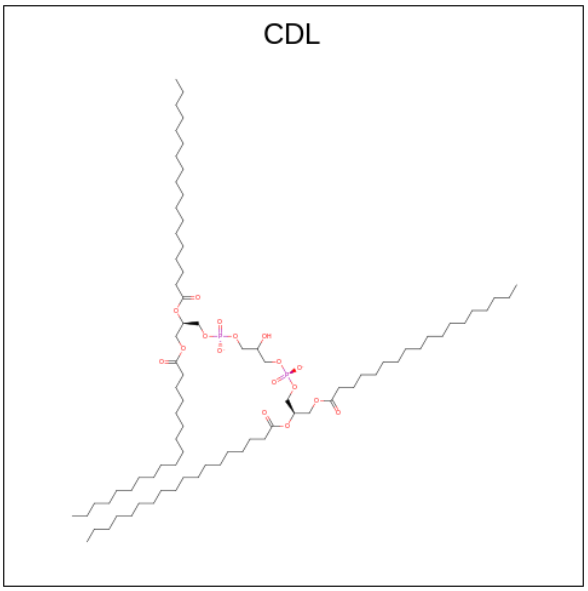
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
26	C	1	1	1	0	0
			Total	X		
26	P	1	1	1	0	0

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 28 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	232	Total	O	0	1
			233	233		
30	B	139	Total	O	0	1
			140	140		
30	C	101	Total	O	0	0
			101	101		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	D	110	Total O 110 110	0	0
30	E	85	Total O 85 85	0	0
30	F	78	Total O 78 78	0	0
30	G	51	Total O 51 51	0	0
30	H	45	Total O 45 45	0	0
30	I	25	Total O 25 25	0	0
30	J	28	Total O 28 28	0	0
30	K	21	Total O 21 21	0	0
30	L	29	Total O 29 29	0	0
30	M	27	Total O 27 27	0	0
30	N	218	Total O 219 219	0	1
30	O	114	Total O 115 115	0	1
30	P	90	Total O 90 90	0	0
30	Q	36	Total O 36 36	0	0
30	R	39	Total O 39 39	0	0
30	S	55	Total O 55 55	0	0
30	T	39	Total O 39 39	0	0
30	U	33	Total O 33 33	0	0
30	V	14	Total O 14 14	0	0
30	W	11	Total O 11 11	0	0
30	X	11	Total O 11 11	0	0

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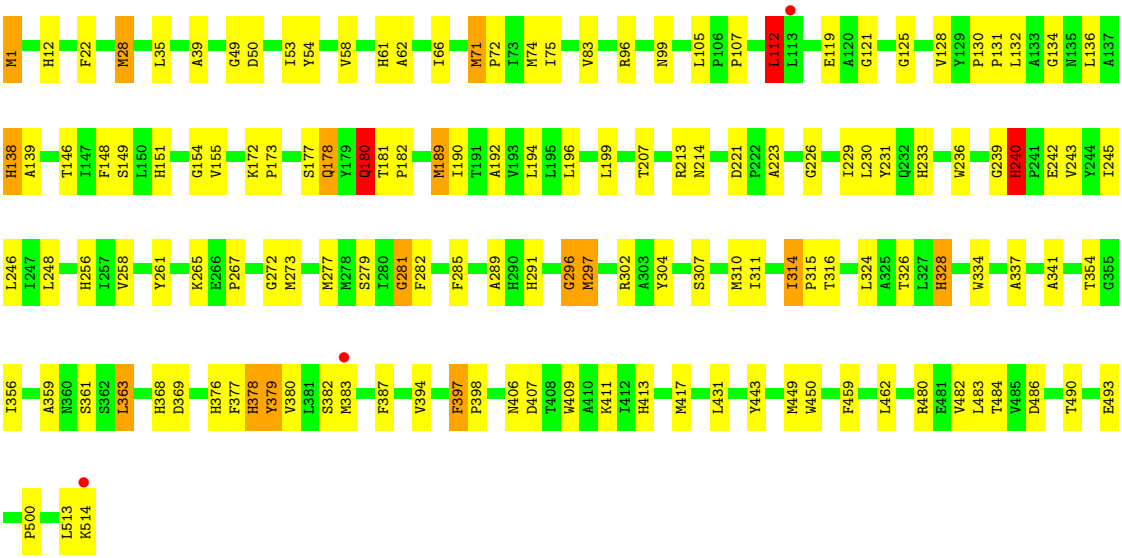
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	Y	14	14	14	0	0
			Total	O		
30	Z	16	16	16	0	0

3 Residue-property plots (i)

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

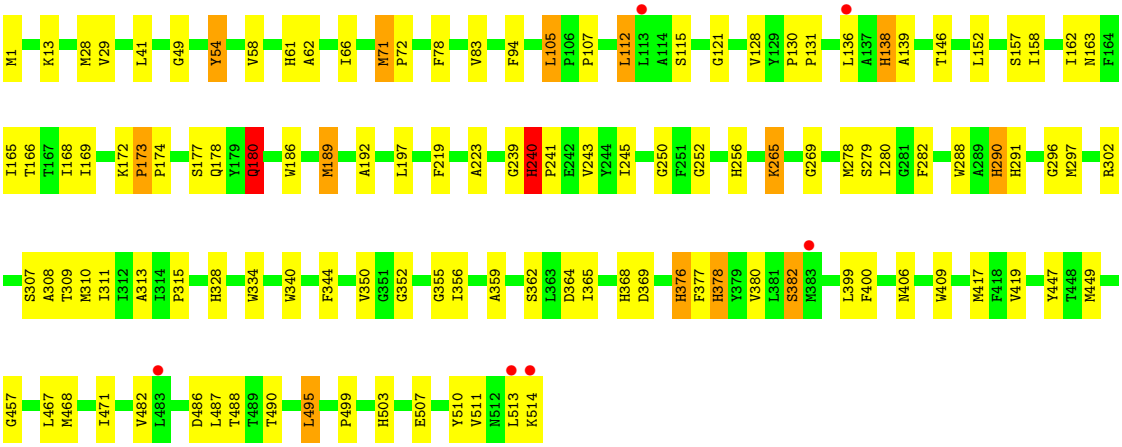
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



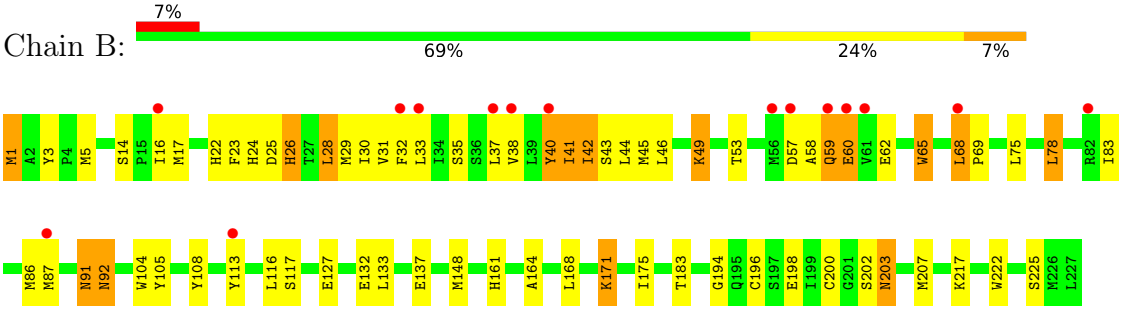
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



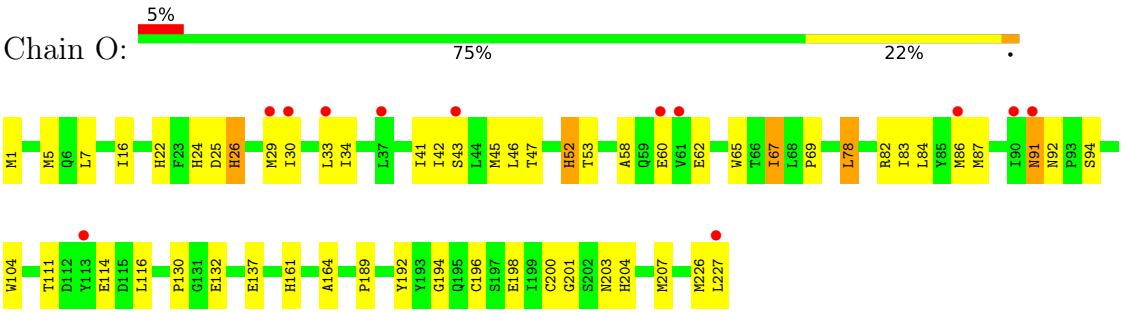
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



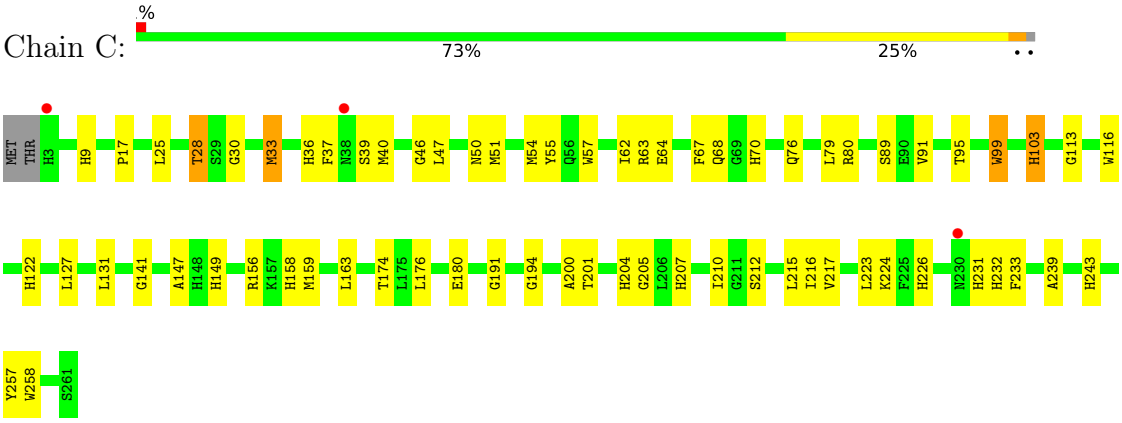
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



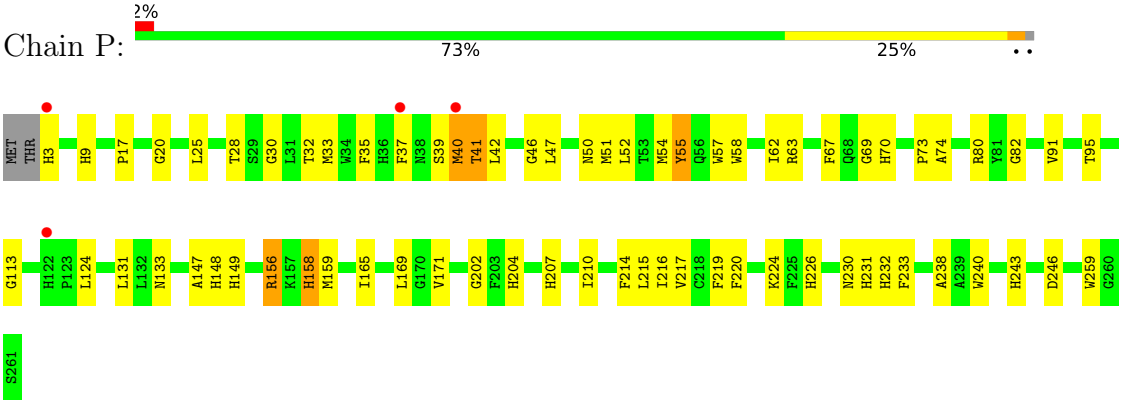
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



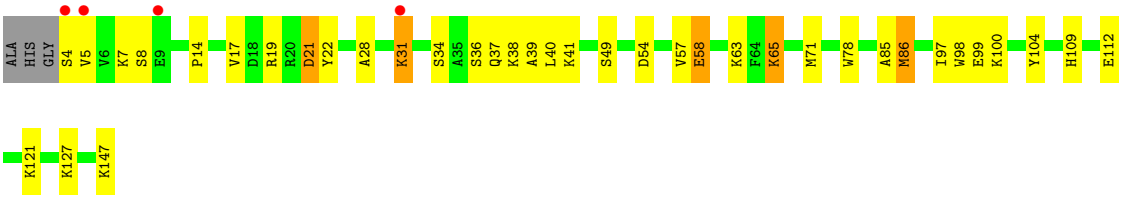
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



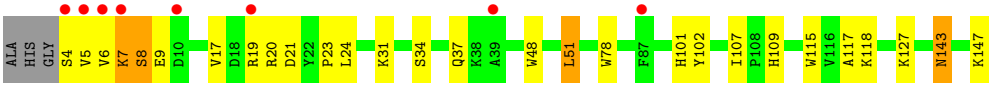
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



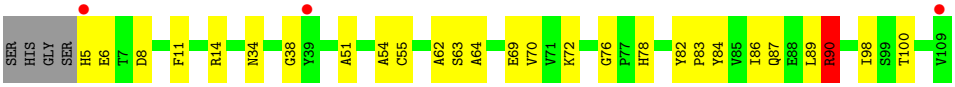
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



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

Chain E:

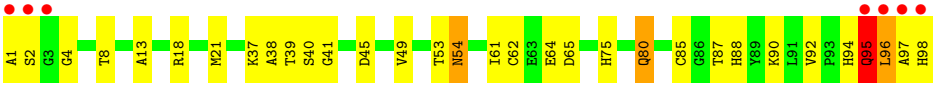


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:

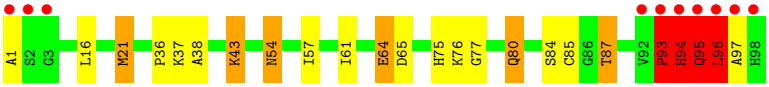
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



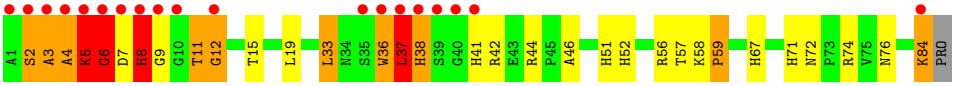
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



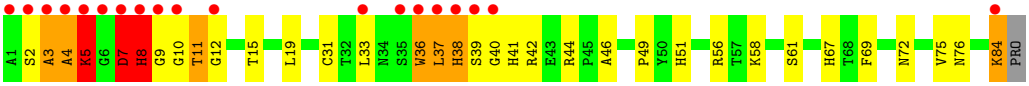
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



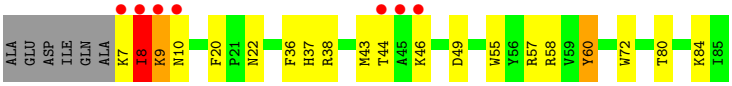
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



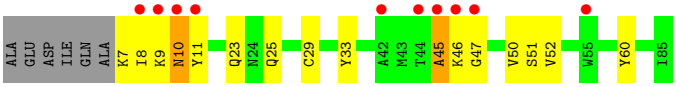
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



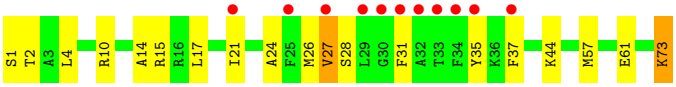
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



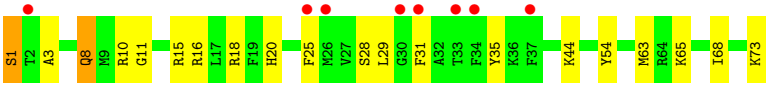
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



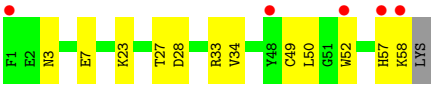
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



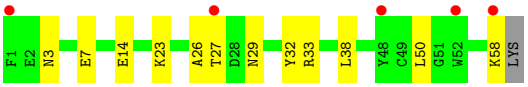
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



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

Chain W:

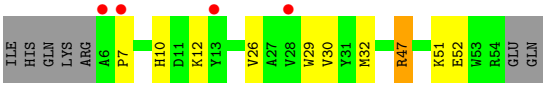


• Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:

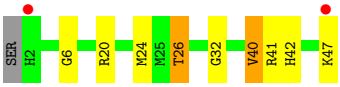
• Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



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

Chain L:

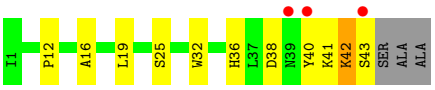


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:

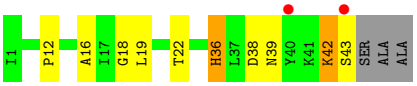
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:


I1
P12
A16
I17
G18
L19
T22
H36
L37
D38
N39
Y40
K41
K42
S43
SER
ALA
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.4 (40.00-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.163 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	28371 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: MG, CDL, PEK, EDO, DMU, CUA, FME, TGL, HEA, CU, ZN, AZI, UNX, TPO, PSC, SAC, PGV, CHD, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.96	84/4322 (1.9%)	1.48	26/5897 (0.4%)
1	N	1.88	63/4308 (1.5%)	1.41	20/5878 (0.3%)
2	B	1.79	28/1945 (1.4%)	1.46	20/2649 (0.8%)
2	O	1.53	12/1896 (0.6%)	1.27	3/2581 (0.1%)
3	C	1.84	38/2272 (1.7%)	1.29	5/3102 (0.2%)
3	P	1.89	42/2272 (1.8%)	1.35	7/3102 (0.2%)
4	D	1.72	14/1265 (1.1%)	1.39	7/1704 (0.4%)
4	Q	1.34	3/1259 (0.2%)	1.17	6/1698 (0.4%)
5	E	1.83	14/871 (1.6%)	1.36	5/1182 (0.4%)
5	R	1.60	5/871 (0.6%)	1.29	4/1182 (0.3%)
6	F	1.65	6/795 (0.8%)	1.46	7/1079 (0.6%)
6	S	1.66	2/780 (0.3%)	1.45	5/1058 (0.5%)
7	G	1.96	12/690 (1.7%)	1.44	10/937 (1.1%)
7	T	1.92	18/702 (2.6%)	1.46	8/953 (0.8%)
8	H	1.55	4/682 (0.6%)	1.32	0/921
8	U	1.32	0/682	1.21	2/921 (0.2%)
9	I	1.48	1/605 (0.2%)	1.32	0/802
9	V	1.27	1/605 (0.2%)	1.32	0/802
10	J	1.61	4/471 (0.8%)	1.31	1/636 (0.2%)
10	W	1.52	1/480 (0.2%)	1.19	0/648
11	K	1.65	4/398 (1.0%)	1.33	2/546 (0.4%)
11	X	1.36	1/405 (0.2%)	1.16	0/556
12	L	1.61	2/401 (0.5%)	1.42	4/536 (0.7%)
12	Y	1.54	2/401 (0.5%)	1.30	2/536 (0.4%)
13	M	1.68	2/345 (0.6%)	1.24	0/470
13	Z	1.48	3/345 (0.9%)	1.21	0/470
All	All	1.75	366/30068 (1.2%)	1.37	144/40846 (0.4%)

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	2
1	N	0	1
6	S	0	1
7	T	0	1
12	Y	0	1
All	All	0	6

The worst 5 of 366 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	49	GLY	C-O	17.10	1.35	1.23
1	A	376	HIS	ND1-CE1	12.01	1.44	1.32
1	A	368	HIS	ND1-CE1	10.98	1.43	1.32
1	A	281	GLY	N-CA	10.25	1.58	1.45
3	P	20	GLY	N-CA	9.87	1.58	1.45

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	71	MET	CG-SD-CE	-11.62	75.34	100.90
1	A	71	MET	CG-SD-CE	-11.29	76.06	100.90
1	A	112	LEU	CD1-CG-CD2	-10.36	88.00	110.80
7	T	7	ASP	N-CA-C	10.30	132.73	110.80
1	A	240	HIS	CA-CB-CG	-8.74	105.06	113.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
7	T	40	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	98	0
1	N	4179	0	4154	92	0
2	B	1904	0	1909	60	0
2	O	1859	0	1860	41	1
3	C	2185	0	2097	53	0
3	P	2185	0	2097	52	0
4	D	1231	0	1227	48	0
4	Q	1224	0	1211	25	1
5	E	852	0	845	9	0
5	R	852	0	845	7	0
6	F	778	0	754	32	0
6	S	763	0	742	33	0
7	G	675	0	643	37	0
7	T	686	0	651	31	0
8	H	662	0	623	20	0
8	U	662	0	623	9	0
9	I	601	0	613	26	0
9	V	601	0	613	17	0
10	J	460	0	459	6	0
10	W	469	0	464	14	0
11	K	384	0	366	5	0
11	X	391	0	374	6	0
12	L	385	0	389	5	0
12	Y	388	0	388	14	0
13	M	335	0	352	11	0
13	Z	335	0	352	7	0
14	A	180	0	162	22	0
14	N	180	0	162	26	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	7	0
18	N	6	0	0	6	0
19	A	63	0	110	3	0
19	D	63	0	110	21	0
19	L	63	0	110	4	0
19	N	63	0	110	8	0
19	Q	63	0	110	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	63	0	110	13	0
20	A	102	0	152	13	0
20	C	102	0	152	11	0
20	G	51	0	76	4	0
20	N	51	0	76	2	0
20	P	51	0	76	4	0
20	Z	51	0	76	12	0
21	A	52	0	78	19	0
21	B	8	0	12	0	0
21	C	36	0	54	4	0
21	D	24	0	36	15	0
21	E	20	0	30	0	0
21	F	16	0	24	3	0
21	G	8	0	12	1	0
21	H	8	0	12	4	0
21	J	4	0	6	0	0
21	L	4	0	6	0	0
21	N	48	0	72	23	0
21	O	12	0	18	2	0
21	P	16	0	24	1	0
21	Q	8	0	12	0	0
21	R	24	0	36	2	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	8	0
22	G	29	0	39	1	0
22	J	29	0	38	2	0
22	P	58	0	78	7	0
22	W	29	0	39	9	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	23	0
24	O	52	0	80	12	0
25	C	99	0	126	18	0
25	L	33	0	42	5	0
25	M	33	0	42	1	0
25	P	99	0	126	18	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	106	0	154	17	0
27	G	53	0	77	10	0
27	P	53	0	77	10	0
27	T	106	0	154	8	0
28	C	100	0	156	28	0
28	N	100	0	156	15	0
28	P	100	0	156	25	0
28	T	100	0	156	20	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	233	0	0	15	0
30	B	140	0	0	13	1
30	C	101	0	0	4	0
30	D	110	0	0	19	1
30	E	85	0	0	4	0
30	F	78	0	0	7	0
30	G	51	0	0	4	0
30	H	45	0	0	3	0
30	I	25	0	0	5	0
30	J	28	0	0	2	0
30	K	21	0	0	4	0
30	L	29	0	0	3	0
30	M	27	0	0	3	0
30	N	219	0	0	18	0
30	O	115	0	0	3	0
30	P	90	0	0	2	0
30	Q	36	0	0	3	0
30	R	39	0	0	0	0
30	S	55	0	0	6	0
30	T	39	0	0	3	0
30	U	33	0	0	0	0
30	V	14	0	0	3	0
30	W	11	0	0	2	0
30	X	11	0	0	0	0
30	Y	14	0	0	1	0
30	Z	16	0	0	1	0
All	All	33735	0	32802	890	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 14.

The worst 5 of 890 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)
21:A:615:EDO:C2	21:A:615:EDO:C1	1.78	1.57
20:Z:101:PGV:C2	20:Z:101:PGV:H011	1.50	1.39
21:A:615:EDO:C1	21:A:615:EDO:O2	1.71	1.36
21:C:316:EDO:H11	30:C:486:HOH:O	1.23	1.29
30:A:705:HOH:O	19:D:201:TGL:HG11	1.32	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)
2:O:226:MET:O	4:Q:5:VAL:O[2_684]	2.13	0.07
30:B:466:HOH:O	30:D:302:HOH:O[2_584]	2.18	0.02

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%)	519 (97%)	15 (3%)	0	100	100
1	N	532/514 (104%)	516 (97%)	16 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	141 (97%)	5 (3%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	4 (3%)	2 (1%)	9	2
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	12	4
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	6	1
6	S	98/98 (100%)	89 (91%)	7 (7%)	2 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	2
8	U	77/85 (91%)	67 (87%)	7 (9%)	3 (4%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3596/3614 (100%)	3454 (96%)	119 (3%)	23 (1%)	18	10

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS
13	M	42	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/426 (105%)	438 (98%)	9 (2%)	48	36
1	N	445/426 (104%)	437 (98%)	8 (2%)	51	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	220/210 (105%)	211 (96%)	9 (4%)	27	12
2	O	214/210 (102%)	209 (98%)	5 (2%)	44	30
3	C	233/226 (103%)	228 (98%)	5 (2%)	47	33
3	P	233/226 (103%)	229 (98%)	4 (2%)	53	42
4	D	132/129 (102%)	126 (96%)	6 (4%)	24	10
4	Q	131/129 (102%)	122 (93%)	9 (7%)	14	3
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	18
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	11
6	F	85/81 (105%)	80 (94%)	5 (6%)	18	5
6	S	83/81 (102%)	72 (87%)	11 (13%)	4	0
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	62 (91%)	6 (9%)	9	1
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	2
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	6
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	3
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	36
10	W	50/50 (100%)	48 (96%)	2 (4%)	28	13
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	22	8
12	L	40/40 (100%)	39 (98%)	1 (2%)	42	27
12	Y	40/40 (100%)	37 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	7
All	All	3130/3082 (102%)	3012 (96%)	118 (4%)	31	14

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
10	W	50	LEU
3	P	230	ASN
10	W	7	GLU
7	T	38	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	68	GLN
6	S	94	HIS
4	Q	32	ASN
5	R	94	ASN
8	U	10	ASN

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	$\#\|Z\| > 2$
9	SAC	I	1	9	7,8,9	1.12	1 (14%)	8,9,11	1.97	2 (25%)
7	TPO	G	11	7	8,10,11	2.02	2 (25%)	10,14,16	1.39	2 (20%)
1	FME	A	1	1	8,9,10	0.87	0	7,9,11	2.27	3 (42%)
7	TPO	T	11	7	8,10,11	1.82	2 (25%)	10,14,16	1.67	2 (20%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	7,9,11	2.29	2 (28%)
1	FME	N	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.61	2 (28%)
2	FME	O	1	2	8,9,10	1.21	1 (12%)	7,9,11	1.88	2 (28%)
9	SAC	V	1	9	7,8,9	1.64	1 (14%)	8,9,11	1.54	3 (37%)

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.17	1.52	1.46
2	B	1	FME	CA-N	3.89	1.51	1.46
1	N	1	FME	CA-N	3.78	1.51	1.46
7	G	11	TPO	P-OG1	3.43	1.65	1.59
7	T	11	TPO	P-O1P	3.08	1.60	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	C-CA-N	-4.23	102.11	109.73
9	I	1	SAC	OG-CB-CA	-4.10	100.50	110.97
7	T	11	TPO	CG2-CB-CA	3.72	120.51	113.16
2	B	1	FME	CG-CB-CA	-3.71	102.63	112.95
2	O	1	FME	CG-CB-CA	-3.32	103.72	112.95

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	A	1	FME	1	0
7	T	11	TPO	1	0
2	B	1	FME	2	0
9	V	1	SAC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 142 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CHD	B	301	-	32,32,32	2.05	10 (31%)	51,51,51	1.93	17 (33%)
21	EDO	N	617	-	3,3,3	1.05	0	2,2,2	0.14	0
25	DMU	P	309	-	34,34,34	0.89	1 (2%)	45,45,45	1.26	3 (6%)
14	HEA	A	601	1	66,67,67	1.94	25 (37%)	78,103,103	2.48	32 (41%)
21	EDO	L	103	-	3,3,3	0.26	0	2,2,2	1.08	0
22	CHD	P	301	-	32,32,32	1.61	8 (25%)	51,51,51	2.01	16 (31%)
21	EDO	A	623	-	3,3,3	0.53	0	2,2,2	0.80	0
22	CHD	W	101	-	32,32,32	1.02	0	51,51,51	3.27	20 (39%)
21	EDO	N	622	-	3,3,3	0.51	0	2,2,2	0.70	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.44	0
21	EDO	A	614	-	3,3,3	0.39	0	2,2,2	1.18	0
21	EDO	E	204	-	3,3,3	0.79	0	2,2,2	0.39	0
22	CHD	C	307	-	32,32,32	1.19	3 (9%)	51,51,51	3.02	21 (41%)
25	DMU	L	102	-	34,34,34	0.96	1 (2%)	45,45,45	1.73	11 (24%)
21	EDO	H	102	-	3,3,3	0.59	0	2,2,2	1.26	0
22	CHD	C	301	-	32,32,32	1.72	6 (18%)	51,51,51	2.40	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	D	202	-	3,3,3	0.55	0	2,2,2	0.74	0
19	TGL	N	610	-	62,62,62	1.16	4 (6%)	65,65,65	1.77	12 (18%)
21	EDO	N	618	-	3,3,3	0.45	0	2,2,2	1.46	0
18	AZI	N	608	14	0,2,2	-	-	0,1,1	-	-
21	EDO	R	203	-	3,3,3	0.54	0	2,2,2	0.82	0
21	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.77	0
21	EDO	N	620	-	3,3,3	0.43	0	2,2,2	0.73	0
21	EDO	E	205	-	3,3,3	0.38	0	2,2,2	0.80	0
21	EDO	C	319	-	3,3,3	0.68	0	2,2,2	0.26	0
22	CHD	G	101	-	32,32,32	1.66	7 (21%)	51,51,51	1.74	10 (19%)
18	AZI	N	607	15	0,2,2	-	-	0,1,1	-	-
20	PGV	P	303	-	50,50,50	0.80	1 (2%)	53,56,56	1.25	8 (15%)
21	EDO	N	616	-	3,3,3	0.56	0	2,2,2	1.11	0
21	EDO	R	205	-	3,3,3	0.32	0	2,2,2	1.05	0
21	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	A	613	-	3,3,3	1.64	1 (33%)	2,2,2	0.92	0
21	EDO	R	206	-	3,3,3	1.02	0	2,2,2	0.48	0
21	EDO	H	101	-	3,3,3	0.24	0	2,2,2	2.63	2 (100%)
21	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.04	0
21	EDO	P	313	-	3,3,3	0.60	0	2,2,2	0.70	0
21	EDO	A	616	-	3,3,3	1.02	0	2,2,2	0.33	0
21	EDO	F	105	-	3,3,3	0.66	0	2,2,2	0.42	0
28	CDL	T	103	-	99,99,99	1.51	14 (14%)	105,111,111	1.72	25 (23%)
14	HEA	A	602[B]	1,18	66,67,67	2.02	21 (31%)	78,103,103	1.98	23 (29%)
21	EDO	T	104	-	3,3,3	1.06	0	2,2,2	0.46	0
27	PEK	C	308	-	52,52,52	1.27	3 (5%)	55,57,57	1.59	9 (16%)
19	TGL	L	101	-	62,62,62	2.03	8 (12%)	65,65,65	2.34	17 (26%)
20	PGV	C	309	-	50,50,50	1.41	3 (6%)	53,56,56	1.48	8 (15%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	1.14	0
20	PGV	A	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.19	5 (9%)
21	EDO	S	102	-	3,3,3	1.13	0	2,2,2	0.39	0
21	EDO	C	320	-	3,3,3	0.79	0	2,2,2	1.30	0
14	HEA	A	602[A]	1,18	66,67,67	1.87	19 (28%)	78,103,103	2.23	27 (34%)
20	PGV	G	103	-	50,50,50	1.25	2 (4%)	53,56,56	1.69	6 (11%)
21	EDO	Q	203	-	3,3,3	0.58	0	2,2,2	0.16	0
21	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.48	0
21	EDO	F	104	-	3,3,3	0.33	0	2,2,2	0.47	0
21	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.23	0
20	PGV	N	609	-	50,50,50	1.13	5 (10%)	53,56,56	1.32	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	B	305	-	3,3,3	1.73	1 (33%)	2,2,2	0.11	0
22	CHD	J	101	-	32,32,32	0.74	0	51,51,51	3.22	28 (54%)
19	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.64	8 (12%)
27	PEK	P	307	-	52,52,52	1.21	2 (3%)	55,57,57	1.32	6 (10%)
21	EDO	D	204	-	3,3,3	0.61	0	2,2,2	0.98	0
21	EDO	G	105	-	3,3,3	0.91	0	2,2,2	0.20	0
21	EDO	R	204	-	3,3,3	0.88	0	2,2,2	0.42	0
25	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.11	9 (20%)
25	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.19	13 (28%)
21	EDO	A	621	-	3,3,3	0.80	0	2,2,2	0.23	0
21	EDO	A	620	-	3,3,3	0.68	0	2,2,2	0.65	0
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	1.09	0
21	EDO	G	104	-	3,3,3	0.58	0	2,2,2	0.47	0
20	PGV	Z	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.36	7 (13%)
27	PEK	G	102	-	52,52,52	1.12	2 (3%)	55,57,57	1.49	5 (9%)
22	CHD	P	305	-	32,32,32	1.32	4 (12%)	51,51,51	3.13	22 (43%)
25	DMU	Z	102	-	34,34,34	0.75	1 (2%)	45,45,45	1.33	5 (11%)
27	PEK	T	102	-	52,52,52	1.18	6 (11%)	55,57,57	2.57	7 (12%)
25	DMU	P	306	-	34,34,34	1.02	1 (2%)	45,45,45	1.38	3 (6%)
21	EDO	U	101	-	3,3,3	0.36	0	2,2,2	0.82	0
20	PGV	A	610	-	50,50,50	1.42	4 (8%)	53,56,56	1.63	8 (15%)
21	EDO	A	617	-	3,3,3	1.21	0	2,2,2	1.28	0
28	CDL	P	304	-	99,99,99	1.61	18 (18%)	105,111,111	1.60	19 (18%)
14	HEA	N	603[B]	1,18	66,67,67	2.05	21 (31%)	78,103,103	1.73	18 (23%)
21	EDO	C	317	-	3,3,3	0.47	0	2,2,2	0.37	0
28	CDL	N	601	-	99,99,99	1.54	14 (14%)	105,111,111	1.60	20 (19%)
21	EDO	O	303	-	3,3,3	0.68	0	2,2,2	0.78	0
20	PGV	C	305	-	50,50,50	1.06	1 (2%)	53,56,56	1.36	7 (13%)
21	EDO	E	203	-	3,3,3	0.31	0	2,2,2	1.26	0
21	EDO	J	102	-	3,3,3	0.39	0	2,2,2	1.78	0
21	EDO	D	206	-	3,3,3	0.26	0	2,2,2	1.32	0
21	EDO	O	304	-	3,3,3	0.35	0	2,2,2	0.92	0
21	EDO	C	315	-	3,3,3	0.68	0	2,2,2	0.51	0
27	PEK	T	101	-	52,52,52	1.30	2 (3%)	55,57,57	1.43	7 (12%)
21	EDO	C	312	-	3,3,3	1.23	0	2,2,2	0.14	0
21	EDO	S	103	-	3,3,3	0.68	0	2,2,2	1.76	1 (50%)
21	EDO	C	313	-	3,3,3	0.36	0	2,2,2	0.80	0
21	EDO	C	318	-	3,3,3	0.66	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	DMU	M	101	-	34,34,34	0.71	0	45,45,45	1.41	6 (13%)
21	EDO	N	614	-	3,3,3	0.40	0	2,2,2	1.22	0
21	EDO	N	611	-	3,3,3	0.36	0	2,2,2	1.12	0
21	EDO	N	612	-	3,3,3	1.36	0	2,2,2	1.62	0
21	EDO	V	101	-	3,3,3	0.39	0	2,2,2	0.90	0
14	HEA	N	602	1	66,67,67	1.90	23 (34%)	78,103,103	2.33	32 (41%)
21	EDO	C	316	-	3,3,3	0.52	0	2,2,2	1.52	0
21	EDO	D	207	-	3,3,3	0.62	0	2,2,2	0.56	0
19	TGL	Y	101	-	62,62,62	1.45	5 (8%)	65,65,65	1.88	11 (16%)
21	EDO	E	202	-	3,3,3	0.53	0	2,2,2	0.84	0
21	EDO	F	103	-	3,3,3	0.64	0	2,2,2	0.54	0
21	EDO	R	201	-	3,3,3	1.14	0	2,2,2	1.17	0
18	AZI	A	606	15	0,2,2	-	-	0,1,1	-	-
18	AZI	A	607	14	0,2,2	-	-	0,1,1	-	-
19	TGL	D	201	-	62,62,62	1.66	5 (8%)	65,65,65	2.26	11 (16%)
21	EDO	P	311	-	3,3,3	0.84	0	2,2,2	0.14	0
21	EDO	P	310	-	3,3,3	0.67	0	2,2,2	2.16	1 (50%)
27	PEK	C	304	-	52,52,52	1.06	5 (9%)	55,57,57	1.28	8 (14%)
21	EDO	O	305	-	3,3,3	0.39	0	2,2,2	0.52	0
21	EDO	A	615	-	3,3,3	2.67	1 (33%)	2,2,2	4.78	1 (50%)
21	EDO	F	102	-	3,3,3	1.06	0	2,2,2	0.29	0
21	EDO	R	202	-	3,3,3	0.18	0	2,2,2	1.29	0
21	EDO	P	312	-	3,3,3	0.59	0	2,2,2	0.63	0
21	EDO	A	618	-	3,3,3	0.23	0	2,2,2	1.43	0
14	HEA	N	603[A]	1,18	66,67,67	2.12	22 (33%)	78,103,103	2.24	25 (32%)
21	EDO	N	615	-	3,3,3	1.57	1 (33%)	2,2,2	0.65	0
25	DMU	C	311	-	34,34,34	1.43	3 (8%)	45,45,45	2.32	11 (24%)
21	EDO	N	613	-	3,3,3	0.54	0	2,2,2	0.44	0
23	CUA	O	301	2	0,1,1	-	-	-		
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.34	4 (7%)
21	EDO	D	203	-	3,3,3	0.45	0	2,2,2	0.71	0
21	EDO	A	619	-	3,3,3	1.55	0	2,2,2	1.69	0
19	TGL	A	608	-	62,62,62	1.37	5 (8%)	65,65,65	2.18	11 (16%)
21	EDO	N	621	-	3,3,3	0.33	0	2,2,2	0.89	0
28	CDL	C	306	-	99,99,99	1.58	17 (17%)	105,111,111	1.66	20 (19%)
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	1.15	0
25	DMU	C	302	-	34,34,34	0.94	0	45,45,45	1.73	14 (31%)
24	PSC	B	303	-	51,51,51	1.46	4 (7%)	57,59,59	1.46	7 (12%)
23	CUA	B	302	2	0,1,1	-	-	-		

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
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
21	EDO	N	617	-	-	0/1/1/1	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
14	HEA	A	601	1	-	5/36/76/76	-
21	EDO	L	103	-	-	1/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	A	623	-	-	0/1/1/1	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
21	EDO	N	622	-	-	1/1/1/1	-
21	EDO	E	201	-	-	1/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	E	204	-	-	1/1/1/1	-
22	CHD	C	307	-	-	8/9/74/74	0/4/4/4
25	DMU	L	102	-	-	12/19/59/59	0/2/2/2
21	EDO	H	102	-	-	1/1/1/1	-
22	CHD	C	301	-	-	3/9/74/74	0/4/4/4
21	EDO	D	202	-	-	1/1/1/1	-
19	TGL	N	610	-	-	39/65/65/65	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	E	205	-	-	0/1/1/1	-
21	EDO	C	319	-	-	1/1/1/1	-
22	CHD	G	101	-	-	2/9/74/74	0/4/4/4
20	PGV	P	303	-	-	11/55/55/55	-
21	EDO	N	616	-	-	1/1/1/1	-
21	EDO	R	205	-	-	1/1/1/1	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	R	206	-	-	1/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	P	313	-	-	1/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CDL	T	103	-	-	63/110/110/110	-
14	HEA	A	602[B]	1,18	-	6/36/76/76	-
21	EDO	T	104	-	-	0/1/1/1	-
27	PEK	C	308	-	-	28/56/56/56	-
19	TGL	L	101	-	-	38/65/65/65	-
20	PGV	C	309	-	-	27/55/55/55	-
21	EDO	A	611	-	-	1/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
14	HEA	A	602[A]	1,18	-	8/36/76/76	-
20	PGV	G	103	-	-	33/55/55/55	-
21	EDO	Q	203	-	-	1/1/1/1	-
21	EDO	A	622	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
20	PGV	N	609	-	-	13/55/55/55	-
21	EDO	B	305	-	-	1/1/1/1	-
22	CHD	J	101	-	-	7/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	37/65/65/65	-
27	PEK	P	307	-	-	27/56/56/56	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	G	105	-	-	1/1/1/1	-
21	EDO	R	204	-	-	0/1/1/1	-
25	DMU	C	310	-	-	6/19/59/59	0/2/2/2
25	DMU	P	308	-	-	7/19/59/59	0/2/2/2
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
20	PGV	Z	101	-	-	31/55/55/55	-
27	PEK	G	102	-	-	34/56/56/56	-
22	CHD	P	305	-	-	6/9/74/74	0/4/4/4
25	DMU	Z	102	-	-	5/19/59/59	0/2/2/2
27	PEK	T	102	-	-	23/56/56/56	-
25	DMU	P	306	-	-	6/19/59/59	0/2/2/2
21	EDO	U	101	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	A	610	-	-	26/55/55/55	-
21	EDO	A	617	-	-	1/1/1/1	-
28	CDL	P	304	-	-	56/110/110/110	-
14	HEA	N	603[B]	1,18	-	7/36/76/76	-
21	EDO	C	317	-	-	1/1/1/1	-
28	CDL	N	601	-	-	53/110/110/110	-
21	EDO	O	303	-	-	0/1/1/1	-
20	PGV	C	305	-	-	14/55/55/55	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	O	304	-	-	1/1/1/1	-
21	EDO	C	315	-	-	1/1/1/1	-
27	PEK	T	101	-	-	29/56/56/56	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	C	313	-	-	1/1/1/1	-
21	EDO	C	318	-	-	1/1/1/1	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	N	611	-	-	1/1/1/1	-
21	EDO	N	612	-	-	1/1/1/1	-
21	EDO	V	101	-	-	0/1/1/1	-
14	HEA	N	602	1	-	7/36/76/76	-
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	D	207	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
19	TGL	D	201	-	-	40/65/65/65	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
27	PEK	C	304	-	-	12/56/56/56	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	R	202	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	603[A]	1,18	-	6/36/76/76	-
21	EDO	N	615	-	-	0/1/1/1	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
21	EDO	N	613	-	-	1/1/1/1	-
24	PSC	O	302	-	-	33/55/55/55	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	N	621	-	-	0/1/1/1	-
28	CDL	C	306	-	-	70/110/110/110	-
21	EDO	A	612	-	-	1/1/1/1	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
24	PSC	B	303	-	-	28/55/55/55	-

The worst 5 of 325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG3-CC1	9.15	1.60	1.33
19	L	101	TGL	OG2-CB1	9.01	1.59	1.34
19	D	201	TGL	OB1-CB1	7.45	1.44	1.22
19	Y	101	TGL	OG2-CB1	6.77	1.53	1.34
20	C	309	PGV	O01-C1	6.53	1.52	1.34

The worst 5 of 653 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	102	PEK	C2-C3-C4	14.82	139.64	113.23
22	P	305	CHD	C23-C22-C20	-12.78	91.17	114.52
22	C	307	CHD	C23-C22-C20	-11.42	93.65	114.52
19	D	201	TGL	OG2-CB1-CB2	-10.77	88.29	111.50
22	J	101	CHD	C14-C8-C9	-10.23	95.67	109.71

There are no chirality outliers.

5 of 1025 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[A]	HEA	C2A-C3A-CMA-OMA
14	A	602[A]	HEA	C4A-C3A-CMA-OMA
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[A]	HEA	C2A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
14	N	603[A]	HEA	C4A-C3A-CMA-OMA

There are no ring outliers.

79 monomers are involved in 458 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	309	DMU	1	0
14	A	601	HEA	8	0
22	P	301	CHD	1	0
22	W	101	CHD	9	0
21	N	622	EDO	7	0
22	C	307	CHD	6	0
25	L	102	DMU	5	0
21	H	102	EDO	1	0
22	C	301	CHD	2	0
21	D	202	EDO	7	0
19	N	610	TGL	8	0
21	N	618	EDO	6	0
18	N	608	AZI	6	0
22	G	101	CHD	1	0
18	N	607	AZI	1	0
20	P	303	PGV	4	0
21	R	205	EDO	1	0
21	A	613	EDO	2	0
21	H	101	EDO	3	0
21	F	105	EDO	3	0
28	T	103	CDL	20	0
14	A	602[B]	HEA	5	0
27	C	308	PEK	9	0
19	L	101	TGL	4	0
20	C	309	PGV	8	0
20	A	609	PGV	6	0
14	A	602[A]	HEA	9	0
20	G	103	PGV	4	0
21	A	622	EDO	1	0
20	N	609	PGV	2	0
22	J	101	CHD	2	0
19	Q	201	TGL	10	0
27	P	307	PEK	10	0
21	D	204	EDO	2	0
25	C	310	DMU	5	0
25	P	308	DMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	621	EDO	5	0
21	G	104	EDO	1	0
20	Z	101	PGV	12	0
27	G	102	PEK	10	0
22	P	305	CHD	6	0
27	T	102	PEK	4	0
25	P	306	DMU	16	0
20	A	610	PGV	7	0
21	A	617	EDO	1	0
28	P	304	CDL	25	0
14	N	603[B]	HEA	9	0
21	C	317	EDO	1	0
28	N	601	CDL	15	0
20	C	305	PGV	3	0
21	D	206	EDO	2	0
21	O	304	EDO	1	0
21	C	315	EDO	1	0
27	T	101	PEK	4	0
25	M	101	DMU	1	0
21	N	612	EDO	3	0
14	N	602	HEA	10	0
21	C	316	EDO	2	0
19	Y	101	TGL	13	0
18	A	606	AZI	2	0
18	A	607	AZI	6	0
19	D	201	TGL	21	0
27	C	304	PEK	8	0
21	O	305	EDO	1	0
21	A	615	EDO	5	0
21	R	202	EDO	1	0
21	P	312	EDO	1	0
21	A	618	EDO	3	0
14	N	603[A]	HEA	7	0
25	C	311	DMU	1	0
21	N	613	EDO	1	0
24	O	302	PSC	12	0
21	D	203	EDO	4	0
21	A	619	EDO	2	0
19	A	608	TGL	3	0
21	N	621	EDO	6	0
28	C	306	CDL	28	0
25	C	302	DMU	12	0

Continued on next page...

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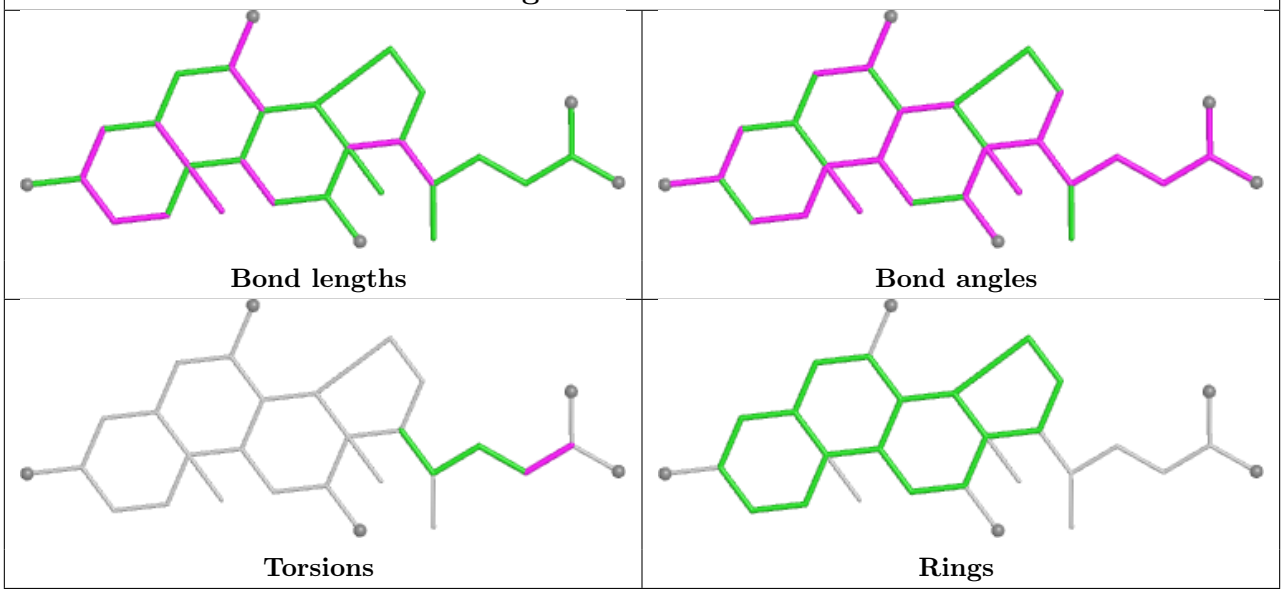
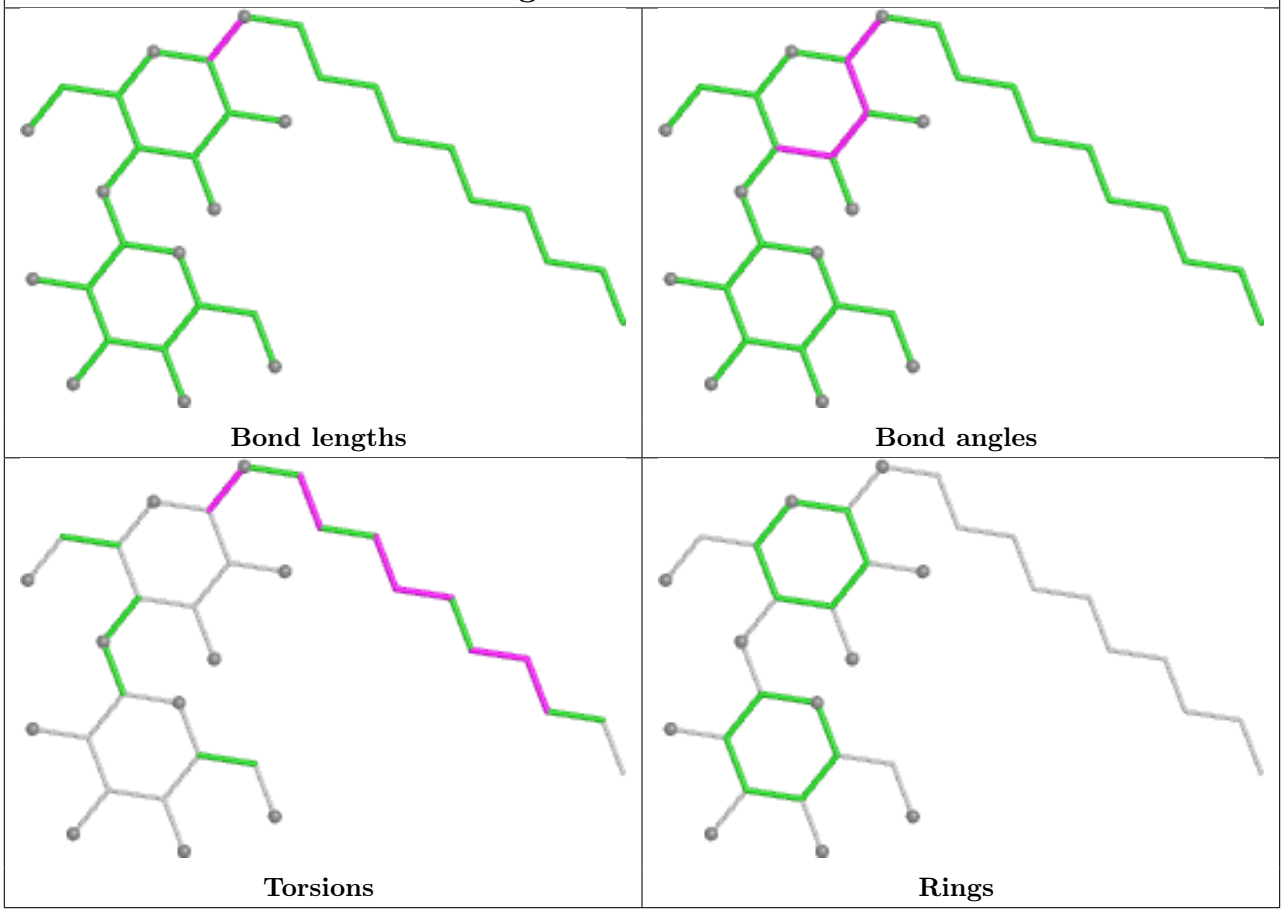
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	303	PSC	23	0

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

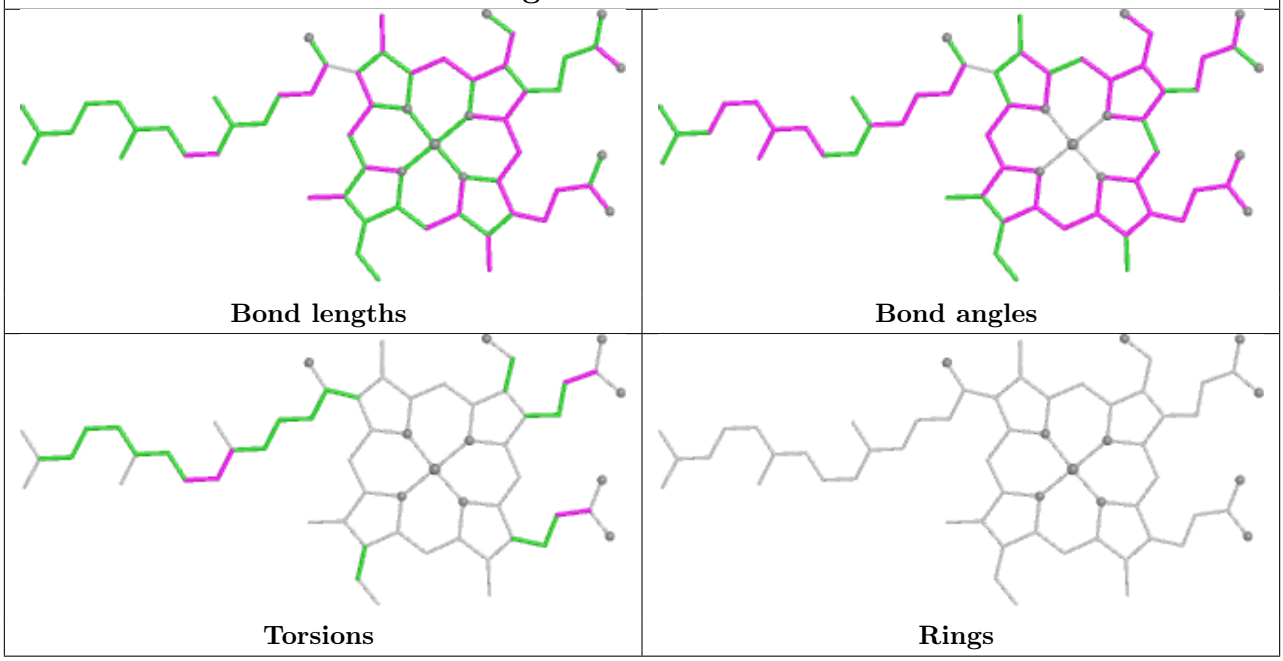
Ligand CHD B 301



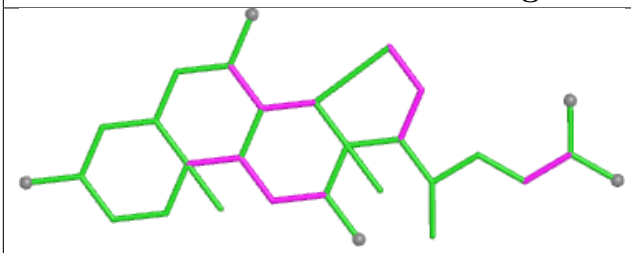
Ligand DMU P 309



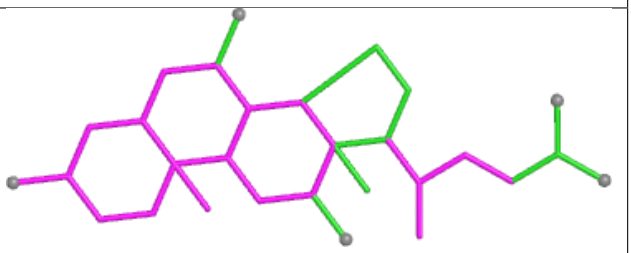
Ligand HEA A 601



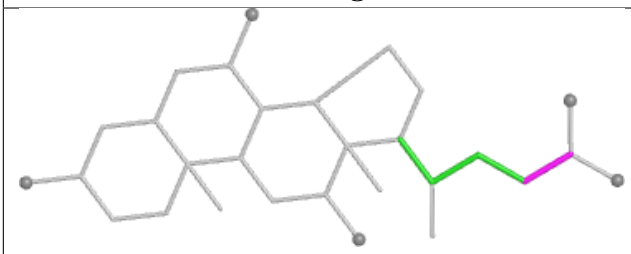
Ligand CHD P 301



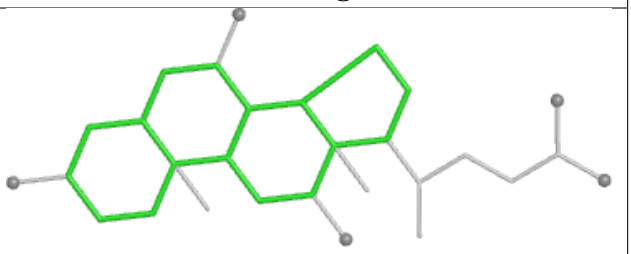
Bond lengths



Bond angles

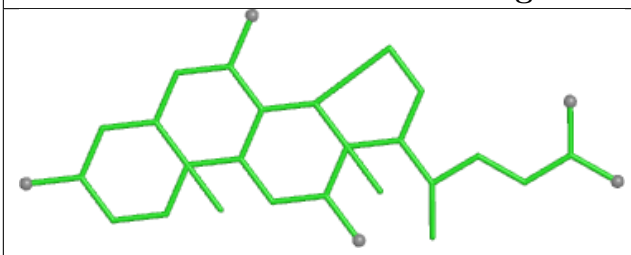


Torsions

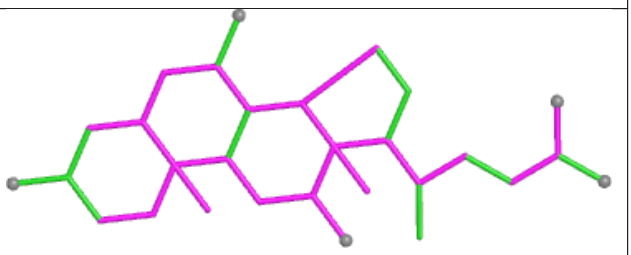


Rings

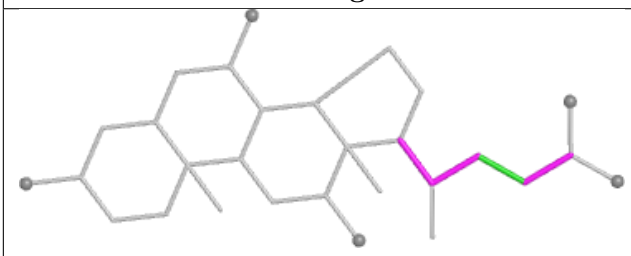
Ligand CHD W 101



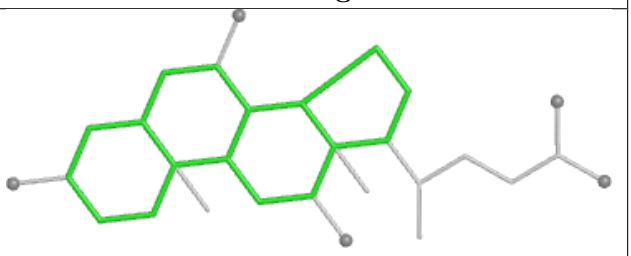
Bond lengths



Bond angles

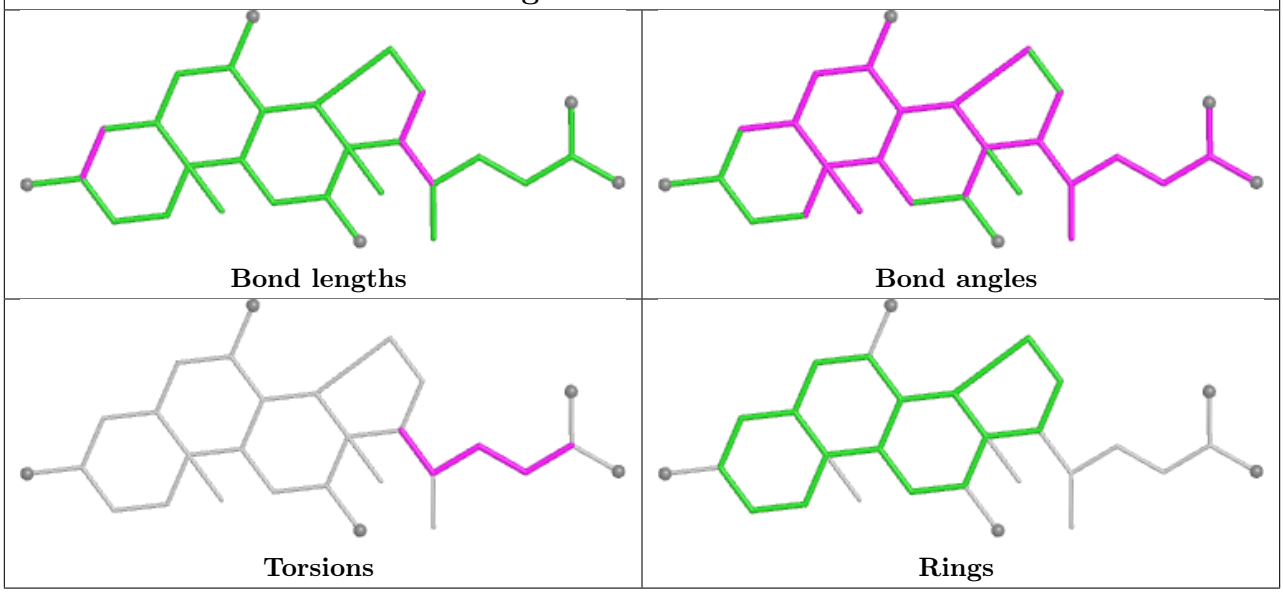


Torsions

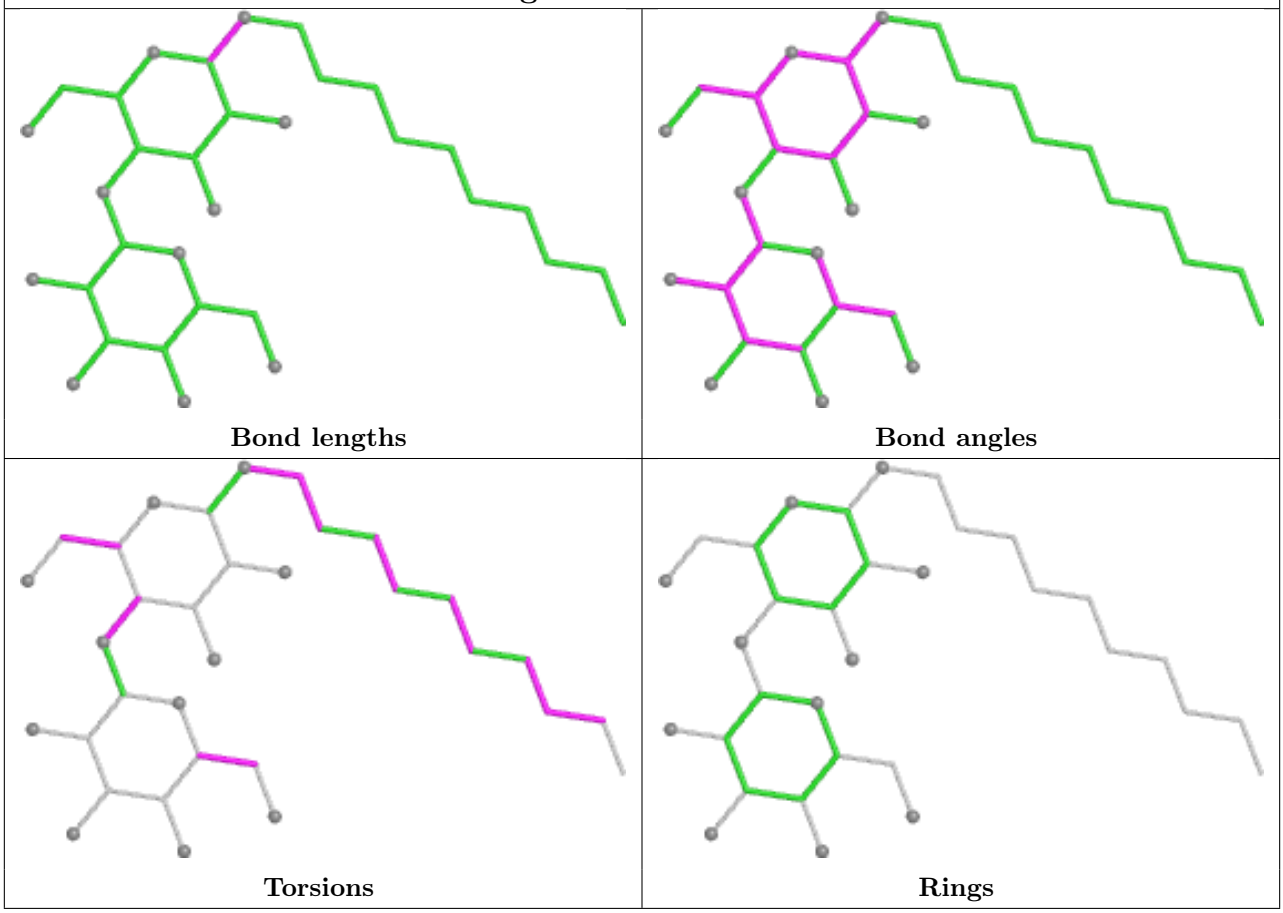


Rings

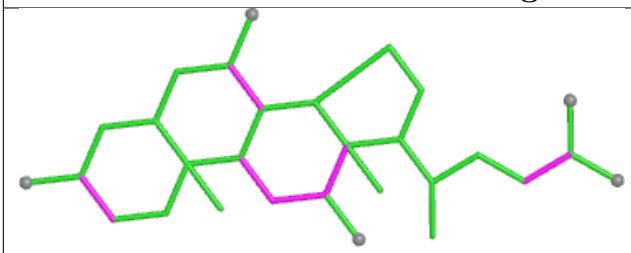
Ligand CHD C 307



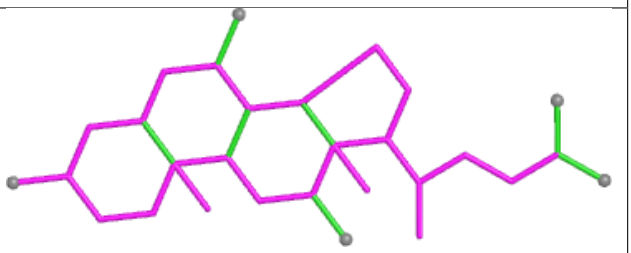
Ligand DMU L 102



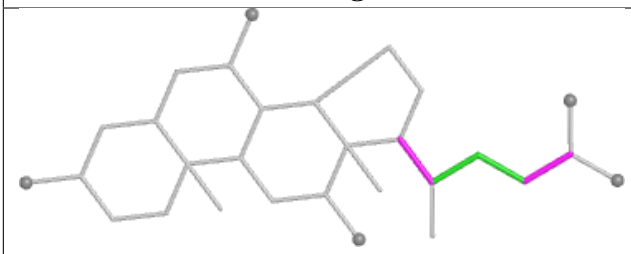
Ligand CHD C 301



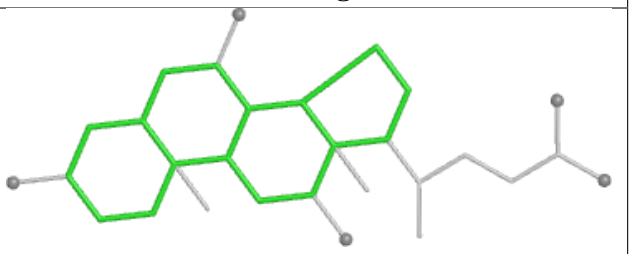
Bond lengths



Bond angles

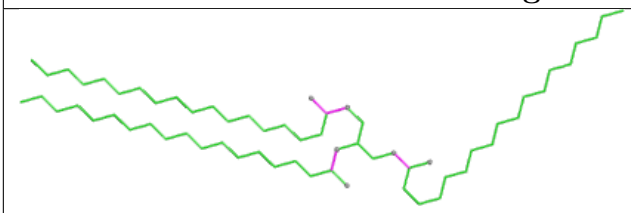


Torsions



Rings

Ligand TGL N 610



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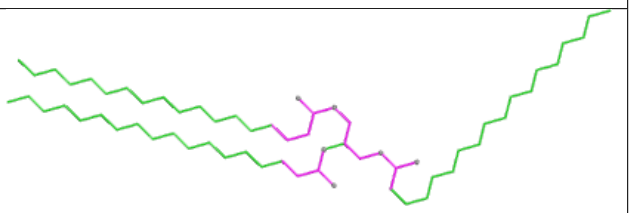
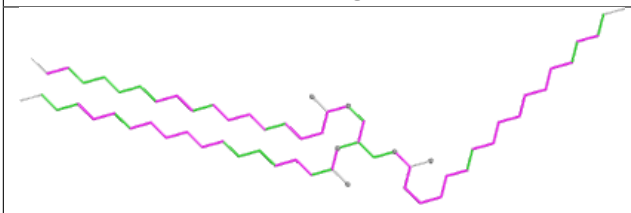
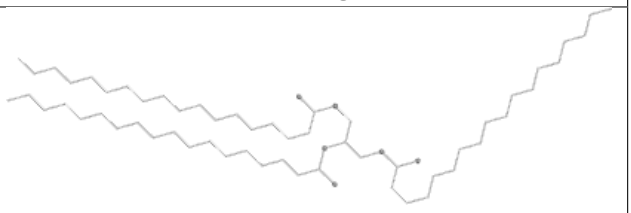


Bond angles

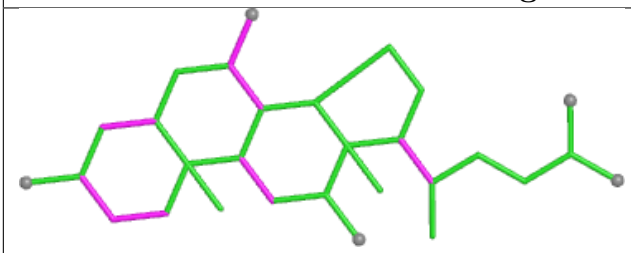


Torsions



Rings

Ligand CHD G 101



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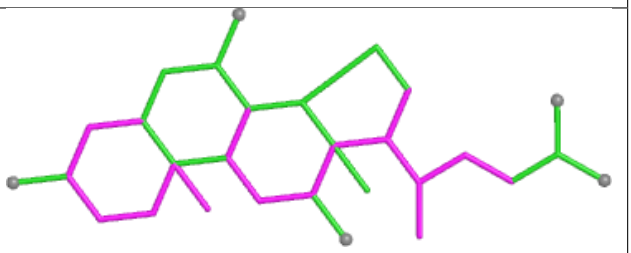
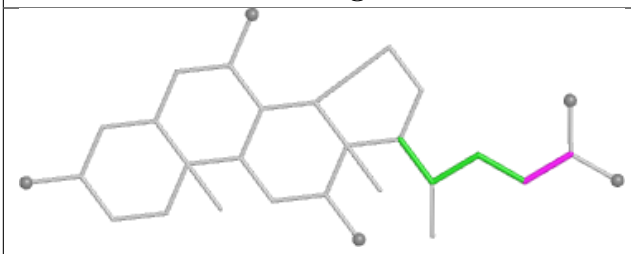


Bond angles



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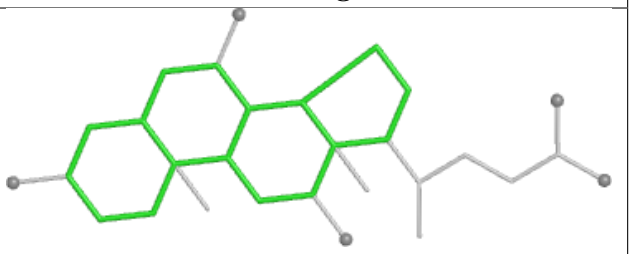
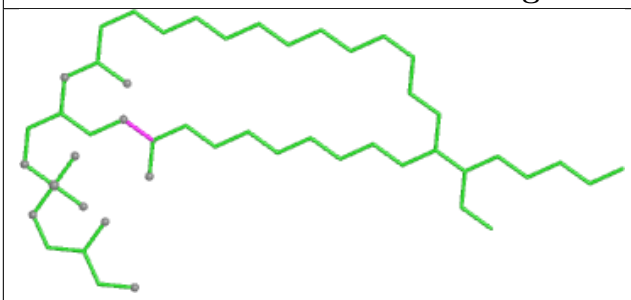
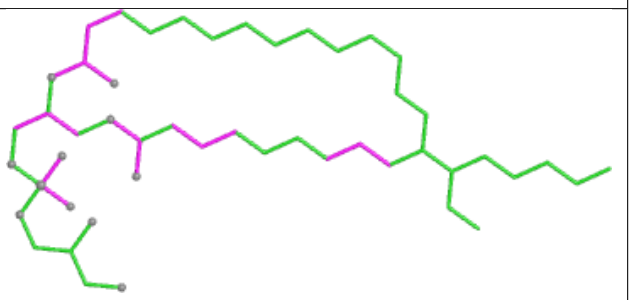


Rings

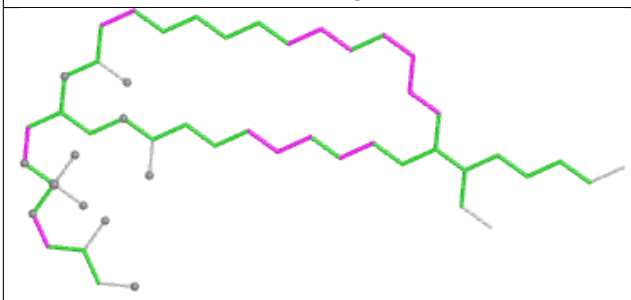
Ligand PGV P 303



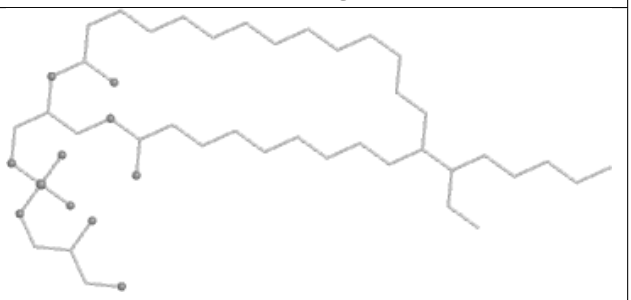
Bond lengths



Bond angles

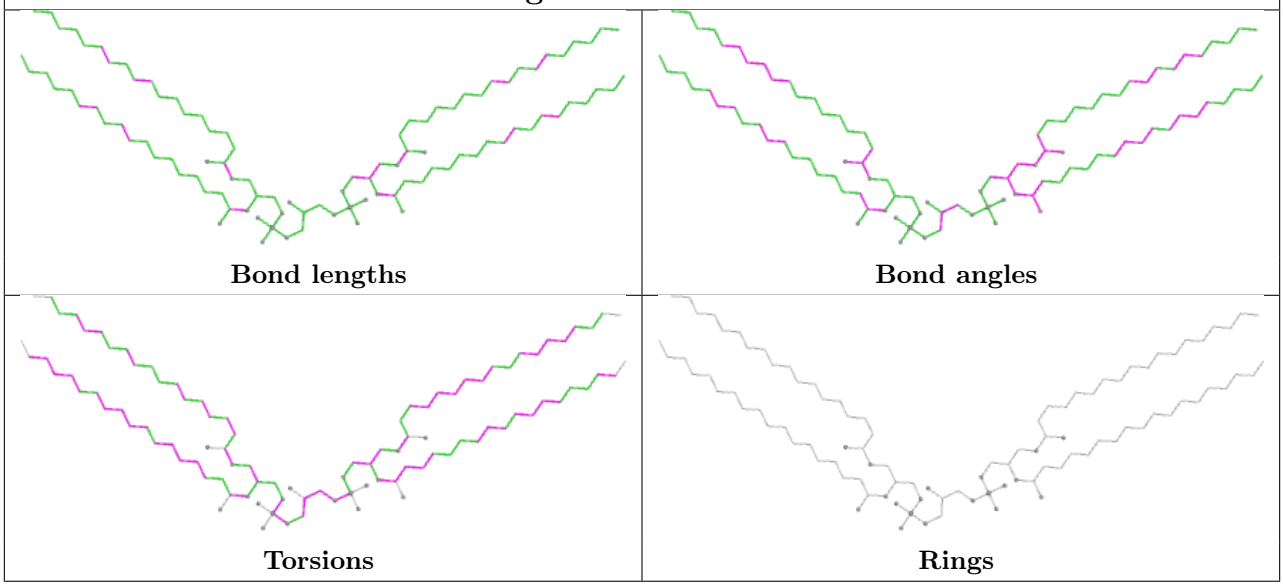


Torsions

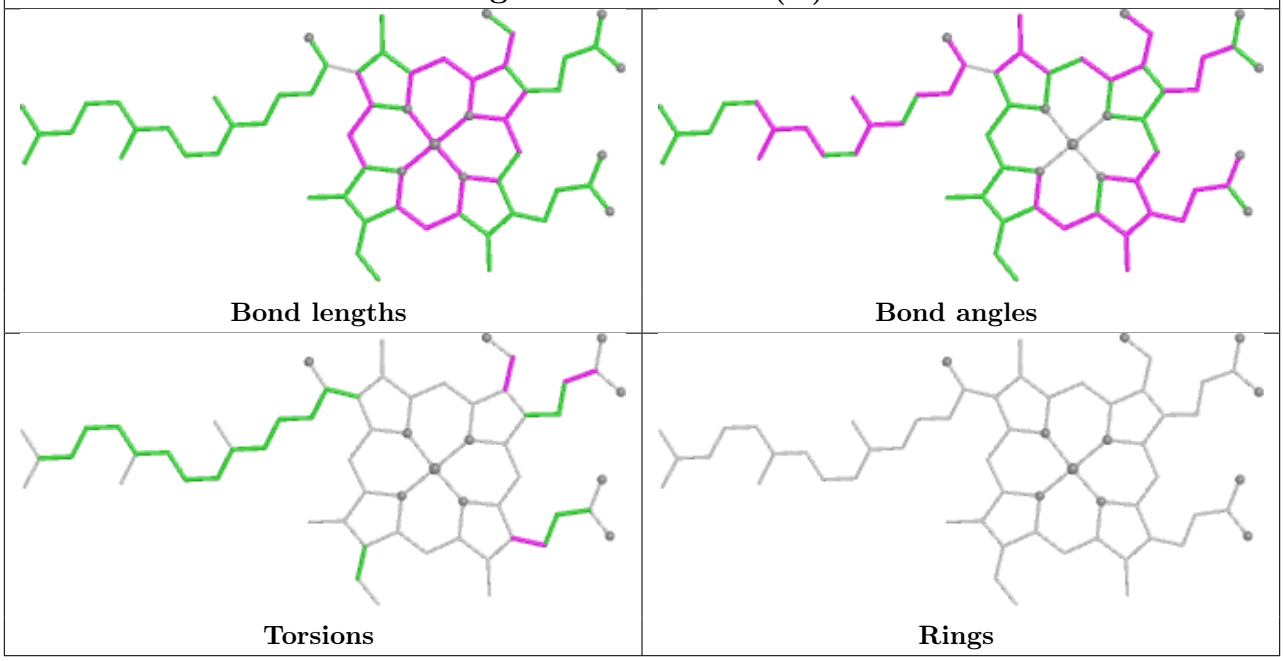


Rings

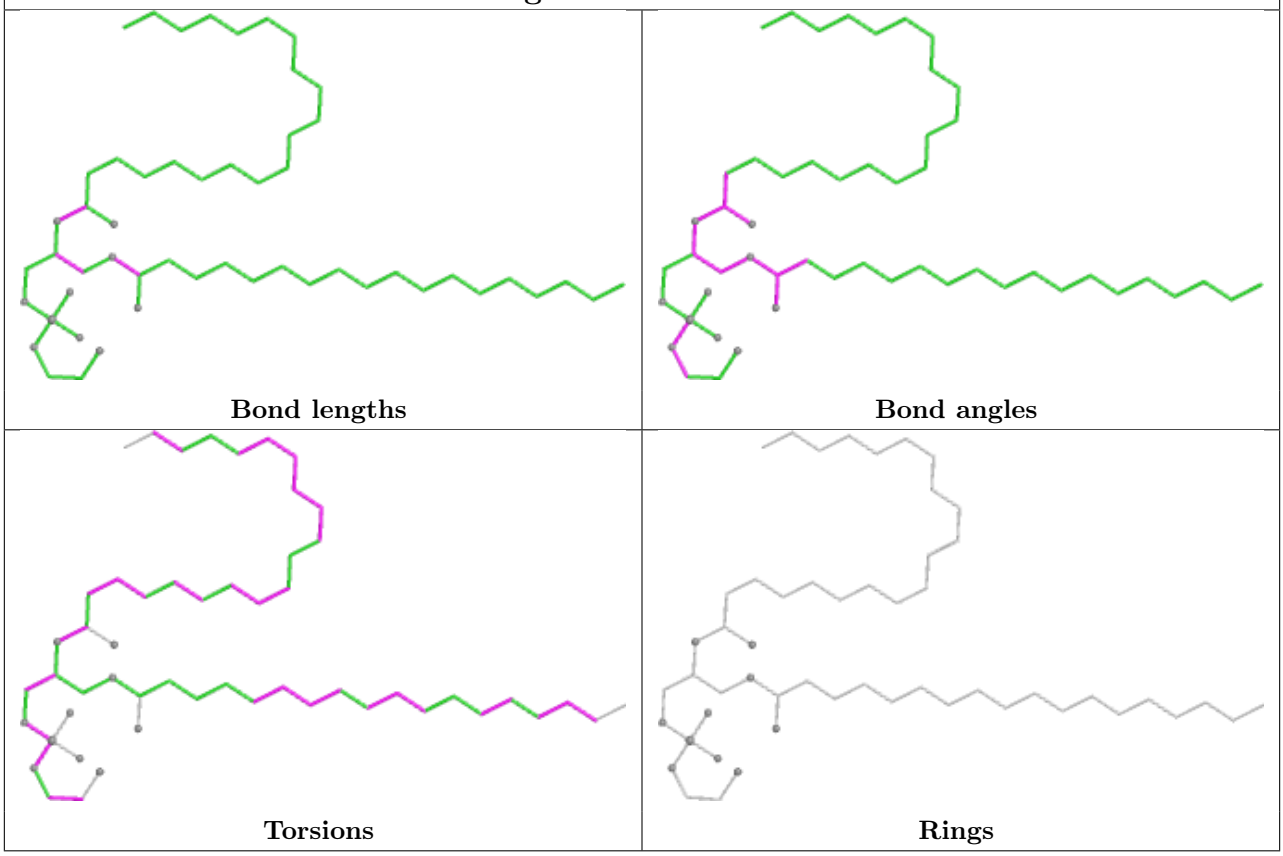
Ligand CDL T 103



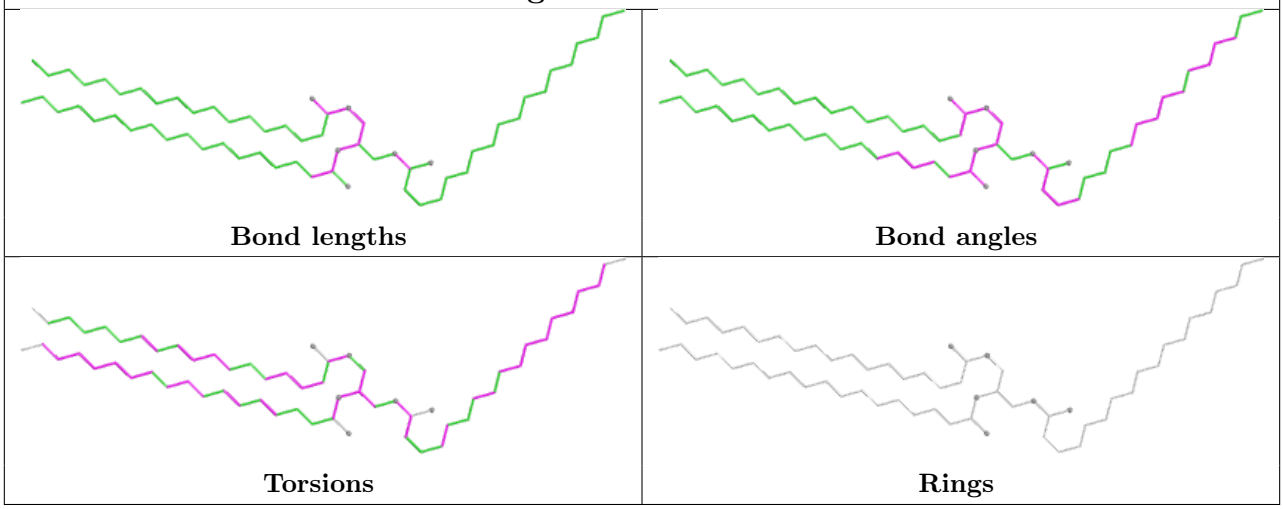
Ligand HEA A 602 (B)



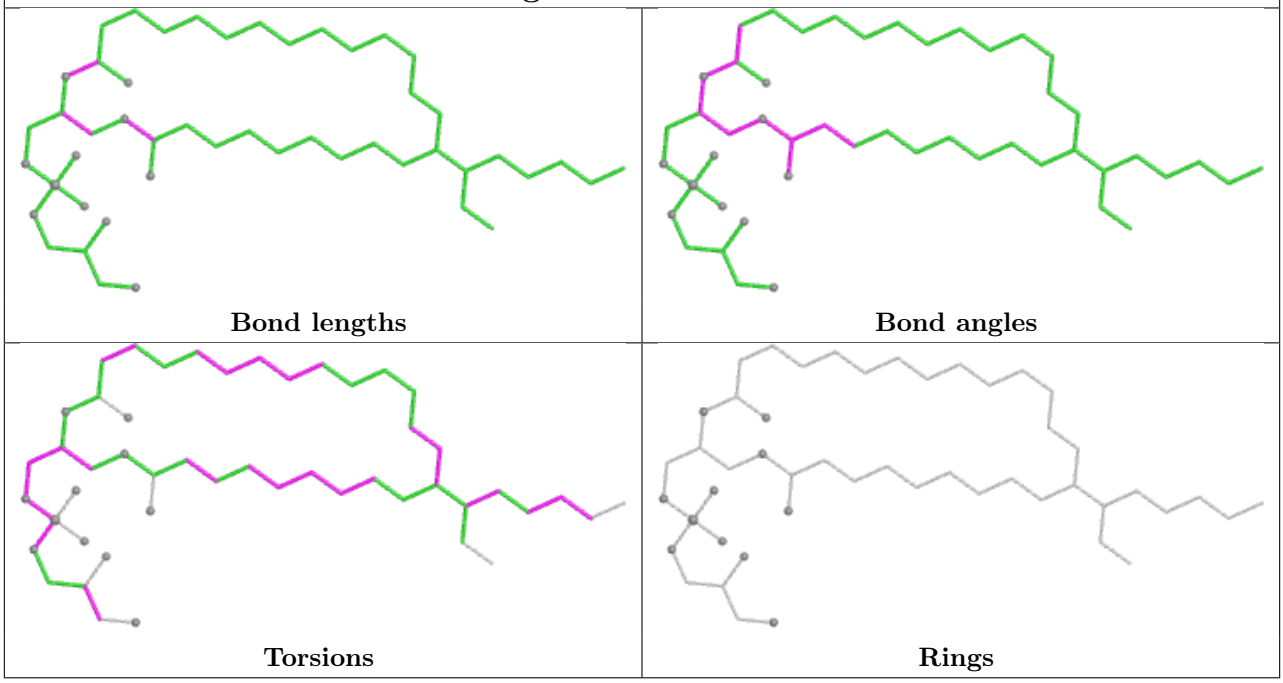
Ligand PEK C 308



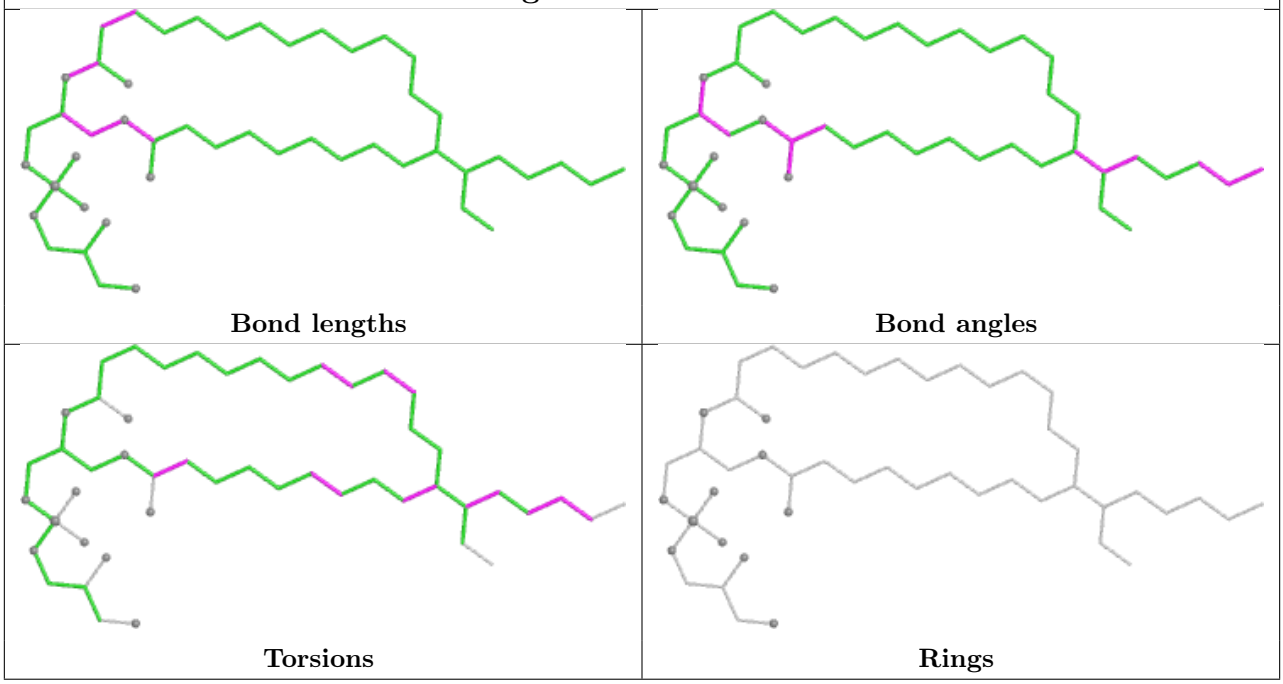
Ligand TGL L 101



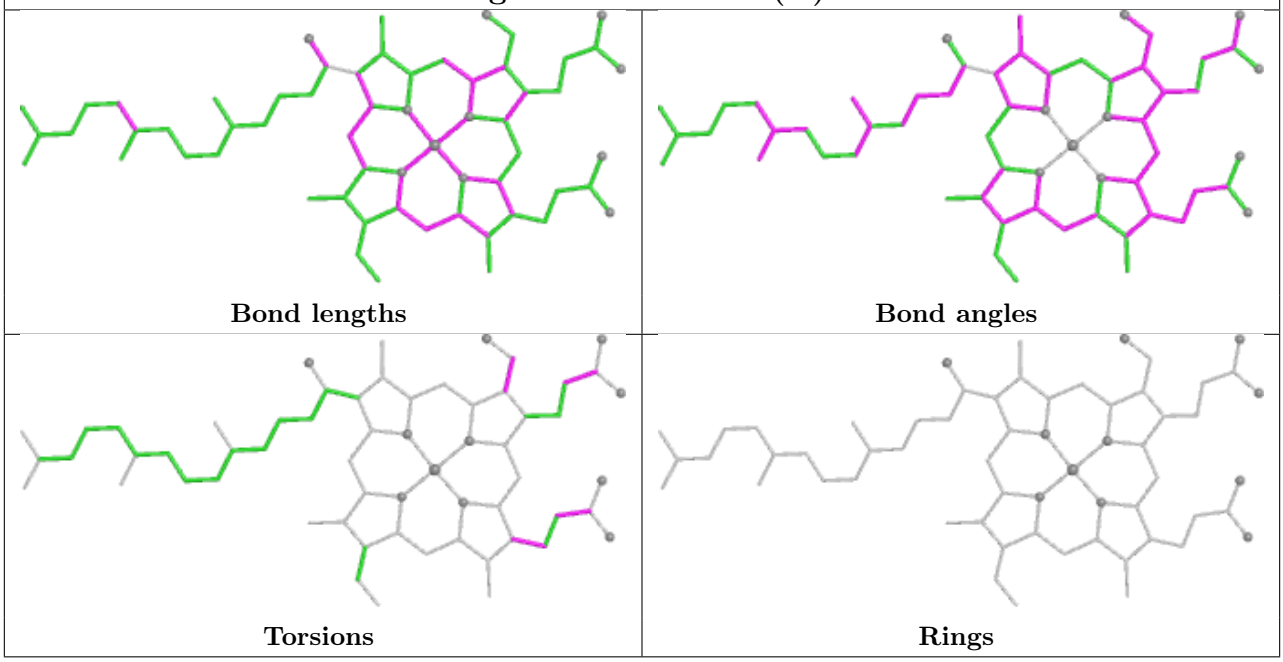
Ligand PGV C 309



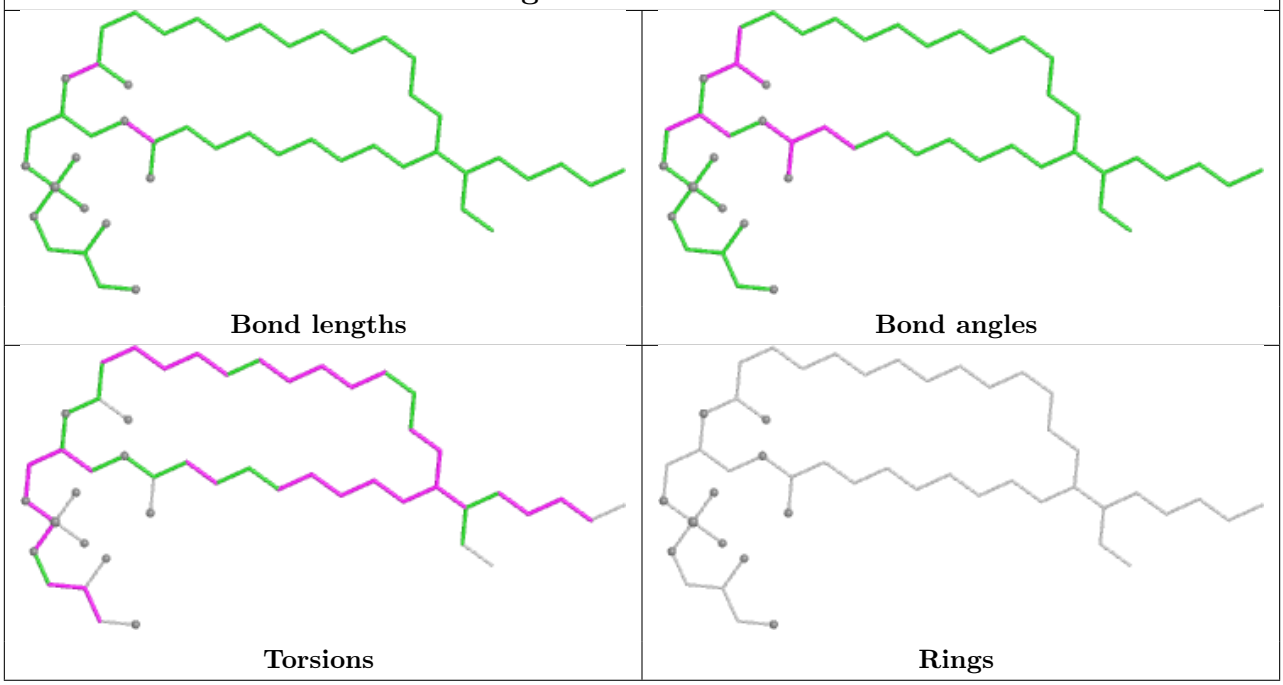
Ligand PGV A 609



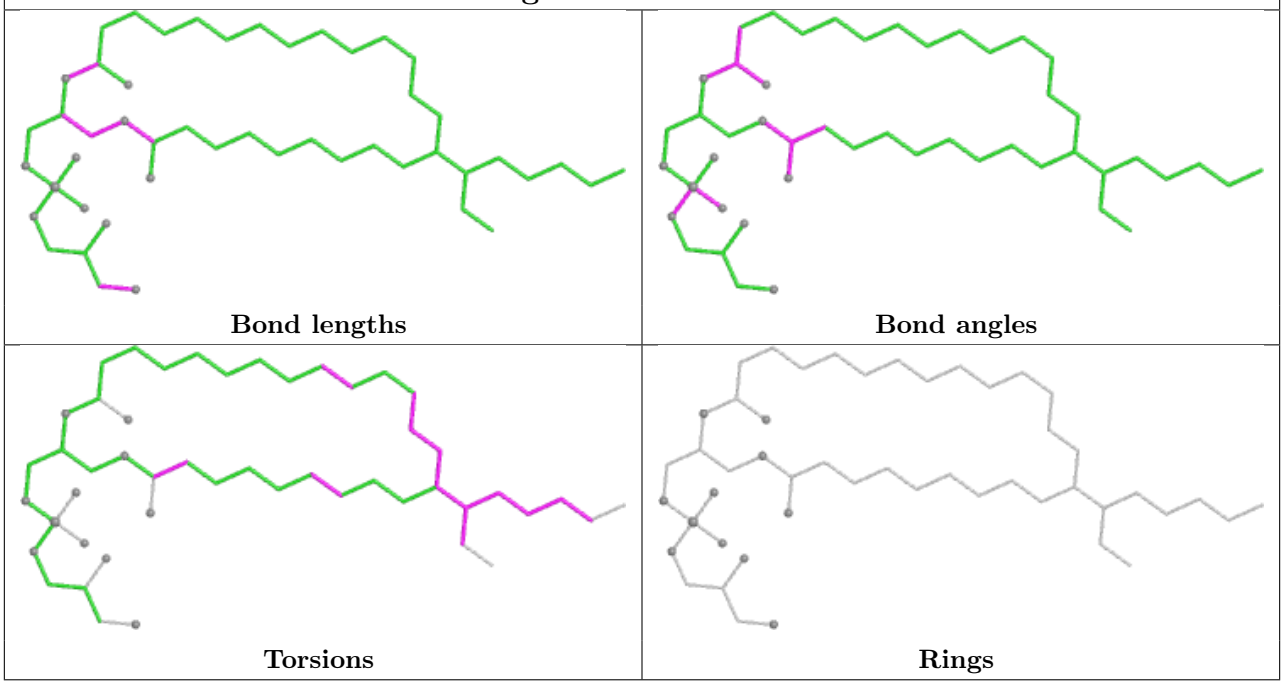
Ligand HEA A 602 (A)



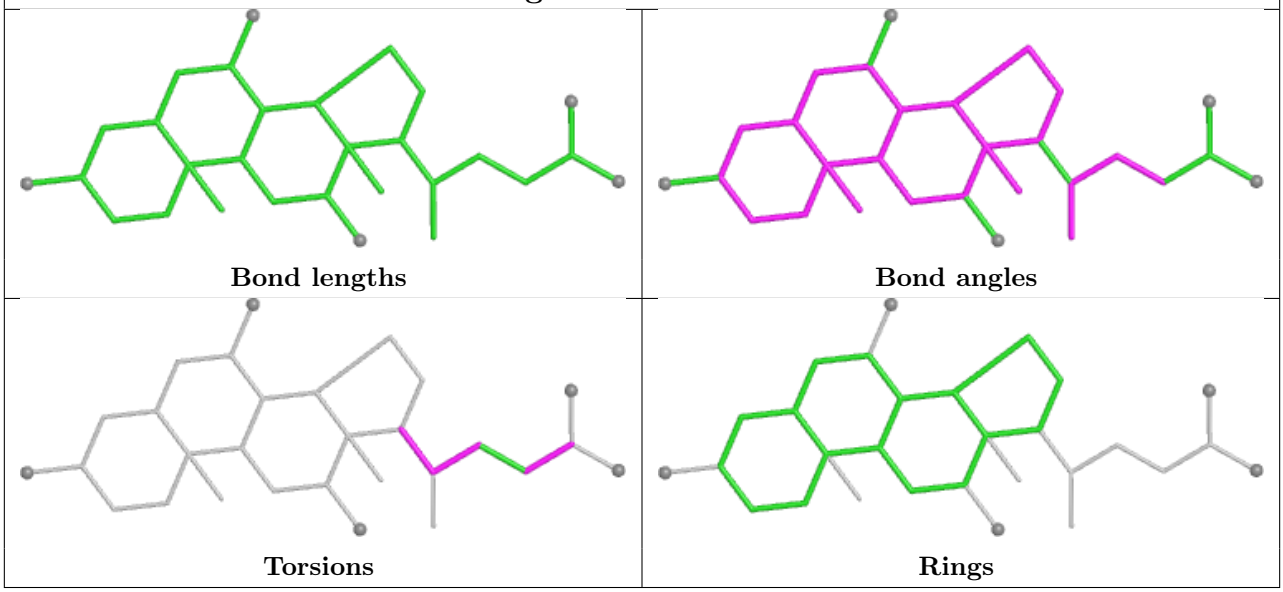
Ligand PGV G 103



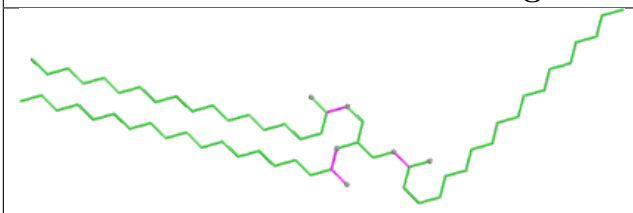
Ligand PGV N 609



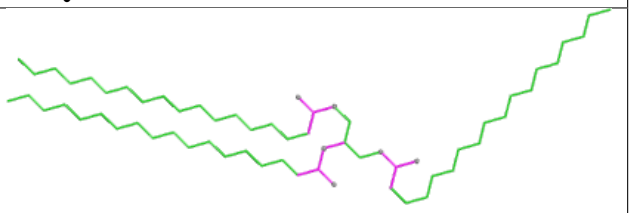
Ligand CHD J 101



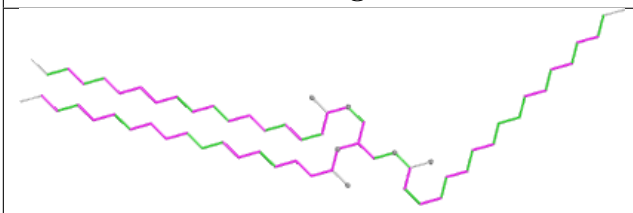
Ligand TGL Q 201



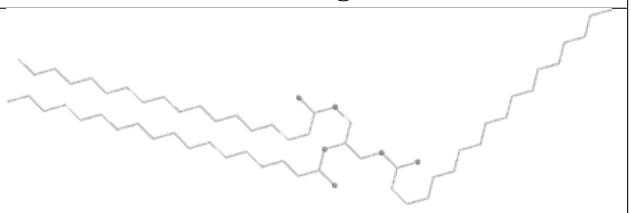
Bond lengths



Bond angles

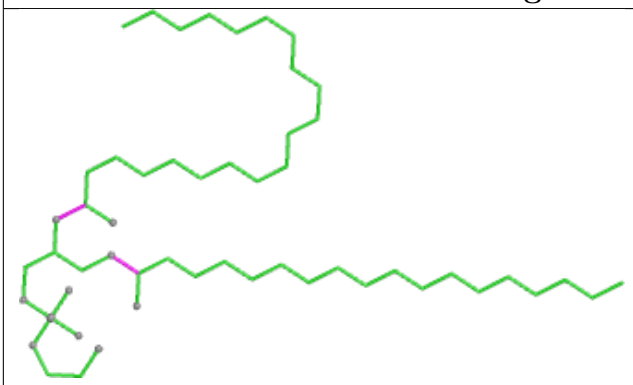


Torsions

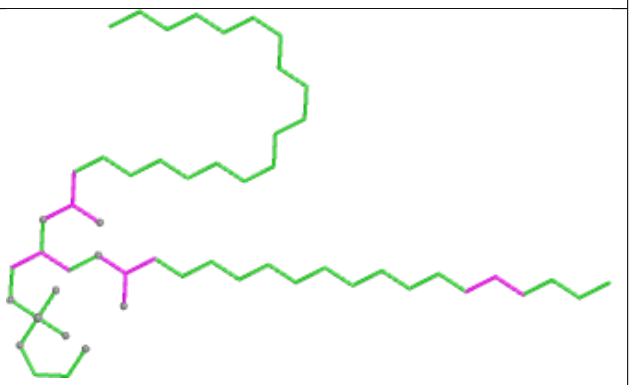


Rings

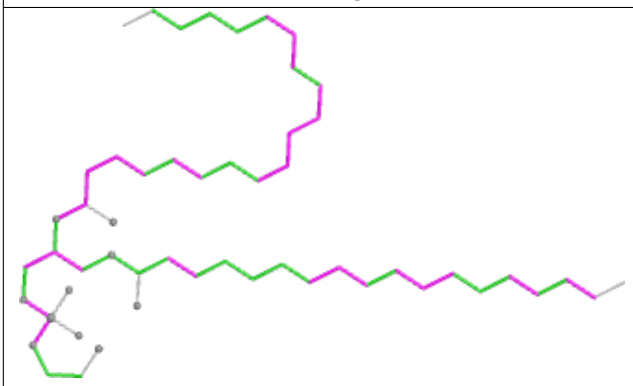
Ligand PEK P 307



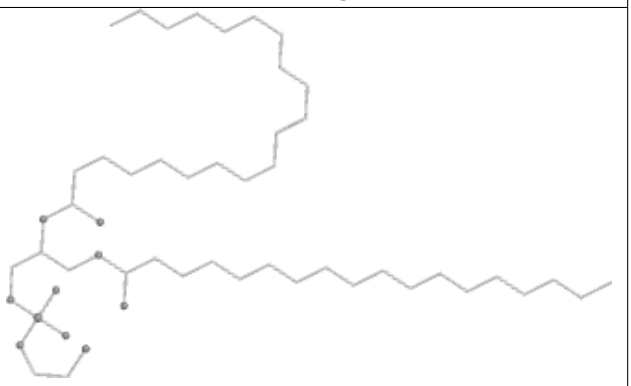
Bond lengths



Bond angles

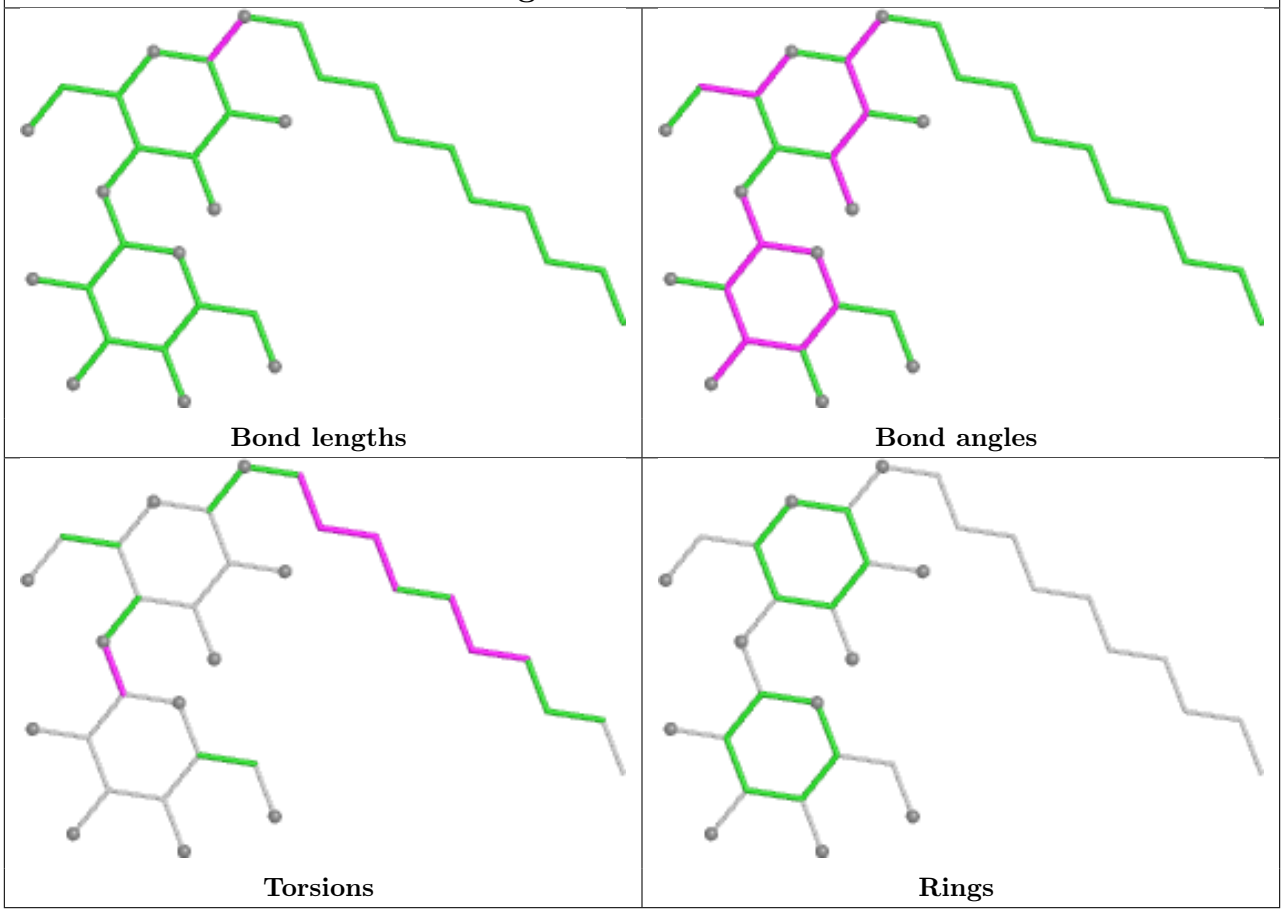


Torsions

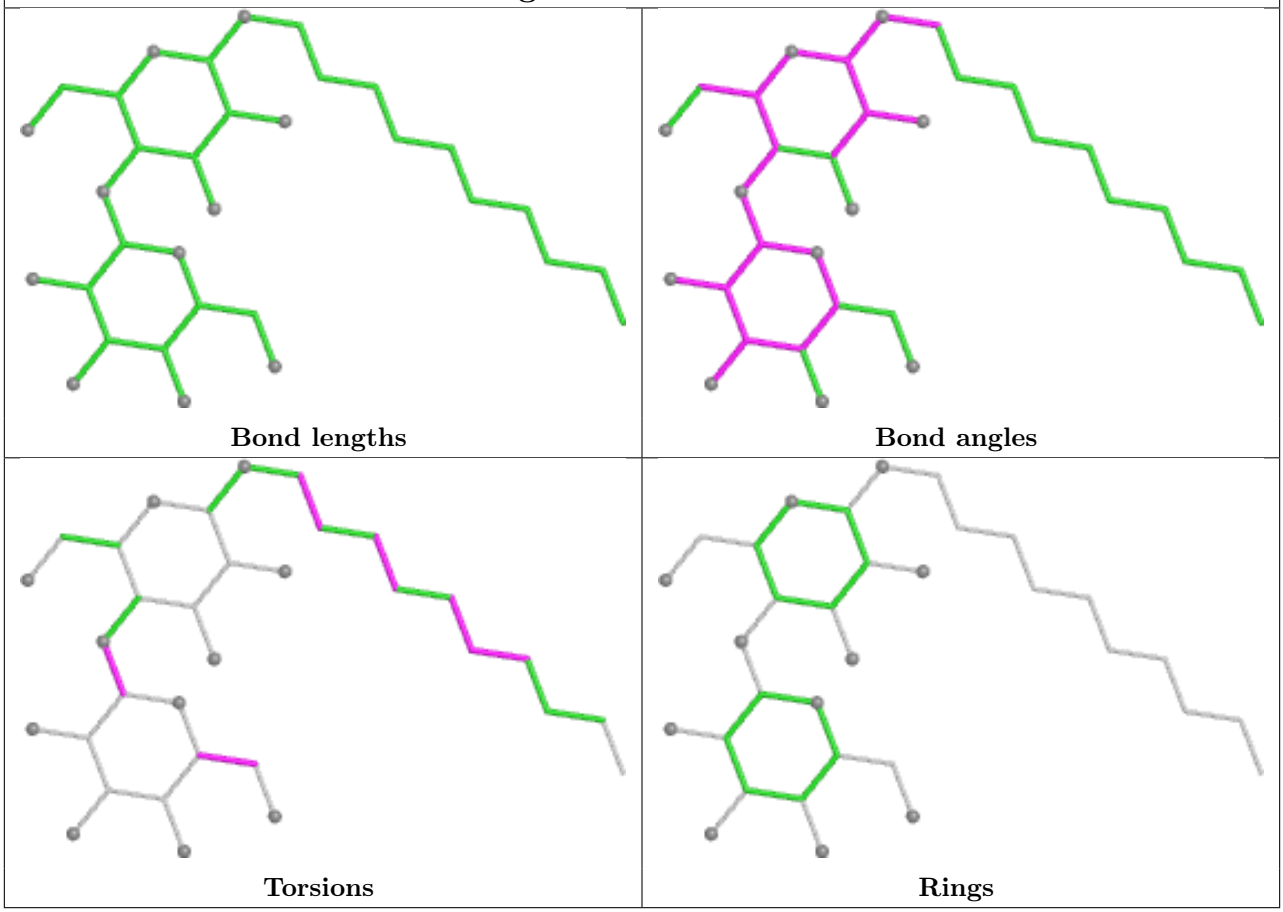


Rings

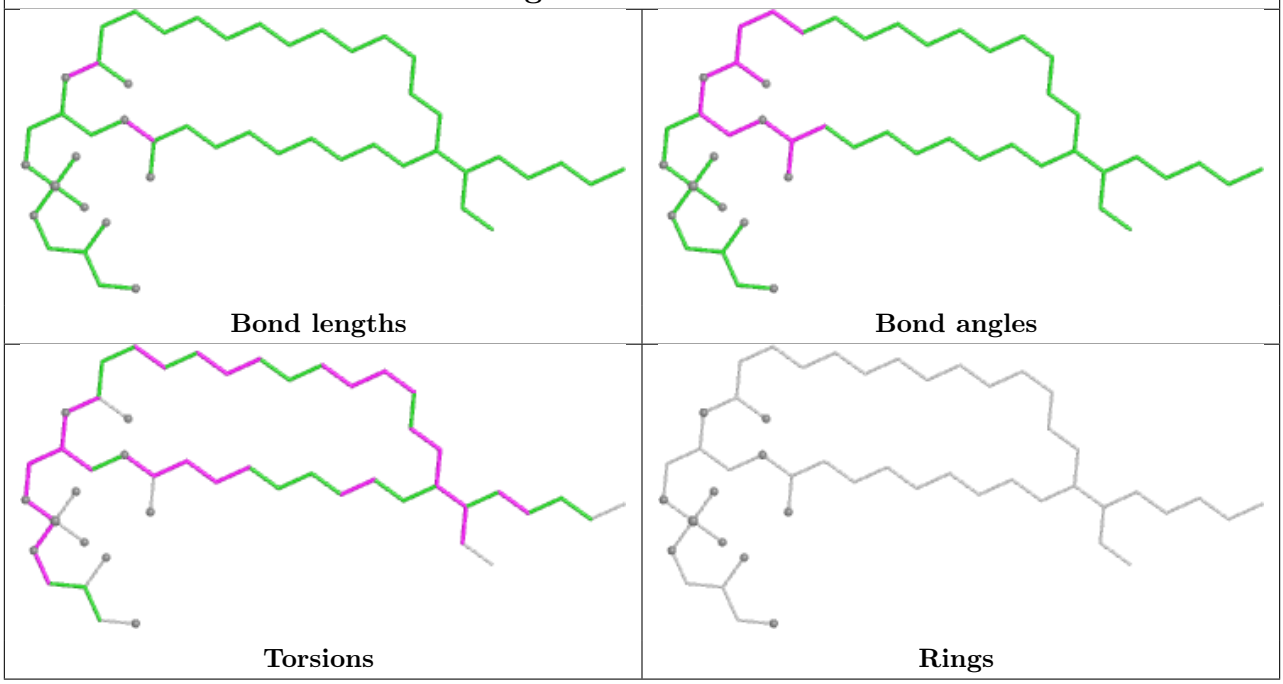
Ligand DMU C 310



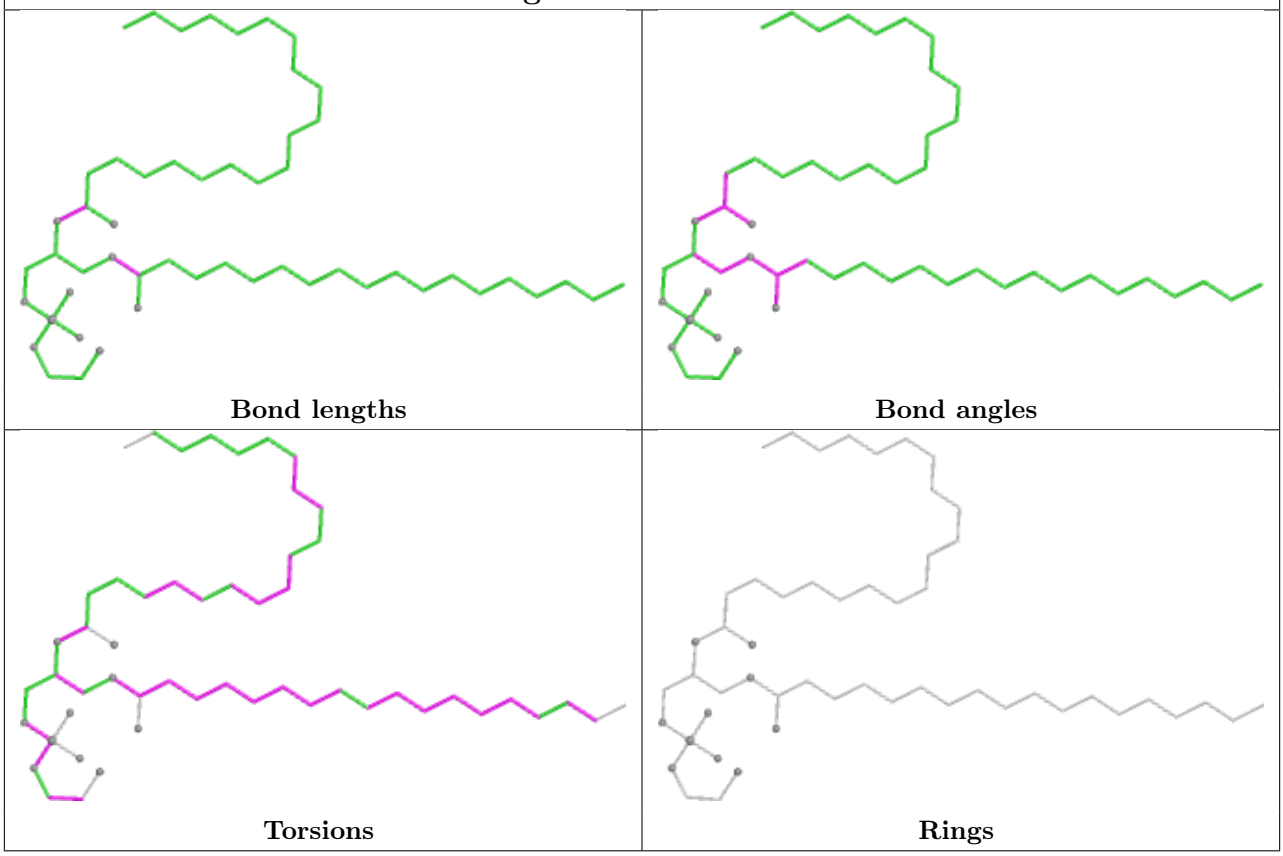
Ligand DMU P 308



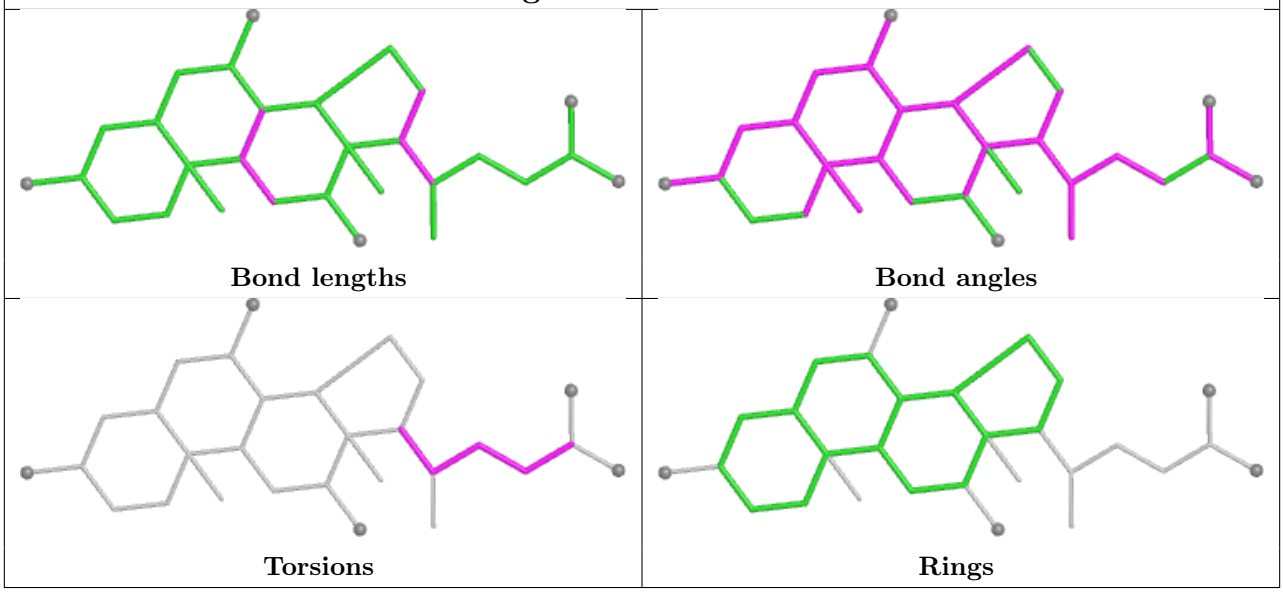
Ligand PGV Z 101



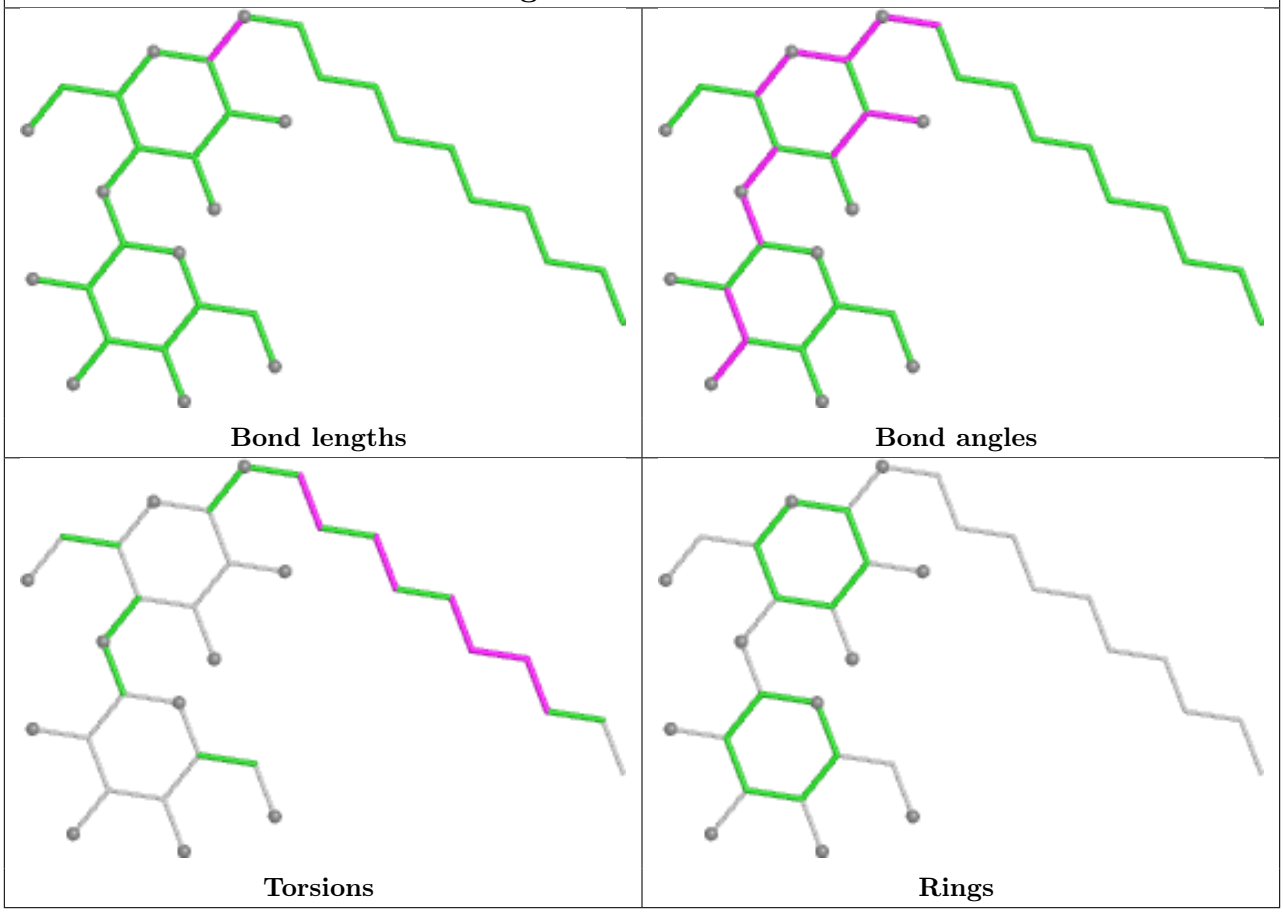
Ligand PEK G 102



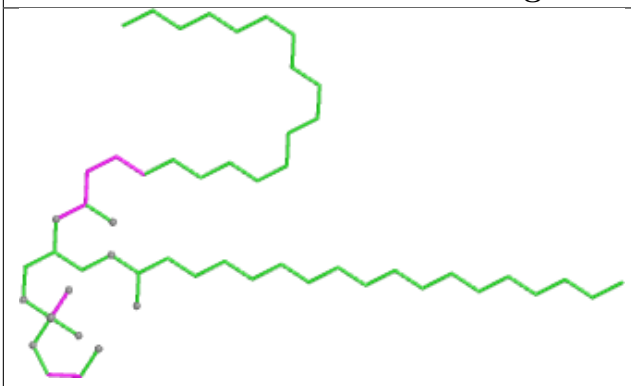
Ligand CHD P 305



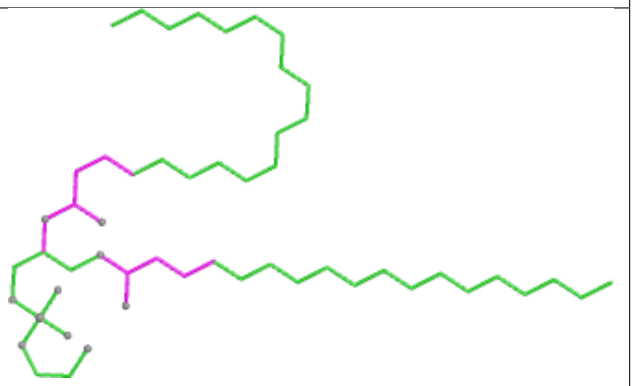
Ligand DMU Z 102



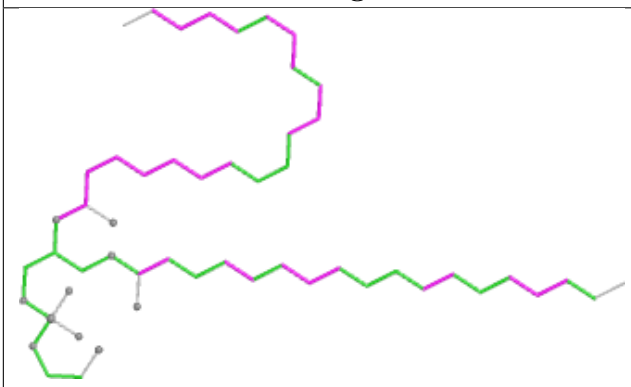
Ligand PEK T 102



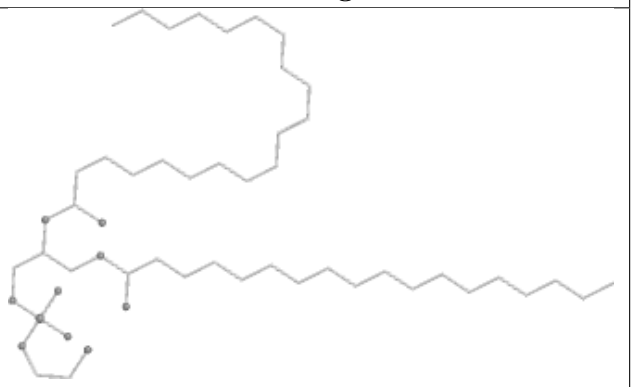
Bond lengths



Bond angles

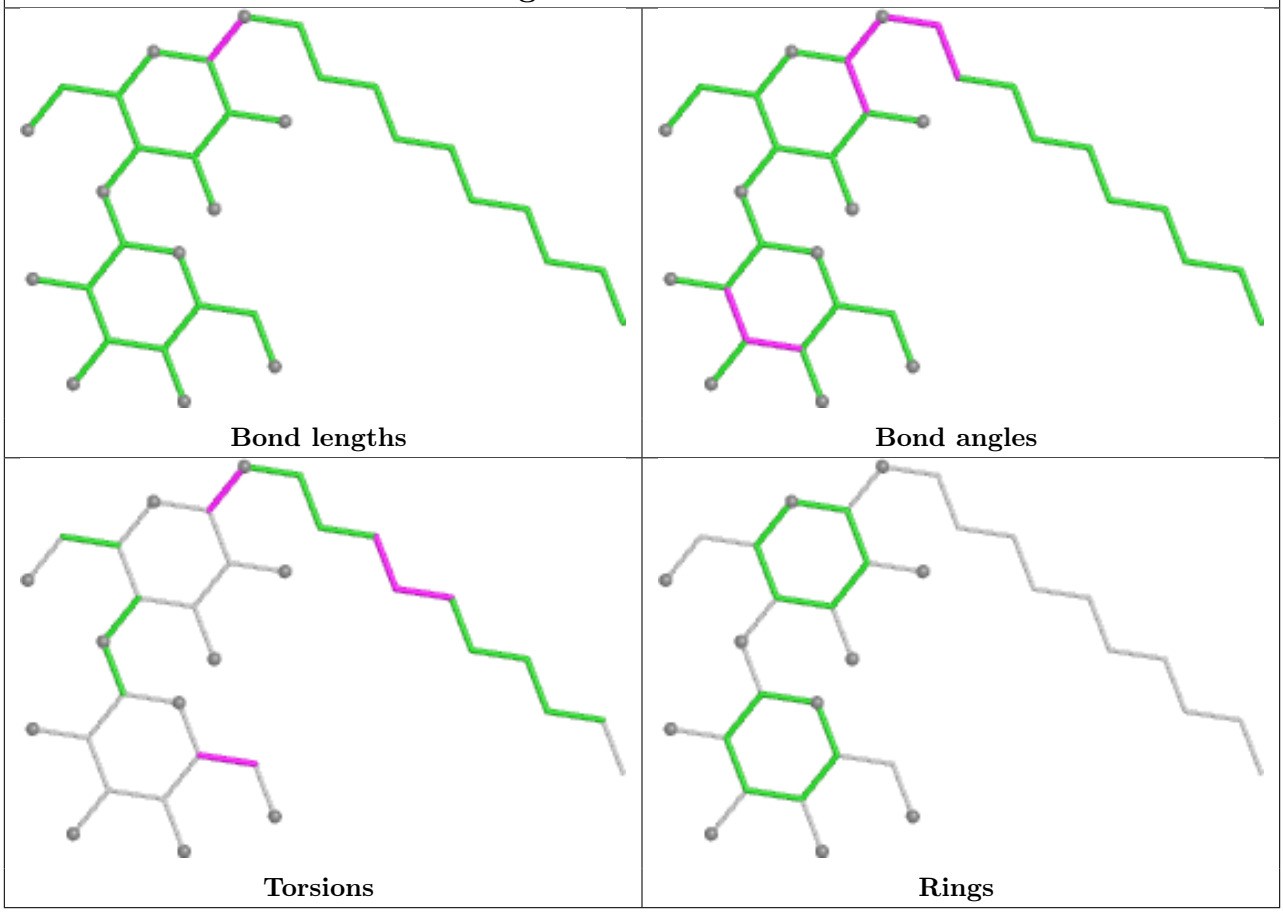


Torsions

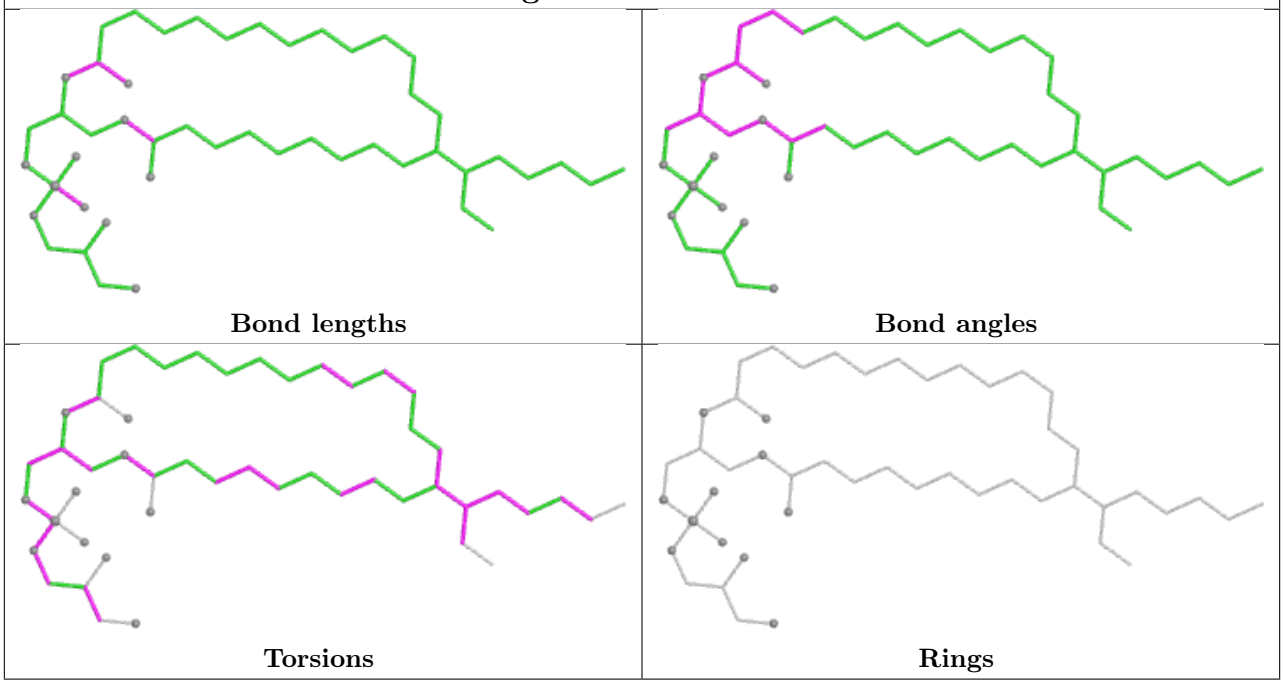


Rings

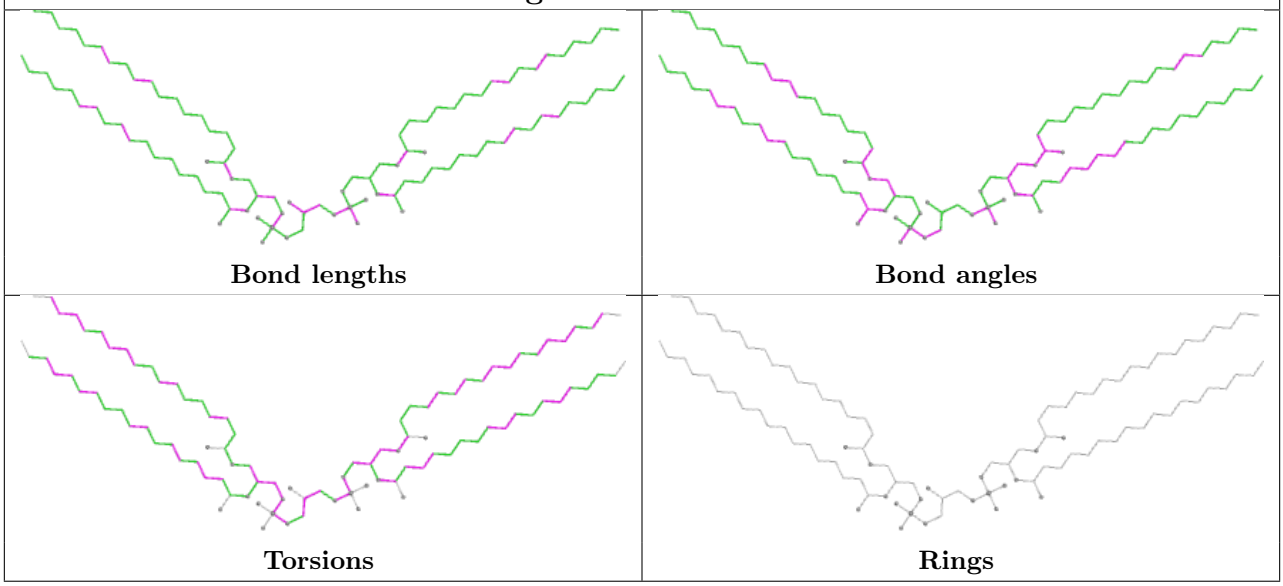
Ligand DMU P 306



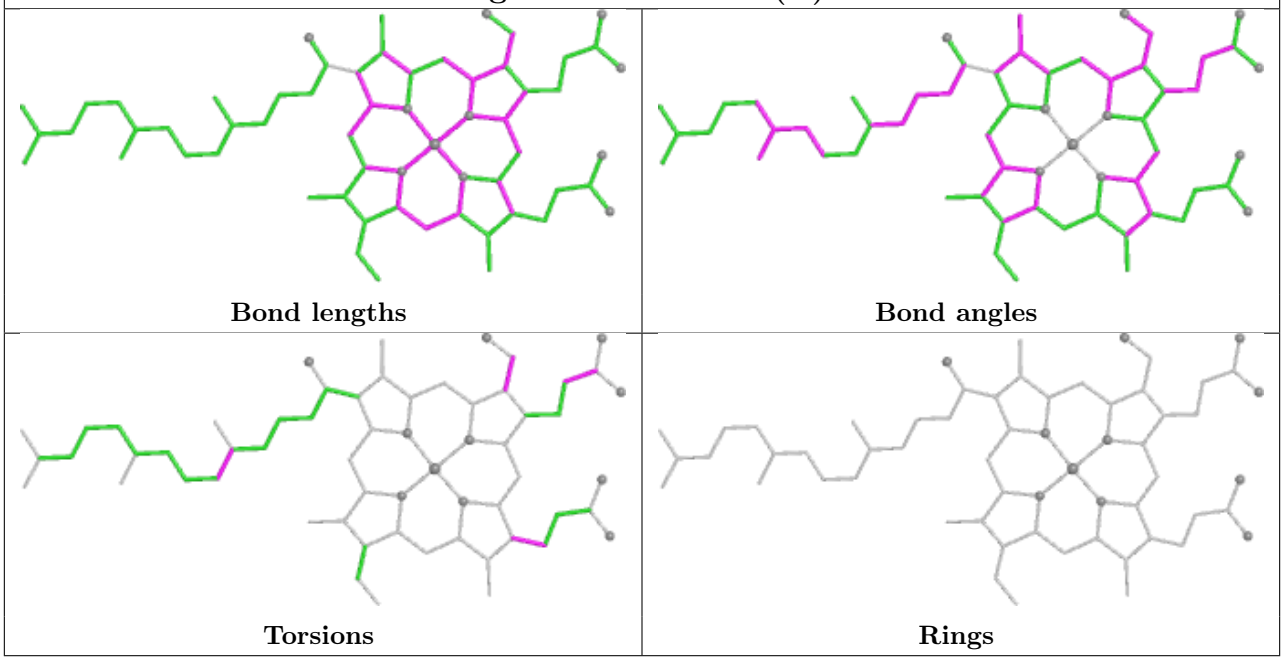
Ligand PGV A 610



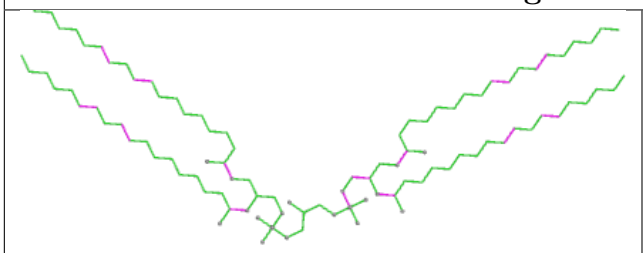
Ligand CDL P 304



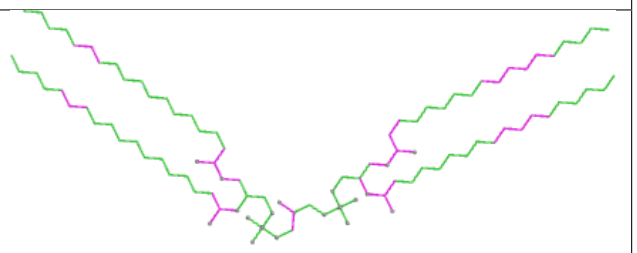
Ligand HEA N 603 (B)



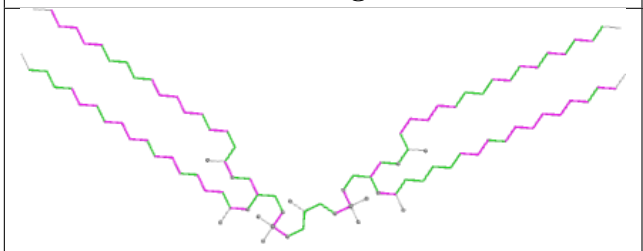
Ligand CDL N 601



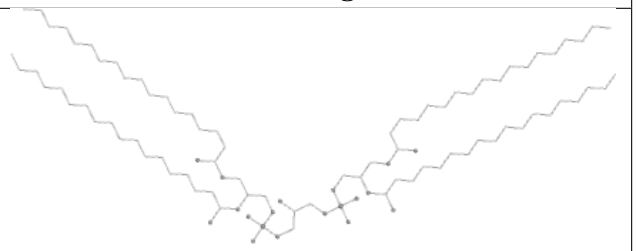
Bond lengths



Bond angles

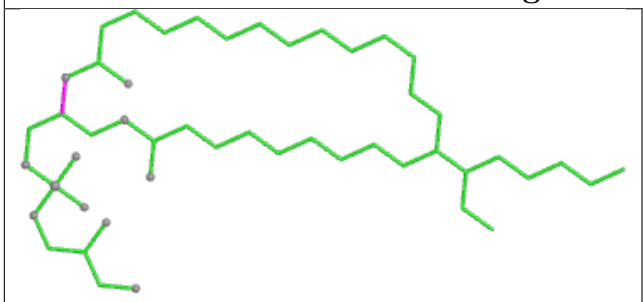


Torsions

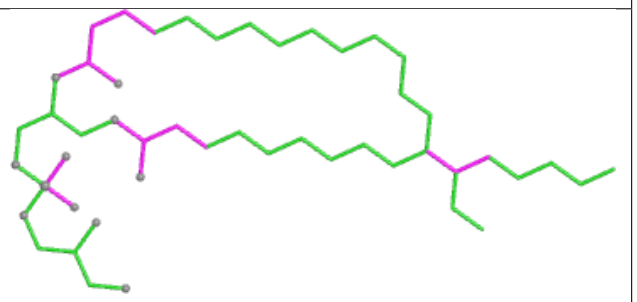


Rings

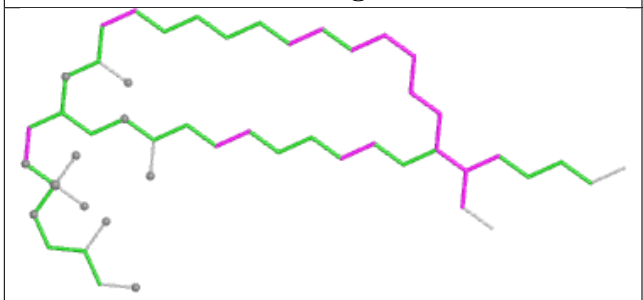
Ligand PGV C 305



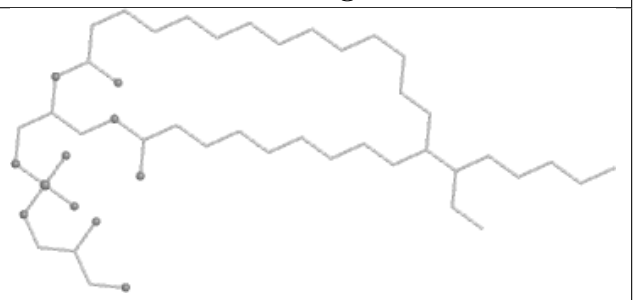
Bond lengths



Bond angles

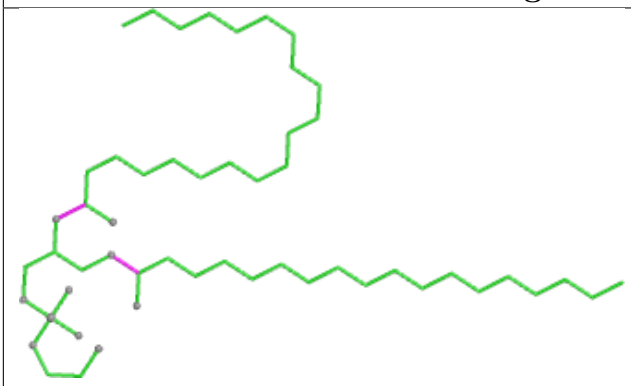


Torsions

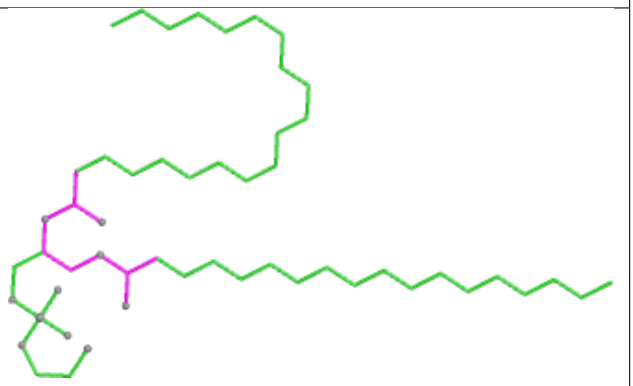


Rings

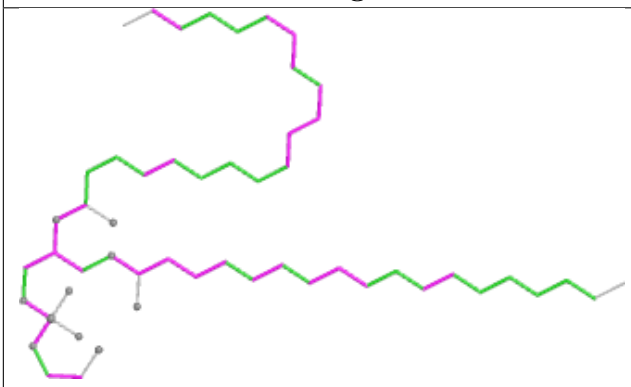
Ligand PEK T 101



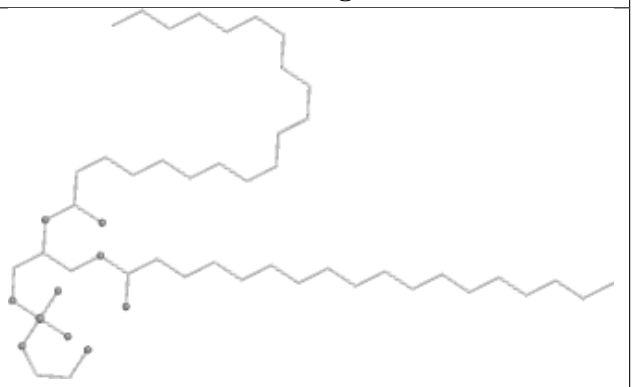
Bond lengths



Bond angles

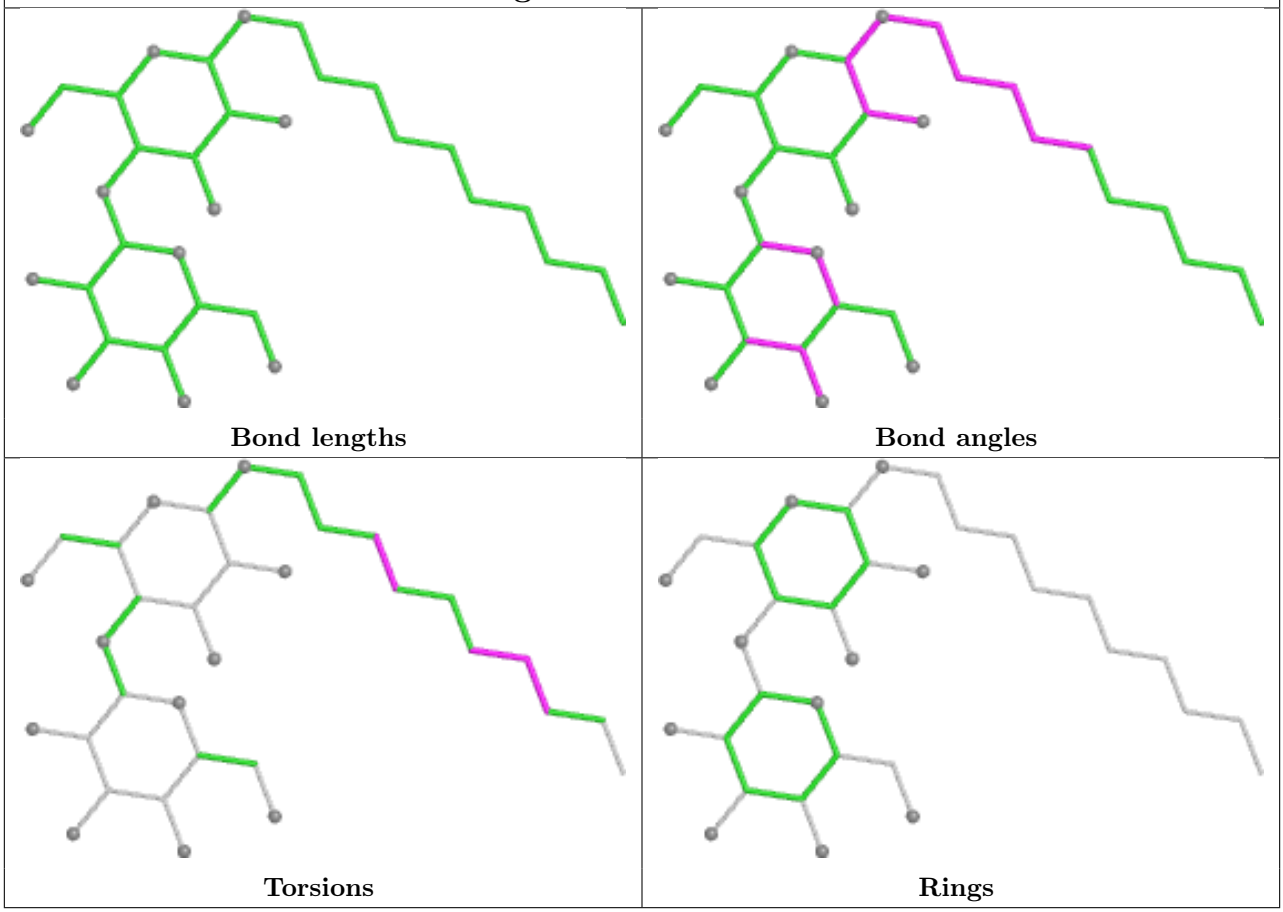


Torsions

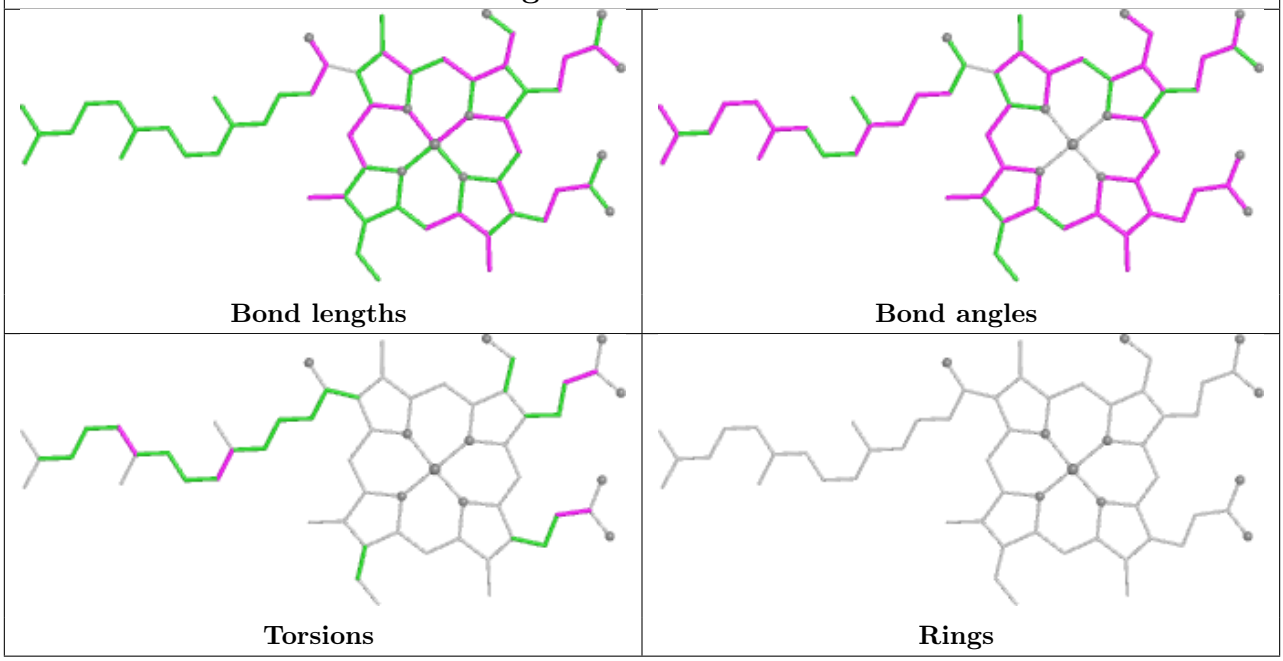


Rings

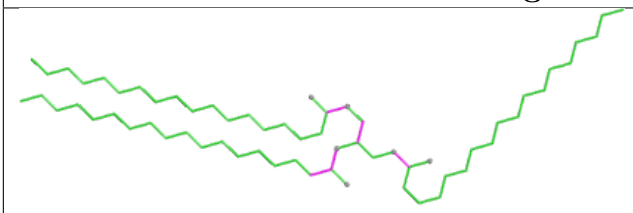
Ligand DMU M 101



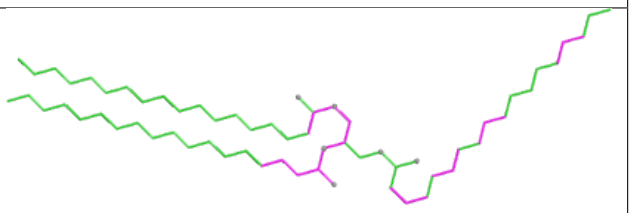
Ligand HEA N 602



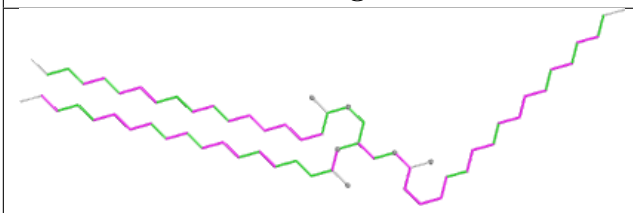
Ligand TGL Y 101



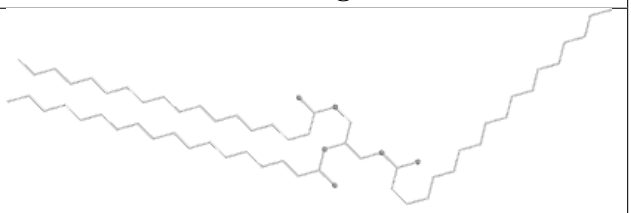
Bond lengths



Bond angles

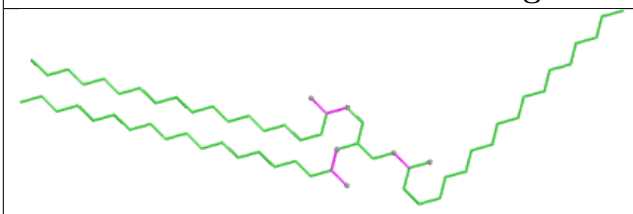


Torsions

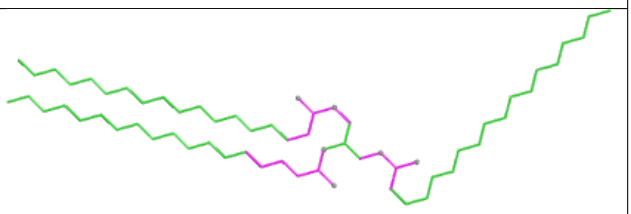


Rings

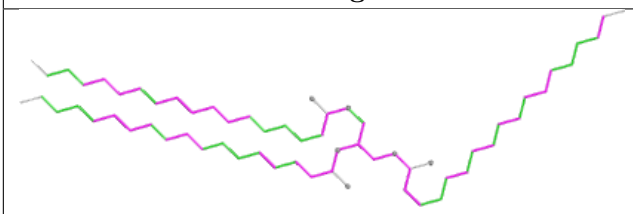
Ligand TGL D 201



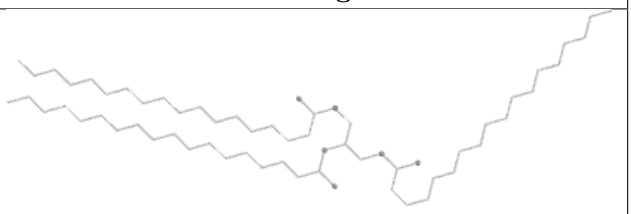
Bond lengths



Bond angles

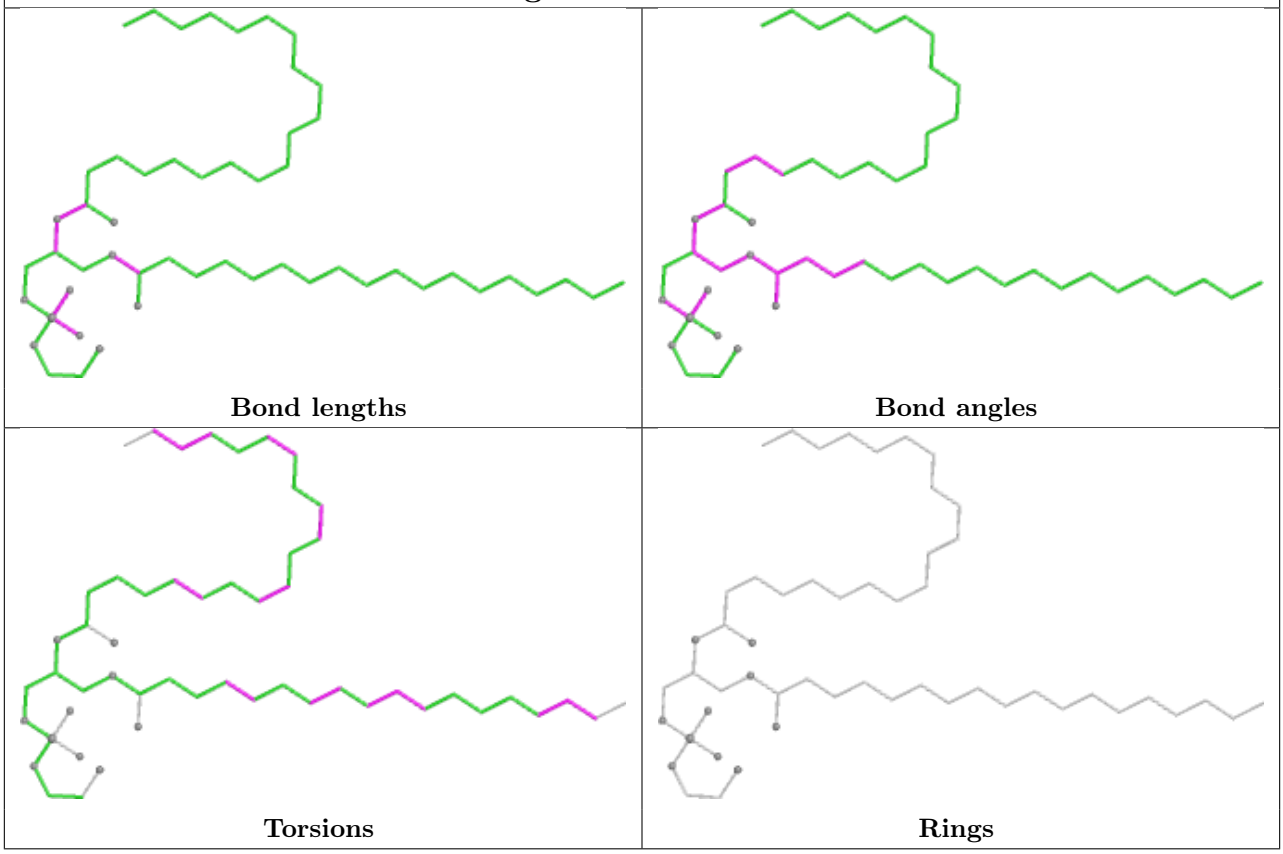


Torsions

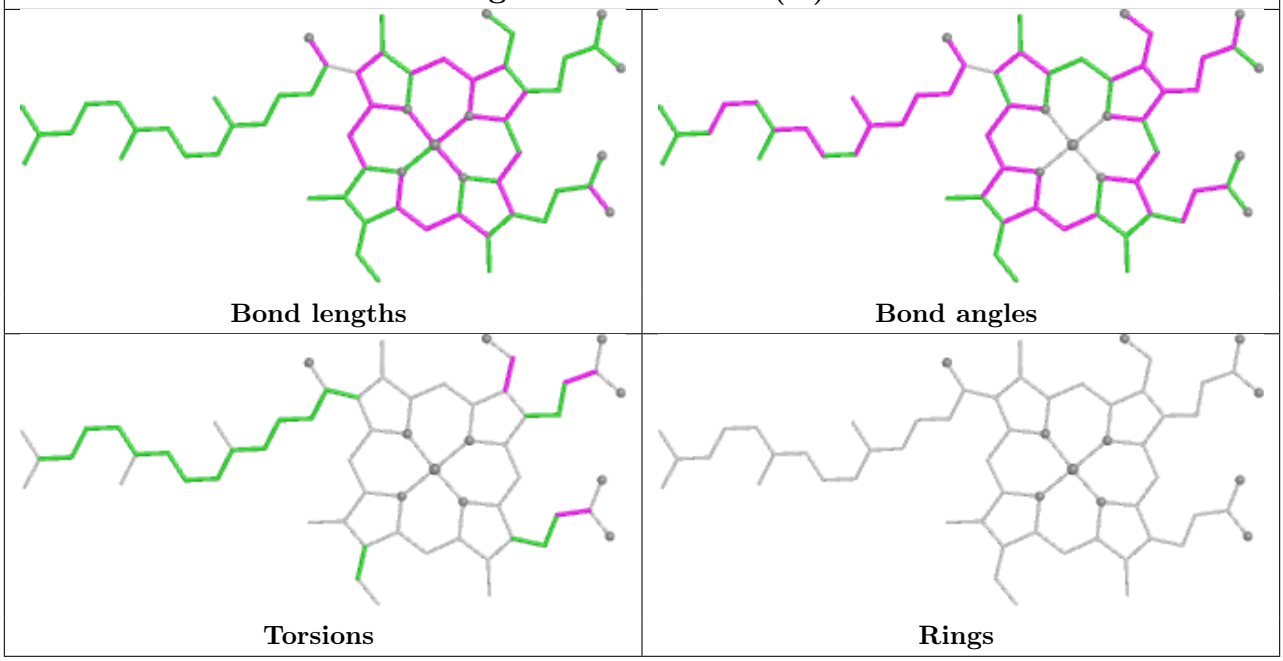


Rings

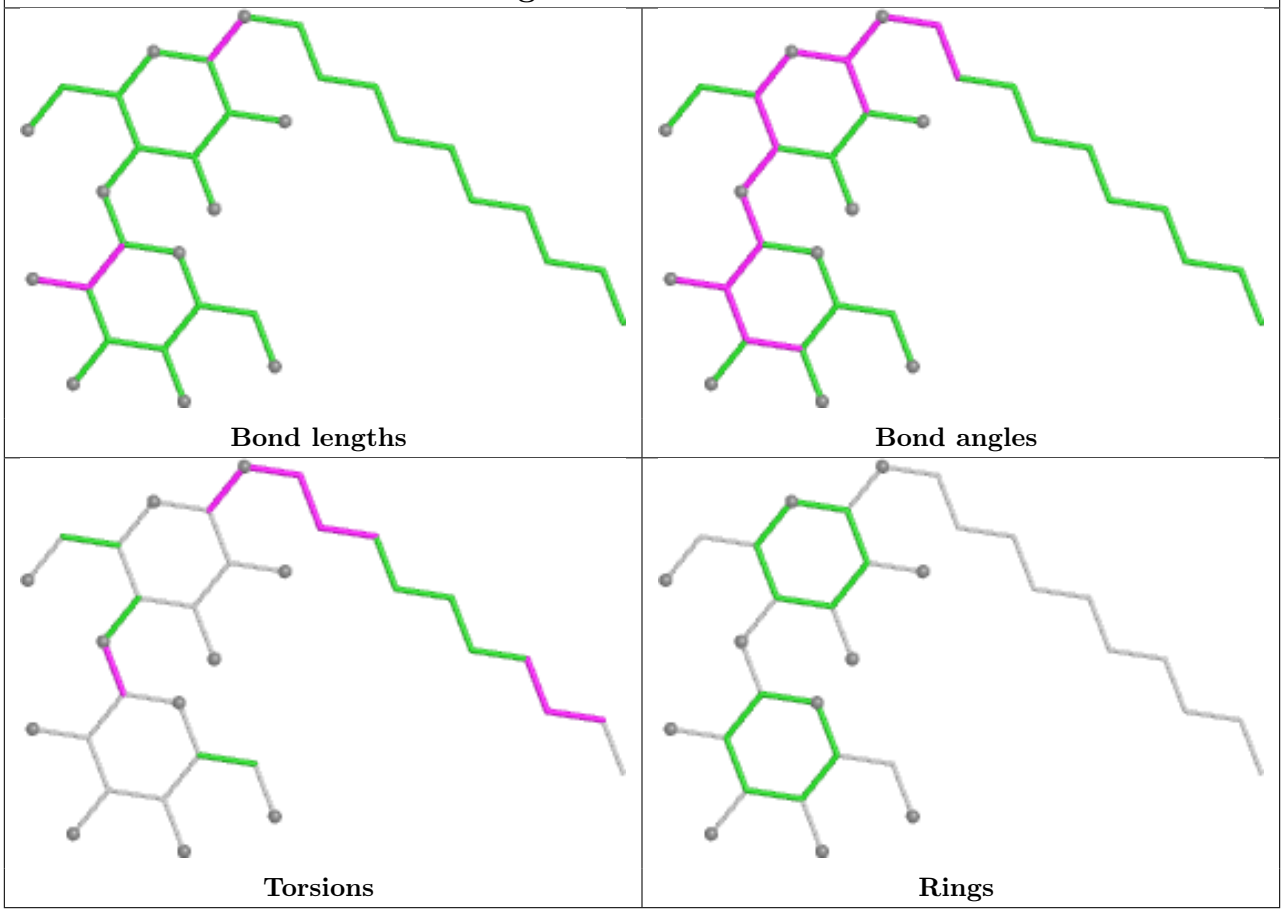
Ligand PEK C 304



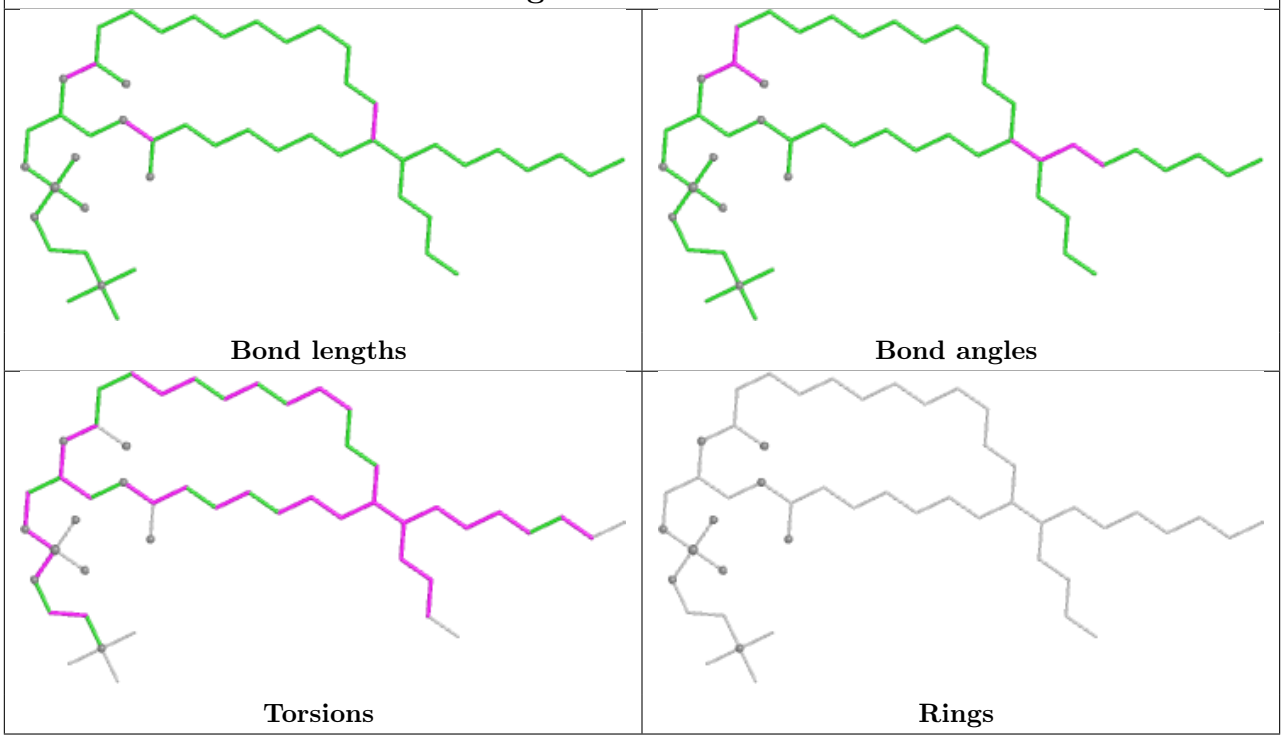
Ligand HEA N 603 (A)



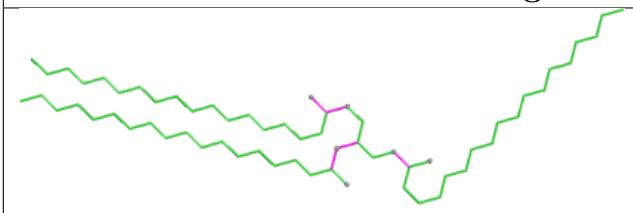
Ligand DMU C 311



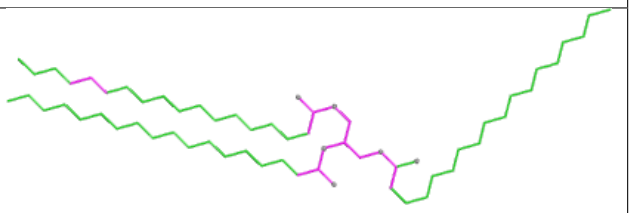
Ligand PSC O 302



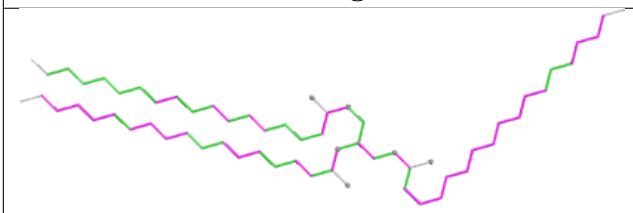
Ligand TGL A 608



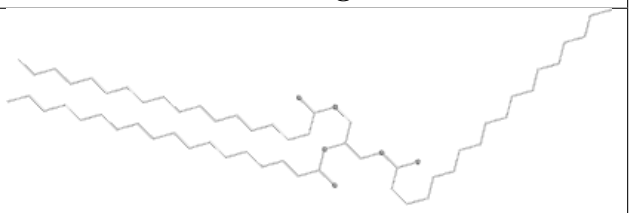
Bond lengths



Bond angles

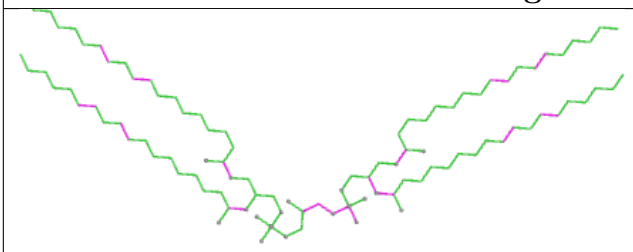


Torsions

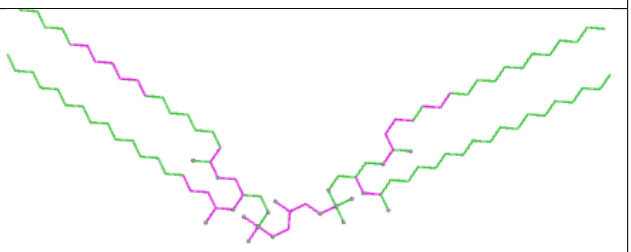


Rings

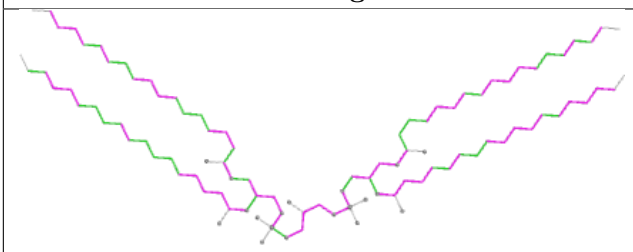
Ligand CDL C 306



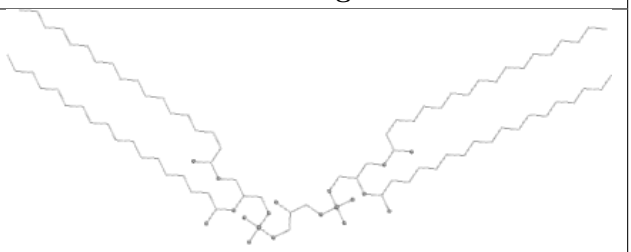
Bond lengths



Bond angles

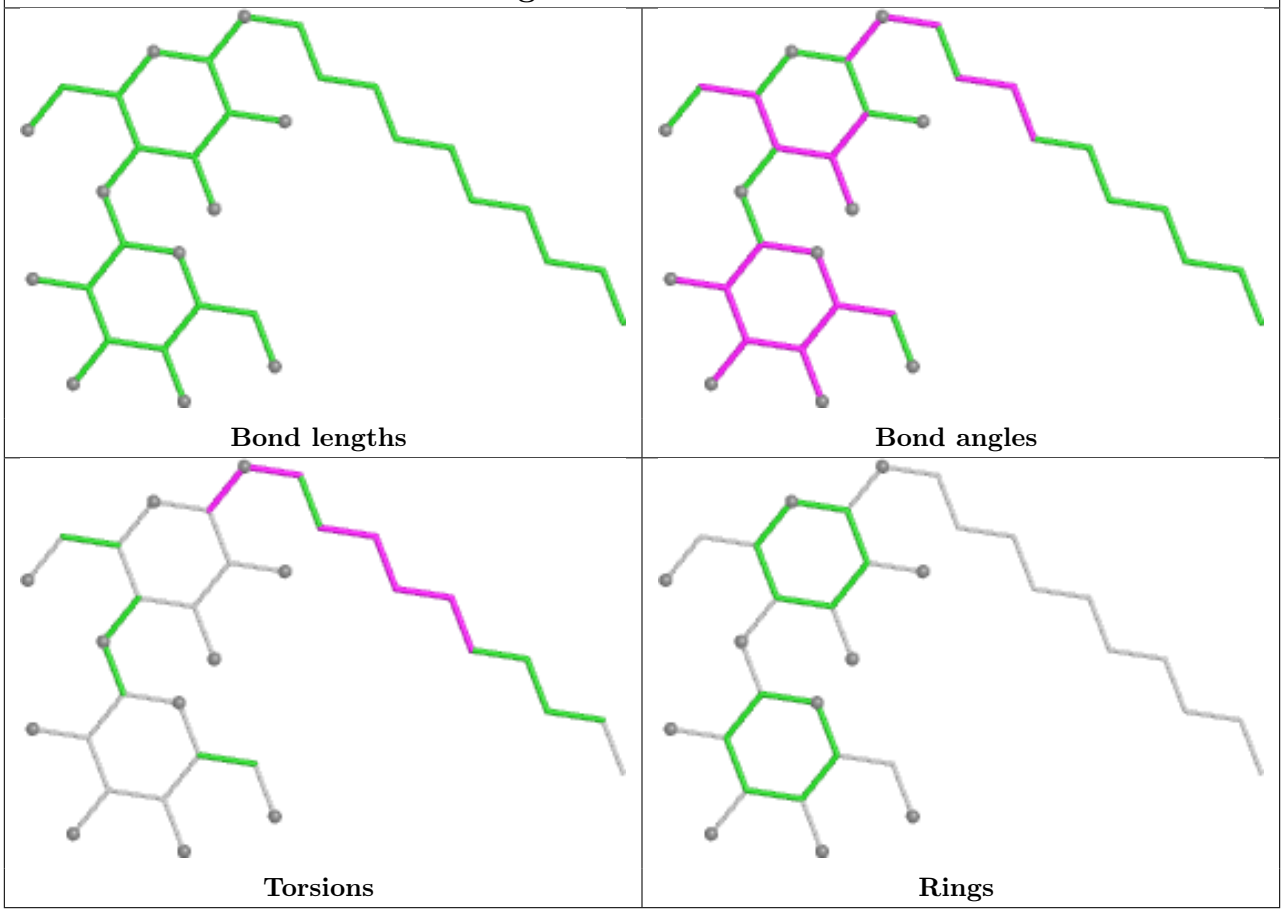


Torsions

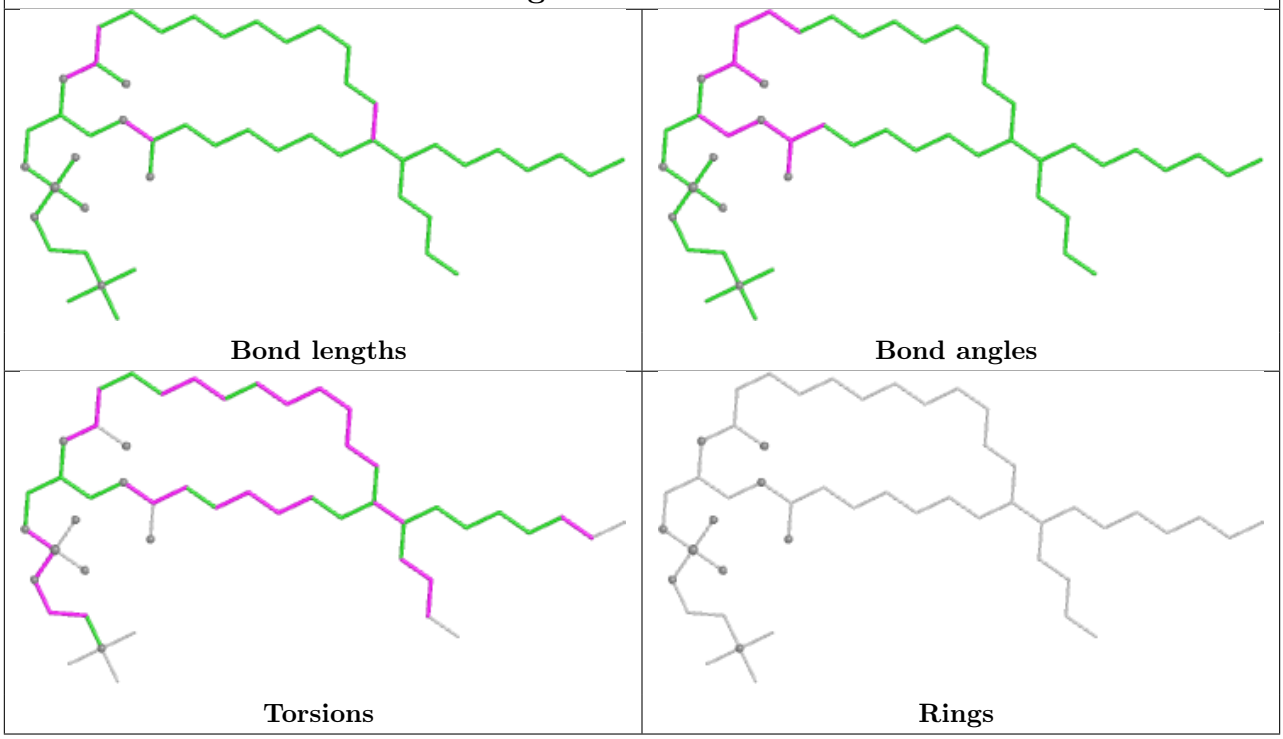


Rings

Ligand DMU C 302



Ligand PSC B 303



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%)	-0.52	3 (0%)	85	88	13, 30, 38, 76	22 (4%)
1	N	513/514 (99%)	-0.29	6 (1%)	76	80	16, 34, 44, 77	20 (3%)
2	B	226/227 (99%)	0.10	15 (6%)	24	26	20, 37, 57, 78	10 (4%)
2	O	226/227 (99%)	0.32	12 (5%)	32	35	23, 45, 69, 89	4 (1%)
3	C	259/261 (99%)	-0.30	3 (1%)	76	80	14, 33, 45, 84	9 (3%)
3	P	259/261 (99%)	-0.23	4 (1%)	72	76	14, 35, 46, 72	9 (3%)
4	D	144/147 (97%)	0.04	4 (2%)	55	58	18, 39, 60, 82	4 (2%)
4	Q	144/147 (97%)	0.71	8 (5%)	30	33	22, 53, 78, 152	3 (2%)
5	E	105/109 (96%)	-0.03	3 (2%)	53	57	31, 38, 63, 113	0
5	R	105/109 (96%)	0.14	2 (1%)	66	70	38, 46, 65, 120	0
6	F	98/98 (100%)	0.38	7 (7%)	22	24	19, 41, 95, 147	4 (4%)
6	S	98/98 (100%)	0.75	10 (10%)	12	12	20, 42, 104, 148	2 (2%)
7	G	83/85 (97%)	0.92	19 (22%)	2	2	32, 43, 113, 127	0
7	T	83/85 (97%)	1.04	19 (22%)	2	2	21, 43, 101, 133	1 (1%)
8	H	79/85 (92%)	0.52	7 (8%)	15	15	35, 45, 91, 104	0
8	U	79/85 (92%)	0.59	10 (12%)	8	7	39, 50, 102, 116	0
9	I	72/73 (98%)	0.81	11 (15%)	5	5	35, 49, 85, 92	0
9	V	72/73 (98%)	0.85	8 (11%)	10	10	36, 58, 83, 102	0
10	J	58/59 (98%)	0.51	5 (8%)	16	16	34, 44, 70, 107	0
10	W	58/59 (98%)	0.55	5 (8%)	16	16	25, 47, 72, 125	1 (1%)
11	K	49/56 (87%)	0.31	3 (6%)	27	29	38, 45, 59, 65	0
11	X	49/56 (87%)	0.62	4 (8%)	17	18	25, 55, 77, 82	1 (2%)
12	L	46/47 (97%)	-0.02	2 (4%)	40	43	25, 36, 56, 86	1 (2%)
12	Y	46/47 (97%)	0.45	2 (4%)	40	43	25, 45, 68, 107	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.16	3 (6%)	22	24	32, 36, 71, 103	0
13	Z	43/46 (93%)	0.44	2 (4%)	36	39	43, 50, 83, 142	0
All	All	3550/3614 (98%)	0.08	177 (4%)	34	37	13, 38, 71, 152	92 (2%)

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	10.4
4	Q	6	VAL	9.2
4	Q	5	VAL	8.4
6	S	96	LEU	7.7
6	F	1	ALA	7.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.60	0.19	101,116,124,132	0
7	TPO	T	11	11/12	0.62	0.23	109,118,139,142	0
7	TPO	G	11	11/12	0.69	0.26	92,121,130,132	0
9	SAC	I	1	9/10	0.72	0.18	70,80,87,89	0
1	FME	N	1	10/11	0.91	0.13	47,56,74,79	0
1	FME	A	1	10/11	0.92	0.12	41,50,81,95	0
2	FME	O	1	10/11	0.96	0.09	41,42,54,65	0
2	FME	B	1	10/11	0.97	0.08	33,35,45,66	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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	J	101	29/29	0.59	0.24	99,135,149,150	0
21	EDO	C	319	4/4	0.69	0.21	81,98,105,107	0
27	PEK	T	101	53/53	0.72	0.26	51,87,154,155	0
22	CHD	W	101	29/29	0.73	0.24	69,124,145,148	0
25	DMU	C	310	33/33	0.77	0.16	56,82,112,121	0
25	DMU	L	102	33/33	0.77	0.19	54,93,139,139	0
27	PEK	G	102	53/53	0.77	0.23	52,95,154,154	0
21	EDO	R	205	4/4	0.77	0.18	57,58,61,75	0
21	EDO	D	204	4/4	0.78	0.23	65,69,81,85	0
21	EDO	A	619	4/4	0.78	0.21	50,57,58,83	0
25	DMU	C	311	33/33	0.79	0.19	56,82,119,129	0
25	DMU	P	306	33/33	0.79	0.16	47,79,120,123	0
28	CDL	P	304	100/100	0.79	0.27	43,87,119,134	0
28	CDL	T	103	100/100	0.79	0.25	54,88,145,159	0
25	DMU	P	308	33/33	0.80	0.16	55,78,101,105	0
21	EDO	C	318	4/4	0.80	0.21	58,86,90,94	0
21	EDO	A	612	4/4	0.80	0.22	52,61,65,67	0
28	CDL	N	601	100/100	0.80	0.27	57,90,140,159	0
20	PGV	G	103	51/51	0.80	0.23	53,83,119,139	0
25	DMU	C	302	33/33	0.80	0.18	35,79,111,124	0
19	TGL	A	608	63/63	0.81	0.24	43,79,109,121	0
25	DMU	P	309	33/33	0.81	0.14	65,87,106,112	0
27	PEK	C	308	53/53	0.81	0.22	49,80,136,148	0
19	TGL	Q	201	63/63	0.81	0.25	52,76,98,109	0
21	EDO	H	101	4/4	0.81	0.21	54,57,67,73	0
21	EDO	Q	203	4/4	0.81	0.21	81,81,88,91	0
19	TGL	Y	101	63/63	0.81	0.26	48,78,110,148	0
20	PGV	C	309	51/51	0.81	0.22	45,78,121,151	0
27	PEK	P	307	53/53	0.82	0.22	45,78,128,145	0
21	EDO	N	622	4/4	0.82	0.21	55,58,81,101	0
24	PSC	B	303	52/52	0.82	0.23	42,85,156,156	0
24	PSC	O	302	52/52	0.82	0.24	48,84,160,160	0
20	PGV	A	610	51/51	0.82	0.23	36,72,112,121	0
21	EDO	C	315	4/4	0.83	0.21	60,75,77,79	0
19	TGL	N	610	63/63	0.83	0.23	52,82,110,122	0
21	EDO	V	101	4/4	0.83	0.19	62,68,74,75	0
28	CDL	C	306	100/100	0.84	0.20	40,80,115,128	0
22	CHD	P	305	29/29	0.84	0.14	53,65,71,76	0
20	PGV	Z	101	51/51	0.84	0.22	51,83,138,144	0
21	EDO	F	105	4/4	0.84	0.23	69,74,77,78	0
19	TGL	L	101	63/63	0.85	0.26	36,64,99,119	0
21	EDO	D	203	4/4	0.85	0.18	55,61,73,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	H	102	4/4	0.85	0.20	68,73,79,94	0
22	CHD	C	307	29/29	0.85	0.14	52,65,72,75	0
21	EDO	C	313	4/4	0.85	0.15	77,84,85,95	0
21	EDO	P	313	4/4	0.85	0.19	54,62,70,73	0
21	EDO	R	201	4/4	0.86	0.20	57,61,66,72	0
19	TGL	D	201	63/63	0.86	0.22	37,67,90,97	0
21	EDO	A	616	4/4	0.87	0.16	46,47,50,50	0
21	EDO	R	202	4/4	0.88	0.17	61,67,72,78	0
21	EDO	A	617	4/4	0.88	0.17	49,53,56,62	0
21	EDO	L	103	4/4	0.88	0.22	71,75,76,99	0
21	EDO	A	614	4/4	0.88	0.21	59,69,74,83	0
21	EDO	R	203	4/4	0.89	0.14	53,63,69,73	0
21	EDO	N	619	4/4	0.89	0.16	50,53,59,62	0
21	EDO	U	101	4/4	0.89	0.17	66,70,70,84	0
21	EDO	G	104	4/4	0.89	0.18	56,67,71,89	0
21	EDO	C	317	4/4	0.89	0.17	68,69,71,84	0
21	EDO	A	621	4/4	0.90	0.15	38,52,62,68	0
21	EDO	D	206	4/4	0.90	0.21	54,62,67,73	0
21	EDO	N	614	4/4	0.90	0.15	56,59,66,69	0
21	EDO	S	103	4/4	0.90	0.13	44,56,72,72	0
25	DMU	Z	102	33/33	0.90	0.12	50,60,75,78	0
26	UNX	C	303	1/1	0.90	0.14	28,28,28,28	0
21	EDO	E	203	4/4	0.90	0.12	50,59,66,70	0
21	EDO	D	202	4/4	0.91	0.13	44,51,52,68	0
21	EDO	E	205	4/4	0.91	0.16	60,63,68,78	0
21	EDO	A	620	4/4	0.91	0.16	64,64,67,70	0
21	EDO	R	206	4/4	0.91	0.13	47,52,58,63	0
21	EDO	D	207	4/4	0.91	0.19	62,66,70,75	0
21	EDO	N	618	4/4	0.91	0.14	60,63,67,70	0
21	EDO	E	201	4/4	0.92	0.12	43,46,56,58	0
21	EDO	C	314	4/4	0.92	0.12	60,64,67,85	0
21	EDO	A	618	4/4	0.92	0.15	43,68,78,83	0
21	EDO	N	617	4/4	0.93	0.13	50,53,53,57	0
21	EDO	A	615	4/4	0.93	0.12	25,30,31,46	0
26	UNX	P	302	1/1	0.93	0.19	28,28,28,28	0
21	EDO	F	104	4/4	0.93	0.12	50,52,62,64	0
21	EDO	J	102	4/4	0.93	0.17	52,75,78,81	0
21	EDO	O	305	4/4	0.93	0.10	67,74,79,79	0
21	EDO	P	310	4/4	0.93	0.15	36,42,48,59	0
21	EDO	P	312	4/4	0.93	0.14	52,60,72,75	0
21	EDO	A	623	4/4	0.93	0.14	55,57,62,63	0
21	EDO	N	611	4/4	0.93	0.16	72,73,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	A	613	4/4	0.93	0.12	35,37,39,41	0
21	EDO	T	104	4/4	0.94	0.13	39,41,42,49	0
21	EDO	O	304	4/4	0.94	0.12	63,67,67,83	0
21	EDO	N	613	4/4	0.94	0.13	42,49,49,54	0
25	DMU	M	101	33/33	0.94	0.10	43,50,62,73	0
21	EDO	N	621	4/4	0.94	0.12	48,51,51,71	0
21	EDO	N	612	4/4	0.94	0.18	36,41,53,64	0
18	AZI	N	608	3/3	0.95	0.10	39,39,39,41	0
18	AZI	A	607	3/3	0.95	0.18	34,34,37,37	0
21	EDO	N	615	4/4	0.95	0.12	38,39,43,47	0
27	PEK	T	102	53/53	0.95	0.14	34,51,84,97	0
21	EDO	N	616	4/4	0.95	0.09	34,37,38,39	0
21	EDO	B	305	4/4	0.95	0.12	35,45,53,55	0
27	PEK	C	304	53/53	0.95	0.12	32,49,84,106	0
21	EDO	C	316	4/4	0.95	0.13	41,61,67,70	0
21	EDO	F	103	4/4	0.96	0.10	40,41,42,45	0
22	CHD	C	301	29/29	0.96	0.07	30,33,37,40	0
21	EDO	A	611	4/4	0.96	0.14	39,44,46,56	0
21	EDO	C	312	4/4	0.96	0.12	42,42,45,45	0
22	CHD	P	301	29/29	0.96	0.07	31,36,39,46	0
20	PGV	N	609	51/51	0.96	0.11	30,40,71,77	0
21	EDO	E	204	4/4	0.96	0.07	43,44,47,50	0
21	EDO	N	620	4/4	0.96	0.11	49,59,67,73	0
21	EDO	Q	202	4/4	0.96	0.12	62,66,69,69	0
21	EDO	C	320	4/4	0.96	0.12	37,45,48,63	0
20	PGV	C	305	51/51	0.97	0.11	29,38,92,108	0
21	EDO	B	304	4/4	0.97	0.08	32,33,38,40	0
21	EDO	P	311	4/4	0.97	0.09	44,44,47,48	0
16	MG	N	605	1/1	0.97	0.05	35,35,35,35	0
21	EDO	D	205	4/4	0.97	0.08	40,41,58,58	0
20	PGV	A	609	51/51	0.97	0.10	27,38,69,73	0
22	CHD	B	301	29/29	0.97	0.07	29,33,36,44	0
18	AZI	N	607	3/3	0.97	0.08	39,39,40,42	0
21	EDO	A	622	4/4	0.97	0.10	37,45,60,64	0
21	EDO	O	303	4/4	0.97	0.11	41,41,42,44	0
21	EDO	E	202	4/4	0.97	0.09	44,46,46,48	0
21	EDO	R	204	4/4	0.97	0.09	45,49,49,50	0
21	EDO	S	102	4/4	0.98	0.08	33,34,36,36	0
14	HEA	N	603[A]	60/60	0.98	0.06	24,27,33,35	60
14	HEA	N	603[B]	60/60	0.98	0.06	26,33,45,47	60
14	HEA	A	602[A]	60/60	0.98	0.06	21,27,31,36	60
21	EDO	G	105	4/4	0.98	0.06	35,38,42,44	0

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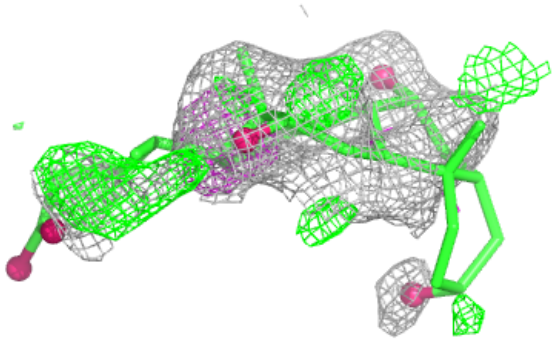
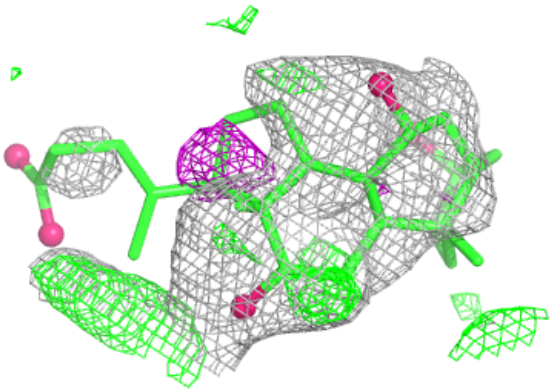
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	AZI	A	606	3/3	0.98	0.10	33,33,36,36	0
20	PGV	P	303	51/51	0.98	0.09	31,40,77,86	0
14	HEA	A	602[B]	60/60	0.98	0.06	21,26,35,39	60
22	CHD	G	101	29/29	0.98	0.05	32,34,38,43	0
17	NA	A	605	1/1	0.99	0.03	32,32,32,32	0
17	NA	N	606	1/1	0.99	0.05	39,39,39,39	0
14	HEA	N	602	60/60	0.99	0.07	28,34,56,65	0
16	MG	A	604	1/1	0.99	0.03	28,28,28,28	0
14	HEA	A	601	60/60	0.99	0.06	23,28,49,51	0
21	EDO	F	102	4/4	0.99	0.06	29,31,31,33	0
23	CUA	O	301	2/2	1.00	0.02	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.01	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.01	30,30,30,30	0
23	CUA	B	302	2/2	1.00	0.02	30,30,30,31	0
29	ZN	F	101	1/1	1.00	0.02	36,36,36,36	0
29	ZN	S	101	1/1	1.00	0.03	38,38,38,38	0

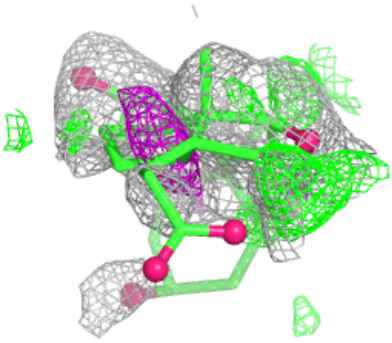
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD 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)

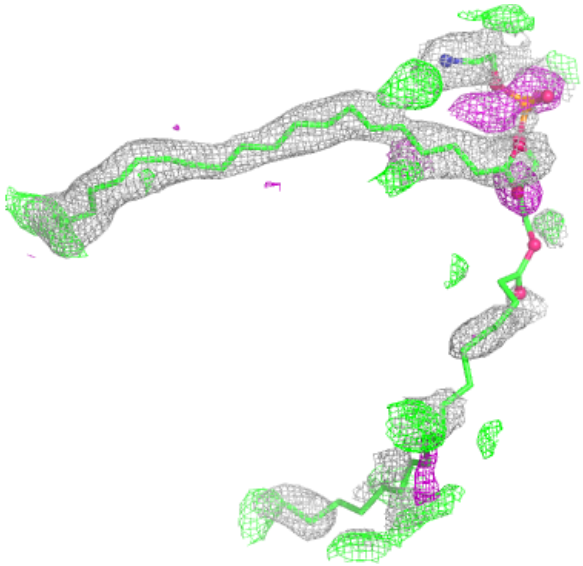


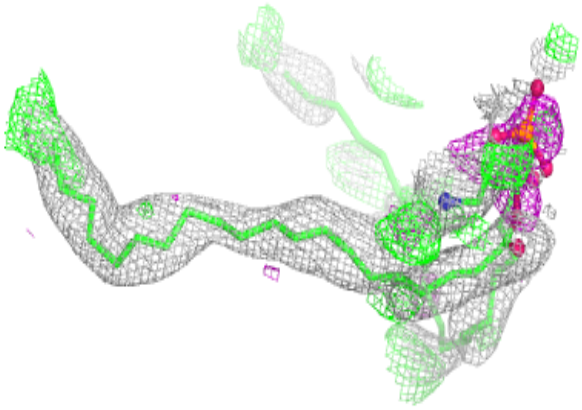


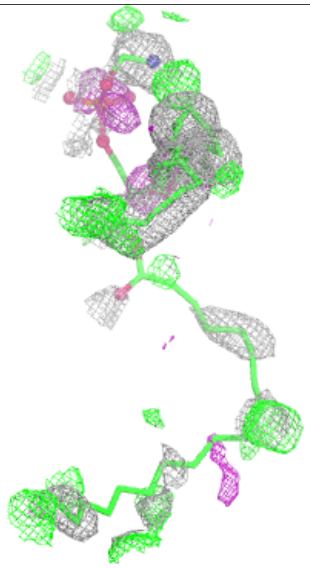


Electron density around PEK T 101:

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

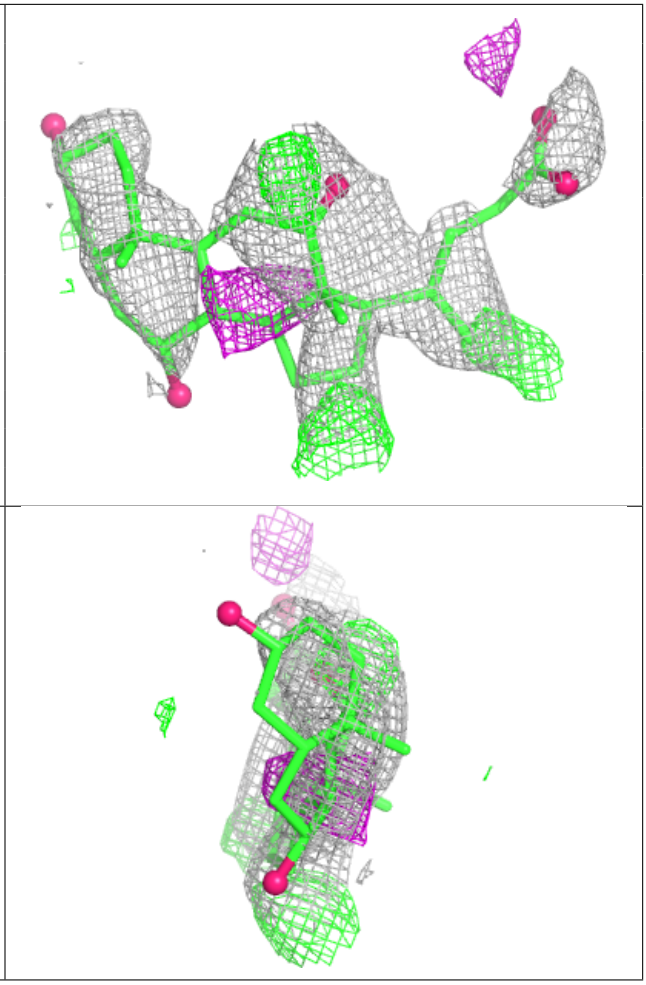






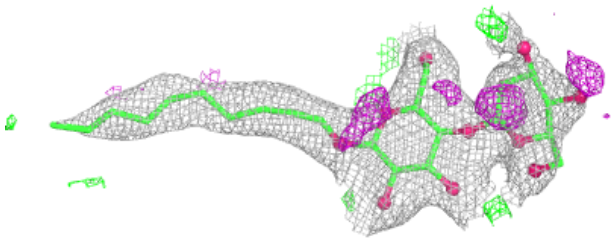
Electron density around CHD W 101:

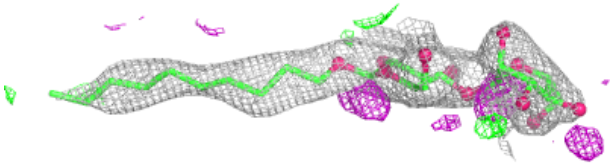
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

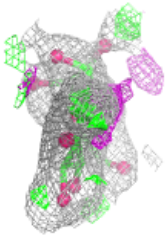


Electron density around DMU C 310:

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

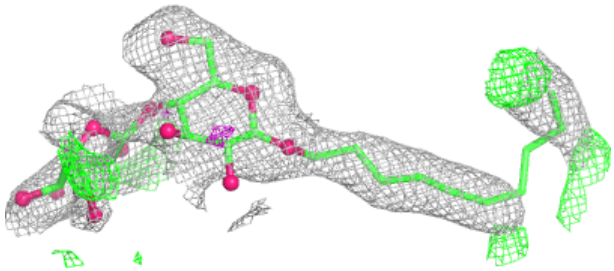


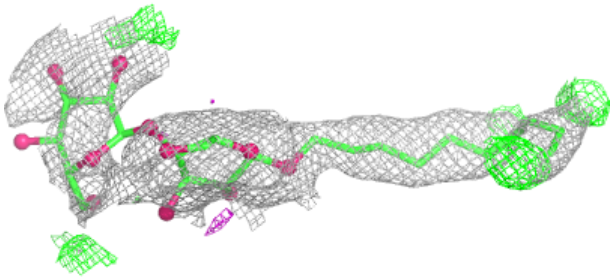


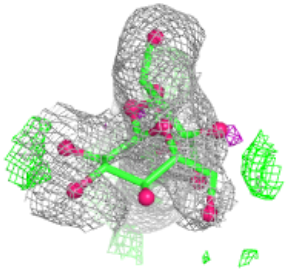


Electron density around DMU L 102:

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

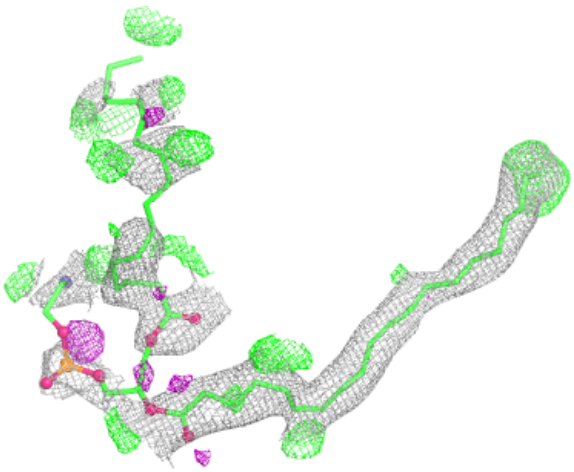


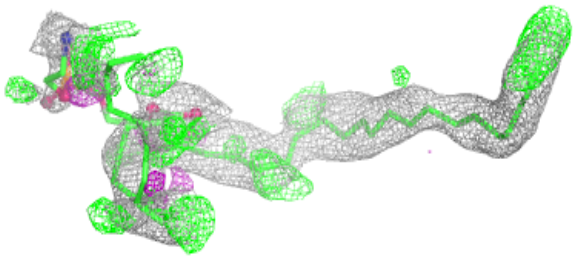


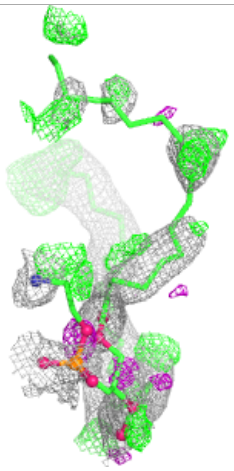


Electron density around PEK G 102:

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

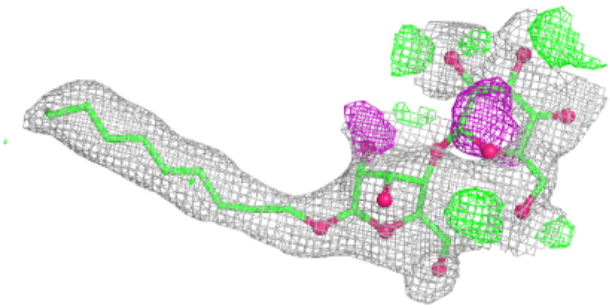


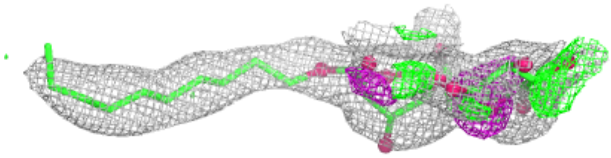


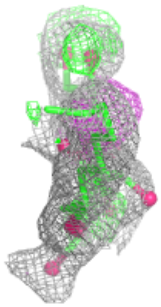


Electron density around DMU C 311:

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

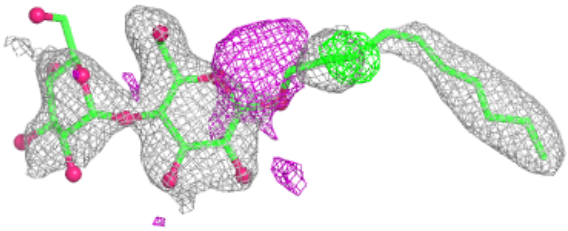


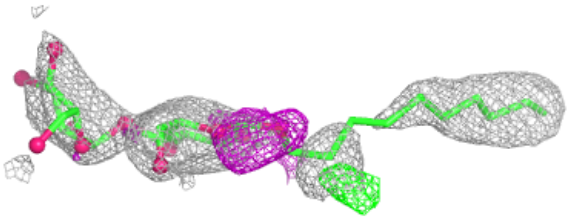


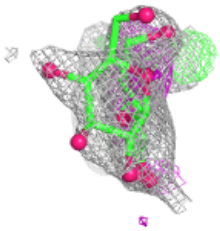


Electron density around DMU P 306:

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

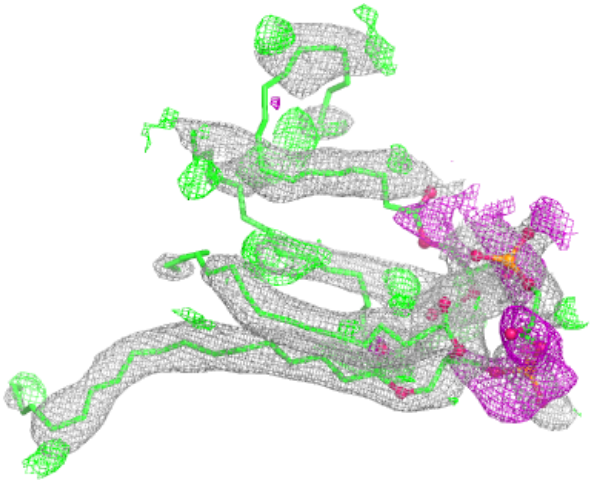


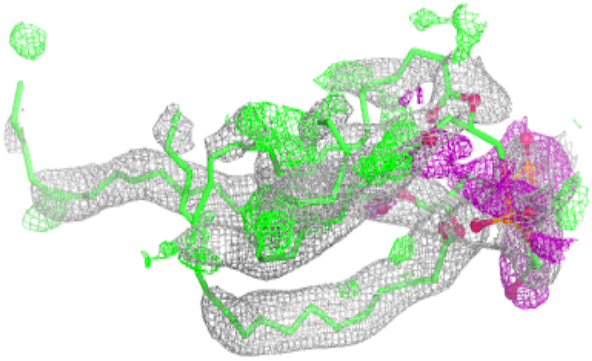


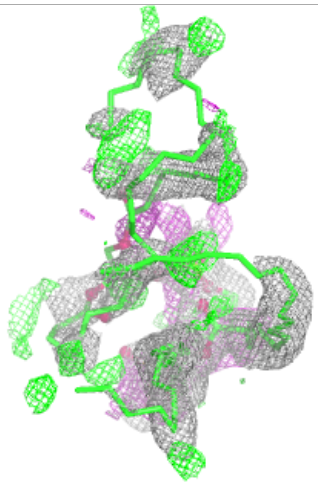


Electron density around CDL P 304:

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

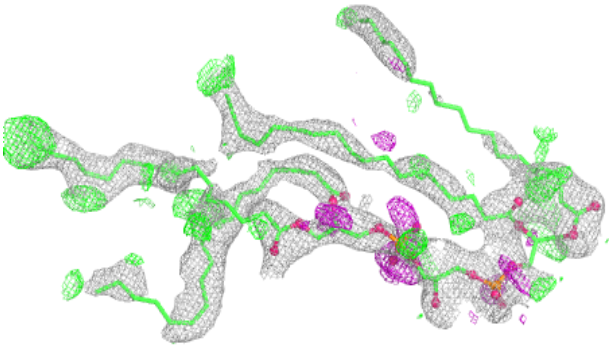


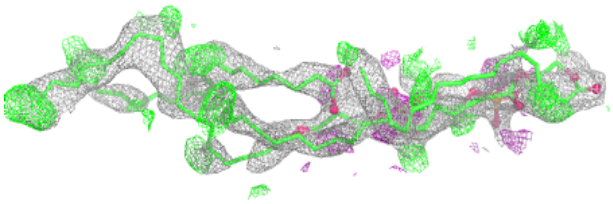


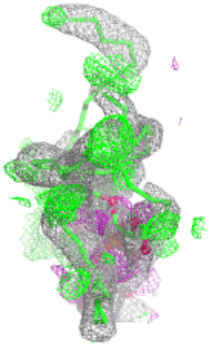


Electron density around CDL T 103:

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

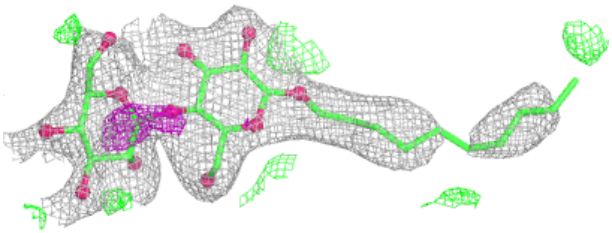


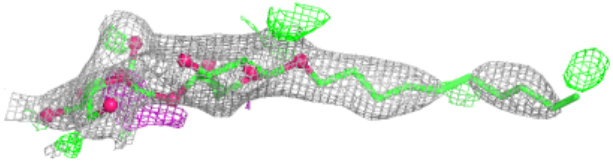


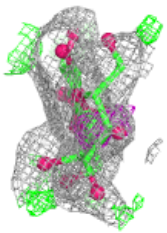


Electron density around DMU P 308:

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

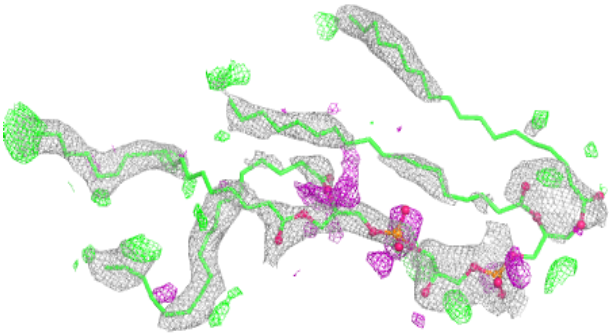


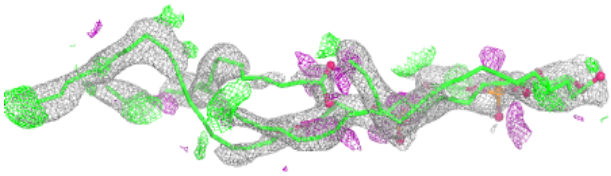


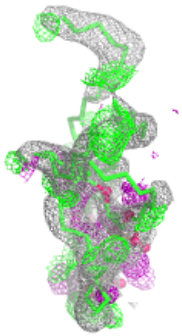


Electron density around CDL N 601:

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

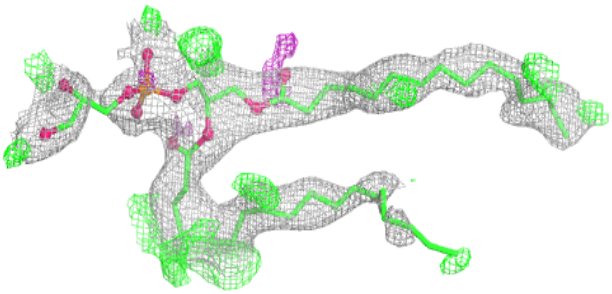


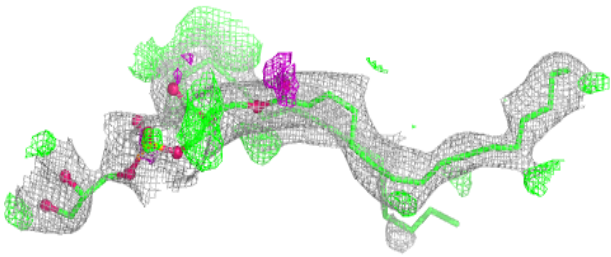


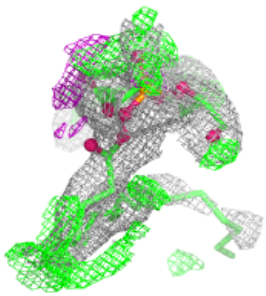


Electron density around PGV G 103:

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

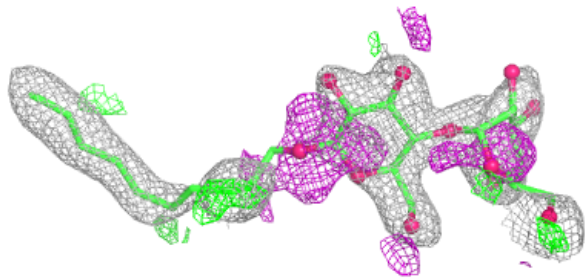


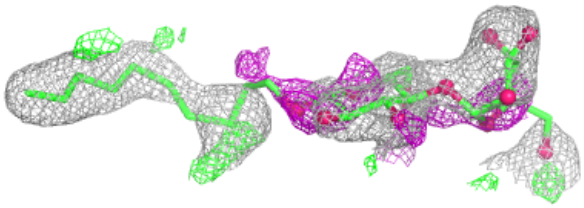


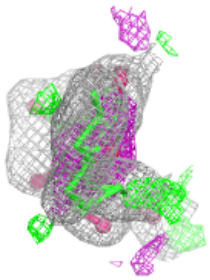


Electron density around DMU C 302:

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

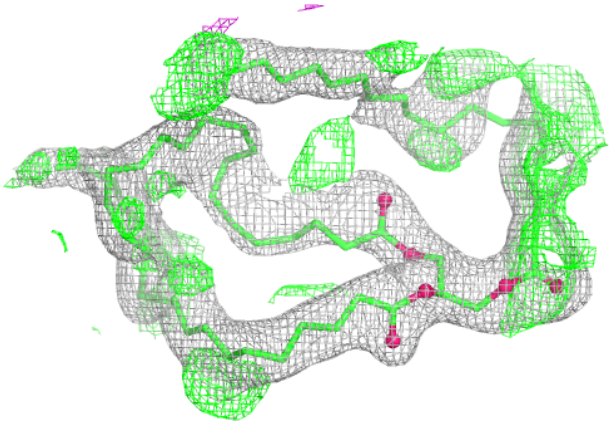


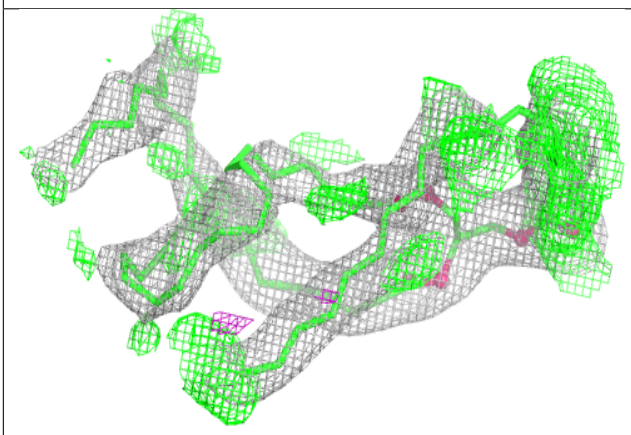


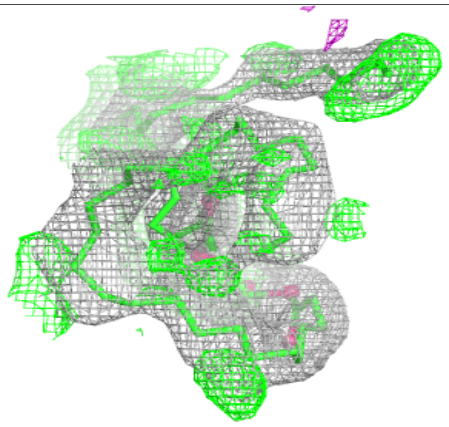


Electron density around TGL A 608:

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

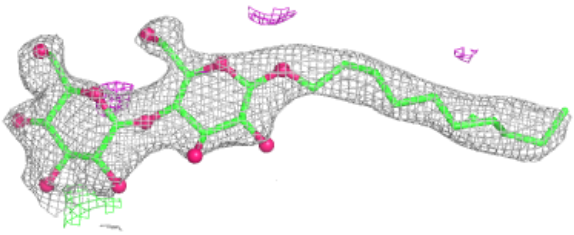


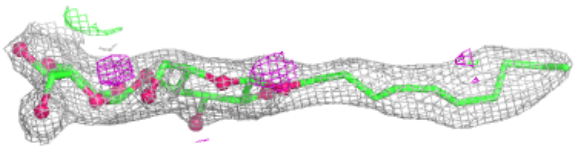




Electron density around DMU P 309:

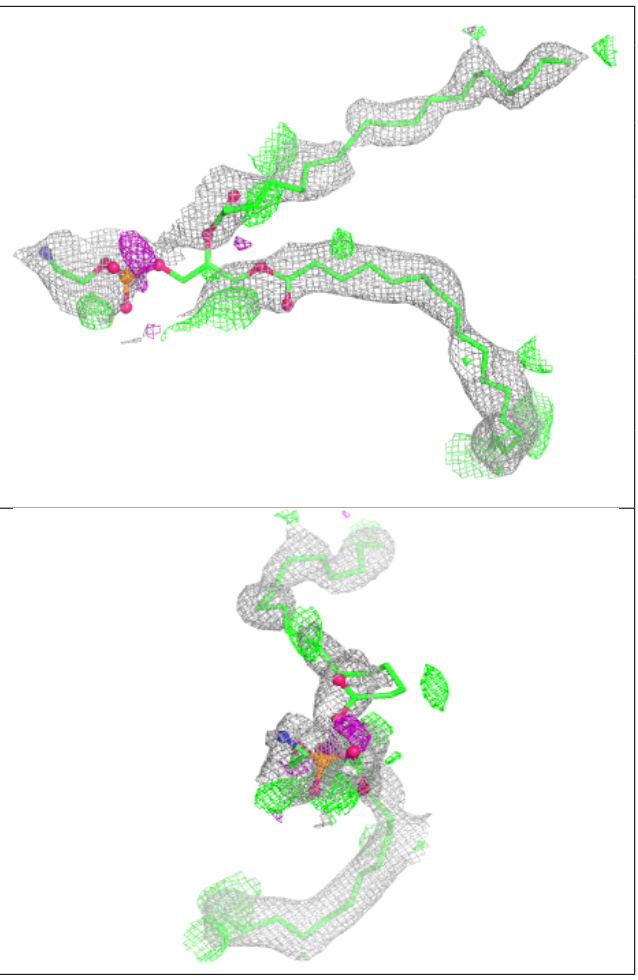
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





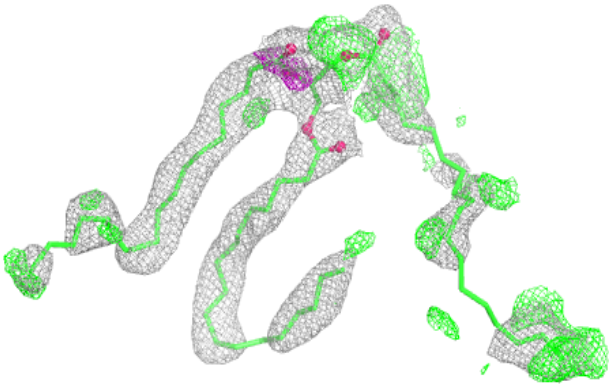
Electron density around PEK C 308:

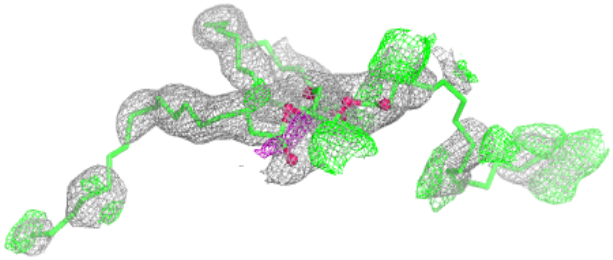
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

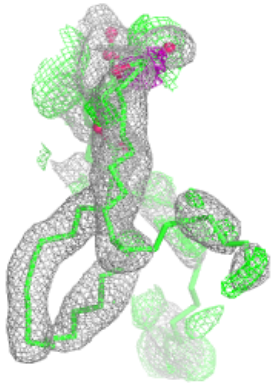


Electron density around TGL Q 201:

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

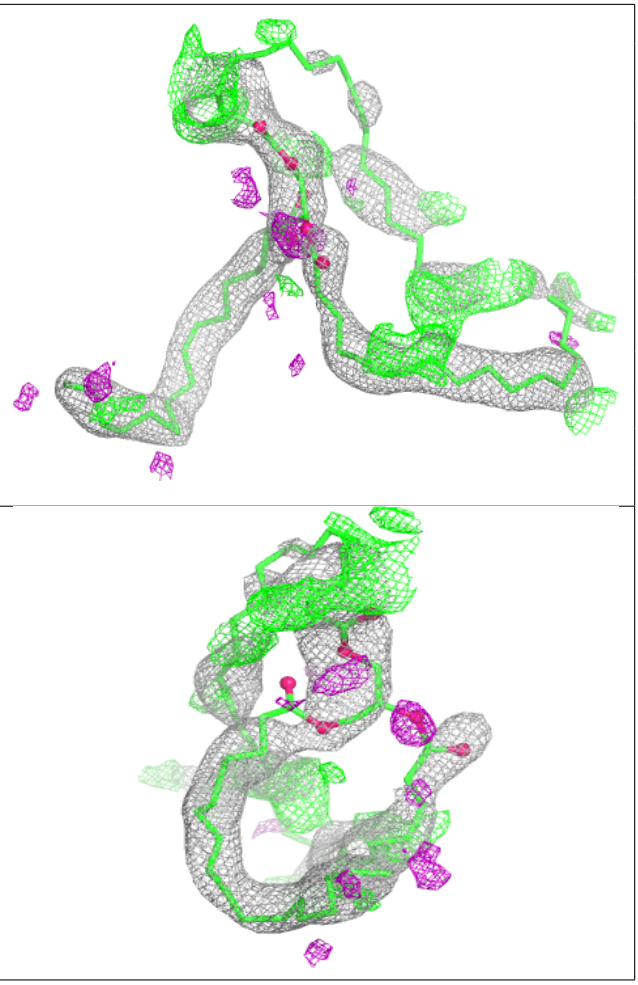






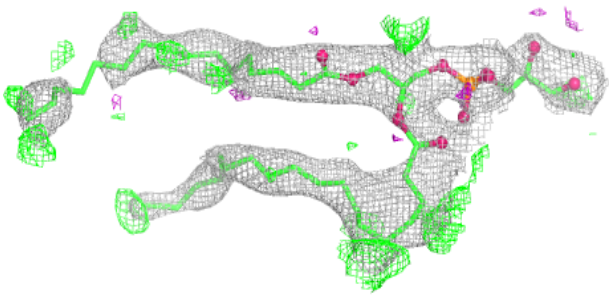
Electron density around TGL Y 101:

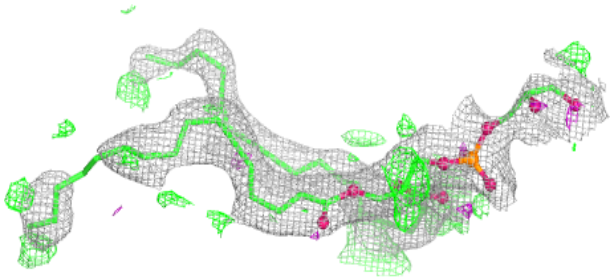
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

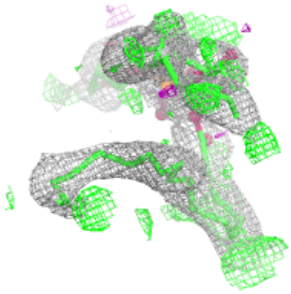


Electron density around PGV C 309:

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

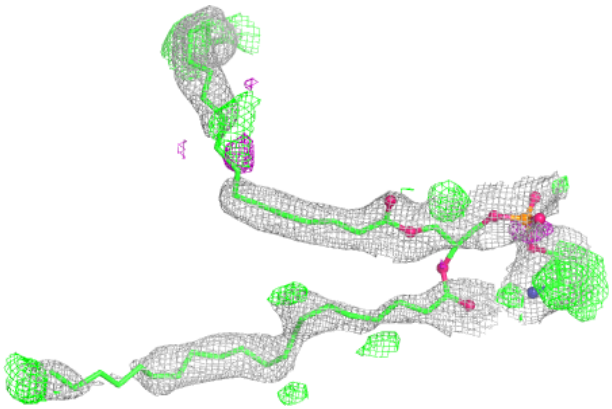


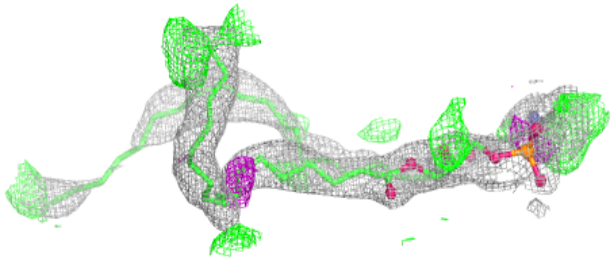


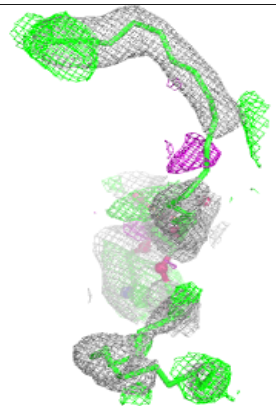


Electron density around PEK P 307:

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

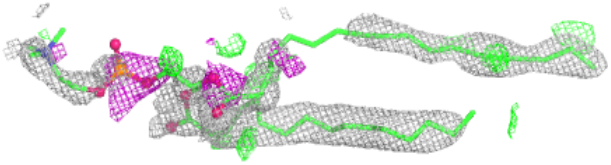


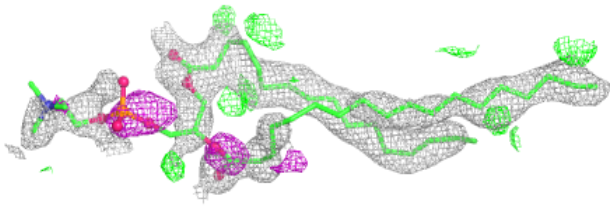


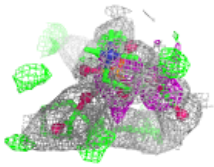


Electron density around PSC B 303:

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

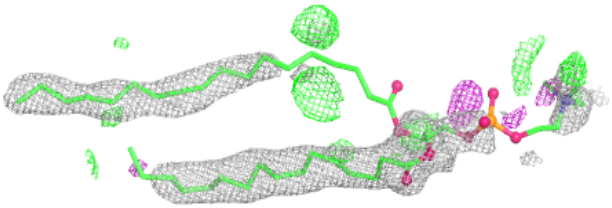


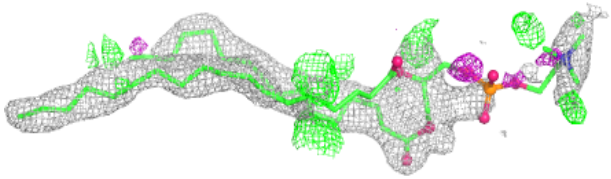


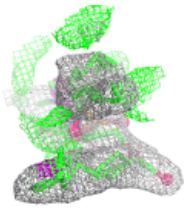


Electron density around PSC O 302:

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

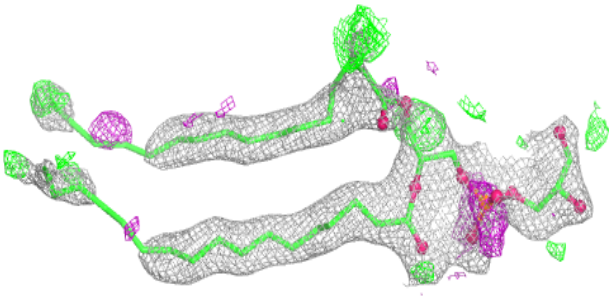


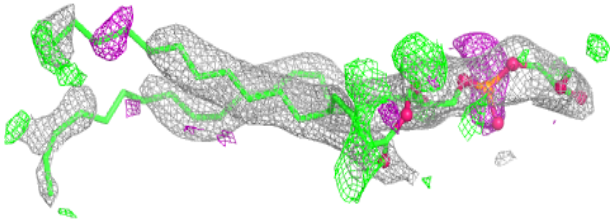


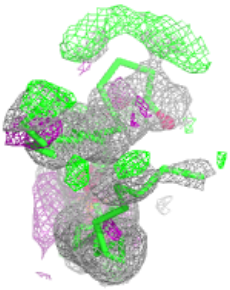


Electron density around PGV A 610:

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

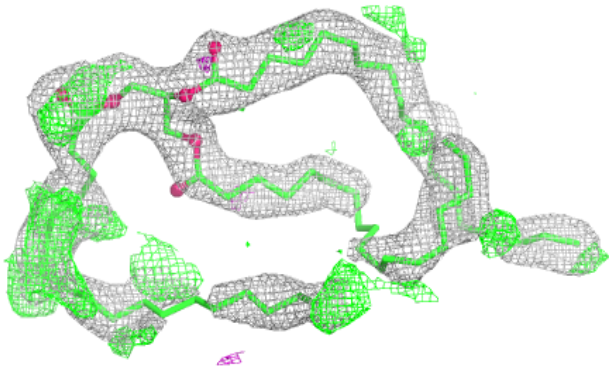


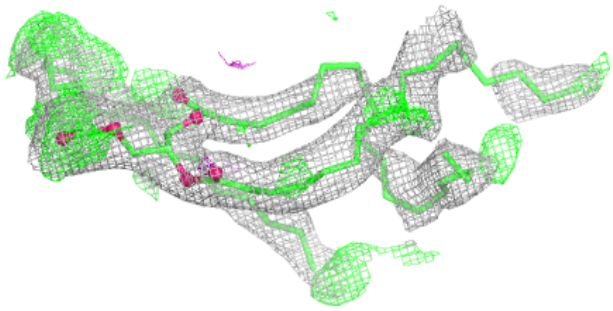


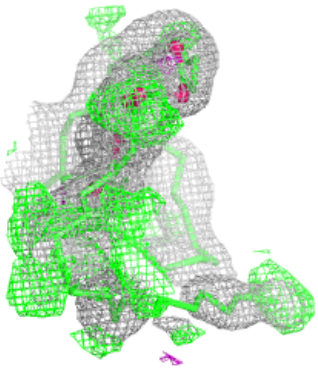


Electron density around TGL N 610:

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

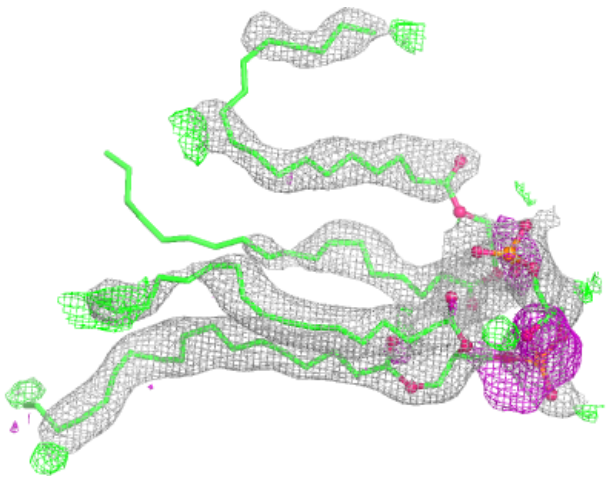


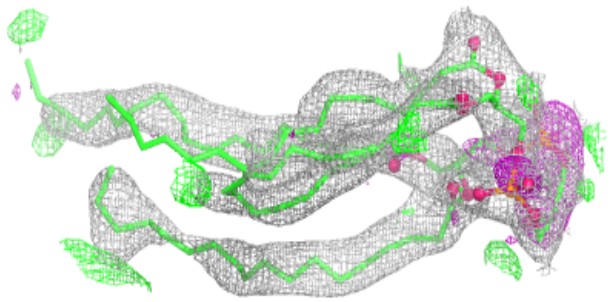


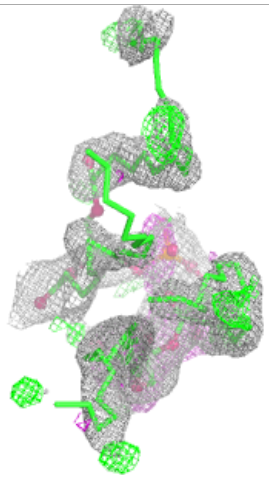


Electron density around CDL C 306:

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

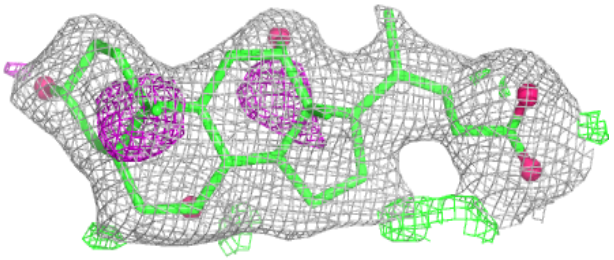


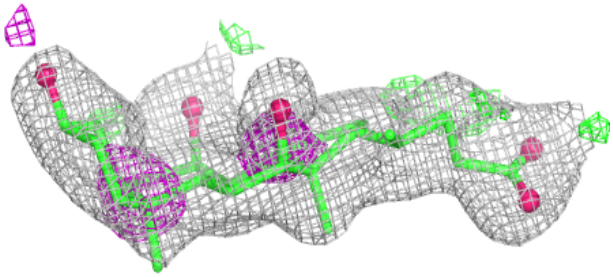


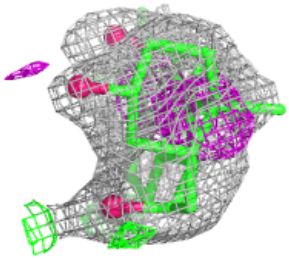


Electron density around CHD P 305:

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

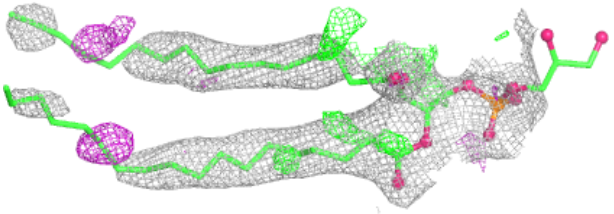


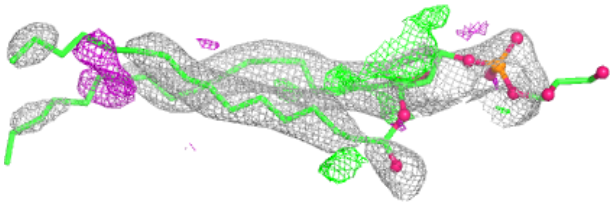


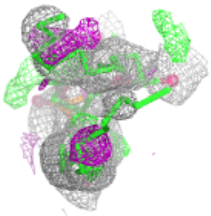


Electron density around PGV Z 101:

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

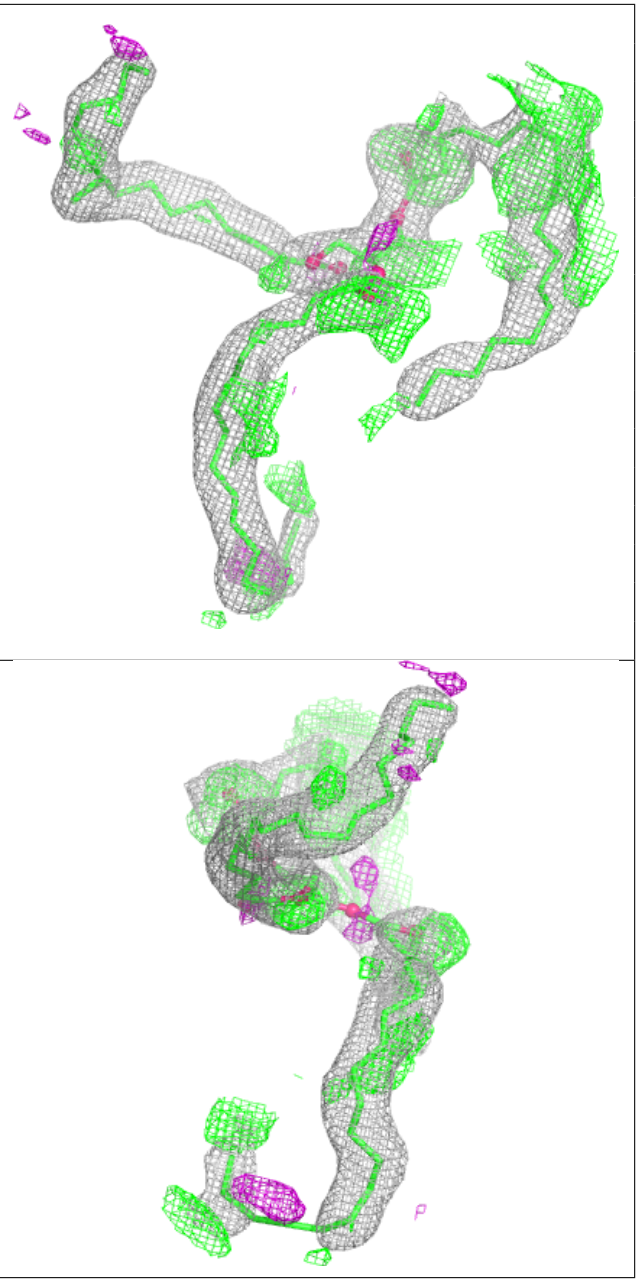






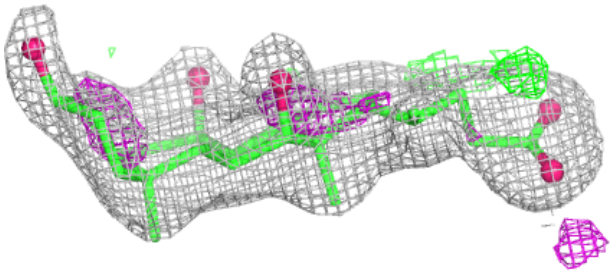
Electron density around TGL L 101:

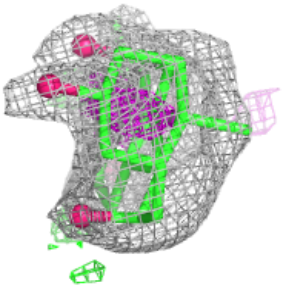
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHD C 307:

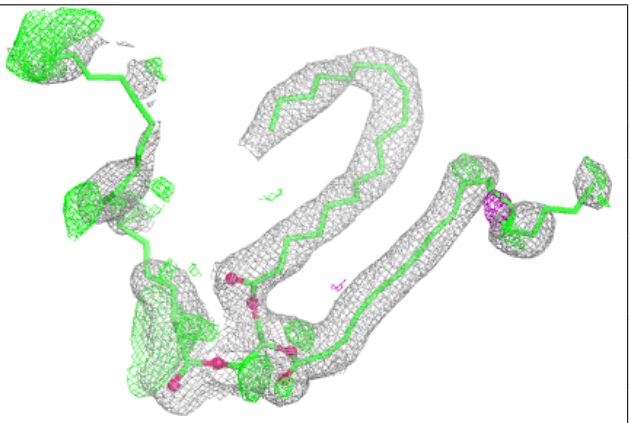
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

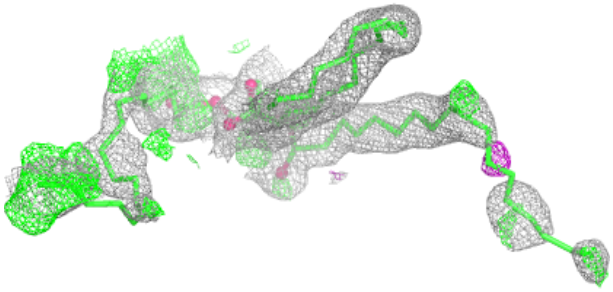


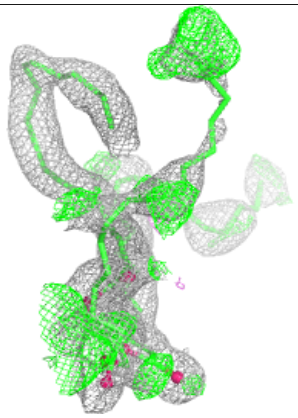


Electron density around TGL D 201:

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

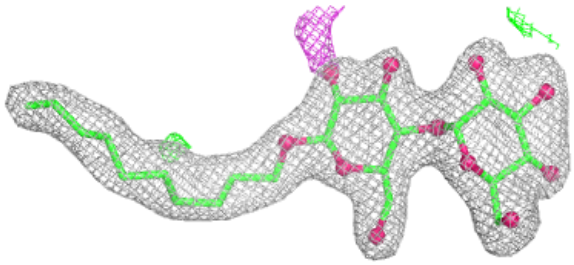


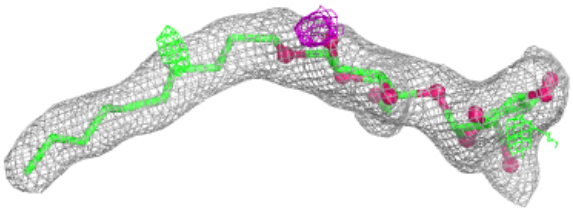


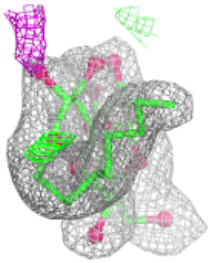


Electron density around DMU Z 102:

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

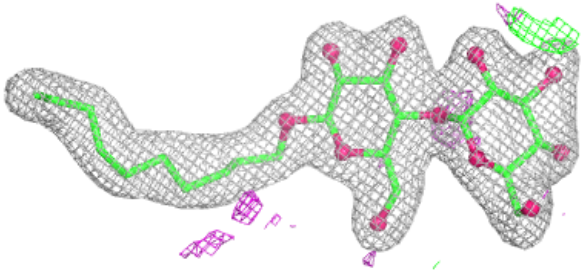


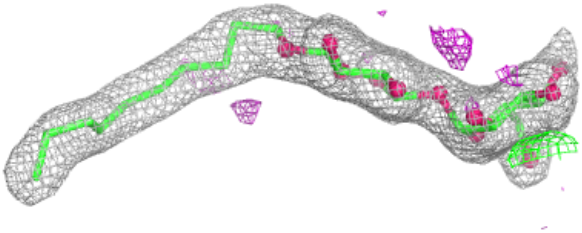


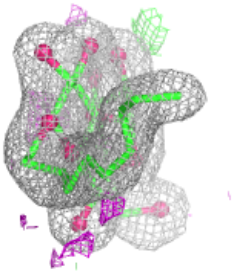


Electron density around DMU M 101:

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

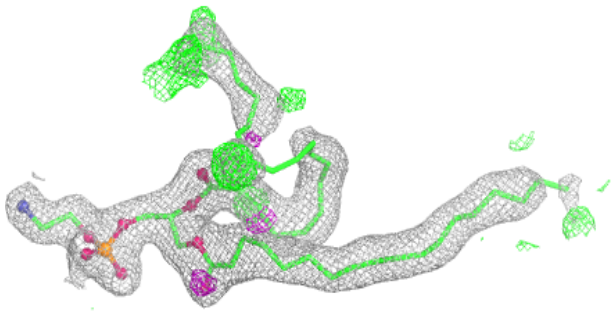


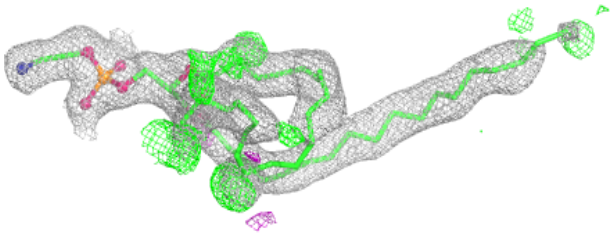


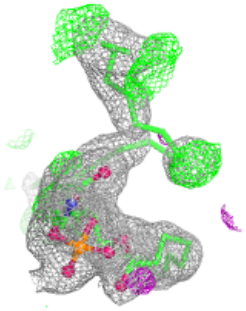


Electron density around PEK T 102:

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

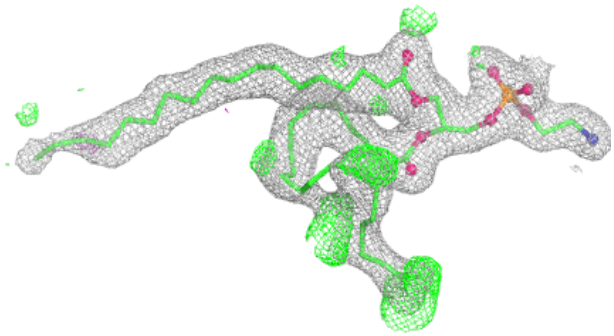


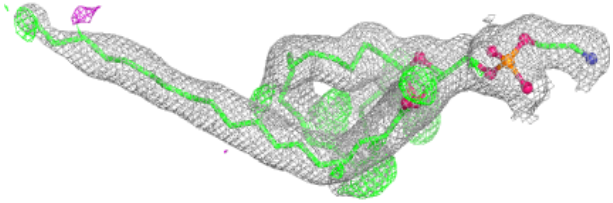


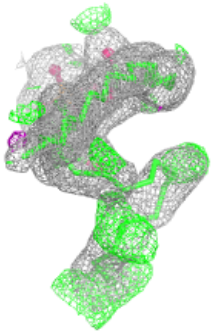


Electron density around PEK C 304:

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

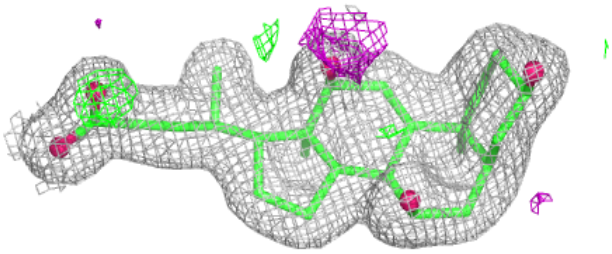


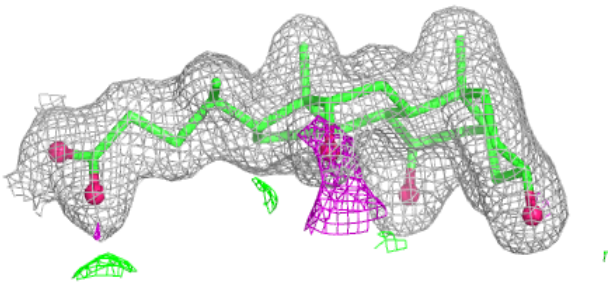


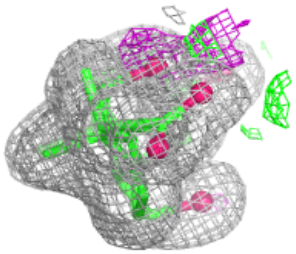


Electron density around CHD C 301:

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

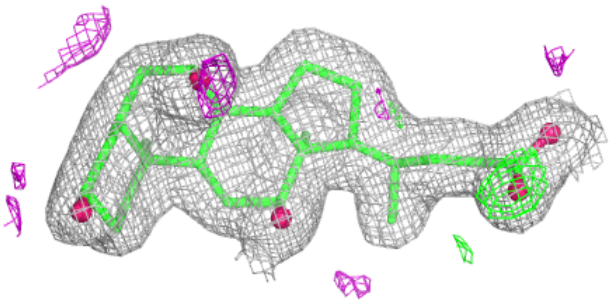


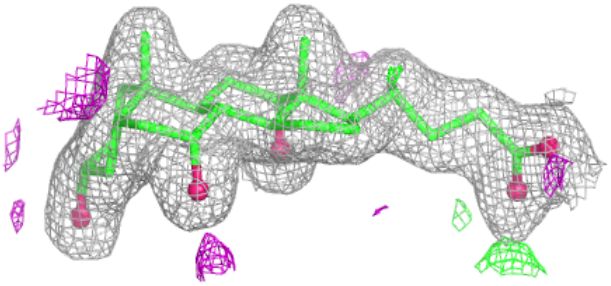


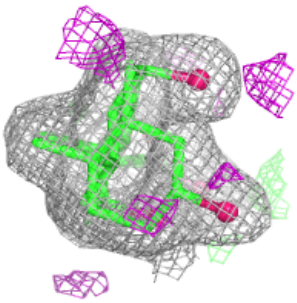


Electron density around CHD P 301:

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

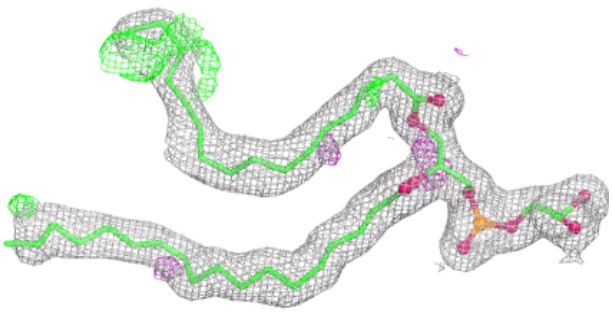


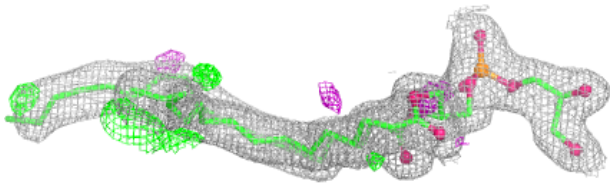




Electron density around PGV N 609:

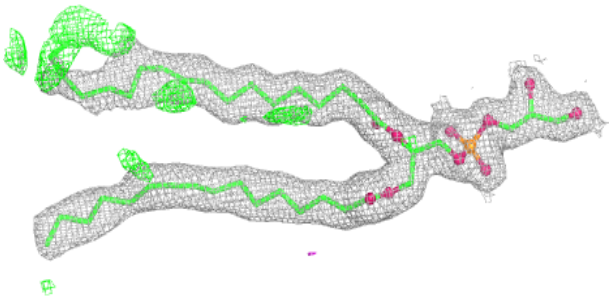
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

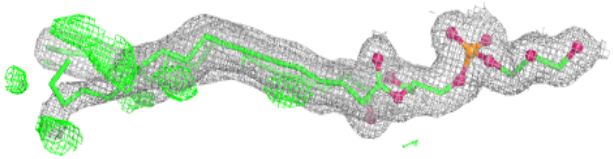


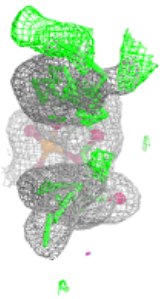


Electron density around PGV C 305:

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

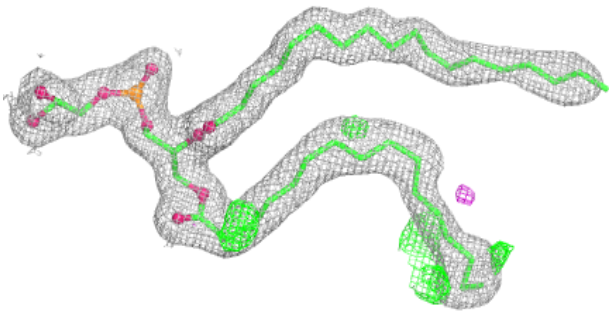


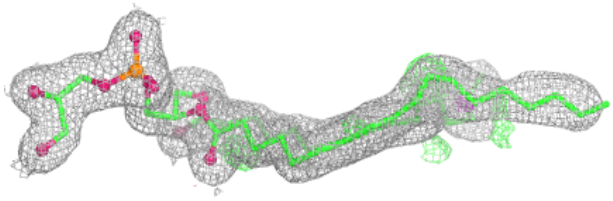


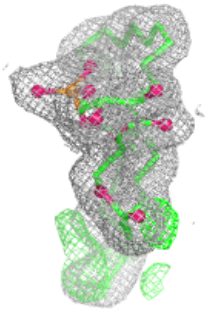


Electron density around PGV A 609:

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

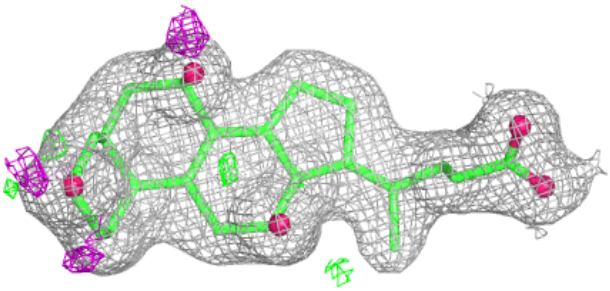


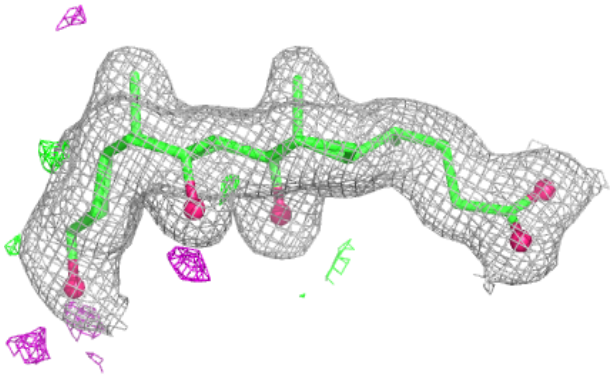


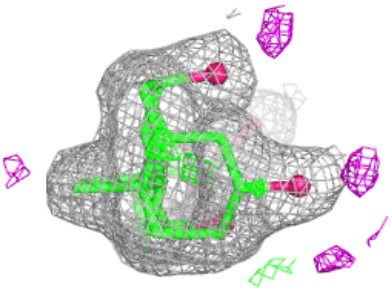


Electron density around CHD B 301:

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

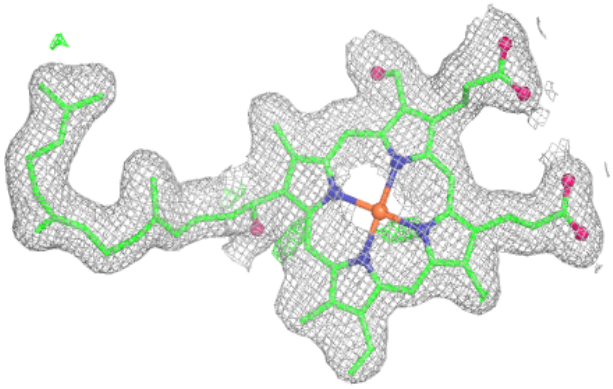


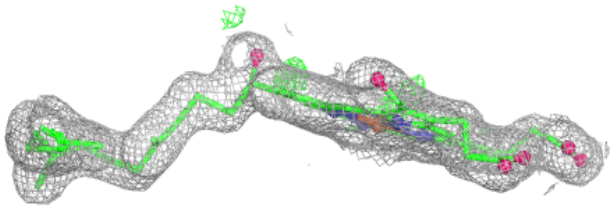


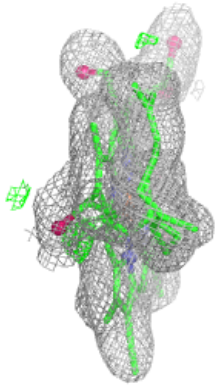


Electron density around HEA N 603 (A):

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

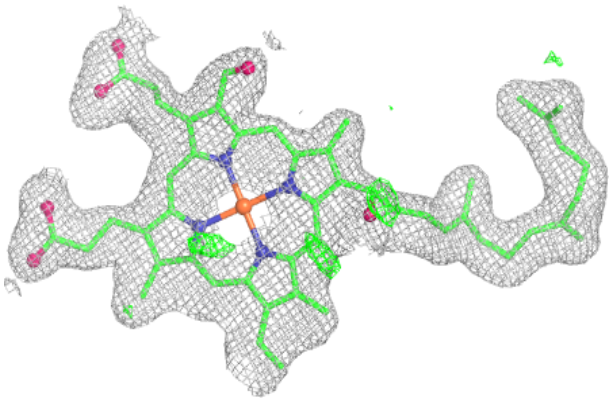


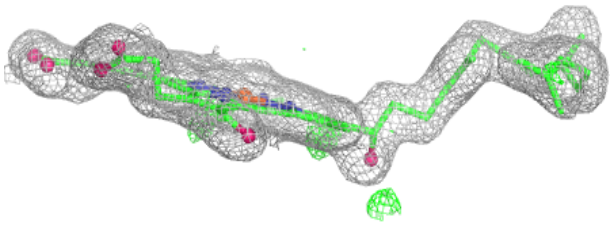


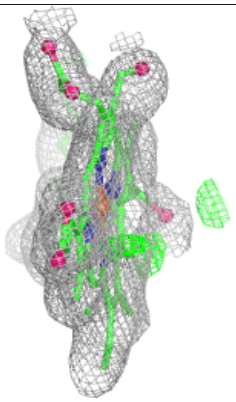


Electron density around HEA N 603 (B):

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

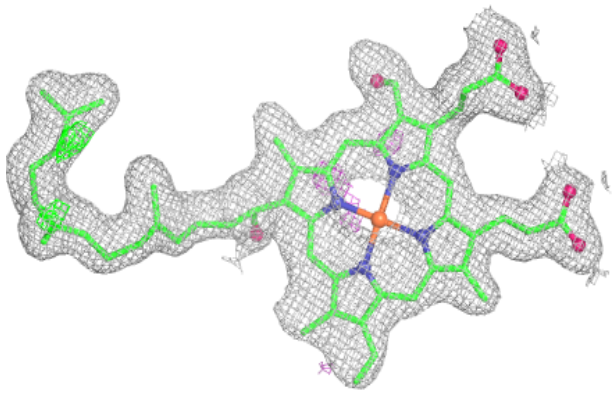


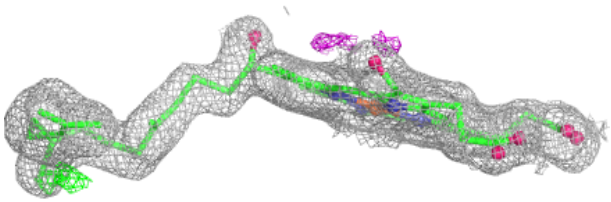


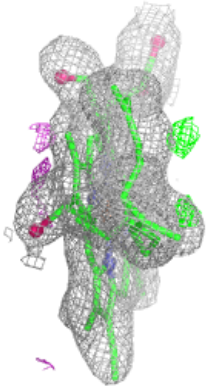


Electron density around HEA A 602 (A):

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

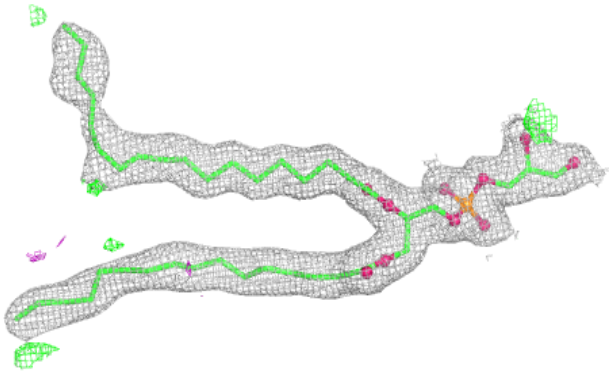


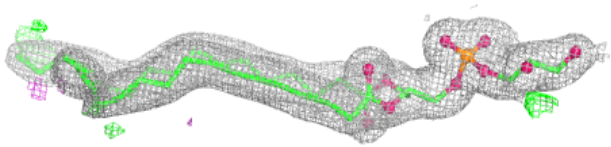


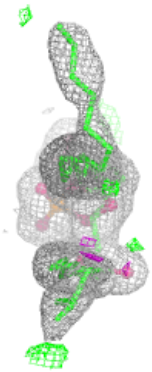


Electron density around PGV P 303:

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

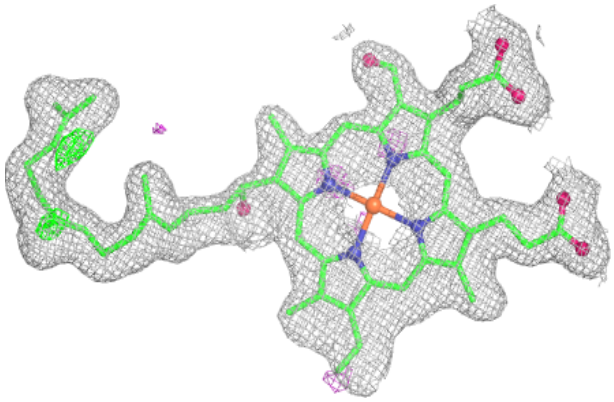


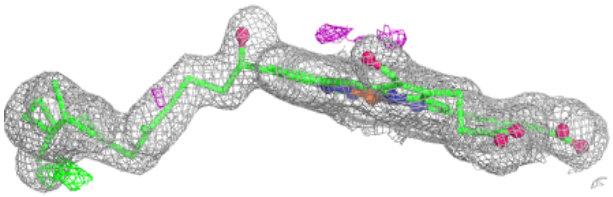


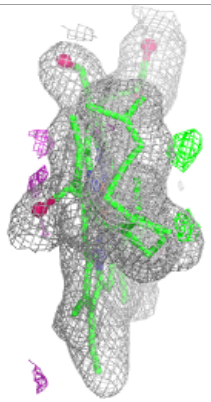


Electron density around HEA A 602 (B):

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

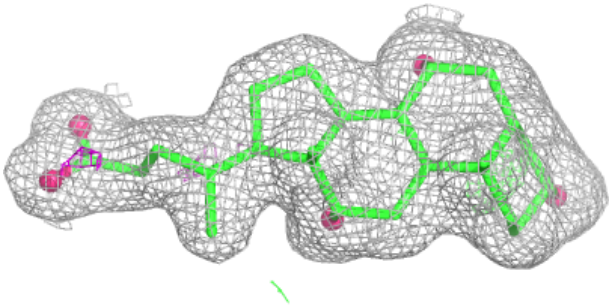


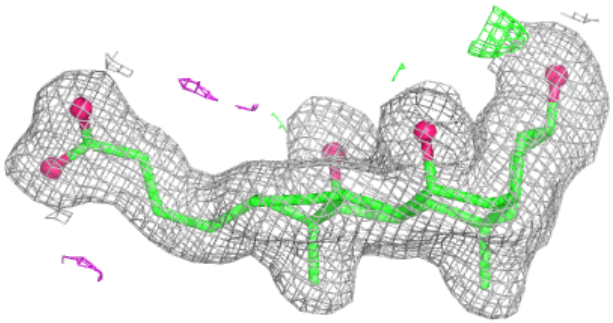


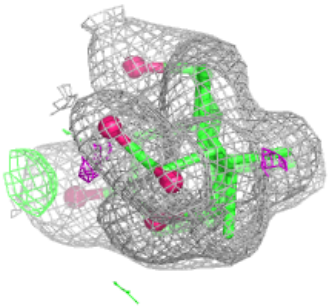


Electron density around CHD G 101:

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

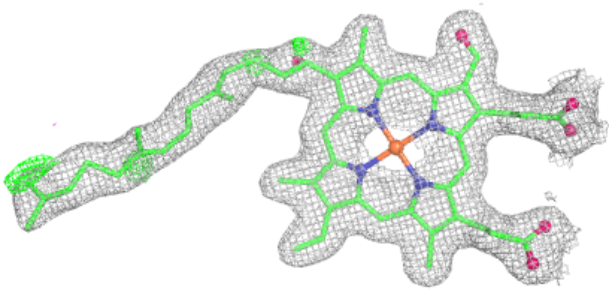


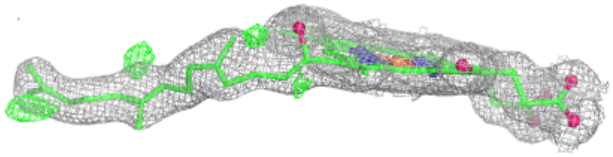




Electron density around HEA N 602:

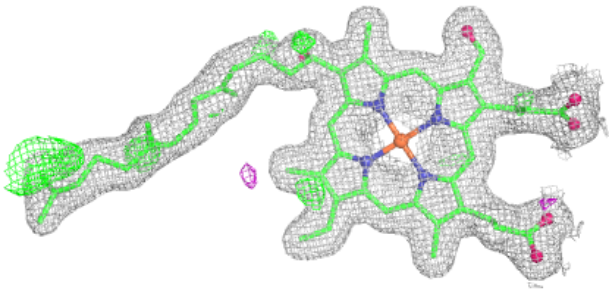
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

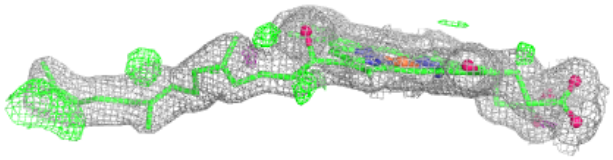




Electron density around HEA A 601:

$2mF_o$-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.