wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 01:29 PM JST

PDB ID	:	6JUW / pdb_00006juw
Title	:	BOVINE HEART CYTOCHROME C OXIDASE IN CATALITIC INTERMEDIATES AT 1.80 ANGSTROM RESOLUTION
Authors	:	Shimada, A.; Muramoto, K.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2019-04-15
Resolution	:	1.80 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:

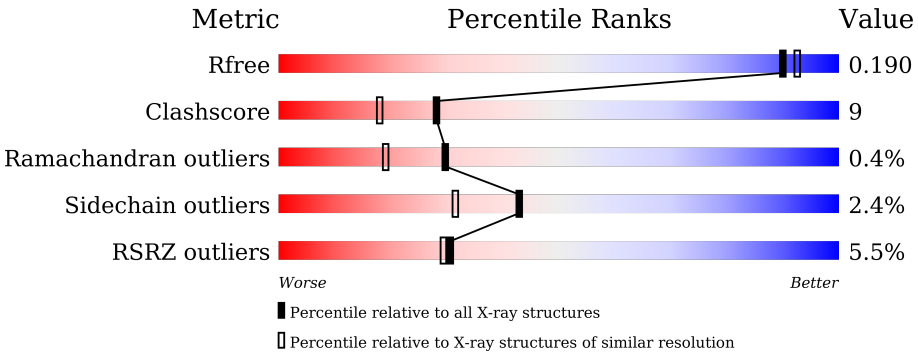
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	87% 13%
1	N	514	86% 14%
2	B	227	5% 81% 17%
2	O	227	5% 75% 22%
3	C	259	89% 11%
3	P	259	3% 88% 12%

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Mol	Chain	Length	Quality of chain
4	D	144	3% 90% 10%
4	Q	144	12% 86% 10%
5	E	105	3% 93% 7%
5	R	105	3% 90% 9%
6	F	98	12% 85% 15%
6	S	98	15% 89% 9%
7	G	84	21% 82% 13% 5%
7	T	84	19% 85% 11% 5%
8	H	79	9% 85% 14%
8	U	79	15% 86% 11%
9	I	73	12% 90% 10%
9	V	73	16% 84% 16%
10	J	58	3% 88% 12%
10	W	58	9% 88% 9%
11	K	49	4% 84% 16%
11	X	49	10% 86% 14%
12	L	46	4% 74% 26%
12	Y	46	7% 76% 22%
13	M	43	5% 95% 5%
13	Z	43	19% 84% 16%

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
22	EDO	N	612	-	-	X	-
22	EDO	N	617	-	-	X	-
22	EDO	U	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CDL	G	102	-	-	X	-
25	CDL	T	102	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 34360 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	37	0
			4192	2794	643	710	45			
1	N	514	Total	C	N	O	S	0	21	0
			4152	2770	639	703	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	4	0
			1839	1196	281	343	19			
2	O	227	Total	C	N	O	S	0	7	0
			1857	1208	287	343	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	5	0
			2122	1417	336	355	14			
3	P	259	Total	C	N	O	S	0	2	0
			2114	1413	336	353	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1198	780	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			751	465	135	146	5			
6	S	98	Total	C	N	O	S	0	1	0
			751	465	134	147	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			676	431	129	114	1	1			
7	T	84	Total	C	N	O	P	S	0	1	0
			685	439	130	114	1	1			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

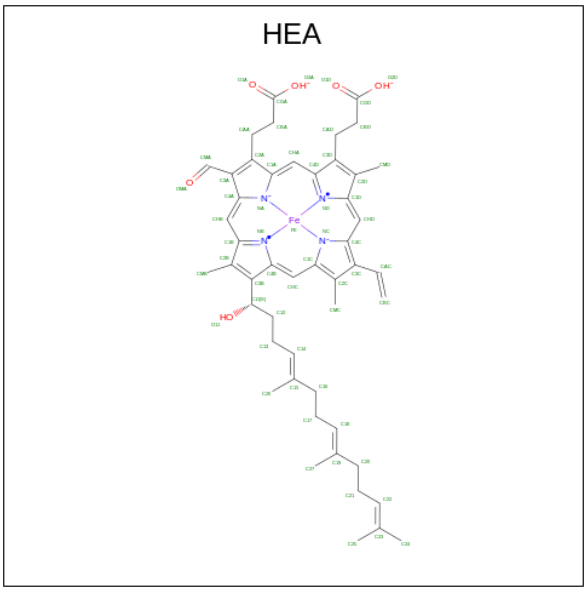
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	1
			72	60	1	4	7		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			72	60	1	4	7		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

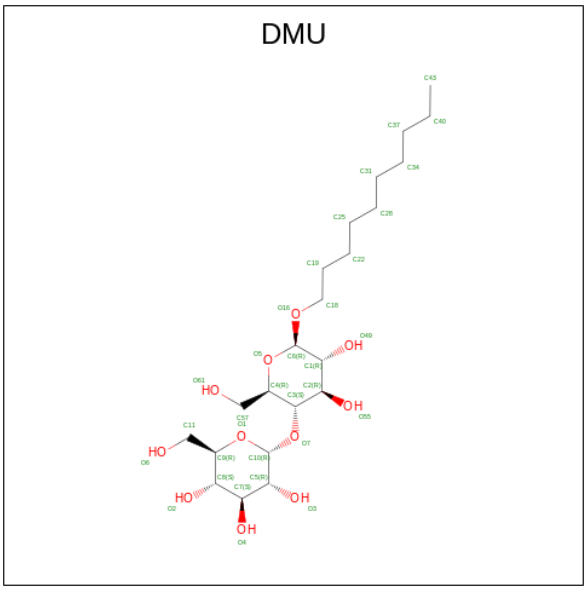
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 18 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



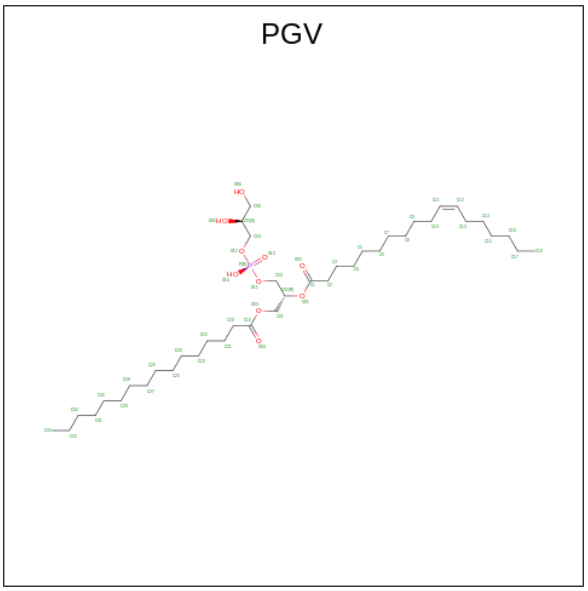
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 13 11 2	0	0
18	B	1	Total C O 11 10 1	0	0
18	C	1	Total C O 33 22 11	0	0
18	C	1	Total C O 22 16 6	0	0
18	C	1	Total C O 11 10 1	0	0
18	D	1	Total C O 21 16 5	0	0
18	J	1	Total C O 21 16 5	0	0

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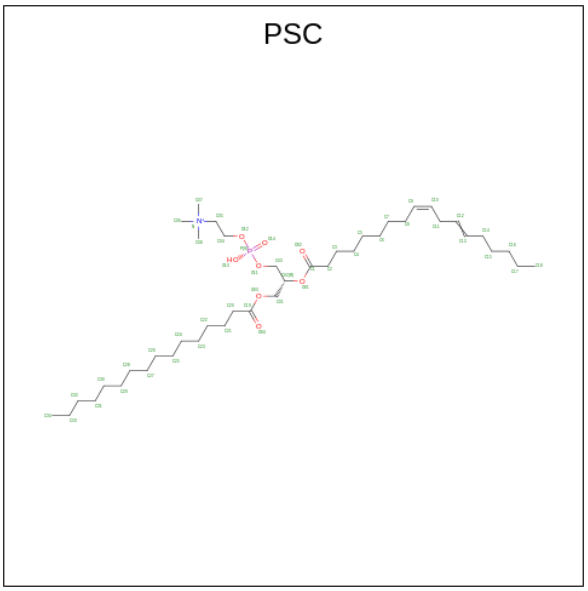
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	K	1	Total	C	O	0	0
			11	10	1		
18	K	1	Total	C	O	0	0
			14	11	3		
18	K	1	Total	C	O	0	0
			22	16	6		
18	K	1	Total	C	O	0	0
			11	10	1		
18	L	1	Total	C	O	0	0
			33	22	11		
18	M	1	Total	C	O	0	0
			33	22	11		
18	O	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			33	22	11		
18	Q	1	Total	C	O	0	0
			23	17	6		
18	W	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	Y	1	Total	C	O	0	0
			33	22	11		
18	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



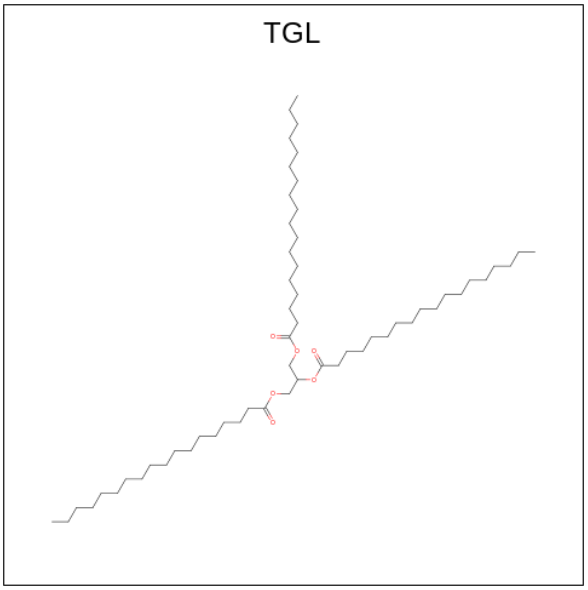
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 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
20	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
20	V	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



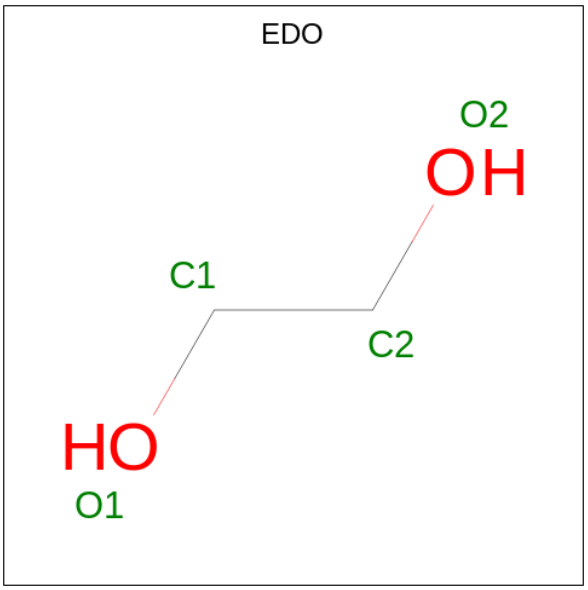
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	O		0	0
			63	57	6			
21	D	1	Total	C	O		0	0
			63	57	6			

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

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

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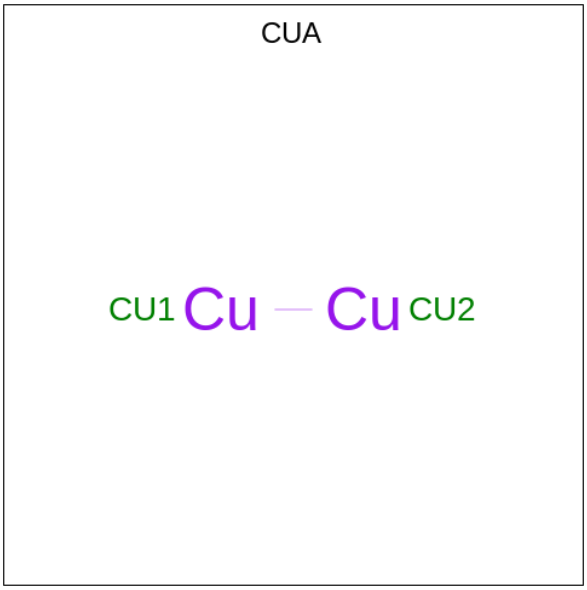
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22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

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

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



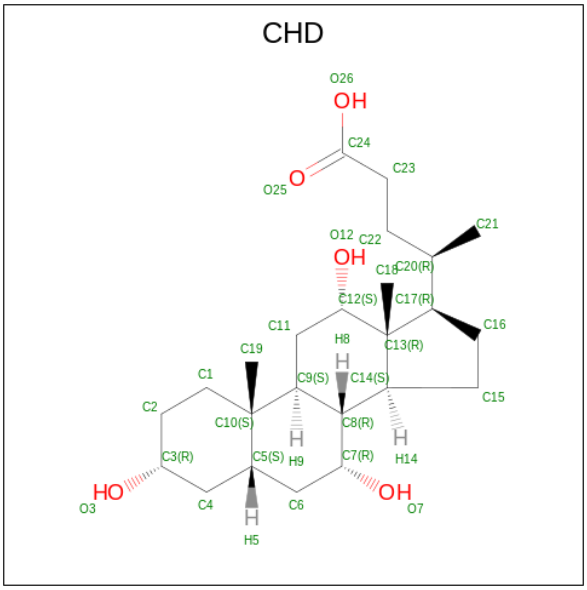
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0

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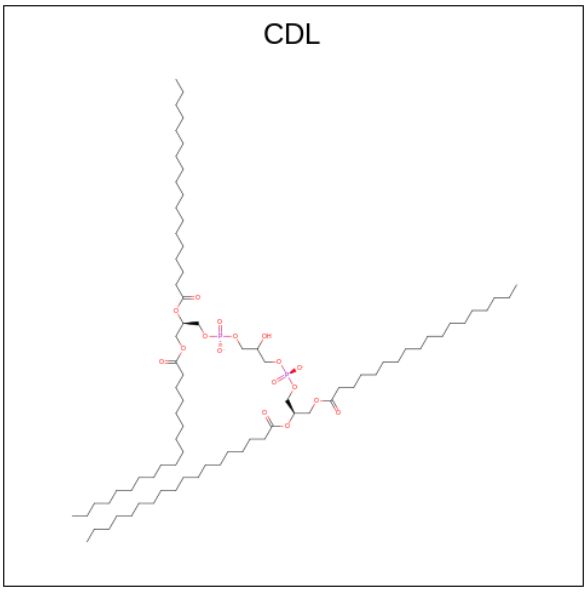
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	O	1	Total Cu 2 2	0	0

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



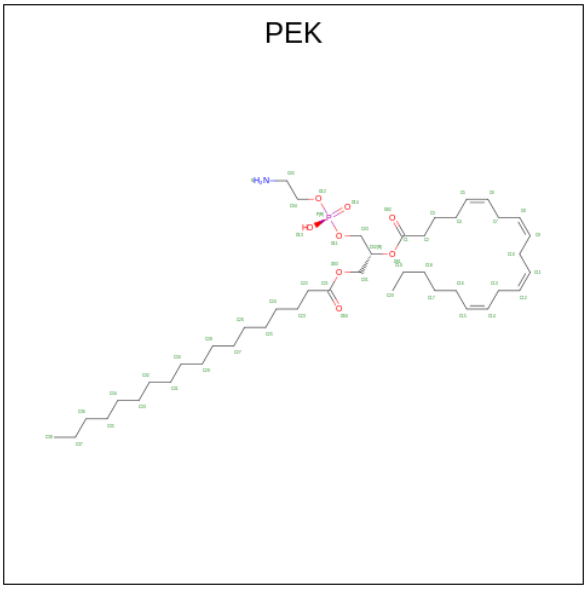
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	J	1	Total C O 29 24 5	0	0
24	L	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	Y	1	Total C O 29 24 5	0	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 is (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: $C_{43}H_{78}NO_8P$).

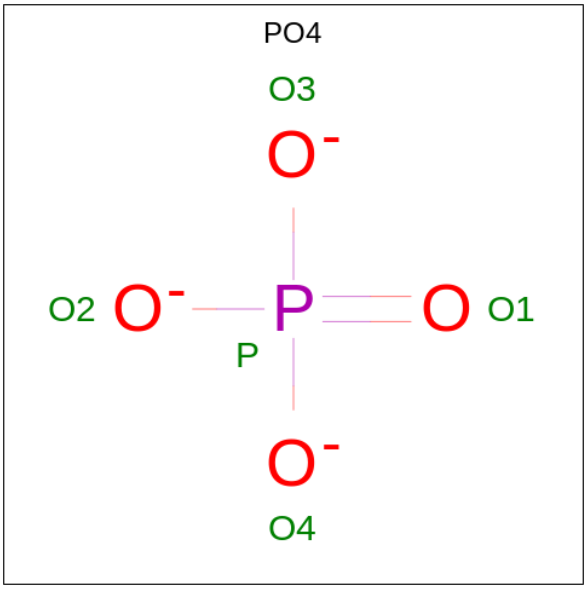


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	F	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	H	1	Total O P 5 4 1	0	0
28	U	1	Total O P 5 4 1	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	247	Total O 250 250	0	4
29	B	200	Total O 200 200	0	0
29	C	136	Total O 136 136	0	0
29	D	174	Total O 174 174	0	0
29	E	133	Total O 133 133	0	0
29	F	117	Total O 117 117	0	0
29	G	72	Total O 72 72	0	0
29	H	79	Total O 79 79	0	0
29	I	56	Total O 56 56	0	0
29	J	44	Total O 44 44	0	0
29	K	36	Total O 36 36	0	0
29	L	42	Total O 42 42	0	0
29	M	34	Total O 34 34	0	0
29	N	245	Total O 247 247	0	3
29	O	166	Total O 166 166	0	0
29	P	132	Total O 132 132	0	0
29	Q	99	Total O 99 99	0	0
29	R	98	Total O 98 98	0	0
29	S	105	Total O 105 105	0	0
29	T	75	Total O 75 75	0	0
29	U	65	Total O 65 65	0	0

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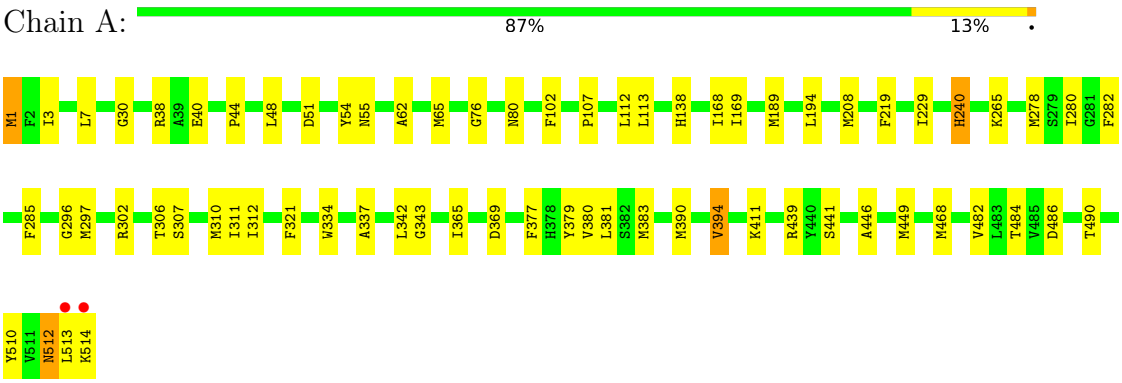
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	48	Total O 48 48	0	0
29	W	27	Total O 27 27	0	0
29	X	28	Total O 28 28	0	0
29	Y	31	Total O 31 31	0	0
29	Z	20	Total O 20 20	0	0

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.

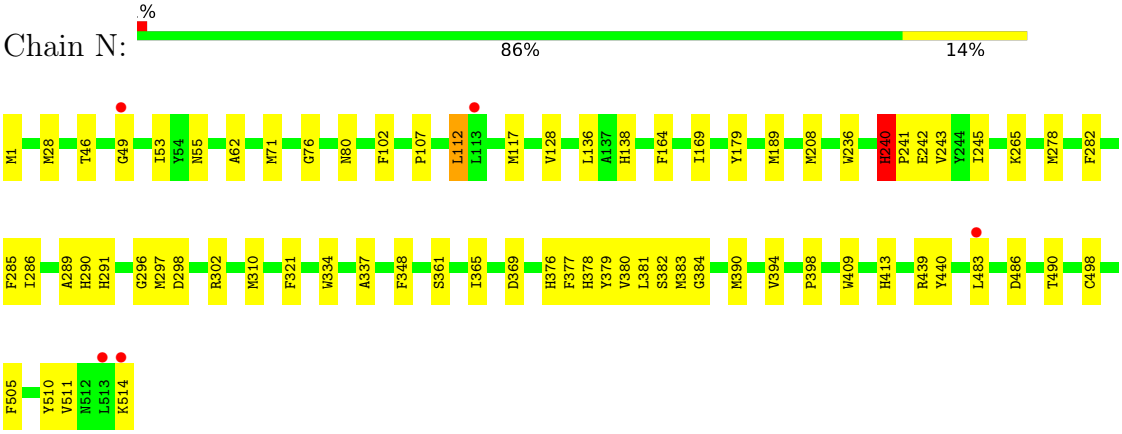
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



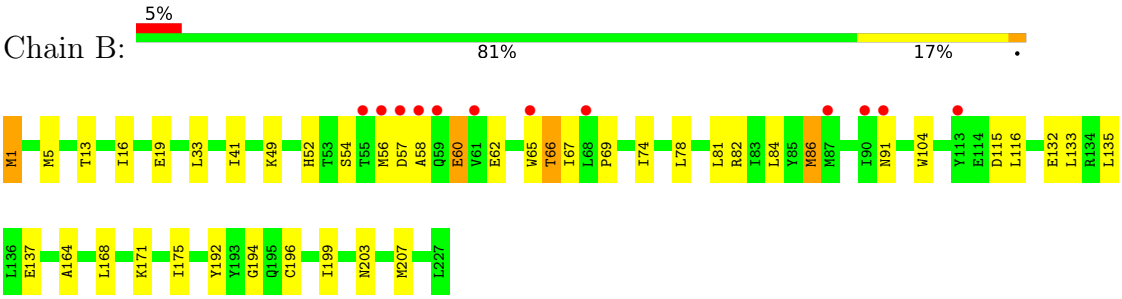
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



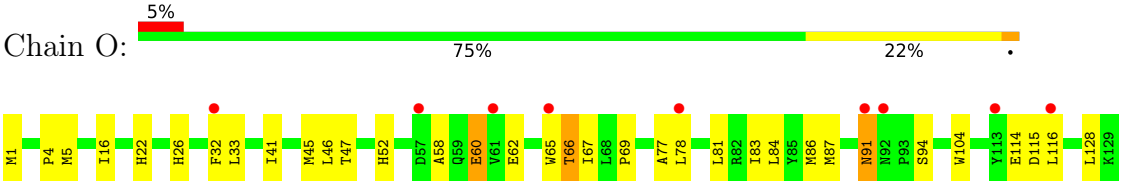
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



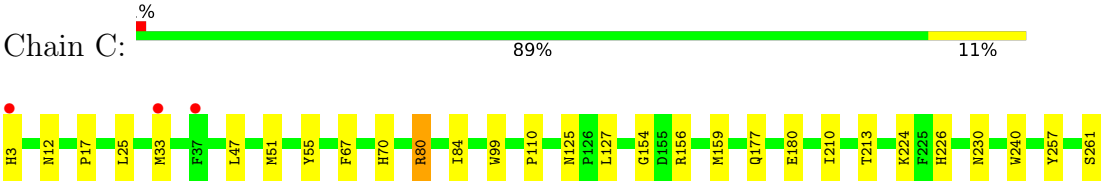
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



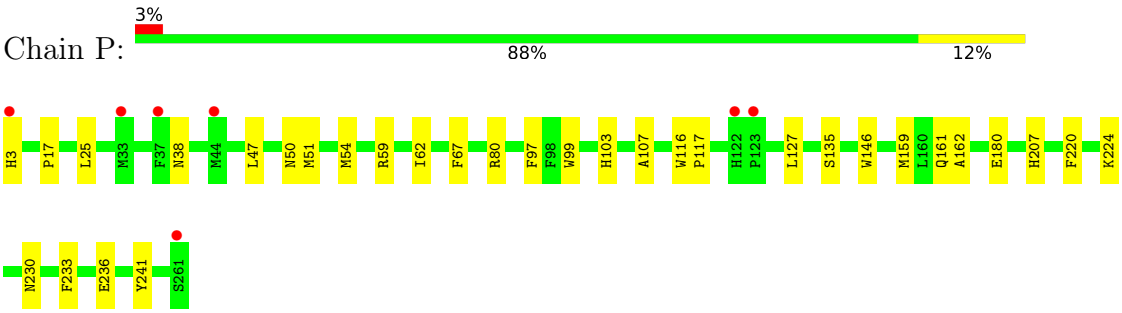
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



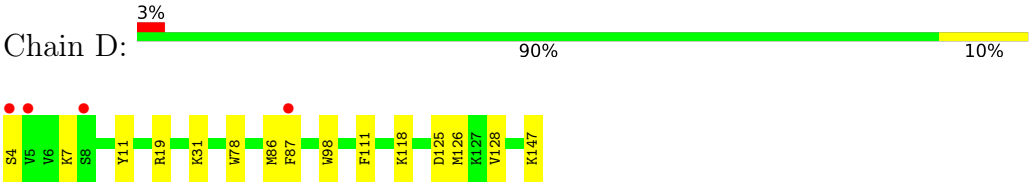
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



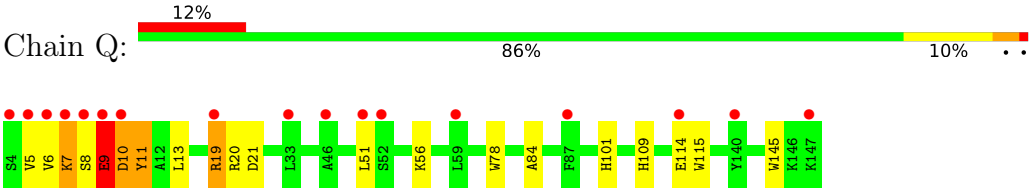
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



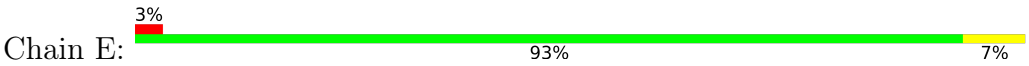
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

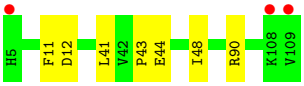
Chain Q:



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

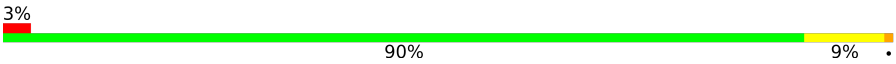
Chain E:

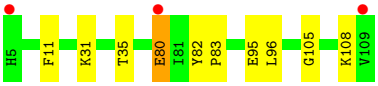




• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:

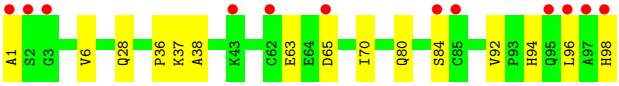




• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:

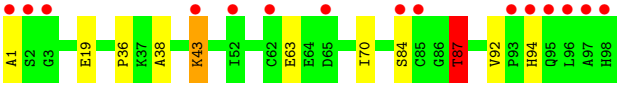




• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:





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

Chain G:

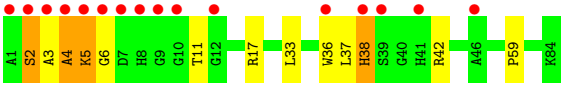




• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:

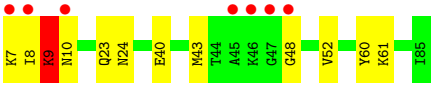




• Molecule 8: Cytochrome c oxidase subunit 6B1

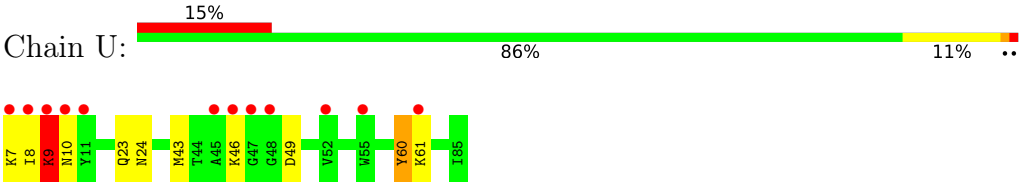
Chain H:





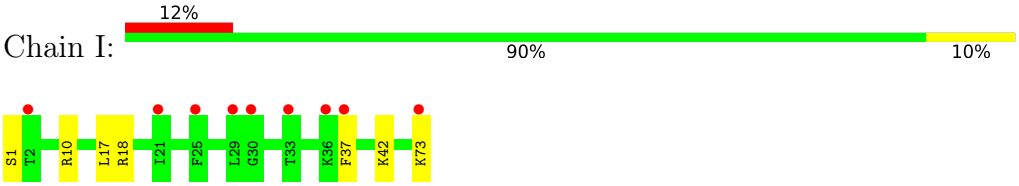
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



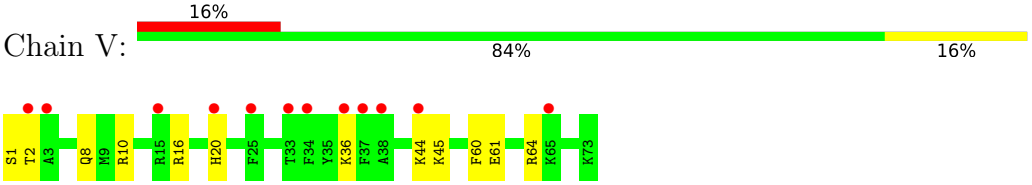
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



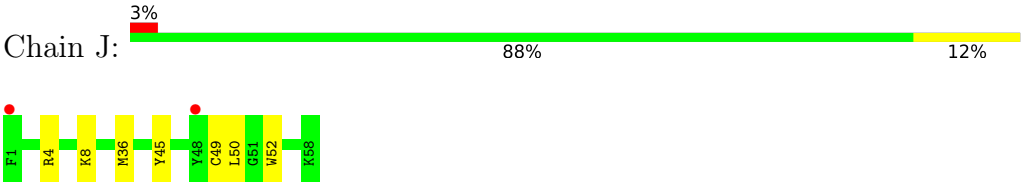
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



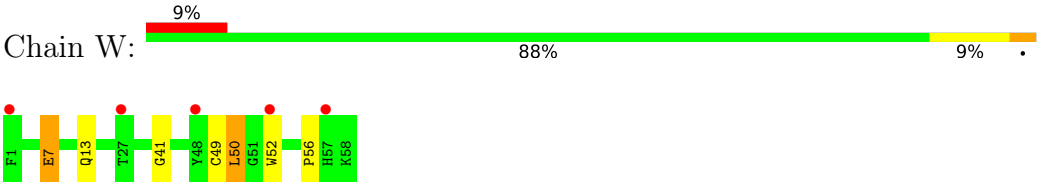
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



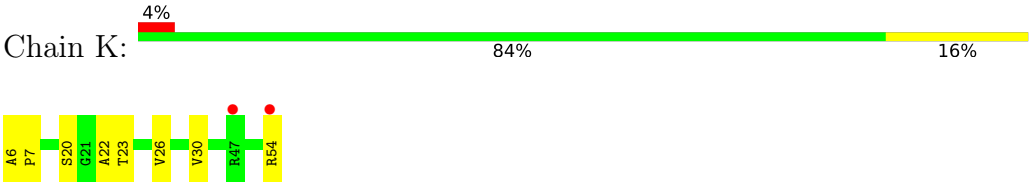
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



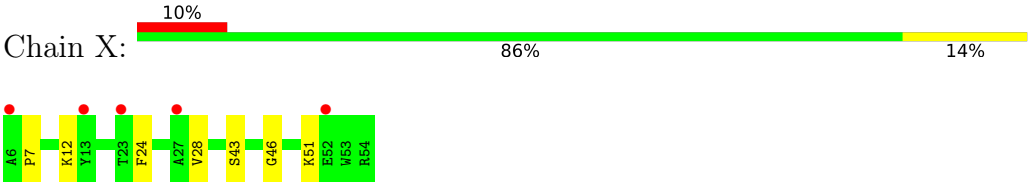
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



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

Chain X:



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

Chain L:

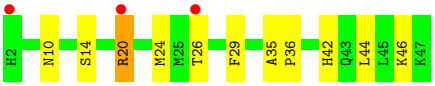




• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

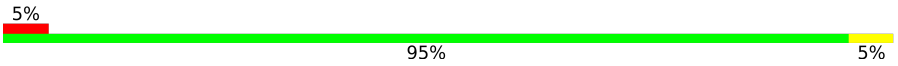
Chain Y:

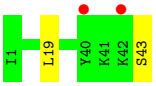




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:

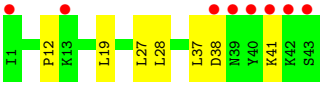




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.22Å 204.65Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 1.80 39.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.88-1.80) 99.8 (39.88-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.157 , 0.188 0.159 , 0.190	Depositor DCC
R_{free} test set	30366 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 79.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	34360	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: PO4, PSC, CHD, TPO, CU, PEK, DMU, ZN, EDO, HEA, PGV, CDL, FME, TGL, MG, NA, CUA, SAC

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	1.06	0/4445	1.00	5/6063 (0.1%)
1	N	0.96	0/4321	0.92	3/5899 (0.1%)
2	B	0.94	0/1896	0.99	1/2582 (0.0%)
2	O	0.77	0/1934	0.92	2/2634 (0.1%)
3	C	0.88	0/2236	0.86	1/3056 (0.0%)
3	P	0.87	0/2211	0.83	0/3024
4	D	0.92	0/1234	0.88	0/1665
4	Q	0.63	0/1229	0.70	0/1658
5	E	0.84	0/871	0.80	0/1182
5	R	0.71	0/871	0.76	0/1182
6	F	0.86	0/774	0.89	0/1050
6	S	0.79	1/774 (0.1%)	0.85	0/1050
7	G	0.79	0/691	0.85	0/937
7	T	0.72	0/707	0.82	0/960
8	H	0.80	0/682	0.87	0/921
8	U	0.70	0/682	0.80	0/921
9	I	0.70	0/605	0.77	0/802
9	V	0.54	0/605	0.70	0/802
10	J	0.64	0/471	0.76	0/636
10	W	0.61	0/471	0.75	0/636
11	K	0.78	0/398	0.81	0/544
11	X	0.55	0/399	0.64	0/546
12	L	0.92	0/393	0.92	0/526
12	Y	0.74	0/393	0.75	0/526
13	M	0.91	0/346	0.85	0/470
13	Z	0.69	0/346	0.67	0/470
All	All	0.87	1/29985 (0.0%)	0.88	12/40742 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	H	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	87	THR	CB-CG2	-5.17	1.35	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	71	MET	CG-SD-CE	-11.77	75.00	100.90
1	A	240	HIS	CA-CB-CG	-6.30	107.50	113.80
1	N	240	HIS	CA-CB-CG	-5.76	108.04	113.80
2	B	192	TYR	CA-CB-CG	-5.62	103.78	113.90
1	N	102	PHE	CA-CB-CG	-5.60	108.20	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain

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	4192	0	4181	75	0
1	N	4152	0	4129	73	0
2	B	1839	0	1848	35	0
2	O	1857	0	1858	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2122	0	2032	38	0
3	P	2114	0	2028	28	0
4	D	1198	0	1189	16	0
4	Q	1195	0	1183	23	0
5	E	852	0	845	5	0
5	R	852	0	845	8	0
6	F	751	0	726	15	0
6	S	751	0	726	12	0
7	G	676	0	644	17	0
7	T	685	0	648	15	0
8	H	662	0	623	9	0
8	U	662	0	623	10	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	9	0
10	W	460	0	459	8	0
11	K	384	0	366	11	0
11	X	385	0	366	6	0
12	L	380	0	380	13	0
12	Y	380	0	380	12	0
13	M	336	0	352	2	0
13	Z	336	0	352	7	0
14	A	132	0	93	5	0
14	N	132	0	93	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	1	0
18	A	13	0	21	2	0
18	B	11	0	21	0	0
18	C	66	0	94	2	0
18	D	21	0	30	0	0
18	J	21	0	30	4	0
18	K	58	0	94	5	0
18	L	33	0	40	2	0
18	M	33	0	42	1	0
18	O	11	0	21	2	0
18	P	44	0	63	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	23	0	31	2	0
18	W	21	0	30	4	0
18	X	65	0	114	1	0
18	Y	33	0	42	3	0
18	Z	33	0	42	2	0
19	A	102	0	152	6	0
19	C	51	0	76	6	0
19	N	102	0	152	9	0
19	P	102	0	152	13	0
19	T	51	0	74	1	0
20	A	52	0	79	17	0
20	V	52	0	78	7	0
21	A	63	0	110	2	0
21	D	63	0	110	15	0
21	L	63	0	110	16	0
21	N	63	0	110	4	0
21	Q	63	0	110	12	0
21	Y	63	0	110	3	0
22	A	36	0	54	9	0
22	B	20	0	30	3	0
22	C	28	0	42	3	0
22	D	20	0	30	3	0
22	E	12	0	18	2	0
22	F	32	0	48	3	0
22	G	4	0	6	0	0
22	H	4	0	6	2	0
22	J	4	0	6	0	0
22	L	8	0	11	1	0
22	M	4	0	6	0	0
22	N	60	0	90	14	0
22	O	8	0	12	1	0
22	P	28	0	42	3	0
22	Q	12	0	18	4	0
22	S	20	0	30	2	0
22	T	8	0	12	1	0
22	U	4	0	6	4	0
22	W	4	0	6	0	0
22	Y	4	0	6	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	58	0	78	3	0
24	G	29	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	29	0	39	1	0
24	L	29	0	39	0	0
24	P	58	0	78	3	0
24	T	29	0	39	1	0
24	Y	29	0	39	1	0
25	C	100	0	156	19	0
25	G	100	0	154	22	0
25	P	100	0	156	11	0
25	T	100	0	154	29	0
26	C	106	0	154	11	0
26	F	53	0	74	6	0
26	P	106	0	154	3	0
26	T	53	0	77	9	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	H	5	0	0	0	0
28	U	5	0	0	0	0
29	A	250	0	0	12	0
29	B	200	0	0	4	2
29	C	136	0	0	8	0
29	D	174	0	0	3	2
29	E	133	0	0	0	0
29	F	117	0	0	2	0
29	G	72	0	0	0	0
29	H	79	0	0	3	0
29	I	56	0	0	5	2
29	J	44	0	0	1	0
29	K	36	0	0	2	0
29	L	42	0	0	2	0
29	M	34	0	0	1	1
29	N	247	0	0	12	0
29	O	166	0	0	4	0
29	P	132	0	0	4	0
29	Q	99	0	0	2	0
29	R	98	0	0	2	0
29	S	105	0	0	4	0
29	T	75	0	0	4	0
29	U	65	0	0	2	0
29	V	48	0	0	1	1
29	W	27	0	0	1	0
29	X	28	0	0	0	0
29	Y	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Z	20	0	0	0	0
All	All	34360	0	32701	576	4

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 9.

The worst 5 of 576 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)
25:G:102:CDL:H512	25:G:102:CDL:H181	1.32	1.09
1:A:55[B]:ASN:ND2	29:A:701:HOH:O	1.87	1.05
25:G:102:CDL:H221	25:G:102:CDL:H551	1.37	1.05
12:L:20:ARG:HH21	21:L:103:TGL:HC51	1.23	1.04
1:A:302[B]:ARG:HH12	1:A:365:ILE:HD11	1.25	1.01

All (4) 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)
29:B:454:HOH:O	29:D:303:HOH:O[2_584]	2.03	0.17
29:I:129:HOH:O	29:V:201:HOH:O[3_647]	2.03	0.17
29:I:132:HOH:O	29:M:226:HOH:O[2_584]	2.09	0.11
29:B:500:HOH:O	29:D:437:HOH:O[2_584]	2.15	0.05

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	550/514 (107%)	537 (98%)	13 (2%)	0	100 100
1	N	534/514 (104%)	517 (97%)	15 (3%)	2 (0%)	30 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	229/227 (101%)	220 (96%)	9 (4%)	0	100	100
2	O	232/227 (102%)	226 (97%)	6 (3%)	0	100	100
3	C	262/259 (101%)	256 (98%)	6 (2%)	0	100	100
3	P	259/259 (100%)	253 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/144 (99%)	135 (95%)	4 (3%)	3 (2%)	5	1
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	97/98 (99%)	95 (98%)	2 (2%)	0	100	100
6	S	97/98 (99%)	93 (96%)	4 (4%)	0	100	100
7	G	81/84 (96%)	71 (88%)	7 (9%)	3 (4%)	2	0
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	1	0
8	H	77/79 (98%)	74 (96%)	2 (3%)	1 (1%)	9	3
8	U	77/79 (98%)	73 (95%)	2 (3%)	2 (3%)	4	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
All	All	3586/3558 (101%)	3474 (97%)	97 (3%)	15 (0%)	30	19

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	6	GLY
4	Q	9	GLU
4	Q	10	ASP
4	Q	11	TYR

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	461/426 (108%)	457 (99%)	4 (1%)	70 67
1	N	445/426 (104%)	441 (99%)	4 (1%)	70 67
2	B	214/210 (102%)	204 (95%)	10 (5%)	23 11
2	O	217/210 (103%)	206 (95%)	11 (5%)	21 9
3	C	229/224 (102%)	225 (98%)	4 (2%)	53 45
3	P	226/224 (101%)	222 (98%)	4 (2%)	51 43
4	D	129/128 (101%)	127 (98%)	2 (2%)	55 47
4	Q	128/128 (100%)	123 (96%)	5 (4%)	28 16
5	E	92/92 (100%)	91 (99%)	1 (1%)	65 60
5	R	92/92 (100%)	91 (99%)	1 (1%)	65 60
6	F	82/81 (101%)	79 (96%)	3 (4%)	30 18
6	S	82/81 (101%)	79 (96%)	3 (4%)	30 18
7	G	67/67 (100%)	62 (92%)	5 (8%)	12 4
7	T	68/67 (102%)	63 (93%)	5 (7%)	13 4
8	H	71/71 (100%)	68 (96%)	3 (4%)	26 14
8	U	71/71 (100%)	68 (96%)	3 (4%)	26 14
9	I	57/57 (100%)	55 (96%)	2 (4%)	32 19
9	V	57/57 (100%)	55 (96%)	2 (4%)	32 19
10	J	49/49 (100%)	49 (100%)	0	100 100
10	W	49/49 (100%)	47 (96%)	2 (4%)	27 15
11	K	39/39 (100%)	39 (100%)	0	100 100
11	X	39/39 (100%)	39 (100%)	0	100 100
12	L	39/39 (100%)	38 (97%)	1 (3%)	40 28
12	Y	39/39 (100%)	37 (95%)	2 (5%)	21 9
13	M	37/37 (100%)	37 (100%)	0	100 100
13	Z	37/37 (100%)	36 (97%)	1 (3%)	39 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3116/3040 (102%)	3038 (98%)	78 (2%)	43 30

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	19	ARG
9	V	8	GLN
5	R	80	GLU
7	T	33	LEU
12	Y	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	38	ASN
4	Q	109	HIS
4	Q	101	HIS
7	T	41	HIS
4	D	109	HIS

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	0.64	0	8,9,11	0.96	0
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.70	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TPO	T	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.23	1 (10%)
7	TPO	G	11	7	8,10,11	1.33	1 (12%)	10,14,16	1.35	1 (10%)
1	FME	N	1	1	8,9,10	0.51	0	7,9,11	1.62	1 (14%)
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	0.61	0
1	FME	A	1	1	8,9,10	0.65	0	7,9,11	1.62	1 (14%)
2	FME	B	1	2	8,9,10	0.96	0	7,9,11	2.08	3 (42%)

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	-	3/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.94	1.60	1.50
7	T	11	TPO	P-O1P	2.73	1.59	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-3.56	103.07	112.95
2	O	1	FME	CG-CB-CA	-3.51	103.19	112.95
1	N	1	FME	CE-SD-CG	3.25	111.55	100.40
7	G	11	TPO	CG2-CB-CA	3.09	119.27	113.16
1	A	1	FME	CE-SD-CG	2.87	110.25	100.40

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 160 ligands modelled in this entry, 10 are monoatomic - leaving 150 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	EDO	N	623	-	3,3,3	0.61	0	2,2,2	0.55	0
22	EDO	N	615	-	3,3,3	0.68	0	2,2,2	0.39	0
22	EDO	F	110	-	3,3,3	0.70	0	2,2,2	0.18	0
26	PEK	C	309	-	52,52,52	0.88	2 (3%)	55,57,57	1.23	6 (10%)
18	DMU	P	302	-	10,10,34	0.44	0	9,9,45	0.38	0
22	EDO	D	207	-	3,3,3	0.58	0	2,2,2	0.31	0
18	DMU	X	102	-	21,21,34	0.57	0	24,25,45	1.40	2 (8%)
22	EDO	P	314	-	3,3,3	0.92	0	2,2,2	0.07	0
22	EDO	J	103	-	3,3,3	0.63	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	A	602	29,1	66,67,67	1.86	20 (30%)	78,103,103	2.47	30 (38%)
22	EDO	A	611	-	3,3,3	0.69	0	2,2,2	0.50	0
21	TGL	N	608	-	62,62,62	1.15	3 (4%)	65,65,65	1.32	6 (9%)
22	EDO	S	102	-	3,3,3	0.74	0	2,2,2	0.65	0
25	CDL	C	307	-	99,99,99	1.40	14 (14%)	105,111,111	1.66	17 (16%)
18	DMU	Y	101	-	34,34,34	0.73	0	45,45,45	1.13	3 (6%)
19	PGV	P	309	-	50,50,50	0.82	4 (8%)	53,56,56	1.08	4 (7%)
22	EDO	P	311	-	3,3,3	0.60	0	2,2,2	0.28	0
18	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.12	4 (8%)
22	EDO	S	104	-	3,3,3	0.76	0	2,2,2	0.34	0
22	EDO	S	105	-	3,3,3	0.36	0	2,2,2	0.28	0
26	PEK	F	102	6,25	52,52,52	1.06	2 (3%)	55,57,57	1.50	5 (9%)
14	HEA	A	601[B]	-	66,67,67	1.94	20 (30%)	78,103,103	2.47	36 (46%)
18	DMU	P	303	-	34,34,34	0.64	0	45,45,45	2.08	15 (33%)
22	EDO	F	103	-	3,3,3	0.72	0	2,2,2	0.55	0
22	EDO	P	315	-	3,3,3	1.08	0	2,2,2	0.66	0
18	DMU	O	302	-	10,10,34	0.40	0	9,9,45	0.40	0
22	EDO	N	618	-	3,3,3	0.83	0	2,2,2	0.36	0
22	EDO	L	104	-	3,3,3	0.68	0	2,2,2	0.54	0
22	EDO	A	616	-	3,3,3	0.61	0	2,2,2	0.27	0
19	PGV	A	608	-	50,50,50	0.89	4 (8%)	53,56,56	1.28	2 (3%)
22	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.57	0
22	EDO	C	313	-	3,3,3	0.38	0	2,2,2	0.68	0
19	PGV	A	607	-	50,50,50	1.10	3 (6%)	53,56,56	1.31	7 (13%)
14	HEA	N	601[B]	-	66,67,67	1.69	20 (30%)	78,103,103	2.06	28 (35%)
14	HEA	N	602	29,1	66,67,67	1.76	17 (25%)	78,103,103	2.26	36 (46%)
22	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.24	0
22	EDO	M	102	-	3,3,3	0.40	0	2,2,2	0.19	0
22	EDO	F	108	-	3,3,3	0.47	0	2,2,2	0.24	0
22	EDO	Q	205	-	3,3,3	0.75	0	2,2,2	0.28	0
18	DMU	X	105	-	10,10,34	0.38	0	9,9,45	0.32	0
18	DMU	X	101	-	10,10,34	0.44	0	9,9,45	0.45	0
24	CHD	G	101	-	32,32,32	0.88	0	51,51,51	1.39	8 (15%)
22	EDO	N	620	-	3,3,3	0.64	0	2,2,2	0.19	0
20	PSC	V	101	9	51,51,51	1.19	4 (7%)	57,59,59	1.56	11 (19%)
26	PEK	P	308	-	52,52,52	0.77	2 (3%)	55,57,57	1.30	5 (9%)
18	DMU	W	101	-	21,21,34	0.92	1 (4%)	24,25,45	1.54	5 (20%)
22	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.55	0
22	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CDL	P	306	-	99,99,99	1.33	12 (12%)	105,111,111	1.58	18 (17%)
22	EDO	C	317	-	3,3,3	0.72	0	2,2,2	0.24	0
22	EDO	N	616	-	3,3,3	0.68	0	2,2,2	0.26	0
22	EDO	H	102	-	3,3,3	0.27	0	2,2,2	0.79	0
22	EDO	U	102	-	3,3,3	0.53	0	2,2,2	0.13	0
24	CHD	C	305	-	32,32,32	1.08	1 (3%)	51,51,51	1.43	6 (11%)
21	TGL	D	202	-	62,62,62	1.33	5 (8%)	65,65,65	1.16	6 (9%)
24	CHD	P	304	-	32,32,32	0.89	0	51,51,51	1.57	7 (13%)
18	DMU	B	302	-	10,10,34	0.42	0	9,9,45	0.44	0
19	PGV	P	310	-	50,50,50	1.04	2 (4%)	53,56,56	1.30	5 (9%)
18	DMU	C	303	-	22,22,34	0.80	1 (4%)	27,27,45	1.56	3 (11%)
22	EDO	F	104	-	3,3,3	0.39	0	2,2,2	0.29	0
22	EDO	P	312	-	3,3,3	0.39	0	2,2,2	0.78	0
26	PEK	C	308	-	52,52,52	1.17	2 (3%)	55,57,57	1.40	6 (10%)
14	HEA	A	601[A]	-	66,67,67	1.95	20 (30%)	78,103,103	2.46	33 (42%)
20	PSC	A	609	1	51,51,51	1.13	3 (5%)	57,59,59	1.53	6 (10%)
22	EDO	B	306	-	3,3,3	0.76	0	2,2,2	0.39	0
22	EDO	N	617	-	3,3,3	0.29	0	2,2,2	0.75	0
22	EDO	E	201	-	3,3,3	0.49	0	2,2,2	0.26	0
22	EDO	A	618	-	3,3,3	0.66	0	2,2,2	0.24	0
19	PGV	C	310	-	50,50,50	0.76	1 (2%)	53,56,56	1.16	5 (9%)
19	PGV	N	606	-	50,50,50	1.02	2 (4%)	53,56,56	1.28	6 (11%)
14	HEA	N	601[A]	-	66,67,67	1.70	19 (28%)	78,103,103	1.92	23 (29%)
18	DMU	D	201	-	21,21,34	0.89	1 (4%)	24,25,45	1.55	5 (20%)
22	EDO	D	205	-	3,3,3	0.55	0	2,2,2	0.37	0
18	DMU	C	302	-	34,34,34	0.51	0	45,45,45	2.14	15 (33%)
18	DMU	A	606	-	11,11,34	0.36	0	9,9,45	0.71	0
24	CHD	P	305	-	32,32,32	0.72	0	51,51,51	1.73	9 (17%)
21	TGL	L	103	-	62,62,62	1.32	4 (6%)	65,65,65	2.12	16 (24%)
22	EDO	P	313	-	3,3,3	0.95	0	2,2,2	0.34	0
22	EDO	A	613	-	3,3,3	0.92	0	2,2,2	0.62	0
18	DMU	C	304	-	10,10,34	0.40	0	9,9,45	0.29	0
22	EDO	Q	203	-	3,3,3	0.48	0	2,2,2	0.27	0
22	EDO	O	304	-	3,3,3	0.60	0	2,2,2	0.24	0
26	PEK	P	307	-	52,52,52	1.09	2 (3%)	55,57,57	1.38	7 (12%)
22	EDO	B	304	-	3,3,3	0.41	0	2,2,2	0.49	0
22	EDO	A	615	-	3,3,3	0.34	0	2,2,2	0.92	0
22	EDO	C	314	-	3,3,3	0.75	0	2,2,2	1.02	0
22	EDO	N	611	-	3,3,3	1.12	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	N	607	-	50,50,50	1.01	2 (4%)	53,56,56	1.37	7 (13%)
22	EDO	N	622	-	3,3,3	1.10	0	2,2,2	1.30	0
18	DMU	L	101	22	34,34,34	0.68	0	45,45,45	1.64	9 (20%)
22	EDO	A	619	-	3,3,3	0.43	0	2,2,2	0.65	0
26	PEK	T	103	-	52,52,52	1.09	2 (3%)	55,57,57	1.48	6 (10%)
22	EDO	F	105	-	3,3,3	0.65	0	2,2,2	0.64	0
18	DMU	K	102	-	12,12,34	0.49	0	10,11,45	0.47	0
22	EDO	T	105	-	3,3,3	0.57	0	2,2,2	0.31	0
22	EDO	C	311	-	3,3,3	0.90	0	2,2,2	0.45	0
24	CHD	C	306	-	32,32,32	0.85	1 (3%)	51,51,51	2.03	16 (31%)
22	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.19	0
22	EDO	N	610	-	3,3,3	0.61	0	2,2,2	0.39	0
18	DMU	J	101	-	21,21,34	0.93	1 (4%)	24,25,45	1.36	4 (16%)
22	EDO	B	303	-	3,3,3	0.67	0	2,2,2	0.65	0
25	CDL	T	102	7	99,99,99	1.36	12 (12%)	105,111,111	1.42	14 (13%)
22	EDO	A	612	-	3,3,3	0.72	0	2,2,2	1.12	0
22	EDO	D	203	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	D	204	-	3,3,3	0.41	0	2,2,2	0.50	0
24	CHD	J	102	-	32,32,32	0.82	0	51,51,51	1.65	13 (25%)
22	EDO	G	103	-	3,3,3	0.88	0	2,2,2	0.54	0
22	EDO	C	315	-	3,3,3	0.50	0	2,2,2	0.57	0
22	EDO	N	614	-	3,3,3	0.54	0	2,2,2	0.22	0
18	DMU	K	103	-	22,22,34	1.01	1 (4%)	27,27,45	1.33	4 (14%)
22	EDO	S	106	-	3,3,3	0.73	0	2,2,2	0.32	0
22	EDO	C	312	-	3,3,3	0.93	0	2,2,2	0.13	0
22	EDO	Y	104	-	3,3,3	0.56	0	2,2,2	0.12	0
22	EDO	P	316	-	3,3,3	0.64	0	2,2,2	0.45	0
23	CUA	O	301	2	0,1,1	-	-	-		
22	EDO	F	109	-	3,3,3	0.59	0	2,2,2	0.30	0
22	EDO	O	303	-	3,3,3	0.71	0	2,2,2	0.62	0
22	EDO	P	317	-	3,3,3	0.69	0	2,2,2	0.60	0
22	EDO	Q	204	-	3,3,3	0.40	0	2,2,2	0.54	0
22	EDO	T	106	-	3,3,3	0.86	0	2,2,2	1.06	0
21	TGL	A	610	-	62,62,62	1.18	3 (4%)	65,65,65	1.34	6 (9%)
22	EDO	B	305	-	3,3,3	0.37	0	2,2,2	0.24	0
28	PO4	H	101	-	4,4,4	0.99	0	6,6,6	0.39	0
22	EDO	B	307	-	3,3,3	0.77	0	2,2,2	0.69	0
18	DMU	Z	101	-	34,34,34	0.63	1 (2%)	45,45,45	1.06	3 (6%)
18	DMU	X	103	-	10,10,34	0.38	0	9,9,45	0.27	0
19	PGV	T	104	7	50,50,50	1.07	2 (4%)	53,56,56	1.50	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	DMU	K	104	-	10,10,34	0.31	0	9,9,45	0.50	0
22	EDO	D	206	-	3,3,3	0.46	0	2,2,2	0.60	0
22	EDO	F	107	-	3,3,3	0.73	0	2,2,2	0.31	0
22	EDO	C	316	-	3,3,3	0.89	0	2,2,2	0.53	0
22	EDO	F	106	-	3,3,3	0.96	0	2,2,2	0.29	0
21	TGL	Q	202	-	62,62,62	1.12	3 (4%)	65,65,65	0.95	5 (7%)
22	EDO	N	619	-	3,3,3	0.54	0	2,2,2	0.41	0
22	EDO	W	102	-	3,3,3	0.47	0	2,2,2	0.41	0
18	DMU	K	101	-	10,10,34	0.27	0	9,9,45	0.78	0
22	EDO	N	609	-	3,3,3	0.58	0	2,2,2	0.87	0
24	CHD	T	101	-	32,32,32	1.10	2 (6%)	51,51,51	1.54	9 (17%)
22	EDO	L	105	18	3,3,3	0.49	0	2,2,2	0.27	0
23	CUA	B	301	2	0,1,1	-	-	-		
24	CHD	Y	102	-	32,32,32	0.64	0	51,51,51	2.18	15 (29%)
21	TGL	Y	103	-	62,62,62	1.33	3 (4%)	65,65,65	1.57	9 (13%)
22	EDO	N	621	-	3,3,3	0.53	0	2,2,2	0.81	0
25	CDL	G	102	26	99,99,99	1.41	12 (12%)	105,111,111	1.25	9 (8%)
22	EDO	A	617	-	3,3,3	0.39	0	2,2,2	0.65	0
24	CHD	L	102	-	32,32,32	0.62	0	51,51,51	2.45	20 (39%)
18	DMU	X	104	-	10,10,34	0.31	0	9,9,45	0.44	0
28	PO4	U	101	-	4,4,4	0.91	0	6,6,6	0.58	0
22	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.40	0
18	DMU	Q	201	-	22,22,34	0.86	1 (4%)	27,27,45	1.74	7 (25%)

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	EDO	N	623	-	-	1/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	F	110	-	-	1/1/1/1	-
26	PEK	C	309	-	-	16/56/56/56	-
18	DMU	P	302	-	-	0/8/8/59	-
22	EDO	D	207	-	-	0/1/1/1	-
18	DMU	X	102	-	-	8/13/29/59	0/1/1/2
22	EDO	P	314	-	-	1/1/1/1	-
22	EDO	J	103	-	-	1/1/1/1	-
14	HEA	A	602	29,1	-	5/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	611	-	-	1/1/1/1	-
21	TGL	N	608	-	-	33/65/65/65	-
22	EDO	S	102	-	-	0/1/1/1	-
25	CDL	C	307	-	-	43/110/110/110	-
18	DMU	Y	101	-	-	5/19/59/59	0/2/2/2
19	PGV	P	309	-	-	10/55/55/55	-
22	EDO	P	311	-	-	0/1/1/1	-
18	DMU	M	101	-	-	7/19/59/59	0/2/2/2
22	EDO	S	104	-	-	0/1/1/1	-
22	EDO	S	105	-	-	0/1/1/1	-
26	PEK	F	102	6,25	-	24/56/56/56	-
14	HEA	A	601[B]	-	-	4/36/76/76	-
18	DMU	P	303	-	-	6/19/59/59	0/2/2/2
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	P	315	-	-	1/1/1/1	-
18	DMU	O	302	-	-	0/8/8/59	-
22	EDO	N	618	-	-	1/1/1/1	-
22	EDO	L	104	-	-	0/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
19	PGV	A	608	-	-	4/55/55/55	-
22	EDO	S	103	-	-	1/1/1/1	-
22	EDO	C	313	-	-	0/1/1/1	-
19	PGV	A	607	-	-	18/55/55/55	-
14	HEA	N	601[B]	-	-	4/36/76/76	-
14	HEA	N	602	29,1	-	6/36/76/76	-
22	EDO	A	614	-	-	0/1/1/1	-
22	EDO	M	102	-	-	0/1/1/1	-
22	EDO	F	108	-	-	0/1/1/1	-
22	EDO	Q	205	-	-	1/1/1/1	-
18	DMU	X	105	-	-	4/8/8/59	-
18	DMU	X	101	-	-	1/8/8/59	-
24	CHD	G	101	-	-	2/9/74/74	0/4/4/4
22	EDO	N	620	-	-	0/1/1/1	-
20	PSC	V	101	9	-	20/55/55/55	-
26	PEK	P	308	-	-	11/56/56/56	-
18	DMU	W	101	-	-	4/13/29/59	0/1/1/2
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	N	613	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	P	306	-	-	42/110/110/110	-
22	EDO	C	317	-	-	1/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
22	EDO	H	102	-	-	0/1/1/1	-
22	EDO	U	102	-	-	1/1/1/1	-
24	CHD	C	305	-	-	1/9/74/74	0/4/4/4
21	TGL	D	202	-	-	21/65/65/65	-
24	CHD	P	304	-	-	2/9/74/74	0/4/4/4
18	DMU	B	302	-	-	3/8/8/59	-
19	PGV	P	310	-	-	16/55/55/55	-
18	DMU	C	303	-	-	7/13/33/59	0/1/1/2
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
26	PEK	C	308	-	-	17/56/56/56	-
14	HEA	A	601[A]	-	-	7/36/76/76	-
20	PSC	A	609	1	-	15/55/55/55	-
22	EDO	B	306	-	-	1/1/1/1	-
22	EDO	N	617	-	-	1/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	A	618	-	-	1/1/1/1	-
19	PGV	C	310	-	-	8/55/55/55	-
19	PGV	N	606	-	-	15/55/55/55	-
14	HEA	N	601[A]	-	-	11/36/76/76	-
18	DMU	D	201	-	-	4/13/29/59	0/1/1/2
22	EDO	D	205	-	-	0/1/1/1	-
18	DMU	C	302	-	-	10/19/59/59	0/2/2/2
18	DMU	A	606	-	-	2/8/8/59	-
24	CHD	P	305	-	-	5/9/74/74	0/4/4/4
21	TGL	L	103	-	-	32/65/65/65	-
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	A	613	-	-	0/1/1/1	-
18	DMU	C	304	-	-	5/8/8/59	-
22	EDO	Q	203	-	-	1/1/1/1	-
22	EDO	O	304	-	-	0/1/1/1	-
26	PEK	P	307	-	-	22/56/56/56	-
22	EDO	B	304	-	-	1/1/1/1	-
22	EDO	A	615	-	-	1/1/1/1	-
22	EDO	C	314	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	N	611	-	-	0/1/1/1	-
19	PGV	N	607	-	-	7/55/55/55	-
22	EDO	N	622	-	-	1/1/1/1	-
18	DMU	L	101	22	-	8/19/59/59	0/2/2/2
22	EDO	A	619	-	-	1/1/1/1	-
26	PEK	T	103	-	-	24/56/56/56	-
22	EDO	F	105	-	-	0/1/1/1	-
18	DMU	K	102	-	-	4/9/10/59	-
22	EDO	T	105	-	-	1/1/1/1	-
22	EDO	C	311	-	-	1/1/1/1	-
24	CHD	C	306	-	-	9/9/74/74	0/4/4/4
22	EDO	N	612	-	-	1/1/1/1	-
22	EDO	N	610	-	-	0/1/1/1	-
18	DMU	J	101	-	-	4/13/29/59	0/1/1/2
22	EDO	B	303	-	-	0/1/1/1	-
25	CDL	T	102	7	-	43/110/110/110	-
22	EDO	A	612	-	-	0/1/1/1	-
22	EDO	D	203	-	-	1/1/1/1	-
22	EDO	D	204	-	-	0/1/1/1	-
24	CHD	J	102	-	-	5/9/74/74	0/4/4/4
22	EDO	G	103	-	-	0/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
18	DMU	K	103	-	-	6/13/33/59	0/1/1/2
22	EDO	S	106	-	-	0/1/1/1	-
22	EDO	C	312	-	-	0/1/1/1	-
22	EDO	Y	104	-	-	1/1/1/1	-
22	EDO	P	316	-	-	0/1/1/1	-
22	EDO	F	109	-	-	1/1/1/1	-
22	EDO	O	303	-	-	0/1/1/1	-
22	EDO	P	317	-	-	1/1/1/1	-
22	EDO	Q	204	-	-	0/1/1/1	-
22	EDO	T	106	-	-	0/1/1/1	-
21	TGL	A	610	-	-	36/65/65/65	-
22	EDO	B	305	-	-	1/1/1/1	-
22	EDO	B	307	-	-	1/1/1/1	-
18	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
18	DMU	X	103	-	-	4/8/8/59	-
19	PGV	T	104	7	-	19/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	DMU	K	104	-	-	4/8/8/59	-
22	EDO	D	206	-	-	0/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
22	EDO	C	316	-	-	1/1/1/1	-
22	EDO	F	106	-	-	0/1/1/1	-
21	TGL	Q	202	-	-	28/65/65/65	-
22	EDO	N	619	-	-	1/1/1/1	-
22	EDO	W	102	-	-	1/1/1/1	-
18	DMU	K	101	-	-	3/8/8/59	-
22	EDO	N	609	-	-	0/1/1/1	-
24	CHD	T	101	-	-	2/9/74/74	0/4/4/4
22	EDO	L	105	18	-	0/1/1/1	-
24	CHD	Y	102	-	-	1/9/74/74	0/4/4/4
21	TGL	Y	103	-	-	32/65/65/65	-
22	EDO	N	621	-	-	0/1/1/1	-
25	CDL	G	102	26	-	40/110/110/110	-
22	EDO	A	617	-	-	0/1/1/1	-
24	CHD	L	102	-	-	5/9/74/74	0/4/4/4
18	DMU	X	104	-	-	3/8/8/59	-
22	EDO	E	202	-	-	1/1/1/1	-
18	DMU	Q	201	-	-	5/13/33/59	0/1/1/2

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	103	TGL	OG2-CB1	6.24	1.51	1.34
21	Y	103	TGL	OG2-CB1	6.12	1.51	1.34
21	Y	103	TGL	OG3-CC1	5.88	1.50	1.33
14	A	602	HEA	CHD-C1D	5.79	1.50	1.38
25	G	102	CDL	OA6-CA5	5.48	1.49	1.34

The worst 5 of 569 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L	102	CHD	C10-C9-C8	7.39	119.75	111.82
21	L	103	TGL	OG2-CB1-CB2	7.35	127.34	111.50
20	A	609	PSC	C03-C02-C01	-7.04	95.14	111.79
21	Y	103	TGL	OG2-CB1-CB2	6.56	125.64	111.50
14	A	602	HEA	C3C-C2C-C1C	-6.49	99.32	107.16

There are no chirality outliers.

5 of 811 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601[A]	HEA	C18-C19-C20-C21
14	N	601[A]	HEA	C27-C19-C20-C21
18	C	302	DMU	C1-C6-O16-C18
18	C	302	DMU	O5-C6-O16-C18
18	W	101	DMU	O5-C6-O16-C18

There are no ring outliers.

89 monomers are involved in 317 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	623	EDO	1	0
22	N	615	EDO	1	0
22	F	110	EDO	1	0
26	C	309	PEK	6	0
18	X	102	DMU	1	0
14	A	602	HEA	3	0
22	A	611	EDO	1	0
21	N	608	TGL	4	0
25	C	307	CDL	19	0
18	Y	101	DMU	3	0
19	P	309	PGV	4	0
18	M	101	DMU	1	0
22	S	105	EDO	2	0
26	F	102	PEK	6	0
14	A	601[B]	HEA	1	0
18	P	303	DMU	3	0
18	O	302	DMU	2	0
22	N	618	EDO	1	0
22	L	104	EDO	1	0
22	A	616	EDO	1	0
19	A	608	PGV	1	0
22	C	313	EDO	1	0
19	A	607	PGV	5	0
14	N	601[B]	HEA	1	0
14	N	602	HEA	5	0
22	A	614	EDO	1	0
22	F	108	EDO	1	0
22	Q	205	EDO	1	0
24	G	101	CHD	1	0
20	V	101	PSC	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	308	PEK	2	0
18	W	101	DMU	4	0
22	E	203	EDO	2	0
22	N	613	EDO	1	0
25	P	306	CDL	11	0
22	H	102	EDO	2	0
22	U	102	EDO	4	0
21	D	202	TGL	15	0
24	P	304	CHD	1	0
19	P	310	PGV	9	0
18	C	303	DMU	1	0
26	C	308	PEK	5	0
14	A	601[A]	HEA	1	0
20	A	609	PSC	17	0
22	N	617	EDO	4	0
22	A	618	EDO	1	0
19	C	310	PGV	6	0
19	N	606	PGV	7	0
14	N	601[A]	HEA	1	0
22	D	205	EDO	1	0
18	C	302	DMU	1	0
18	A	606	DMU	2	0
24	P	305	CHD	2	0
21	L	103	TGL	16	0
22	P	313	EDO	1	0
22	Q	203	EDO	1	0
22	O	304	EDO	1	0
26	P	307	PEK	1	0
22	A	615	EDO	2	0
19	N	607	PGV	2	0
22	N	622	EDO	2	0
18	L	101	DMU	2	0
26	T	103	PEK	9	0
22	T	105	EDO	1	0
22	C	311	EDO	1	0
24	C	306	CHD	3	0
22	N	612	EDO	4	0
18	J	101	DMU	4	0
25	T	102	CDL	29	0
22	D	203	EDO	1	0
24	J	102	CHD	1	0
18	K	103	DMU	5	0

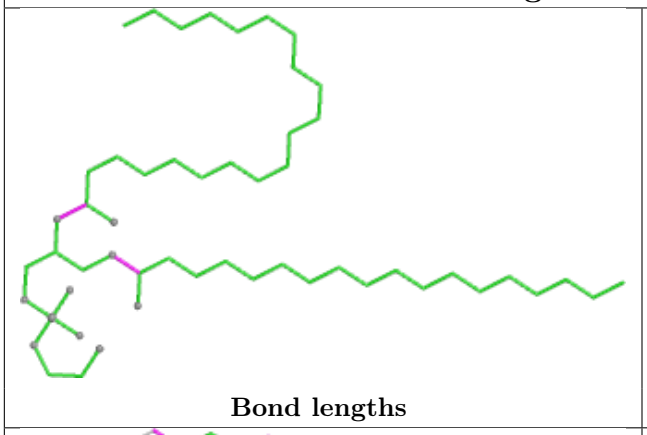
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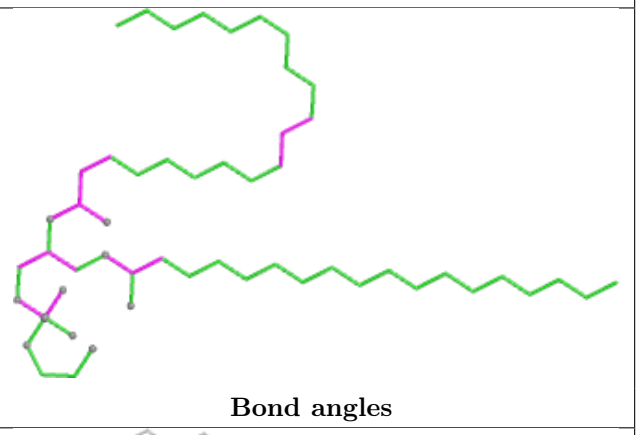
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	316	EDO	2	0
22	F	109	EDO	1	0
22	Q	204	EDO	2	0
21	A	610	TGL	2	0
22	B	305	EDO	2	0
22	B	307	EDO	1	0
18	Z	101	DMU	2	0
19	T	104	PGV	1	0
22	D	206	EDO	1	0
22	C	316	EDO	1	0
21	Q	202	TGL	12	0
24	T	101	CHD	1	0
24	Y	102	CHD	1	0
21	Y	103	TGL	3	0
25	G	102	CDL	22	0
22	A	617	EDO	3	0
18	Q	201	DMU	2	0

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

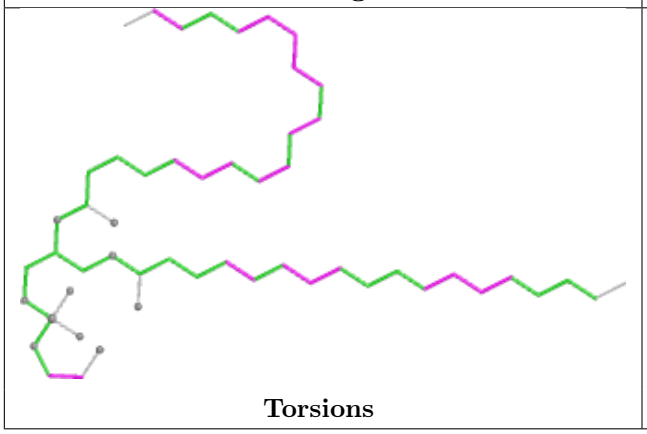
Ligand PEK C 309



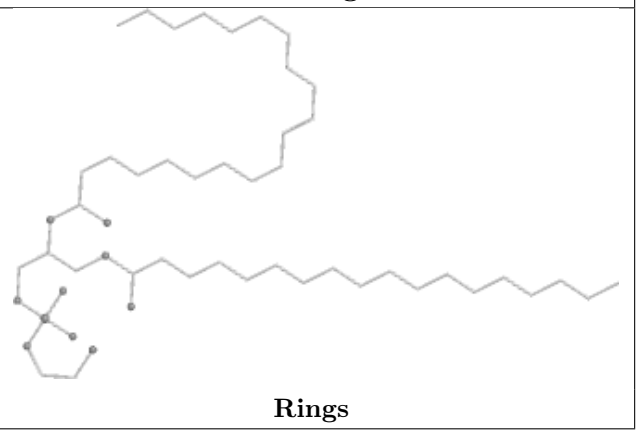
Bond lengths



Bond angles

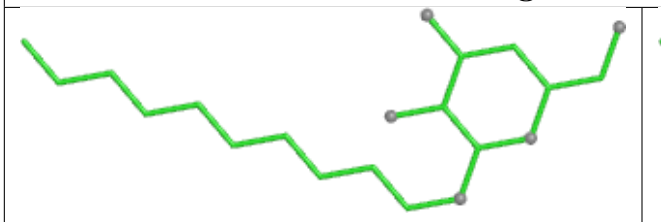


Torsions

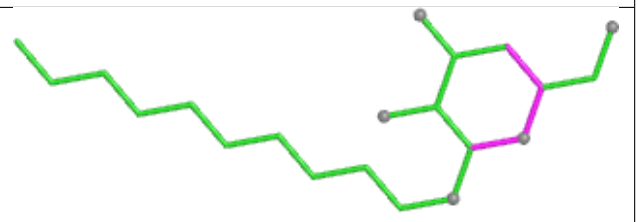


Rings

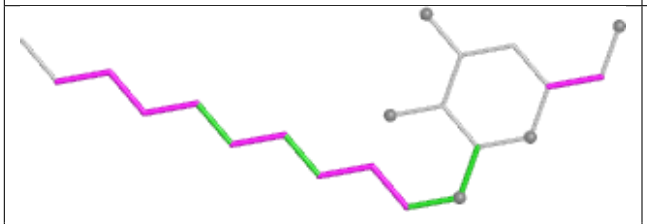
Ligand DMU X 102



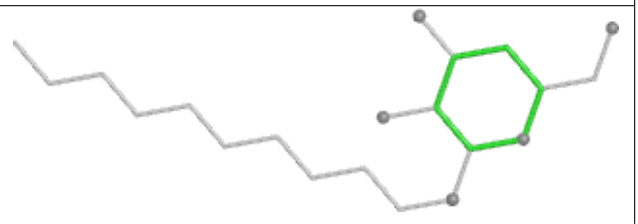
Bond lengths



Bond angles

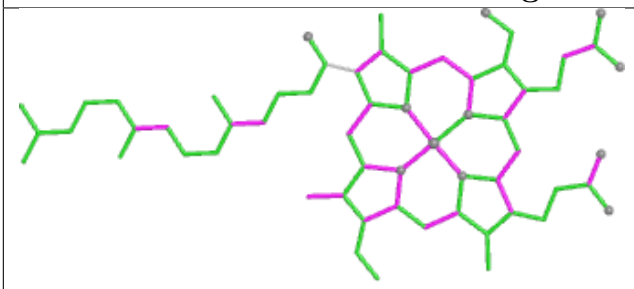


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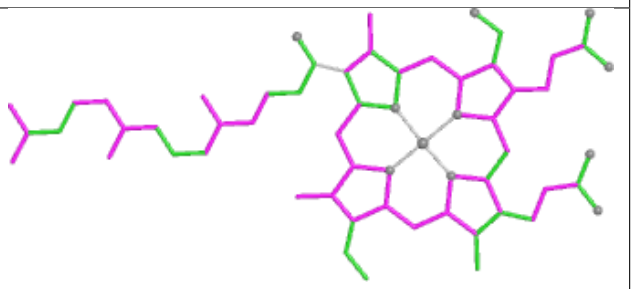


Rings

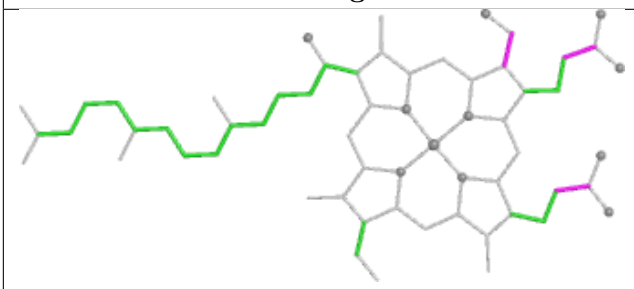
Ligand HEA A 602



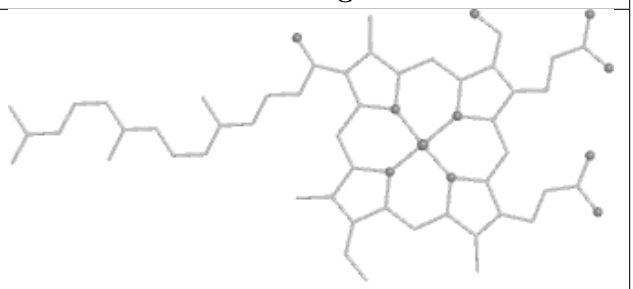
Bond lengths



Bond angles

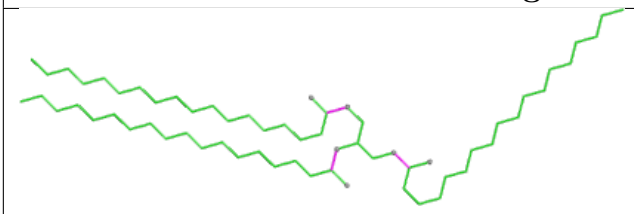


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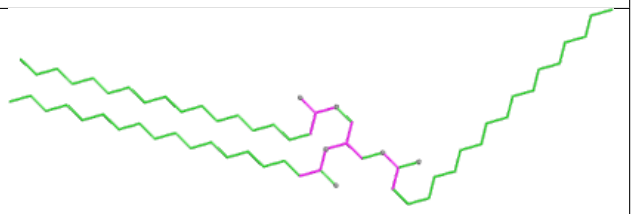


Rings

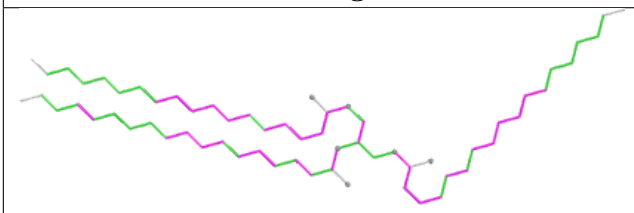
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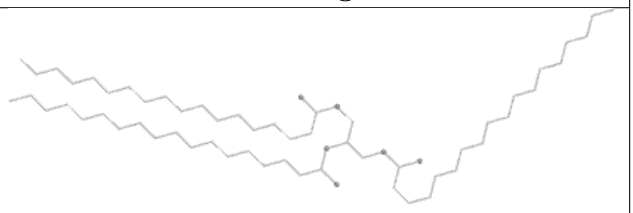
Bond lengths



Bond angles

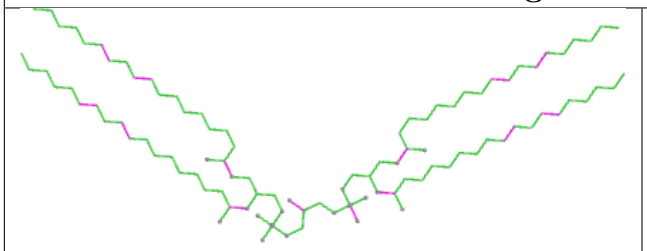


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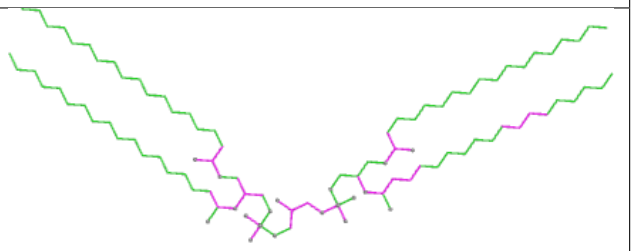


Rings

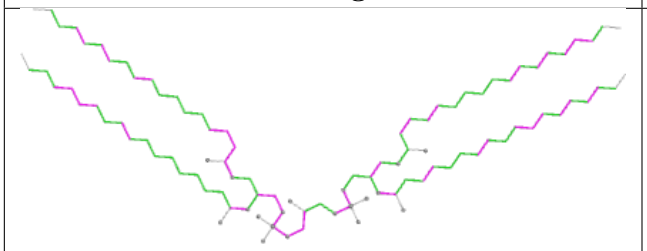
Ligand CDL C 307



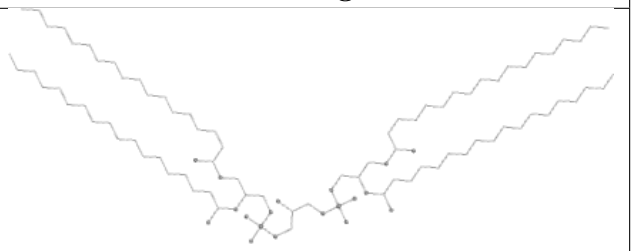
Bond lengths



Bond angles

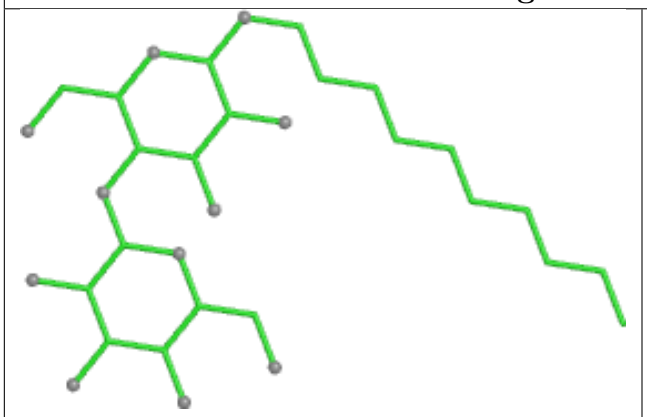


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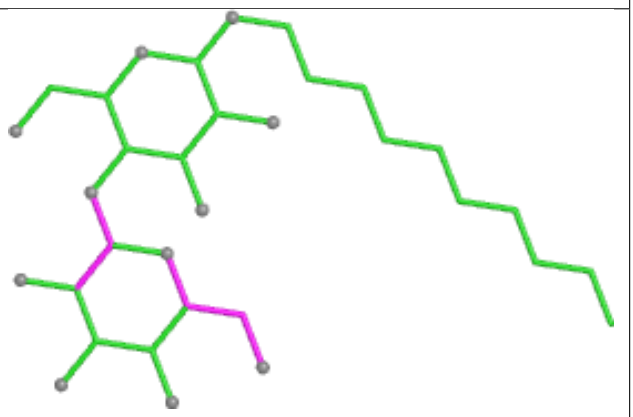


Rings

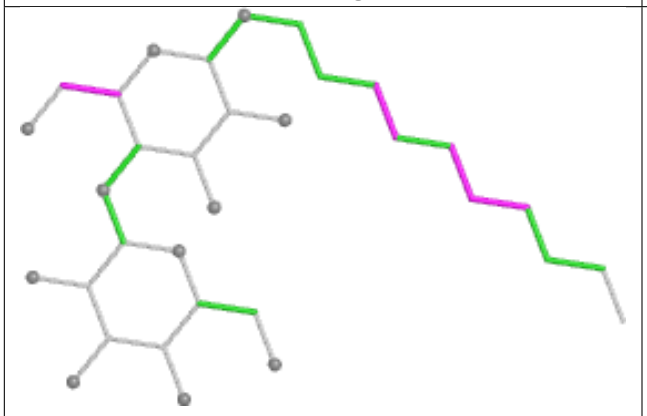
Ligand DMU Y 101



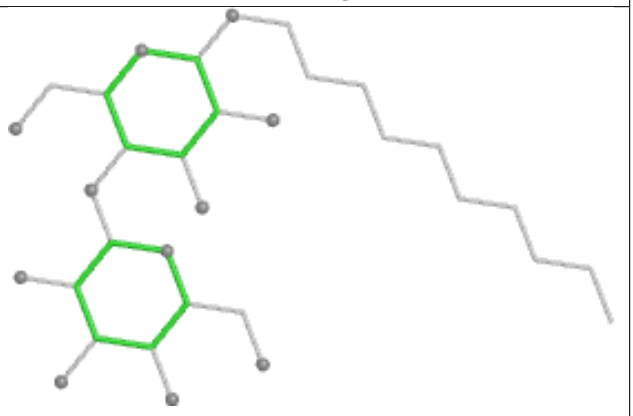
Bond lengths



Bond angles

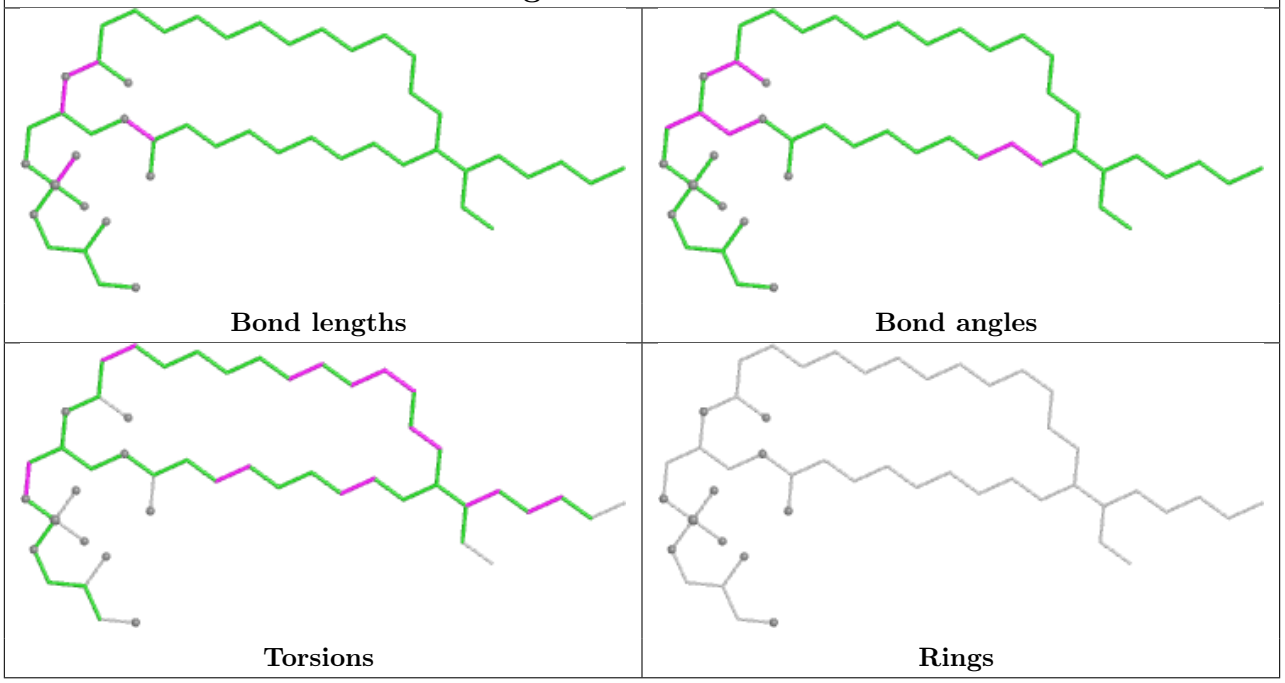


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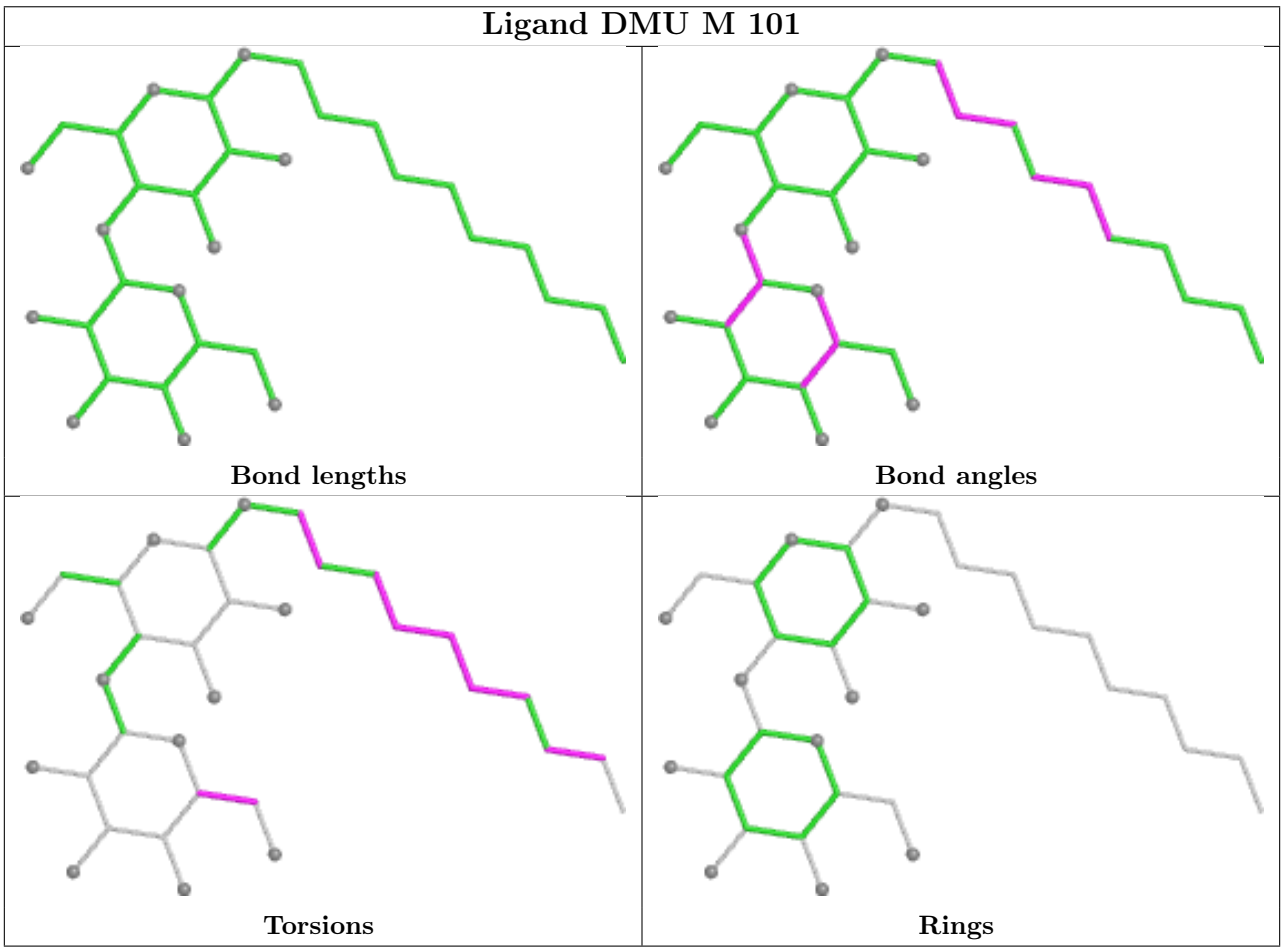


Rings

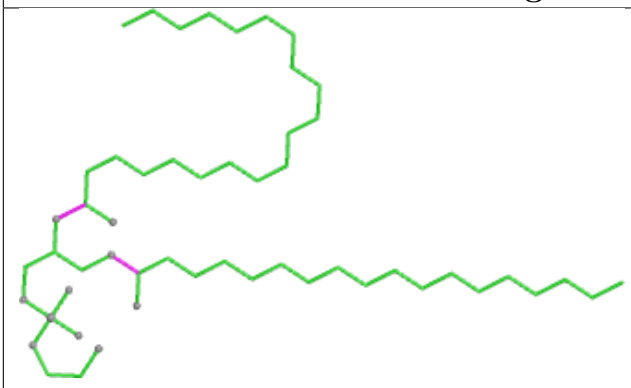
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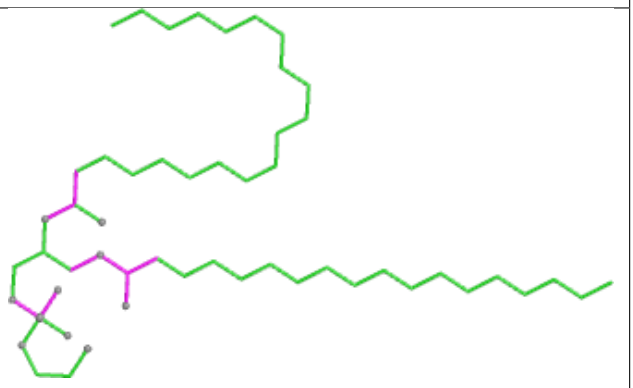
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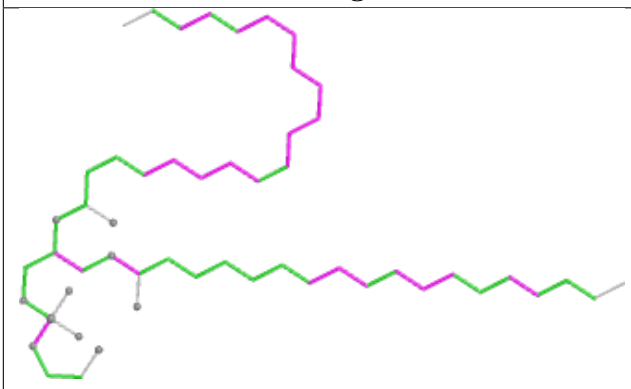
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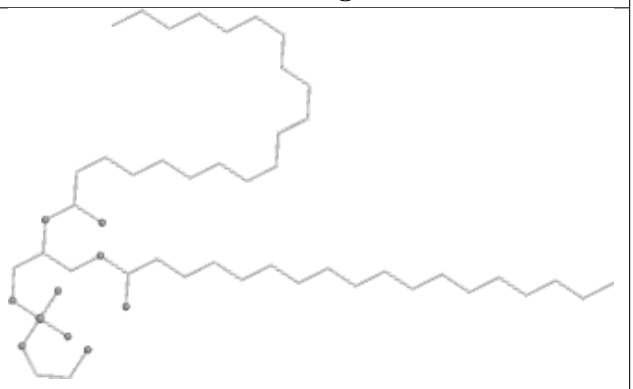
Bond lengths



Bond angles

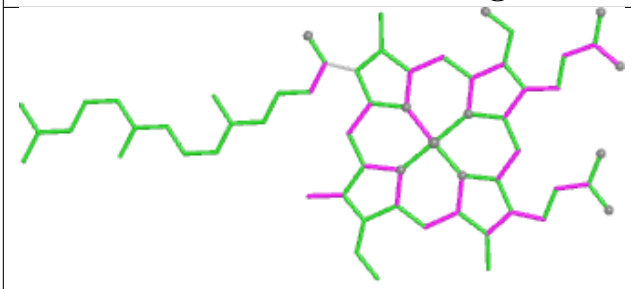


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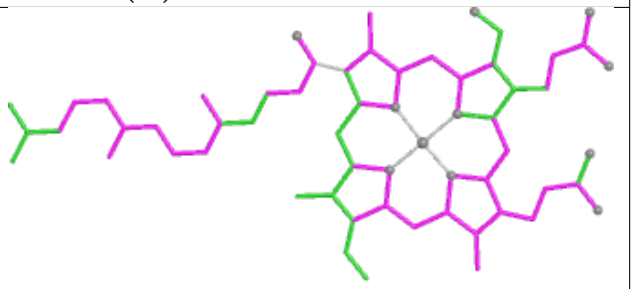


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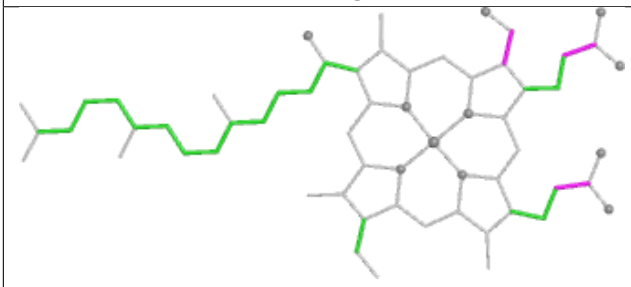
Ligand HEA A 601 (B)



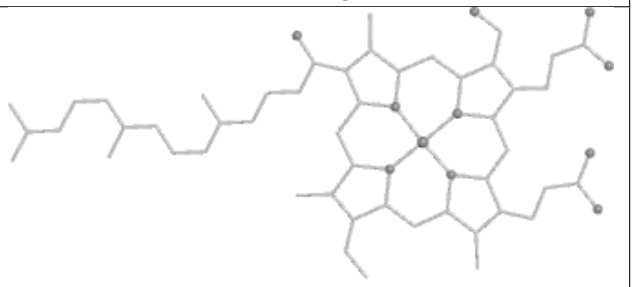
Bond lengths



Bond angles

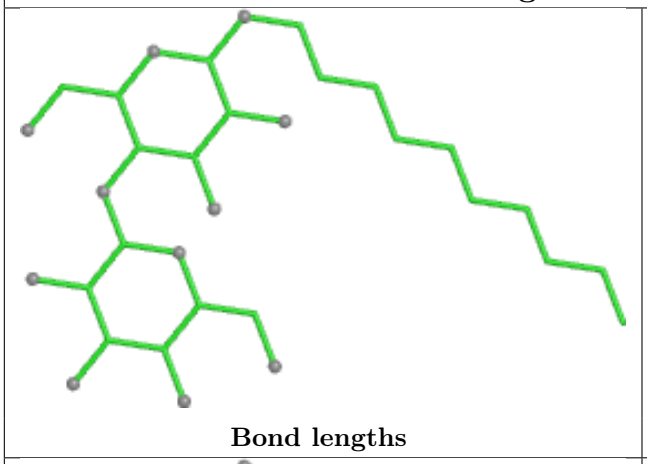


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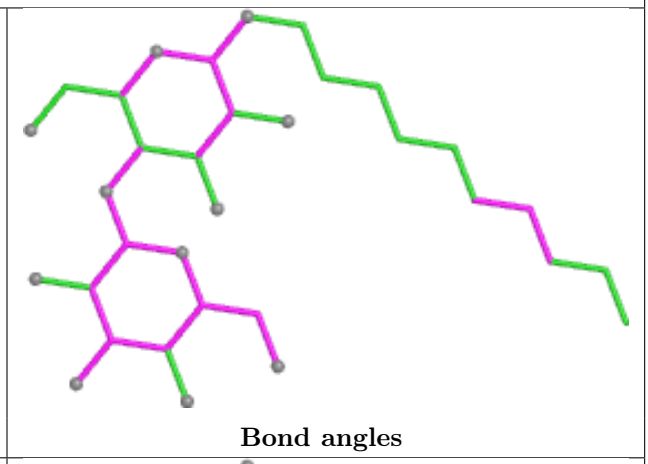


Rings

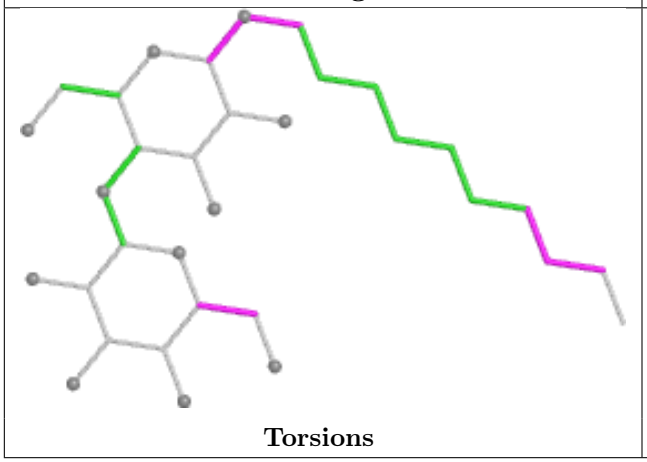
Ligand DMU P 303



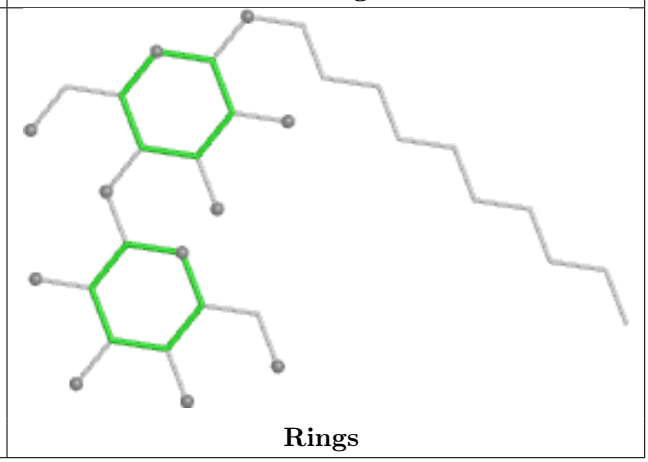
Bond lengths



Bond angles

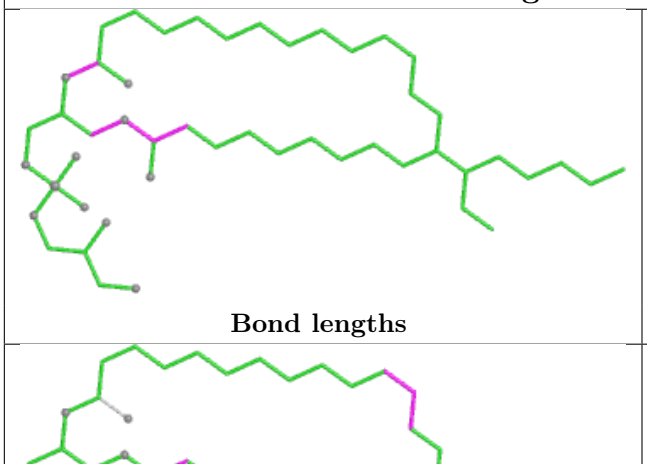


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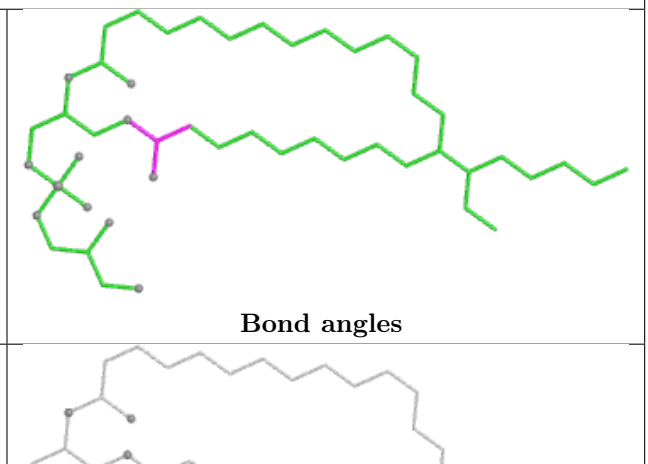


Rings

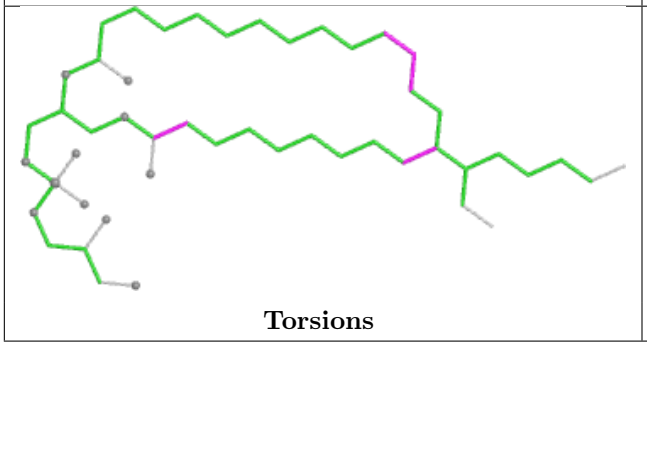
Ligand PGV A 608



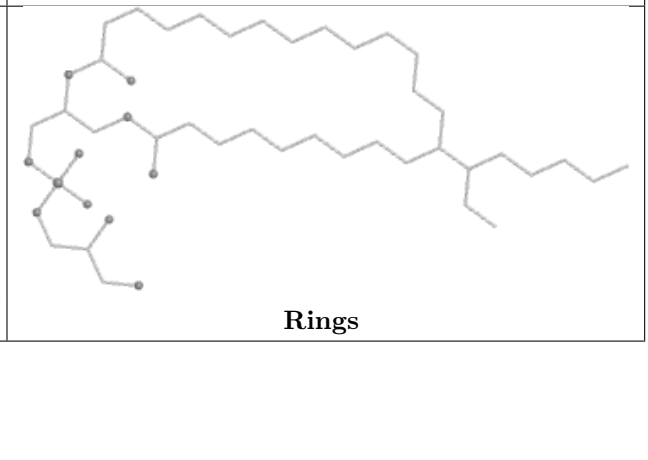
Bond lengths



Bond angles

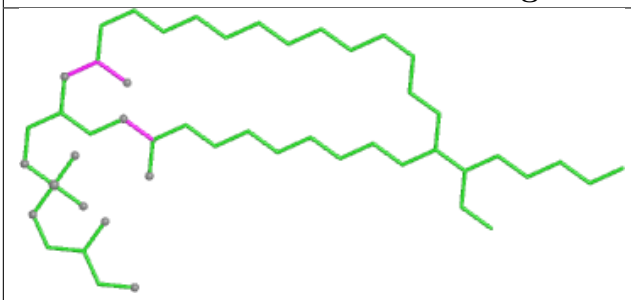


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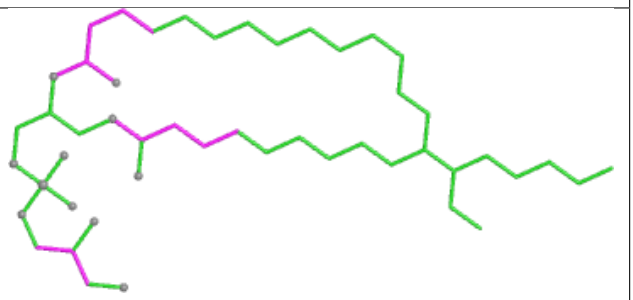


Rings

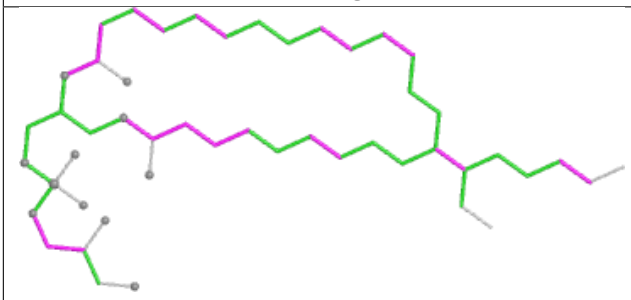
Ligand PGV A 607



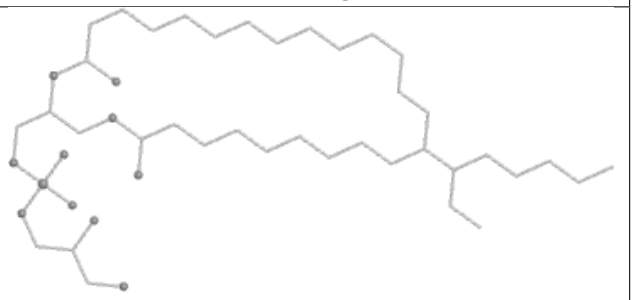
Bond lengths



Bond angles

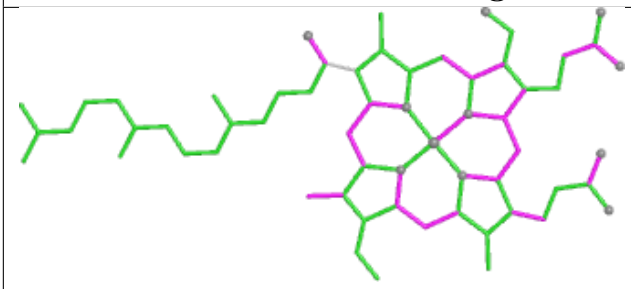


Torsions

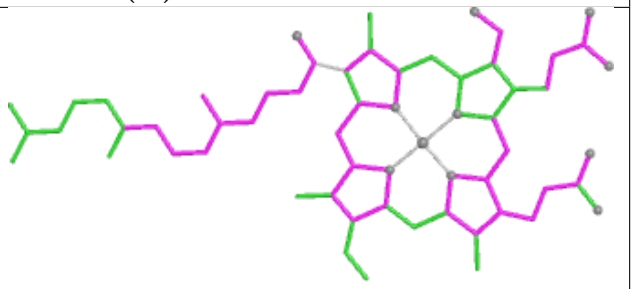


Rings

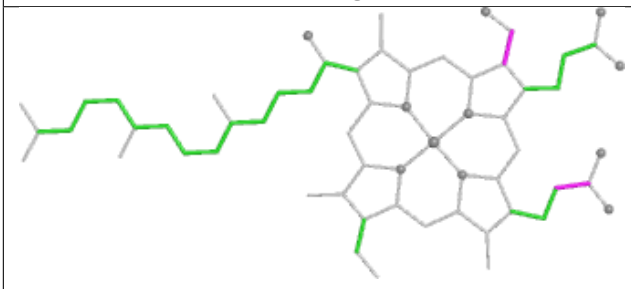
Ligand HEA N 601 (B)



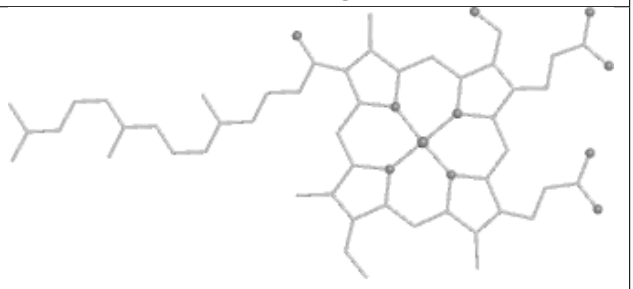
Bond lengths



Bond angles

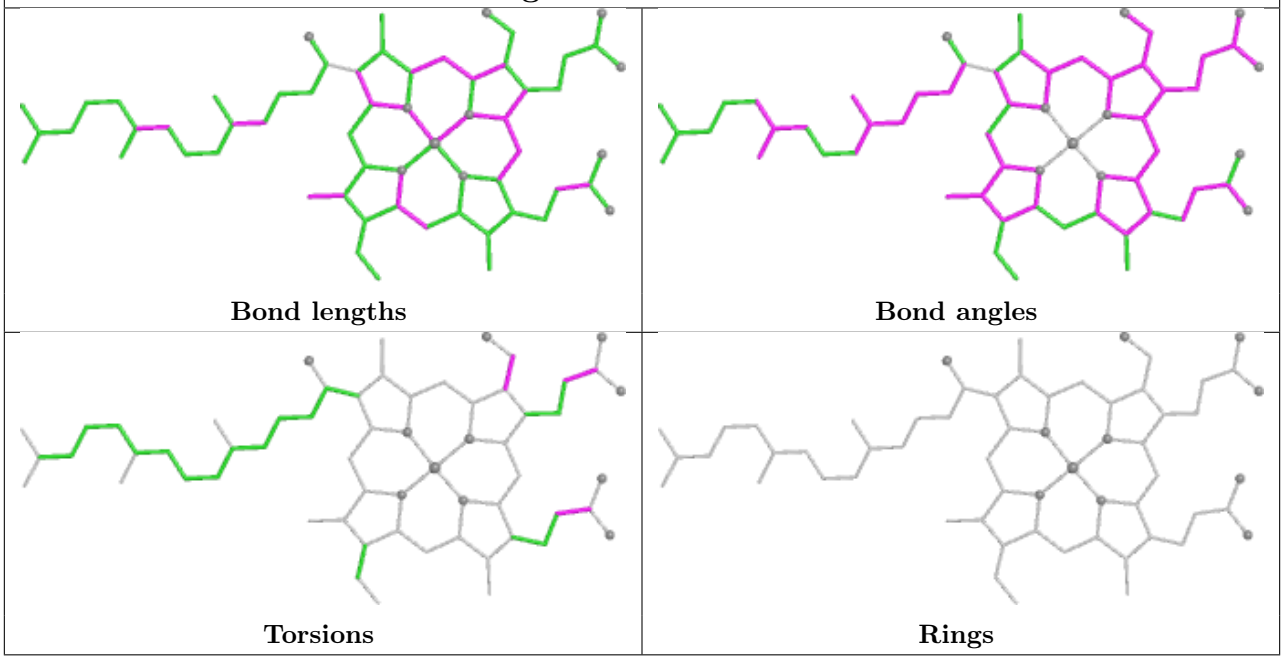


Torsions

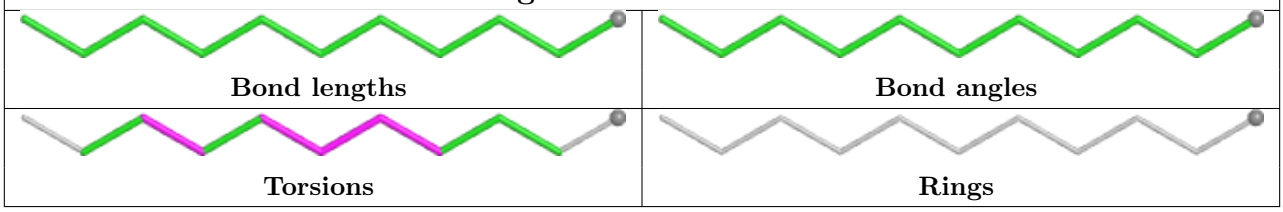


Rings

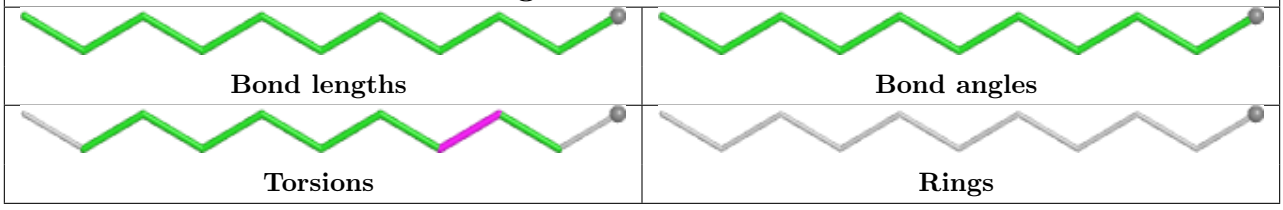
Ligand HEA N 602



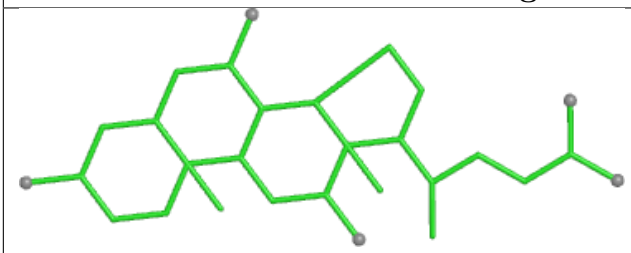
Ligand DMU X 105



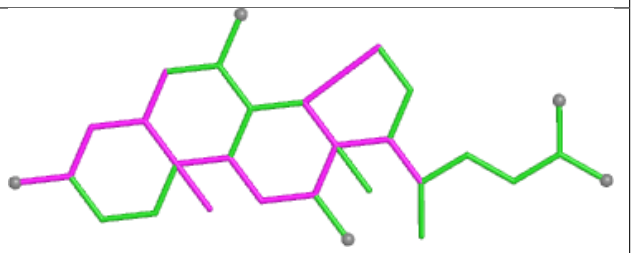
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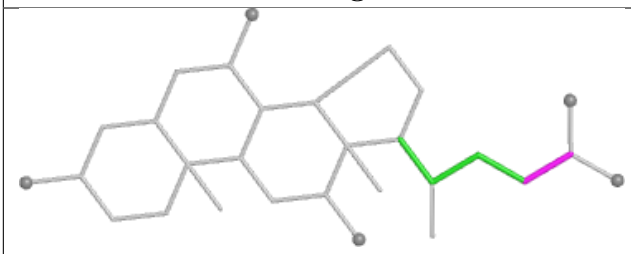
Ligand CHD G 101



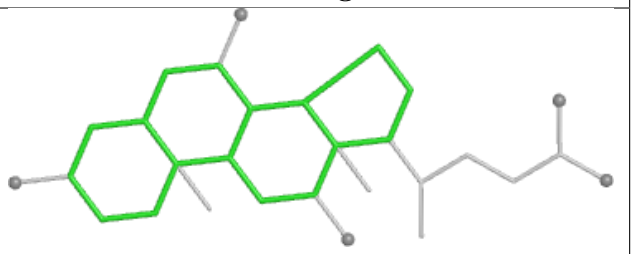
Bond lengths



Bond angles

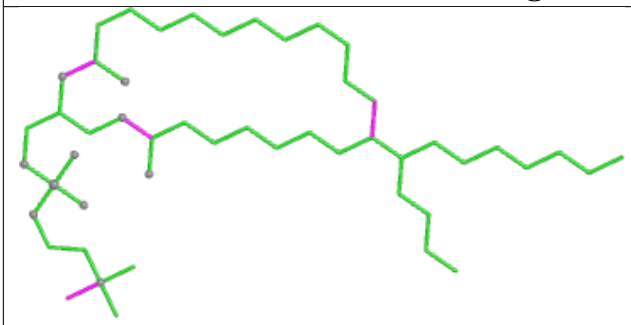


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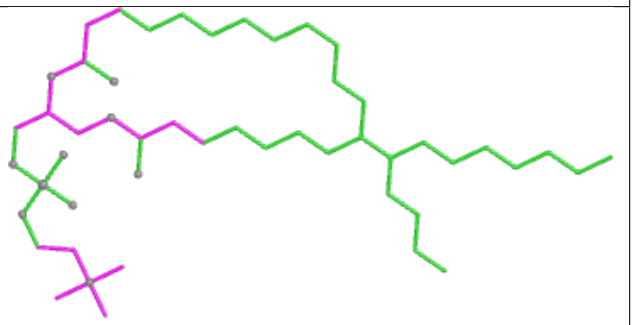


Rings

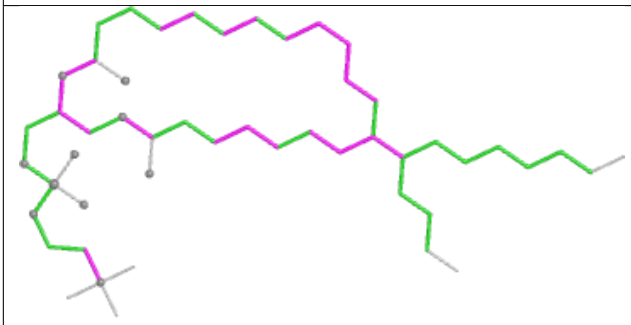
Ligand PSC V 101



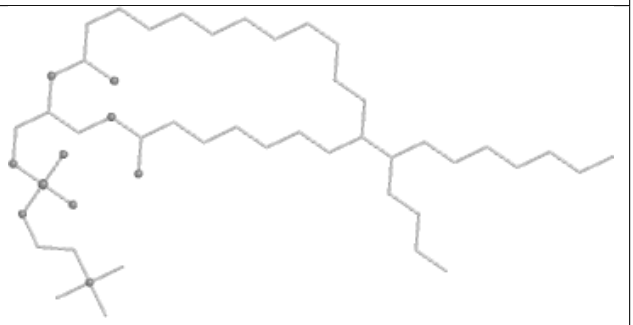
Bond lengths



Bond angles

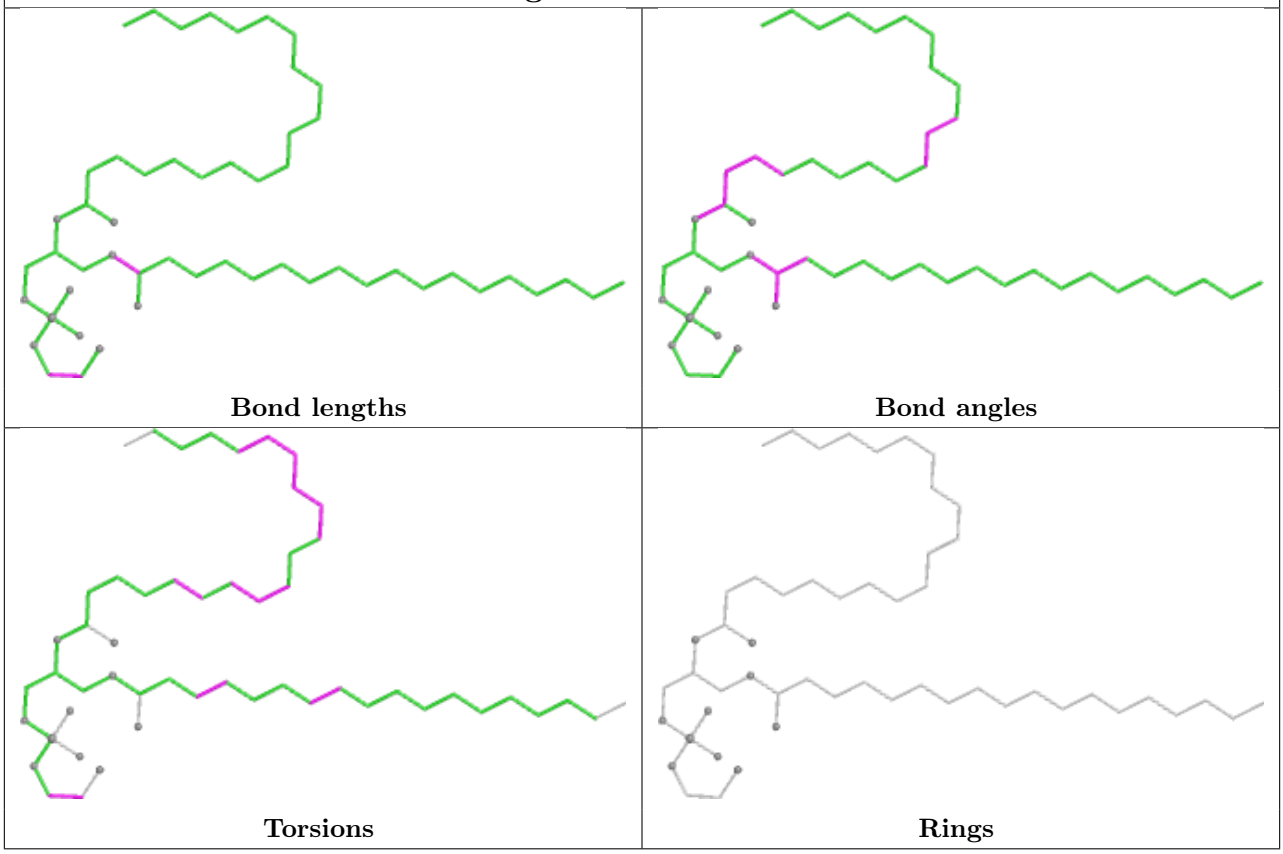


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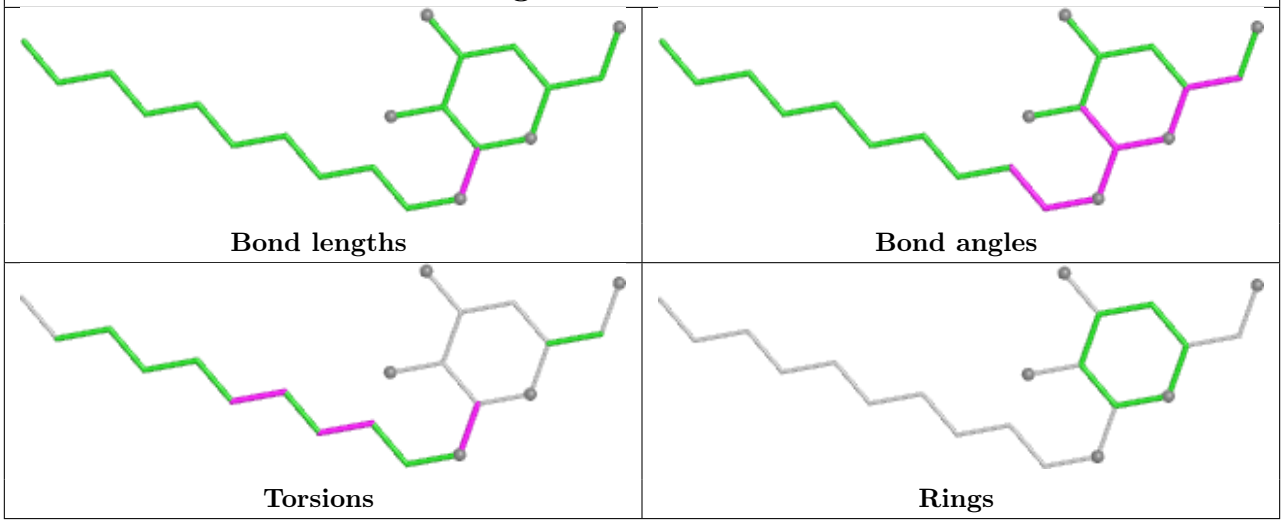


Rings

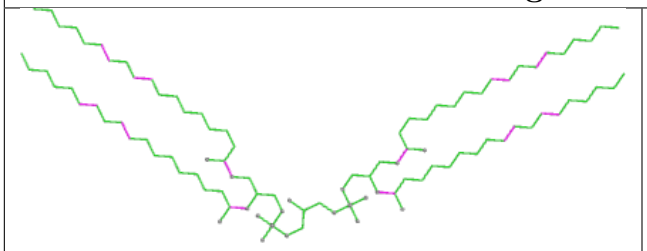
Ligand PEK P 308

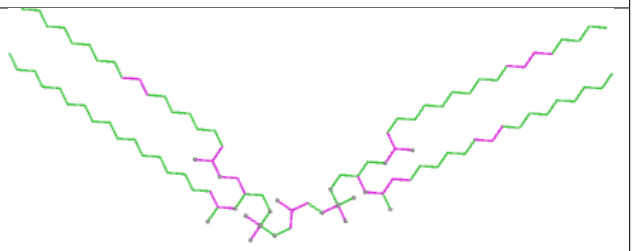


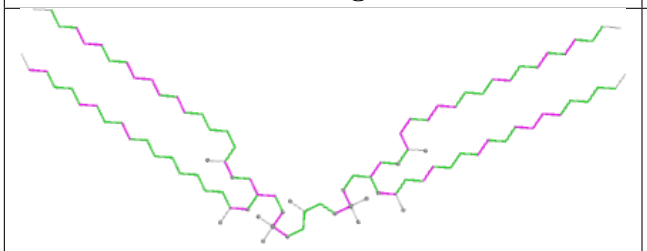
Ligand DMU W 101

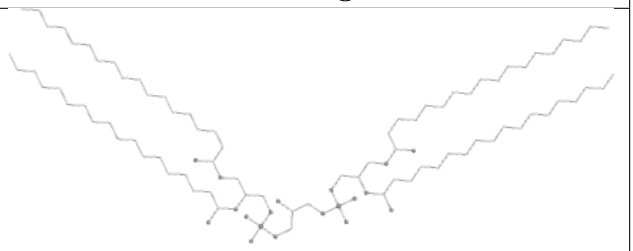


Ligand CDL P 306

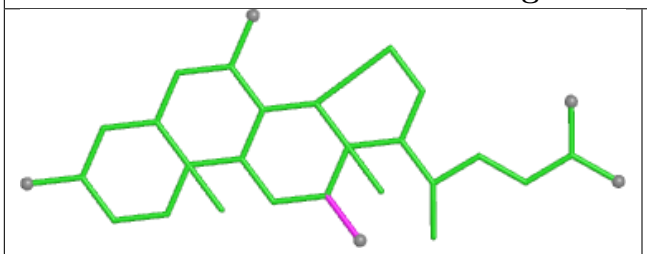

Bond lengths

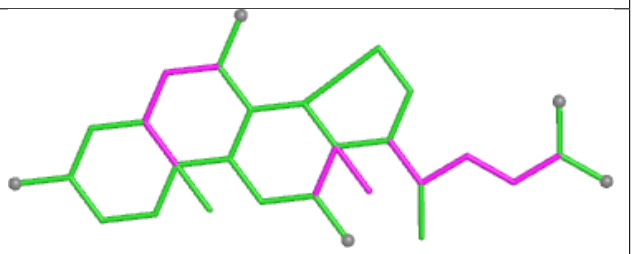

Bond angles

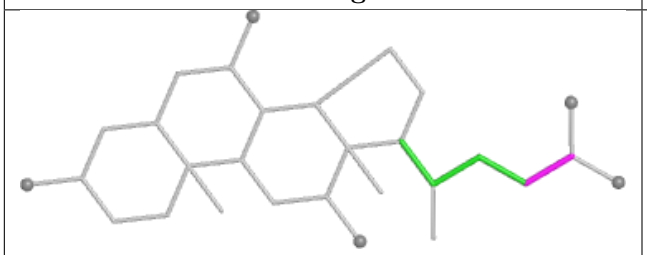

Torsions

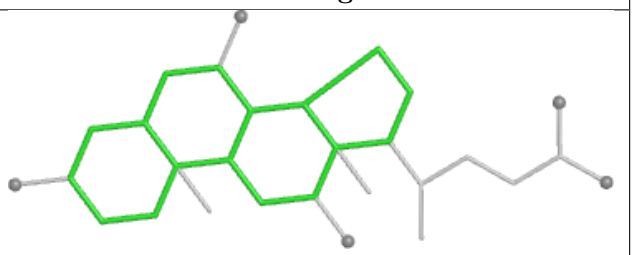

Rings

Ligand CHD C 305

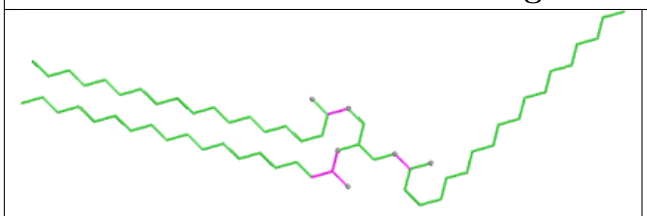

Bond lengths

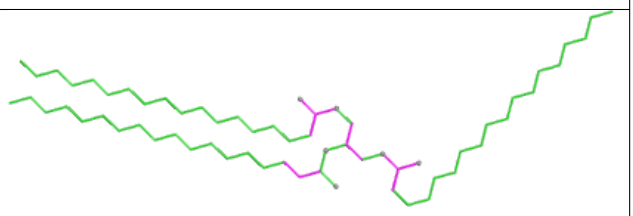

Bond angles

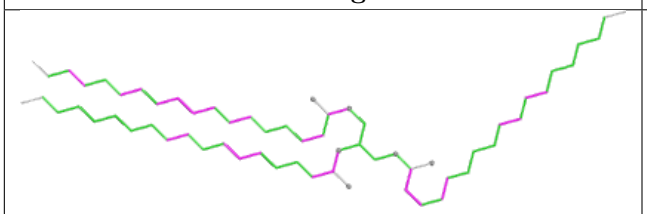

Torsions

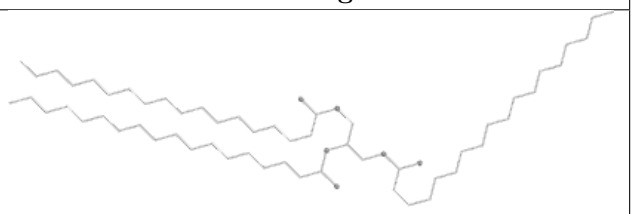

Rings

Ligand TGL D 202

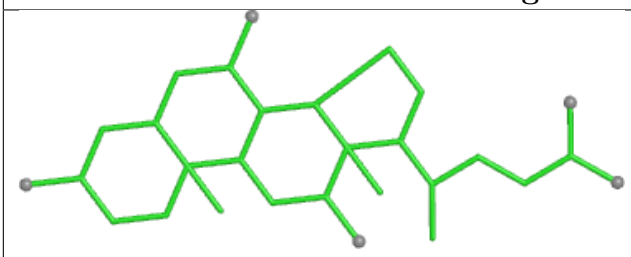

Bond lengths


Bond angles

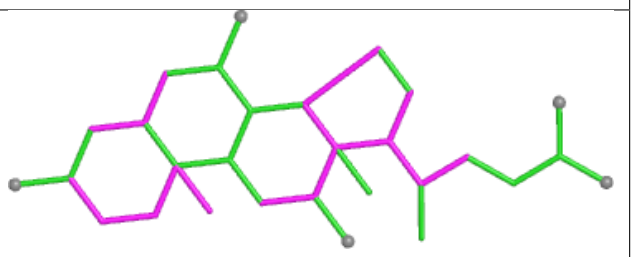

Torsions


Rings

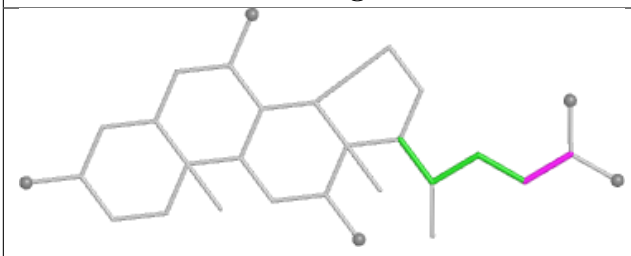
Ligand CHD P 304



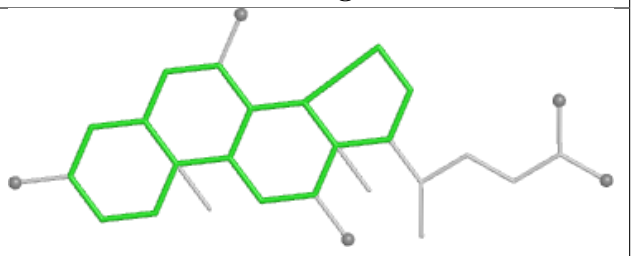
Bond lengths



Bond angles

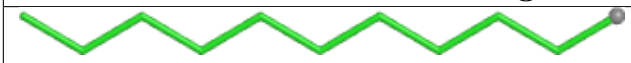


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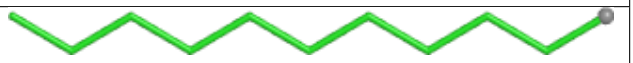


Rings

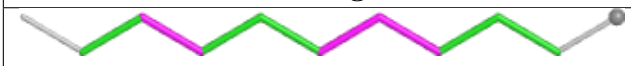
Ligand DMU B 302



Bond lengths



Bond angles

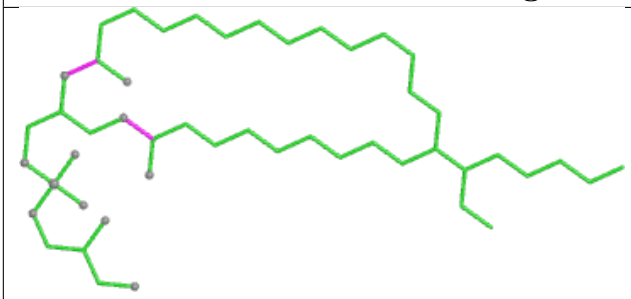


Torsions



Rings

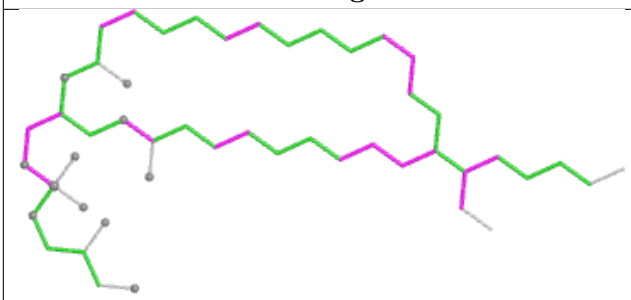
Ligand PGV P 310



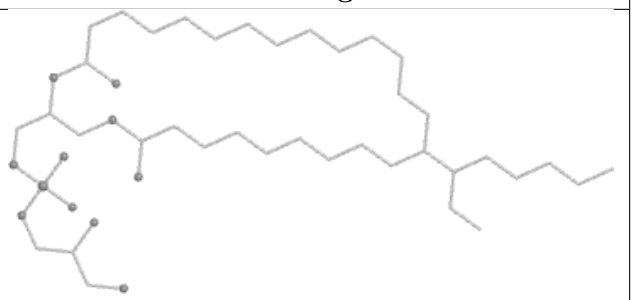
Bond lengths



Bond angles

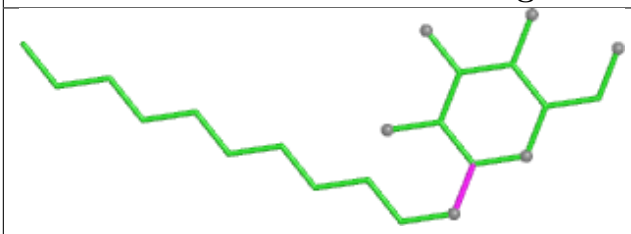


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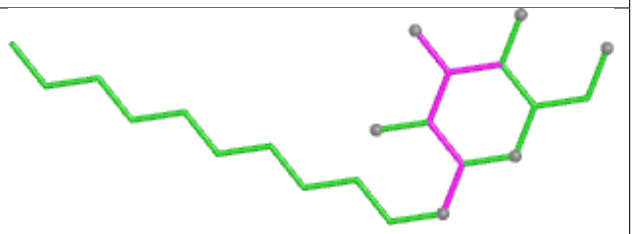


Rings

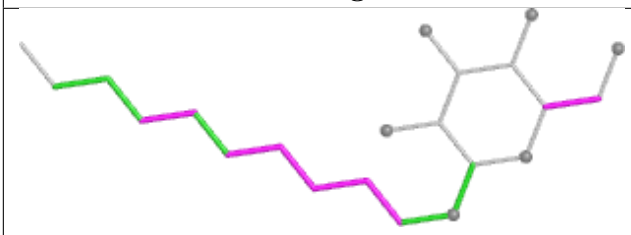
Ligand DMU C 303



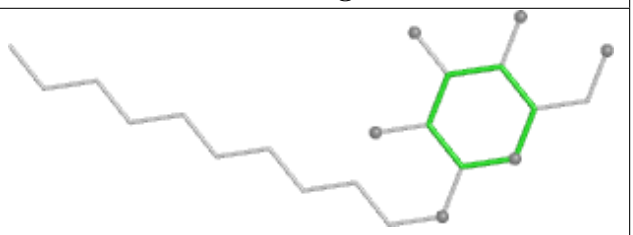
Bond lengths



Bond angles

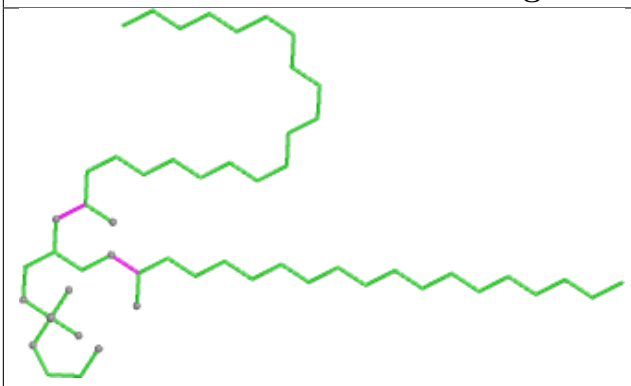


Torsions

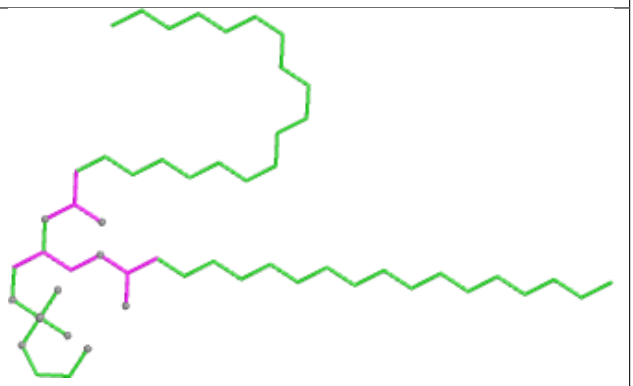


Rings

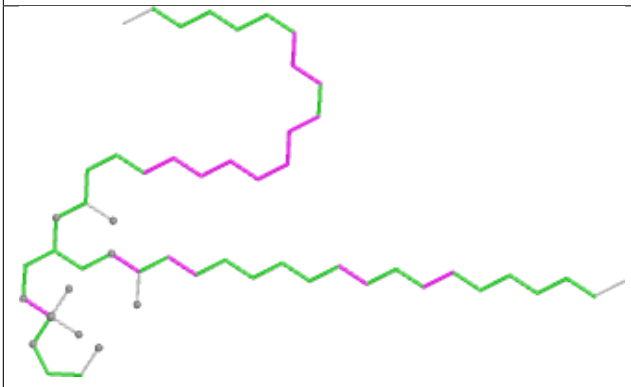
Ligand PEK C 308



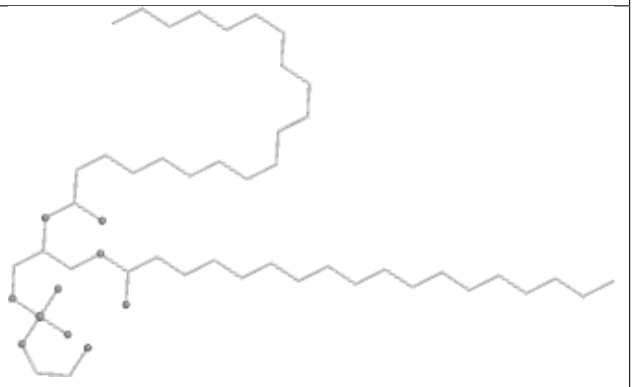
Bond lengths



Bond angles

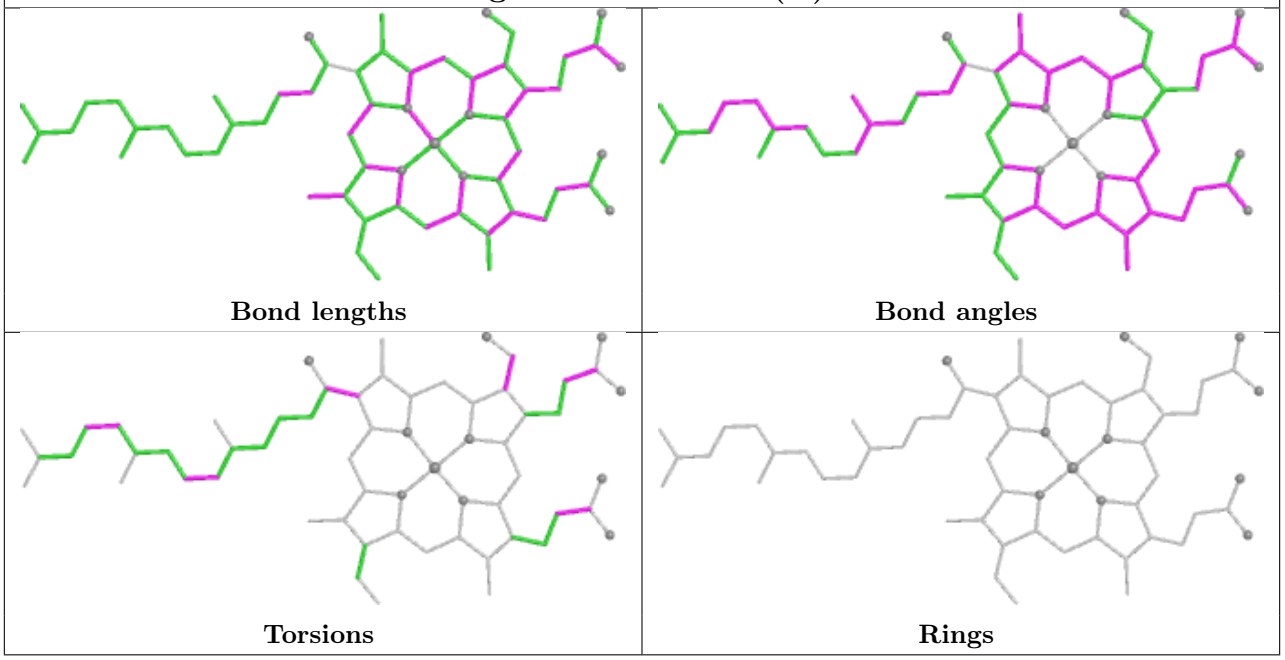


Torsions

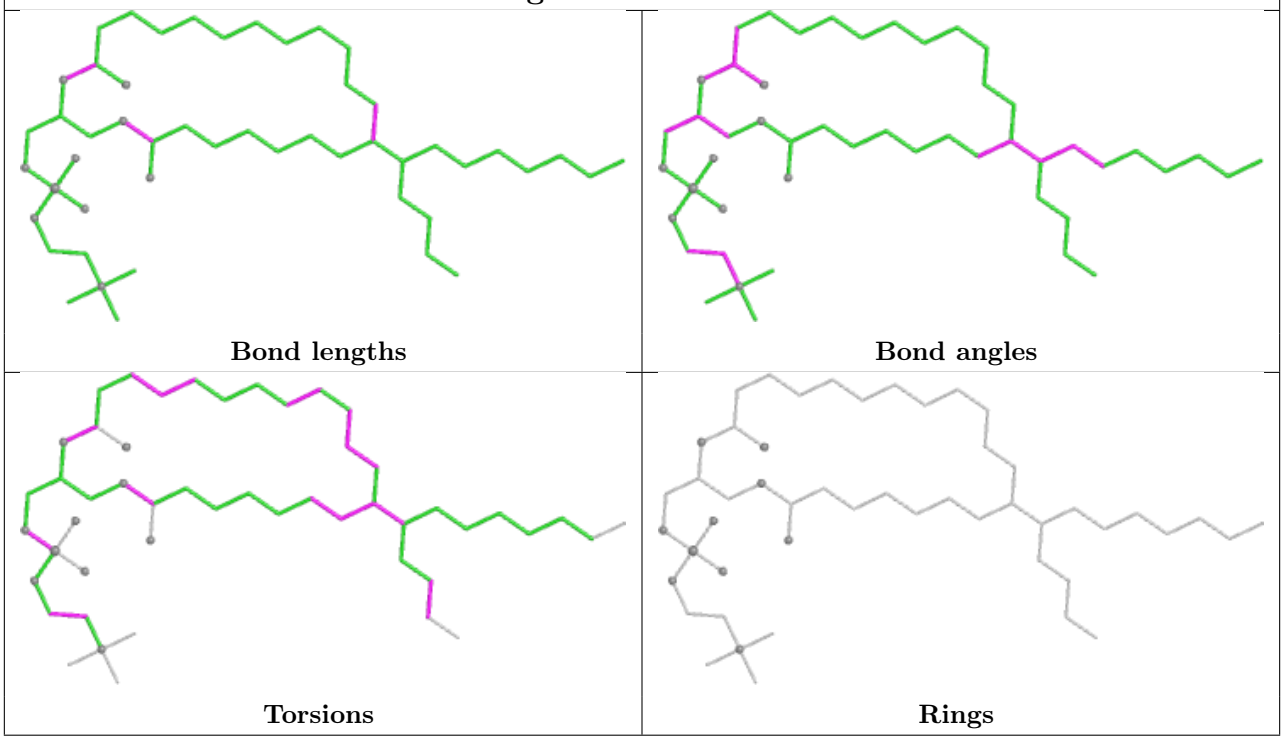


Rings

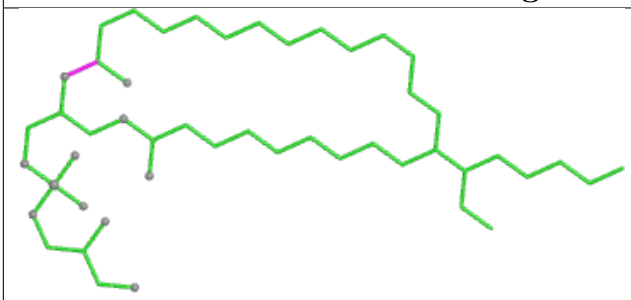
Ligand HEA A 601 (A)



Ligand PSC A 609



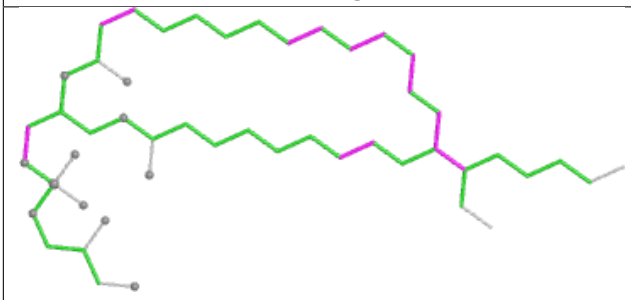
Ligand PGV C 310



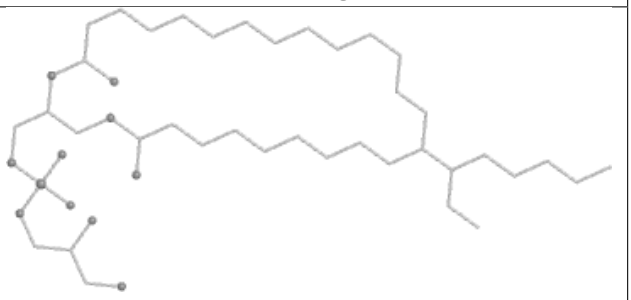
Bond lengths



Bond angles

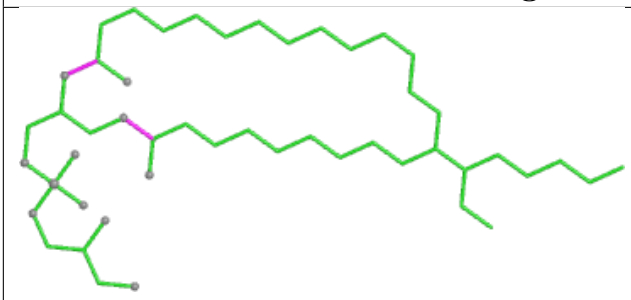


Torsions

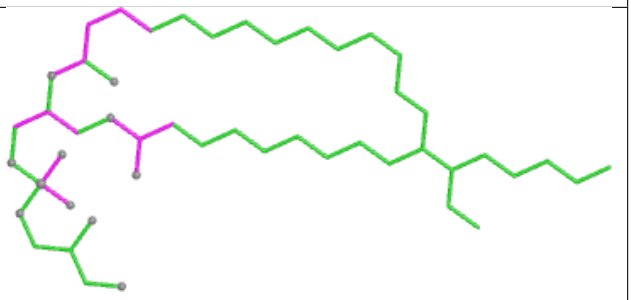


Rings

Ligand PGV N 606



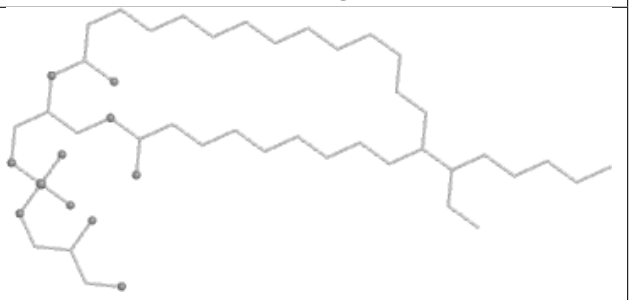
Bond lengths



Bond angles

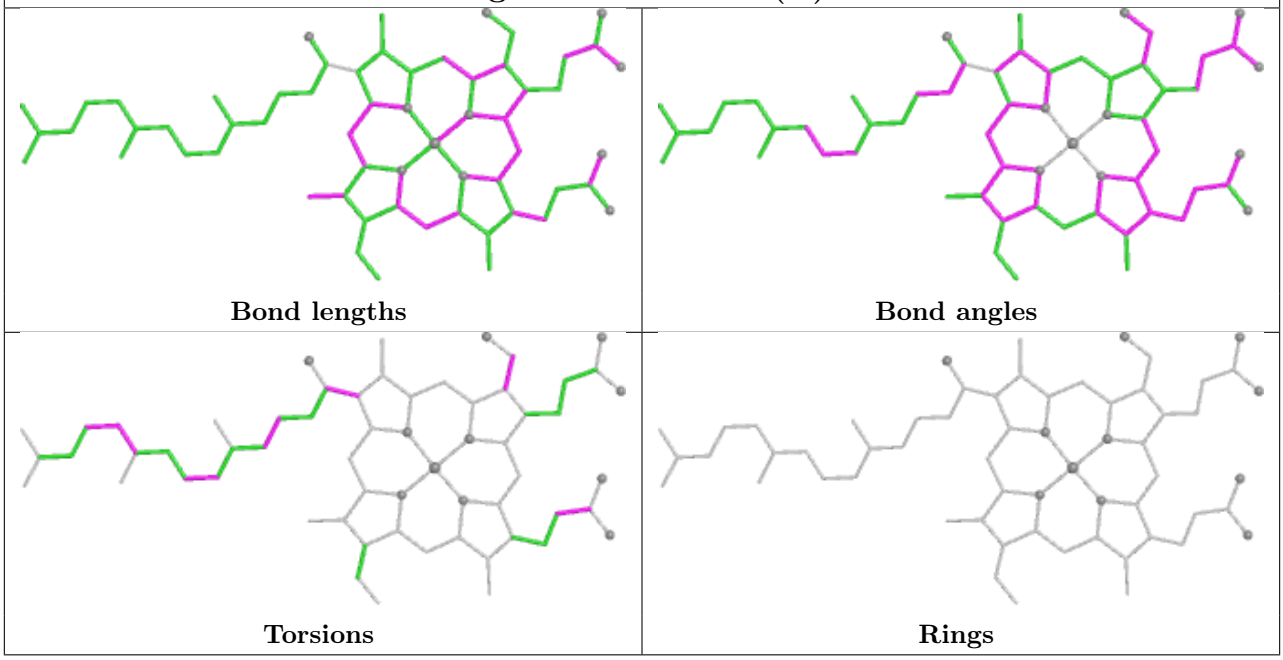


Torsions

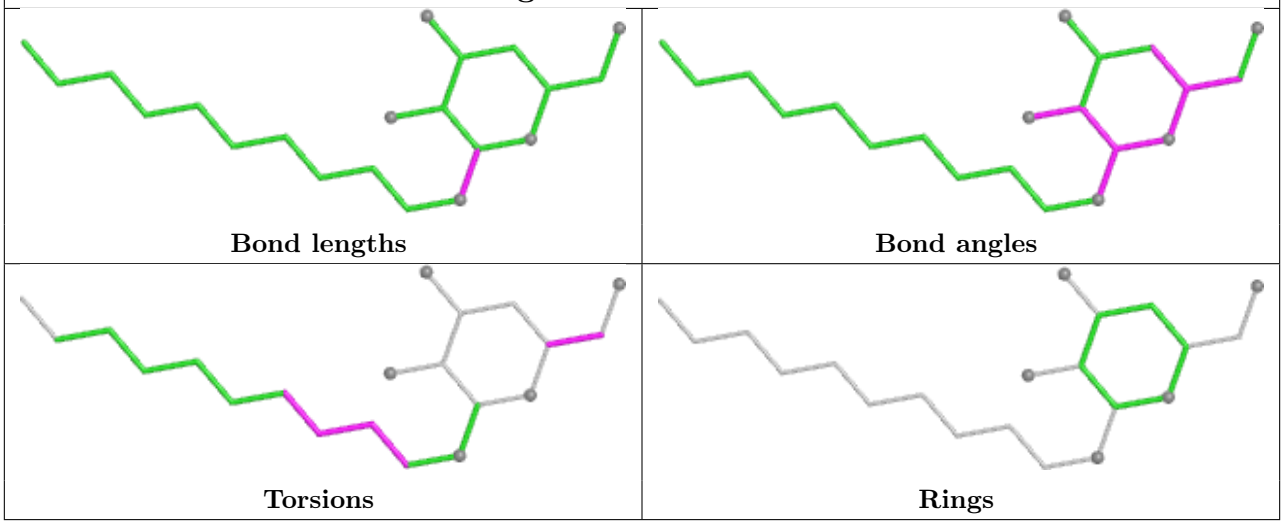


Rings

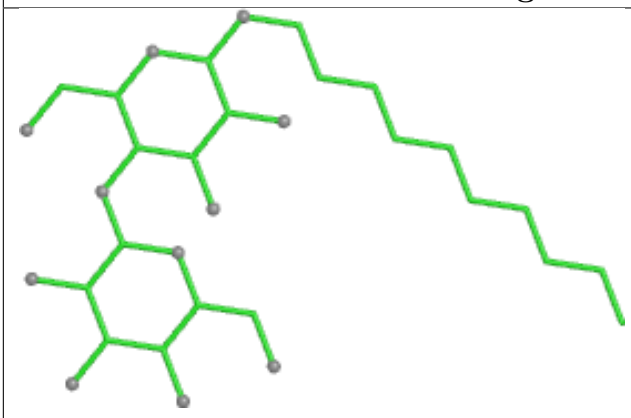
Ligand HEA N 601 (A)



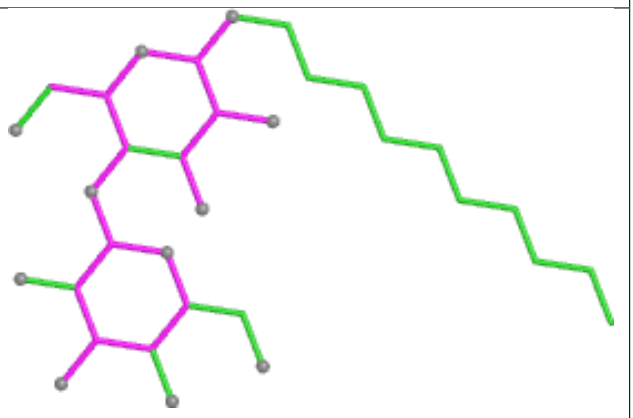
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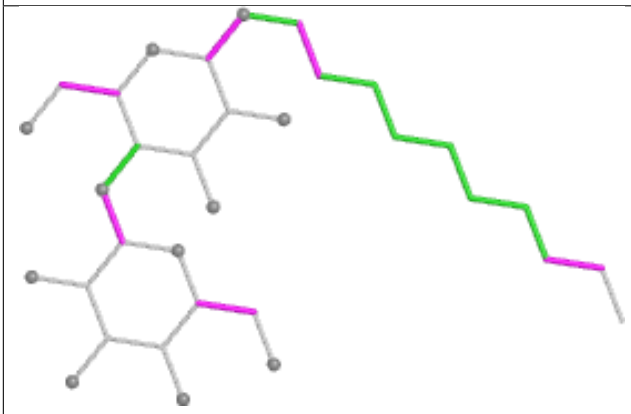
Ligand DMU C 302



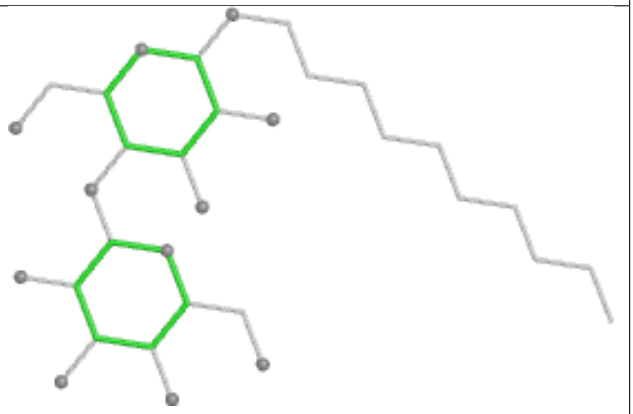
Bond lengths



Bond angles

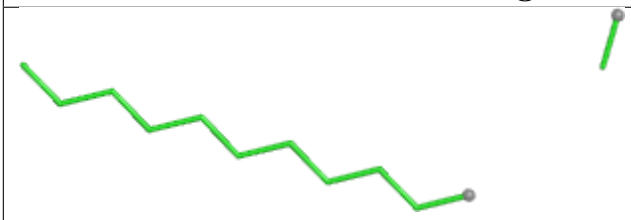


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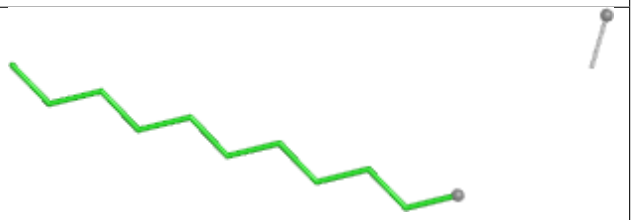


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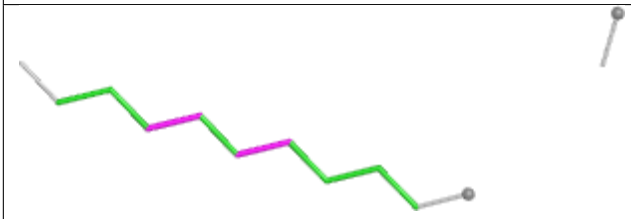
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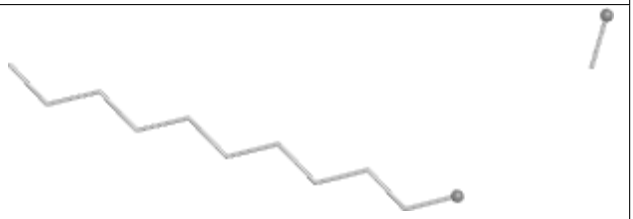
Bond lengths



Bond angles

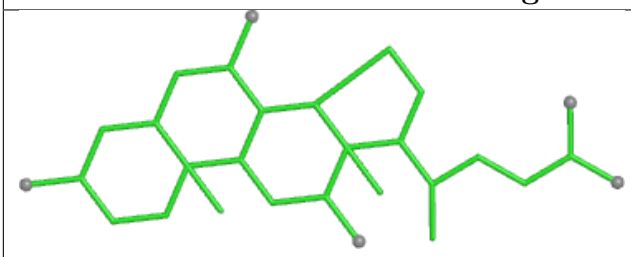


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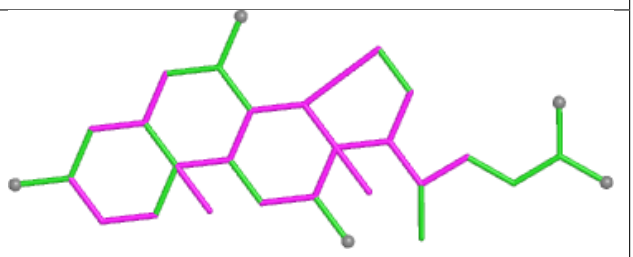


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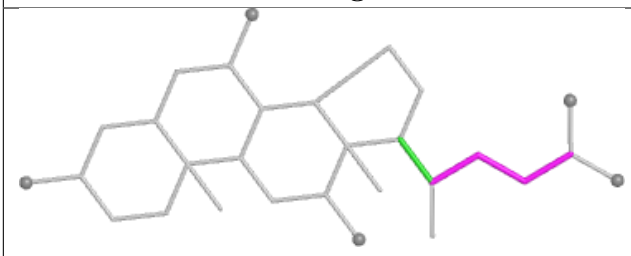
Ligand CHD P 305



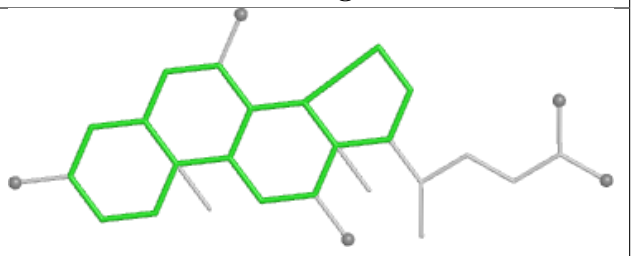
Bond lengths



Bond angles

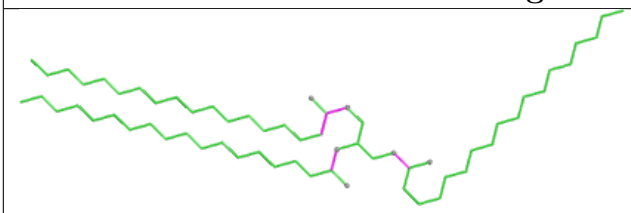


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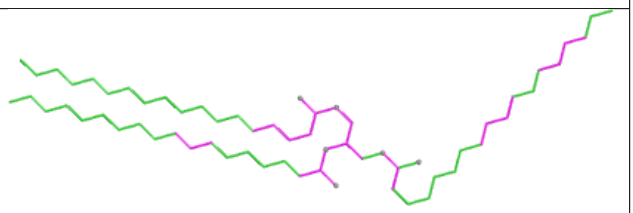


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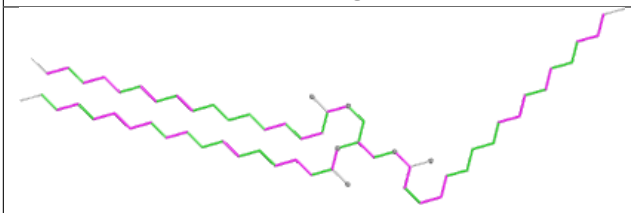
Ligand TGL L 103



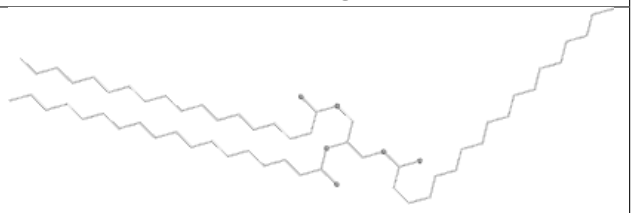
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU C 304



Bond lengths



Bond angles

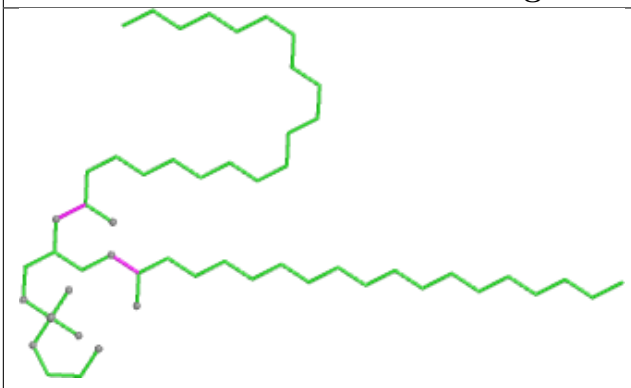


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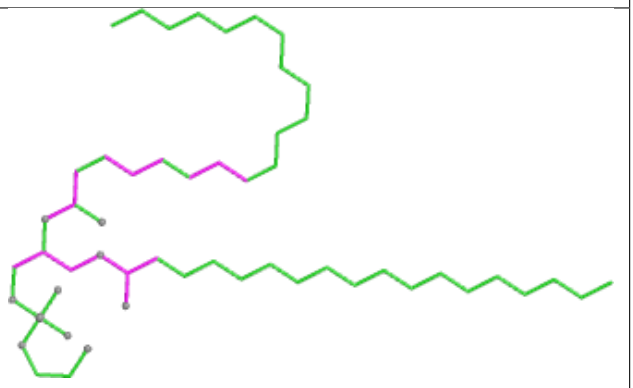


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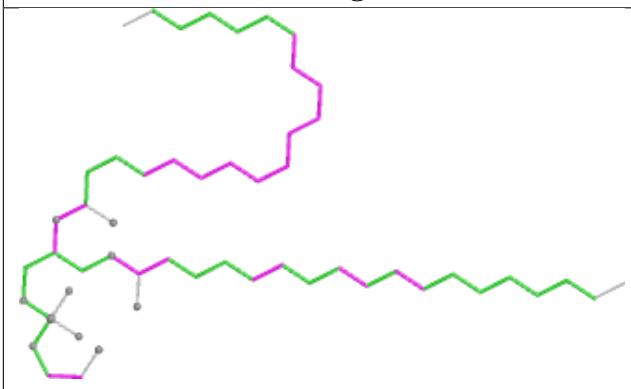
Ligand PEK P 307



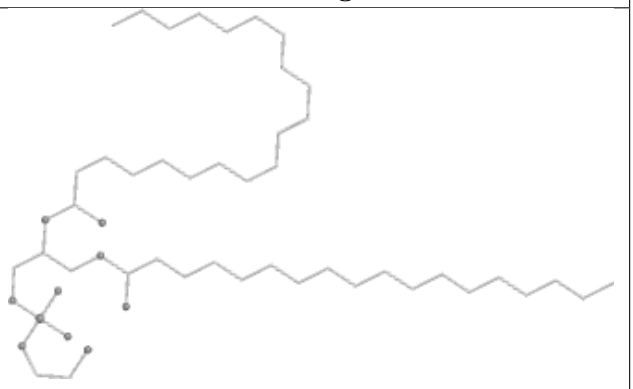
Bond lengths



Bond angles

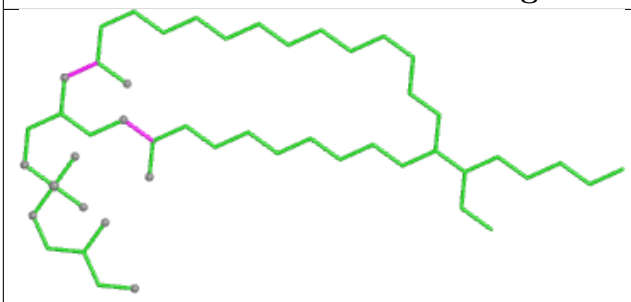


Torsions



Rings

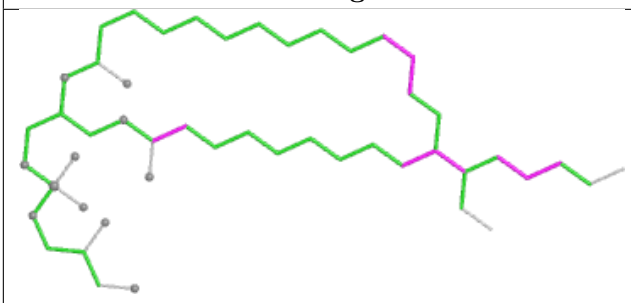
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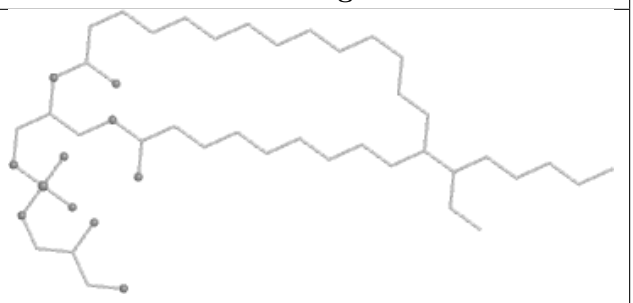
Bond lengths



Bond angles

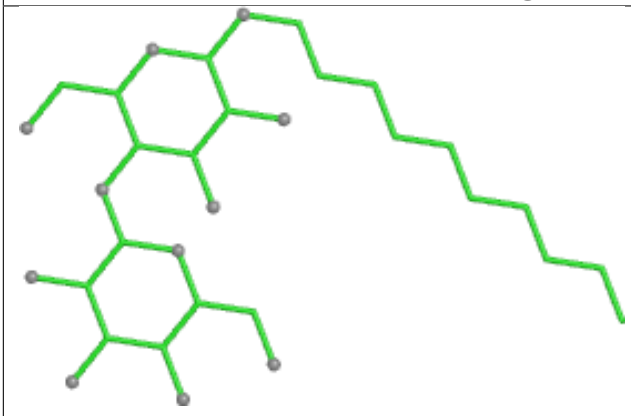


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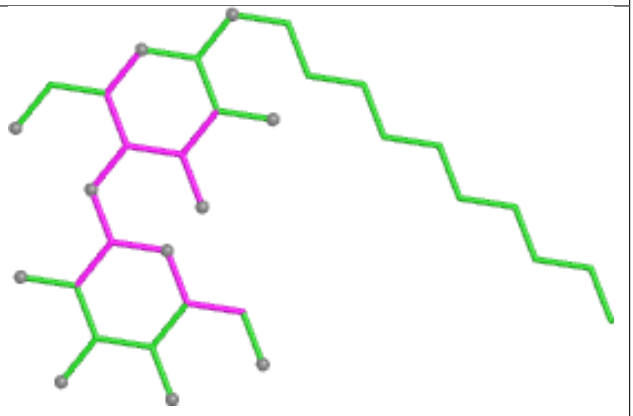


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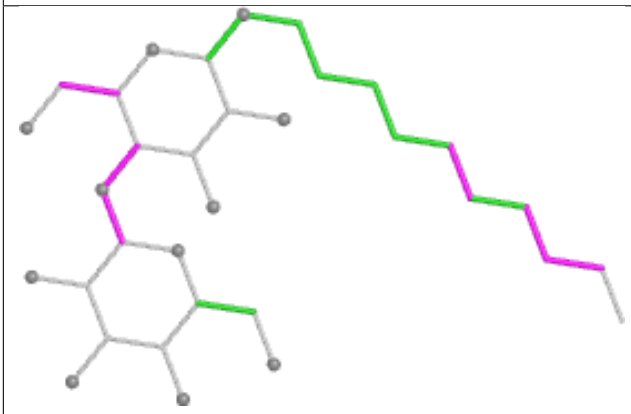
Ligand DMU L 101



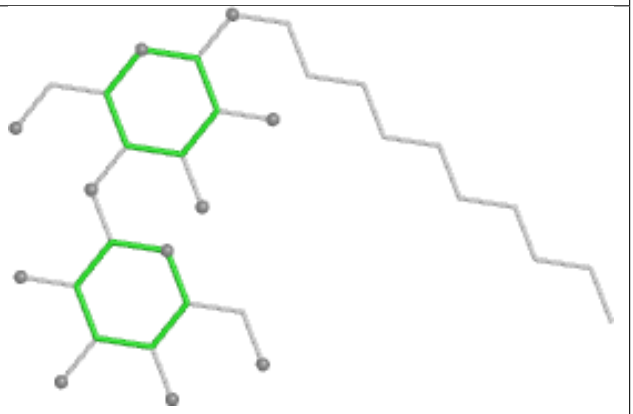
Bond lengths



Bond angles

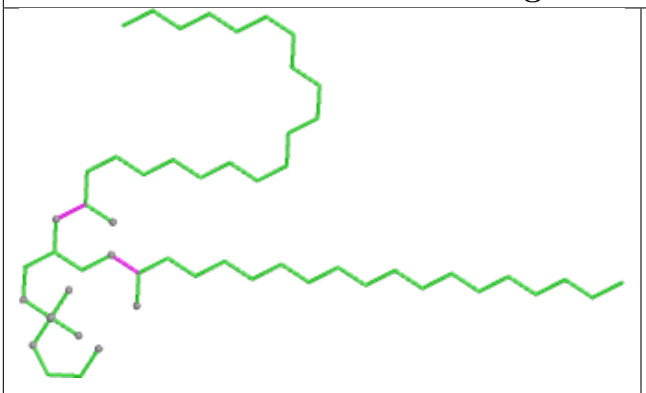


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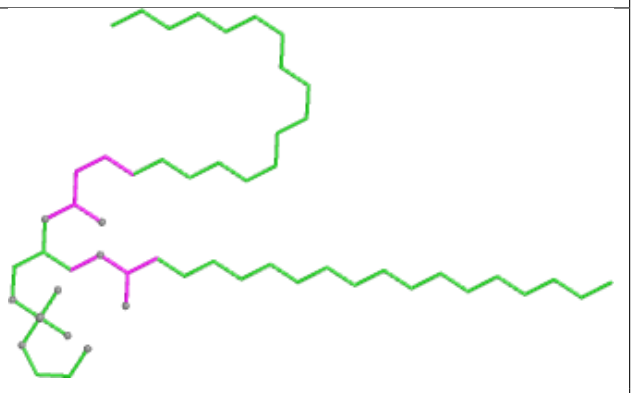


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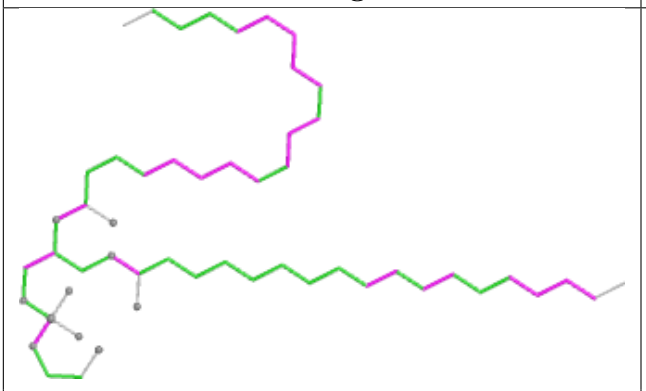
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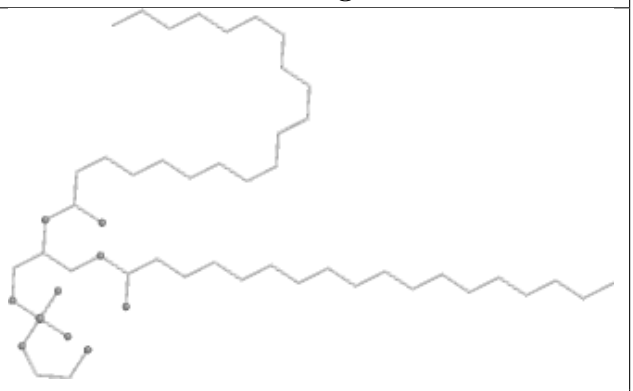
Bond lengths



Bond angles



Torsions



Rings

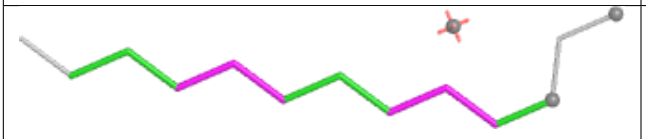
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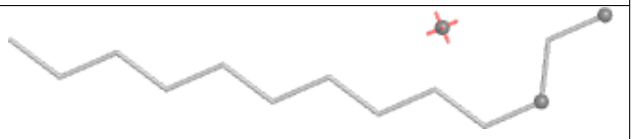
Bond lengths



Bond angles

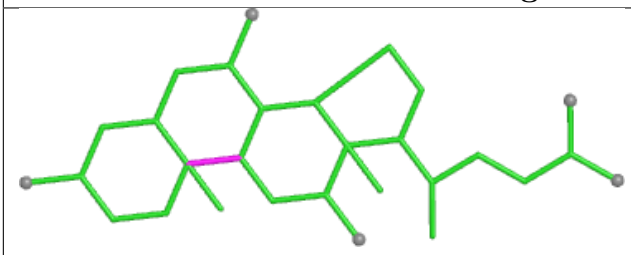


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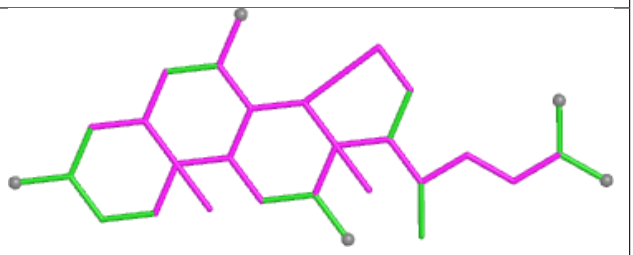


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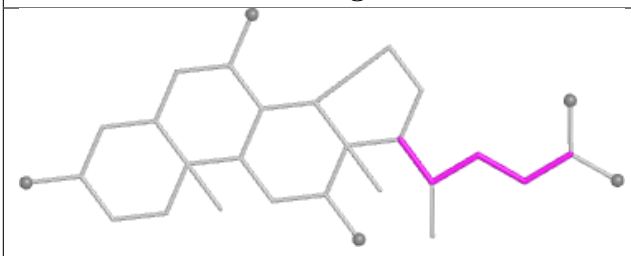
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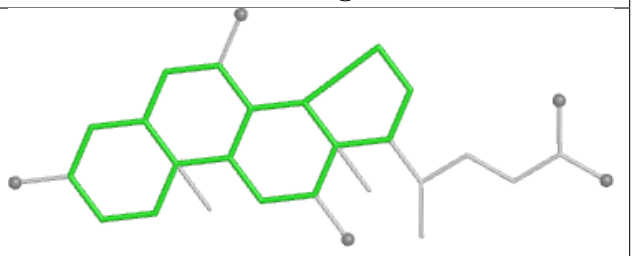
Bond lengths



Bond angles

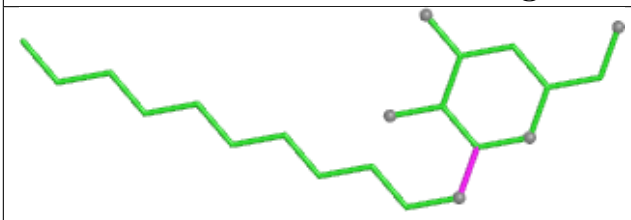


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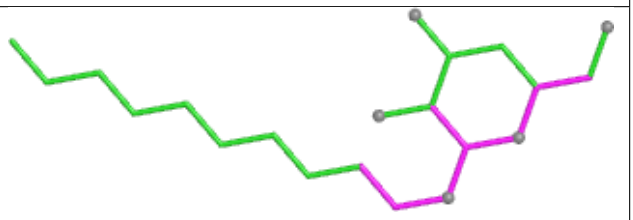


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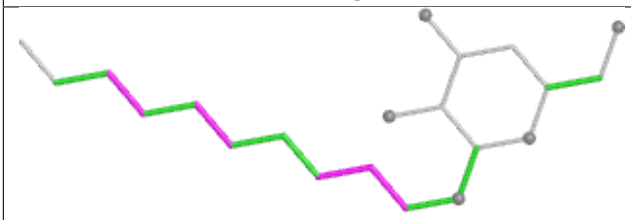
Ligand DMU J 101



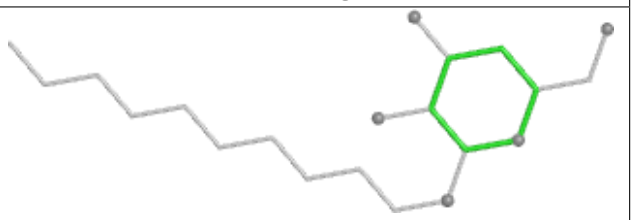
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Bond angles

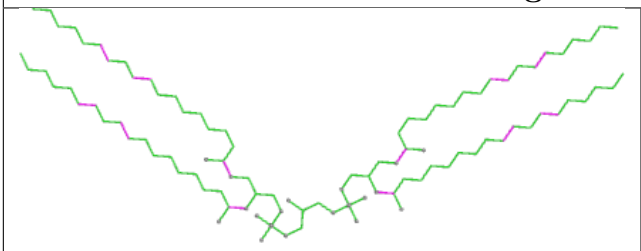


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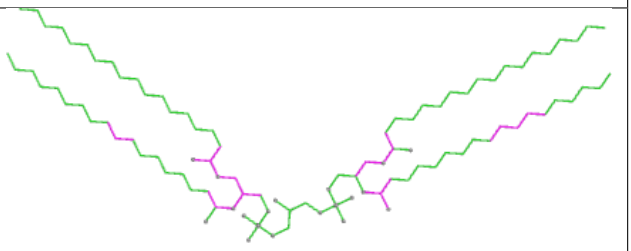


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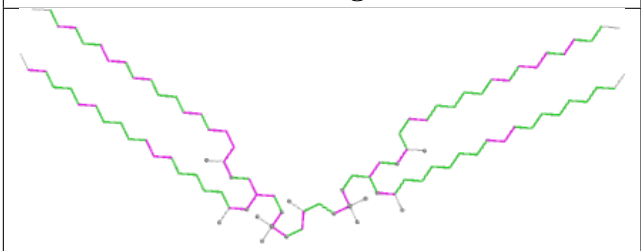
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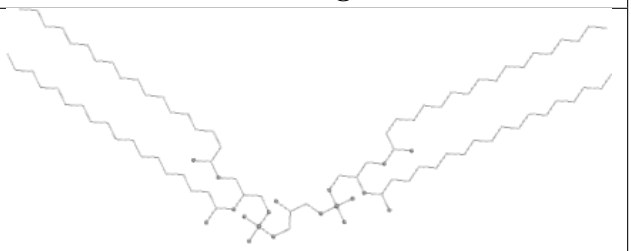
Bond lengths



Bond angles

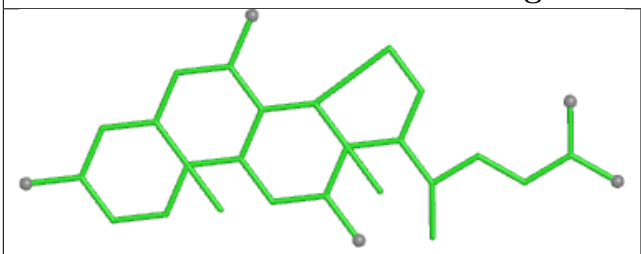


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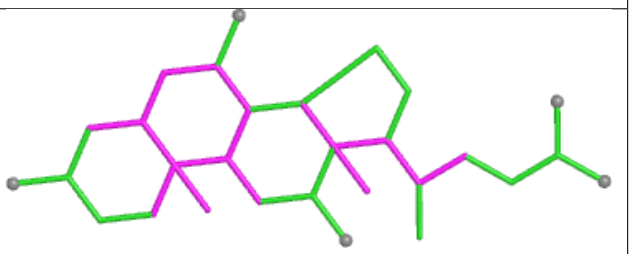


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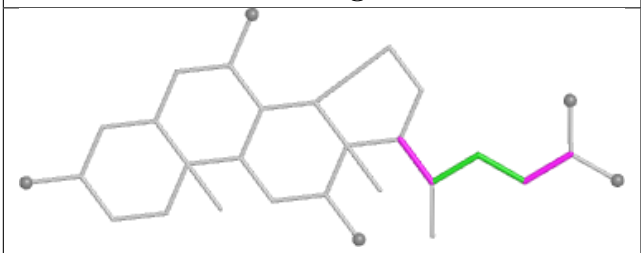
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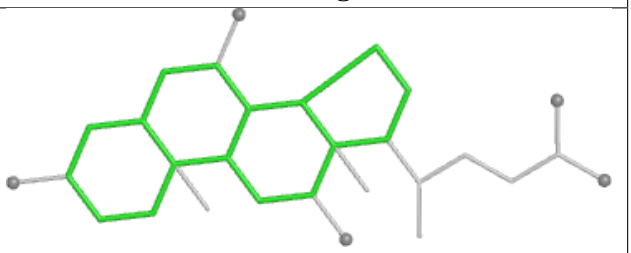
Bond lengths



Bond angles

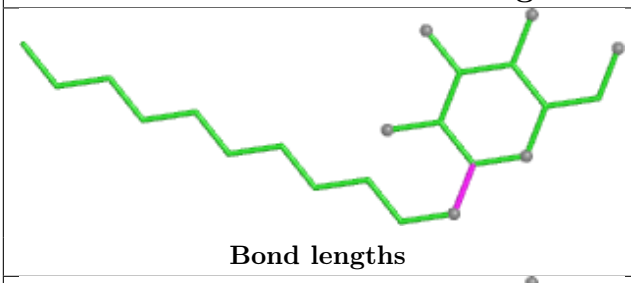


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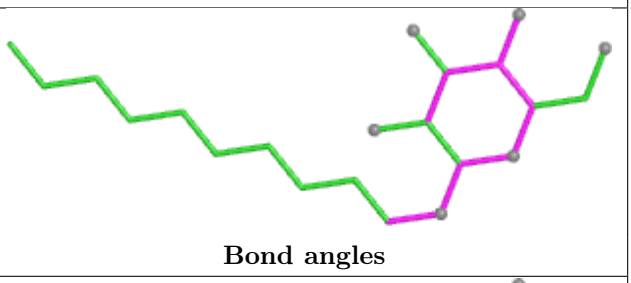


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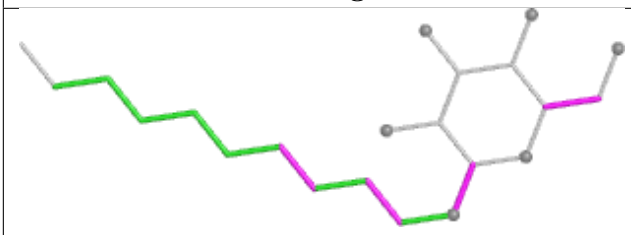
Ligand DMU K 103



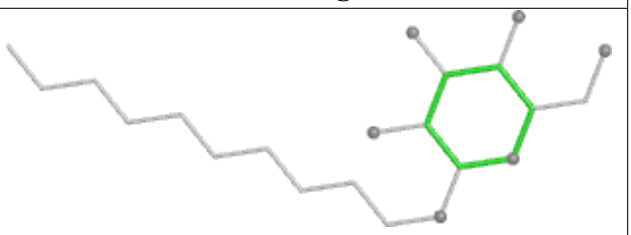
Bond lengths



Bond angles

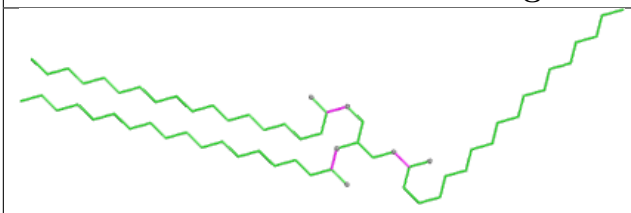


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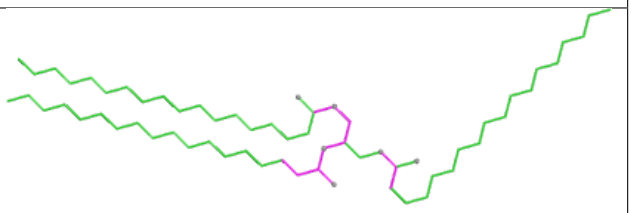


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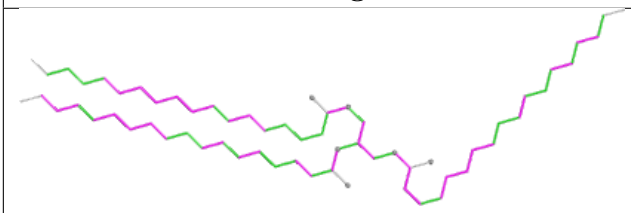
Ligand TGL A 610



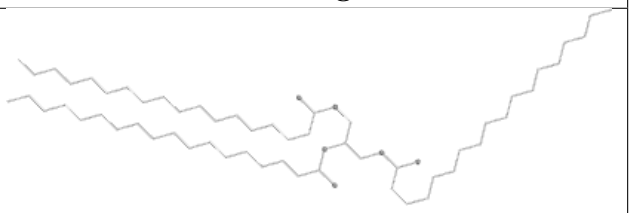
Bond lengths



Bond angles

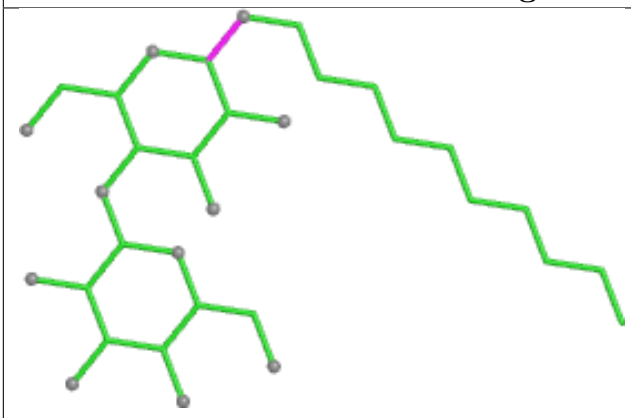


Torsions

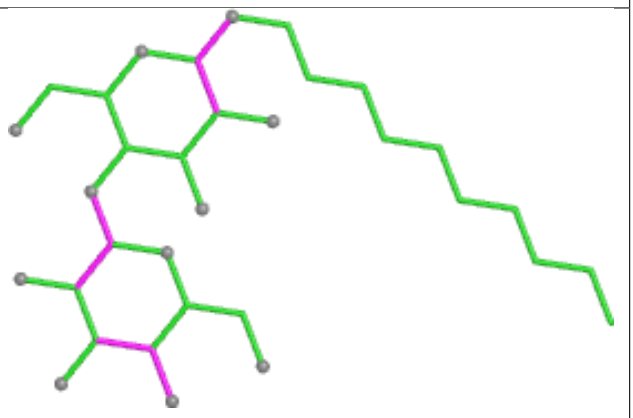


Rings

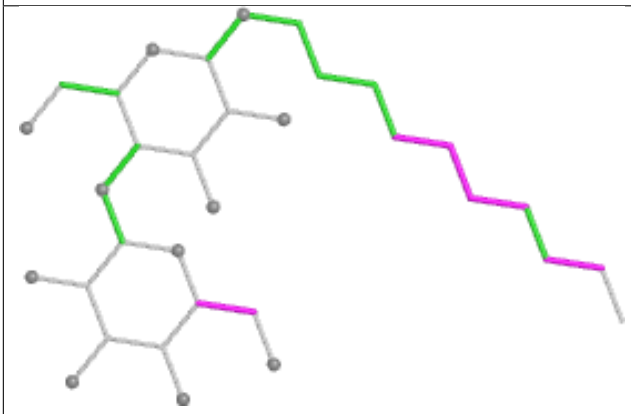
Ligand DMU Z 101



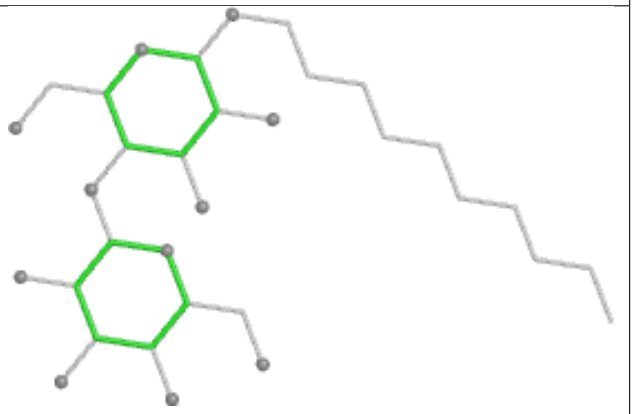
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU X 103



Bond lengths



Bond angles

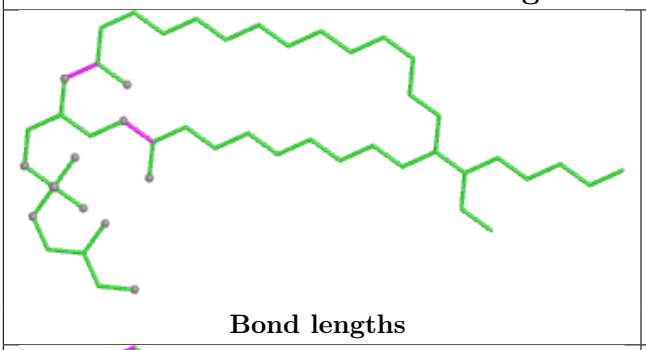


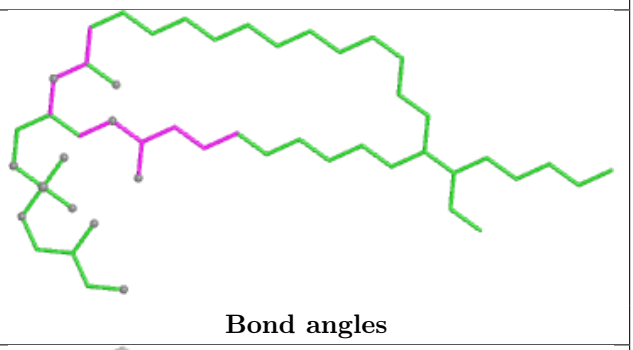
Torsions

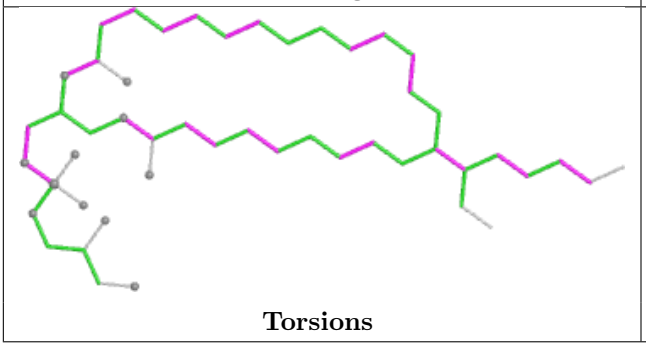


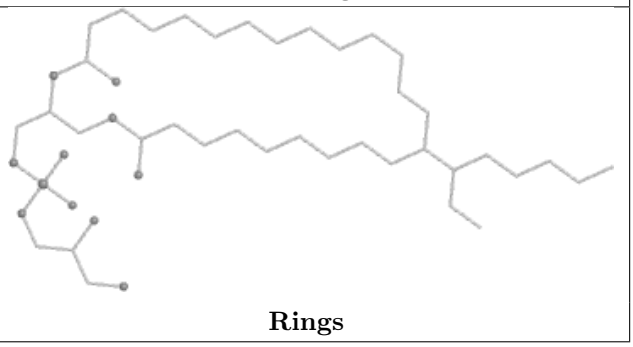
Rings

Ligand PGV T 104


Bond lengths


Bond angles


Torsions


Rings

Ligand DMU K 104

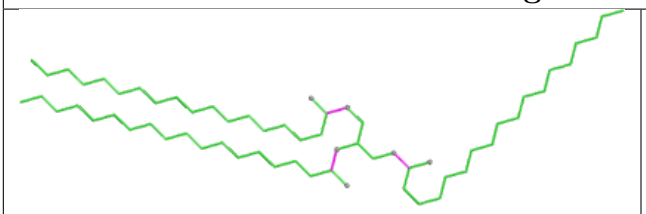

Bond lengths

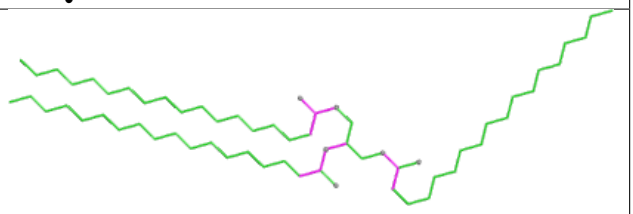

Bond angles

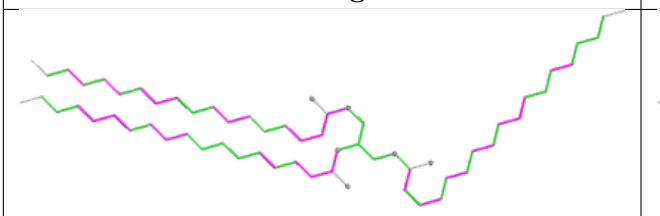

Torsions

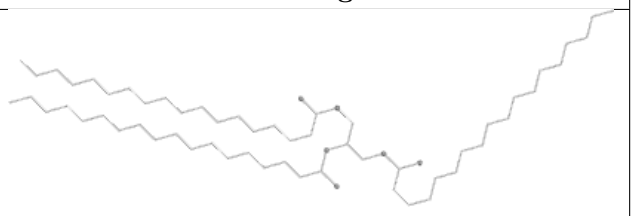

Rings

Ligand TGL Q 202


Bond lengths


Bond angles


Torsions


Rings

Ligand DMU K 101

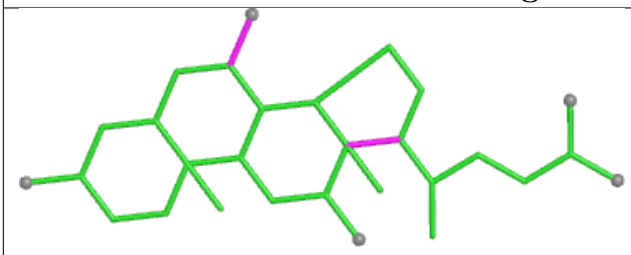

Bond lengths


Bond angles

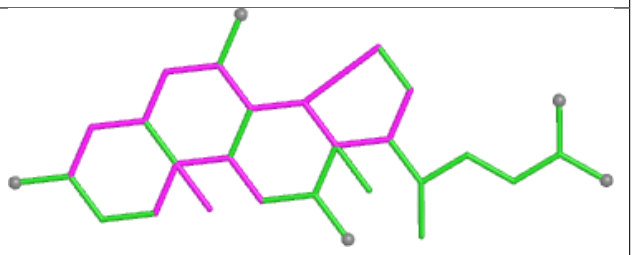

Torsions


Rings

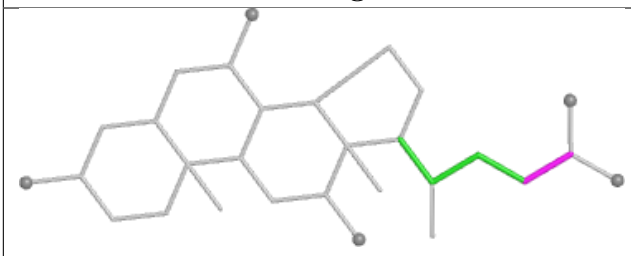
Ligand CHD T 101



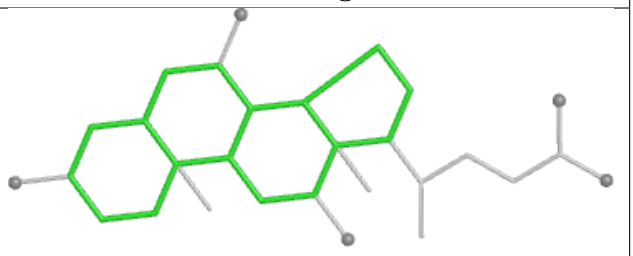
Bond lengths



Bond angles

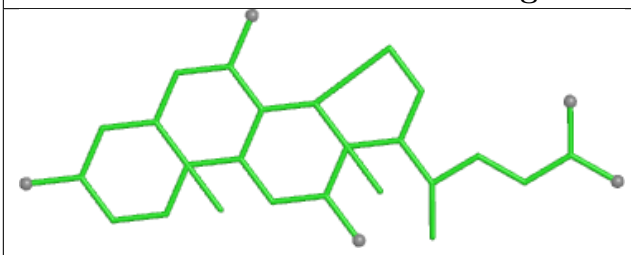


Torsions

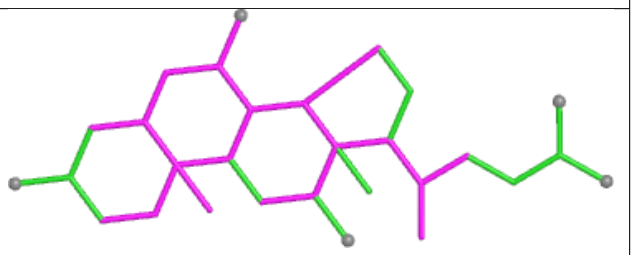


Rings

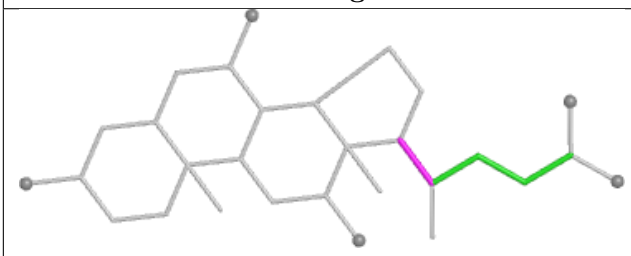
Ligand CHD Y 102



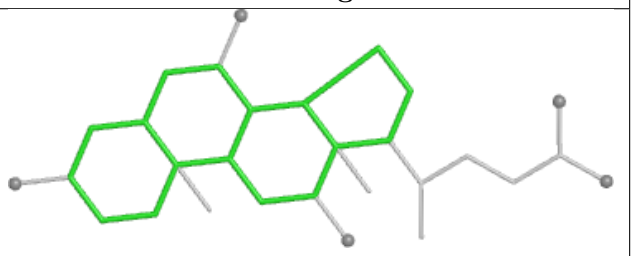
Bond lengths



Bond angles

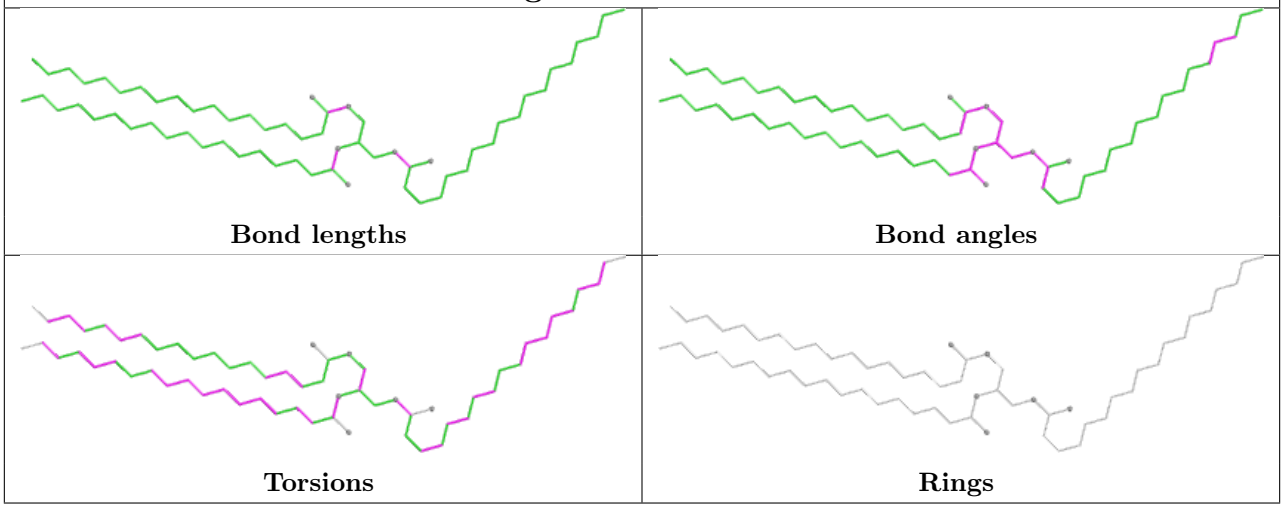


Torsions

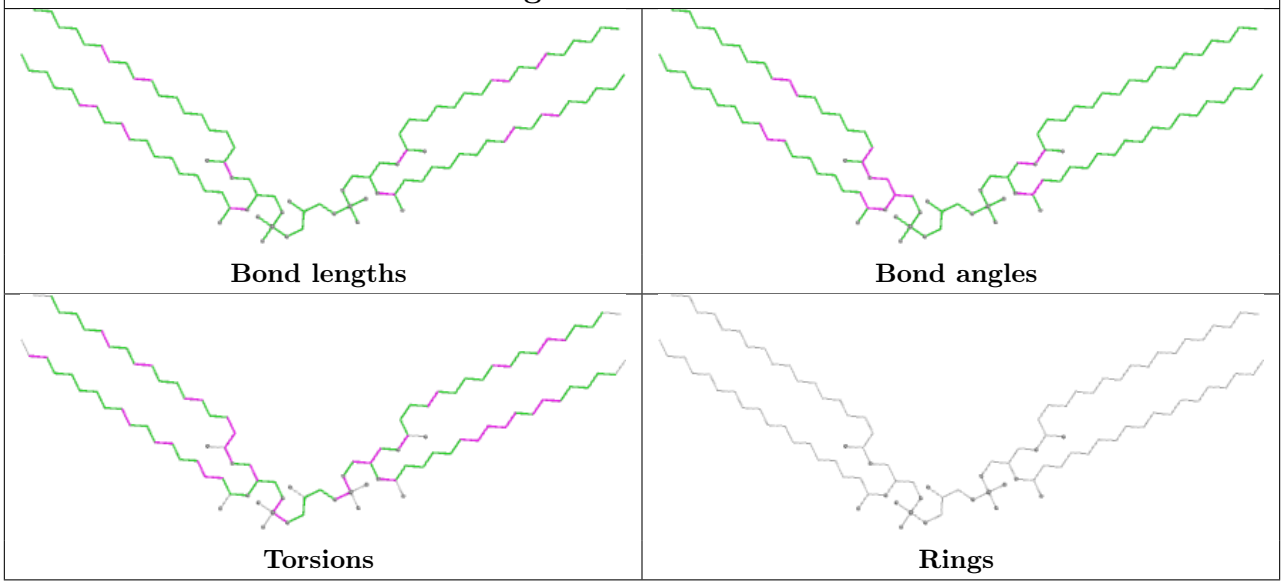


Rings

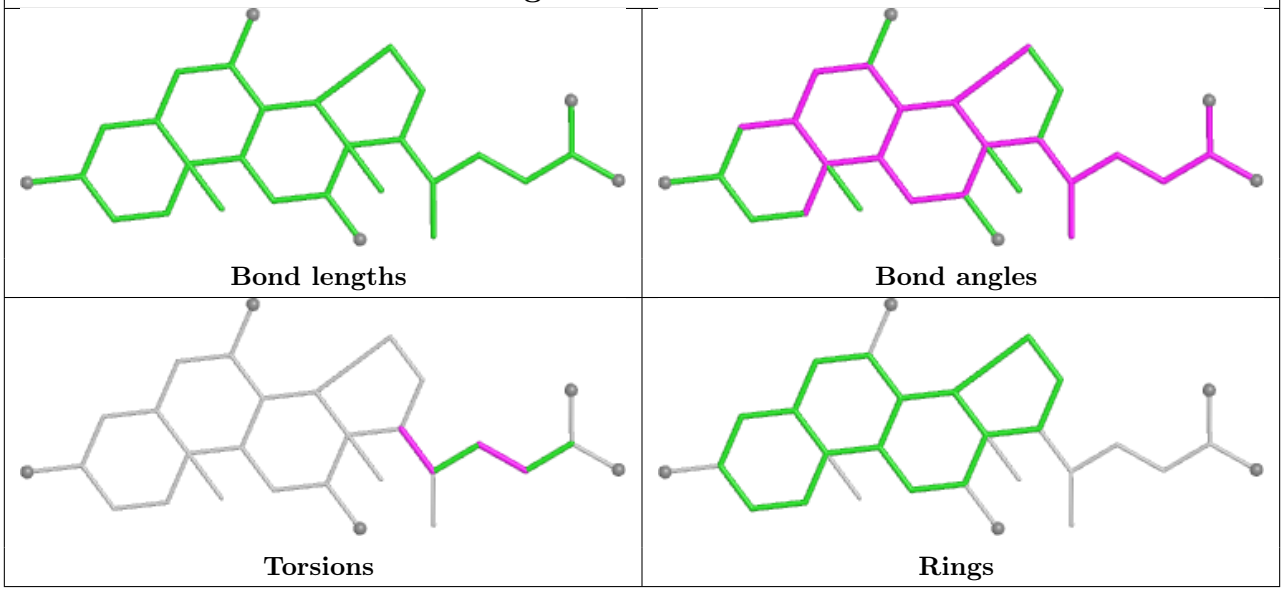
Ligand TGL Y 103

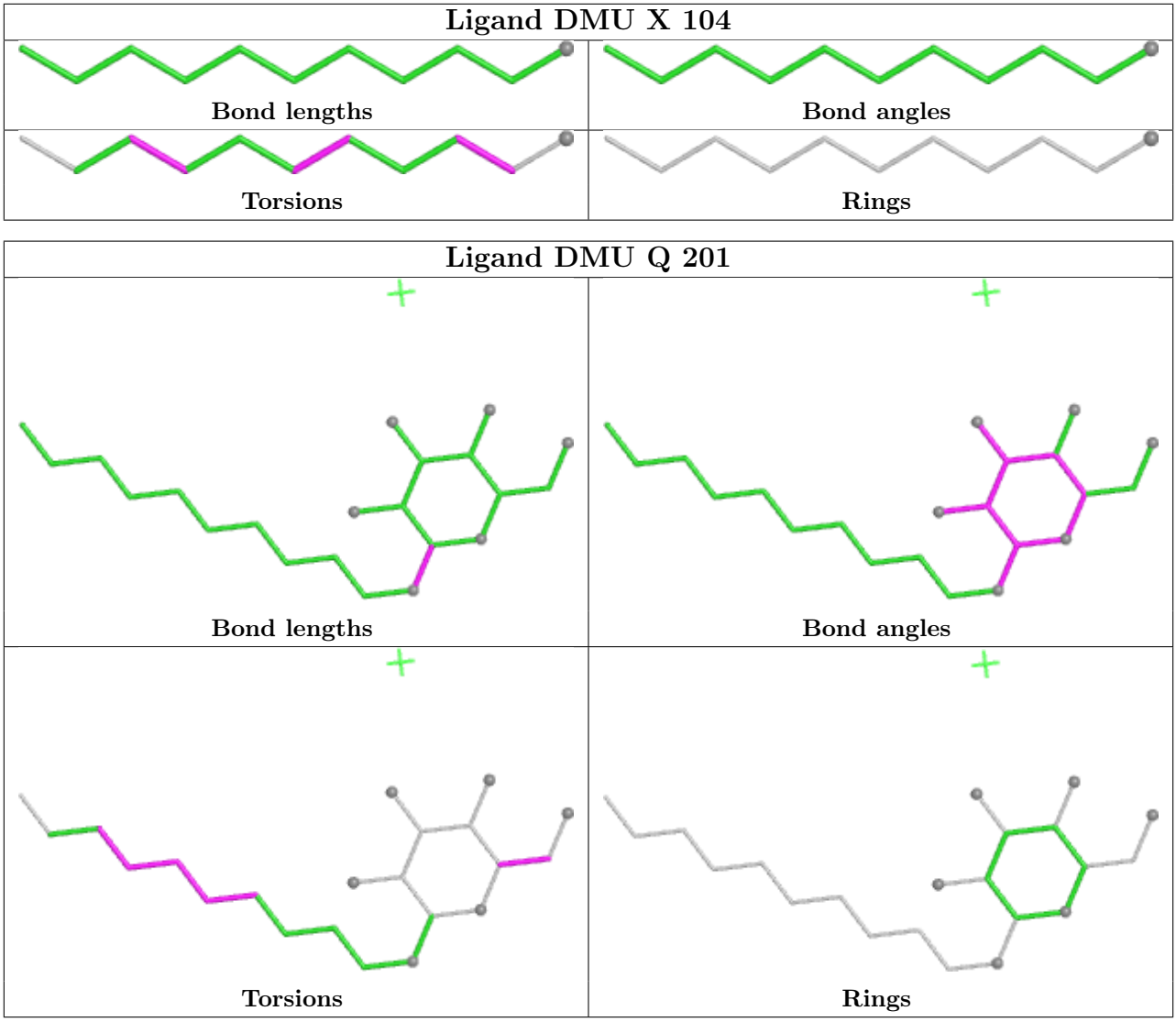


Ligand CDL G 102



Ligand CHD L 102





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.37	2 (0%) 88 89	12, 28, 36, 103	37 (7%)
1	N	513/514 (99%)	-0.33	5 (0%) 79 80	13, 31, 42, 111	21 (4%)
2	B	226/227 (99%)	0.21	12 (5%) 32 31	26, 37, 73, 143	4 (1%)
2	O	226/227 (99%)	0.29	11 (4%) 35 33	29, 42, 81, 124	7 (3%)
3	C	259/259 (100%)	-0.12	3 (1%) 76 77	25, 32, 50, 99	5 (1%)
3	P	259/259 (100%)	-0.05	7 (2%) 56 56	26, 33, 55, 94	2 (0%)
4	D	144/144 (100%)	0.09	4 (2%) 55 55	23, 39, 64, 120	1 (0%)
4	Q	144/144 (100%)	0.82	17 (11%) 9 7	36, 52, 106, 286	0
5	E	105/105 (100%)	0.02	3 (2%) 53 53	29, 37, 72, 132	0
5	R	105/105 (100%)	0.29	3 (2%) 53 53	33, 47, 83, 161	0
6	F	98/98 (100%)	0.64	12 (12%) 8 7	28, 41, 147, 232	1 (1%)
6	S	98/98 (100%)	0.68	15 (15%) 5 4	29, 42, 130, 198	1 (1%)
7	G	83/84 (98%)	1.38	18 (21%) 2 2	29, 41, 129, 212	0
7	T	83/84 (98%)	0.99	16 (19%) 3 2	28, 45, 138, 226	1 (1%)
8	H	79/79 (100%)	0.65	7 (8%) 15 13	33, 45, 118, 155	0
8	U	79/79 (100%)	0.76	12 (15%) 5 4	36, 48, 144, 220	0
9	I	72/73 (98%)	0.88	9 (12%) 8 6	34, 54, 87, 116	0
9	V	72/73 (98%)	1.12	12 (16%) 4 3	34, 61, 104, 191	0
10	J	58/58 (100%)	0.41	2 (3%) 48 48	31, 43, 94, 131	0
10	W	58/58 (100%)	0.60	5 (8%) 16 14	33, 47, 94, 161	0
11	K	49/49 (100%)	0.35	2 (4%) 41 41	35, 43, 67, 78	0
11	X	49/49 (100%)	0.67	5 (10%) 12 10	43, 54, 93, 113	0
12	L	46/46 (100%)	0.20	2 (4%) 40 39	29, 33, 62, 118	0
12	Y	46/46 (100%)	0.28	3 (6%) 25 23	34, 42, 87, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/43 (100%)	0.14	2 (4%) 36 35	29, 34, 83, 143	0
13	Z	43/43 (100%)	0.64	8 (18%) 3 2	40, 46, 123, 185	0
All	All	3550/3558 (99%)	0.17	197 (5%) 30 29	12, 37, 85, 286	80 (2%)

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	10.7
6	S	1	ALA	10.4
7	G	3	ALA	10.0
6	F	1	ALA	9.9
7	G	1	ALA	9.3

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	0.44	0.18	210,249,270,285	0
7	TPO	T	11	11/12	0.67	0.25	124,161,188,220	0
9	SAC	I	1	9/10	0.67	0.21	131,136,147,157	0
7	TPO	G	11	11/12	0.73	0.26	137,171,213,223	0
1	FME	N	1	10/11	0.92	0.13	38,54,95,119	0
1	FME	A	1	10/11	0.93	0.14	39,52,94,106	0
2	FME	B	1	10/11	0.97	0.09	32,35,43,114	0
2	FME	O	1	10/11	0.97	0.09	35,40,46,125	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
18	DMU	K	104	11/33	0.68	0.17	73,94,107,107	0
18	DMU	K	103	22/33	0.69	0.21	66,110,139,152	0
22	EDO	E	203	4/4	0.69	0.17	67,79,81,82	0
18	DMU	Q	201	23/33	0.70	0.24	52,92,138,154	0
24	CHD	Y	102	29/29	0.71	0.22	68,98,143,174	0
18	DMU	X	103	11/33	0.72	0.19	67,83,110,113	0
18	DMU	X	105	11/33	0.72	0.20	80,95,123,124	0
26	PEK	C	308	53/53	0.72	0.22	48,101,182,205	0
18	DMU	C	302	33/33	0.75	0.16	53,103,152,162	0
18	DMU	C	303	22/33	0.75	0.19	53,89,148,160	0
18	DMU	P	303	33/33	0.75	0.15	49,107,135,152	0
22	EDO	C	317	4/4	0.77	0.25	45,73,80,84	0
24	CHD	J	102	29/29	0.78	0.17	61,109,143,153	0
22	EDO	D	203	4/4	0.78	0.27	45,66,83,84	0
19	PGV	T	104	51/51	0.78	0.22	50,97,182,229	0
19	PGV	P	310	51/51	0.79	0.20	51,97,153,200	0
21	TGL	A	610	63/63	0.79	0.20	36,73,112,133	0
26	PEK	T	103	53/53	0.79	0.22	49,78,169,233	0
18	DMU	C	304	11/33	0.80	0.16	56,65,86,100	0
18	DMU	L	101	33/33	0.80	0.15	49,102,136,160	0
25	CDL	T	102	100/100	0.80	0.22	42,103,168,206	0
18	DMU	Y	101	33/33	0.80	0.14	52,105,145,149	0
22	EDO	N	618	4/4	0.80	0.22	41,54,66,72	0
21	TGL	N	608	63/63	0.81	0.20	48,70,116,129	0
20	PSC	V	101	52/52	0.81	0.24	43,92,191,241	0
20	PSC	A	609	52/52	0.81	0.21	42,101,181,243	0
26	PEK	P	307	53/53	0.81	0.21	50,74,159,190	0
24	CHD	L	102	29/29	0.81	0.21	51,91,123,145	0
19	PGV	N	606	51/51	0.82	0.21	41,94,148,194	0
22	EDO	C	311	4/4	0.82	0.23	35,61,78,103	0
24	CHD	P	305	29/29	0.82	0.14	59,75,113,132	0
18	DMU	D	201	21/33	0.82	0.21	51,85,132,140	0
18	DMU	X	102	21/33	0.83	0.15	68,102,136,151	0
18	DMU	K	102	14/33	0.83	0.19	60,80,119,123	0
22	EDO	C	314	4/4	0.83	0.21	41,45,49,59	0
22	EDO	F	110	4/4	0.83	0.20	66,70,80,81	0
25	CDL	G	102	100/100	0.83	0.20	51,99,177,197	0
25	CDL	P	306	100/100	0.83	0.23	40,100,173,211	0
22	EDO	C	316	4/4	0.83	0.29	52,60,77,128	0
22	EDO	P	317	4/4	0.83	0.16	61,66,67,80	0
22	EDO	S	103	4/4	0.83	0.18	61,71,80,83	0
22	EDO	S	105	4/4	0.83	0.19	73,85,94,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	DMU	A	606	13/33	0.84	0.17	43,67,113,117	0
22	EDO	C	315	4/4	0.84	0.23	51,65,79,108	0
21	TGL	D	202	63/63	0.84	0.21	34,68,120,140	0
22	EDO	Q	203	4/4	0.84	0.19	78,86,87,105	0
19	PGV	A	607	51/51	0.85	0.22	31,70,159,167	0
26	PEK	F	102	53/53	0.85	0.20	46,79,162,232	0
24	CHD	C	306	29/29	0.85	0.15	51,80,118,135	0
21	TGL	Q	202	63/63	0.85	0.20	37,73,125,139	0
21	TGL	Y	103	63/63	0.86	0.20	39,73,128,179	0
22	EDO	L	104	4/4	0.86	0.21	41,94,96,97	0
21	TGL	L	103	63/63	0.86	0.20	29,63,125,169	0
22	EDO	P	315	4/4	0.86	0.20	41,52,78,113	0
18	DMU	X	101	11/33	0.86	0.16	48,75,115,125	0
18	DMU	X	104	11/33	0.86	0.20	56,71,105,109	0
22	EDO	Q	205	4/4	0.86	0.24	67,78,84,107	0
22	EDO	A	613	4/4	0.87	0.21	39,40,46,80	0
22	EDO	F	107	4/4	0.87	0.18	54,60,63,83	0
22	EDO	F	109	4/4	0.87	0.22	53,57,67,98	0
22	EDO	B	304	4/4	0.87	0.21	59,73,85,88	0
18	DMU	J	101	21/33	0.87	0.18	32,68,123,131	0
18	DMU	W	101	21/33	0.87	0.17	42,75,111,128	0
25	CDL	C	307	100/100	0.88	0.17	39,85,148,175	0
22	EDO	T	105	4/4	0.88	0.21	58,81,89,108	0
22	EDO	D	206	4/4	0.88	0.19	46,59,99,113	0
22	EDO	P	314	4/4	0.88	0.19	46,48,65,82	0
22	EDO	P	313	4/4	0.89	0.19	50,57,70,84	0
22	EDO	W	102	4/4	0.89	0.18	53,80,80,128	0
18	DMU	O	302	11/33	0.89	0.15	57,67,89,89	0
22	EDO	D	205	4/4	0.89	0.16	53,58,60,87	0
18	DMU	P	302	11/33	0.89	0.14	52,60,93,94	0
28	PO4	H	101	5/5	0.89	0.09	63,70,118,149	0
22	EDO	N	623	4/4	0.90	0.24	67,76,79,96	0
18	DMU	K	101	11/33	0.90	0.14	47,70,93,99	0
18	DMU	Z	101	33/33	0.90	0.13	44,58,89,96	0
24	CHD	C	305	29/29	0.90	0.11	35,42,60,67	0
22	EDO	M	102	4/4	0.90	0.16	71,76,76,93	0
22	EDO	N	611	4/4	0.90	0.19	37,37,43,56	0
22	EDO	D	207	4/4	0.90	0.17	42,70,72,108	0
22	EDO	N	620	4/4	0.90	0.17	45,56,92,96	0
22	EDO	N	622	4/4	0.90	0.20	29,50,67,70	0
22	EDO	F	106	4/4	0.91	0.12	43,43,53,54	0
22	EDO	A	617	4/4	0.91	0.25	49,69,96,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	EDO	N	613	4/4	0.91	0.16	52,55,73,74	0
22	EDO	D	204	4/4	0.91	0.14	54,55,56,95	0
22	EDO	A	619	4/4	0.91	0.14	59,67,69,89	0
22	EDO	Y	104	4/4	0.91	0.16	56,71,73,83	0
22	EDO	F	104	4/4	0.91	0.20	60,66,79,83	0
28	PO4	U	101	5/5	0.91	0.09	59,65,141,151	0
22	EDO	N	616	4/4	0.92	0.14	49,54,55,66	0
22	EDO	B	305	4/4	0.92	0.16	44,56,58,76	0
22	EDO	J	103	4/4	0.92	0.15	44,70,75,83	0
22	EDO	A	618	4/4	0.92	0.17	38,57,68,73	0
22	EDO	A	611	4/4	0.93	0.16	37,41,41,94	0
22	EDO	Q	204	4/4	0.93	0.14	35,64,73,77	0
22	EDO	N	619	4/4	0.93	0.15	49,65,71,83	0
22	EDO	L	105	4/4	0.93	0.11	56,59,64,85	0
22	EDO	B	306	4/4	0.93	0.16	35,46,51,94	0
18	DMU	B	302	11/33	0.93	0.13	61,78,97,105	0
22	EDO	T	106	4/4	0.93	0.13	38,40,45,52	0
22	EDO	U	102	4/4	0.93	0.15	42,53,67,72	0
22	EDO	N	612	4/4	0.93	0.15	40,55,59,61	0
22	EDO	C	312	4/4	0.93	0.13	38,46,49,49	0
22	EDO	N	615	4/4	0.93	0.17	40,56,59,88	0
22	EDO	P	316	4/4	0.93	0.19	32,52,92,94	0
18	DMU	M	101	33/33	0.93	0.10	36,46,68,80	0
22	EDO	A	614	4/4	0.94	0.14	36,57,62,82	0
22	EDO	N	621	4/4	0.94	0.15	37,47,53,79	0
22	EDO	H	102	4/4	0.94	0.12	41,41,57,84	0
22	EDO	N	610	4/4	0.94	0.15	33,57,77,86	0
22	EDO	O	303	4/4	0.94	0.09	33,35,37,38	0
22	EDO	O	304	4/4	0.94	0.17	56,64,81,84	0
22	EDO	N	617	4/4	0.94	0.14	48,48,58,79	0
24	CHD	P	304	29/29	0.94	0.09	34,44,64,70	0
22	EDO	F	108	4/4	0.94	0.12	74,76,86,88	0
22	EDO	A	616	4/4	0.94	0.16	48,53,72,112	0
22	EDO	A	615	4/4	0.95	0.18	30,61,69,139	0
26	PEK	C	309	53/53	0.95	0.12	31,48,111,119	0
22	EDO	B	307	4/4	0.95	0.15	36,57,74,101	0
22	EDO	C	313	4/4	0.95	0.12	34,41,56,57	0
26	PEK	P	308	53/53	0.95	0.12	31,50,93,125	0
22	EDO	E	201	4/4	0.95	0.09	44,47,50,56	0
22	EDO	E	202	4/4	0.95	0.10	37,40,47,53	0
22	EDO	S	102	4/4	0.95	0.13	33,33,35,39	0
22	EDO	B	303	4/4	0.96	0.08	30,31,32,40	0

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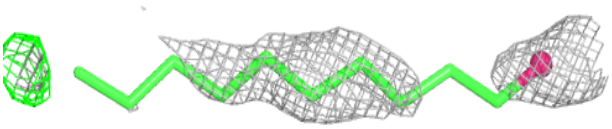
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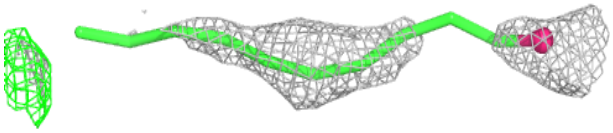
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	EDO	G	103	4/4	0.96	0.08	31,37,40,44	0
22	EDO	F	105	4/4	0.96	0.11	36,39,40,42	0
22	EDO	A	612	4/4	0.96	0.08	24,28,31,31	0
22	EDO	N	614	4/4	0.96	0.11	38,45,67,71	0
19	PGV	N	607	51/51	0.96	0.10	26,38,64,78	0
19	PGV	C	310	51/51	0.96	0.11	26,33,93,120	0
22	EDO	P	312	4/4	0.96	0.12	37,43,47,68	0
19	PGV	A	608	51/51	0.96	0.11	26,33,69,92	0
22	EDO	S	106	4/4	0.96	0.11	38,45,59,63	0
27	ZN	F	101	1/1	0.96	0.32	55,55,55,55	0
27	ZN	S	101	1/1	0.96	0.31	55,55,55,55	0
24	CHD	T	101	29/29	0.96	0.07	28,33,41,65	0
22	EDO	N	609	4/4	0.96	0.08	29,32,35,37	0
19	PGV	P	309	51/51	0.97	0.10	26,37,83,126	0
22	EDO	F	103	4/4	0.97	0.09	31,35,37,40	0
22	EDO	S	104	4/4	0.97	0.07	32,35,38,42	0
22	EDO	P	311	4/4	0.97	0.09	40,46,48,56	0
24	CHD	G	101	29/29	0.97	0.06	27,32,38,49	0
14	HEA	A	602	60/60	0.98	0.07	22,27,38,47	0
14	HEA	N	602	60/60	0.98	0.07	24,28,33,47	0
16	MG	A	604	1/1	0.98	0.06	29,29,29,29	0
17	NA	P	301	1/1	0.98	0.15	22,22,22,22	0
14	HEA	N	601[B]	60/60	0.99	0.06	24,30,48,56	12
14	HEA	A	601[B]	60/60	0.99	0.06	20,24,41,51	12
15	CU	N	603	1/1	0.99	0.02	30,30,30,30	0
14	HEA	A	601[A]	60/60	0.99	0.06	20,24,41,51	12
16	MG	N	604	1/1	0.99	0.05	31,31,31,31	0
17	NA	A	605	1/1	0.99	0.05	29,29,29,29	0
17	NA	C	301	1/1	0.99	0.13	22,22,22,22	0
17	NA	N	605	1/1	0.99	0.06	34,34,34,34	0
14	HEA	N	601[A]	60/60	0.99	0.06	23,30,48,53	12
23	CUA	O	301	2/2	1.00	0.01	32,32,32,33	0
15	CU	A	603	1/1	1.00	0.03	29,29,29,29	0
23	CUA	B	301	2/2	1.00	0.02	28,28,28,29	0

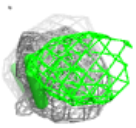
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU K 104:

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

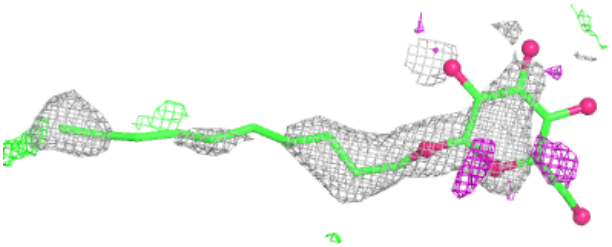


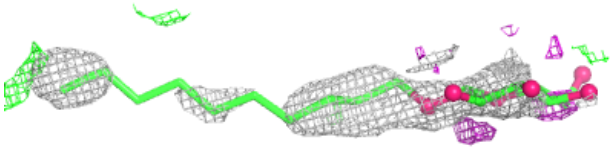


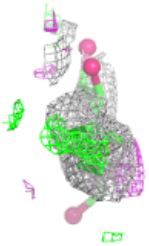


Electron density around DMU K 103:

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

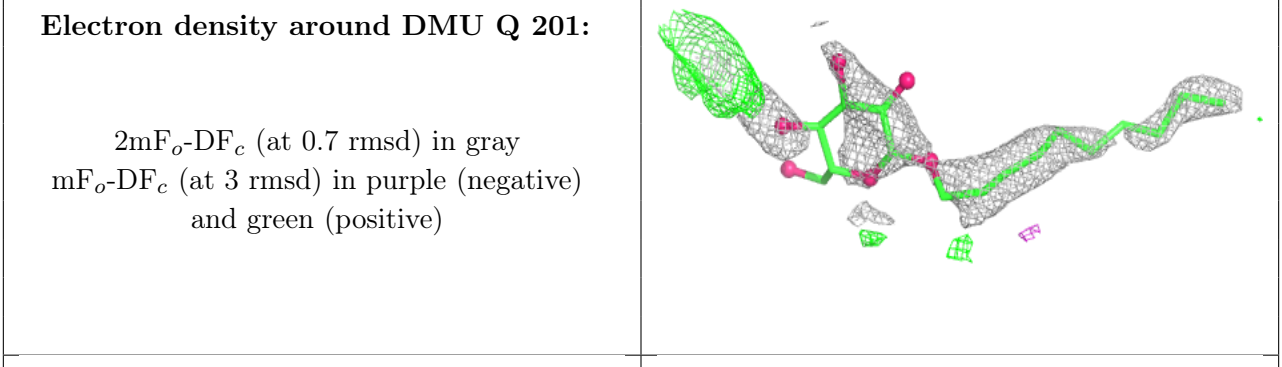






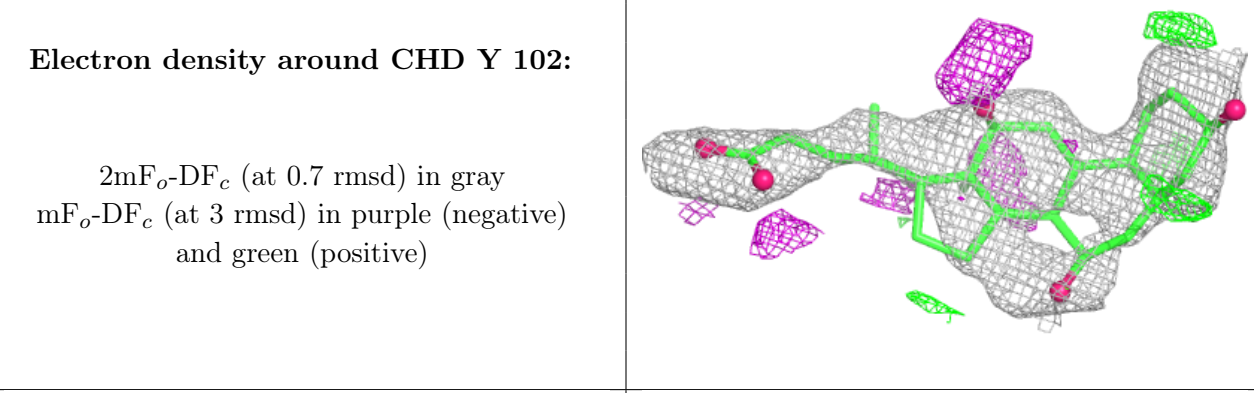
Electron density around DMU Q 201:

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



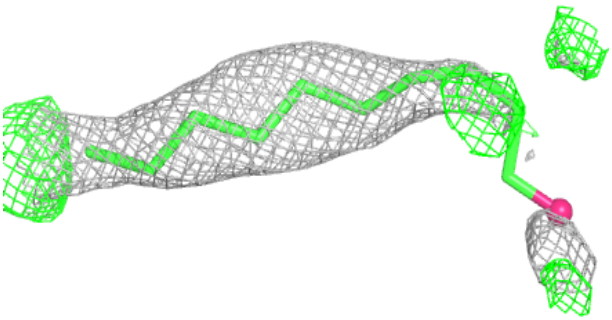
Electron density around CHD Y 102:

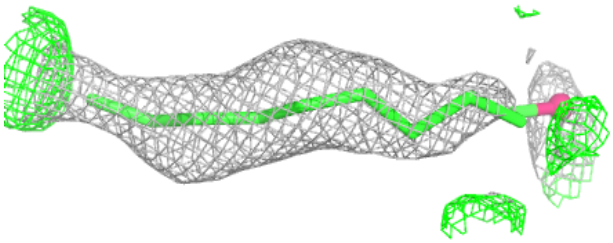
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

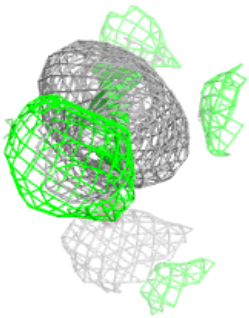


Electron density around DMU X 103:

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

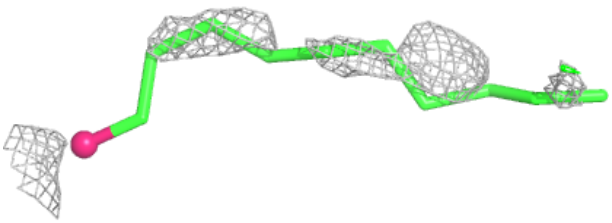


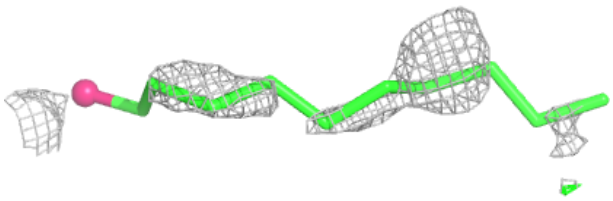


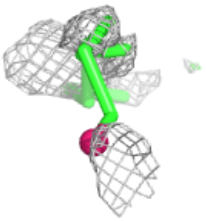


Electron density around DMU X 105:

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

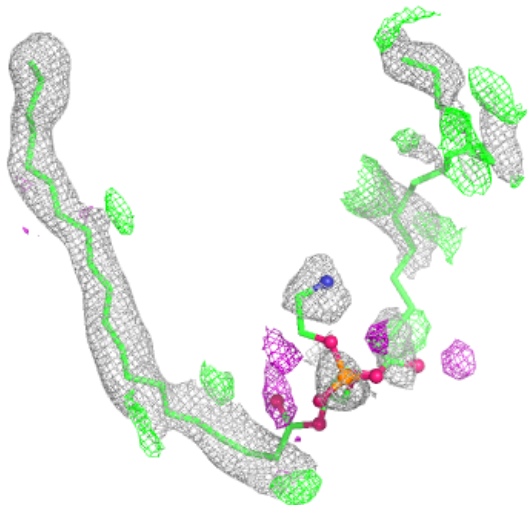


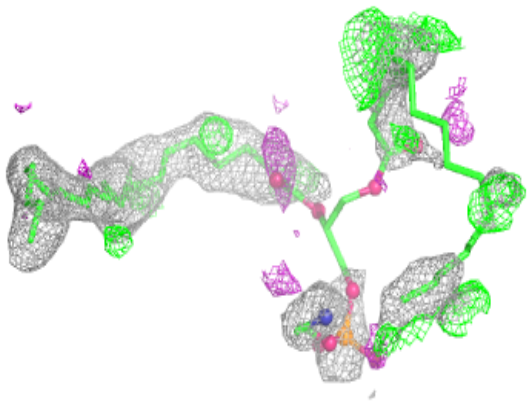


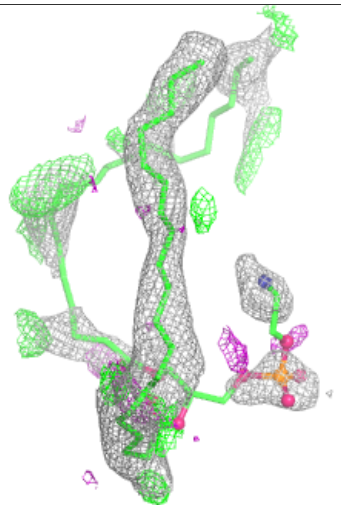


Electron density around PEK C 308:

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

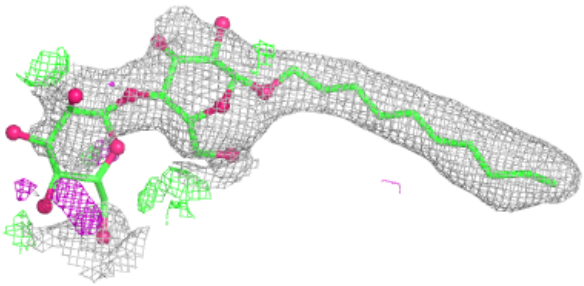


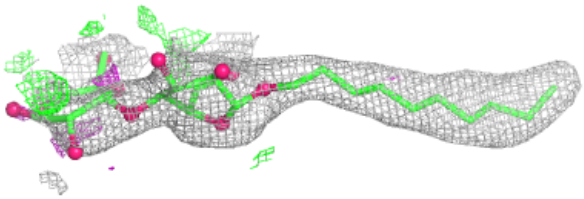


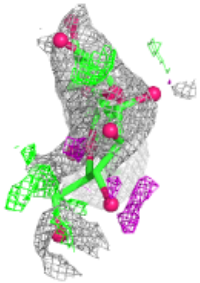


Electron density around DMU C 302:

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

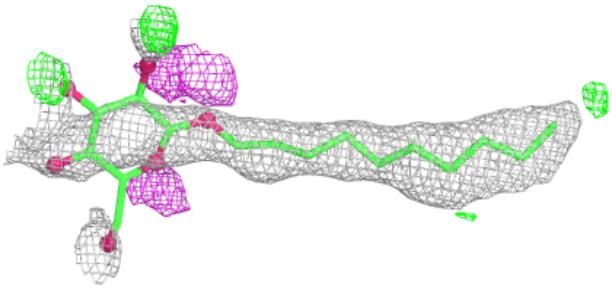


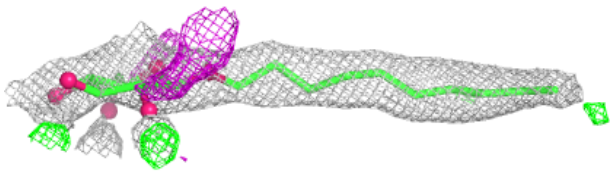


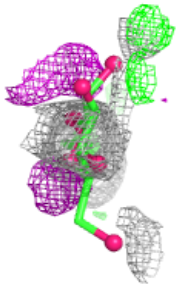


Electron density around DMU C 303:

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

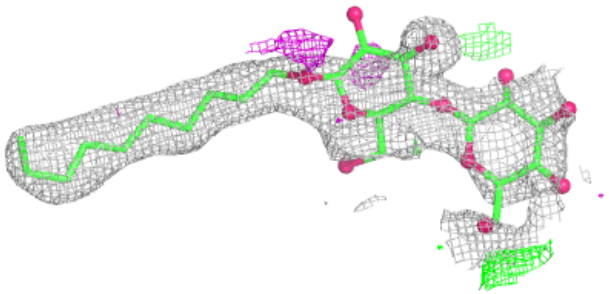


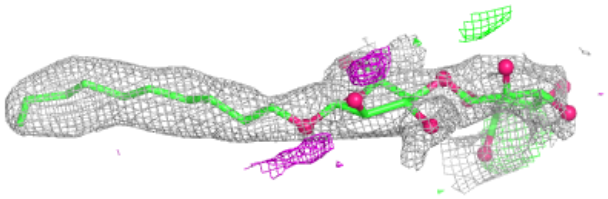


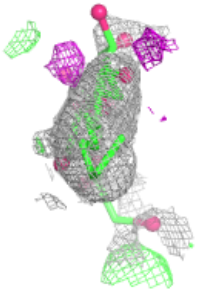


Electron density around DMU P 303:

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

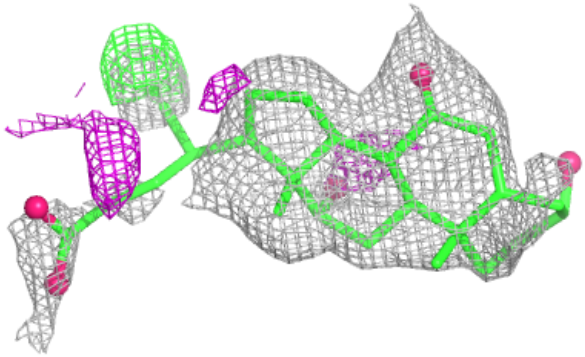


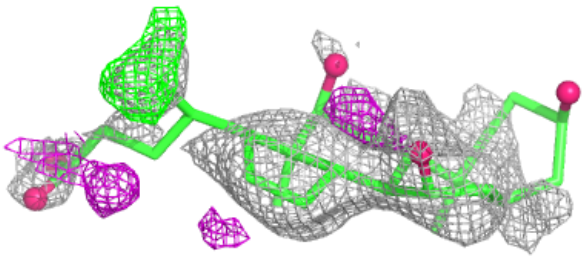


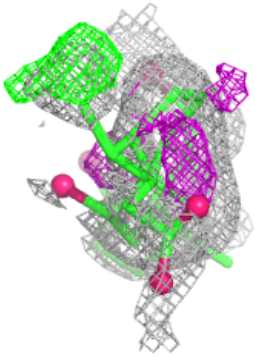


Electron density around CHD J 102:

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

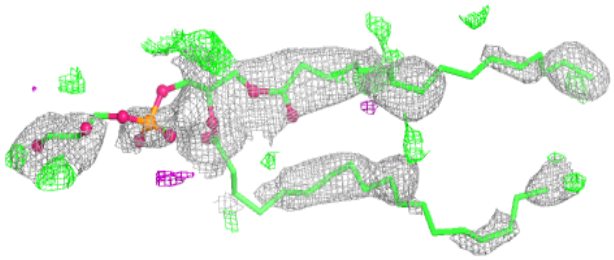


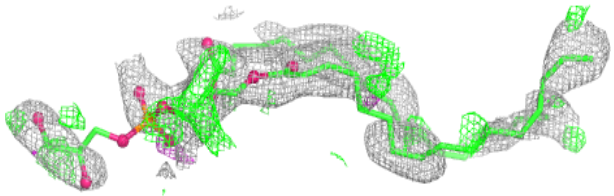


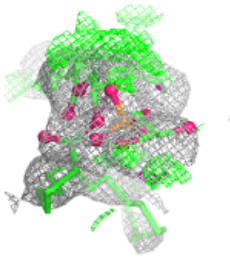


Electron density around PGV T 104:

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

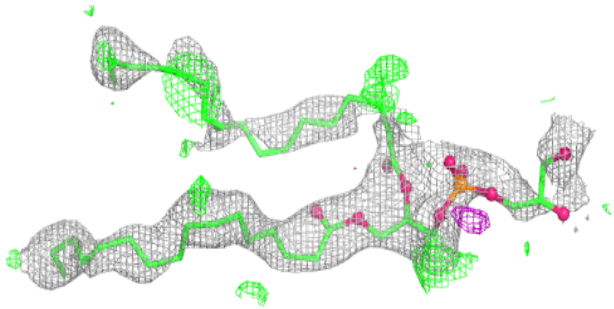


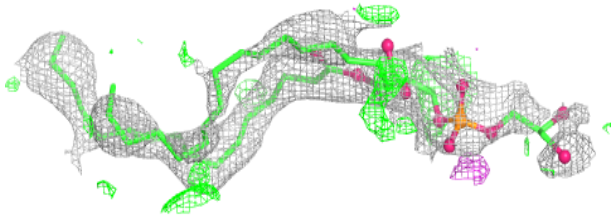


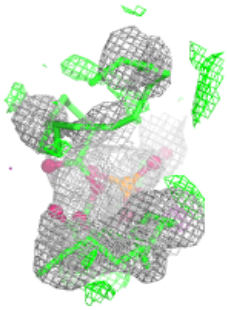


Electron density around PGV P 310:

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

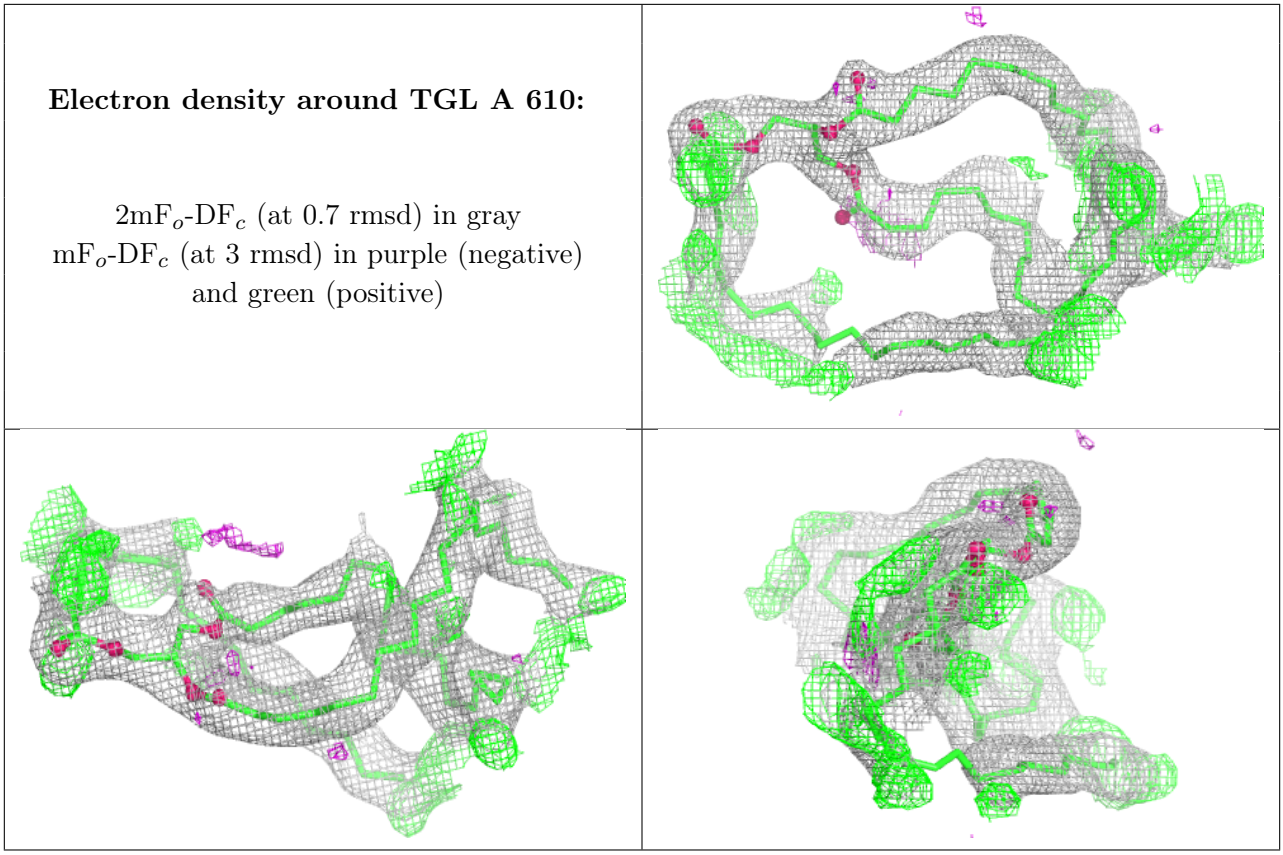






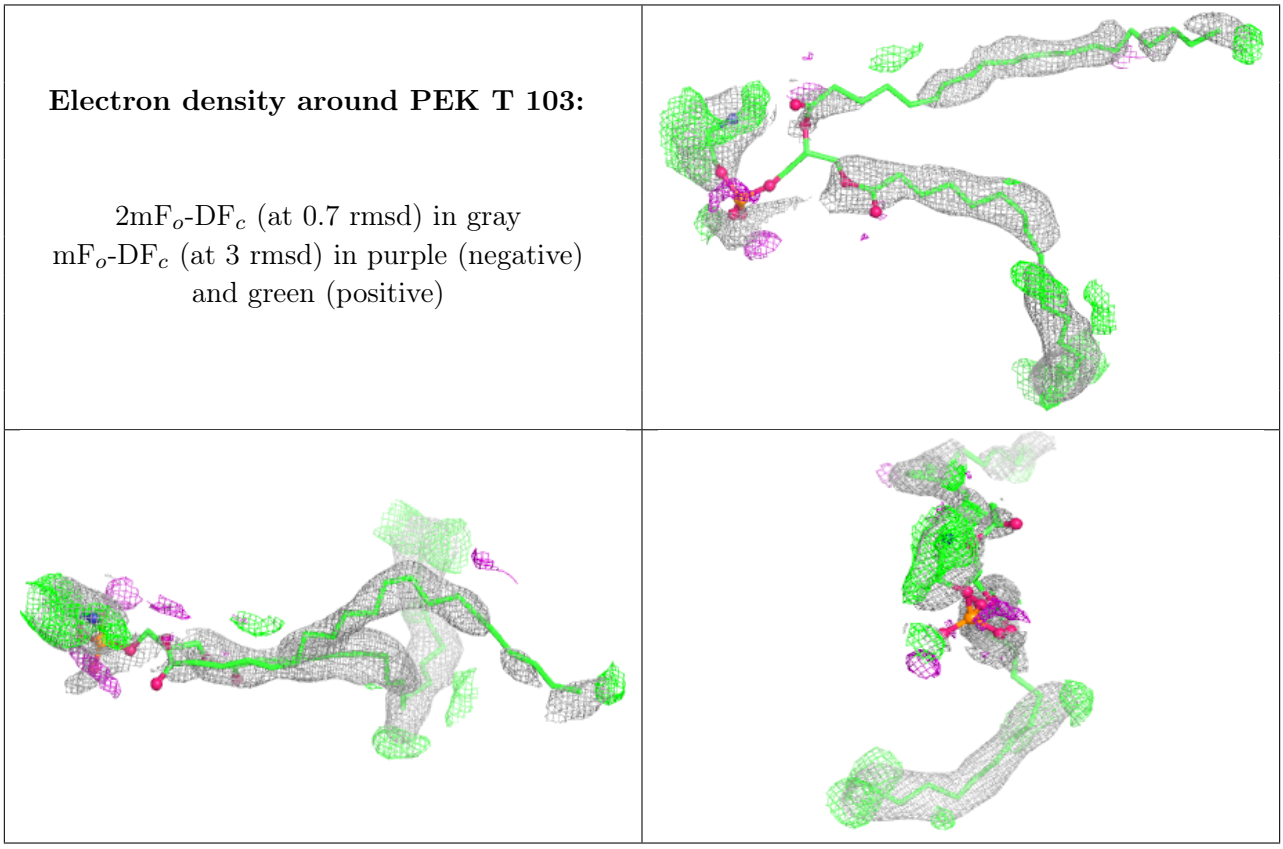
Electron density around TGL A 610:

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



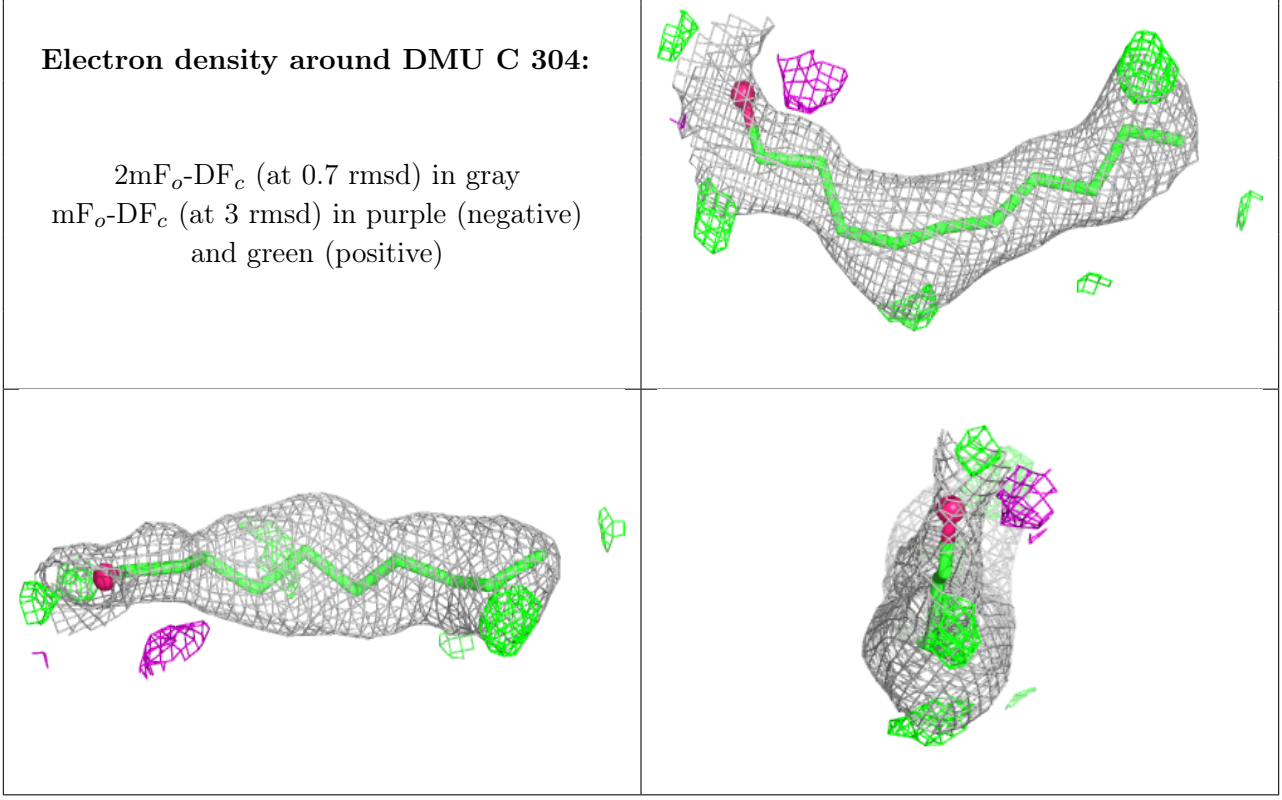
Electron density around PEK T 103:

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



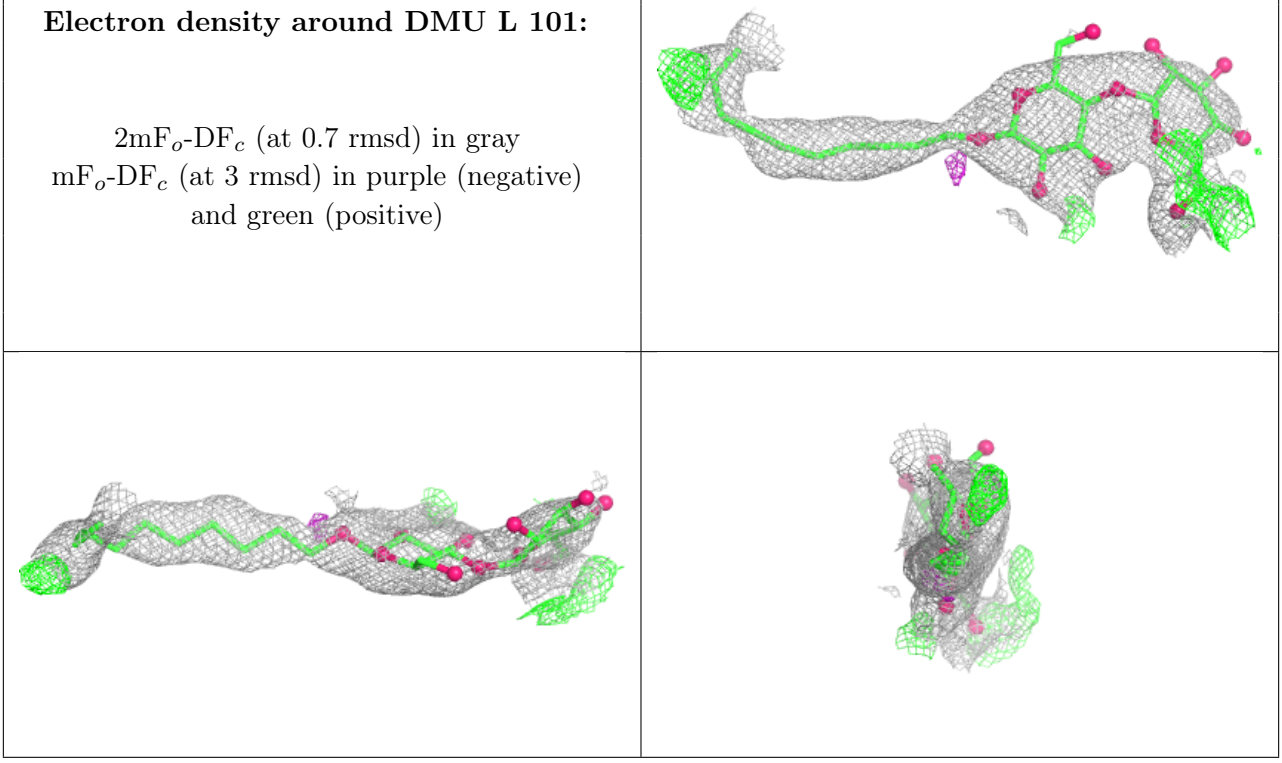
Electron density around DMU C 304:

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



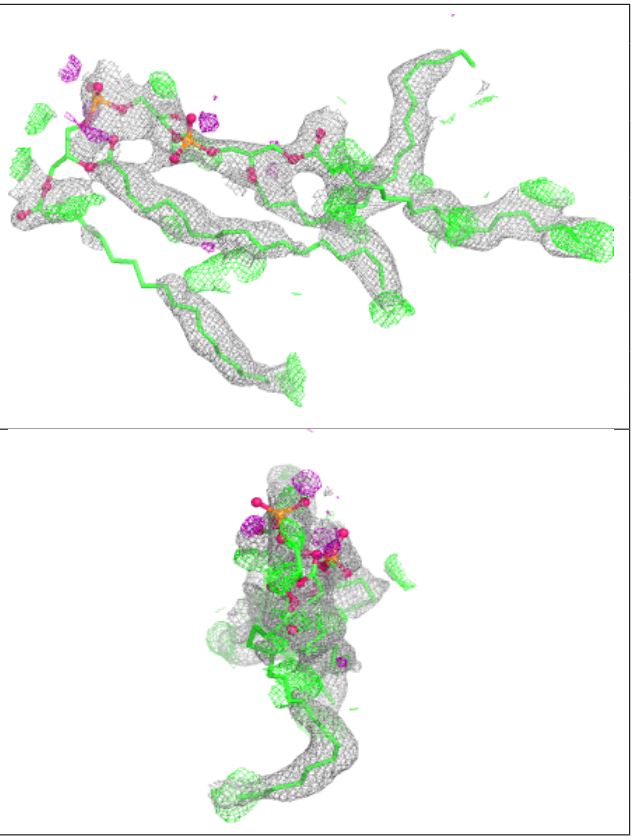
Electron density around DMU L 101:

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



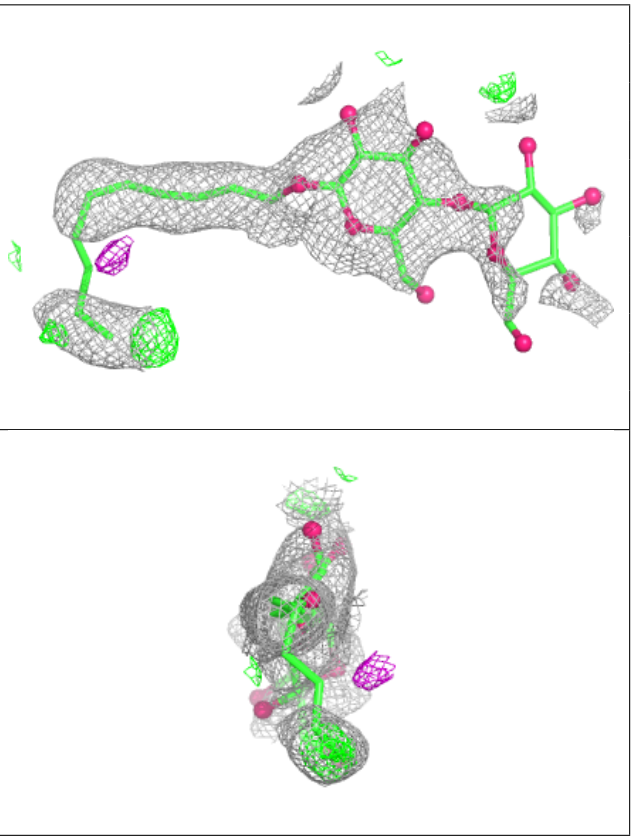
Electron density around CDL T 102:

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



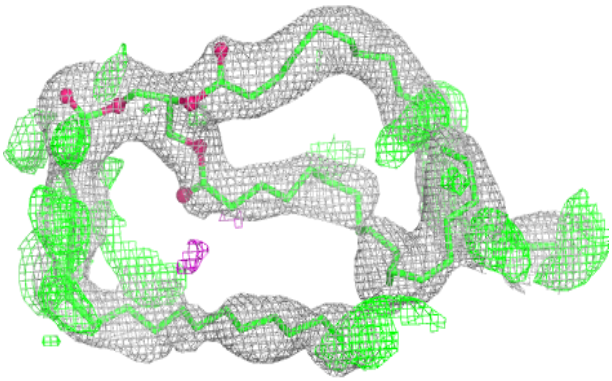
Electron density around DMU Y 101:

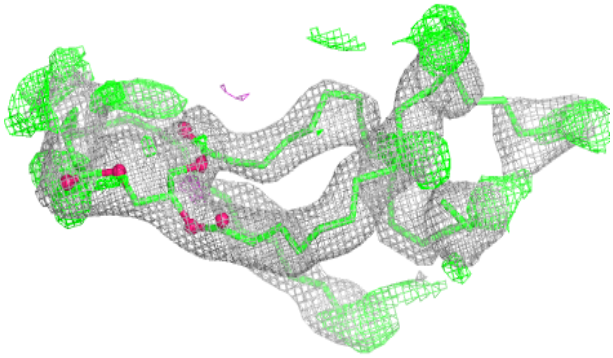
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

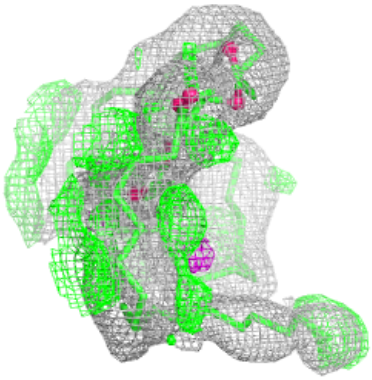


Electron density around TGL N 608:

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

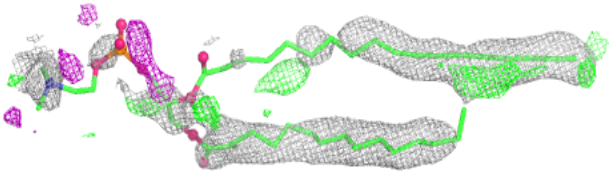


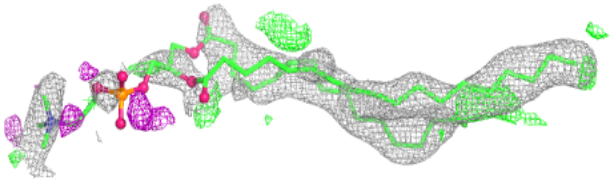


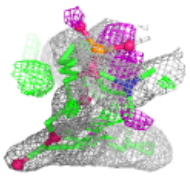


Electron density around PSC V 101:

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

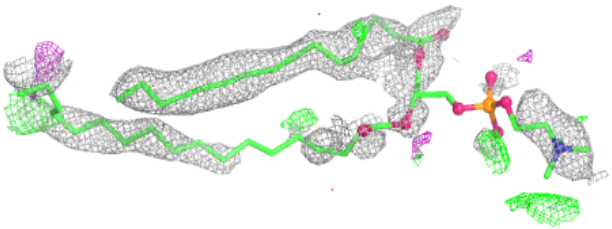


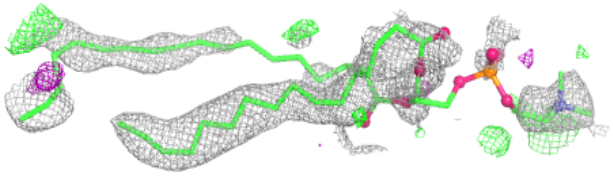


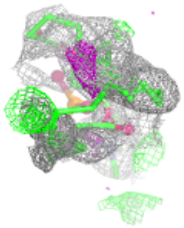


Electron density around PSC A 609:

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

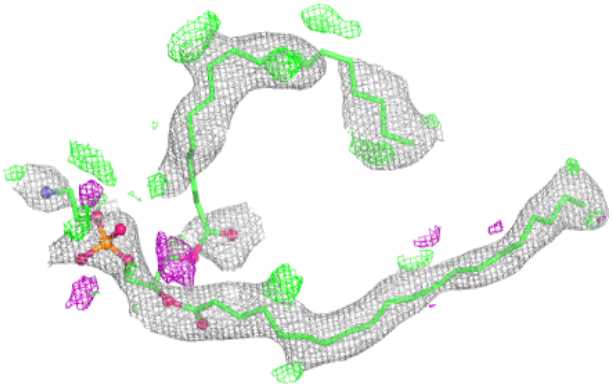


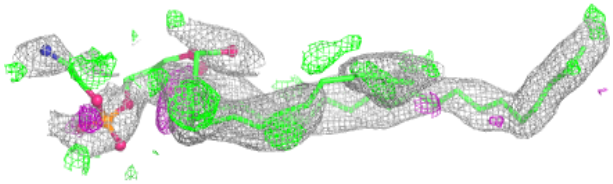


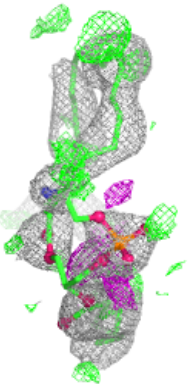


Electron density around PEK P 307:

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

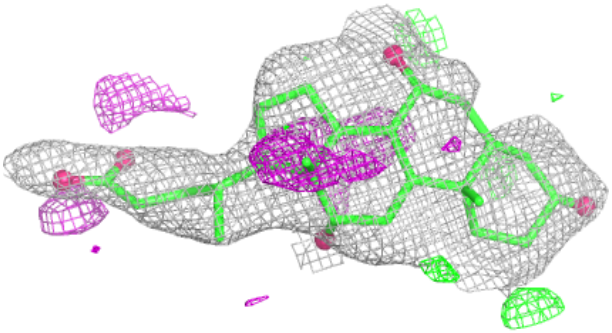


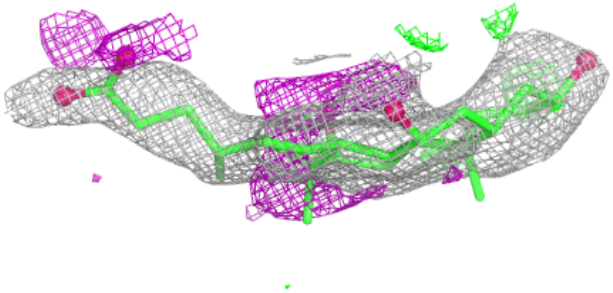


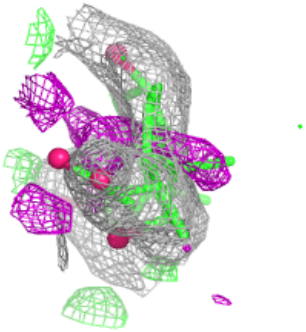


Electron density around CHD L 102:

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

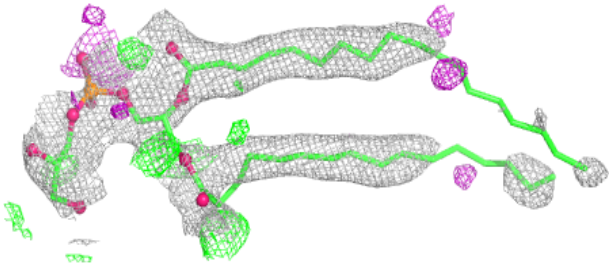


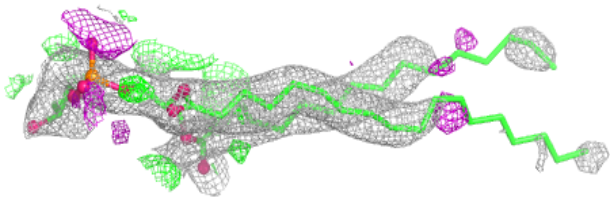


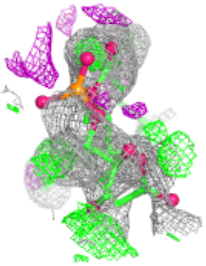


Electron density around PGV N 606:

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

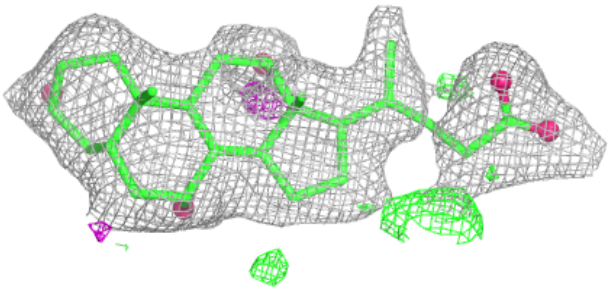


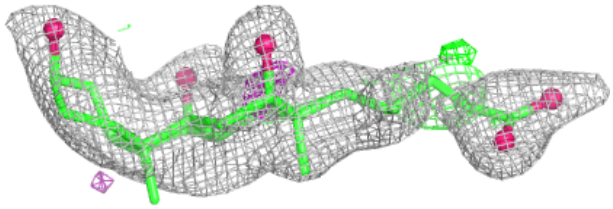


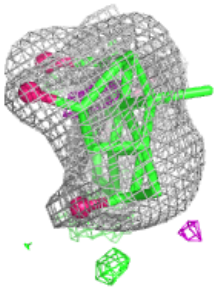


Electron density around CHD P 305:

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

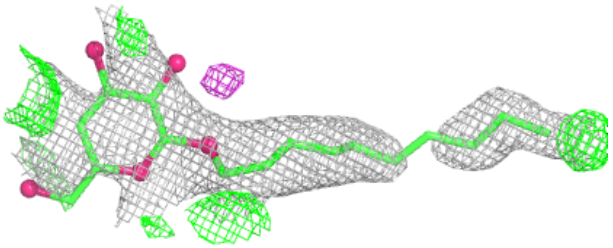


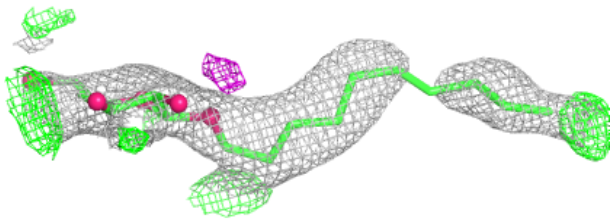


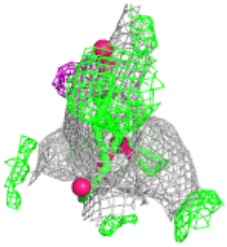


Electron density around DMU D 201:

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

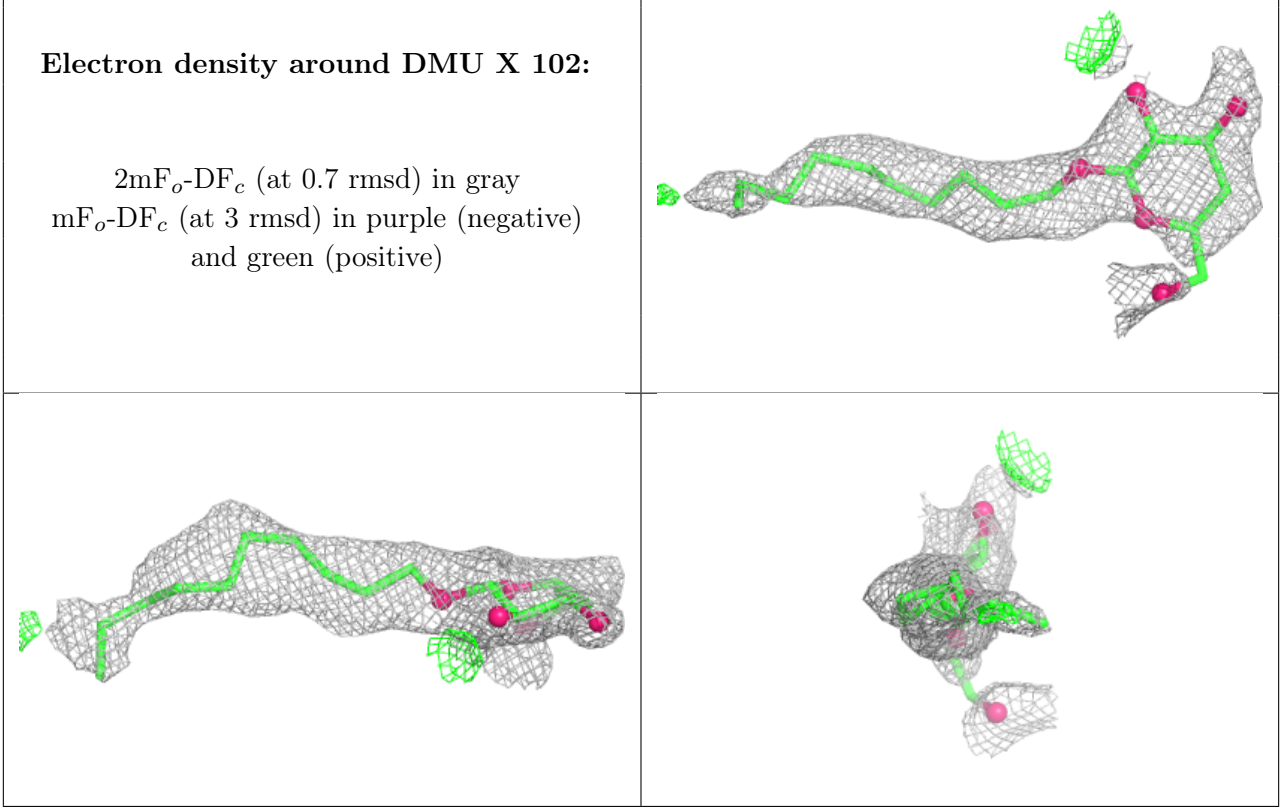






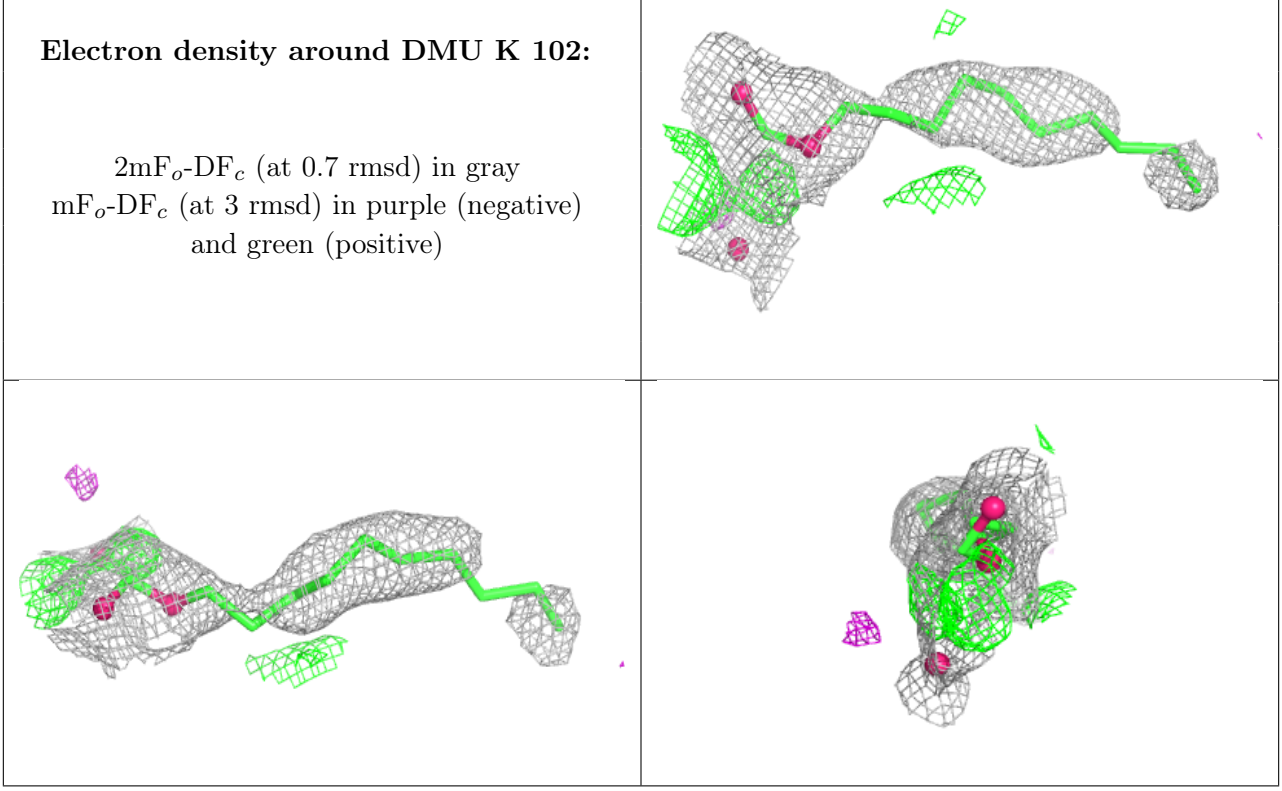
Electron density around DMU X 102:

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



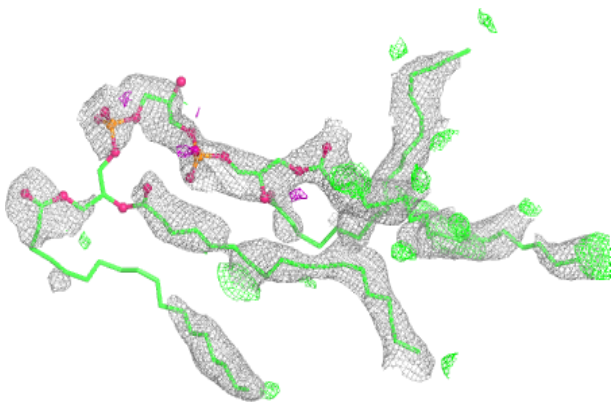
Electron density around DMU K 102:

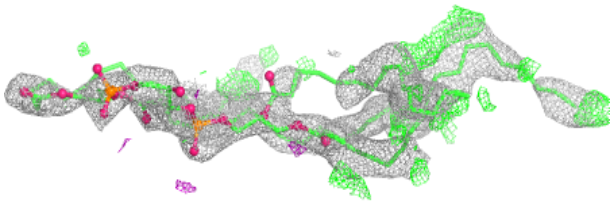
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

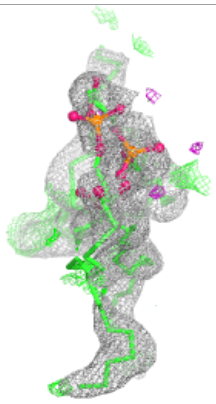


Electron density around CDL G 102:

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

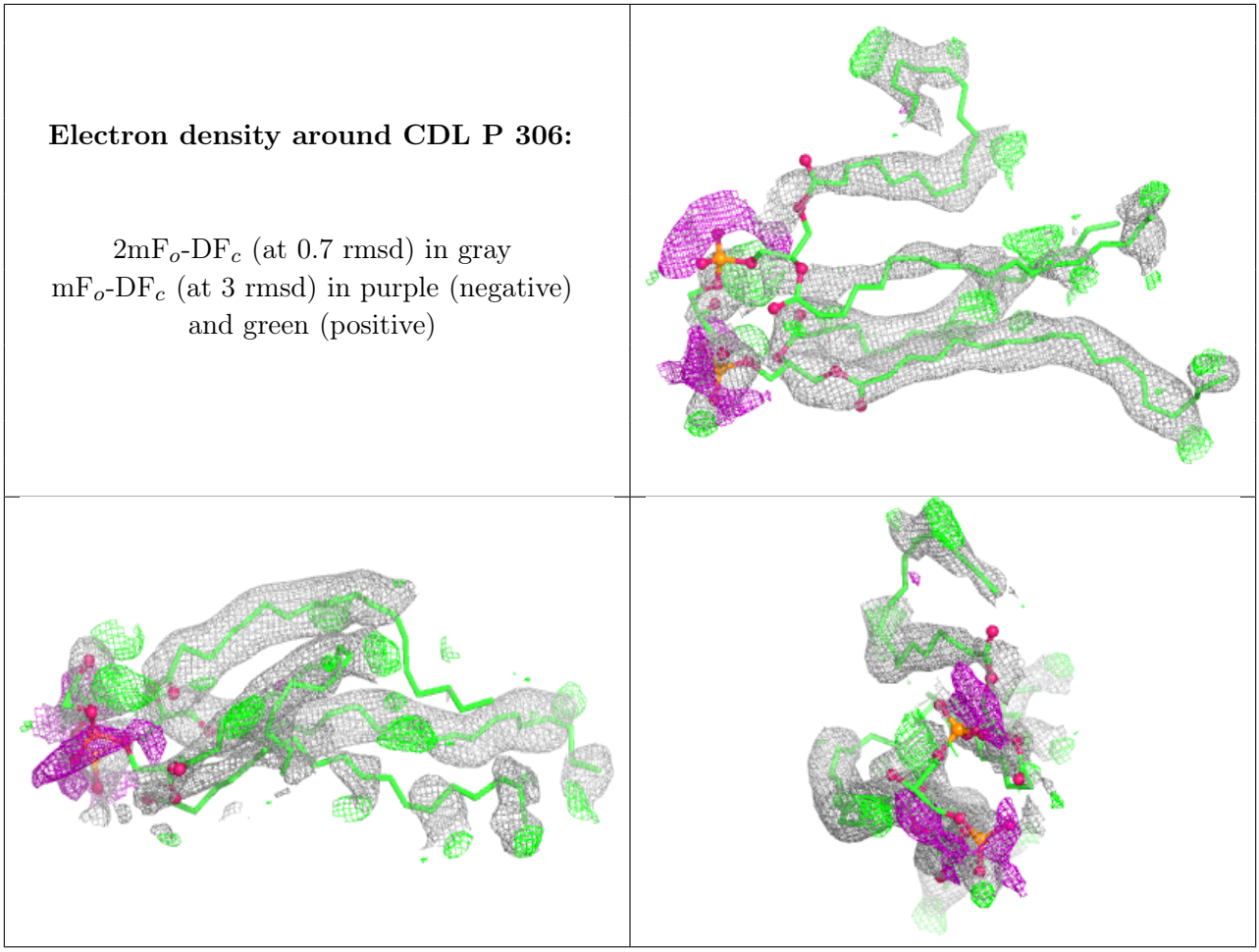






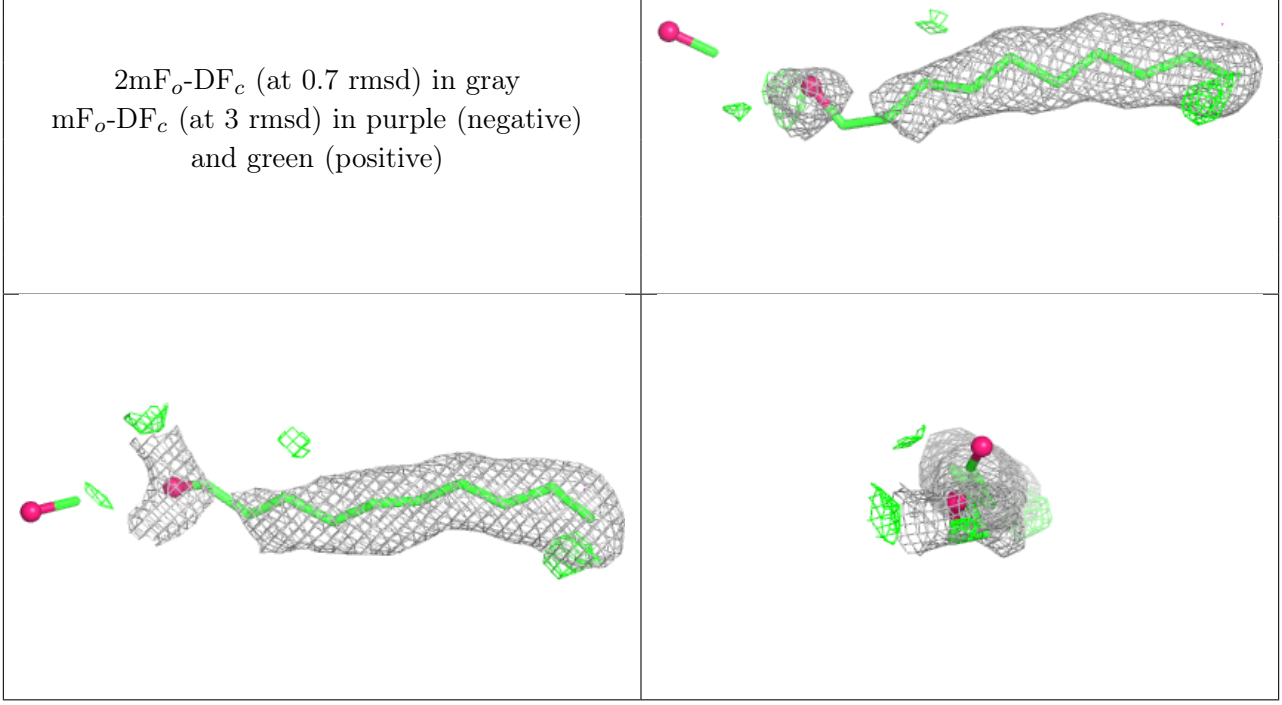
Electron density around CDL P 306:

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



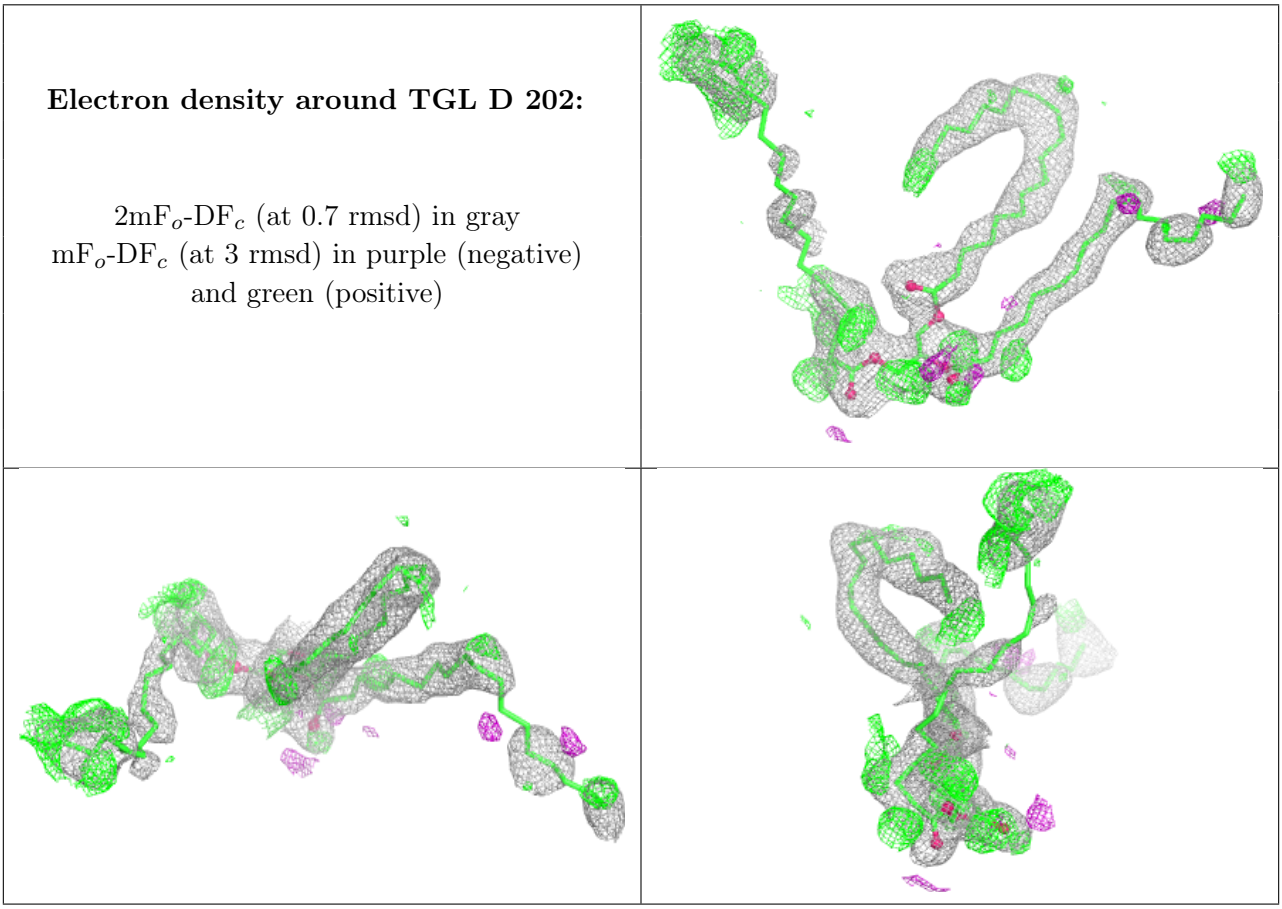
Electron density around DMU A 606:

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



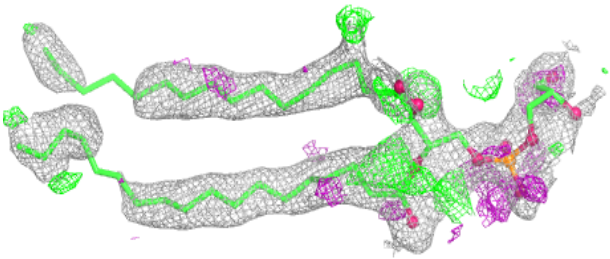
Electron density around TGL D 202:

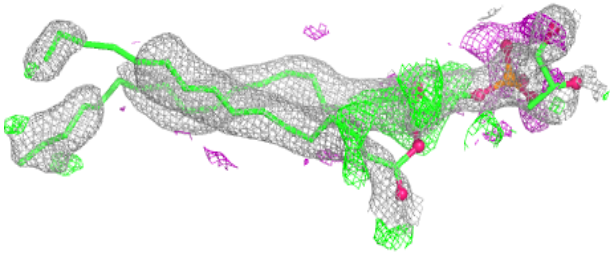
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

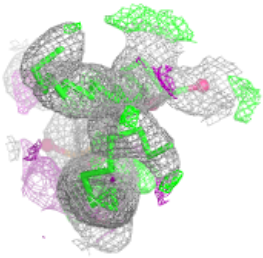


Electron density around PGV A 607:

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

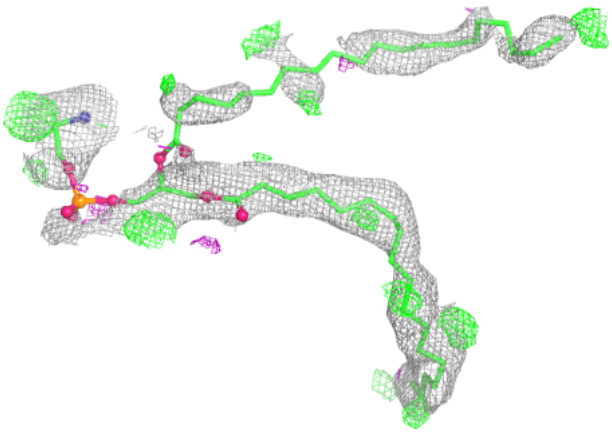


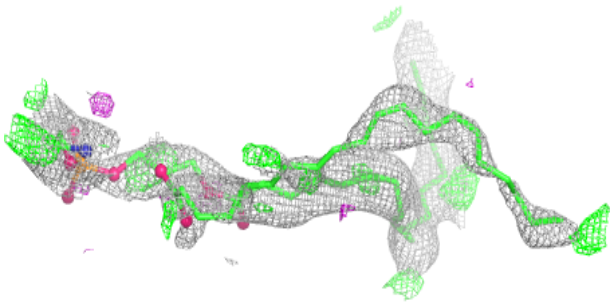


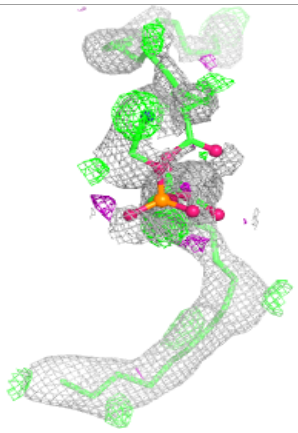


Electron density around PEK F 102:

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

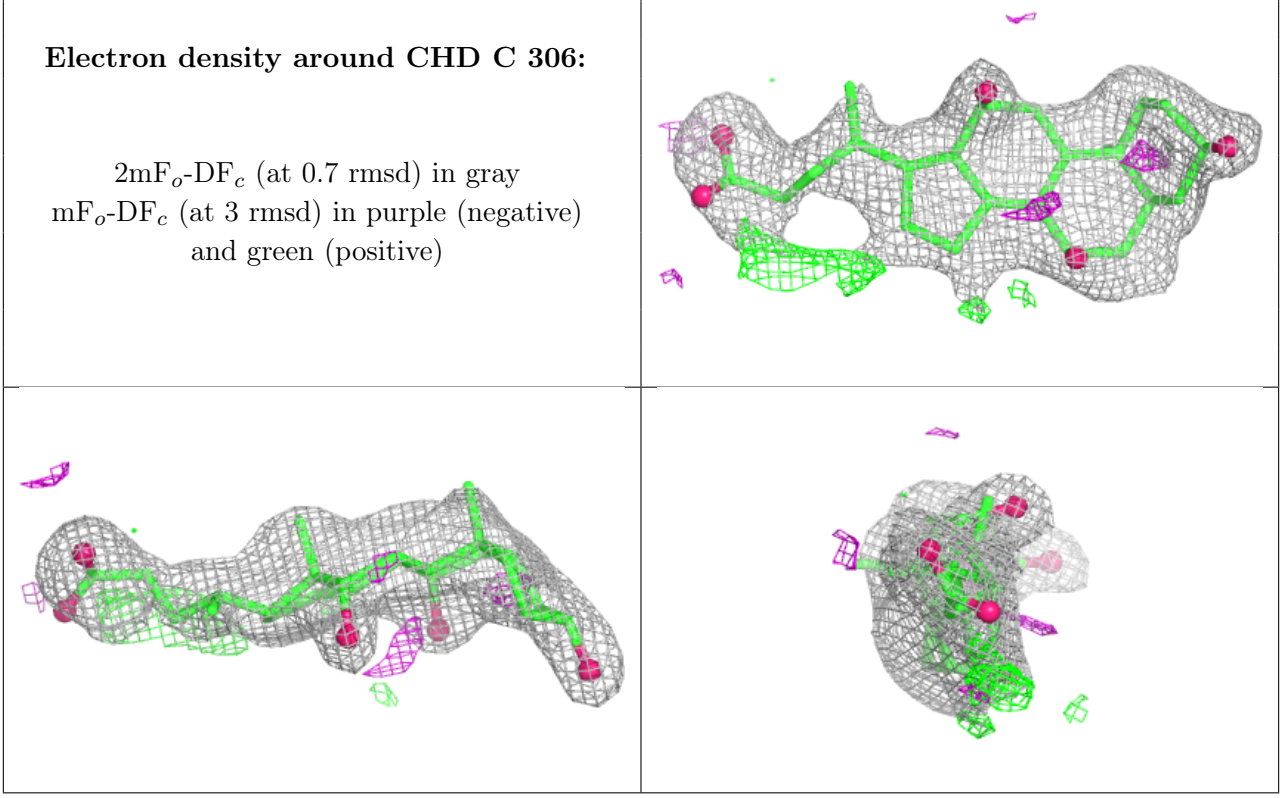






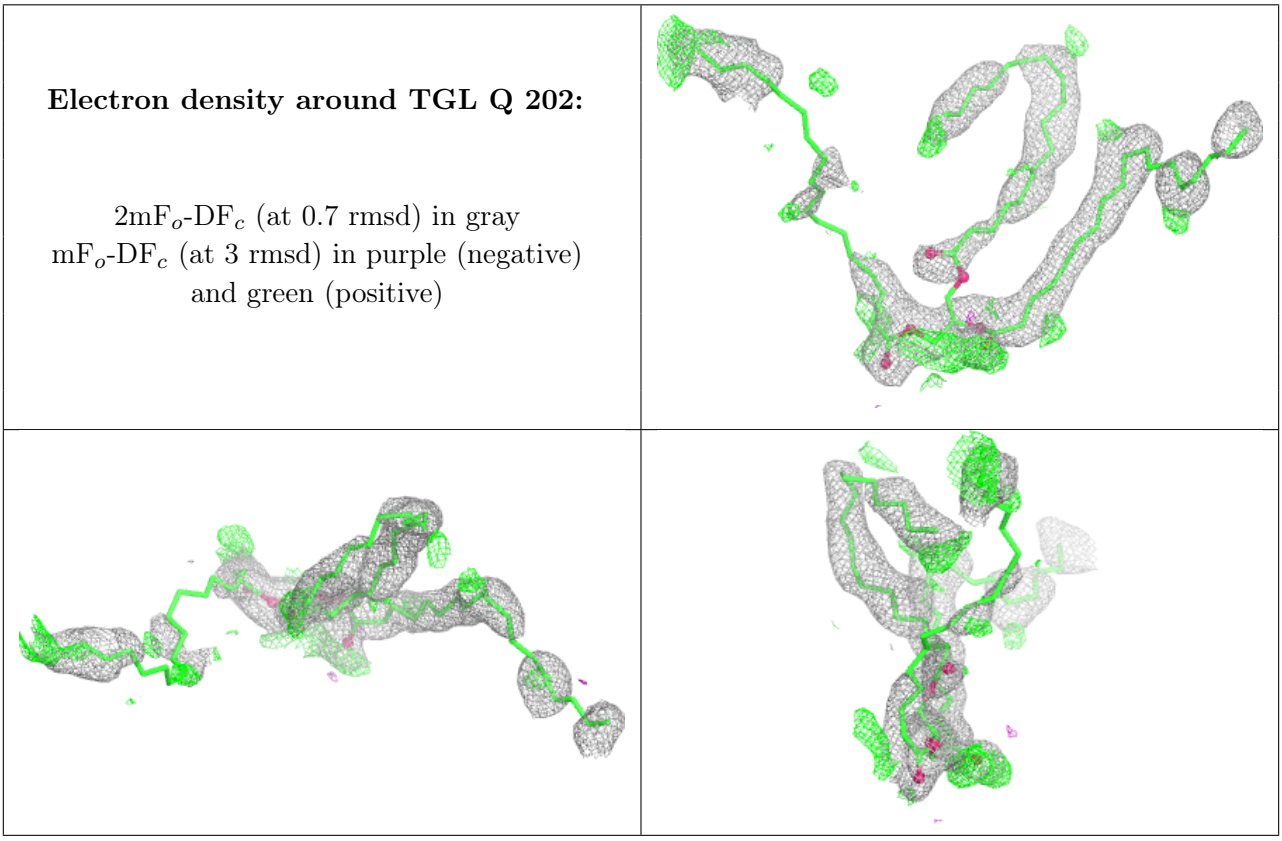
Electron density around CHD C 306:

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



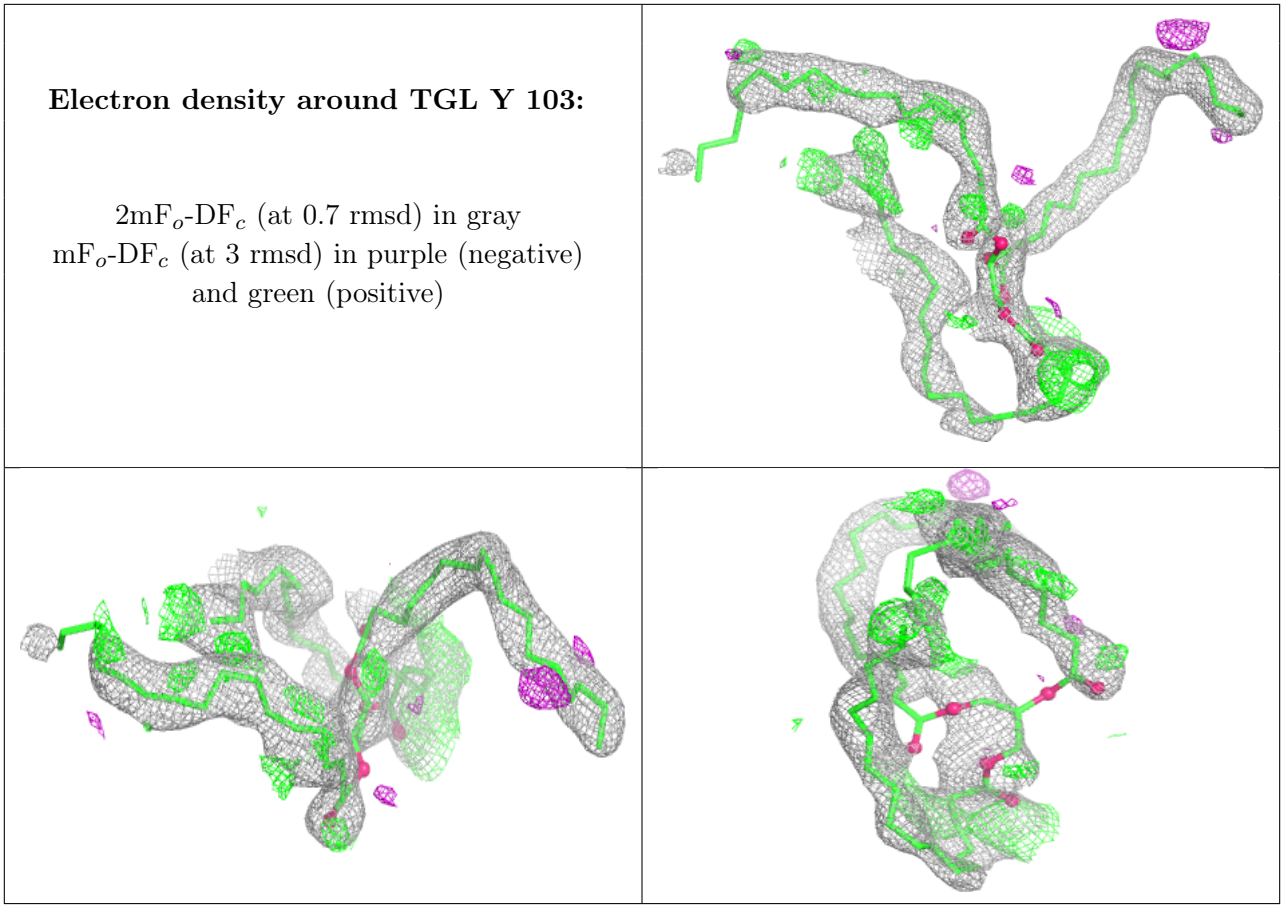
Electron density around TGL Q 202:

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



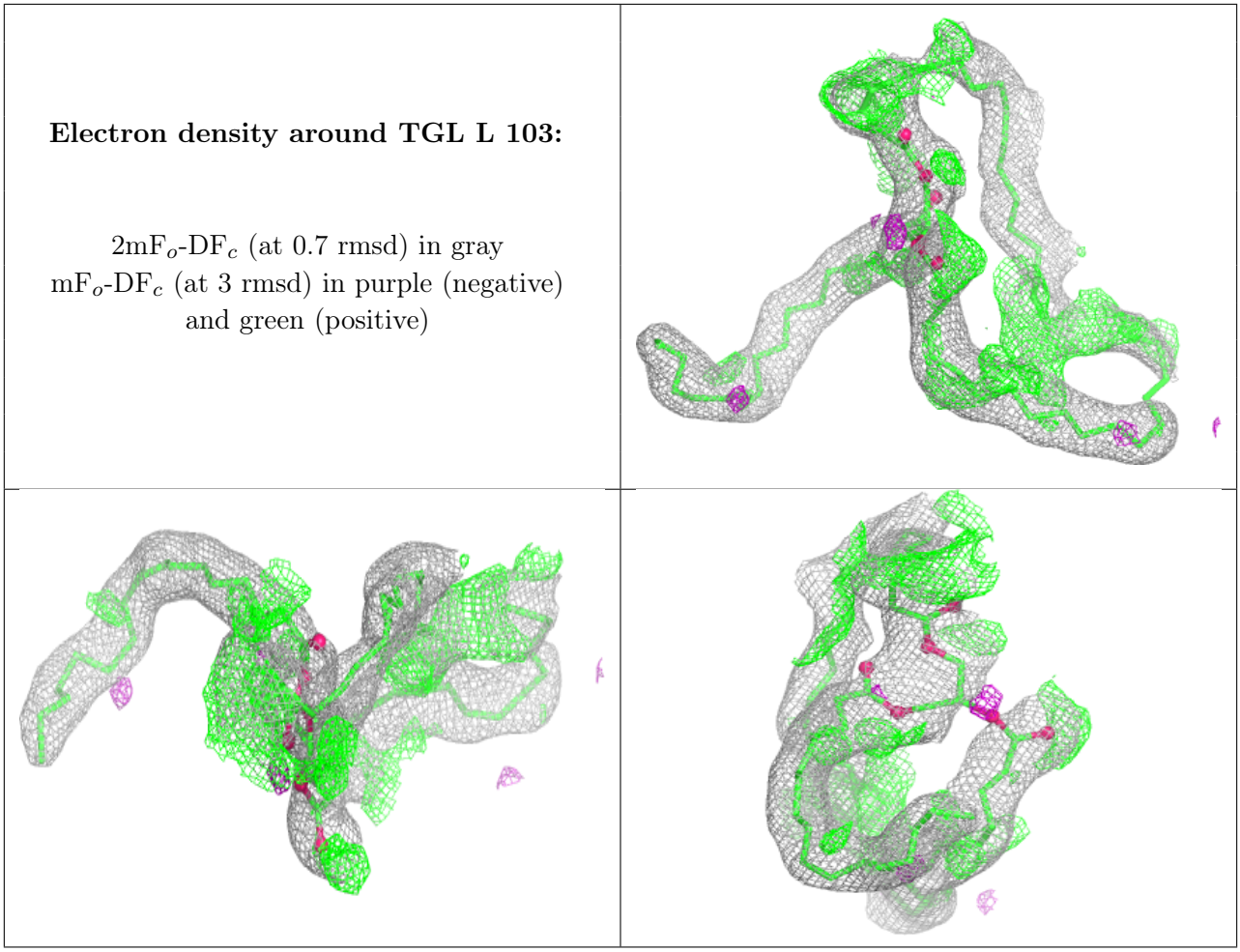
Electron density around TGL Y 103:

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



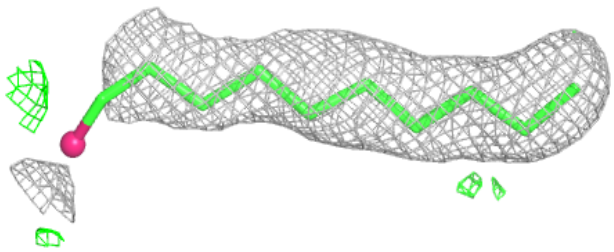
Electron density around TGL L 103:

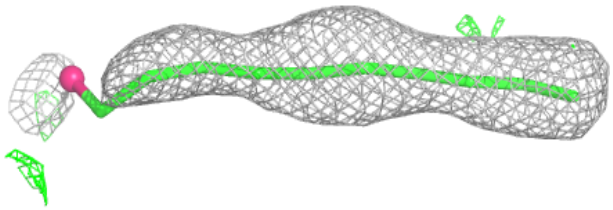
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

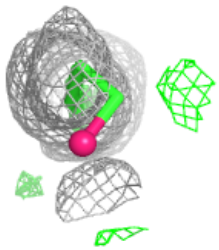


Electron density around DMU X 101:

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

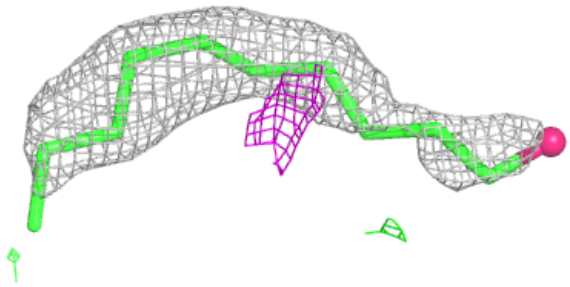


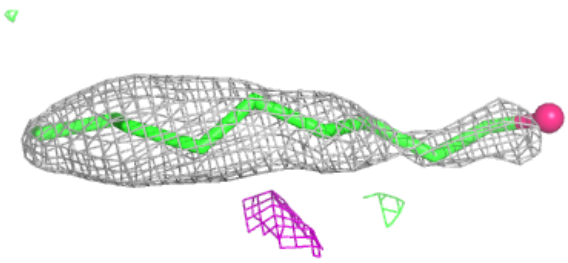


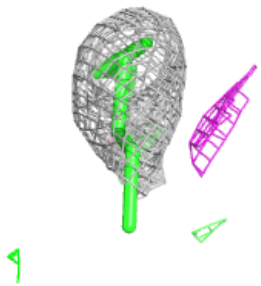


Electron density around DMU X 104:

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

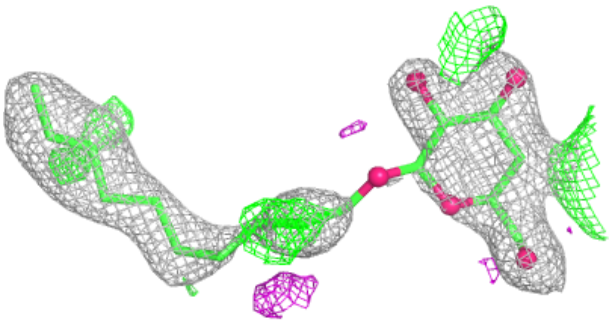


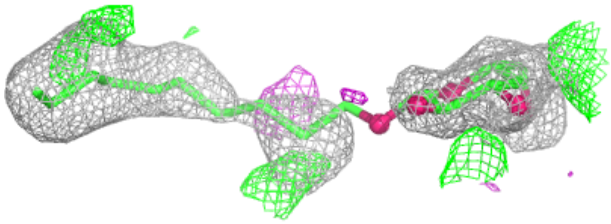


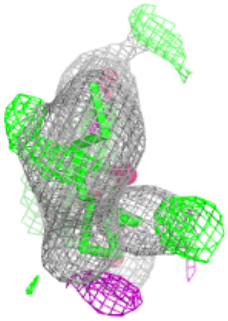


Electron density around DMU J 101:

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

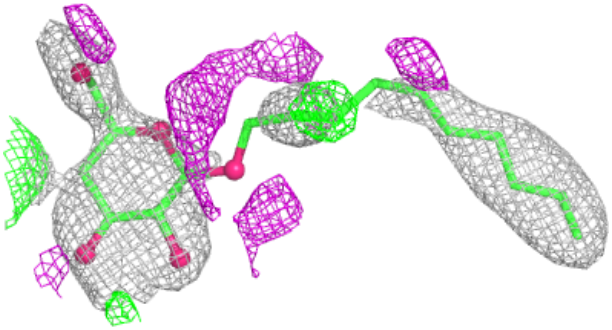


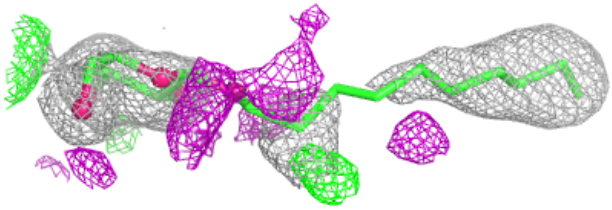


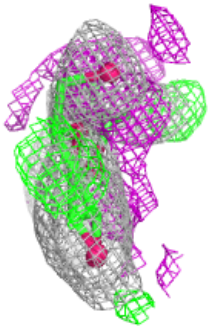


Electron density around DMU W 101:

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

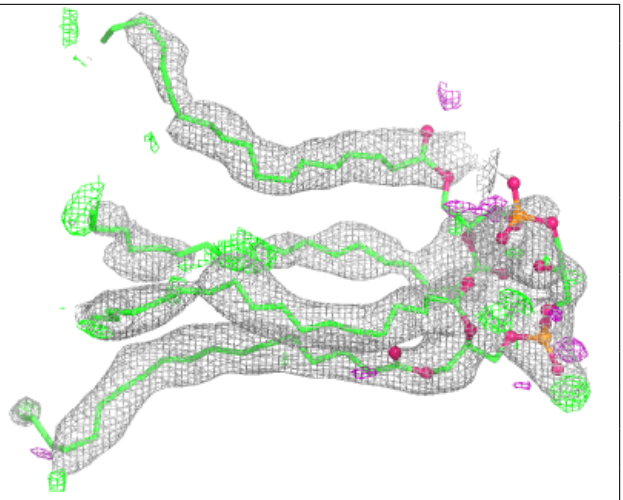


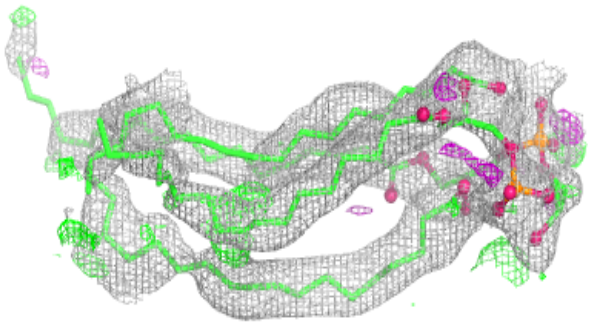


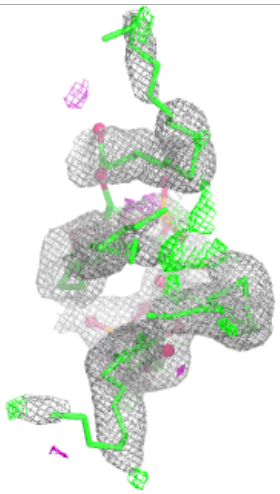


Electron density around CDL C 307:

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

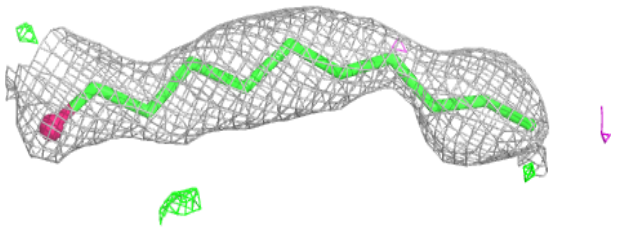


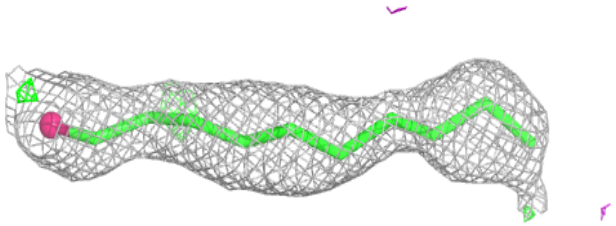


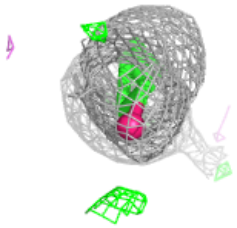


Electron density around DMU K 101:

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

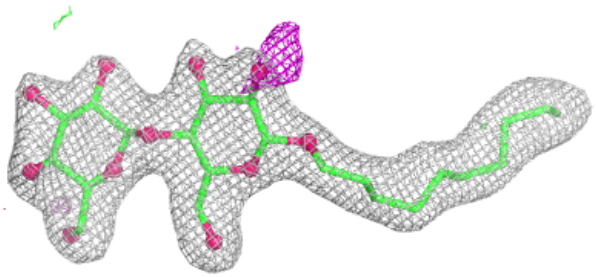


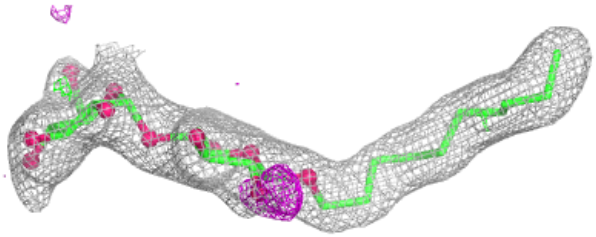


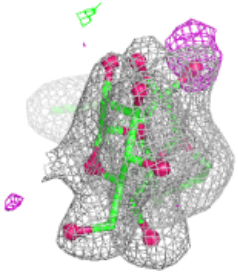


Electron density around DMU Z 101:

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

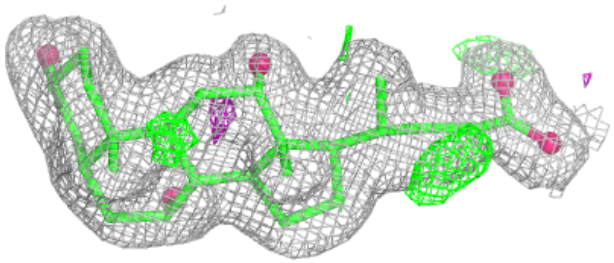


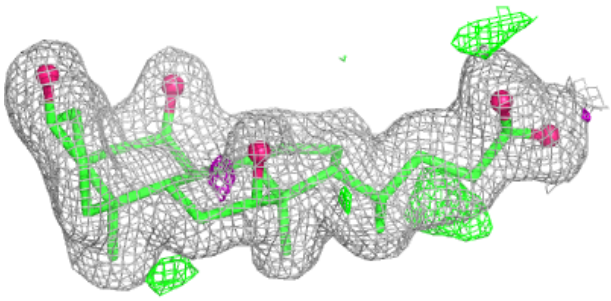


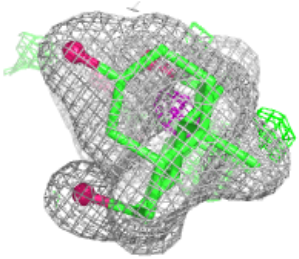


Electron density around CHD C 305:

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

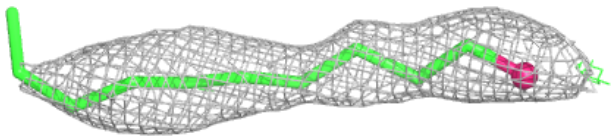


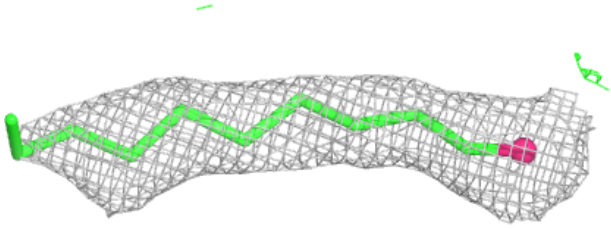


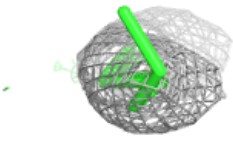


Electron density around DMU B 302:

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

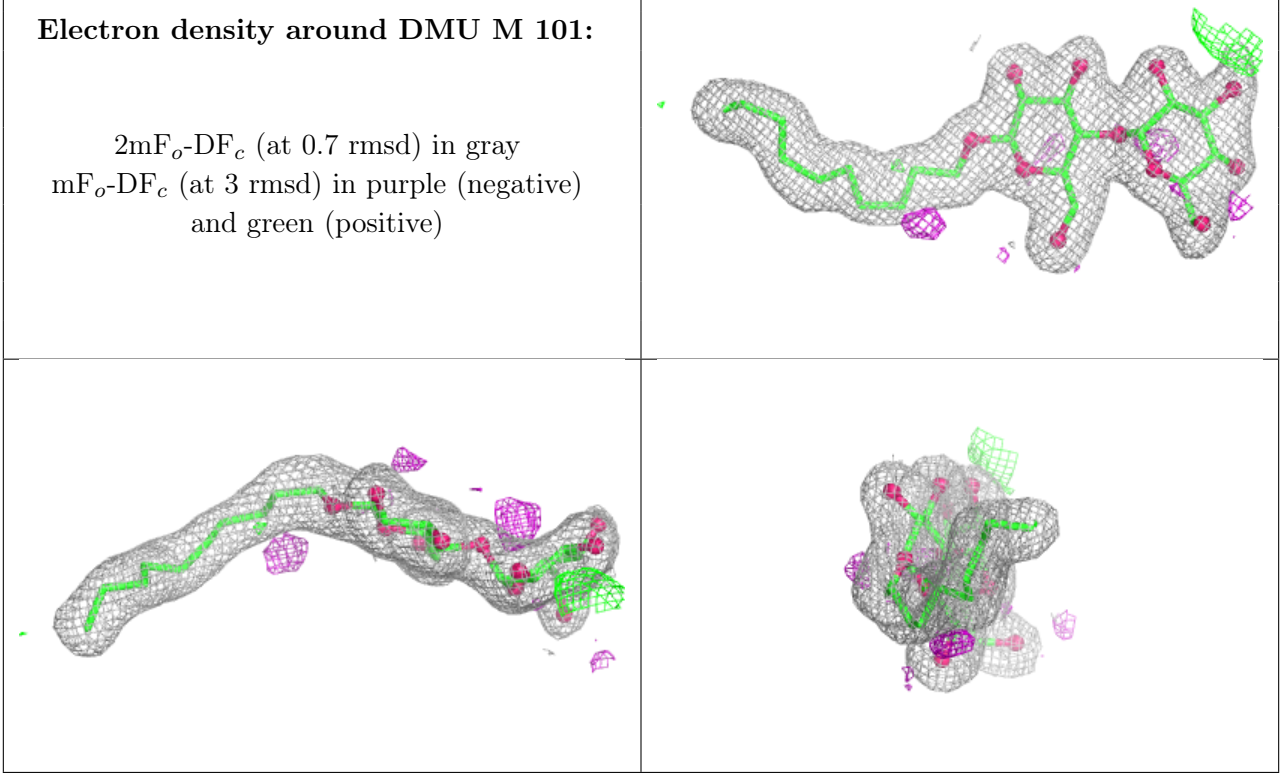






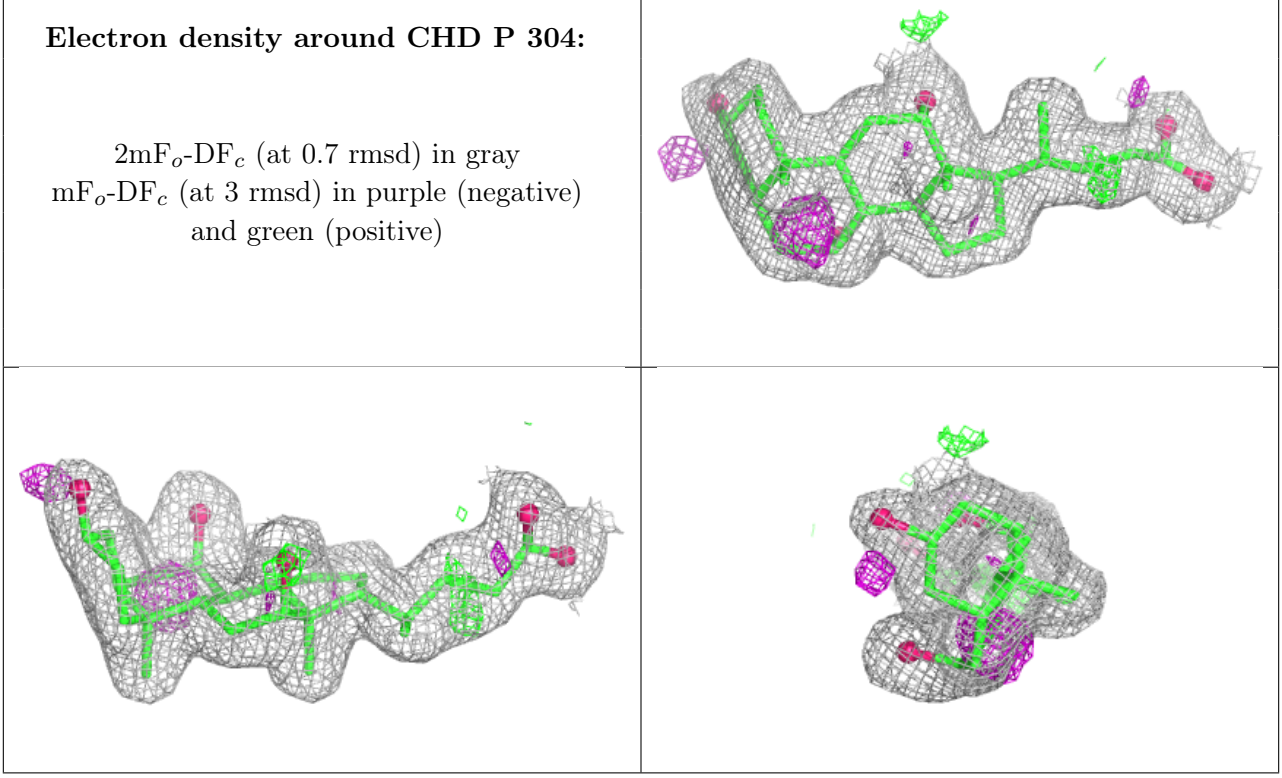
Electron density around DMU M 101:

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



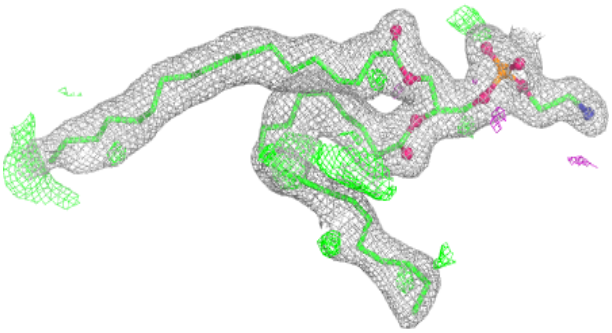
Electron density around CHD P 304:

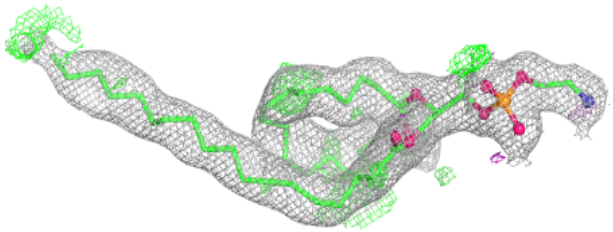
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

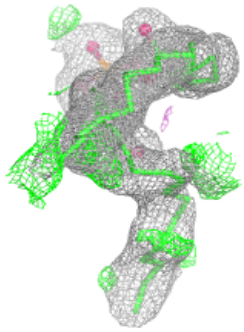


Electron density around PEK C 309:

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

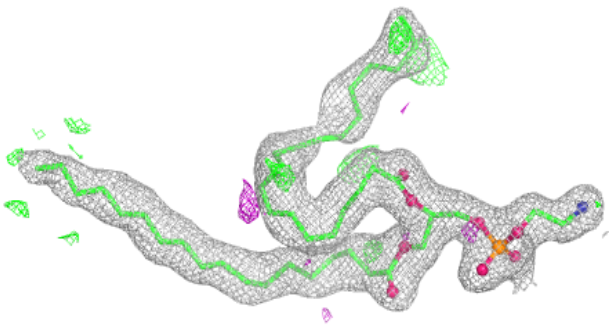


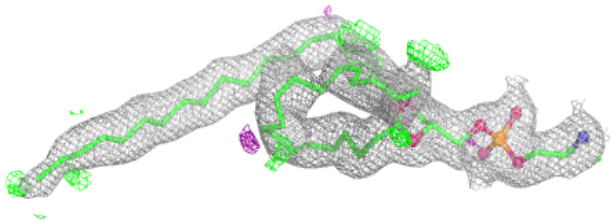


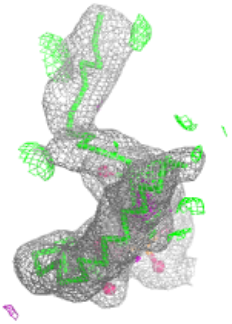


Electron density around PEK P 308:

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

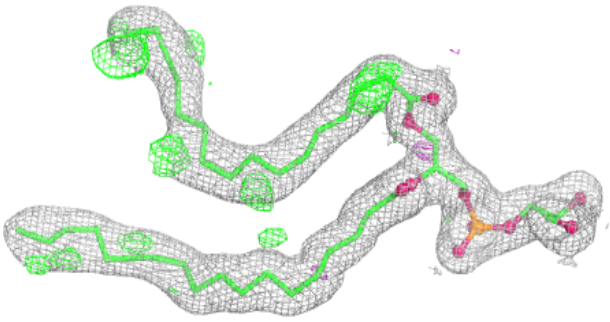


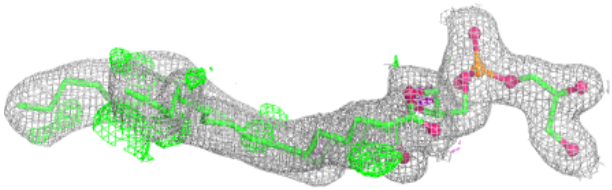


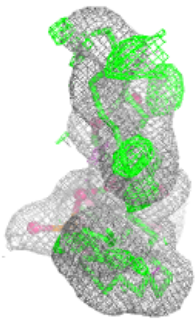


Electron density around PGV N 607:

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

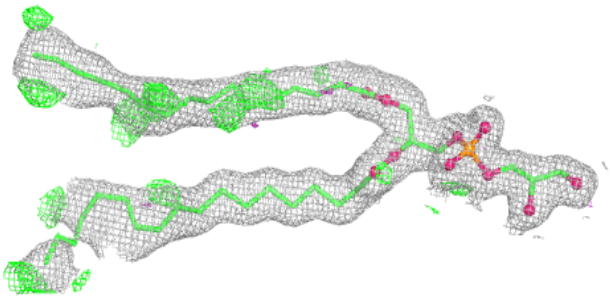


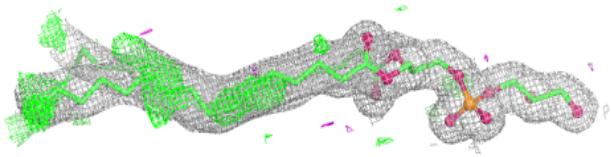




Electron density around PGV C 310:

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

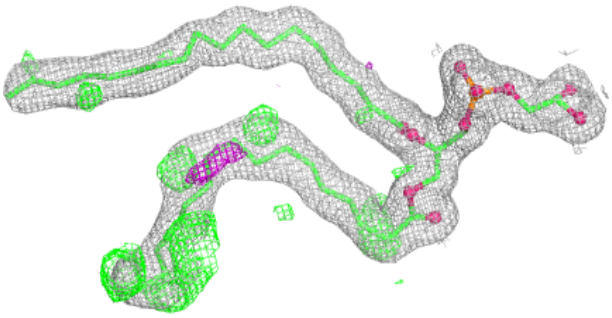


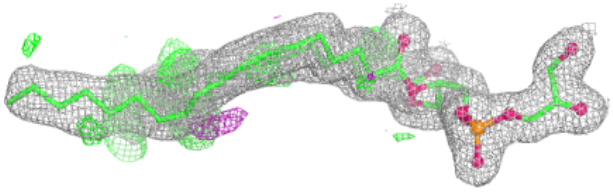




Electron density around PGV A 608:

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

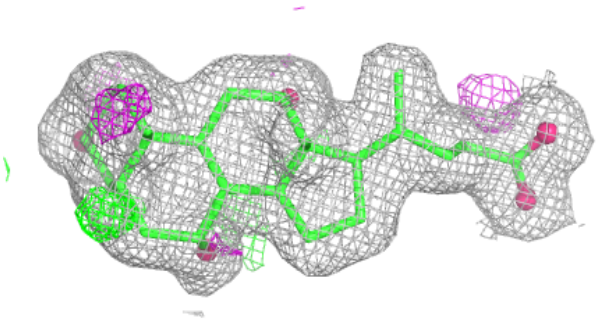


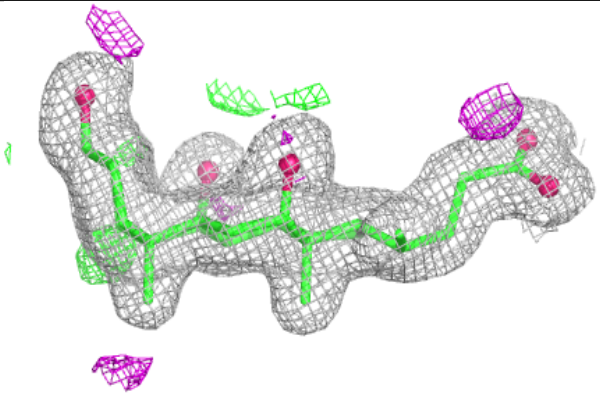


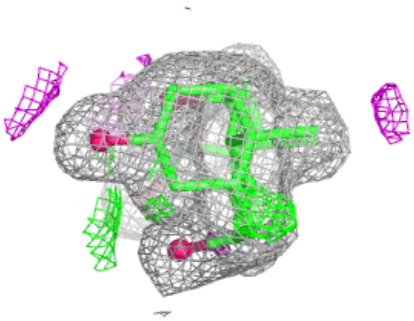


Electron density around CHD T 101:

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

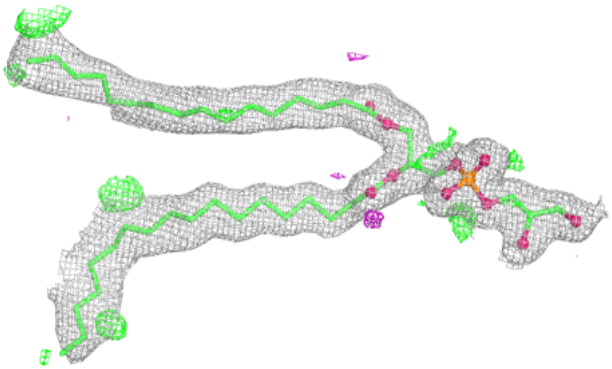


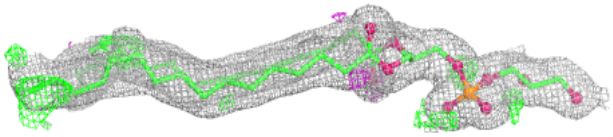


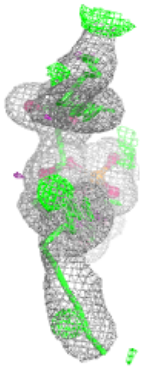


Electron density around PGV P 309:

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

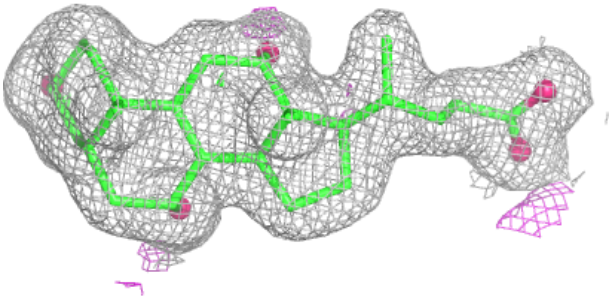


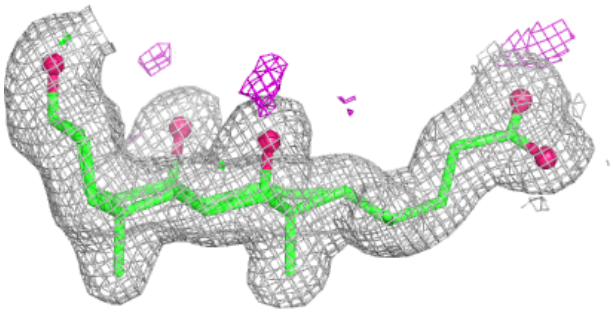


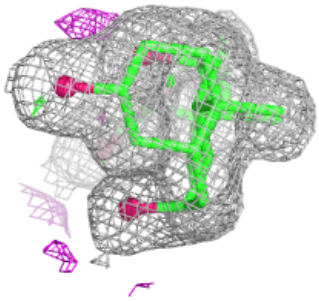


Electron density around CHD G 101:

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

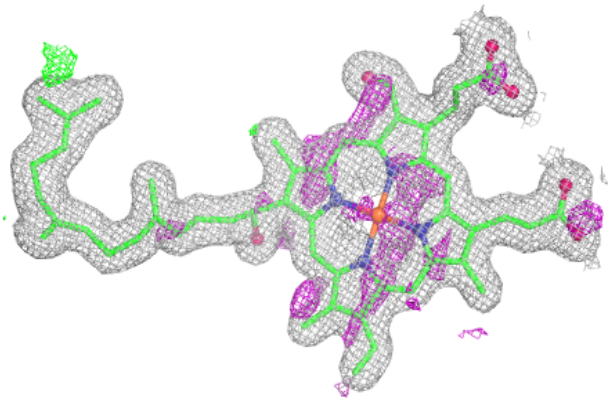


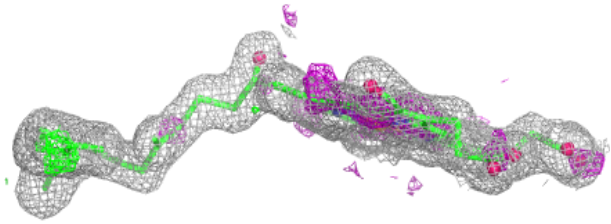


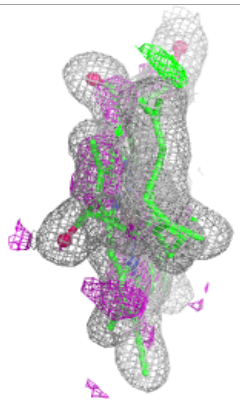


Electron density around HEA A 602:

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

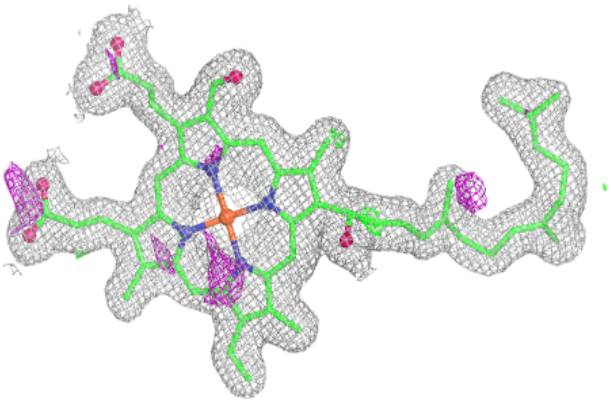


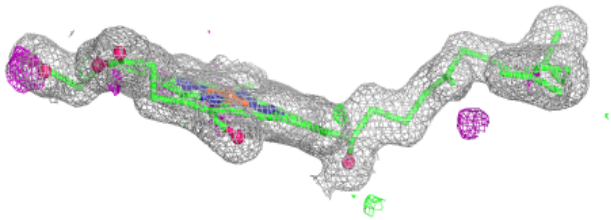


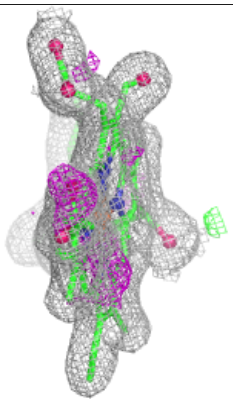


Electron density around HEA N 602:

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

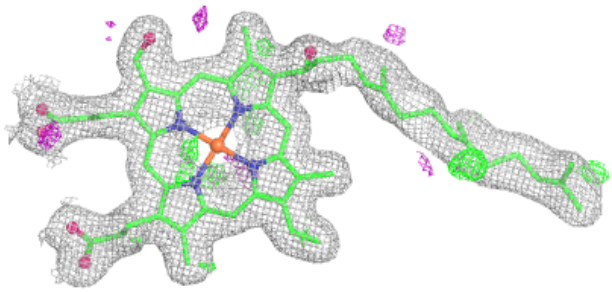


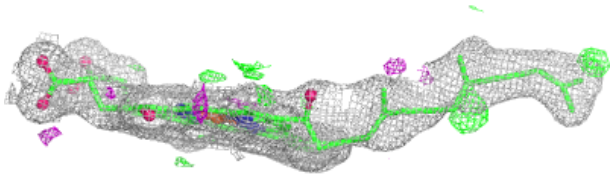


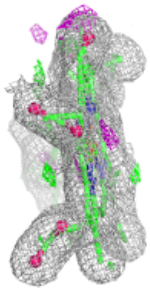


Electron density around HEA N 601 (B):

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

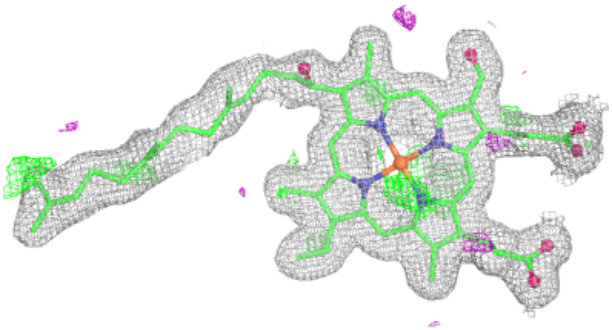


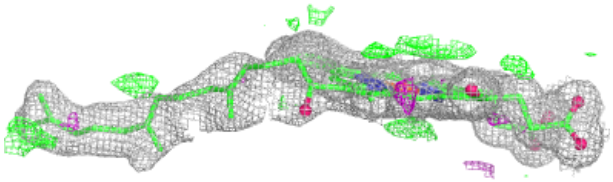


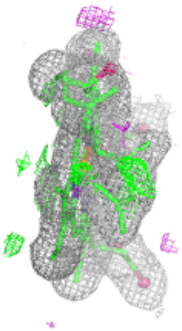


Electron density around HEA A 601 (B):

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

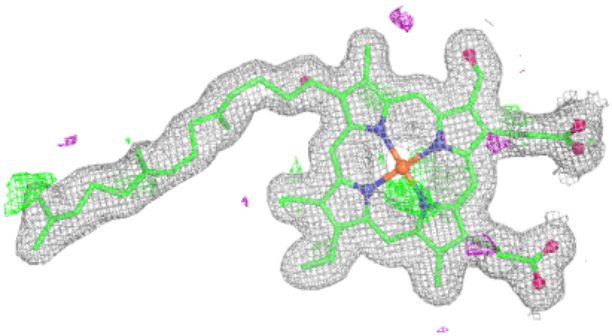


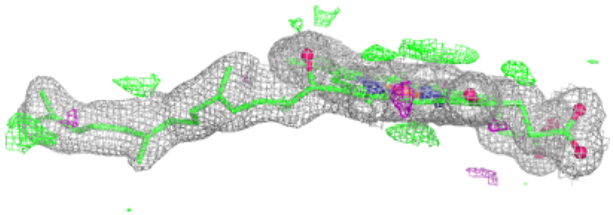


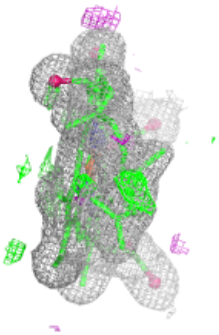


Electron density around HEA A 601 (A):

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

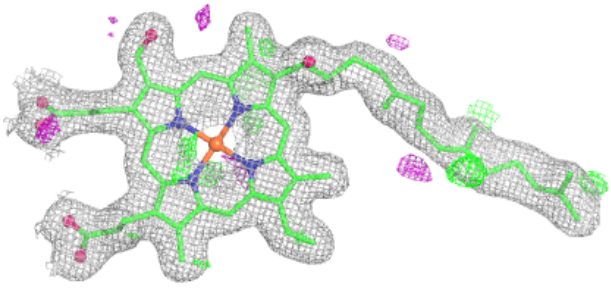


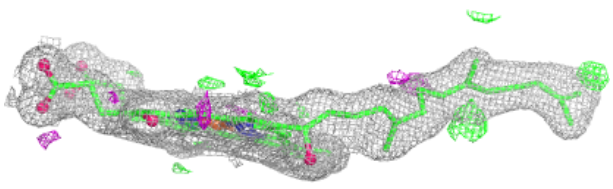


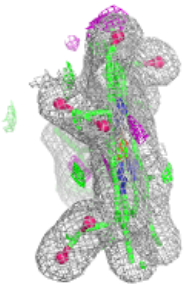


Electron density around HEA N 601 (A):

$2mF_o$-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.