Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 09:55 AM EDT

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

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

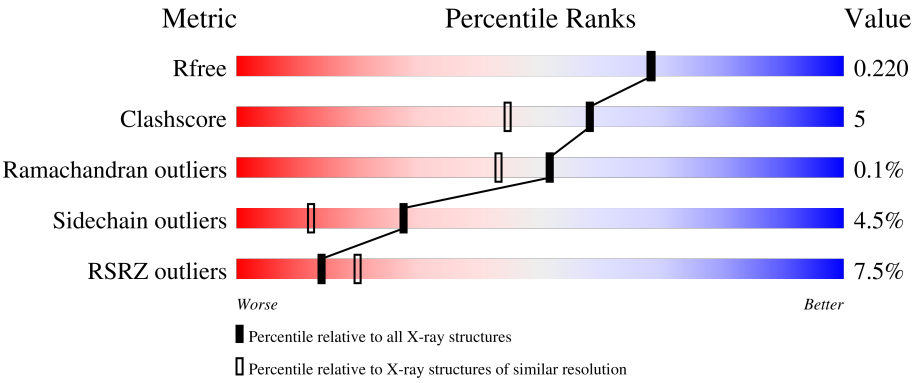
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	514	5% 89% 10%
1	N	514	4% 88% 11%
2	B	227	2% 87% 11%
2	O	227	4% 85% 15%
3	C	261	91% 8%

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

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

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

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

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32695 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			
11	X	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			

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

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

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

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

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

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

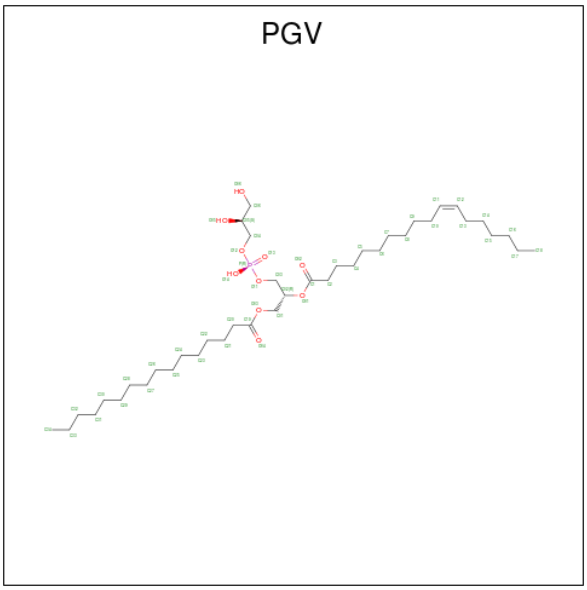
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

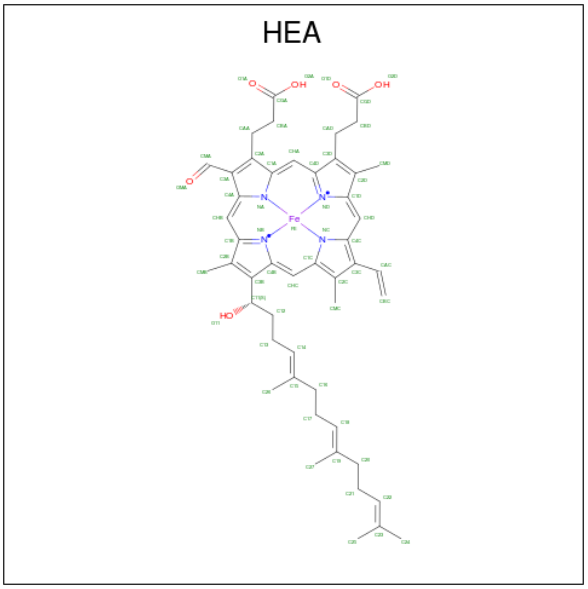
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

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



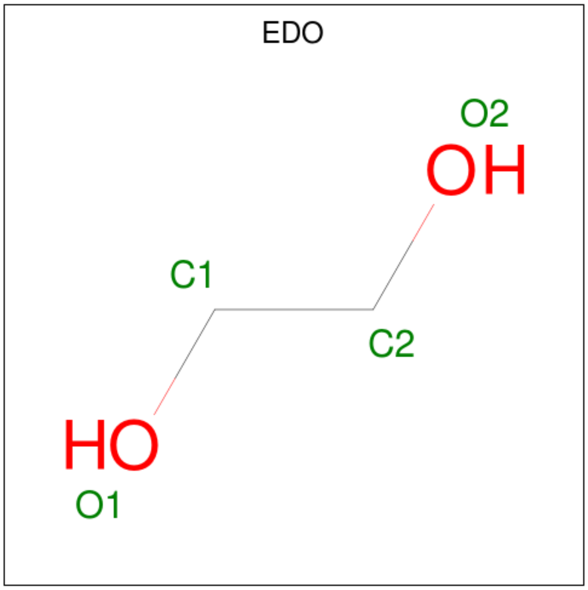
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C O P 51 40 10 1	0	0
17	A	1	Total C O P 51 40 10 1	0	0
17	C	1	Total C O P 51 40 10 1	0	0
17	N	1	Total C O P 51 40 10 1	0	0
17	N	1	Total C O P 51 40 10 1	0	0
17	P	1	Total C O P 51 40 10 1	0	0
17	T	1	Total C O P 51 40 10 1	0	0
17	Z	1	Total C O P 51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

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



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

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



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

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

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

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

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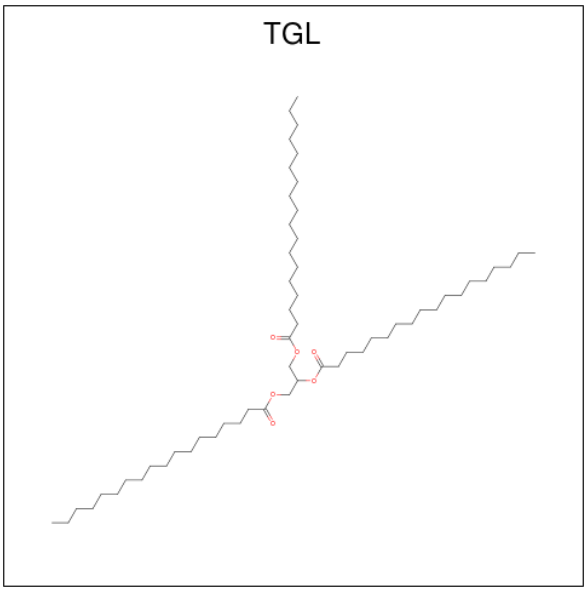
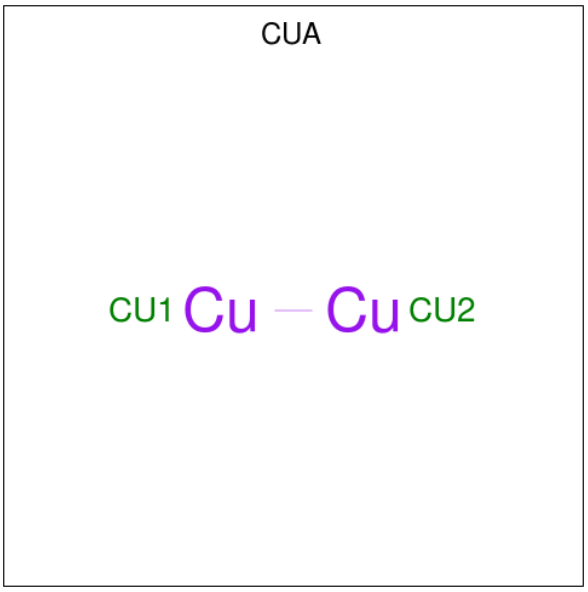
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	U	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4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

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



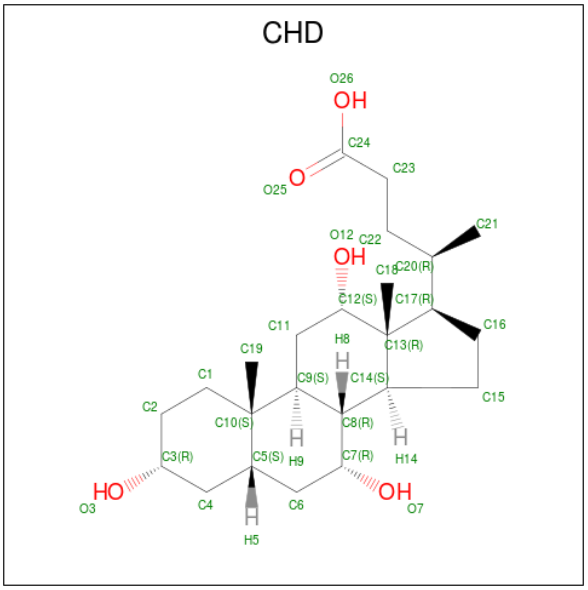
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 63 57 6	0	0
20	D	1	Total C O 63 57 6	0	0
20	L	1	Total C O 63 57 6	0	0
20	N	1	Total C O 63 57 6	0	0
20	Q	1	Total C O 63 57 6	0	0
20	Y	1	Total C O 63 57 6	0	0

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



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

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



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

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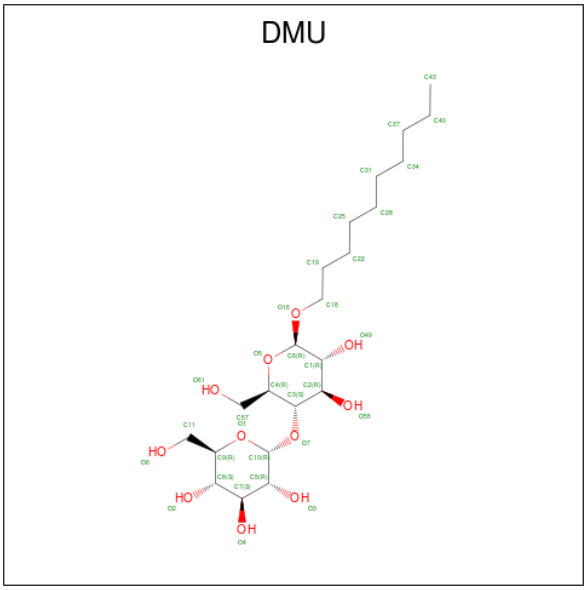
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	T	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0
22	Y	1	Total C O 29 24 5	0	0

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



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

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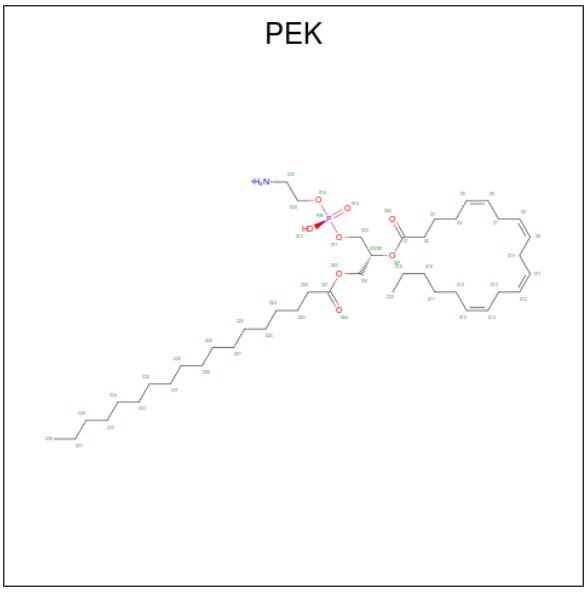
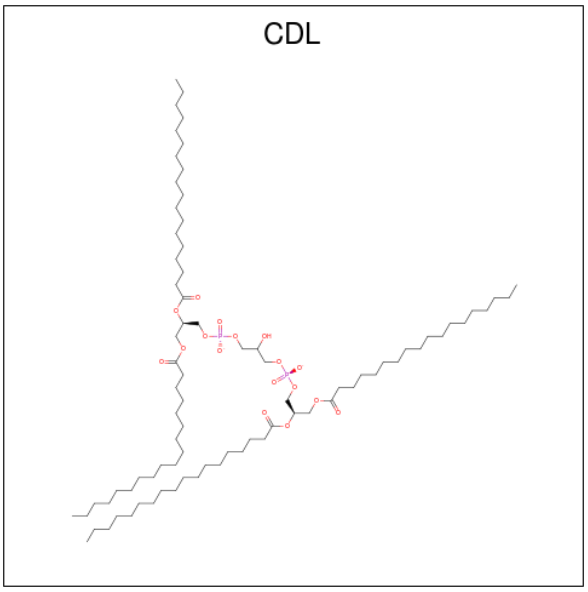
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	M	1	Total C O 33 22 11	0	0
23	P	1	Total C O 33 22 11	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



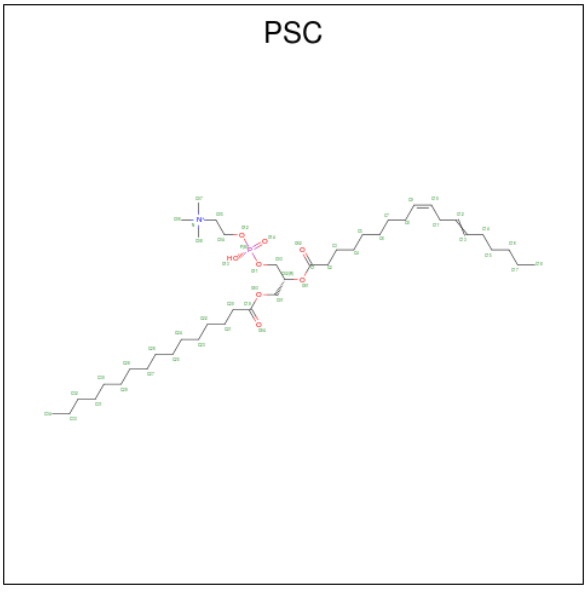
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0

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



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

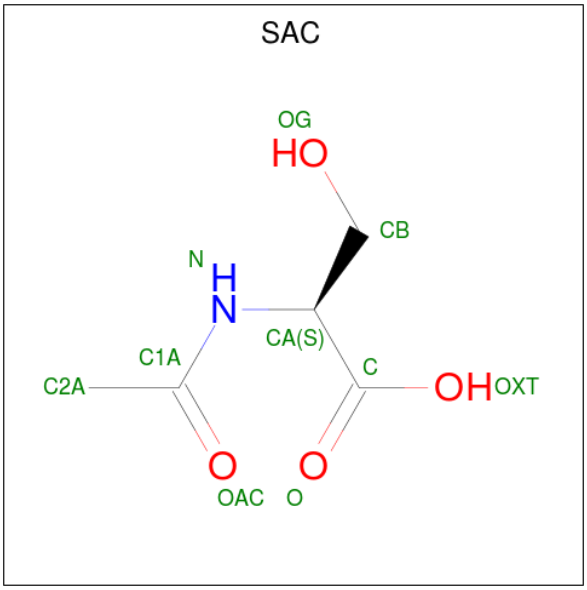


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

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



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

- Molecule 29 is water.

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

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

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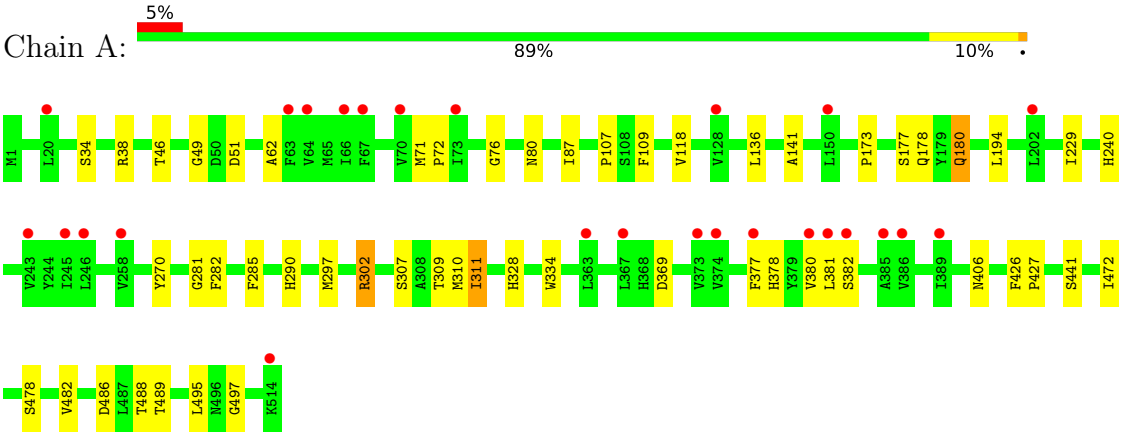
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	W	17	Total O 17 17	0	0
29	X	11	Total O 11 11	0	0
29	Y	18	Total O 18 18	0	0
29	Z	5	Total O 5 5	0	0

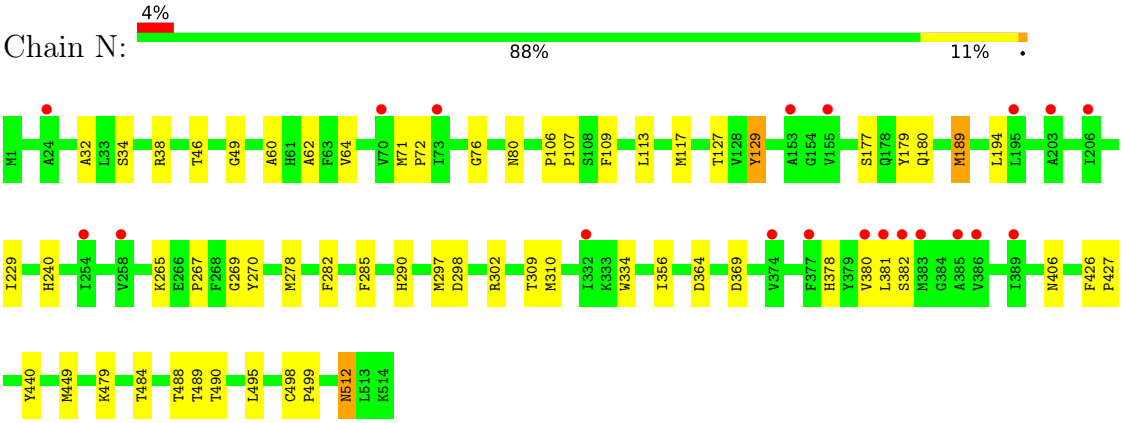
3 Residue-property plots (i)

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

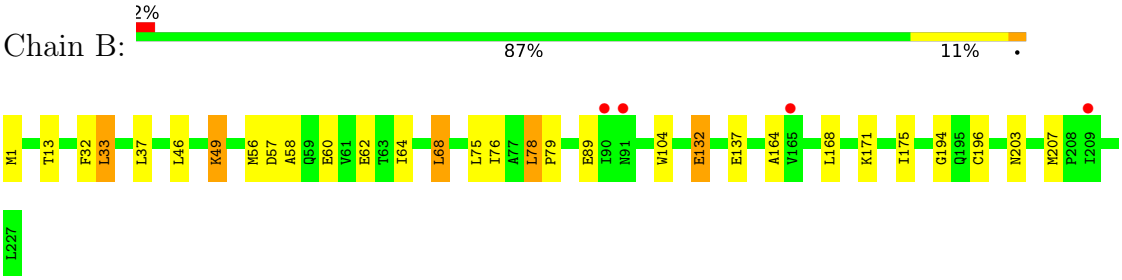
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

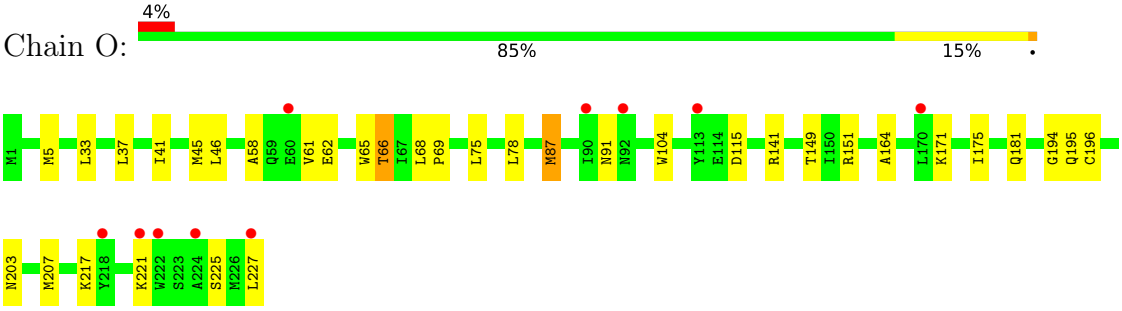


• Molecule 2: Cytochrome c oxidase subunit 2



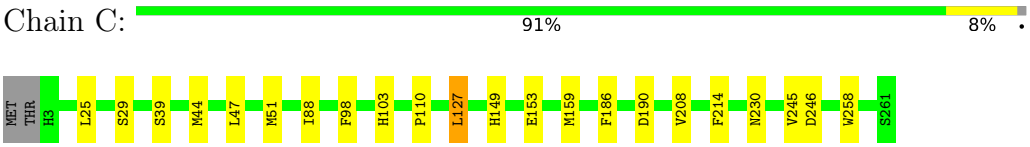
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



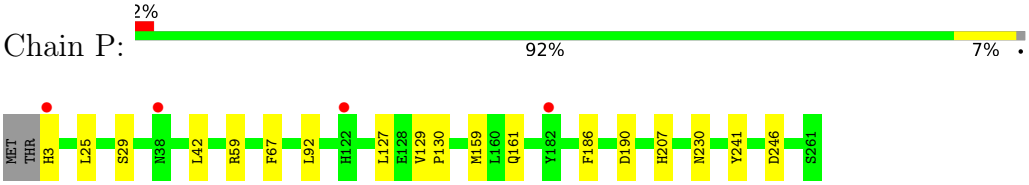
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



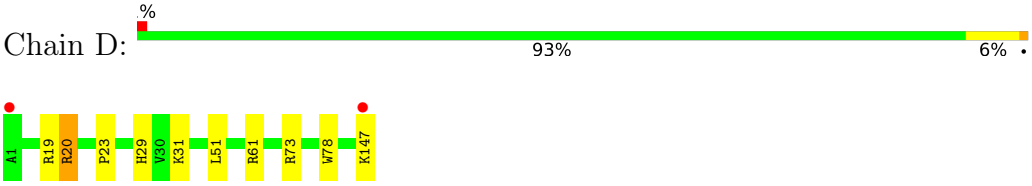
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



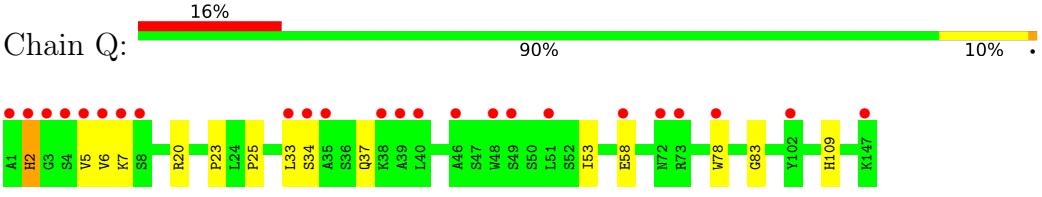
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



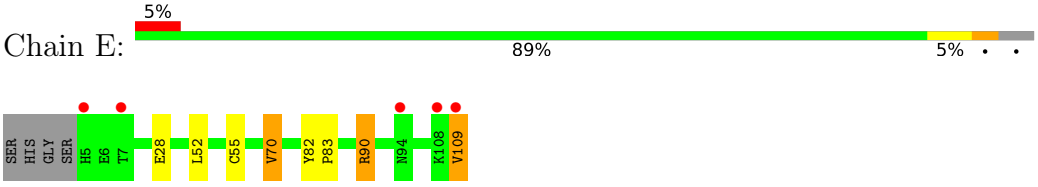
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



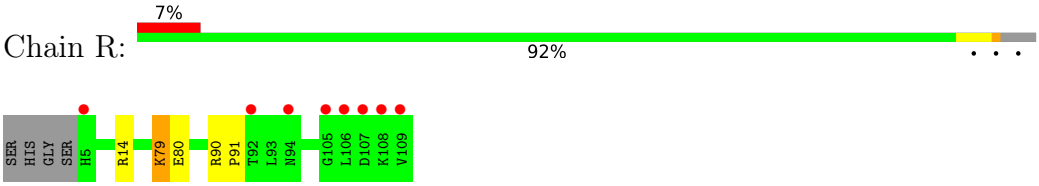
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



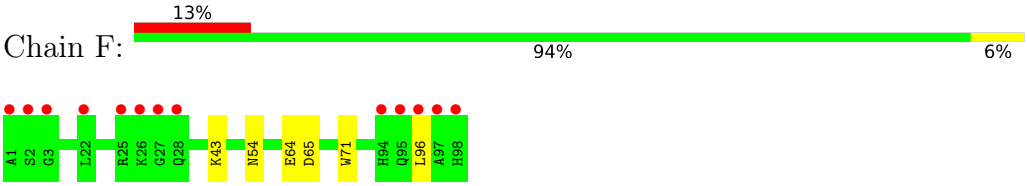
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



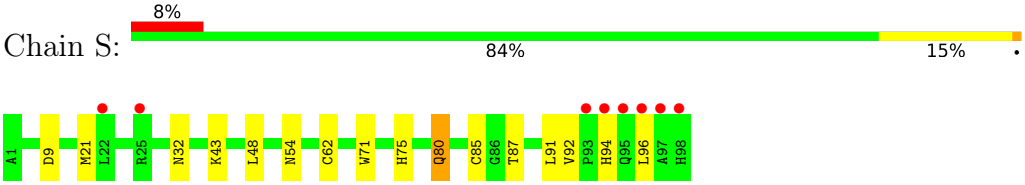
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



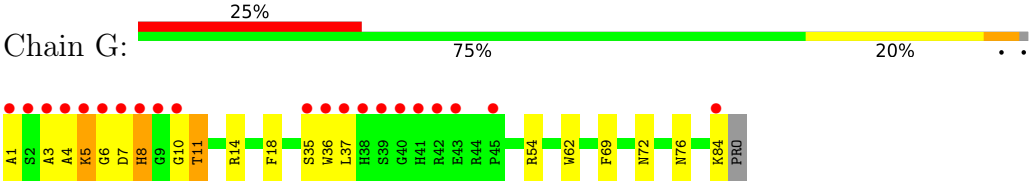
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



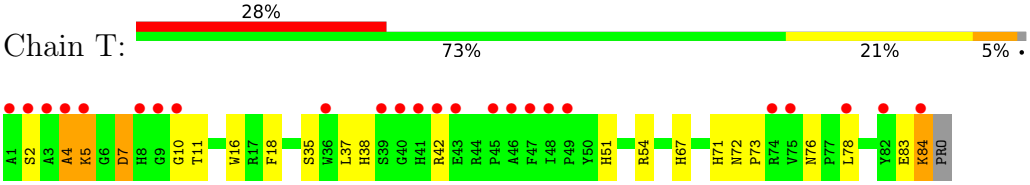
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



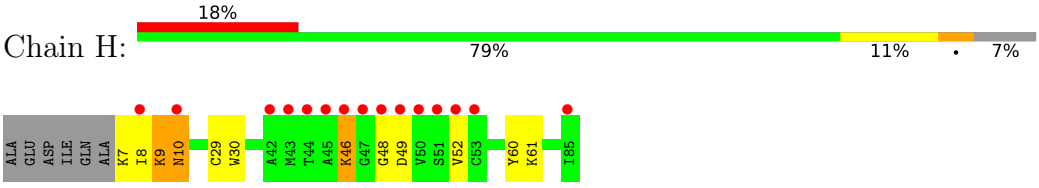
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



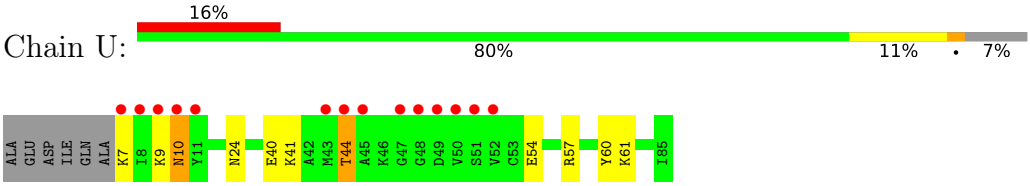
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



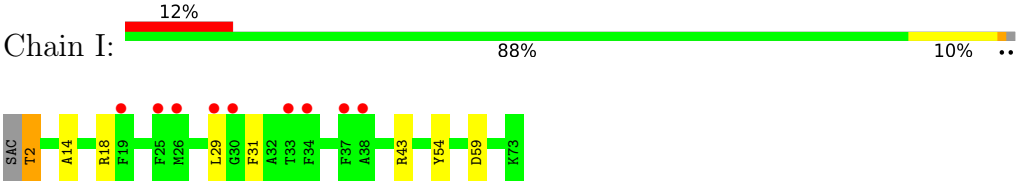
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



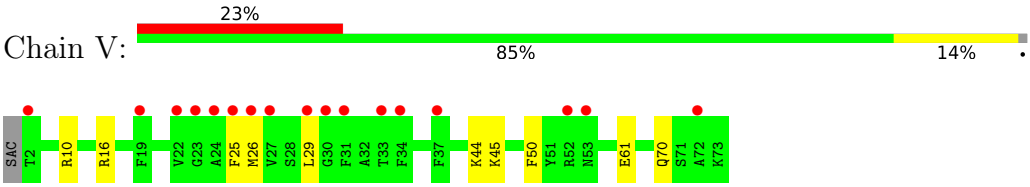
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



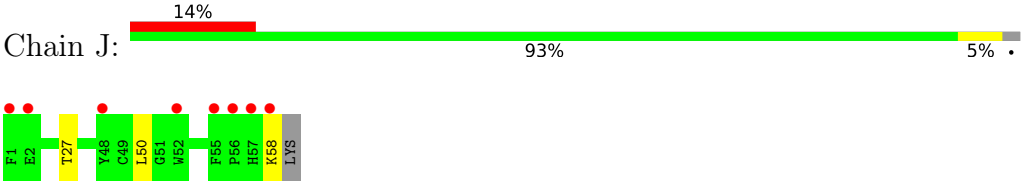
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



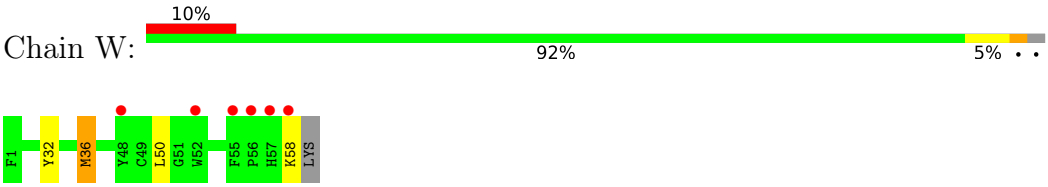
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



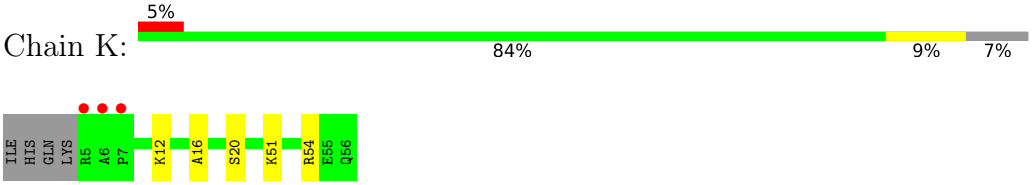
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



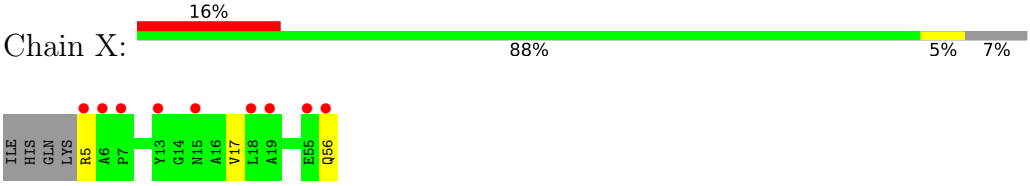
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



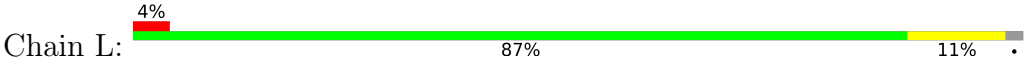
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

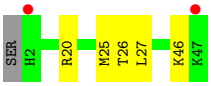
Chain X:



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

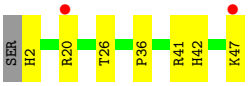
Chain L:





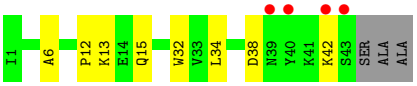
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



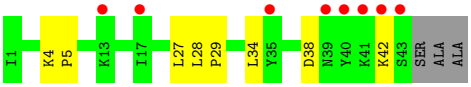
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	178.18Å 182.28Å 208.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93 39.97 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.93) 99.1 (39.97-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.184 , 0.212 0.194 , 0.220	Depositor DCC
R_{free} test set	24681 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32695	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

All (1) bond length outliers are listed below:

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

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	20	ARG	NE-CZ-NH2	-7.15	116.73	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	N	240	HIS	CA-CB-CG	-5.73	103.85	113.60
4	D	20	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	302	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	240	HIS	CA-CB-CG	-5.28	104.62	113.60
1	N	129	TYR	CB-CG-CD2	5.16	124.10	121.00
4	D	20	ARG	CG-CD-NE	-5.07	101.16	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	43	0
1	N	4027	0	4001	58	0
2	B	1824	0	1833	20	0
2	O	1824	0	1833	18	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	13	0
4	D	1214	0	1201	10	0
4	Q	1214	0	1201	9	0
5	E	852	0	845	6	0
5	R	852	0	845	2	0
6	F	748	0	728	2	0
6	S	748	0	728	10	0
7	G	675	0	644	26	0
7	T	675	0	644	20	0
8	H	662	0	623	8	0
8	U	662	0	623	6	0
9	I	592	0	604	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	592	0	604	7	0
10	J	460	0	459	1	0
10	W	460	0	459	1	0
11	K	413	0	393	1	0
11	X	413	0	393	1	0
12	L	380	0	380	2	0
12	Y	380	0	380	3	0
13	M	335	0	352	5	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	102	0	152	4	0
17	C	51	0	76	0	0
17	N	102	0	152	2	0
17	P	51	0	76	0	0
17	T	51	0	76	1	0
17	Z	51	0	76	2	0
18	A	120	0	108	5	0
18	N	120	0	108	9	0
19	A	48	0	72	6	0
19	B	28	0	42	0	0
19	C	20	0	30	0	0
19	D	28	0	42	0	0
19	E	16	0	24	0	0
19	F	16	0	24	1	0
19	G	16	0	24	2	0
19	I	8	0	12	0	0
19	J	16	0	24	2	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	48	0	72	11	0
19	O	8	0	12	0	0
19	P	12	0	18	0	0
19	Q	12	0	18	0	0
19	R	8	0	12	0	0
19	S	24	0	36	4	0
19	T	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	12	0	18	0	0
19	Z	4	0	6	0	0
20	A	63	0	110	1	0
20	D	63	0	110	7	0
20	L	63	0	110	2	0
20	N	63	0	110	0	0
20	Q	63	0	110	5	0
20	Y	63	0	110	2	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	G	29	0	39	1	0
22	J	29	0	39	0	0
22	P	58	0	78	1	0
22	T	29	0	39	7	0
22	W	29	0	39	0	0
22	Y	29	0	39	4	0
23	C	66	0	84	1	0
23	G	33	0	42	2	0
23	M	33	0	41	0	0
23	P	33	0	42	0	0
23	Z	33	0	42	1	0
24	C	159	0	231	8	0
24	P	159	0	231	6	0
25	C	200	0	312	15	0
25	P	100	0	156	4	0
25	T	100	0	156	3	0
26	E	52	0	80	5	0
26	O	52	0	80	5	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	2	0
28	V	9	0	8	1	0
29	A	190	0	0	0	0
29	B	125	0	0	0	0
29	C	96	0	0	7	0
29	D	68	0	0	0	0
29	E	53	0	0	0	0
29	F	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	G	35	0	0	0	0
29	H	39	0	0	1	0
29	I	24	0	0	0	0
29	J	17	0	0	0	0
29	K	9	0	0	0	0
29	L	21	0	0	2	0
29	M	14	0	0	0	0
29	N	179	0	0	7	0
29	O	85	0	0	3	0
29	P	80	0	0	1	0
29	Q	46	0	0	1	0
29	R	46	0	0	0	0
29	S	64	0	0	2	0
29	T	23	0	0	4	0
29	U	30	0	0	1	0
29	V	16	0	0	0	0
29	W	17	0	0	0	0
29	X	11	0	0	0	0
29	Y	18	0	0	1	0
29	Z	5	0	0	1	0
All	All	32695	0	32113	307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:MET:HG3	29:C:496:HOH:O	1.38	1.19
9:I:2:THR:N	28:I:101:SAC:HG	1.47	1.12
1:A:270:TYR:H	19:A:614:EDO:H11	1.21	1.04
24:P:305:PEK:C38	25:T:102:CDL:H271	1.91	1.00
7:T:73:PRO:HG3	7:T:84:LYS:HE2	1.49	0.94
1:N:270:TYR:H	19:N:614:EDO:H21	1.31	0.93
1:N:270:TYR:HB2	19:N:614:EDO:H11	1.51	0.93
7:G:72:ASN:H	7:G:76:ASN:HD22	1.15	0.89
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.69	0.88
24:P:305:PEK:H383	25:T:102:CDL:H271	1.59	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.28	0.82
25:C:306:CDL:OA5	25:C:306:CDL:H1	1.78	0.81
6:S:94:HIS:HB2	29:S:2301:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:267:PRO:O	19:N:614:EDO:H12	1.79	0.81
22:T:104:CHD:H22	29:T:203:HOH:O	1.80	0.81
3:P:246:ASP:HB2	29:P:474:HOH:O	1.81	0.80
18:N:607:HEA:HMC1	18:N:607:HEA:HBC1	1.63	0.78
7:G:11:TPO:HG23	7:G:14:ARG:H	1.46	0.78
24:P:304:PEK:HN2	7:T:76:ASN:HD21	1.32	0.77
8:U:10:ASN:HA	29:U:1603:HOH:O	1.84	0.77
7:G:10:GLY:HA2	1:N:177:SER:HB2	1.66	0.76
6:S:94:HIS:CB	29:S:2301:HOH:O	2.33	0.76
3:C:149:HIS:NE2	23:G:1302:DMU:H5	2.01	0.76
1:N:270:TYR:N	19:N:614:EDO:H21	2.01	0.76
24:C:303:PEK:HN2	7:G:76:ASN:HD21	1.32	0.75
19:N:613:EDO:H11	29:N:793:HOH:O	1.86	0.75
9:V:50:PHE:O	19:V:103:EDO:H21	1.87	0.75
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.75
1:N:297:MET:HG3	1:N:302:ARG:HG3	1.68	0.74
7:T:5:LYS:NZ	29:T:201:HOH:O	1.99	0.73
7:G:4:ALA:HB1	1:N:194:LEU:CD2	2.20	0.72
1:A:46:THR:HG22	1:A:49:GLY:H	1.55	0.71
1:A:270:TYR:H	19:A:614:EDO:C1	2.00	0.71
1:A:486:ASP:OD1	4:D:19:ARG:HD2	1.90	0.70
8:H:9:LYS:HZ2	8:H:9:LYS:HA	1.56	0.70
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.21	0.70
8:U:24:ASN:HD21	19:U:1501:EDO:C1	2.04	0.70
8:U:24:ASN:HD21	19:U:1501:EDO:H11	1.58	0.68
3:C:258:TRP:CD1	25:C:312:CDL:H562	2.28	0.68
1:A:51:ASP:OD1	1:A:441:SER:OG	2.12	0.68
20:Q:201:TGL:HG31	20:Q:201:TGL:HC31	1.75	0.68
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.77	0.66
2:O:141:ARG:H	9:V:70:GLN:NE2	1.94	0.66
17:Z:102:PGV:H031	29:Z:201:HOH:O	1.96	0.66
7:G:72:ASN:H	7:G:76:ASN:ND2	1.92	0.65
25:C:312:CDL:H371	29:C:488:HOH:O	1.97	0.65
22:P:308:CHD:H183	22:P:308:CHD:H212	1.79	0.64
1:A:281:GLY:C	7:T:4:ALA:HB3	2.18	0.64
29:N:743:HOH:O	20:Q:201:TGL:HB32	1.98	0.63
3:C:127:LEU:CD1	25:C:312:CDL:H552	2.29	0.63
1:A:194:LEU:HD21	7:T:4:ALA:HB1	1.81	0.63
3:C:258:TRP:CE2	25:C:312:CDL:H542	2.34	0.63
1:N:270:TYR:H	19:N:614:EDO:C2	2.11	0.62
18:A:607:HEA:HBC1	18:A:607:HEA:HMC1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:46:THR:HG22	1:N:49:GLY:H	1.64	0.62
7:G:4:ALA:HB1	1:N:194:LEU:HD23	1.82	0.61
12:Y:41:ARG:HH22	22:Y:102:CHD:H191	1.65	0.61
8:H:46:LYS:NZ	29:H:101:HOH:O	2.32	0.61
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.35	0.61
17:A:604:PGV:H11	13:M:15:GLN:HE22	1.66	0.61
1:N:76:GLY:O	1:N:80:ASN:HB2	2.00	0.61
7:T:78:LEU:HD22	7:T:84:LYS:HA	1.81	0.60
8:H:9:LYS:HA	8:H:9:LYS:CE	2.31	0.60
2:O:62:GLU:O	2:O:66:THR:HB	2.01	0.60
22:T:104:CHD:H192	29:T:203:HOH:O	2.02	0.59
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.37	0.59
24:C:304:PEK:H052	19:S:2206:EDO:H11	1.83	0.59
7:T:71:HIS:NE2	7:T:84:LYS:HD2	2.16	0.59
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.38	0.59
4:Q:5:VAL:HG13	4:Q:5:VAL:O	2.03	0.59
1:A:87:ILE:O	1:A:173:PRO:HD3	2.03	0.58
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.85	0.58
29:L:220:HOH:O	13:M:32:TRP:HH2	1.85	0.58
18:N:606:HEA:HMC1	18:N:606:HEA:HBC1	1.85	0.58
19:A:616:EDO:H21	2:B:58:ALA:HB3	1.86	0.58
7:G:8:HIS:H	7:G:8:HIS:CD2	2.21	0.58
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.33	0.57
3:C:127:LEU:HD13	25:C:312:CDL:H552	1.86	0.57
24:P:305:PEK:H382	25:T:102:CDL:H271	1.84	0.57
4:D:78:TRP:N	20:D:201:TGL:HB32	2.20	0.57
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.19	0.56
26:O:302:PSC:H081	9:V:10:ARG:HE	1.71	0.56
2:O:141:ARG:H	9:V:70:GLN:HE22	1.52	0.56
1:A:297:MET:SD	1:A:302:ARG:HG2	2.46	0.56
26:E:201:PSC:H32	9:I:14:ALA:CB	2.35	0.56
3:C:98:PHE:CD2	24:C:315:PEK:H12	2.41	0.56
1:N:46:THR:HG21	1:N:49:GLY:HA2	1.88	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.55
1:N:62:ALA:HB2	18:N:607:HEA:HBD1	1.89	0.55
1:N:488:THR:HB	1:N:495:LEU:HD13	1.89	0.55
7:T:67:HIS:NE2	7:T:84:LYS:HB2	2.22	0.55
1:N:267:PRO:O	19:N:614:EDO:C1	2.53	0.54
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.90	0.54
19:N:619:EDO:H21	6:S:32:ASN:HD21	1.72	0.54
25:C:312:CDL:H351	29:C:488:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.89	0.54
7:T:73:PRO:CG	7:T:84:LYS:HE2	2.32	0.54
25:C:312:CDL:H381	29:O:422:HOH:O	2.07	0.53
4:D:78:TRP:H	20:D:201:TGL:HB32	1.74	0.53
1:N:34:SER:HB2	18:N:607:HEA:C2B	2.39	0.53
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.43	0.53
22:G:1305:CHD:H3	2:O:66:THR:HG21	1.90	0.53
29:N:782:HOH:O	19:S:2201:EDO:C1	2.55	0.53
2:B:57:ASP:H	26:E:201:PSC:H222	1.74	0.53
10:W:32:TYR:CE1	10:W:36:MET:HG3	2.44	0.53
1:N:270:TYR:CB	19:N:614:EDO:H11	2.33	0.53
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.44	0.52
1:A:482:VAL:O	19:A:613:EDO:H21	2.08	0.52
11:K:16:ALA:O	11:K:20:SER:OG	2.26	0.52
24:C:304:PEK:H011	24:C:304:PEK:H21	1.91	0.52
4:D:78:TRP:HA	20:D:201:TGL:HB52	1.91	0.52
7:T:16:TRP:HE1	22:T:104:CHD:H152	1.74	0.52
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.92	0.52
22:T:104:CHD:H151	22:T:104:CHD:O7	2.10	0.52
7:G:8:HIS:CB	1:N:179:TYR:OH	2.58	0.52
12:L:25:MET:HG2	20:L:101:TGL:HA71	1.91	0.52
25:C:312:CDL:C35	29:C:488:HOH:O	2.58	0.51
8:U:24:ASN:HD21	19:U:1501:EDO:H12	1.75	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.51
7:G:8:HIS:HB3	1:N:179:TYR:OH	2.10	0.51
22:Y:102:CHD:H41	29:Y:218:HOH:O	2.10	0.51
1:A:62:ALA:HB2	18:A:607:HEA:HBD1	1.91	0.51
17:A:604:PGV:H11	13:M:15:GLN:NE2	2.25	0.51
26:E:201:PSC:H32	9:I:14:ALA:HA	1.93	0.51
24:C:303:PEK:C12	24:C:303:PEK:H162	2.41	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.50
1:A:46:THR:HG21	1:A:49:GLY:HA2	1.91	0.50
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.76	0.50
8:H:9:LYS:HD3	8:H:10:ASN:H	1.77	0.50
7:G:5:LYS:HB3	1:N:278:MET:CG	2.42	0.50
3:C:246:ASP:HB2	29:C:479:HOH:O	2.12	0.50
1:N:406:ASN:HD21	17:Z:102:PGV:H71	1.77	0.50
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.93	0.50
3:C:153:GLU:OE2	7:G:11:TPO:HG22	2.11	0.49
22:C:302:CHD:H183	22:C:302:CHD:H212	1.93	0.49
7:G:69:PHE:O	19:G:1303:EDO:H11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:MET:HA	26:E:201:PSC:H222	1.94	0.49
2:O:227:LEU:HD12	2:O:227:LEU:OXT	2.13	0.49
29:N:782:HOH:O	19:S:2201:EDO:H11	2.12	0.49
1:A:282:PHE:N	7:T:4:ALA:HB3	2.27	0.49
1:N:113:LEU:HB2	20:Y:101:TGL:H323	1.94	0.49
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.66	0.49
13:Z:27:LEU:HD22	23:Z:101:DMU:H14	1.94	0.49
20:D:201:TGL:HB42	20:D:201:TGL:HG11	1.94	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
3:C:127:LEU:HD11	25:C:312:CDL:H552	1.95	0.48
9:I:2:THR:N	28:I:101:SAC:OG	2.28	0.48
6:S:92:VAL:O	6:S:92:VAL:HG23	2.13	0.48
1:N:302:ARG:HD3	29:N:728:HOH:O	2.12	0.48
3:P:59:ARG:HA	25:P:307:CDL:H512	1.94	0.48
9:V:25:PHE:CD2	9:V:26:MET:CE	2.97	0.48
22:Y:102:CHD:H192	22:Y:102:CHD:H3	1.95	0.48
1:A:178:GLN:HG3	7:T:7:ASP:HB2	1.93	0.48
3:C:29:SER:HB2	19:J:1104:EDO:H12	1.95	0.48
24:C:303:PEK:C12	24:C:303:PEK:C16	2.91	0.48
2:B:49:LYS:O	4:D:20:ARG:NH2	2.42	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.95	0.48
1:N:298:ASP:OD2	17:N:616:PGV:O06	2.27	0.48
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.96	0.48
1:N:449:MET:SD	2:O:5:MET:HG2	2.54	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
1:N:512:ASN:C	1:N:512:ASN:HD22	2.16	0.48
12:Y:42:HIS:ND1	22:Y:102:CHD:H151	2.29	0.48
10:J:27:THR:HG22	19:J:1101:EDO:H22	1.94	0.48
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.96	0.48
7:G:6:GLY:HA3	1:N:189:MET:HG2	1.96	0.48
5:R:79:LYS:HE3	5:R:79:LYS:HA	1.94	0.48
1:N:297:MET:CG	1:N:302:ARG:HG3	2.40	0.47
7:G:62:TRP:CD1	19:G:1303:EDO:H22	2.49	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.79	0.47
3:C:258:TRP:CZ2	25:C:312:CDL:H542	2.49	0.47
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.97	0.47
3:C:39:SER:OG	23:C:313:DMU:H30	2.14	0.47
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.95	0.47
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.13	0.47
20:Y:101:TGL:HB21	20:Y:101:TGL:HG12	1.95	0.47
1:A:478:SER:O	13:M:6:ALA:HB1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:72:ASN:N	7:T:76:ASN:HD22	2.06	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.14	0.47
26:O:302:PSC:H262	26:O:302:PSC:H221	1.97	0.47
1:A:76:GLY:O	1:A:80:ASN:HB2	2.15	0.47
1:A:377:PHE:O	1:A:381:LEU:HB3	2.15	0.47
1:A:488:THR:HB	1:A:495:LEU:HD13	1.97	0.47
2:B:49:LYS:HE2	4:D:20:ARG:CZ	2.45	0.46
25:C:312:CDL:C37	29:C:488:HOH:O	2.57	0.46
7:G:5:LYS:HB3	1:N:278:MET:HG2	1.98	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.46
1:A:489:THR:HA	6:F:71:TRP:O	2.15	0.46
7:G:1:ALA:CB	3:P:92:LEU:HD21	2.46	0.46
1:N:489:THR:HA	6:S:71:TRP:O	2.15	0.46
25:P:307:CDL:H711	25:P:307:CDL:H131	1.97	0.46
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.96	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
3:C:88:ILE:HG12	24:C:315:PEK:H231	1.98	0.46
25:C:312:CDL:H471	29:O:484:HOH:O	2.16	0.46
20:Q:201:TGL:HC22	20:Q:201:TGL:HG11	1.98	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.45
25:P:307:CDL:OA7	25:P:307:CDL:H673	2.16	0.45
2:B:64:ILE:HG23	2:B:68:LEU:HD22	1.98	0.45
1:N:426:PHE:N	1:N:427:PRO:CD	2.79	0.45
1:A:307:SER:O	1:A:311:ILE:HG23	2.15	0.45
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.45
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.29	0.45
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.45
1:A:270:TYR:N	19:A:614:EDO:H11	2.06	0.45
7:G:1:ALA:HB2	3:P:92:LEU:HD21	1.99	0.45
20:D:201:TGL:HC42	20:D:201:TGL:HG31	1.98	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.45
8:H:8:ILE:O	8:H:8:ILE:HG22	2.17	0.45
1:N:309:THR:HG22	18:N:606:HEA:HMB2	1.97	0.45
1:A:281:GLY:C	7:T:4:ALA:CB	2.86	0.44
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.48	0.44
5:E:52:LEU:O	5:E:55:CYS:HB2	2.17	0.44
4:Q:7:LYS:HE3	13:Z:4:LYS:HG2	1.98	0.44
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.97	0.44
29:C:484:HOH:O	7:G:11:TPO:HG21	2.17	0.44
4:Q:78:TRP:HB3	20:Q:201:TGL:HB42	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:109:HIS:HD2	29:Q:331:HOH:O	2.00	0.44
6:S:85:CYS:SG	6:S:87:THR:HG23	2.57	0.44
8:U:40:GLU:O	8:U:44:THR:HB	2.18	0.44
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.17	0.44
6:S:9:ASP:HB3	6:S:21:MET:HE1	2.00	0.44
1:A:309:THR:HG22	18:A:606:HEA:HMB2	1.99	0.44
5:E:90:ARG:HD3	5:E:90:ARG:HA	1.83	0.43
12:L:46:LYS:HD2	29:L:217:HOH:O	2.18	0.43
28:V:101:SAC:C	28:V:101:SAC:H2A1	2.48	0.43
1:A:497:GLY:HA2	19:A:608:EDO:H11	2.00	0.43
1:N:309:THR:CG2	18:N:606:HEA:HMB2	2.48	0.43
29:N:782:HOH:O	19:S:2201:EDO:H12	2.17	0.43
1:N:46:THR:CG2	1:N:49:GLY:H	2.31	0.43
22:T:104:CHD:H181	22:T:104:CHD:C22	2.48	0.43
1:A:328:HIS:NE2	26:E:201:PSC:H22	2.33	0.43
26:O:302:PSC:C08	9:V:10:ARG:HH21	2.32	0.43
3:P:67:PHE:CE1	25:P:307:CDL:HB22	2.53	0.43
17:N:605:PGV:H101	17:N:605:PGV:H132	1.77	0.43
19:N:614:EDO:H22	29:O:431:HOH:O	2.18	0.43
1:A:472:ILE:HG21	20:L:101:TGL:H202	2.01	0.43
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.18	0.43
7:T:67:HIS:NE2	7:T:84:LYS:HG3	2.33	0.43
1:N:364:ASP:OD2	18:N:606:HEA:O2A	2.36	0.43
18:N:606:HEA:HMC1	18:N:606:HEA:CBC	2.48	0.43
1:N:479:LYS:NZ	29:N:706:HOH:O	2.49	0.43
4:D:29:HIS:HD2	4:D:61:ARG:O	2.02	0.42
4:D:73:ARG:HB3	5:E:109:VAL:HG11	2.00	0.42
26:O:302:PSC:H211	26:O:302:PSC:H252	2.00	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.01	0.42
1:A:34:SER:HB2	18:A:607:HEA:C2B	2.49	0.42
1:A:378:HIS:HA	1:A:382:SER:OG	2.19	0.42
24:C:303:PEK:H221	24:C:303:PEK:H251	1.90	0.42
3:P:186:PHE:HA	3:P:190:ASP:OD2	2.20	0.42
17:A:604:PGV:H142	13:M:12:PRO:HG3	2.00	0.42
25:C:306:CDL:CB2	25:C:306:CDL:CB3	2.96	0.42
4:D:78:TRP:CA	20:D:201:TGL:HB52	2.49	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.54	0.42
18:N:607:HEA:HMC1	18:N:607:HEA:CBC	2.44	0.42
4:Q:2:HIS:O	4:Q:2:HIS:CG	2.72	0.42
22:T:104:CHD:H181	22:T:104:CHD:C23	2.50	0.42
5:E:28:GLU:OE1	19:F:702:EDO:C1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:378:HIS:HA	1:N:382:SER:OG	2.19	0.42
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.68	0.42
1:A:118:VAL:HG11	1:A:141:ALA:HB3	2.02	0.42
9:I:54:TYR:OH	9:I:59:ASP:OD1	2.31	0.42
24:P:305:PEK:H012	24:P:305:PEK:O14	2.20	0.42
2:B:32:PHE:CD1	9:I:31:PHE:CZ	3.08	0.42
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.55	0.42
3:C:47:LEU:O	3:C:51:MET:HG2	2.19	0.42
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.42
26:O:302:PSC:H222	26:O:302:PSC:C1	2.49	0.42
1:A:406:ASN:HD21	17:A:604:PGV:H02	1.84	0.42
1:N:60:ALA:O	1:N:64:VAL:HG23	2.20	0.42
7:T:51:HIS:ND1	29:T:204:HOH:O	2.37	0.42
7:G:4:ALA:CB	1:N:285:PHE:CE2	3.02	0.41
6:S:96:LEU:HD23	6:S:96:LEU:C	2.40	0.41
7:G:3:ALA:HA	1:N:282:PHE:CD1	2.55	0.41
1:N:302:ARG:HH12	2:O:87:MET:HE1	1.85	0.41
3:C:103:HIS:HA	17:T:101:PGV:H012	2.02	0.41
22:T:104:CHD:O7	22:T:104:CHD:C15	2.68	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.97	0.41
18:A:606:HEA:HBC1	18:A:606:HEA:HMC1	2.03	0.41
20:A:615:TGL:H283	20:A:615:TGL:H121	2.02	0.41
2:O:65:TRP:O	2:O:69:PRO:HG2	2.21	0.41
3:P:161:GLN:HE22	24:P:305:PEK:H31	1.85	0.41
8:U:54:GLU:OE2	8:U:57:ARG:NH2	2.44	0.41
1:A:46:THR:CG2	1:A:49:GLY:H	2.29	0.41
1:A:426:PHE:N	1:A:427:PRO:CD	2.82	0.41
3:C:149:HIS:CE1	23:G:1302:DMU:H5	2.55	0.41
3:C:186:PHE:HA	3:C:190:ASP:OD2	2.21	0.41
7:G:1:ALA:HB1	3:P:92:LEU:HD11	2.02	0.41
7:G:4:ALA:CB	1:N:285:PHE:HE2	2.34	0.41
1:N:269:GLY:N	19:N:614:EDO:H21	2.35	0.41
3:P:29:SER:HB2	3:P:42:LEU:HD13	2.03	0.41
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.56	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.94	0.41
7:G:4:ALA:CB	1:N:194:LEU:CD2	2.95	0.40
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.56	0.40
2:B:13:THR:HB	2:B:168:LEU:HD23	2.02	0.40
3:C:258:TRP:NE1	25:C:312:CDL:C56	2.84	0.40
1:N:310:MET:HE2	1:N:356:ILE:HG23	2.03	0.40
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.56	0.40
3:P:129:VAL:N	3:P:130:PRO:CD	2.84	0.40
20:D:201:TGL:CC3	20:D:201:TGL:CG3	3.00	0.40
20:Q:201:TGL:H352	9:V:16:ARG:HE	1.86	0.40
8:H:49:ASP:O	8:H:52:VAL:HG22	2.21	0.40
1:N:127:THR:HB	1:N:129:TYR:CE2	2.57	0.40
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
2	O	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	G	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
7	T	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	12 4
8	U	77/85 (91%)	71 (92%)	6 (8%)	0	100 100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100 100
9	V	70/73 (96%)	68 (97%)	2 (3%)	0	100 100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
11	K	50/56 (89%)	48 (96%)	2 (4%)	0	100 100
11	X	50/56 (89%)	48 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	41 (100%)	0	0	100 100
All	All	3514/3614 (97%)	3412 (97%)	100 (3%)	2 (0%)	51 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
7	T	4	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/426 (100%)	418 (98%)	8 (2%)	57 45
1	N	426/426 (100%)	415 (97%)	11 (3%)	46 32
2	B	210/210 (100%)	201 (96%)	9 (4%)	29 14
2	O	210/210 (100%)	197 (94%)	13 (6%)	18 6
3	C	224/226 (99%)	220 (98%)	4 (2%)	59 47
3	P	224/226 (99%)	220 (98%)	4 (2%)	59 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	129/129 (100%)	126 (98%)	3 (2%)	50 38
4	Q	129/129 (100%)	124 (96%)	5 (4%)	32 17
5	E	92/95 (97%)	89 (97%)	3 (3%)	38 24
5	R	92/95 (97%)	89 (97%)	3 (3%)	38 24
6	F	81/81 (100%)	78 (96%)	3 (4%)	34 19
6	S	81/81 (100%)	76 (94%)	5 (6%)	18 6
7	G	67/68 (98%)	58 (87%)	9 (13%)	4 0
7	T	67/68 (98%)	56 (84%)	11 (16%)	2 0
8	H	71/75 (95%)	64 (90%)	7 (10%)	8 1
8	U	71/75 (95%)	64 (90%)	7 (10%)	8 1
9	I	57/57 (100%)	53 (93%)	4 (7%)	15 4
9	V	57/57 (100%)	53 (93%)	4 (7%)	15 4
10	J	49/50 (98%)	47 (96%)	2 (4%)	30 15
10	W	49/50 (98%)	46 (94%)	3 (6%)	18 6
11	K	42/46 (91%)	39 (93%)	3 (7%)	14 4
11	X	42/46 (91%)	40 (95%)	2 (5%)	25 10
12	L	39/40 (98%)	36 (92%)	3 (8%)	13 3
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7 1
13	M	37/38 (97%)	33 (89%)	4 (11%)	6 1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6 1
All	All	3048/3082 (99%)	2910 (96%)	138 (4%)	27 12

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	136	LEU
1	A	180	GLN
1	A	290	HIS
1	A	311	ILE
1	A	369	ASP
1	A	380	VAL
2	B	33	LEU
2	B	37	LEU

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Mol	Chain	Res	Type
2	B	49	LYS
2	B	60	GLU
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	89	GLU
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	31	LYS
4	D	51	LEU
4	D	147	LYS
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	43	LYS
6	F	54	ASN
6	F	96	LEU
7	G	5	LYS
7	G	7	ASP
7	G	8	HIS
7	G	18	PHE
7	G	35	SER
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	10	ASN
8	H	29	CYS
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	18	ARG
9	I	29	LEU
9	I	43	ARG
10	J	50	LEU
10	J	58	LYS

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Mol	Chain	Res	Type
11	K	12	LYS
11	K	51	LYS
11	K	54	ARG
12	L	20	ARG
12	L	26	THR
12	L	27	LEU
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	117	MET
1	N	180	GLN
1	N	189	MET
1	N	290	HIS
1	N	369	ASP
1	N	380	VAL
1	N	381	LEU
1	N	484	THR
1	N	512	ASN
2	O	33	LEU
2	O	37	LEU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	87	MET
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
2	O	221	LYS
2	O	225	SER
3	P	3	HIS
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	2	HIS
4	Q	6	VAL
4	Q	33	LEU
4	Q	53	ILE

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Mol	Chain	Res	Type
4	Q	58	GLU
5	R	14	ARG
5	R	79	LYS
5	R	80	GLU
6	S	43	LYS
6	S	48	LEU
6	S	54	ASN
6	S	80	GLN
6	S	91	LEU
7	T	2	SER
7	T	5	LYS
7	T	7	ASP
7	T	18	PHE
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	54	ARG
7	T	83	GLU
7	T	84	LYS
8	U	7	LYS
8	U	9	LYS
8	U	10	ASN
8	U	41	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
9	V	29	LEU
9	V	44	LYS
9	V	45	LYS
9	V	61	GLU
10	W	36	MET
10	W	50	LEU
10	W	58	LYS
11	X	5	ARG
11	X	56	GLN
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
12	Y	47	LYS
13	Z	5	PRO
13	Z	34	LEU

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Mol	Chain	Res	Type
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	360	ASN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
4	D	29	HIS
5	E	94	ASN
6	F	54	ASN
7	G	8	HIS
7	G	76	ASN
8	H	23	GLN
10	J	29	ASN
11	K	35	GLN
1	N	178	GLN
1	N	232	GLN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	8	HIS
7	T	76	ASN

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Mol	Chain	Res	Type
9	V	8	GLN
9	V	70	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.30	0	7,9,11	0.83	0
7	TPO	T	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.93	0
1	FME	N	1	1	8,9,10	0.59	0	7,9,11	1.09	0
2	FME	B	1	2	8,9,10	0.80	0	7,9,11	1.26	2 (28%)
2	FME	O	1	2	8,9,10	0.43	0	7,9,11	0.91	0
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	1.25	1 (10%)

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

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

All (2) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	O-C-CA-CB
7	T	11	TPO	CA-CB-OG1-P
1	N	1	FME	CA-CB-CG-SD
1	A	1	FME	CA-CB-CG-SD
7	G	11	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 149 ligands modelled in this entry, 8 are monoatomic - leaving 141 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	EDO	M	102	-	3,3,3	0.13	0	2,2,2	0.13	0
24	PEK	C	303	-	52,52,52	0.49	0	55,57,57	0.79	0
18	HEA	A	607	1	57,67,67	1.77	12 (21%)	61,103,103	2.76	21 (34%)
19	EDO	W	301	-	3,3,3	0.18	0	2,2,2	0.42	0
19	EDO	A	609	-	3,3,3	0.20	0	2,2,2	0.12	0
23	DMU	G	1302	-	34,34,34	1.85	10 (29%)	45,45,45	1.43	7 (15%)
19	EDO	W	304	-	3,3,3	0.18	0	2,2,2	0.24	0
25	CDL	P	307	-	99,99,99	0.34	0	105,111,111	0.51	1 (0%)
19	EDO	A	618	-	3,3,3	0.16	0	2,2,2	0.58	0
26	PSC	E	201	-	51,51,51	0.44	0	57,59,59	0.51	0
19	EDO	B	309	-	3,3,3	0.11	0	2,2,2	0.30	0
19	EDO	P	311	-	3,3,3	0.37	0	2,2,2	0.44	0
20	TGL	Y	101	-	62,62,62	0.32	0	65,65,65	0.52	1 (1%)
24	PEK	P	304	-	52,52,52	0.42	0	55,57,57	0.72	2 (3%)
19	EDO	A	616	-	3,3,3	0.08	0	2,2,2	0.23	0
17	PGV	A	604	-	50,50,50	1.18	2 (4%)	53,56,56	1.59	5 (9%)
23	DMU	C	301	-	34,34,34	1.54	5 (14%)	45,45,45	1.86	9 (20%)
19	EDO	A	611	-	3,3,3	0.14	0	2,2,2	0.10	0
19	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.24	0
17	PGV	T	101	-	50,50,50	1.14	2 (4%)	53,56,56	1.19	4 (7%)
19	EDO	V	104	-	3,3,3	0.37	0	2,2,2	0.48	0
19	EDO	N	619	-	3,3,3	0.11	0	2,2,2	0.20	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.55	2 (3%)
19	EDO	G	1306	-	3,3,3	0.12	0	2,2,2	0.25	0
19	EDO	G	1303	-	3,3,3	0.07	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PEK	C	304	-	52,52,52	0.35	0	55,57,57	0.51	0
19	EDO	N	615	-	3,3,3	0.11	0	2,2,2	0.31	0
18	HEA	A	606	1	57,67,67	1.59	10 (17%)	61,103,103	2.47	21 (34%)
25	CDL	C	306	-	99,99,99	0.38	0	105,111,111	0.59	2 (1%)
25	CDL	T	102	-	99,99,99	0.36	0	105,111,111	0.46	0
19	EDO	B	305	-	3,3,3	0.13	0	2,2,2	0.31	0
19	EDO	C	309	-	3,3,3	0.03	0	2,2,2	0.21	0
26	PSC	O	302	-	51,51,51	0.40	0	57,59,59	0.42	0
19	EDO	L	102	-	3,3,3	0.25	0	2,2,2	0.42	0
19	EDO	A	610	-	3,3,3	0.26	0	2,2,2	0.18	0
19	EDO	R	202	-	3,3,3	0.14	0	2,2,2	0.28	0
22	CHD	P	308	-	32,32,32	0.59	0	51,51,51	1.09	2 (3%)
19	EDO	C	314	-	3,3,3	0.11	0	2,2,2	0.19	0
19	EDO	C	308	-	3,3,3	0.36	0	2,2,2	0.12	0
19	EDO	B	303	-	3,3,3	0.41	0	2,2,2	0.31	0
19	EDO	T	105	-	3,3,3	0.05	0	2,2,2	0.36	0
19	EDO	D	203	-	3,3,3	0.09	0	2,2,2	0.12	0
24	PEK	P	305	-	52,52,52	0.33	0	55,57,57	0.40	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.34	0
19	EDO	D	207	-	3,3,3	0.24	0	2,2,2	0.12	0
19	EDO	A	620	-	3,3,3	0.30	0	2,2,2	0.13	0
19	EDO	E	205	-	3,3,3	0.07	0	2,2,2	0.22	0
19	EDO	S	2206	-	3,3,3	0.19	0	2,2,2	0.12	0
20	TGL	A	615	-	62,62,62	0.35	0	65,65,65	0.48	1 (1%)
19	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.43	0
19	EDO	B	308	-	3,3,3	0.08	0	2,2,2	0.08	0
19	EDO	S	2205	-	3,3,3	0.11	0	2,2,2	0.08	0
22	CHD	Y	102	-	32,32,32	0.57	0	51,51,51	0.98	3 (5%)
17	PGV	N	605	-	50,50,50	0.82	2 (4%)	53,56,56	1.29	4 (7%)
20	TGL	L	101	-	62,62,62	0.33	0	65,65,65	0.27	0
17	PGV	C	305	-	50,50,50	0.73	2 (4%)	53,56,56	0.82	1 (1%)
19	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.41	0
19	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.81	0
19	EDO	S	2204	-	3,3,3	0.32	0	2,2,2	0.48	0
19	EDO	F	702	-	3,3,3	0.17	0	2,2,2	0.13	0
19	EDO	D	205	-	3,3,3	0.31	0	2,2,2	0.33	0
19	EDO	D	206	-	3,3,3	0.19	0	2,2,2	0.33	0
17	PGV	P	306	-	50,50,50	0.76	2 (4%)	53,56,56	0.98	4 (7%)
19	EDO	D	204	-	3,3,3	0.09	0	2,2,2	0.15	0
19	EDO	F	701	-	3,3,3	0.14	0	2,2,2	0.44	0
19	EDO	P	310	-	3,3,3	0.32	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	EDO	S	2201	-	3,3,3	0.41	0	2,2,2	0.60	0
19	EDO	J	1103	-	3,3,3	0.09	0	2,2,2	0.15	0
23	DMU	Z	101	-	34,34,34	1.19	4 (11%)	45,45,45	1.55	7 (15%)
19	EDO	J	1105	-	3,3,3	0.23	0	2,2,2	0.43	0
19	EDO	N	617	-	3,3,3	0.04	0	2,2,2	0.24	0
19	EDO	P	309	-	3,3,3	0.17	0	2,2,2	0.32	0
23	DMU	M	101	-	34,34,34	1.11	3 (8%)	45,45,45	1.26	5 (11%)
28	SAC	I	101	-	7,8,9	0.52	0	8,9,11	1.04	1 (12%)
19	EDO	C	311	-	3,3,3	0.12	0	2,2,2	0.19	0
19	EDO	J	1104	-	3,3,3	0.49	0	2,2,2	0.73	0
20	TGL	Q	201	-	62,62,62	0.29	0	65,65,65	0.30	0
19	EDO	E	202	-	3,3,3	0.13	0	2,2,2	0.15	0
19	EDO	F	704	-	3,3,3	0.15	0	2,2,2	0.31	0
19	EDO	G	1304	-	3,3,3	0.17	0	2,2,2	0.39	0
19	EDO	S	2203	-	3,3,3	0.35	0	2,2,2	0.28	0
19	EDO	G	1301	-	3,3,3	0.22	0	2,2,2	0.51	0
19	EDO	C	310	-	3,3,3	0.08	0	2,2,2	0.16	0
19	EDO	N	608	-	3,3,3	0.25	0	2,2,2	0.46	0
19	EDO	N	610	-	3,3,3	0.38	0	2,2,2	0.77	0
19	EDO	Z	103	-	3,3,3	0.24	0	2,2,2	0.34	0
19	EDO	O	303	-	3,3,3	0.47	0	2,2,2	0.76	0
19	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.38	0
19	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.57	0
19	EDO	J	1101	-	3,3,3	0.47	0	2,2,2	0.29	0
22	CHD	C	302	-	32,32,32	0.64	1 (3%)	51,51,51	0.79	1 (1%)
17	PGV	A	605	-	50,50,50	0.84	2 (4%)	53,56,56	1.22	2 (3%)
23	DMU	P	302	-	34,34,34	1.12	2 (5%)	45,45,45	1.96	11 (24%)
19	EDO	T	103	-	3,3,3	0.37	0	2,2,2	0.19	0
24	PEK	C	315	-	52,52,52	0.43	0	55,57,57	0.57	0
22	CHD	T	104	-	32,32,32	0.70	0	51,51,51	1.26	6 (11%)
19	EDO	S	2207	-	3,3,3	0.12	0	2,2,2	0.39	0
21	CUA	B	301	2	0,1,1	-	-	-		
19	EDO	A	612	-	3,3,3	0.20	0	2,2,2	0.19	0
19	EDO	K	101	-	3,3,3	0.09	0	2,2,2	0.22	0
19	EDO	N	609	-	3,3,3	0.18	0	2,2,2	0.16	0
22	CHD	B	302	-	32,32,32	0.60	0	51,51,51	0.85	1 (1%)
19	EDO	N	614	-	3,3,3	0.53	0	2,2,2	0.69	0
19	EDO	U	1501	-	3,3,3	0.27	0	2,2,2	0.54	0
19	EDO	D	208	-	3,3,3	0.16	0	2,2,2	0.16	0
22	CHD	C	307	-	32,32,32	0.60	0	51,51,51	0.78	0
19	EDO	A	617	-	3,3,3	0.15	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CUA	O	301	2	0,1,1	-	-	-		
20	TGL	N	604	-	62,62,62	0.27	0	65,65,65	0.46	1 (1%)
19	EDO	N	620	-	3,3,3	0.34	0	2,2,2	0.55	0
18	HEA	N	607	1	57,67,67	2.03	14 (24%)	61,103,103	2.60	23 (37%)
19	EDO	A	608	-	3,3,3	0.31	0	2,2,2	0.34	0
24	PEK	P	301	-	52,52,52	0.32	0	55,57,57	0.49	0
19	EDO	V	103	-	3,3,3	0.16	0	2,2,2	0.36	0
22	CHD	P	303	-	32,32,32	0.68	1 (3%)	51,51,51	0.73	0
19	EDO	O	304	-	3,3,3	0.28	0	2,2,2	0.39	0
19	EDO	N	618	-	3,3,3	0.18	0	2,2,2	0.13	0
17	PGV	Z	102	-	50,50,50	1.09	2 (4%)	53,56,56	1.16	5 (9%)
19	EDO	N	612	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	B	306	-	3,3,3	0.22	0	2,2,2	0.30	0
19	EDO	I	103	-	3,3,3	0.17	0	2,2,2	0.43	0
19	EDO	W	303	-	3,3,3	0.40	0	2,2,2	0.49	0
19	EDO	I	102	-	3,3,3	0.10	0	2,2,2	0.24	0
19	EDO	N	611	-	3,3,3	0.18	0	2,2,2	0.09	0
19	EDO	E	204	-	3,3,3	0.11	0	2,2,2	0.24	0
22	CHD	G	1305	-	32,32,32	0.56	0	51,51,51	0.80	0
19	EDO	Q	204	-	3,3,3	0.22	0	2,2,2	0.06	0
23	DMU	C	313	-	34,34,34	1.81	7 (20%)	45,45,45	1.93	10 (22%)
28	SAC	V	101	-	7,8,9	0.49	0	8,9,11	1.10	1 (12%)
19	EDO	Q	202	-	3,3,3	0.18	0	2,2,2	0.24	0
19	EDO	F	705	-	3,3,3	0.33	0	2,2,2	0.39	0
19	EDO	D	202	-	3,3,3	0.12	0	2,2,2	0.21	0
25	CDL	C	312	-	99,99,99	0.37	0	105,111,111	0.45	0
18	HEA	N	606	1	57,67,67	1.68	14 (24%)	61,103,103	2.51	25 (40%)
19	EDO	K	102	-	3,3,3	0.11	0	2,2,2	0.29	0
19	EDO	B	304	-	3,3,3	0.22	0	2,2,2	0.28	0
19	EDO	Q	203	-	3,3,3	0.20	0	2,2,2	0.16	0
17	PGV	N	616	-	50,50,50	1.04	2 (4%)	53,56,56	1.04	3 (5%)
22	CHD	J	1102	-	32,32,32	0.63	1 (3%)	51,51,51	0.77	0
22	CHD	W	302	-	32,32,32	0.55	0	51,51,51	0.74	0
19	EDO	R	201	-	3,3,3	0.10	0	2,2,2	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	M	102	-	-	0/1/1/1	-
24	PEK	C	303	-	-	22/56/56/56	-
18	HEA	A	607	1	3/3/7/16	7/32/76/76	-
19	EDO	W	301	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
23	DMU	G	1302	-	-	11/19/59/59	0/2/2/2
19	EDO	W	304	-	-	1/1/1/1	-
25	CDL	P	307	-	-	49/110/110/110	-
19	EDO	A	618	-	-	0/1/1/1	-
26	PSC	E	201	-	-	27/55/55/55	-
19	EDO	B	309	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
20	TGL	Y	101	-	-	30/65/65/65	-
24	PEK	P	304	-	-	20/56/56/56	-
19	EDO	A	616	-	-	0/1/1/1	-
17	PGV	A	604	-	-	30/55/55/55	-
23	DMU	C	301	-	-	11/19/59/59	0/2/2/2
19	EDO	A	611	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
17	PGV	T	101	-	-	26/55/55/55	-
19	EDO	V	104	-	-	0/1/1/1	-
19	EDO	N	619	-	-	1/1/1/1	-
20	TGL	D	201	-	-	36/65/65/65	-
19	EDO	G	1306	-	-	1/1/1/1	-
19	EDO	G	1303	-	-	1/1/1/1	-
24	PEK	C	304	-	-	29/56/56/56	-
19	EDO	N	615	-	-	1/1/1/1	-
18	HEA	A	606	1	3/3/7/16	6/32/76/76	-
25	CDL	C	306	-	-	59/110/110/110	-
25	CDL	T	102	-	-	63/110/110/110	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
26	PSC	O	302	-	-	37/55/55/55	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	A	610	-	-	0/1/1/1	-
19	EDO	R	202	-	-	1/1/1/1	-
22	CHD	P	308	-	-	4/9/74/74	0/4/4/4
19	EDO	C	314	-	-	1/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	B	303	-	-	0/1/1/1	-
19	EDO	T	105	-	-	1/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
24	PEK	P	305	-	-	31/56/56/56	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	D	207	-	-	1/1/1/1	-
19	EDO	A	620	-	-	0/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
19	EDO	S	2206	-	-	1/1/1/1	-
20	TGL	A	615	-	-	42/65/65/65	-
19	EDO	A	613	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	S	2205	-	-	0/1/1/1	-
22	CHD	Y	102	-	-	8/9/74/74	1/4/4/4
17	PGV	N	605	-	-	14/55/55/55	-
20	TGL	L	101	-	-	35/65/65/65	-
17	PGV	C	305	-	-	13/55/55/55	-
19	EDO	E	203	-	-	0/1/1/1	-
19	EDO	N	613	-	-	0/1/1/1	-
19	EDO	S	2204	-	-	1/1/1/1	-
19	EDO	F	702	-	-	0/1/1/1	-
19	EDO	D	205	-	-	1/1/1/1	-
19	EDO	D	206	-	-	1/1/1/1	-
17	PGV	P	306	-	-	9/55/55/55	-
19	EDO	D	204	-	-	1/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
19	EDO	P	310	-	-	0/1/1/1	-
19	EDO	S	2201	-	-	1/1/1/1	-
19	EDO	J	1103	-	-	0/1/1/1	-
23	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
19	EDO	J	1105	-	-	1/1/1/1	-
19	EDO	N	617	-	-	0/1/1/1	-
19	EDO	P	309	-	-	1/1/1/1	-
23	DMU	M	101	-	-	6/19/59/59	0/2/2/2
28	SAC	I	101	-	-	7/7/8/10	-
19	EDO	C	311	-	-	0/1/1/1	-
19	EDO	J	1104	-	-	0/1/1/1	-
20	TGL	Q	201	-	-	32/65/65/65	-
19	EDO	E	202	-	-	1/1/1/1	-
19	EDO	F	704	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	G	1304	-	-	1/1/1/1	-
19	EDO	S	2203	-	-	0/1/1/1	-
19	EDO	G	1301	-	-	0/1/1/1	-
19	EDO	C	310	-	-	1/1/1/1	-
19	EDO	N	608	-	-	1/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	Z	103	-	-	0/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
19	EDO	A	619	-	-	1/1/1/1	-
19	EDO	J	1101	-	-	0/1/1/1	-
22	CHD	C	302	-	-	2/9/74/74	0/4/4/4
17	PGV	A	605	-	-	15/55/55/55	-
23	DMU	P	302	-	-	6/19/59/59	0/2/2/2
19	EDO	T	103	-	-	1/1/1/1	-
24	PEK	C	315	-	-	27/56/56/56	-
22	CHD	T	104	-	-	6/9/74/74	1/4/4/4
19	EDO	S	2207	-	-	1/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	N	609	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	U	1501	-	-	0/1/1/1	-
19	EDO	D	208	-	-	0/1/1/1	-
22	CHD	C	307	-	-	2/9/74/74	0/4/4/4
19	EDO	A	617	-	-	1/1/1/1	-
20	TGL	N	604	-	-	33/65/65/65	-
19	EDO	N	620	-	-	1/1/1/1	-
18	HEA	N	607	1	3/3/7/16	4/32/76/76	-
19	EDO	A	608	-	-	0/1/1/1	-
24	PEK	P	301	-	-	29/56/56/56	-
19	EDO	V	103	-	-	0/1/1/1	-
22	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	O	304	-	-	0/1/1/1	-
19	EDO	N	618	-	-	0/1/1/1	-
17	PGV	Z	102	-	-	25/55/55/55	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	B	306	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	I	103	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	I	102	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
22	CHD	G	1305	-	-	2/9/74/74	0/4/4/4
19	EDO	Q	204	-	-	0/1/1/1	-
23	DMU	C	313	-	-	6/19/59/59	0/2/2/2
28	SAC	V	101	-	-	2/7/8/10	-
19	EDO	Q	202	-	-	1/1/1/1	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	D	202	-	-	0/1/1/1	-
25	CDL	C	312	-	-	63/110/110/110	-
18	HEA	N	606	1	3/3/7/16	4/32/76/76	-
19	EDO	K	102	-	-	1/1/1/1	-
19	EDO	B	304	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	1/1/1/1	-
17	PGV	N	616	-	-	24/55/55/55	-
22	CHD	J	1102	-	-	2/9/74/74	0/4/4/4
22	CHD	W	302	-	-	2/9/74/74	0/4/4/4
19	EDO	R	201	-	-	1/1/1/1	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C1D-ND	-5.88	1.30	1.40
23	G	1302	DMU	O16-C6	5.73	1.50	1.40
23	C	313	DMU	O16-C6	5.56	1.49	1.40
18	A	607	HEA	C1D-ND	-5.54	1.30	1.40
18	N	607	HEA	C4B-NB	-5.33	1.31	1.40
17	A	604	PGV	O01-C1	5.23	1.49	1.34
17	Z	102	PGV	O03-C19	5.19	1.48	1.33
23	C	301	DMU	O16-C6	5.16	1.49	1.40
17	T	101	PGV	O03-C19	5.13	1.48	1.33
17	A	604	PGV	O03-C19	4.98	1.47	1.33
17	T	101	PGV	O01-C1	4.94	1.48	1.34
17	N	616	PGV	O01-C1	4.88	1.48	1.34
23	C	313	DMU	O1-C9	4.70	1.55	1.44
18	N	607	HEA	C3A-C2A	4.59	1.46	1.40
17	Z	102	PGV	O01-C1	4.50	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C3B-C2B	4.47	1.44	1.34
18	N	606	HEA	C1D-ND	-4.36	1.32	1.40
17	N	616	PGV	O03-C19	4.30	1.45	1.33
18	A	607	HEA	C4B-NB	-4.21	1.33	1.40
23	Z	101	DMU	O16-C6	4.00	1.47	1.40
18	A	606	HEA	CHD-C1D	3.99	1.45	1.35
18	N	606	HEA	C3A-C2A	3.80	1.45	1.40
23	G	1302	DMU	O7-C3	3.77	1.53	1.43
23	C	313	DMU	O1-C10	3.76	1.51	1.41
18	A	606	HEA	C3B-C2B	3.76	1.43	1.34
18	A	607	HEA	C3D-C2D	3.71	1.44	1.36
18	A	606	HEA	C3D-C2D	3.63	1.44	1.36
18	N	607	HEA	FE-ND	3.47	2.14	1.96
18	N	606	HEA	C4B-NB	-3.45	1.34	1.40
18	N	606	HEA	CHD-C1D	3.41	1.43	1.35
17	N	605	PGV	O03-C19	3.36	1.43	1.33
18	N	606	HEA	C3B-C2B	3.36	1.42	1.34
23	G	1302	DMU	O7-C10	3.34	1.51	1.41
18	A	607	HEA	C3A-C2A	3.33	1.45	1.40
18	N	607	HEA	C3D-C2D	3.17	1.43	1.36
18	A	607	HEA	CHD-C1D	3.16	1.43	1.35
18	A	607	HEA	C3B-C2B	3.16	1.41	1.34
18	N	607	HEA	C3C-C2C	3.14	1.44	1.40
17	A	605	PGV	O03-C19	3.14	1.42	1.33
18	A	606	HEA	C1D-ND	-3.13	1.34	1.40
23	M	101	DMU	O16-C6	3.12	1.45	1.40
23	C	301	DMU	O5-C4	3.11	1.51	1.44
23	P	302	DMU	O16-C6	3.10	1.45	1.40
23	M	101	DMU	O1-C9	3.04	1.51	1.44
18	N	606	HEA	CHC-C4B	3.04	1.42	1.35
18	A	606	HEA	C3C-C2C	3.03	1.44	1.40
18	N	607	HEA	FE-NB	3.03	2.11	1.96
18	A	606	HEA	C4B-C3B	3.01	1.49	1.44
23	Z	101	DMU	O1-C9	2.99	1.51	1.44
18	A	606	HEA	CHC-C4B	2.95	1.42	1.35
18	N	607	HEA	CMC-C2C	-2.85	1.45	1.51
18	A	607	HEA	CHC-C4B	2.81	1.42	1.35
18	N	607	HEA	CHD-C1D	2.81	1.42	1.35
18	A	607	HEA	C1B-NB	2.78	1.44	1.38
17	A	605	PGV	O01-C1	2.78	1.42	1.34
23	C	301	DMU	C7-C5	2.76	1.59	1.52
23	C	301	DMU	O5-C6	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	101	DMU	O49-C1	-2.69	1.36	1.43
18	N	606	HEA	FE-ND	2.67	2.10	1.96
17	P	306	PGV	O03-C19	2.66	1.41	1.33
17	P	306	PGV	O01-C1	2.66	1.41	1.34
17	C	305	PGV	O03-C19	2.63	1.41	1.33
18	A	606	HEA	C4B-NB	-2.62	1.35	1.40
17	N	605	PGV	O01-C1	2.61	1.41	1.34
17	C	305	PGV	O01-C1	2.56	1.41	1.34
18	A	606	HEA	C3A-C2A	2.55	1.43	1.40
18	A	607	HEA	CAA-C2A	-2.54	1.47	1.52
18	N	607	HEA	CHB-C1B	2.53	1.48	1.41
18	N	606	HEA	FE-NB	2.53	2.09	1.96
23	C	313	DMU	C8-C7	2.47	1.58	1.52
23	C	301	DMU	O3-C5	2.45	1.48	1.43
23	C	313	DMU	O5-C4	2.45	1.50	1.44
23	G	1302	DMU	O5-C4	2.44	1.50	1.44
23	G	1302	DMU	C7-C5	2.42	1.58	1.52
18	A	607	HEA	C4C-NC	-2.33	1.31	1.36
23	G	1302	DMU	O1-C10	2.32	1.47	1.41
18	N	606	HEA	CHB-C1B	2.29	1.47	1.41
23	G	1302	DMU	O1-C9	2.27	1.49	1.44
23	G	1302	DMU	C10-C5	2.25	1.59	1.52
23	C	313	DMU	O7-C10	2.24	1.48	1.41
18	N	607	HEA	CHC-C4B	2.23	1.40	1.35
22	P	303	CHD	O26-C24	-2.23	1.23	1.30
23	G	1302	DMU	C2-C1	2.22	1.58	1.52
18	N	606	HEA	O2A-CGA	-2.20	1.23	1.30
18	N	607	HEA	C4D-C3D	2.20	1.48	1.45
23	Z	101	DMU	O7-C10	2.20	1.47	1.41
18	A	607	HEA	C3C-C2C	2.18	1.43	1.40
18	N	606	HEA	C2A-C1A	2.17	1.47	1.42
18	N	606	HEA	CHA-C4D	2.15	1.47	1.41
23	C	313	DMU	C11-C9	2.15	1.59	1.51
18	N	607	HEA	C1D-C2D	2.15	1.48	1.44
18	A	607	HEA	C4D-ND	2.14	1.43	1.38
18	N	606	HEA	C4B-C3B	2.12	1.48	1.44
18	A	606	HEA	C1B-NB	2.09	1.43	1.38
23	Z	101	DMU	O1-C10	2.09	1.47	1.41
18	N	606	HEA	C1D-C2D	2.08	1.48	1.44
22	C	302	CHD	O26-C24	-2.06	1.23	1.30
23	G	1302	DMU	C3-C4	2.04	1.58	1.52
23	P	302	DMU	O5-C4	2.04	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	1102	CHD	O26-C24	-2.03	1.23	1.30

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	607	HEA	C16-C15-C14	9.20	139.74	121.12
18	A	607	HEA	C26-C15-C14	-8.38	102.19	123.68
23	P	302	DMU	C18-O16-C6	7.96	127.05	113.84
23	C	313	DMU	O1-C9-C11	7.14	124.19	106.44
18	A	606	HEA	C1D-C2D-C3D	-7.12	99.47	106.96
18	N	606	HEA	C1D-C2D-C3D	-7.03	99.57	106.96
23	C	301	DMU	C18-O16-C6	6.71	124.97	113.84
17	A	604	PGV	O01-C1-C2	6.20	124.87	111.50
18	A	607	HEA	C1D-C2D-C3D	-6.11	100.53	106.96
18	N	607	HEA	C3D-C4D-ND	-6.01	104.53	110.36
18	N	607	HEA	CMB-C2B-C1B	-5.90	116.05	125.04
18	N	606	HEA	CHB-C1B-NB	5.90	130.84	124.43
18	N	606	HEA	C2D-C1D-ND	5.82	116.73	109.84
17	A	604	PGV	C02-O01-C1	5.71	131.86	117.79
18	N	607	HEA	C13-C12-C11	-5.58	105.97	114.35
18	A	606	HEA	C2D-C1D-ND	5.33	116.15	109.84
18	N	607	HEA	C1D-C2D-C3D	-5.28	101.41	106.96
18	N	607	HEA	C2B-C1B-NB	-5.21	103.64	109.88
17	A	605	PGV	O03-C19-O04	-5.16	110.56	123.59
18	A	606	HEA	CHB-C1B-NB	5.12	129.99	124.43
18	N	607	HEA	C3C-C4C-NC	5.12	115.83	109.21
18	A	606	HEA	C3C-C4C-NC	4.94	115.60	109.21
17	N	605	PGV	O03-C19-C20	4.94	127.42	111.91
18	A	606	HEA	CMD-C2D-C1D	4.92	132.53	125.04
18	N	606	HEA	C3C-C4C-NC	4.86	115.50	109.21
17	T	101	PGV	O01-C1-C2	4.74	121.72	111.50
17	A	605	PGV	O03-C19-C20	4.71	126.67	111.91
17	N	605	PGV	O03-C19-O04	-4.65	111.84	123.59
23	C	301	DMU	C6-O5-C4	4.59	122.69	113.69
18	A	607	HEA	C3C-C4C-NC	4.53	115.07	109.21
18	A	607	HEA	C3D-C4D-ND	-4.52	105.98	110.36
18	A	606	HEA	C4B-C3B-C2B	-4.51	99.71	107.41
23	C	313	DMU	C6-O5-C4	4.41	122.34	113.69
18	A	606	HEA	C1B-C2B-C3B	4.39	112.06	106.80
23	C	301	DMU	O5-C4-C57	4.39	117.34	106.44
17	A	604	PGV	O03-C19-C20	4.39	125.67	111.91
18	N	607	HEA	C4B-C3B-C2B	-4.38	99.92	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	607	HEA	CMC-C2C-C3C	4.36	132.83	124.68
18	A	606	HEA	C3D-C4D-ND	-4.35	106.14	110.36
18	N	606	HEA	C2B-C1B-NB	-4.34	104.68	109.88
17	T	101	PGV	O03-C19-C20	4.32	125.45	111.91
18	N	606	HEA	C1B-C2B-C3B	4.28	111.93	106.80
18	N	607	HEA	C1D-ND-C4D	4.28	109.49	105.07
17	N	616	PGV	O03-C19-C20	4.26	125.28	111.91
18	A	607	HEA	C2D-C1D-ND	4.19	114.81	109.84
18	N	606	HEA	CMB-C2B-C1B	-4.18	118.67	125.04
23	P	302	DMU	O5-C6-O16	4.16	119.82	109.97
18	N	607	HEA	C3B-C4B-NB	4.16	114.77	109.84
17	Z	102	PGV	O01-C1-C2	4.13	120.41	111.50
22	P	308	CHD	C1-C2-C3	4.12	115.75	110.47
18	N	607	HEA	C26-C15-C16	4.11	122.18	115.27
18	A	607	HEA	C13-C14-C15	4.06	137.44	127.66
18	N	606	HEA	CAD-CBD-CGD	-4.00	105.00	113.60
18	A	606	HEA	C3B-C4B-NB	3.97	114.54	109.84
18	N	607	HEA	CAA-CBA-CGA	-3.90	102.82	113.76
18	N	606	HEA	C4B-C3B-C2B	-3.88	100.78	107.41
22	Y	102	CHD	C5-C6-C7	-3.85	110.22	114.46
23	C	301	DMU	C8-C7-C5	3.81	117.47	110.82
18	A	607	HEA	C2B-C1B-NB	-3.77	105.36	109.88
18	A	606	HEA	CMC-C2C-C3C	3.75	131.70	124.68
18	N	607	HEA	CHA-C4D-ND	3.73	128.48	124.43
23	Z	101	DMU	O16-C6-C1	3.71	114.10	108.30
18	N	607	HEA	C4B-NB-C1B	3.71	108.90	105.07
18	N	606	HEA	CMD-C2D-C1D	3.70	130.68	125.04
17	Z	102	PGV	O03-C19-C20	3.65	123.36	111.91
18	A	607	HEA	C3B-C4B-NB	3.64	114.15	109.84
23	P	302	DMU	C6-C1-C2	-3.60	102.50	110.00
18	N	606	HEA	C4B-NB-C1B	3.50	108.68	105.07
23	Z	101	DMU	C11-C9-C8	-3.45	104.91	113.00
23	M	101	DMU	O1-C9-C11	3.43	114.97	106.44
17	A	604	PGV	O01-C1-O02	-3.40	115.49	123.70
18	A	607	HEA	C4B-C3B-C2B	-3.39	101.61	107.41
18	N	606	HEA	C13-C12-C11	-3.39	109.26	114.35
23	C	313	DMU	O5-C4-C3	3.37	116.85	109.75
25	C	306	CDL	OA6-CA5-C11	3.30	118.61	111.50
18	N	607	HEA	CHB-C1B-NB	3.30	128.01	124.43
18	N	606	HEA	C3B-C4B-NB	3.25	113.69	109.84
17	N	616	PGV	O01-C1-C2	3.25	118.50	111.50
18	A	606	HEA	C4D-C3D-C2D	3.25	111.63	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Z	101	DMU	O1-C9-C11	3.24	114.50	106.44
18	N	607	HEA	C2D-C1D-ND	3.22	113.66	109.84
18	A	606	HEA	C26-C15-C16	3.22	120.69	115.27
23	M	101	DMU	C22-C19-C18	-3.21	99.28	113.49
20	Y	101	TGL	OG2-CB1-CB2	3.20	118.40	111.50
18	A	606	HEA	CMB-C2B-C1B	-3.20	120.17	125.04
22	T	104	CHD	C17-C13-C14	3.19	103.31	100.09
22	C	302	CHD	C6-C7-C8	3.17	114.87	111.48
18	A	607	HEA	CMD-C2D-C1D	3.10	129.77	125.04
18	A	607	HEA	CHA-C4D-ND	3.10	127.80	124.43
23	G	1302	DMU	C18-O16-C6	3.06	118.92	113.84
18	N	606	HEA	C27-C19-C20	3.03	120.37	115.27
23	M	101	DMU	C34-C31-C28	-3.02	99.12	114.42
18	A	607	HEA	C17-C18-C19	-2.99	120.45	127.66
18	A	607	HEA	CMB-C2B-C1B	-2.97	120.52	125.04
20	N	604	TGL	OG2-CB1-CB2	2.97	117.89	111.50
23	P	302	DMU	O16-C18-C19	-2.96	99.19	109.56
17	N	605	PGV	O01-C1-O02	-2.95	116.58	123.70
18	A	607	HEA	C1B-C2B-C3B	2.93	110.30	106.80
18	A	607	HEA	C16-C17-C18	2.93	121.50	111.88
17	P	306	PGV	O01-C1-C2	2.90	117.76	111.50
20	D	201	TGL	OG2-CB1-CB2	2.89	117.73	111.50
23	C	313	DMU	O7-C10-O1	2.86	118.65	110.67
18	N	606	HEA	C4D-C3D-C2D	2.85	111.05	106.90
17	A	604	PGV	O04-C19-C20	-2.85	112.62	123.73
18	N	606	HEA	CHD-C1D-C2D	-2.84	118.86	126.72
17	P	306	PGV	O14-P-O13	2.83	126.22	112.24
23	G	1302	DMU	C10-O1-C9	2.82	119.23	113.69
23	C	313	DMU	C25-C22-C19	-2.81	100.14	114.42
23	G	1302	DMU	O16-C6-C1	2.81	112.68	108.30
20	A	615	TGL	OG2-CB1-CB2	2.80	117.54	111.50
18	A	606	HEA	CHD-C1D-C2D	-2.80	118.98	126.72
23	Z	101	DMU	O1-C9-C8	2.79	114.76	109.69
18	A	607	HEA	CAA-CBA-CGA	-2.79	105.94	113.76
17	P	306	PGV	O01-C1-O02	-2.78	116.99	123.70
23	G	1302	DMU	O7-C3-C2	2.74	114.56	107.28
22	T	104	CHD	C14-C8-C7	2.74	115.44	111.81
18	N	607	HEA	C1B-C2B-C3B	2.74	110.08	106.80
28	I	101	SAC	O-C-CA	-2.73	117.64	124.78
23	P	302	DMU	C10-O7-C3	-2.71	111.27	117.96
23	C	313	DMU	C34-C31-C28	-2.68	100.82	114.42
18	A	606	HEA	C2B-C1B-NB	-2.68	106.67	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	N	607	HEA	C4A-CHB-C1B	2.68	126.09	122.56
18	A	607	HEA	O11-C11-C12	2.65	116.83	109.42
18	A	606	HEA	C4A-CHB-C1B	-2.64	119.08	122.56
22	P	308	CHD	C2-C1-C10	2.63	117.30	112.78
18	N	606	HEA	C3D-C4D-ND	-2.61	107.83	110.36
23	G	1302	DMU	O5-C4-C3	2.60	115.23	109.75
28	V	101	SAC	O-C-CA	-2.59	117.98	124.78
18	N	606	HEA	C25-C23-C24	2.59	120.33	114.60
18	N	607	HEA	CAD-CBD-CGD	-2.59	108.04	113.60
18	N	606	HEA	O2D-CGD-CBD	2.55	122.23	114.03
23	P	302	DMU	C37-C34-C31	-2.55	101.47	114.42
24	P	304	PEK	O01-C1-O02	-2.55	117.54	123.70
17	N	616	PGV	O03-C19-O04	-2.53	117.20	123.59
23	C	301	DMU	C7-C8-C9	2.51	114.72	110.24
23	C	313	DMU	C7-C8-C9	-2.50	105.77	110.24
18	A	606	HEA	CBD-CAD-C3D	2.50	119.57	112.63
18	A	606	HEA	CAD-C3D-C4D	-2.48	120.32	124.66
18	N	606	HEA	C26-C15-C16	2.44	119.37	115.27
18	N	607	HEA	C17-C18-C19	-2.43	121.80	127.66
17	Z	102	PGV	C7-C6-C5	-2.42	102.13	114.42
18	A	607	HEA	C1D-ND-C4D	2.41	107.56	105.07
18	N	607	HEA	CMD-C2D-C1D	2.41	128.71	125.04
23	Z	101	DMU	C10-C5-C7	-2.39	105.02	110.00
23	M	101	DMU	O49-C1-C6	-2.37	104.28	110.05
18	N	607	HEA	C13-C14-C15	-2.36	121.97	127.66
23	C	313	DMU	O2-C8-C7	2.35	115.79	110.35
17	T	101	PGV	O03-C01-C02	2.35	115.27	108.43
25	P	307	CDL	OB6-CB5-OB7	-2.34	118.06	123.70
23	C	301	DMU	C57-C4-C3	-2.33	106.54	113.33
17	C	305	PGV	O14-P-O13	2.32	123.72	112.24
20	D	201	TGL	OG2-CB1-OB1	-2.32	118.10	123.70
22	T	104	CHD	C15-C14-C8	2.31	121.56	118.33
23	C	301	DMU	C10-C5-C7	2.31	114.80	110.00
25	C	306	CDL	OB2-PB2-OB3	2.30	118.06	109.07
18	N	607	HEA	CAD-C3D-C4D	-2.30	120.64	124.66
22	T	104	CHD	C22-C23-C24	2.29	118.59	112.51
18	N	606	HEA	O1D-CGD-CBD	-2.29	115.74	123.08
22	Y	102	CHD	C16-C17-C13	-2.28	101.32	103.55
17	T	101	PGV	O04-C19-C20	-2.26	114.92	123.73
18	A	606	HEA	C27-C19-C20	2.25	119.06	115.27
23	C	313	DMU	C10-O1-C9	2.23	118.07	113.69
17	Z	102	PGV	O03-C01-C02	2.23	114.92	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Z	101	DMU	C10-O1-C9	2.21	118.03	113.69
23	G	1302	DMU	O1-C9-C11	2.19	111.89	106.44
18	N	606	HEA	CAD-C3D-C4D	-2.19	120.83	124.66
18	N	606	HEA	CBA-CAA-C2A	-2.18	108.93	112.60
23	C	301	DMU	C1-C2-C3	2.16	114.61	109.68
23	C	313	DMU	C10-O7-C3	-2.16	112.63	117.96
18	A	606	HEA	C4D-CHA-C1A	2.14	125.38	122.56
18	N	606	HEA	OMA-CMA-C3A	-2.14	120.25	124.91
23	G	1302	DMU	C6-O5-C4	2.14	117.89	113.69
23	P	302	DMU	C6-O5-C4	2.13	117.88	113.69
23	Z	101	DMU	C34-C31-C28	-2.12	103.68	114.42
18	A	606	HEA	CBA-CAA-C2A	-2.12	109.04	112.60
17	P	306	PGV	C22-C21-C20	-2.11	105.61	113.19
22	B	302	CHD	C17-C13-C14	2.10	102.21	100.09
22	Y	102	CHD	C9-C11-C12	2.08	117.05	114.30
18	N	606	HEA	CMC-C2C-C3C	2.07	128.55	124.68
17	N	605	PGV	O12-P-O13	2.07	117.15	109.07
23	M	101	DMU	C37-C34-C31	-2.07	103.93	114.42
23	P	302	DMU	C31-C28-C25	-2.07	103.93	114.42
22	T	104	CHD	C2-C1-C10	2.06	116.32	112.78
23	C	301	DMU	O7-C10-C5	2.06	113.43	108.10
23	P	302	DMU	O7-C10-C5	2.05	113.41	108.10
18	A	607	HEA	C25-C23-C24	2.05	119.12	114.60
18	N	607	HEA	C3A-C4A-NA	2.03	114.77	110.94
24	P	304	PEK	O11-P-O14	-2.03	101.14	109.07
17	Z	102	PGV	C01-O03-C19	2.02	124.61	117.12
23	P	302	DMU	O2-C8-C7	-2.02	105.68	110.35
23	P	302	DMU	C7-C8-C9	2.01	113.83	110.24
22	T	104	CHD	C18-C13-C12	-2.01	107.02	109.07

All (12) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
18	N	607	HEA	ND
18	N	607	HEA	NA
18	N	607	HEA	NB

All (980) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C03-O11-P-O14
17	A	604	PGV	C04-C05-C06-O06
17	A	604	PGV	O02-C1-O01-C02
17	A	604	PGV	C2-C1-O01-C02
17	N	616	PGV	C03-O11-P-O13
17	N	616	PGV	C04-O12-P-O13
17	N	616	PGV	O12-C04-C05-O05
17	N	616	PGV	O02-C1-O01-C02
17	T	101	PGV	O12-C04-C05-C06
17	Z	102	PGV	O02-C1-O01-C02
18	A	607	HEA	C11-C12-C13-C14
20	D	201	TGL	CB2-CB1-OG2-CG2
20	L	101	TGL	OB1-CB1-OG2-CG2
20	Y	101	TGL	CB2-CB1-OG2-CG2
20	Y	101	TGL	OB1-CB1-OG2-CG2
23	C	301	DMU	C1-C6-O16-C18
23	C	301	DMU	O5-C6-O16-C18
23	C	301	DMU	C19-C18-O16-C6
23	C	313	DMU	O5-C6-O16-C18
23	C	313	DMU	C19-C18-O16-C6
23	G	1302	DMU	C19-C18-O16-C6
24	C	303	PEK	O12-C04-C05-N
24	C	303	PEK	C6-C7-C8-C9
24	C	304	PEK	C04-O12-P-O14
24	C	304	PEK	O12-C04-C05-N
24	C	304	PEK	C2-C1-O01-C02
24	C	304	PEK	C9-C10-C11-C12
24	C	315	PEK	C03-O11-P-O12
24	C	315	PEK	C03-O11-P-O13
24	C	315	PEK	C03-O11-P-O14
24	C	315	PEK	C11-C12-C13-C14
24	P	301	PEK	C03-O11-P-O14
24	P	301	PEK	C2-C1-O01-C02
24	P	305	PEK	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
24	P	305	PEK	C03-O11-P-O14
24	P	305	PEK	C04-O12-P-O14
24	P	305	PEK	O12-C04-C05-N
24	P	305	PEK	O02-C1-O01-C02
25	C	306	CDL	O1-C1-CB2-OB2
25	C	306	CDL	C1-CA2-OA2-PA1
25	C	306	CDL	OA7-CA5-OA6-CA4
25	C	306	CDL	C11-CA5-OA6-CA4
25	C	306	CDL	CB2-OB2-PB2-OB3
25	C	312	CDL	CA2-OA2-PA1-OA5
25	C	312	CDL	CB2-OB2-PB2-OB3
25	C	312	CDL	CB2-OB2-PB2-OB4
25	C	312	CDL	C51-CB5-OB6-CB4
25	P	307	CDL	CB2-C1-CA2-OA2
25	P	307	CDL	C1-CA2-OA2-PA1
25	P	307	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	CA3-OA5-PA1-OA3
25	T	102	CDL	CB2-OB2-PB2-OB5
26	E	201	PSC	C03-O11-P-O13
26	E	201	PSC	C04-O12-P-O14
26	O	302	PSC	C03-O11-P-O13
26	O	302	PSC	C04-O12-P-O11
26	O	302	PSC	C04-O12-P-O14
26	O	302	PSC	O12-C04-C05-N
28	I	101	SAC	C2A-C1A-N-CA
28	I	101	SAC	OAC-C1A-N-CA
28	I	101	SAC	C-CA-N-C1A
28	I	101	SAC	CB-CA-N-C1A
28	I	101	SAC	O-C-CA-CB
28	V	101	SAC	C2A-C1A-N-CA
28	V	101	SAC	OAC-C1A-N-CA
23	G	1302	DMU	O1-C10-O7-C3
20	Q	201	TGL	OC1-CC1-OG3-CG3
23	P	302	DMU	C3-C4-C57-O61
17	A	604	PGV	O04-C19-O03-C01
20	D	201	TGL	OC1-CC1-OG3-CG3
24	C	304	PEK	O04-C21-O03-C01
25	C	312	CDL	OB9-CB7-OB8-CB6
25	P	307	CDL	OA9-CA7-OA8-CA6
26	O	302	PSC	O04-C19-O03-C01
20	D	201	TGL	OB1-CB1-OG2-CG2
24	C	304	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
24	P	301	PEK	O02-C1-O01-C02
25	C	312	CDL	OB7-CB5-OB6-CB4
20	D	201	TGL	CC2-CC1-OG3-CG3
24	C	304	PEK	C22-C21-O03-C01
25	C	312	CDL	C71-CB7-OB8-CB6
25	P	307	CDL	C31-CA7-OA8-CA6
17	N	616	PGV	C2-C1-O01-C02
17	Z	102	PGV	C2-C1-O01-C02
20	L	101	TGL	CB2-CB1-OG2-CG2
24	P	305	PEK	C2-C1-O01-C02
18	A	607	HEA	C26-C15-C16-C17
22	J	1102	CHD	C20-C22-C23-C24
22	P	308	CHD	C20-C22-C23-C24
22	T	104	CHD	C20-C22-C23-C24
17	A	604	PGV	C20-C19-O03-C01
20	Q	201	TGL	CC2-CC1-OG3-CG3
25	T	102	CDL	C31-CA7-OA8-CA6
26	O	302	PSC	C20-C19-O03-C01
17	Z	102	PGV	O04-C19-O03-C01
20	Y	101	TGL	OA1-CA1-OG1-CG1
17	T	101	PGV	O12-C04-C05-O05
17	Z	102	PGV	O12-C04-C05-O05
25	C	312	CDL	O1-C1-CB2-OB2
26	E	201	PSC	C20-C19-O03-C01
25	C	306	CDL	C51-CB5-OB6-CB4
23	G	1302	DMU	O5-C4-C57-O61
23	P	302	DMU	O5-C4-C57-O61
20	L	101	TGL	CA3-CA4-CA5-CA6
24	C	315	PEK	C26-C27-C28-C29
25	T	102	CDL	C79-C80-C81-C82
26	E	201	PSC	O04-C19-O03-C01
22	Y	102	CHD	C13-C17-C20-C22
20	D	201	TGL	C14-C29-C30-C31
24	C	303	PEK	C22-C23-C24-C25
25	T	102	CDL	C42-C43-C44-C45
23	C	301	DMU	C5-C10-O7-C3
17	Z	102	PGV	C20-C19-O03-C01
20	Y	101	TGL	CA2-CA1-OG1-CG1
25	T	102	CDL	OA9-CA7-OA8-CA6
23	C	301	DMU	O6-C11-C9-O1
26	E	201	PSC	C30-C31-C32-C33
17	N	616	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
25	C	306	CDL	CA2-C1-CB2-OB2
17	N	616	PGV	C20-C19-O03-C01
25	T	102	CDL	C71-CB7-OB8-CB6
23	G	1302	DMU	O6-C11-C9-C8
24	C	304	PEK	C24-C25-C26-C27
22	T	104	CHD	C16-C17-C20-C21
22	T	104	CHD	C13-C17-C20-C22
20	Q	201	TGL	CA1-CA2-CA3-CA4
24	P	305	PEK	C1-C2-C3-C4
25	T	102	CDL	CB7-C71-C72-C73
23	C	301	DMU	O6-C11-C9-C8
23	C	301	DMU	O1-C10-O7-C3
25	P	307	CDL	O1-C1-CA2-OA2
23	C	313	DMU	C1-C6-O16-C18
23	P	302	DMU	C1-C6-O16-C18
23	M	101	DMU	O6-C11-C9-C8
23	G	1302	DMU	O6-C11-C9-O1
25	C	306	CDL	OB7-CB5-OB6-CB4
17	A	604	PGV	C19-C20-C21-C22
24	C	315	PEK	C21-C22-C23-C24
17	N	616	PGV	O04-C19-O03-C01
25	T	102	CDL	OB9-CB7-OB8-CB6
22	T	104	CHD	C17-C20-C22-C23
23	M	101	DMU	O6-C11-C9-O1
23	G	1302	DMU	C3-C4-C57-O61
17	Z	102	PGV	C1-C2-C3-C4
20	N	604	TGL	CA1-CA2-CA3-CA4
24	P	301	PEK	C21-C22-C23-C24
26	O	302	PSC	C1-C2-C3-C4
17	C	305	PGV	C12-C13-C14-C15
20	Q	201	TGL	CB1-CB2-CB3-CB4
24	C	303	PEK	C1-C2-C3-C4
24	C	315	PEK	C1-C2-C3-C4
25	C	306	CDL	CB7-C71-C72-C73
25	C	312	CDL	CB7-C71-C72-C73
25	T	102	CDL	CA5-C11-C12-C13
25	T	102	CDL	CA7-C31-C32-C33
22	Y	102	CHD	C17-C20-C22-C23
17	A	605	PGV	C26-C27-C28-C29
26	O	302	PSC	C20-C21-C22-C23
22	T	104	CHD	C21-C20-C22-C23
20	D	201	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C04-C05-N-C07
17	Z	102	PGV	C19-C20-C21-C22
19	W	304	EDO	O1-C1-C2-O2
25	C	312	CDL	C11-CA5-OA6-CA4
22	T	104	CHD	C13-C17-C20-C21
22	Y	102	CHD	C21-C20-C22-C23
23	P	302	DMU	O16-C18-C19-C22
20	D	201	TGL	CC1-CC2-CC3-CC4
26	O	302	PSC	C19-C20-C21-C22
25	C	306	CDL	O1-C1-CA2-OA2
25	T	102	CDL	O1-C1-CB2-OB2
25	C	312	CDL	OA7-CA5-OA6-CA4
22	Y	102	CHD	C13-C17-C20-C21
20	N	604	TGL	CB1-CB2-CB3-CB4
17	A	604	PGV	C03-O11-P-O12
17	A	604	PGV	C04-O12-P-O11
17	T	101	PGV	C04-O12-P-O11
24	C	304	PEK	C04-O12-P-O11
24	P	305	PEK	C04-O12-P-O11
25	C	306	CDL	CA3-OA5-PA1-OA2
25	C	312	CDL	CA3-OA5-PA1-OA2
25	C	312	CDL	CB2-OB2-PB2-OB5
25	P	307	CDL	CA3-OA5-PA1-OA2
25	P	307	CDL	CB2-OB2-PB2-OB5
26	O	302	PSC	C03-O11-P-O12
24	P	304	PEK	C1-C2-C3-C4
20	N	604	TGL	CC1-CC2-CC3-CC4
25	C	306	CDL	CB2-C1-CA2-OA2
25	T	102	CDL	CA2-C1-CB2-OB2
26	E	201	PSC	C04-C05-N-C08
20	N	604	TGL	CA2-CA1-OG1-CG1
20	A	615	TGL	CB9-C10-C11-C12
23	M	101	DMU	O16-C18-C19-C22
25	C	306	CDL	C52-C53-C54-C55
26	O	302	PSC	C2-C1-O01-C02
17	A	604	PGV	C7-C8-C9-C10
17	N	616	PGV	C28-C29-C30-C31
17	P	306	PGV	C7-C8-C9-C10
17	T	101	PGV	C3-C4-C5-C6
20	A	615	TGL	CA3-CA4-CA5-CA6
20	A	615	TGL	CB7-CB8-CB9-C10
20	D	201	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
20	L	101	TGL	CB6-CB7-CB8-CB9
20	N	604	TGL	C10-C11-C12-C13
24	C	303	PEK	C31-C32-C33-C34
24	P	301	PEK	C25-C26-C27-C28
25	C	312	CDL	C37-C38-C39-C40
25	C	312	CDL	C57-C58-C59-C60
25	C	312	CDL	C59-C60-C61-C62
25	P	307	CDL	C36-C37-C38-C39
26	O	302	PSC	C25-C26-C27-C28
17	A	604	PGV	C6-C7-C8-C9
17	A	605	PGV	C4-C5-C6-C7
17	T	101	PGV	C23-C24-C25-C26
20	L	101	TGL	CC9-C15-C16-C17
20	N	604	TGL	CB5-CB6-CB7-CB8
24	C	303	PEK	C24-C25-C26-C27
25	C	306	CDL	C14-C15-C16-C17
25	C	312	CDL	C20-C21-C22-C23
25	P	307	CDL	C12-C13-C14-C15
25	P	307	CDL	C43-C44-C45-C46
25	T	102	CDL	C63-C64-C65-C66
26	O	302	PSC	O02-C1-O01-C02
17	N	616	PGV	C3-C4-C5-C6
20	Y	101	TGL	CC2-CC3-CC4-CC5
24	P	301	PEK	C26-C27-C28-C29
24	P	305	PEK	C32-C33-C34-C35
26	O	302	PSC	C02-C03-O11-P
24	C	315	PEK	C10-C11-C12-C13
24	C	315	PEK	C13-C14-C15-C16
17	C	305	PGV	C24-C25-C26-C27
23	Z	101	DMU	C28-C31-C34-C37
25	P	307	CDL	C81-C82-C83-C84
17	A	604	PGV	O12-C04-C05-O05
20	L	101	TGL	CB7-CB8-CB9-C10
25	C	312	CDL	C56-C57-C58-C59
25	P	307	CDL	C19-C20-C21-C22
26	E	201	PSC	C4-C5-C6-C7
25	C	312	CDL	CB5-C51-C52-C53
24	P	301	PEK	C22-C21-O03-C01
17	N	605	PGV	C4-C5-C6-C7
17	N	605	PGV	C5-C6-C7-C8
20	N	604	TGL	C22-C23-C24-C25
20	Q	201	TGL	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
20	Q	201	TGL	CB4-CB5-CB6-CB7
23	G	1302	DMU	C31-C34-C37-C40
25	P	307	CDL	C77-C78-C79-C80
25	P	307	CDL	C78-C79-C80-C81
20	D	201	TGL	C16-C17-C18-C19
20	N	604	TGL	CA7-CA8-CA9-C20
20	Q	201	TGL	C21-C20-CA9-CA8
20	Q	201	TGL	CB2-CB3-CB4-CB5
20	Q	201	TGL	C16-C17-C18-C19
25	C	306	CDL	C56-C57-C58-C59
17	N	605	PGV	C30-C31-C32-C33
20	A	615	TGL	C11-C10-CB9-CB8
20	D	201	TGL	CC7-CC8-CC9-C15
20	D	201	TGL	C16-C15-CC9-CC8
20	N	604	TGL	CC7-CC8-CC9-C15
20	Q	201	TGL	C10-C11-C12-C13
24	C	315	PEK	C29-C30-C31-C32
25	C	306	CDL	C39-C40-C41-C42
25	C	312	CDL	C31-C32-C33-C34
26	O	302	PSC	C14-C15-C16-C17
17	T	101	PGV	C28-C29-C30-C31
20	L	101	TGL	C16-C17-C18-C19
20	Q	201	TGL	C16-C15-CC9-CC8
24	C	315	PEK	C28-C29-C30-C31
25	T	102	CDL	C36-C37-C38-C39
26	O	302	PSC	C22-C23-C24-C25
17	Z	102	PGV	C04-C05-C06-O06
20	D	201	TGL	C21-C20-CA9-CA8
20	Y	101	TGL	C23-C24-C25-C26
25	C	306	CDL	C81-C82-C83-C84
25	P	307	CDL	C22-C23-C24-C25
17	A	604	PGV	C11-C10-C9-C8
24	C	304	PEK	C21-C22-C23-C24
26	E	201	PSC	C19-C20-C21-C22
17	A	605	PGV	C6-C7-C8-C9
17	A	605	PGV	C29-C30-C31-C32
17	N	616	PGV	C29-C30-C31-C32
17	Z	102	PGV	C6-C7-C8-C9
17	Z	102	PGV	C21-C22-C23-C24
20	A	615	TGL	C17-C18-C19-C33
20	D	201	TGL	C24-C25-C26-C27
20	L	101	TGL	CA9-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
20	Y	101	TGL	C13-C14-C29-C30
24	P	305	PEK	C27-C28-C29-C30
25	P	307	CDL	C55-C56-C57-C58
25	T	102	CDL	C12-C13-C14-C15
17	N	605	PGV	C23-C24-C25-C26
17	P	306	PGV	C6-C7-C8-C9
17	Z	102	PGV	C26-C27-C28-C29
20	D	201	TGL	CB4-CB5-CB6-CB7
20	L	101	TGL	C18-C19-C33-C34
24	C	304	PEK	C33-C34-C35-C36
25	T	102	CDL	C18-C19-C20-C21
25	T	102	CDL	C56-C57-C58-C59
17	A	604	PGV	C4-C5-C6-C7
20	L	101	TGL	CC6-CC7-CC8-CC9
20	N	604	TGL	CB3-CB4-CB5-CB6
20	N	604	TGL	C11-C10-CB9-CB8
20	Y	101	TGL	CA9-C20-C21-C22
24	C	304	PEK	C26-C27-C28-C29
24	C	315	PEK	C16-C17-C18-C19
25	C	306	CDL	C43-C44-C45-C46
25	C	312	CDL	C15-C16-C17-C18
20	N	604	TGL	OA1-CA1-OG1-CG1
20	A	615	TGL	CB6-CB7-CB8-CB9
20	D	201	TGL	CA6-CA7-CA8-CA9
25	C	306	CDL	C73-C74-C75-C76
25	C	306	CDL	C77-C78-C79-C80
17	A	604	PGV	C5-C6-C7-C8
17	A	604	PGV	C26-C27-C28-C29
20	A	615	TGL	CB3-CB4-CB5-CB6
20	A	615	TGL	CC6-CC7-CC8-CC9
25	C	306	CDL	C36-C37-C38-C39
25	P	307	CDL	C37-C38-C39-C40
22	Y	102	CHD	C16-C17-C20-C22
17	A	605	PGV	C5-C6-C7-C8
23	G	1302	DMU	C22-C25-C28-C31
25	C	312	CDL	C75-C76-C77-C78
20	A	615	TGL	CA9-C20-C21-C22
20	Y	101	TGL	C19-C33-C34-C35
23	C	301	DMU	C19-C22-C25-C28
20	N	604	TGL	CA9-C20-C21-C22
20	Q	201	TGL	C12-C13-C14-C29
24	C	315	PEK	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	C	312	CDL	C80-C81-C82-C83
25	T	102	CDL	C32-C33-C34-C35
17	T	101	PGV	C14-C15-C16-C17
20	A	615	TGL	CB2-CB1-OG2-CG2
25	T	102	CDL	C11-CA5-OA6-CA4
24	P	304	PEK	C23-C24-C25-C26
22	Y	102	CHD	C16-C17-C20-C21
17	A	604	PGV	O05-C05-C06-O06
20	A	615	TGL	CC4-CC5-CC6-CC7
20	N	604	TGL	C20-C21-C22-C23
25	T	102	CDL	C51-C52-C53-C54
17	T	101	PGV	C12-C13-C14-C15
24	P	304	PEK	C15-C16-C17-C18
26	O	302	PSC	C13-C14-C15-C16
17	T	101	PGV	C25-C26-C27-C28
20	N	604	TGL	C15-C16-C17-C18
24	P	301	PEK	O04-C21-O03-C01
25	C	312	CDL	CA2-C1-CB2-OB2
17	N	605	PGV	C6-C7-C8-C9
20	N	604	TGL	CC3-CC4-CC5-CC6
24	C	304	PEK	C29-C30-C31-C32
24	P	304	PEK	C34-C35-C36-C37
25	T	102	CDL	OA7-CA5-OA6-CA4
23	G	1302	DMU	C2-C3-O7-C10
24	P	304	PEK	C28-C29-C30-C31
20	N	604	TGL	CA5-CA6-CA7-CA8
20	Y	101	TGL	C11-C12-C13-C14
26	E	201	PSC	C5-C6-C7-C8
26	E	201	PSC	C04-C05-N-C06
19	A	611	EDO	O1-C1-C2-O2
19	A	614	EDO	O1-C1-C2-O2
19	A	619	EDO	O1-C1-C2-O2
19	B	306	EDO	O1-C1-C2-O2
19	B	307	EDO	O1-C1-C2-O2
19	B	308	EDO	O1-C1-C2-O2
19	C	310	EDO	O1-C1-C2-O2
19	D	205	EDO	O1-C1-C2-O2
19	D	206	EDO	O1-C1-C2-O2
19	N	619	EDO	O1-C1-C2-O2
19	Q	203	EDO	O1-C1-C2-O2
19	S	2207	EDO	O1-C1-C2-O2
19	T	103	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	V	102	EDO	O1-C1-C2-O2
20	D	201	TGL	C19-C33-C34-C35
25	C	312	CDL	C52-C53-C54-C55
25	C	312	CDL	C73-C74-C75-C76
25	P	307	CDL	C58-C59-C60-C61
25	P	307	CDL	C51-CB5-OB6-CB4
25	T	102	CDL	C51-CB5-OB6-CB4
17	T	101	PGV	C22-C23-C24-C25
20	N	604	TGL	C16-C15-CC9-CC8
24	C	303	PEK	C16-C17-C18-C19
25	C	306	CDL	C76-C77-C78-C79
25	C	306	CDL	C78-C79-C80-C81
17	P	306	PGV	C1-C2-C3-C4
20	L	101	TGL	C21-C22-C23-C24
18	A	607	HEA	C14-C15-C16-C17
20	Q	201	TGL	C18-C19-C33-C34
25	T	102	CDL	C34-C35-C36-C37
24	C	304	PEK	C15-C16-C17-C18
24	P	305	PEK	C15-C16-C17-C18
20	N	604	TGL	OB1-CB1-OG2-CG2
24	P	305	PEK	C22-C21-O03-C01
17	Z	102	PGV	C13-C14-C15-C16
17	N	616	PGV	C24-C25-C26-C27
20	D	201	TGL	CC5-CC6-CC7-CC8
25	C	312	CDL	C60-C61-C62-C63
20	A	615	TGL	CB1-CB2-CB3-CB4
17	N	605	PGV	C7-C8-C9-C10
20	A	615	TGL	CA6-CA7-CA8-CA9
20	Q	201	TGL	CC3-CC4-CC5-CC6
25	T	102	CDL	C37-C38-C39-C40
17	T	101	PGV	C2-C1-O01-C02
20	N	604	TGL	CB2-CB1-OG2-CG2
20	Q	201	TGL	CB2-CB1-OG2-CG2
25	P	307	CDL	C11-CA5-OA6-CA4
20	L	101	TGL	C12-C13-C14-C29
20	Q	201	TGL	CA3-CA4-CA5-CA6
24	P	305	PEK	C33-C34-C35-C36
17	T	101	PGV	O02-C1-O01-C02
20	A	615	TGL	OB1-CB1-OG2-CG2
20	Q	201	TGL	OB1-CB1-OG2-CG2
25	P	307	CDL	OB7-CB5-OB6-CB4
25	T	102	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	N	604	TGL	C21-C22-C23-C24
25	T	102	CDL	C38-C39-C40-C41
20	A	615	TGL	CA5-CA6-CA7-CA8
20	L	101	TGL	CC3-CC4-CC5-CC6
24	C	303	PEK	C33-C34-C35-C36
17	Z	102	PGV	C11-C10-C9-C8
18	N	607	HEA	C14-C15-C16-C17
20	N	604	TGL	CB4-CB5-CB6-CB7
20	Y	101	TGL	C20-C21-C22-C23
17	T	101	PGV	C30-C31-C32-C33
17	N	616	PGV	C25-C26-C27-C28
17	T	101	PGV	C4-C5-C6-C7
20	Y	101	TGL	C10-C11-C12-C13
24	C	304	PEK	C30-C31-C32-C33
25	P	307	CDL	C75-C76-C77-C78
25	P	307	CDL	OA7-CA5-OA6-CA4
25	C	306	CDL	C11-C12-C13-C14
26	O	302	PSC	C27-C28-C29-C30
17	N	616	PGV	C03-O11-P-O12
17	N	616	PGV	C04-O12-P-O11
24	P	301	PEK	C03-O11-P-O12
25	C	306	CDL	CB2-OB2-PB2-OB5
26	E	201	PSC	C03-O11-P-O12
25	C	306	CDL	C21-C22-C23-C24
17	Z	102	PGV	C2-C3-C4-C5
23	C	301	DMU	C22-C25-C28-C31
18	A	607	HEA	O11-C11-C12-C13
20	D	201	TGL	C12-C13-C14-C29
23	G	1302	DMU	C4-C3-O7-C10
25	T	102	CDL	C20-C21-C22-C23
26	E	201	PSC	C13-C14-C15-C16
20	N	604	TGL	CC4-CC5-CC6-CC7
25	C	306	CDL	C62-C63-C64-C65
18	N	607	HEA	C26-C15-C16-C17
20	A	615	TGL	C11-C12-C13-C14
20	A	615	TGL	CC2-CC3-CC4-CC5
25	T	102	CDL	C55-C56-C57-C58
17	C	305	PGV	C22-C23-C24-C25
17	Z	102	PGV	C15-C16-C17-C18
20	N	604	TGL	CA2-CA3-CA4-CA5
20	D	201	TGL	CG1-CG2-CG3-OG3
20	Y	101	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
23	Z	101	DMU	C22-C25-C28-C31
24	P	301	PEK	O03-C01-C02-C03
24	P	301	PEK	C17-C18-C19-C20
24	P	305	PEK	O03-C01-C02-C03
25	T	102	CDL	CB3-CB4-CB6-OB8
26	E	201	PSC	O03-C01-C02-C03
17	C	305	PGV	C27-C28-C29-C30
20	A	615	TGL	C25-C26-C27-C28
20	L	101	TGL	CC4-CC5-CC6-CC7
23	C	313	DMU	C34-C37-C40-C43
24	P	305	PEK	O04-C21-O03-C01
20	L	101	TGL	C22-C23-C24-C25
25	T	102	CDL	C35-C36-C37-C38
25	T	102	CDL	C72-C73-C74-C75
17	C	305	PGV	C31-C32-C33-C34
25	T	102	CDL	C82-C83-C84-C85
24	P	305	PEK	C35-C36-C37-C38
25	C	306	CDL	C34-C35-C36-C37
17	A	605	PGV	C7-C8-C9-C10
17	C	305	PGV	C7-C8-C9-C10
24	P	301	PEK	C35-C36-C37-C38
17	Z	102	PGV	O05-C05-C06-O06
20	L	101	TGL	C33-C34-C35-C36
20	Y	101	TGL	CB2-CB3-CB4-CB5
24	C	315	PEK	C34-C35-C36-C37
24	P	304	PEK	C30-C31-C32-C33
25	C	312	CDL	C35-C36-C37-C38
24	P	304	PEK	C2-C3-C4-C5
17	N	605	PGV	C29-C30-C31-C32
24	C	303	PEK	C2-C1-O01-C02
20	A	615	TGL	CC9-C15-C16-C17
25	P	307	CDL	C11-C12-C13-C14
20	Y	101	TGL	CA3-CA4-CA5-CA6
20	L	101	TGL	CC7-CC8-CC9-C15
24	P	305	PEK	C17-C18-C19-C20
24	P	301	PEK	C31-C32-C33-C34
25	T	102	CDL	C40-C41-C42-C43
26	O	302	PSC	C15-C16-C17-C18
17	A	605	PGV	C31-C32-C33-C34
20	Q	201	TGL	CB5-CB6-CB7-CB8
25	C	312	CDL	C44-C45-C46-C47
24	P	301	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	P	306	PGV	C20-C21-C22-C23
24	C	303	PEK	C17-C18-C19-C20
25	T	102	CDL	C75-C76-C77-C78
20	A	615	TGL	CA2-CA1-OG1-CG1
24	P	301	PEK	O01-C02-C03-O11
18	A	606	HEA	C4D-C3D-CAD-CBD
19	O	303	EDO	O1-C1-C2-O2
17	T	101	PGV	C15-C16-C17-C18
20	Y	101	TGL	CC4-CC5-CC6-CC7
25	C	312	CDL	C13-C14-C15-C16
17	T	101	PGV	C29-C30-C31-C32
20	D	201	TGL	CG2-CG1-OG1-CA1
20	D	201	TGL	OG2-CG2-CG3-OG3
20	L	101	TGL	OG2-CG2-CG3-OG3
20	Q	201	TGL	OG2-CG2-CG3-OG3
24	C	304	PEK	O03-C01-C02-O01
25	T	102	CDL	OB6-CB4-CB6-OB8
17	Z	102	PGV	C30-C31-C32-C33
25	P	307	CDL	C52-C53-C54-C55
25	P	307	CDL	C57-C58-C59-C60
20	A	615	TGL	CB4-CB5-CB6-CB7
25	C	306	CDL	C37-C38-C39-C40
25	T	102	CDL	C22-C23-C24-C25
18	A	606	HEA	C2D-C3D-CAD-CBD
17	P	306	PGV	C15-C16-C17-C18
20	L	101	TGL	C29-C30-C31-C32
26	O	302	PSC	C26-C27-C28-C29
20	D	201	TGL	CB2-CB3-CB4-CB5
23	M	101	DMU	C34-C37-C40-C43
25	C	312	CDL	C74-C75-C76-C77
20	A	615	TGL	CC2-CC1-OG3-CG3
20	A	615	TGL	CA2-CA3-CA4-CA5
25	C	312	CDL	C71-C72-C73-C74
20	A	615	TGL	C15-C16-C17-C18
25	T	102	CDL	C73-C74-C75-C76
17	N	616	PGV	C22-C23-C24-C25
25	C	312	CDL	C72-C73-C74-C75
25	C	306	CDL	OA5-CA3-CA4-CA6
25	C	312	CDL	OB5-CB3-CB4-CB6
17	N	616	PGV	C20-C21-C22-C23
17	A	604	PGV	C29-C30-C31-C32
23	C	301	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
20	A	615	TGL	C16-C17-C18-C19
25	P	307	CDL	C72-C73-C74-C75
23	Z	101	DMU	C34-C37-C40-C43
24	P	301	PEK	C02-C03-O11-P
25	T	102	CDL	CA4-CA3-OA5-PA1
20	N	604	TGL	CA3-CA4-CA5-CA6
25	C	306	CDL	C15-C16-C17-C18
20	N	604	TGL	C23-C24-C25-C26
25	C	306	CDL	C79-C80-C81-C82
20	A	615	TGL	CB5-CB6-CB7-CB8
20	L	101	TGL	CG1-CG2-CG3-OG3
24	C	304	PEK	O03-C01-C02-C03
25	C	306	CDL	CA3-CA4-CA6-OA8
25	C	306	CDL	CB3-CB4-CB6-OB8
25	P	307	CDL	CB3-CB4-CB6-OB8
17	C	305	PGV	C1-C2-C3-C4
24	C	303	PEK	C4-C5-C6-C7
20	Y	101	TGL	C17-C18-C19-C33
25	C	312	CDL	C76-C77-C78-C79
20	Q	201	TGL	C33-C34-C35-C36
24	P	301	PEK	C5-C6-C7-C8
24	P	301	PEK	C9-C10-C11-C12
24	P	301	PEK	C11-C12-C13-C14
24	P	304	PEK	C9-C10-C11-C12
24	P	305	PEK	C5-C6-C7-C8
24	P	305	PEK	C9-C10-C11-C12
25	T	102	CDL	CA3-OA5-PA1-OA2
26	E	201	PSC	C04-O12-P-O11
26	E	201	PSC	C9-C10-C11-C12
26	E	201	PSC	C10-C11-C12-C13
26	O	302	PSC	C10-C11-C12-C13
20	A	615	TGL	OA1-CA1-OG1-CG1
24	C	303	PEK	C28-C29-C30-C31
24	C	303	PEK	C35-C36-C37-C38
24	C	315	PEK	C24-C25-C26-C27
24	P	301	PEK	C30-C31-C32-C33
25	C	306	CDL	OB5-CB3-CB4-OB6
25	T	102	CDL	OA5-CA3-CA4-OA6
20	A	615	TGL	OC1-CC1-OG3-CG3
25	C	306	CDL	C44-C45-C46-C47
20	L	101	TGL	CA1-CA2-CA3-CA4
24	P	305	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	OG1-CG1-CG2-OG2
25	C	306	CDL	OA6-CA4-CA6-OA8
25	C	306	CDL	OB6-CB4-CB6-OB8
25	C	312	CDL	OA6-CA4-CA6-OA8
25	P	307	CDL	OB6-CB4-CB6-OB8
26	E	201	PSC	O03-C01-C02-O01
24	P	305	PEK	C34-C35-C36-C37
24	P	304	PEK	C2-C1-O01-C02
25	C	306	CDL	C23-C24-C25-C26
17	A	604	PGV	O12-C04-C05-C06
17	Z	102	PGV	O12-C04-C05-C06
25	P	307	CDL	CA2-C1-CB2-OB2
20	Q	201	TGL	CA4-CA5-CA6-CA7
24	C	315	PEK	O02-C1-O01-C02
20	D	201	TGL	C17-C18-C19-C33
17	A	604	PGV	C05-C04-O12-P
20	D	201	TGL	C13-C14-C29-C30
25	C	312	CDL	C34-C35-C36-C37
25	P	307	CDL	C84-C85-C86-C87
28	I	101	SAC	N-CA-CB-OG
17	N	616	PGV	C31-C32-C33-C34
19	B	304	EDO	O1-C1-C2-O2
19	G	1304	EDO	O1-C1-C2-O2
19	G	1306	EDO	O1-C1-C2-O2
19	I	103	EDO	O1-C1-C2-O2
24	P	305	PEK	C23-C24-C25-C26
26	E	201	PSC	C3-C4-C5-C6
25	C	312	CDL	C43-C44-C45-C46
25	T	102	CDL	OB5-CB3-CB4-CB6
20	N	604	TGL	CC5-CC6-CC7-CC8
25	C	306	CDL	C60-C61-C62-C63
20	A	615	TGL	CC3-CC4-CC5-CC6
20	L	101	TGL	CA6-CA7-CA8-CA9
25	C	306	CDL	C31-CA7-OA8-CA6
17	A	604	PGV	C03-C02-O01-C1
25	T	102	CDL	CA3-CA4-OA6-CA5
20	D	201	TGL	C33-C34-C35-C36
25	T	102	CDL	C57-C58-C59-C60
20	A	615	TGL	CG1-CG2-CG3-OG3
20	Q	201	TGL	OG1-CG1-CG2-CG3
20	Q	201	TGL	CG1-CG2-CG3-OG3
25	C	312	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
28	I	101	SAC	C-CA-CB-OG
25	P	307	CDL	C74-C75-C76-C77
25	C	306	CDL	OA5-CA3-CA4-OA6
17	A	605	PGV	C30-C31-C32-C33
20	A	615	TGL	C13-C14-C29-C30
20	A	615	TGL	C14-C29-C30-C31
25	C	312	CDL	C54-C55-C56-C57
24	C	303	PEK	C3-C4-C5-C6
25	T	102	CDL	C77-C78-C79-C80
20	Y	101	TGL	OG1-CG1-CG2-OG2
24	P	305	PEK	O03-C01-C02-O01
20	D	201	TGL	CC4-CC5-CC6-CC7
20	L	101	TGL	C11-C10-CB9-CB8
20	N	604	TGL	C25-C26-C27-C28
24	C	304	PEK	C35-C36-C37-C38
24	C	303	PEK	O02-C1-O01-C02
25	C	306	CDL	C35-C36-C37-C38
20	Y	101	TGL	C16-C17-C18-C19
25	C	312	CDL	C23-C24-C25-C26
26	O	302	PSC	C3-C4-C5-C6
24	C	315	PEK	C2-C1-O01-C02
17	Z	102	PGV	C3-C4-C5-C6
20	A	615	TGL	C29-C30-C31-C32
20	Q	201	TGL	C23-C24-C25-C26
24	C	304	PEK	C03-O11-P-O12
20	Y	101	TGL	CB3-CB4-CB5-CB6
17	C	305	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
24	C	315	PEK	C02-C03-O11-P
25	C	306	CDL	OA9-CA7-OA8-CA6
17	A	604	PGV	C04-O12-P-O14
17	N	616	PGV	C03-O11-P-O14
17	N	616	PGV	C04-O12-P-O14
17	T	101	PGV	C04-O12-P-O13
24	C	304	PEK	C04-O12-P-O13
24	P	301	PEK	C03-O11-P-O13
24	P	305	PEK	C04-O12-P-O13
25	C	306	CDL	CA3-OA5-PA1-OA3
25	C	306	CDL	CB2-OB2-PB2-OB4
25	C	312	CDL	CA2-OA2-PA1-OA4
25	C	312	CDL	CA3-OA5-PA1-OA3
25	P	307	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
25	P	307	CDL	CB2-OB2-PB2-OB4
25	T	102	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	CB2-OB2-PB2-OB3
26	E	201	PSC	C03-O11-P-O14
26	E	201	PSC	C04-O12-P-O13
26	O	302	PSC	C04-C05-N-C07
26	O	302	PSC	C04-C05-N-C08
23	P	302	DMU	O5-C6-O16-C18
24	P	301	PEK	C01-C02-C03-O11
25	C	306	CDL	OB5-CB3-CB4-CB6
25	P	307	CDL	OB5-CB3-CB4-CB6
25	T	102	CDL	OA5-CA3-CA4-CA6
24	P	304	PEK	C29-C30-C31-C32
24	P	304	PEK	O12-C04-C05-N
19	D	207	EDO	O1-C1-C2-O2
19	E	205	EDO	O1-C1-C2-O2
19	I	102	EDO	O1-C1-C2-O2
19	K	102	EDO	O1-C1-C2-O2
19	N	612	EDO	O1-C1-C2-O2
19	N	615	EDO	O1-C1-C2-O2
19	N	620	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
19	R	202	EDO	O1-C1-C2-O2
23	G	1302	DMU	C34-C37-C40-C43
25	C	312	CDL	C51-C52-C53-C54
24	P	301	PEK	C13-C14-C15-C16
24	P	305	PEK	C7-C8-C9-C10
17	C	305	PGV	C25-C26-C27-C28
23	P	302	DMU	C34-C37-C40-C43
18	A	607	HEA	C3B-C11-C12-C13
25	C	306	CDL	C40-C41-C42-C43
20	Y	101	TGL	C18-C19-C33-C34
17	N	605	PGV	C12-C13-C14-C15
20	L	101	TGL	CB4-CB5-CB6-CB7
25	C	306	CDL	C74-C75-C76-C77
25	P	307	CDL	OB5-CB3-CB4-OB6
26	O	302	PSC	O01-C02-C03-O11
24	P	304	PEK	C3-C4-C5-C6
26	O	302	PSC	C2-C3-C4-C5
17	T	101	PGV	O04-C19-O03-C01
20	L	101	TGL	C16-C15-CC9-CC8
24	P	305	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
20	N	604	TGL	OG1-CA1-CA2-CA3
20	D	201	TGL	OG1-CG1-CG2-CG3
20	N	604	TGL	C14-C29-C30-C31
25	C	306	CDL	C82-C83-C84-C85
26	E	201	PSC	O12-C04-C05-N
20	A	615	TGL	OG2-CG2-CG3-OG3
24	P	301	PEK	O03-C01-C02-O01
20	Q	201	TGL	CA9-C20-C21-C22
24	P	305	PEK	C2-C3-C4-C5
17	T	101	PGV	C7-C8-C9-C10
17	A	604	PGV	C9-C10-C11-C12
24	P	305	PEK	C02-C03-O11-P
25	C	306	CDL	CA4-CA3-OA5-PA1
25	P	307	CDL	C1-CB2-OB2-PB2
17	Z	102	PGV	C31-C32-C33-C34
22	J	1102	CHD	C17-C20-C22-C23
24	C	304	PEK	C23-C24-C25-C26
25	C	312	CDL	C63-C64-C65-C66
25	C	312	CDL	C81-C82-C83-C84
26	O	302	PSC	C30-C31-C32-C33
17	P	306	PGV	C28-C29-C30-C31
20	D	201	TGL	CA4-CA5-CA6-CA7
20	A	615	TGL	CC5-CC6-CC7-CC8
17	A	604	PGV	C13-C14-C15-C16
26	O	302	PSC	C04-C05-N-C06
17	T	101	PGV	C11-C12-C13-C14
17	A	604	PGV	C24-C25-C26-C27
25	C	312	CDL	C18-C19-C20-C21
24	P	305	PEK	C03-C02-O01-C1
25	C	312	CDL	CB3-CB4-OB6-CB5
26	O	302	PSC	C01-C02-C03-O11
20	N	604	TGL	C16-C17-C18-C19
17	A	604	PGV	C28-C29-C30-C31
20	Y	101	TGL	CC6-CC7-CC8-CC9
25	C	306	CDL	C22-C23-C24-C25
20	L	101	TGL	C20-C21-C22-C23
25	C	312	CDL	OB5-CB3-CB4-OB6
17	T	101	PGV	C27-C28-C29-C30
24	P	305	PEK	C30-C31-C32-C33
19	A	617	EDO	O1-C1-C2-O2
19	C	314	EDO	O1-C1-C2-O2
19	E	204	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	J	1105	EDO	O1-C1-C2-O2
19	S	2201	EDO	O1-C1-C2-O2
19	S	2204	EDO	O1-C1-C2-O2
19	W	301	EDO	O1-C1-C2-O2
19	W	303	EDO	O1-C1-C2-O2
25	C	312	CDL	C79-C80-C81-C82
25	T	102	CDL	C61-C62-C63-C64
17	T	101	PGV	C20-C19-O03-C01
20	D	201	TGL	OG3-CC1-CC2-CC3
25	T	102	CDL	C52-C51-CB5-OB6
25	C	306	CDL	C51-C52-C53-C54
26	E	201	PSC	C24-C25-C26-C27
24	P	304	PEK	C14-C15-C16-C17
24	C	315	PEK	C04-O12-P-O11
25	C	312	CDL	CB3-OB5-PB2-OB2
25	T	102	CDL	CB3-OB5-PB2-OB2
20	L	101	TGL	C14-C29-C30-C31
26	E	201	PSC	C15-C16-C17-C18
17	A	604	PGV	C20-C21-C22-C23
17	N	605	PGV	C25-C26-C27-C28
25	T	102	CDL	CB5-C51-C52-C53
20	Q	201	TGL	C24-C25-C26-C27
23	M	101	DMU	C19-C22-C25-C28
20	Y	101	TGL	CB6-CB7-CB8-CB9
17	A	604	PGV	C11-C12-C13-C14
20	D	201	TGL	CA2-CA3-CA4-CA5
25	T	102	CDL	C60-C61-C62-C63
20	A	615	TGL	C21-C20-CA9-CA8
24	C	315	PEK	C22-C23-C24-C25
25	C	312	CDL	C58-C59-C60-C61
24	P	301	PEK	C33-C34-C35-C36
22	G	1305	CHD	C22-C23-C24-O26
20	A	615	TGL	OG1-CG1-CG2-OG2
24	C	315	PEK	O03-C01-C02-O01
20	A	615	TGL	CA4-CA5-CA6-CA7
25	P	307	CDL	C56-C57-C58-C59
25	T	102	CDL	C1-CA2-OA2-PA1
22	P	308	CHD	C13-C17-C20-C21
17	T	101	PGV	C24-C25-C26-C27
20	D	201	TGL	CC6-CC7-CC8-CC9
18	A	606	HEA	CAA-CBA-CGA-O1A
22	G	1305	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
17	N	605	PGV	C11-C10-C9-C8
19	D	203	EDO	O1-C1-C2-O2
19	G	1303	EDO	O1-C1-C2-O2
19	S	2206	EDO	O1-C1-C2-O2
17	T	101	PGV	C1-C2-C3-C4
24	C	304	PEK	C31-C32-C33-C34
24	P	301	PEK	C29-C30-C31-C32
20	L	101	TGL	C11-C12-C13-C14
25	P	307	CDL	C51-C52-C53-C54
25	T	102	CDL	C81-C82-C83-C84
23	C	313	DMU	O6-C11-C9-C8
26	O	302	PSC	C31-C32-C33-C34
22	B	302	CHD	C22-C23-C24-O26
26	O	302	PSC	C4-C5-C6-C7
22	C	307	CHD	C22-C23-C24-O25
20	L	101	TGL	C13-C14-C29-C30
17	N	616	PGV	C4-C5-C6-C7
17	A	605	PGV	C11-C10-C9-C8
25	P	307	CDL	CA7-C31-C32-C33
22	P	308	CHD	C22-C23-C24-O25
17	Z	102	PGV	C03-C02-O01-C1
25	C	312	CDL	CB6-CB4-OB6-CB5
18	N	606	HEA	CAD-CBD-CGD-O2D
22	B	302	CHD	C22-C23-C24-O25
22	C	302	CHD	C16-C17-C20-C22
24	C	315	PEK	C5-C6-C7-C8
24	C	315	PEK	C11-C10-C9-C8
24	C	315	PEK	C12-C13-C14-C15
24	P	304	PEK	C5-C6-C7-C8
24	P	304	PEK	C11-C10-C9-C8
24	P	304	PEK	C11-C12-C13-C14
26	O	302	PSC	C9-C10-C11-C12
17	N	605	PGV	C26-C27-C28-C29
25	C	312	CDL	C62-C63-C64-C65
26	E	201	PSC	C22-C23-C24-C25
17	C	305	PGV	C05-C04-O12-P
24	C	304	PEK	C1-C2-C3-C4
23	Z	101	DMU	O6-C11-C9-O1
18	A	606	HEA	CAA-CBA-CGA-O2A
25	P	307	CDL	OA5-CA3-CA4-CA6
18	N	606	HEA	CAD-CBD-CGD-O1D
22	C	307	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
22	Y	102	CHD	C22-C23-C24-O25
22	Y	102	CHD	C22-C23-C24-O26
24	P	301	PEK	C32-C33-C34-C35
20	L	101	TGL	CC2-CC1-OG3-CG3
24	C	304	PEK	C16-C17-C18-C19
24	C	303	PEK	C10-C11-C12-C13
17	N	616	PGV	C23-C24-C25-C26
25	T	102	CDL	C13-C14-C15-C16
25	C	312	CDL	C53-C54-C55-C56
18	A	606	HEA	CAD-CBD-CGD-O1D
22	P	308	CHD	C22-C23-C24-O26
17	C	305	PGV	C11-C12-C13-C14
17	A	605	PGV	C23-C24-C25-C26
20	L	101	TGL	CB3-CB4-CB5-CB6
17	A	605	PGV	O03-C19-C20-C21
17	N	605	PGV	O03-C19-C20-C21
24	C	303	PEK	O03-C21-C22-C23
18	N	606	HEA	CAA-CBA-CGA-O2A
19	C	309	EDO	O1-C1-C2-O2
19	F	701	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
20	N	604	TGL	OC1-CC1-OG3-CG3
24	C	304	PEK	C17-C18-C19-C20
25	C	306	CDL	C72-C73-C74-C75
20	D	201	TGL	CA9-C20-C21-C22
17	C	305	PGV	C14-C15-C16-C17
20	A	615	TGL	C10-C11-C12-C13
20	L	101	TGL	CB2-CB3-CB4-CB5
17	N	616	PGV	C9-C10-C11-C12
17	N	616	PGV	C11-C12-C13-C14
24	C	304	PEK	C3-C4-C5-C6
26	E	201	PSC	C7-C8-C9-C10
25	T	102	CDL	OB5-CB3-CB4-OB6
22	P	303	CHD	C22-C23-C24-O26
25	P	307	CDL	C39-C40-C41-C42
18	A	606	HEA	CAD-CBD-CGD-O2D
25	T	102	CDL	C62-C63-C64-C65
23	C	301	DMU	C18-C19-C22-C25
20	Q	201	TGL	C21-C22-C23-C24
25	C	306	CDL	CB4-CB3-OB5-PB2
20	L	101	TGL	OG1-CG1-CG2-OG2
20	Y	101	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	A	605	PGV	C11-C12-C13-C14
24	C	304	PEK	O03-C21-C22-C23
20	L	101	TGL	OC1-CC1-OG3-CG3
20	Q	201	TGL	OG3-CC1-CC2-CC3
24	P	304	PEK	O01-C1-C2-C3
17	C	305	PGV	C26-C27-C28-C29
20	D	201	TGL	OG2-CB1-CB2-CB3
17	Z	102	PGV	C9-C10-C11-C12
24	P	301	PEK	C3-C4-C5-C6
24	C	304	PEK	C22-C23-C24-C25
26	O	302	PSC	C21-C22-C23-C24
24	P	304	PEK	O02-C1-O01-C02
24	C	303	PEK	C32-C33-C34-C35
24	C	303	PEK	O01-C1-C2-C3
25	P	307	CDL	C16-C17-C18-C19
22	W	302	CHD	C22-C23-C24-O26
17	Z	102	PGV	O01-C1-C2-C3
24	C	303	PEK	C14-C15-C16-C17
20	Y	101	TGL	OG1-CG1-CG2-CG3
17	T	101	PGV	O01-C02-C03-O11
22	P	303	CHD	C22-C23-C24-O25
20	D	201	TGL	CC9-C15-C16-C17
19	B	309	EDO	O1-C1-C2-O2
19	F	704	EDO	O1-C1-C2-O2
19	K	101	EDO	O1-C1-C2-O2
19	P	309	EDO	O1-C1-C2-O2
18	N	606	HEA	CAA-CBA-CGA-O1A
25	P	307	CDL	C31-C32-C33-C34
25	T	102	CDL	O1-C1-CA2-OA2
20	D	201	TGL	C29-C30-C31-C32
18	A	607	HEA	CAD-CBD-CGD-O2D
25	C	306	CDL	C58-C59-C60-C61
20	Y	101	TGL	OG2-CB1-CB2-CB3
26	O	302	PSC	C23-C24-C25-C26
17	N	605	PGV	C9-C10-C11-C12
26	O	302	PSC	O03-C19-C20-C21
25	P	307	CDL	C21-C22-C23-C24
20	N	604	TGL	C24-C25-C26-C27
26	O	302	PSC	C12-C13-C14-C15
20	A	615	TGL	OG3-CC1-CC2-CC3
25	C	306	CDL	C57-C58-C59-C60
24	C	303	PEK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	Q	201	TGL	CA6-CA7-CA8-CA9
22	W	302	CHD	C22-C23-C24-O25
20	Q	201	TGL	C11-C10-CB9-CB8
24	P	304	PEK	C35-C36-C37-C38
17	A	605	PGV	C9-C10-C11-C12
25	P	307	CDL	C64-C65-C66-C67
24	C	304	PEK	O04-C21-C22-C23
24	P	304	PEK	O02-C1-C2-C3
17	A	605	PGV	C22-C23-C24-C25
20	Q	201	TGL	OC1-CC1-CC2-CC3
23	M	101	DMU	C22-C25-C28-C31
18	N	607	HEA	CAD-CBD-CGD-O1D
25	C	312	CDL	CB3-CB4-CB6-OB8
18	N	607	HEA	CAD-CBD-CGD-O2D
25	C	306	CDL	C72-C71-CB7-OB8
24	C	315	PEK	C04-O12-P-O14
25	T	102	CDL	CA2-OA2-PA1-OA3
25	T	102	CDL	CB3-OB5-PB2-OB3
17	Z	102	PGV	O02-C1-C2-C3
24	C	303	PEK	O02-C1-C2-C3
25	T	102	CDL	C16-C17-C18-C19
19	D	204	EDO	O1-C1-C2-O2
19	E	202	EDO	O1-C1-C2-O2
19	N	608	EDO	O1-C1-C2-O2
19	N	609	EDO	O1-C1-C2-O2
19	Q	202	EDO	O1-C1-C2-O2
19	R	201	EDO	O1-C1-C2-O2
19	T	105	EDO	O1-C1-C2-O2
24	C	315	PEK	O01-C1-C2-C3
25	C	312	CDL	C12-C11-CA5-OA6
25	P	307	CDL	C61-C62-C63-C64
20	L	101	TGL	C23-C24-C25-C26
25	C	312	CDL	C21-C22-C23-C24
18	A	607	HEA	CAD-CBD-CGD-O1D
17	A	604	PGV	C27-C28-C29-C30
24	P	301	PEK	C24-C25-C26-C27
25	C	312	CDL	CA3-CA4-OA6-CA5
25	C	312	CDL	CA6-CA4-OA6-CA5
26	E	201	PSC	C05-C04-O12-P
23	C	313	DMU	C3-C4-C57-O61
24	C	315	PEK	O02-C1-C2-C3
17	T	101	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	P	305	PEK	C22-C23-C24-C25
25	P	307	CDL	C63-C64-C65-C66
20	A	615	TGL	OG1-CA1-CA2-CA3
17	N	605	PGV	C15-C16-C17-C18
20	Y	101	TGL	CC5-CC6-CC7-CC8
17	A	605	PGV	C19-C20-C21-C22
25	T	102	CDL	C58-C59-C60-C61
17	P	306	PGV	C27-C28-C29-C30
26	O	302	PSC	O04-C19-C20-C21
20	Q	201	TGL	CB7-CB8-CB9-C10
17	Z	102	PGV	O01-C02-C03-O11
20	A	615	TGL	OC1-CC1-CC2-CC3
20	Y	101	TGL	OB1-CB1-CB2-CB3
25	C	312	CDL	C40-C41-C42-C43
25	C	306	CDL	C72-C71-CB7-OB9
20	Y	101	TGL	OG3-CC1-CC2-CC3
25	C	312	CDL	C72-C71-CB7-OB8
22	C	302	CHD	C13-C17-C20-C21
25	C	312	CDL	C72-C71-CB7-OB9
17	P	306	PGV	C13-C14-C15-C16
20	Y	101	TGL	OC1-CC1-CC2-CC3

All (2) ring outliers are listed below:

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

50 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	303	PEK	4	0
18	A	607	HEA	3	0
23	G	1302	DMU	2	0
25	P	307	CDL	4	0
26	E	201	PSC	5	0
20	Y	101	TGL	2	0
24	P	304	PEK	1	0
19	A	616	EDO	1	0
17	A	604	PGV	4	0
17	T	101	PGV	1	0
19	N	619	EDO	1	0

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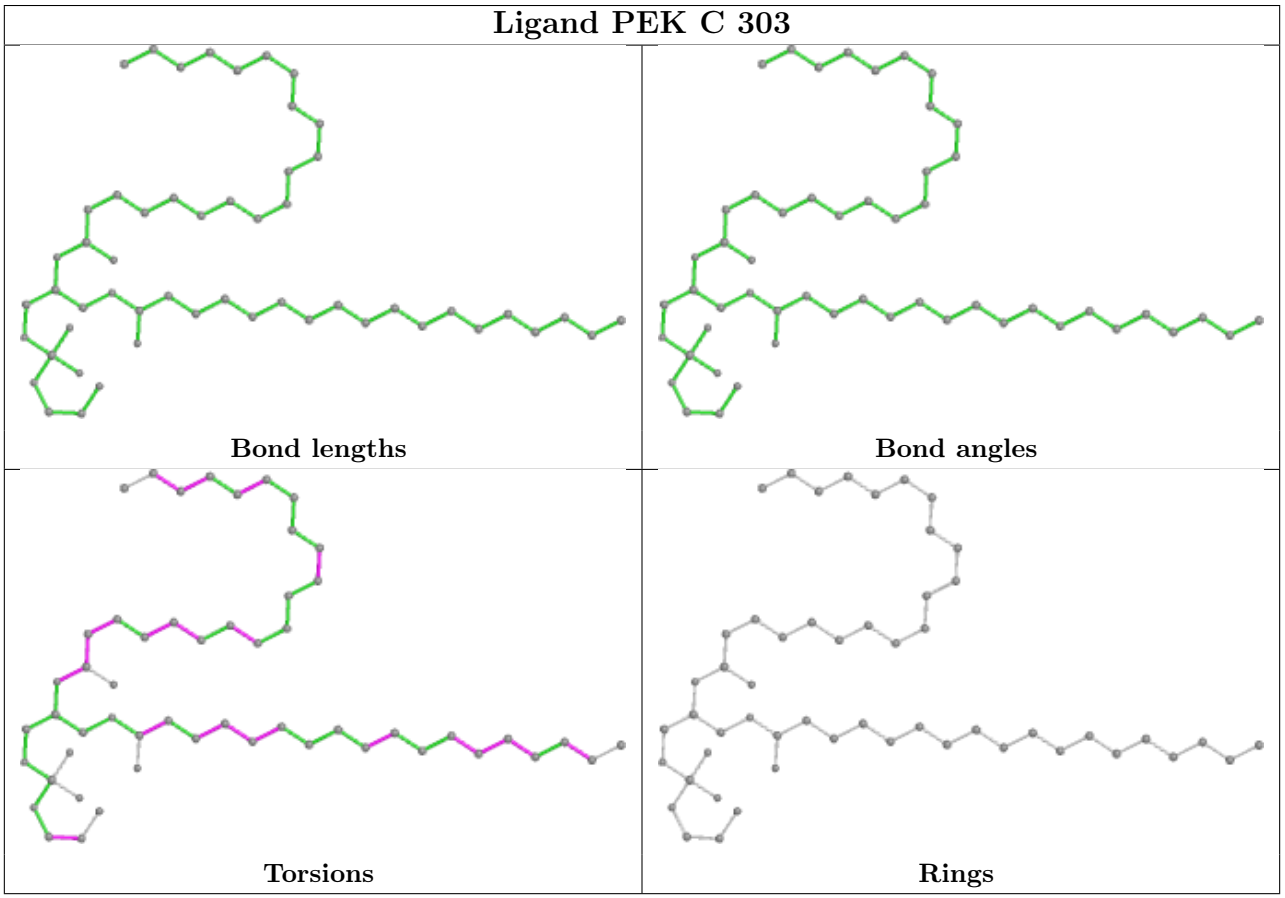
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	201	TGL	7	0
19	G	1303	EDO	2	0
24	C	304	PEK	2	0
18	A	606	HEA	2	0
25	C	306	CDL	2	0
25	T	102	CDL	3	0
26	O	302	PSC	5	0
22	P	308	CHD	1	0
24	P	305	PEK	5	0
19	S	2206	EDO	1	0
20	A	615	TGL	1	0
19	A	613	EDO	1	0
22	Y	102	CHD	4	0
17	N	605	PGV	1	0
20	L	101	TGL	2	0
19	N	613	EDO	1	0
19	F	702	EDO	1	0
19	S	2201	EDO	3	0
23	Z	101	DMU	1	0
28	I	101	SAC	2	0
19	J	1104	EDO	1	0
20	Q	201	TGL	5	0
19	A	614	EDO	3	0
19	J	1101	EDO	1	0
22	C	302	CHD	1	0
24	C	315	PEK	2	0
22	T	104	CHD	7	0
19	N	614	EDO	9	0
19	U	1501	EDO	3	0
18	N	607	HEA	4	0
19	A	608	EDO	1	0
19	V	103	EDO	1	0
17	Z	102	PGV	2	0
22	G	1305	CHD	1	0
23	C	313	DMU	1	0
28	V	101	SAC	1	0
25	C	312	CDL	13	0
18	N	606	HEA	5	0
17	N	616	PGV	1	0

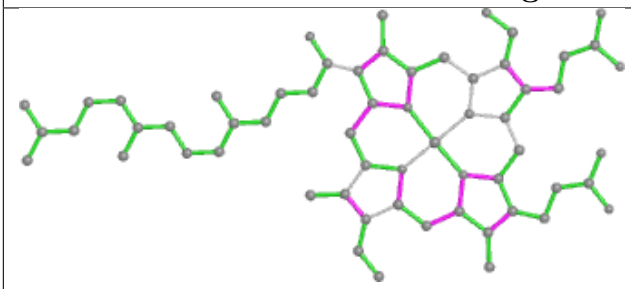
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

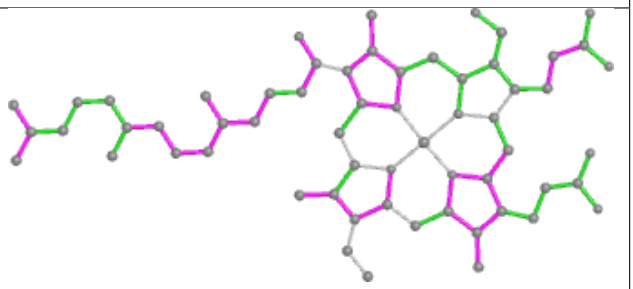
Ligand PEK C 303



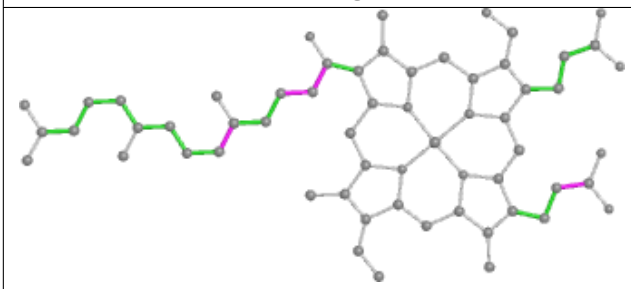
Ligand HEA A 607



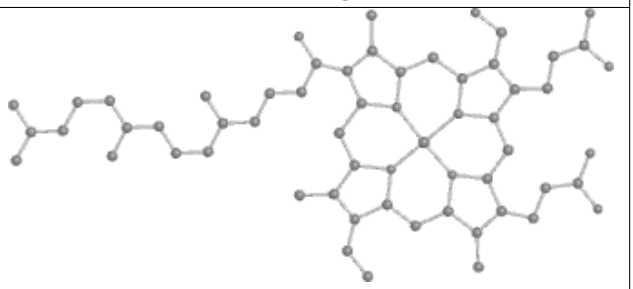
Bond lengths



Bond angles

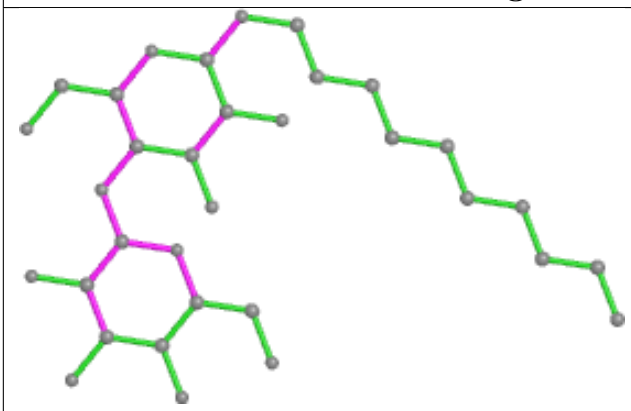


Torsions

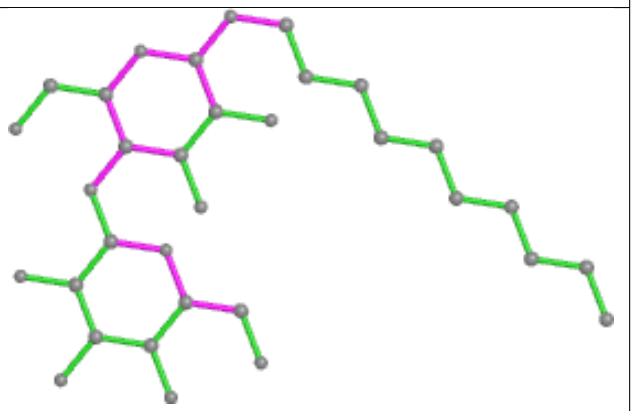


Rings

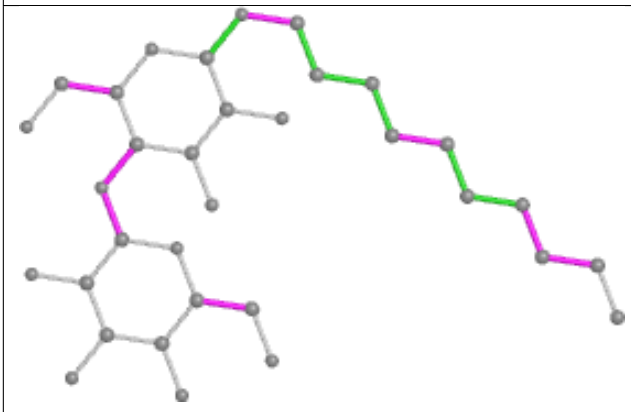
Ligand DMU G 1302



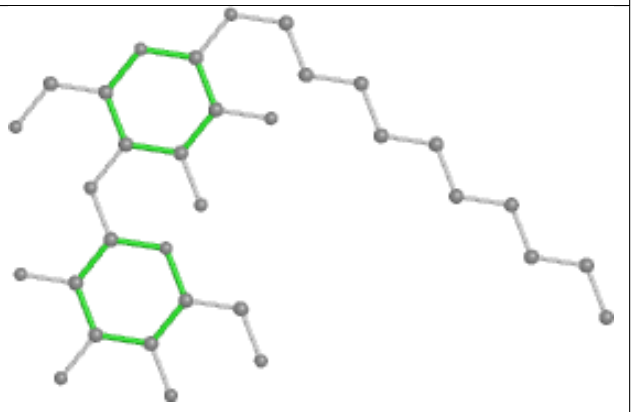
Bond lengths



Bond angles

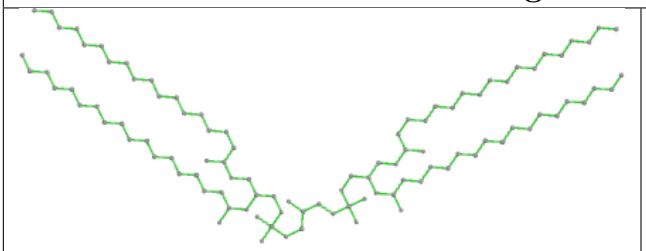


Torsions



Rings

Ligand CDL P 307



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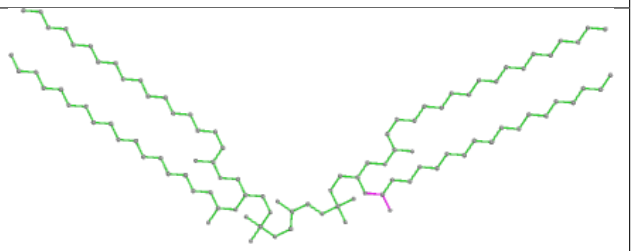
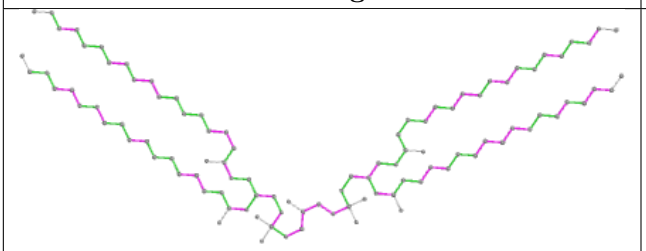


Bond angles



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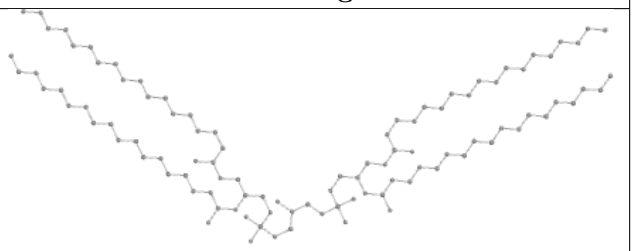
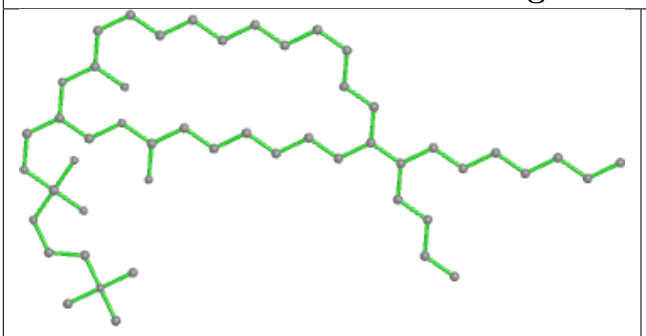
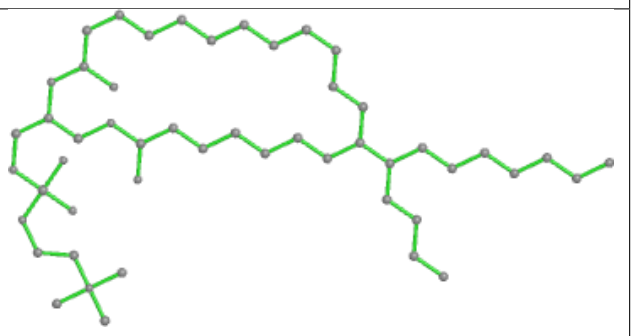


Rings

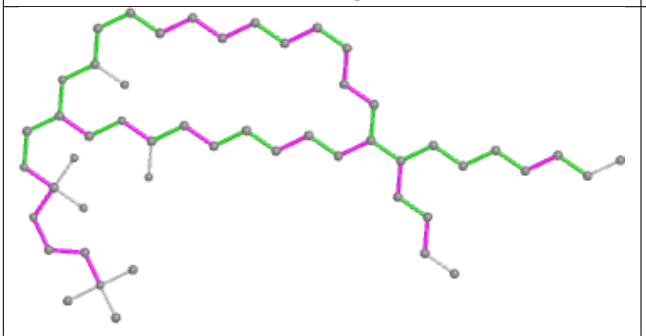
Ligand PSC E 201



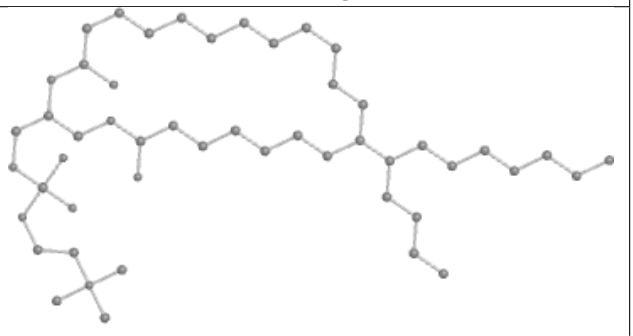
Bond lengths



Bond angles

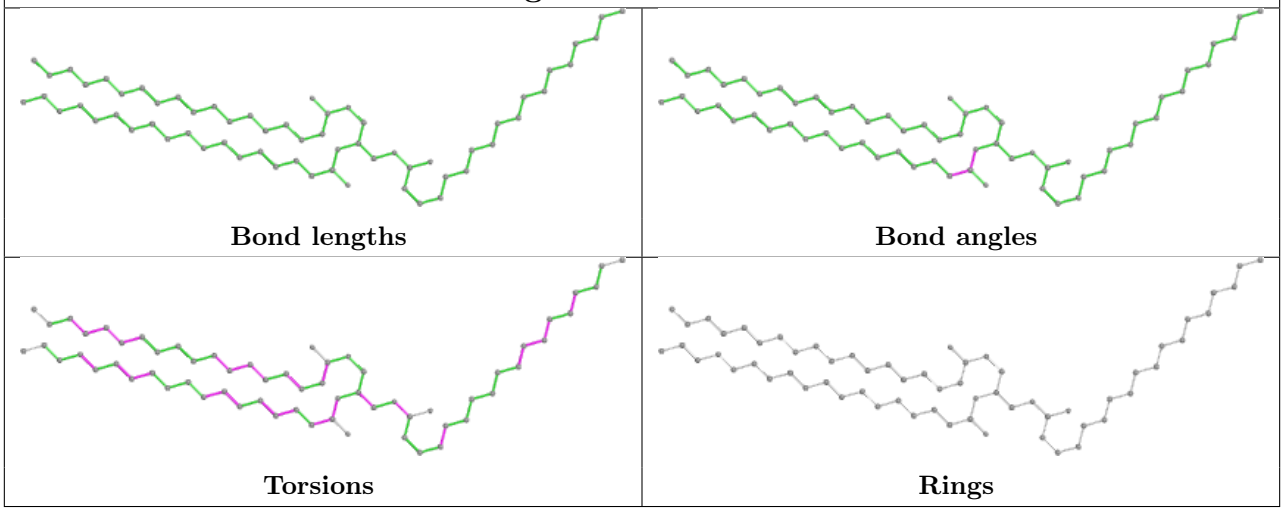


Torsions

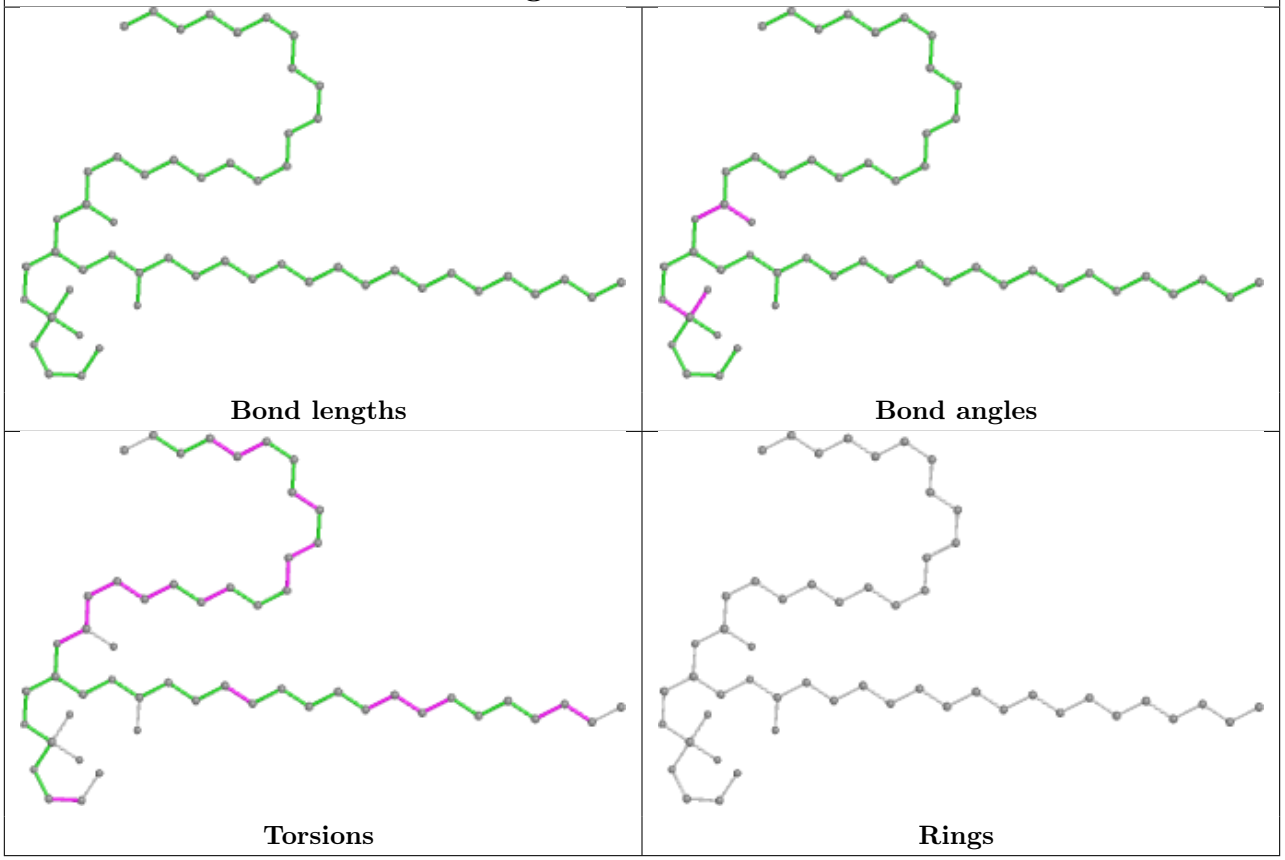


Rings

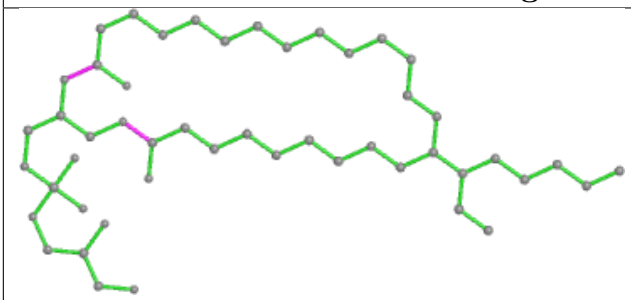
Ligand TGL Y 101



Ligand PEK P 304



Ligand PGV A 604



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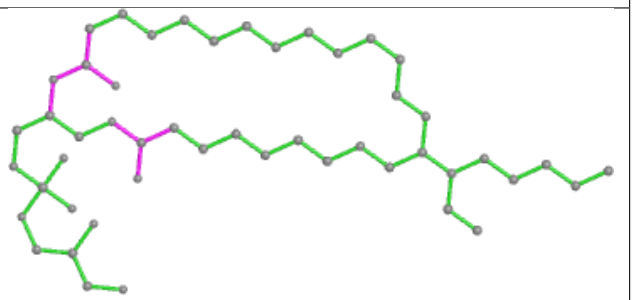
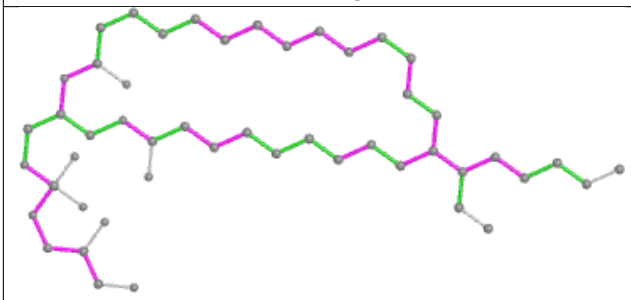


Bond angles



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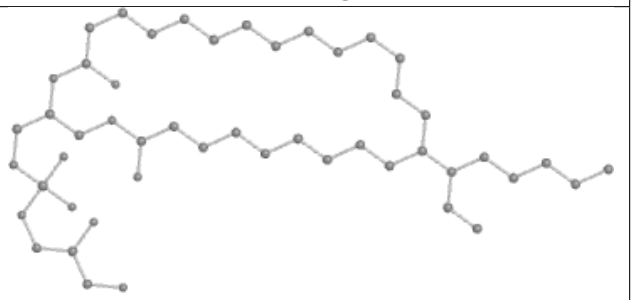
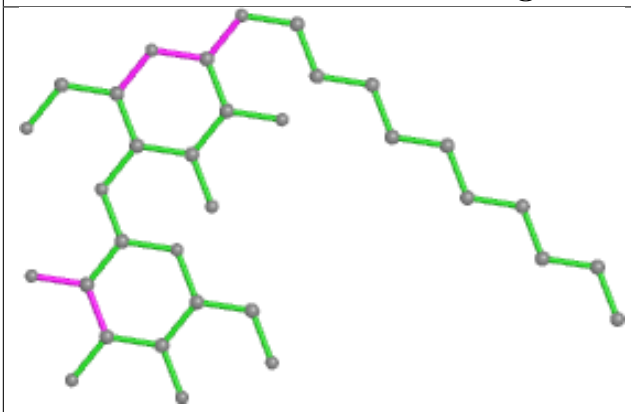


Rings

Ligand DMU C 301



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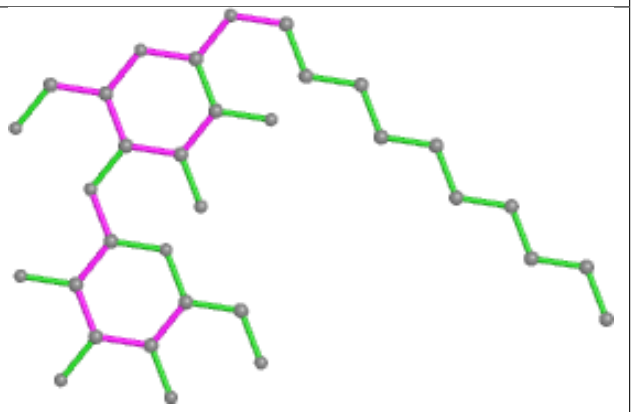
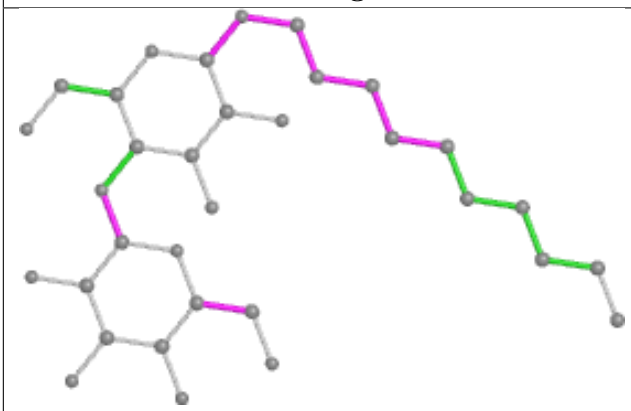


Bond angles



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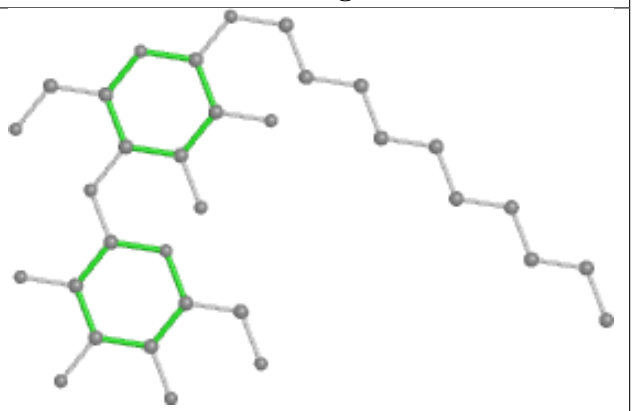
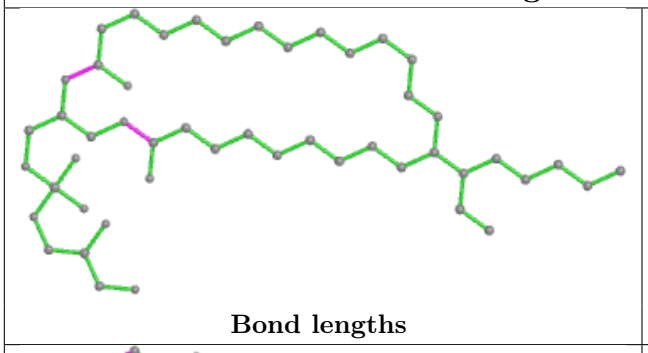


Rings

Ligand PGV T 101



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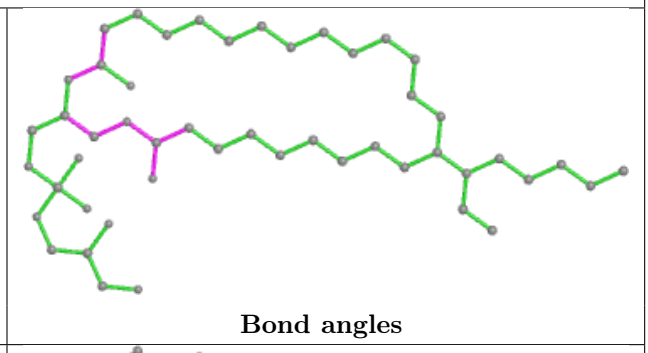

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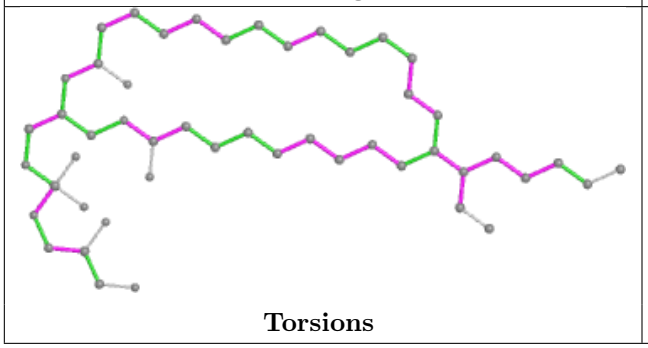

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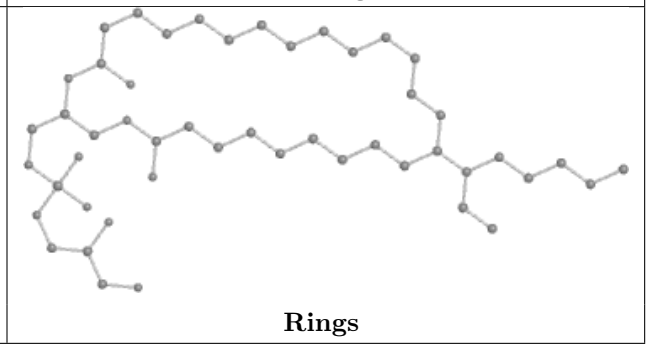
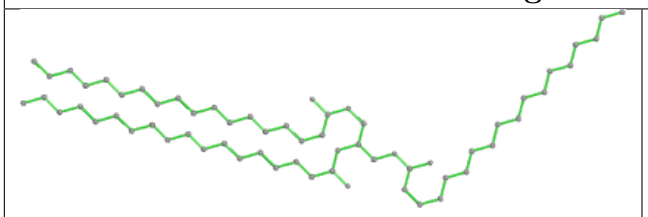


Rings

Ligand TGL D 201



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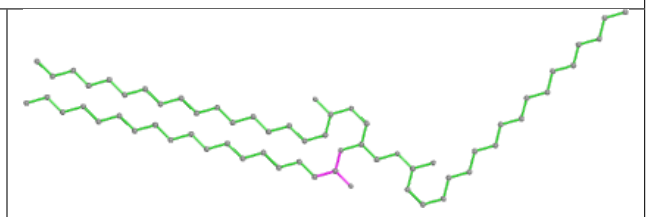
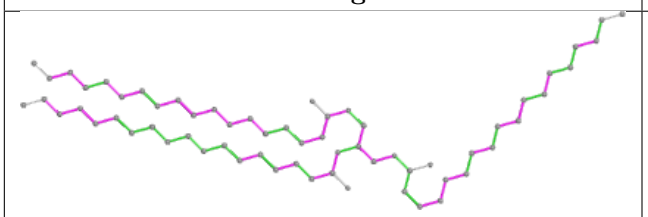
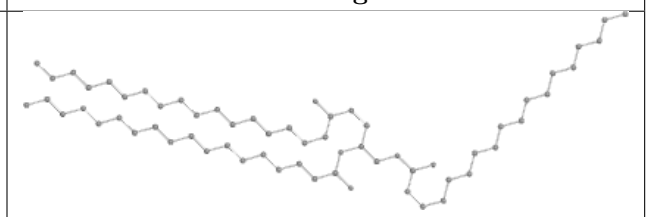


Bond angles

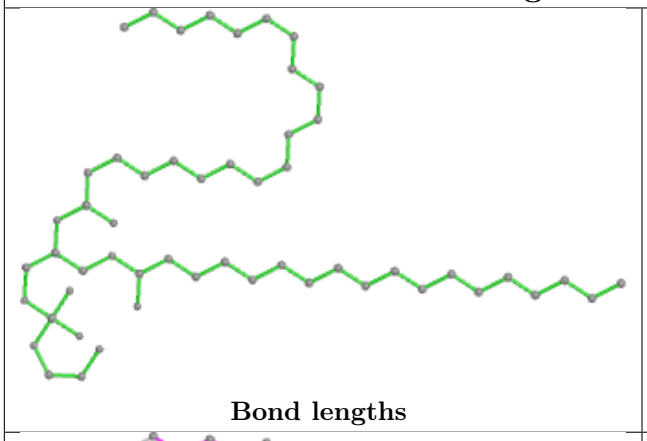


Torsions

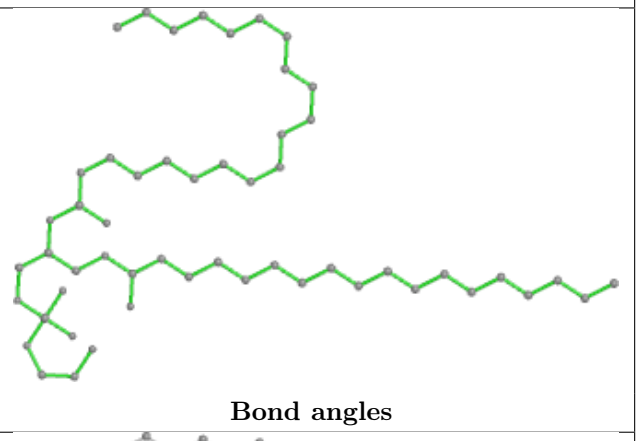


Rings

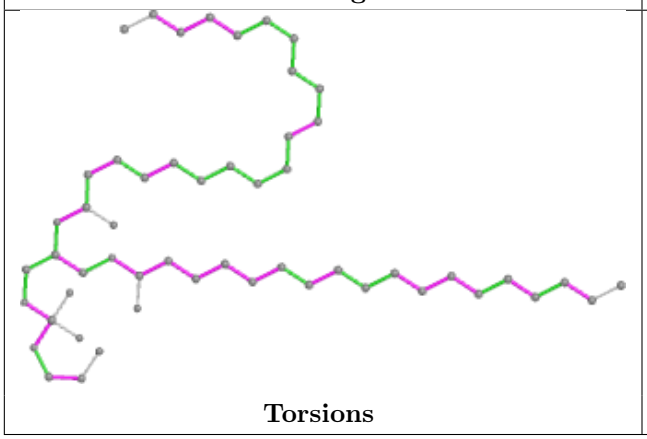
Ligand PEK C 304



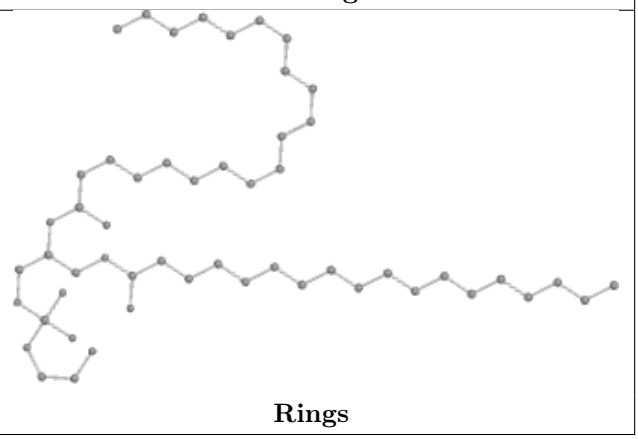
Bond lengths



Bond angles

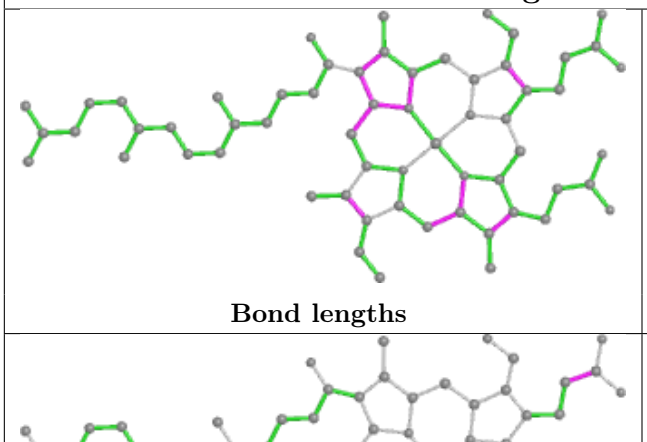


Torsions



Rings

Ligand HEA A 606



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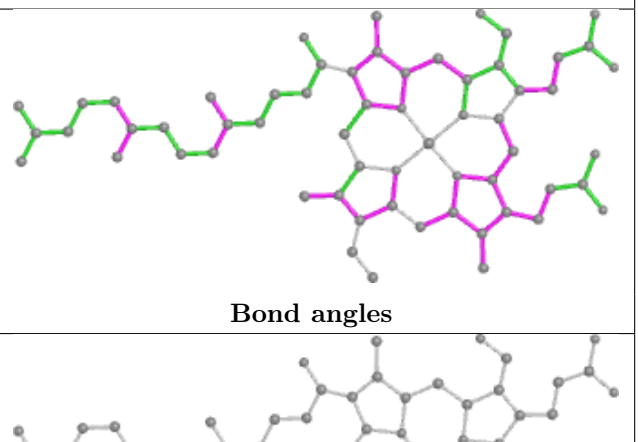
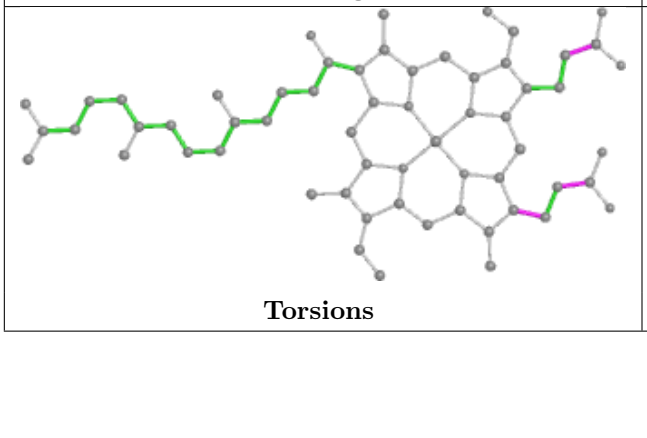
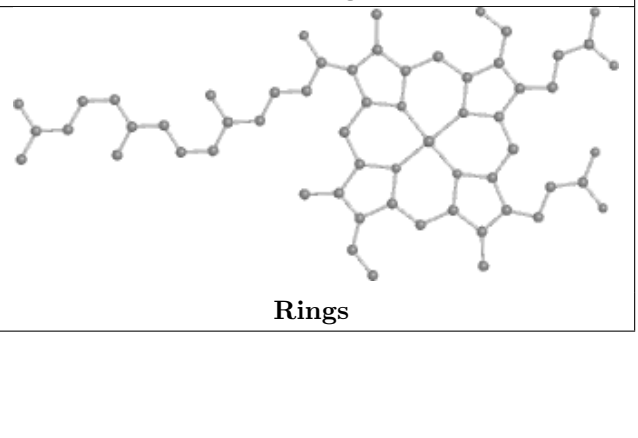


Bond angles

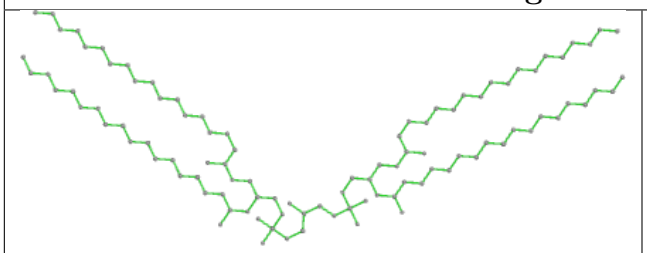


Torsions

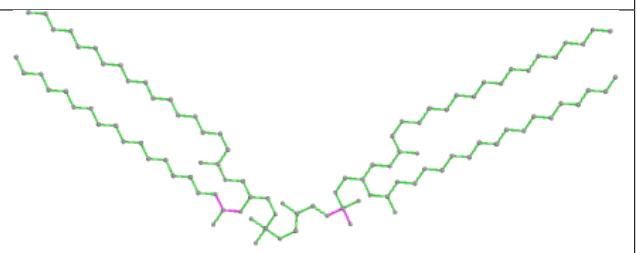


Rings

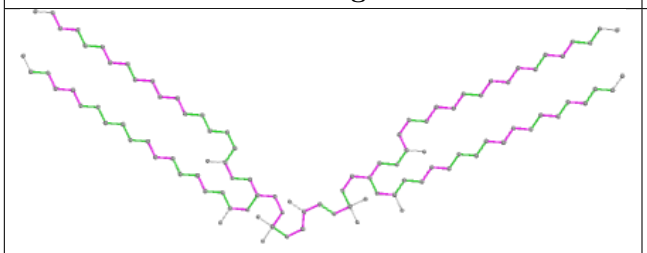
Ligand CDL C 306



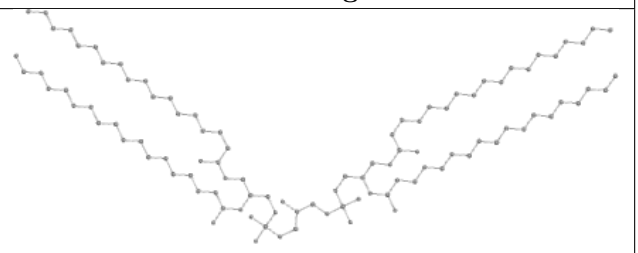
Bond lengths



Bond angles

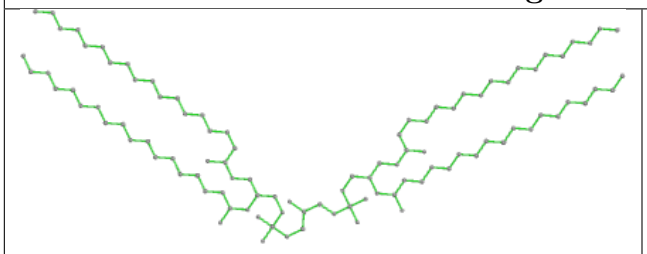


Torsions

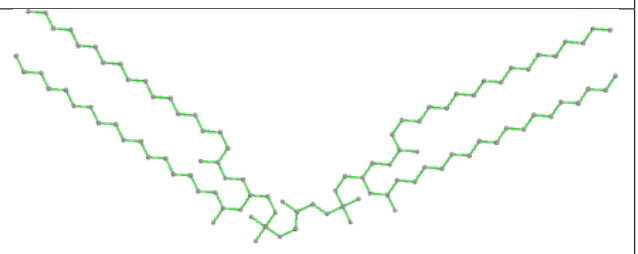


Rings

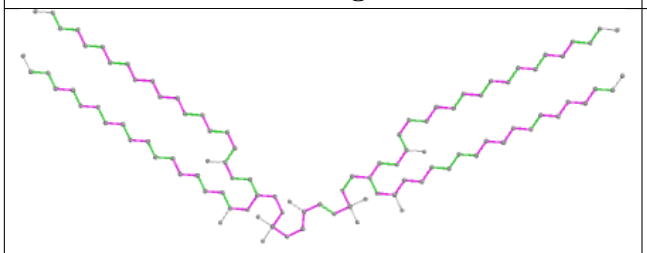
Ligand CDL T 102



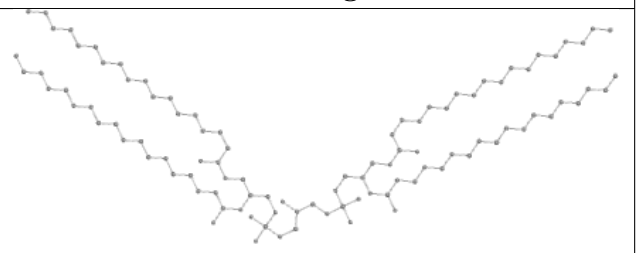
Bond lengths



Bond angles

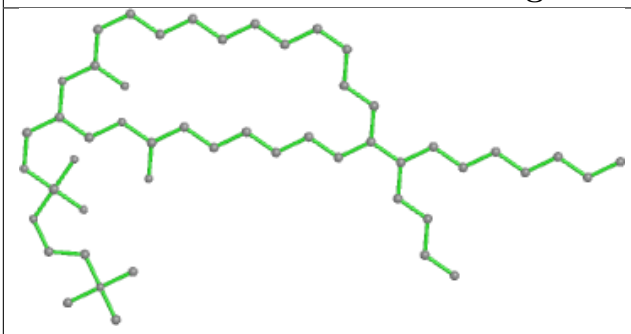


Torsions

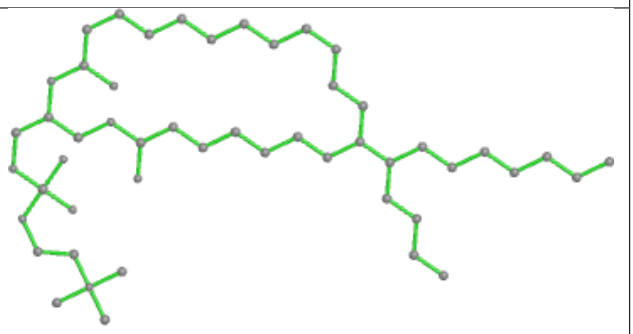


Rings

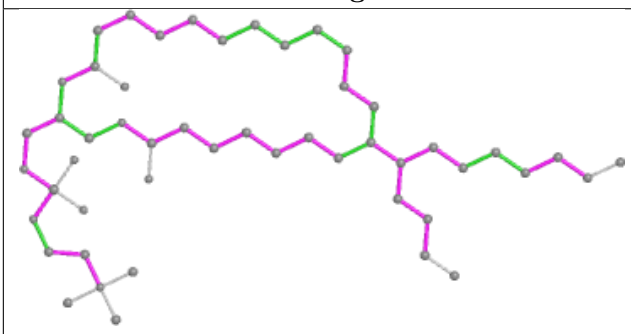
Ligand PSC O 302



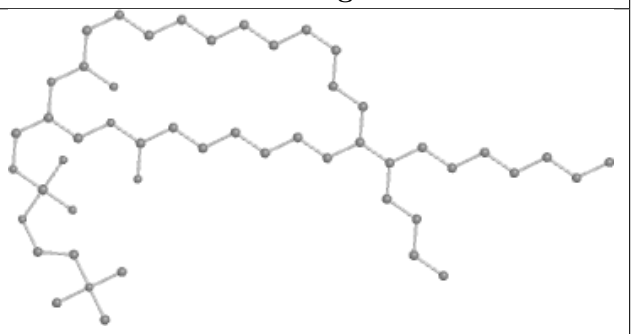
Bond lengths



Bond angles

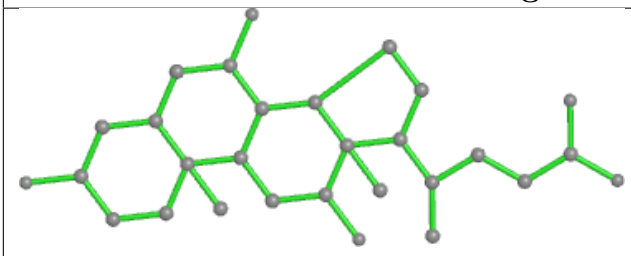


Torsions

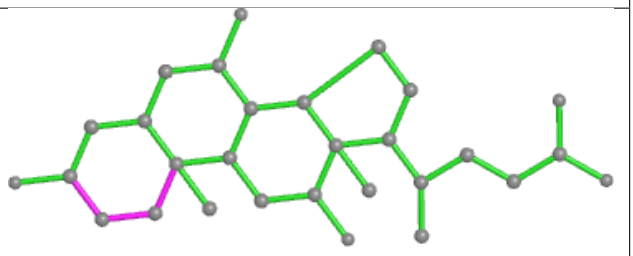


Rings

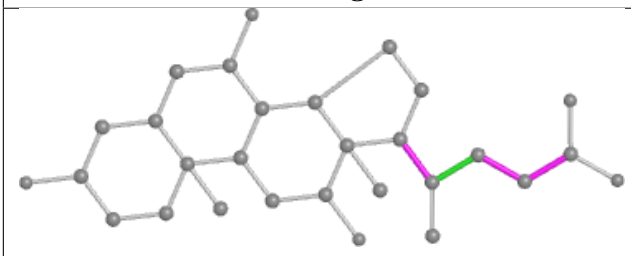
Ligand CHD P 308



Bond lengths



Bond angles



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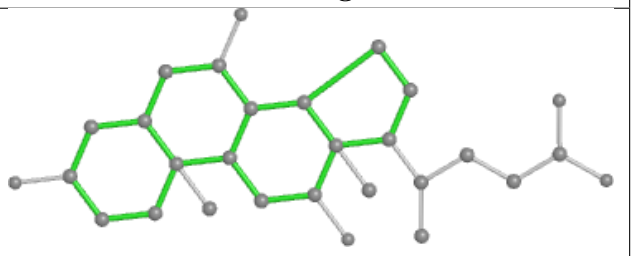
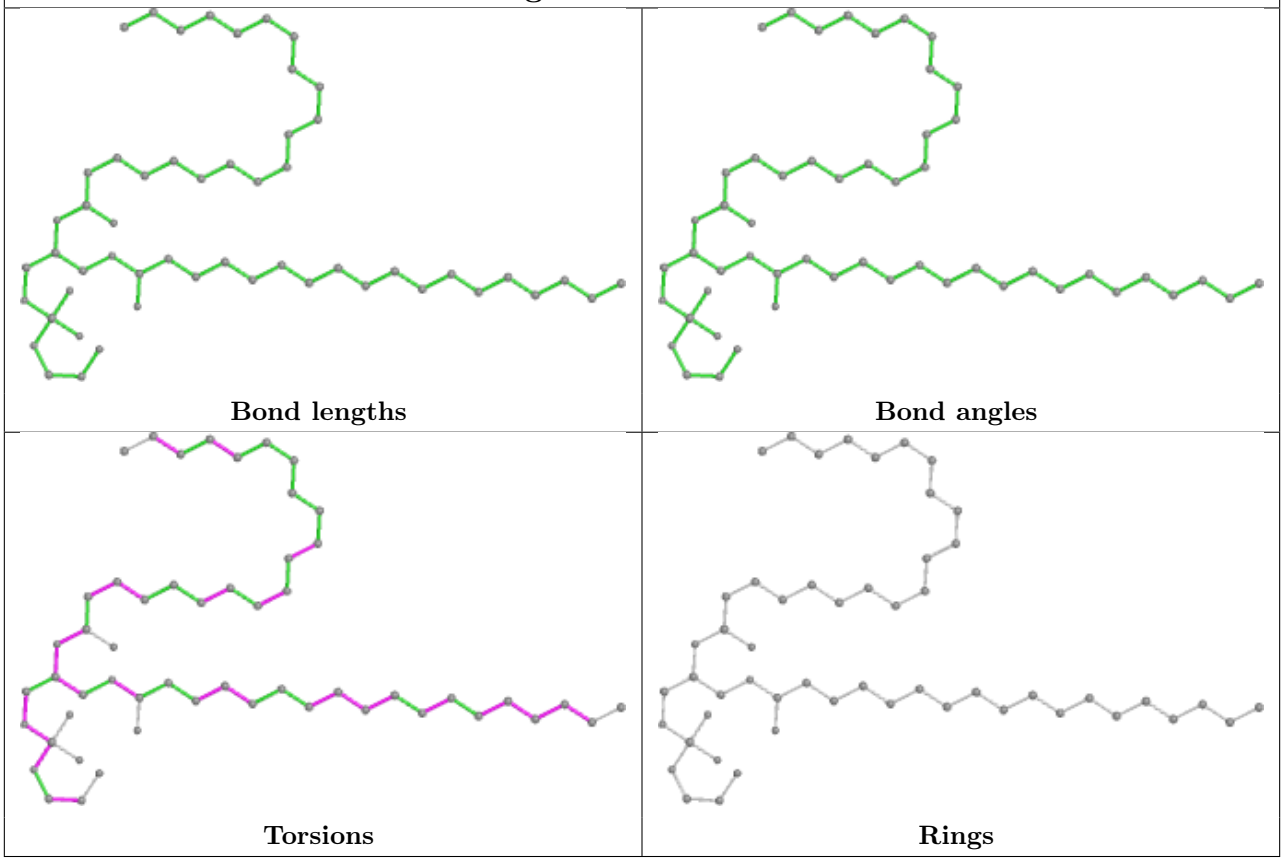
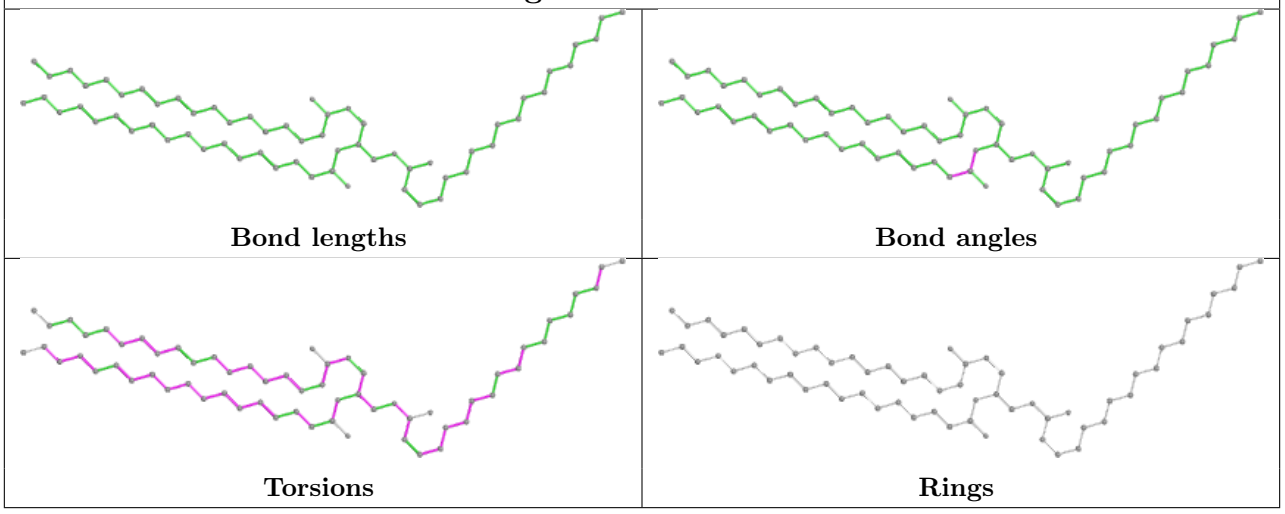


Rings

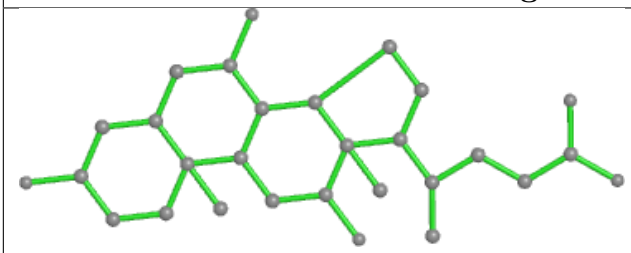
Ligand PEK P 305



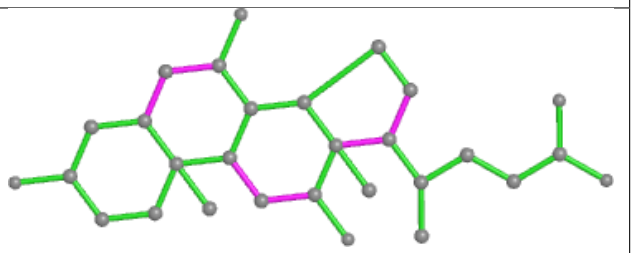
Ligand TGL A 615



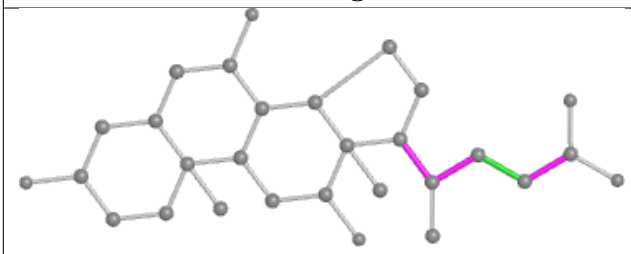
Ligand CHD Y 102



Bond lengths



Bond angles



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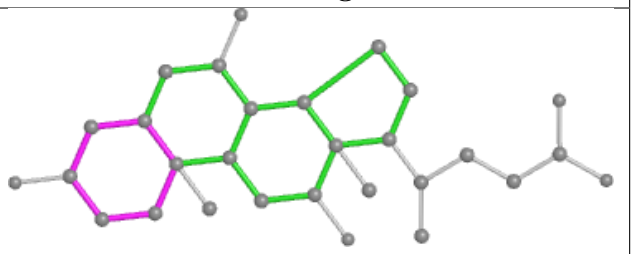
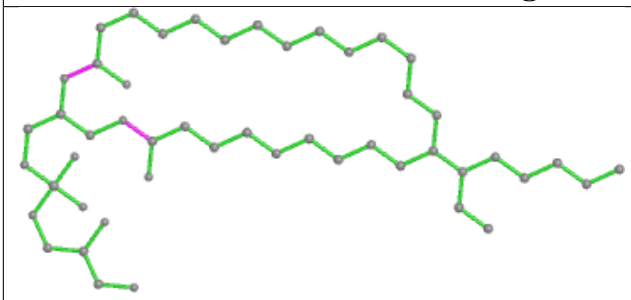
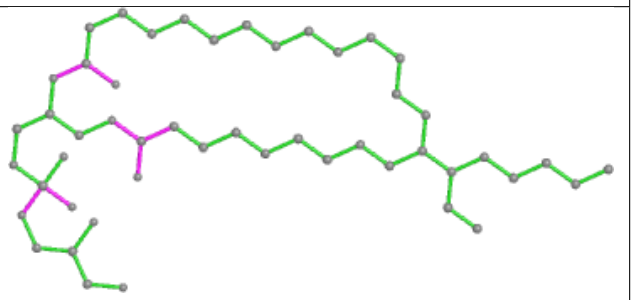


Rings

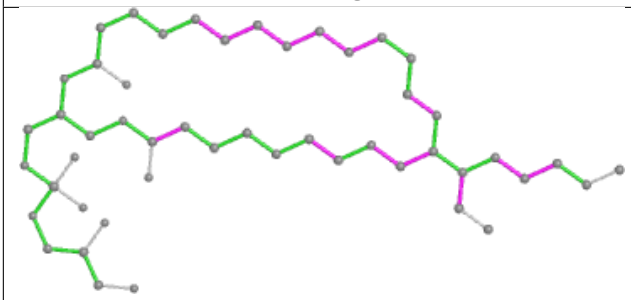
Ligand PGV N 605



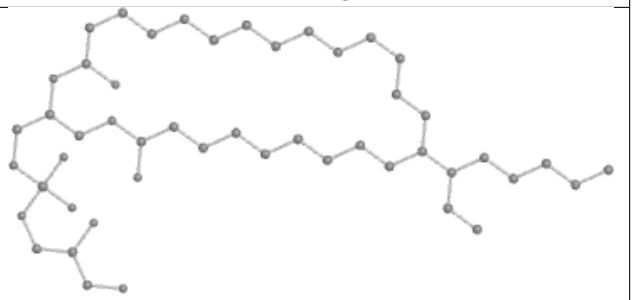
Bond lengths



Bond angles

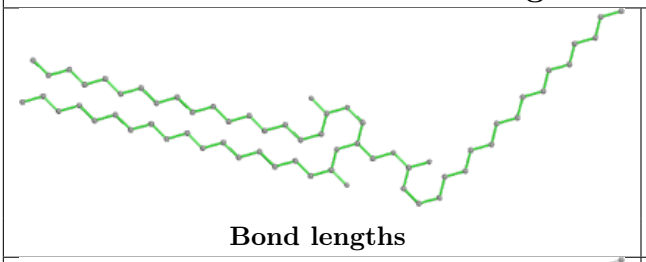


Torsions



Rings

Ligand TGL L 101



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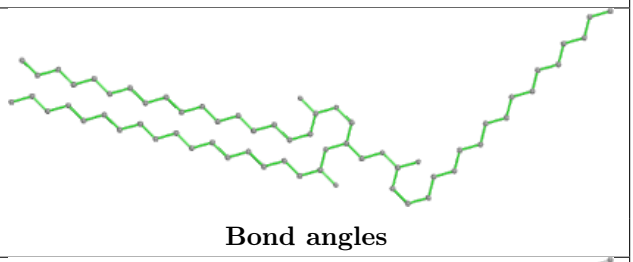
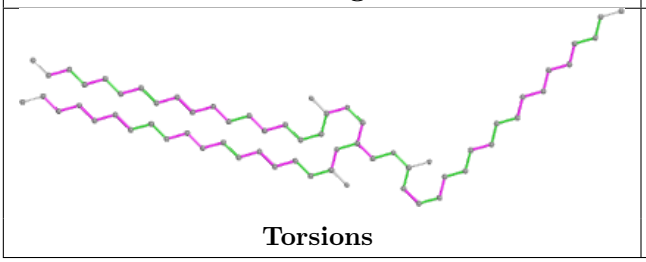
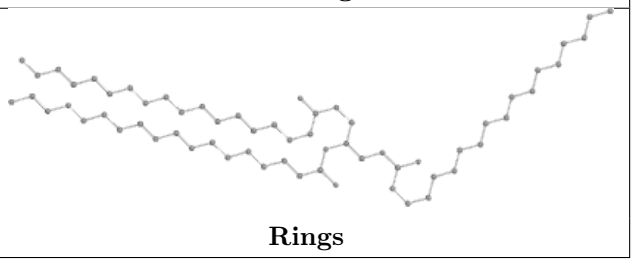


Bond angles

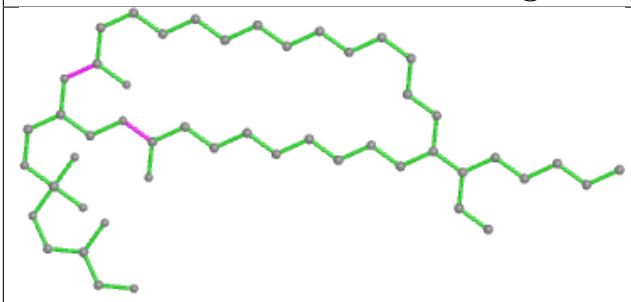


Torsions



Rings

Ligand PGV C 305



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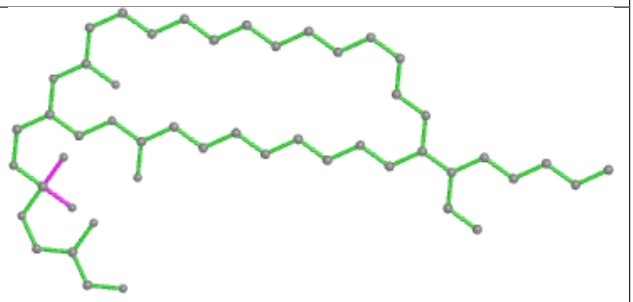
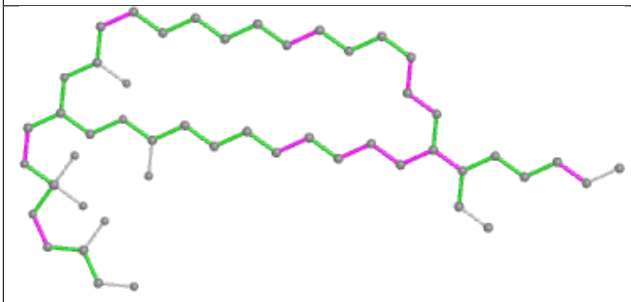
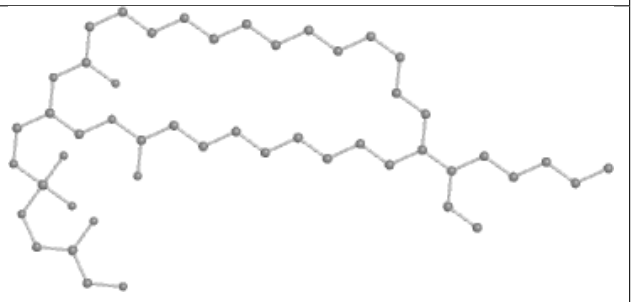


Bond angles

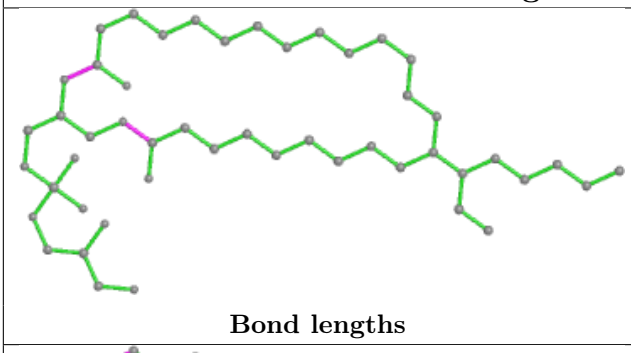


Torsions

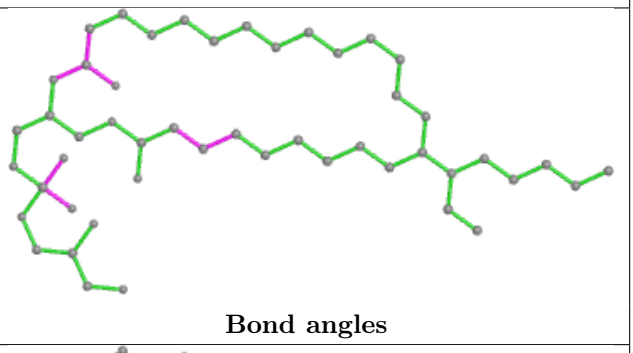


Rings

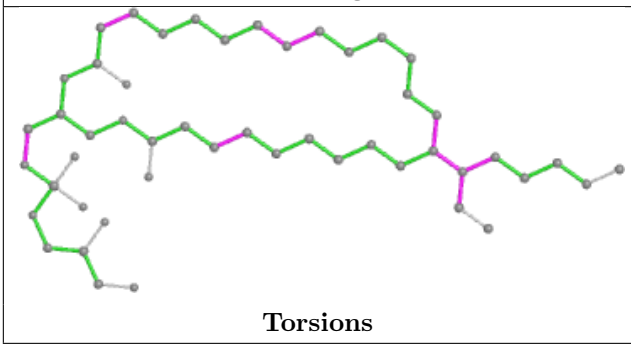
Ligand PGV P 306



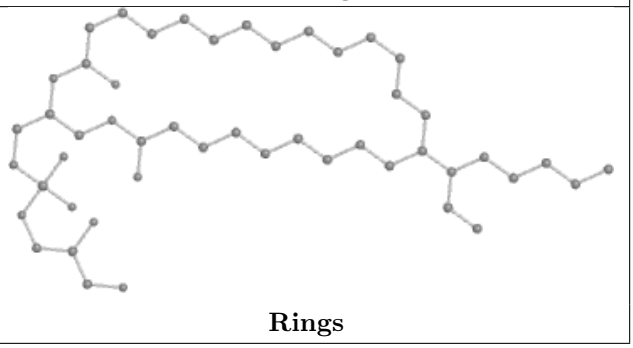
Bond lengths



Bond angles

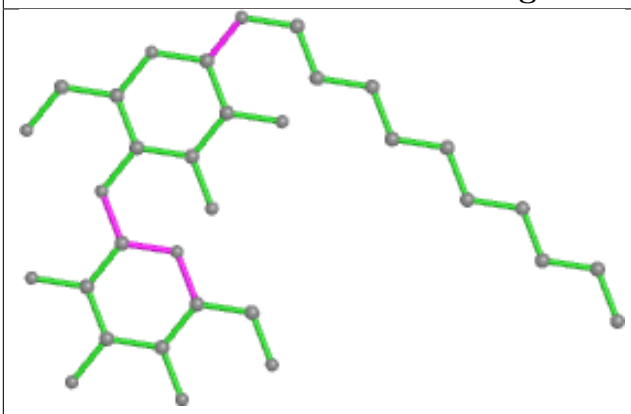


Torsions

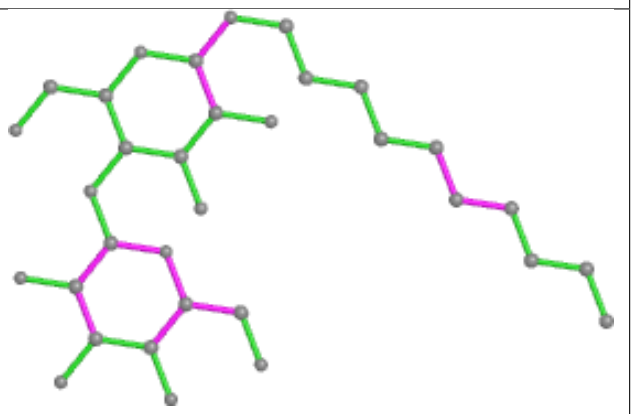


Rings

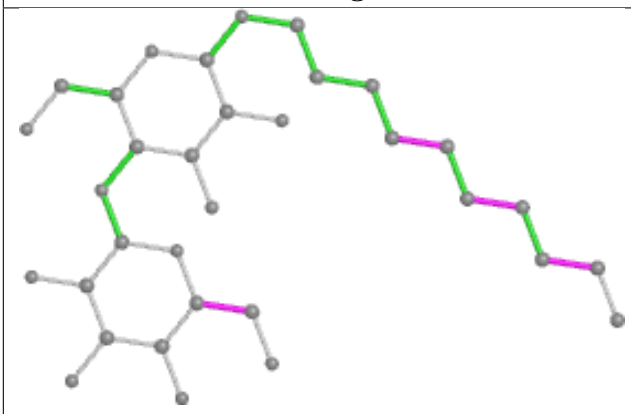
Ligand DMU Z 101



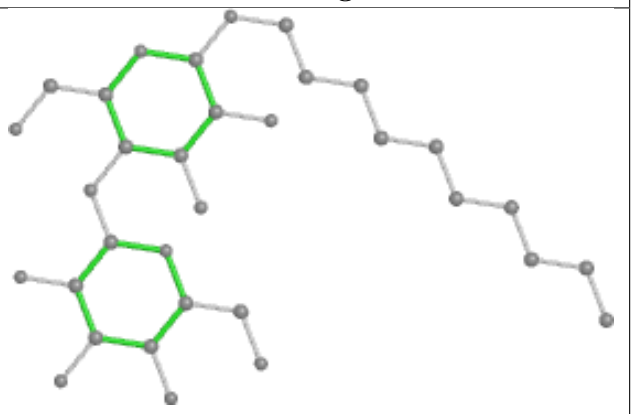
Bond lengths



Bond angles

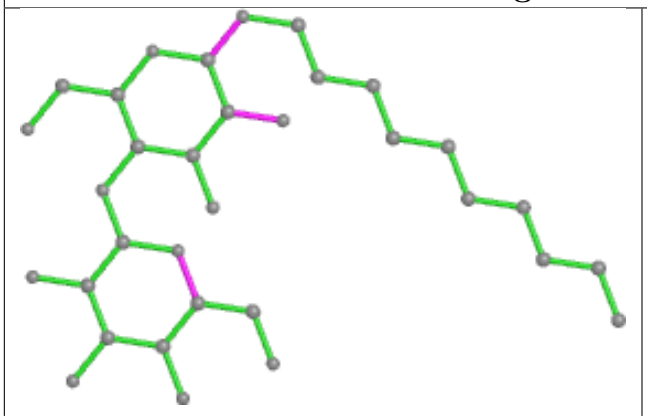


Torsions



Rings

Ligand DMU M 101



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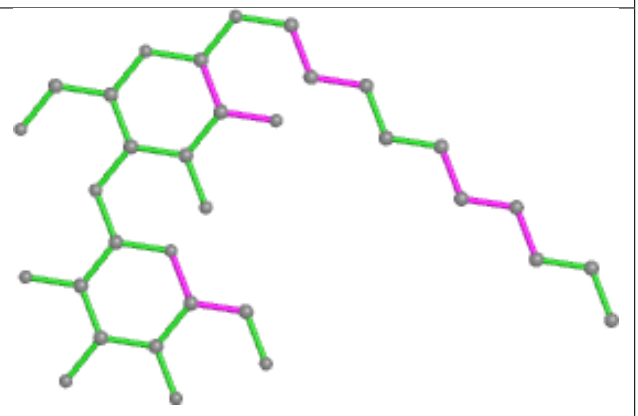
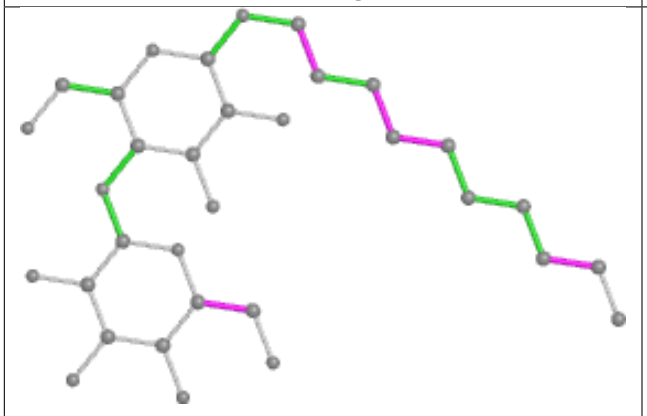
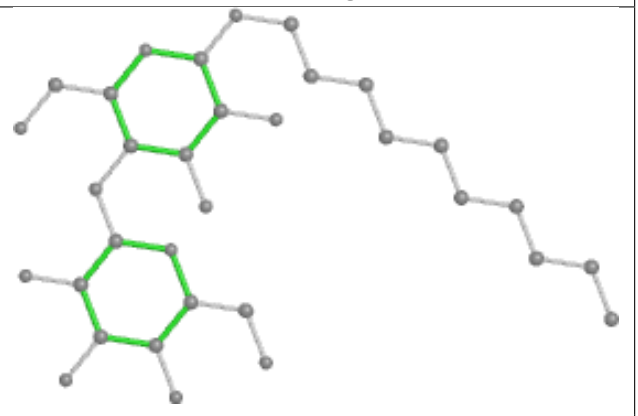


Bond angles

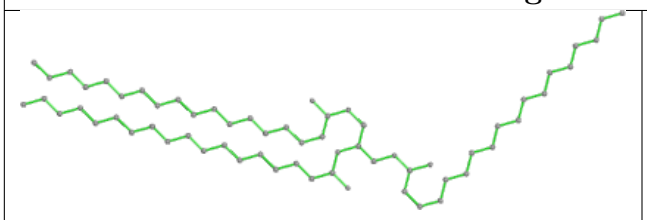


Torsions

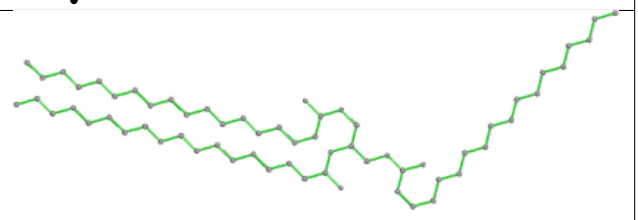


Rings

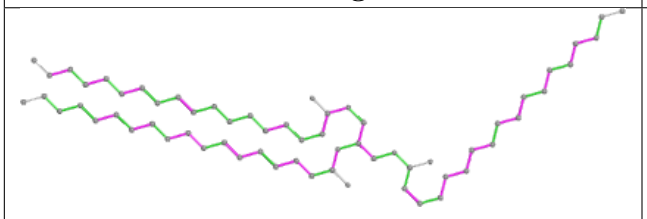
Ligand TGL Q 201



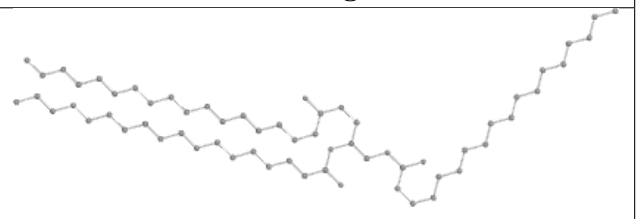
Bond lengths



Bond angles

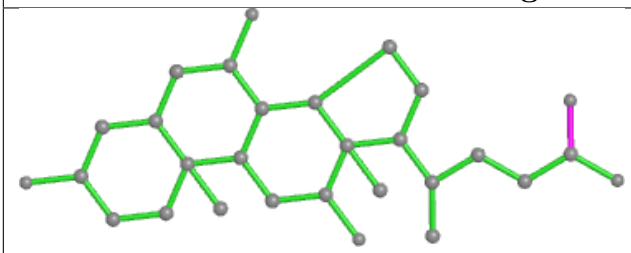


Torsions

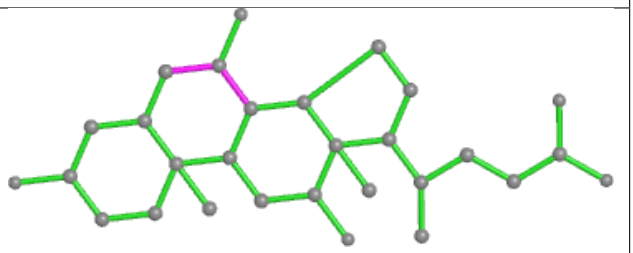


Rings

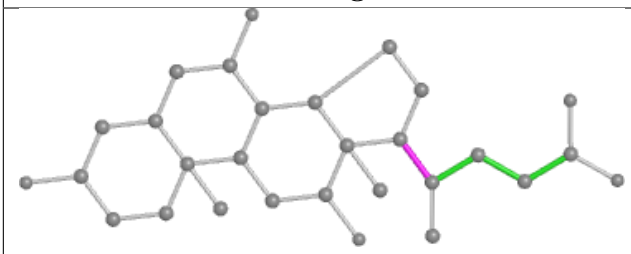
Ligand CHD C 302



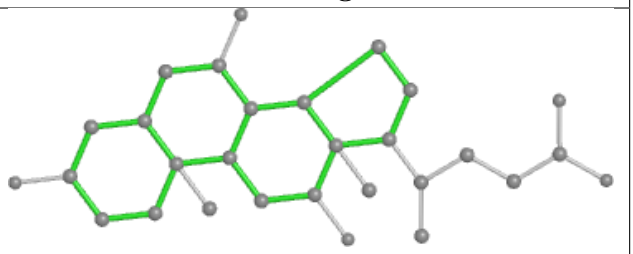
Bond lengths



Bond angles

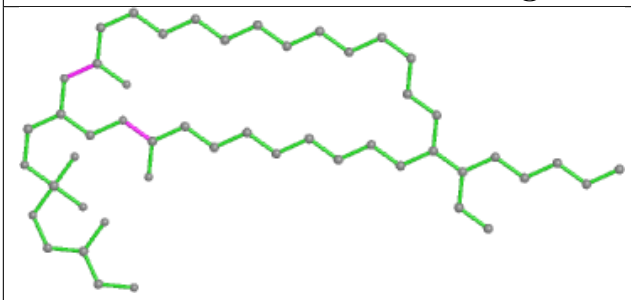


Torsions

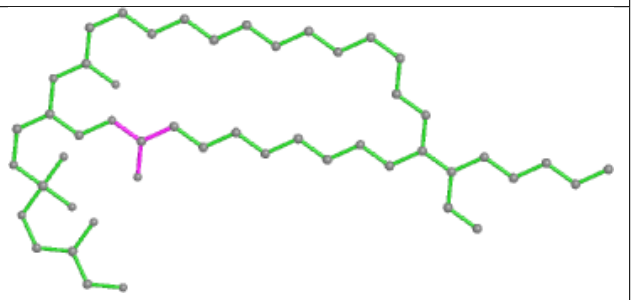


Rings

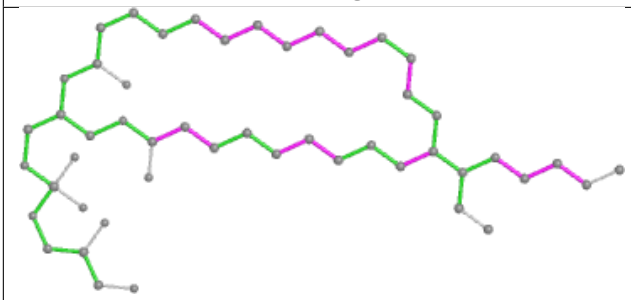
Ligand PGV A 605



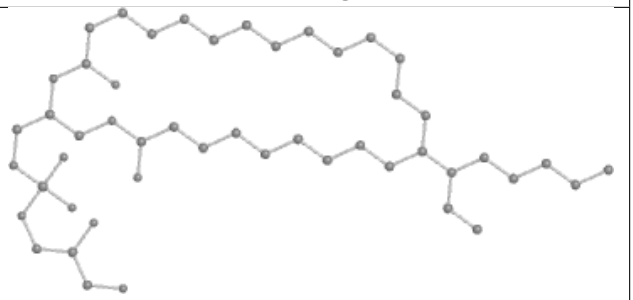
Bond lengths



Bond angles

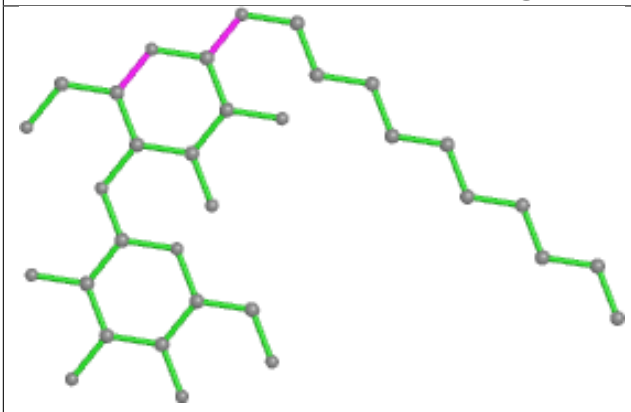


Torsions

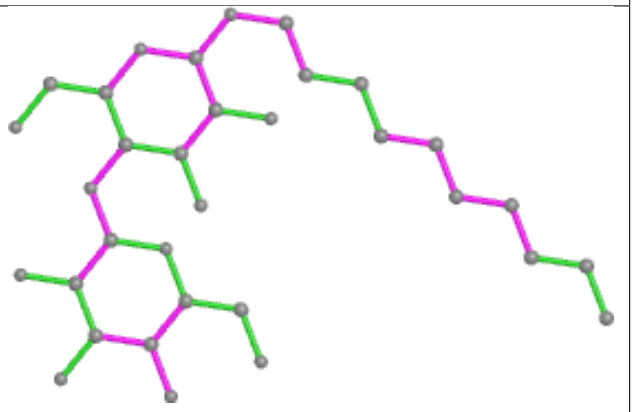


Rings

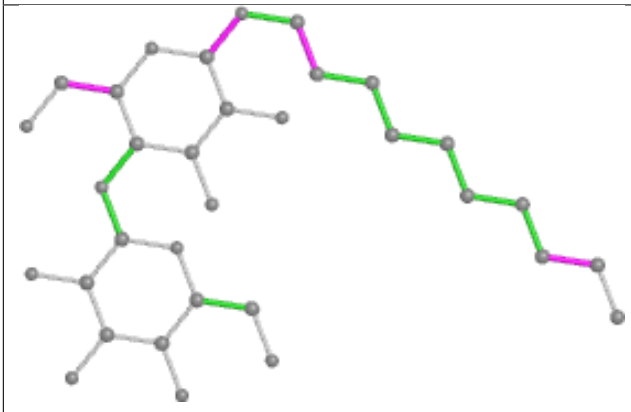
Ligand DMU P 302



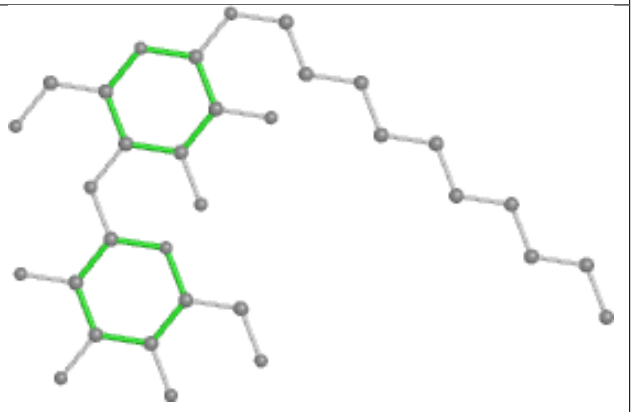
Bond lengths



Bond angles

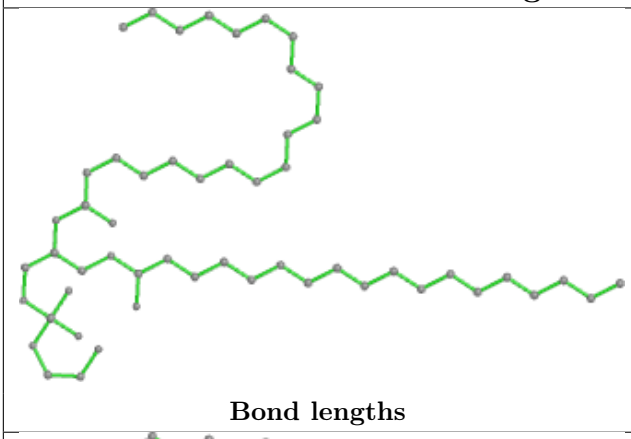


Torsions

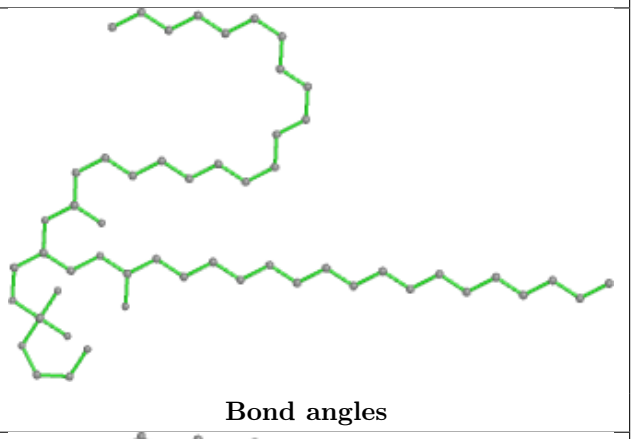


Rings

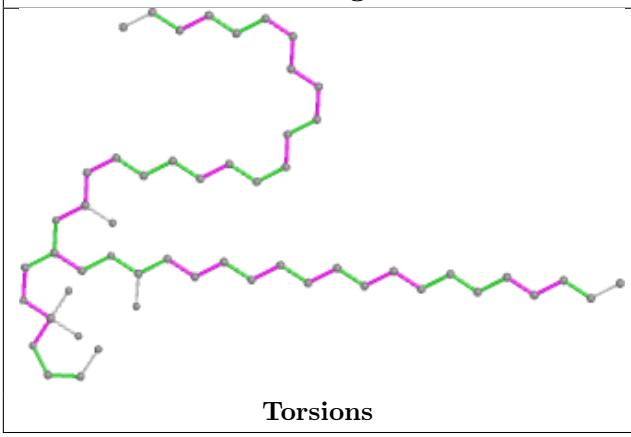
Ligand PEK C 315



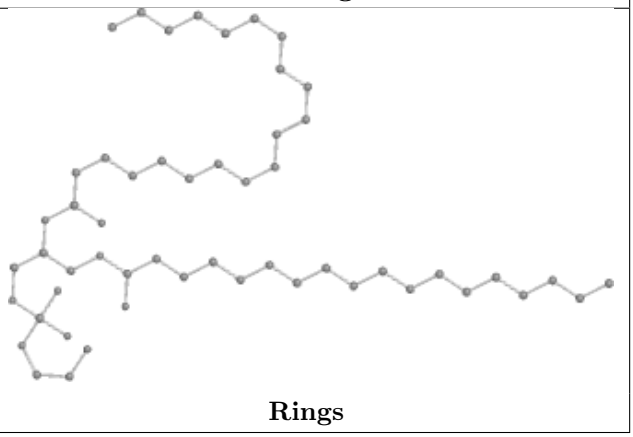
Bond lengths



Bond angles

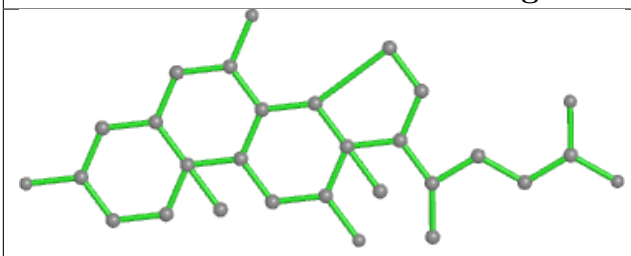


Torsions

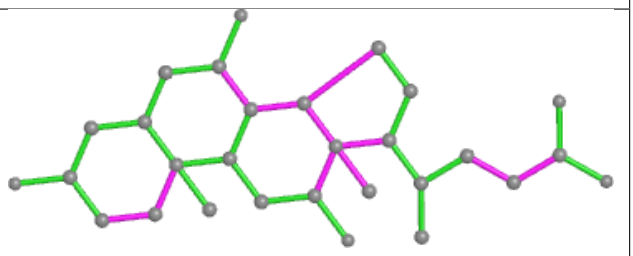


Rings

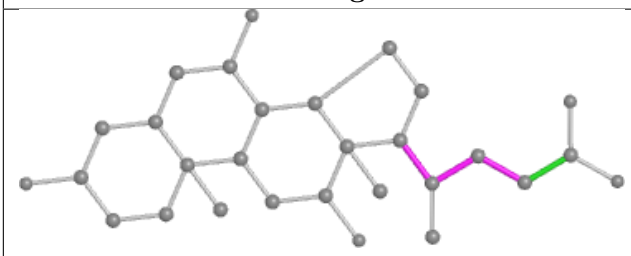
Ligand CHD T 104



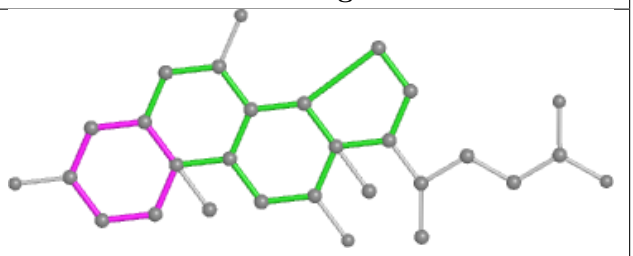
Bond lengths



Bond angles

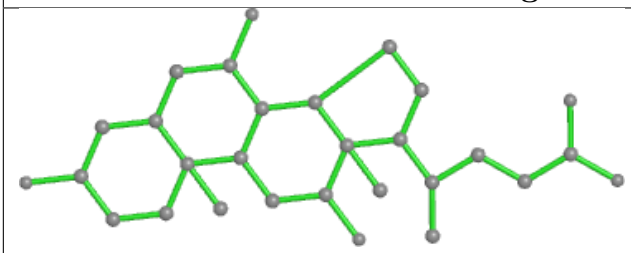


Torsions

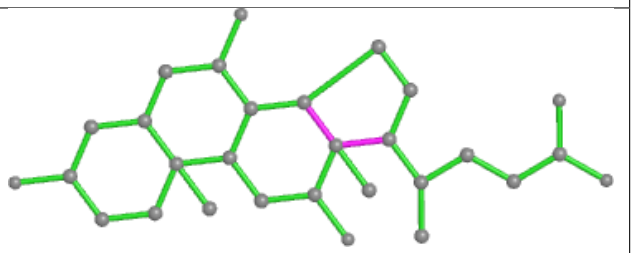


Rings

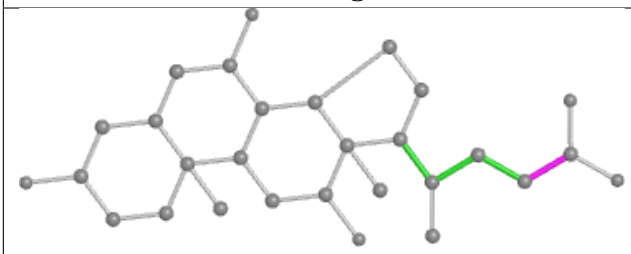
Ligand CHD B 302



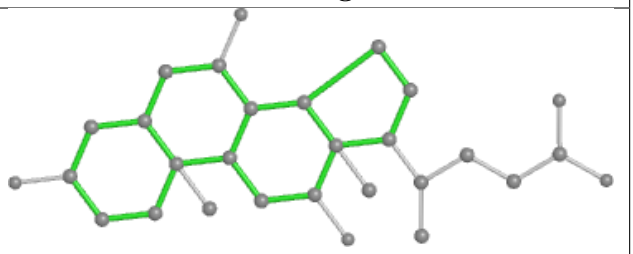
Bond lengths



Bond angles

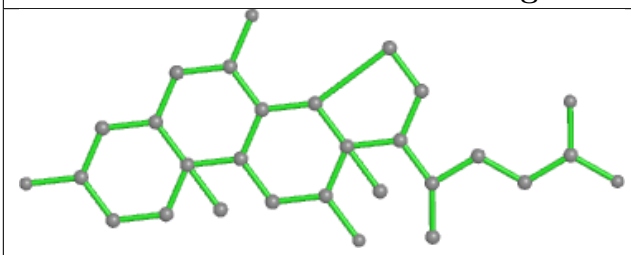


Torsions

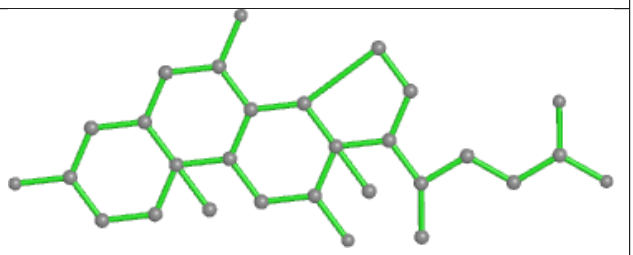


Rings

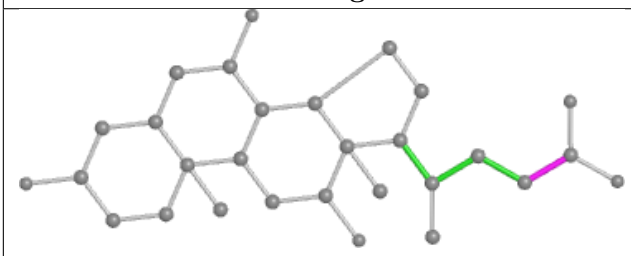
Ligand CHD C 307



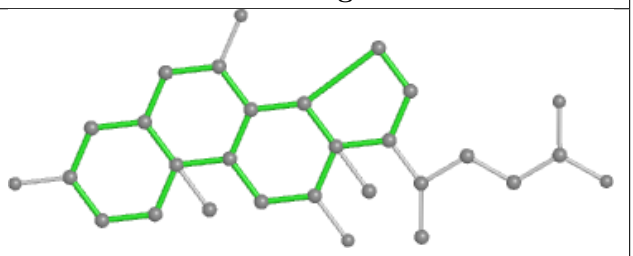
Bond lengths



Bond angles

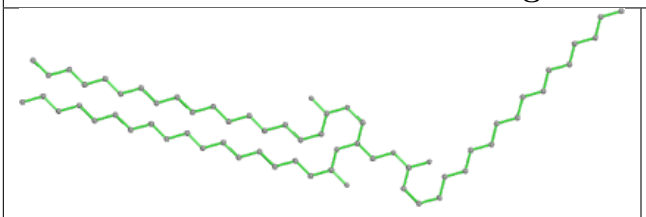


Torsions

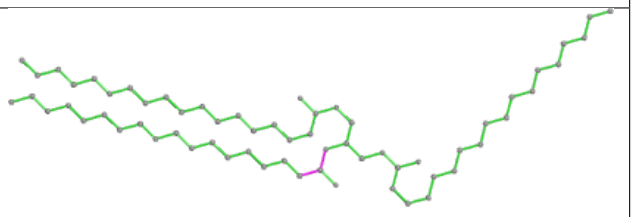


Rings

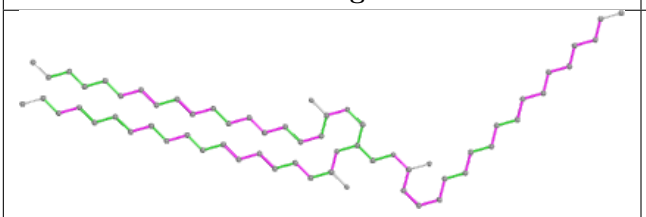
Ligand TGL N 604



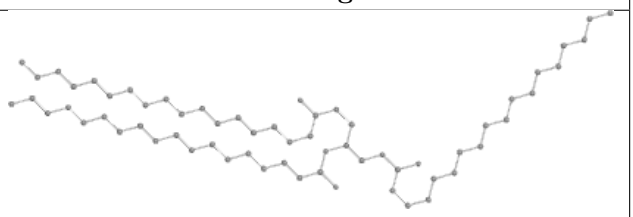
Bond lengths



Bond angles

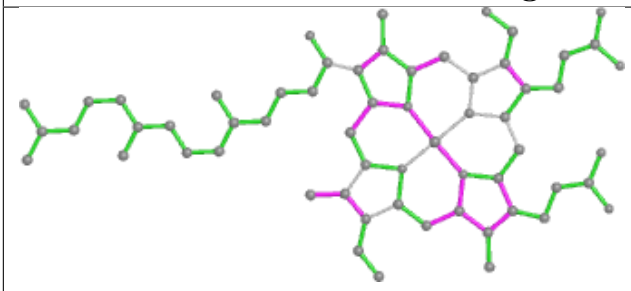


Torsions

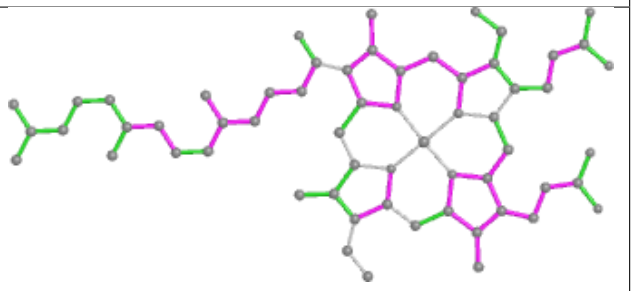


Rings

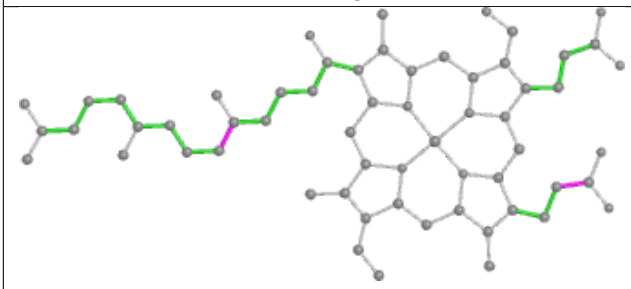
Ligand HEA N 607



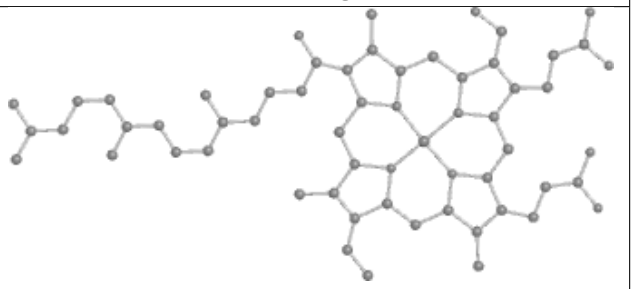
Bond lengths



Bond angles

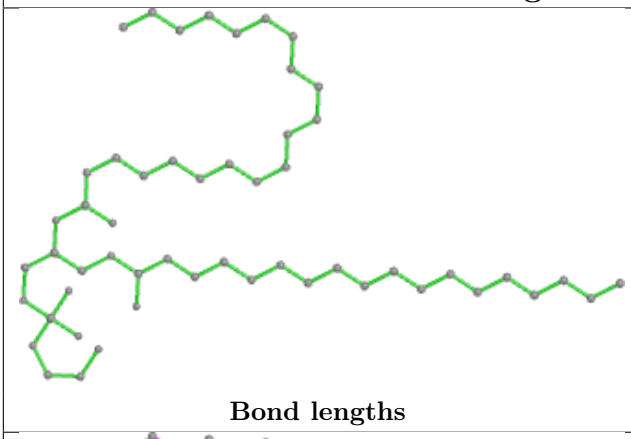


Torsions

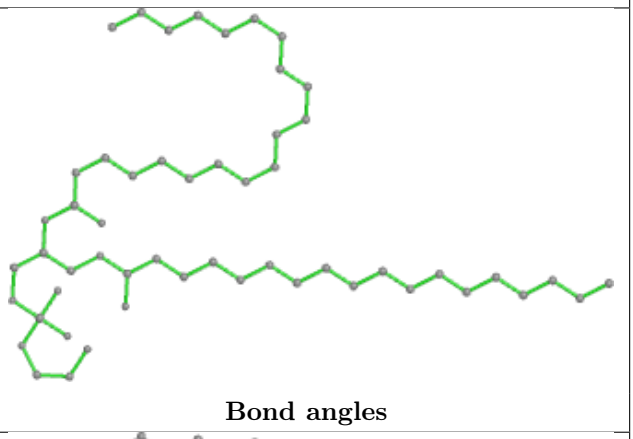


Rings

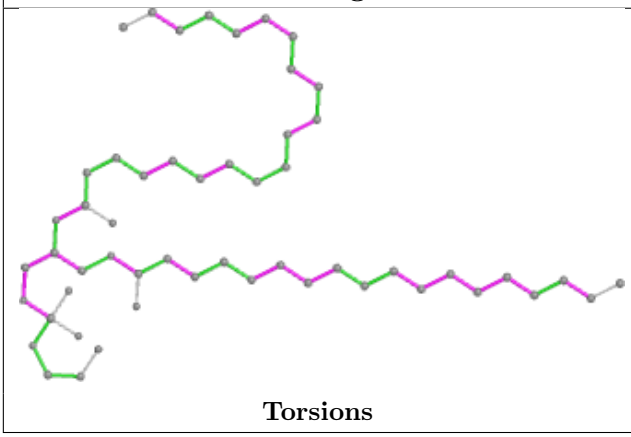
Ligand PEK P 301



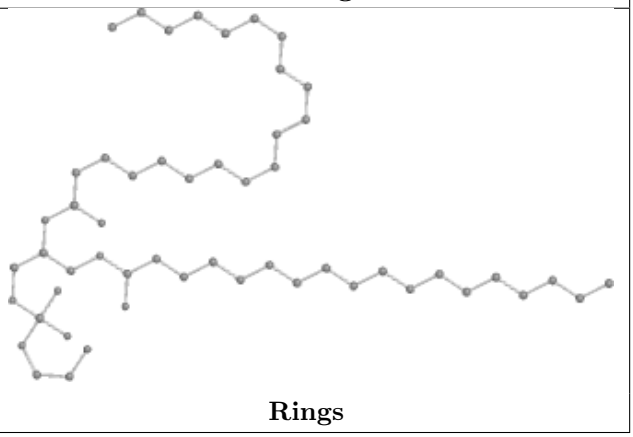
Bond lengths



Bond angles

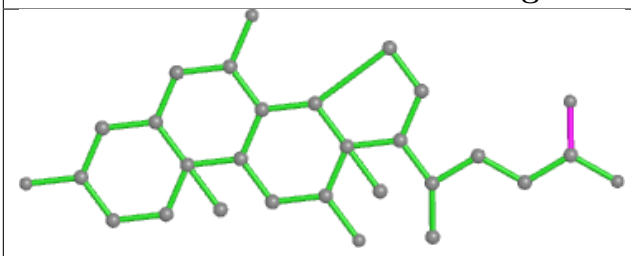


Torsions

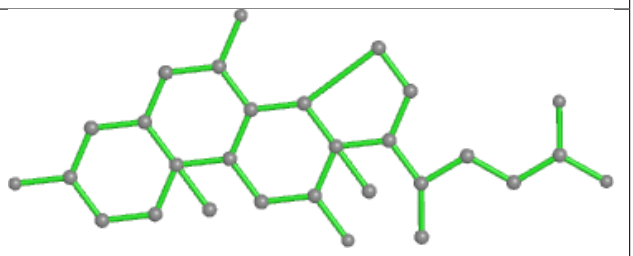


Rings

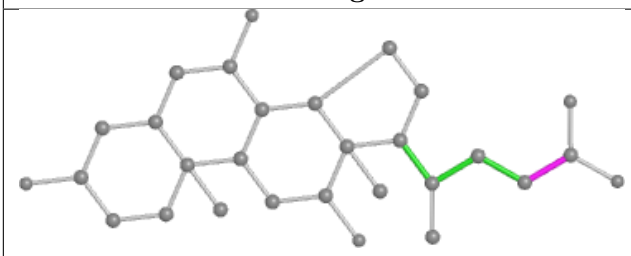
Ligand CHD P 303



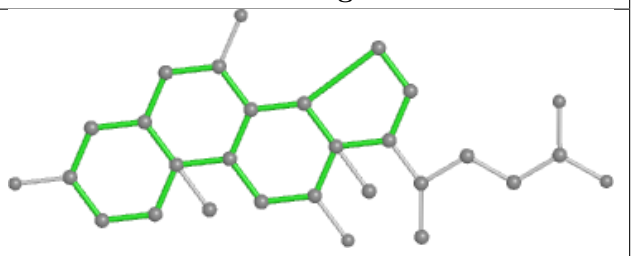
Bond lengths



Bond angles

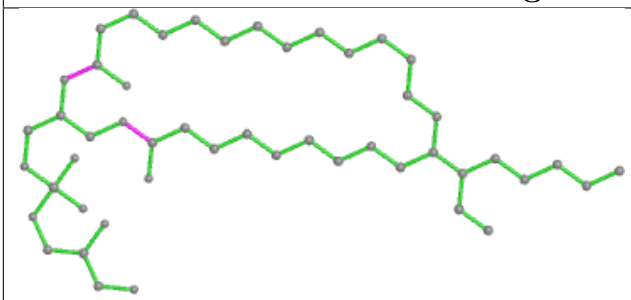


Torsions



Rings

Ligand PGV Z 102



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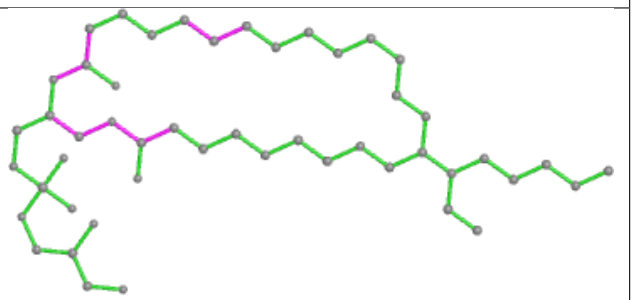
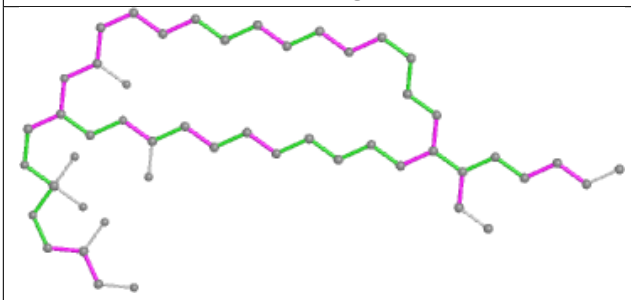
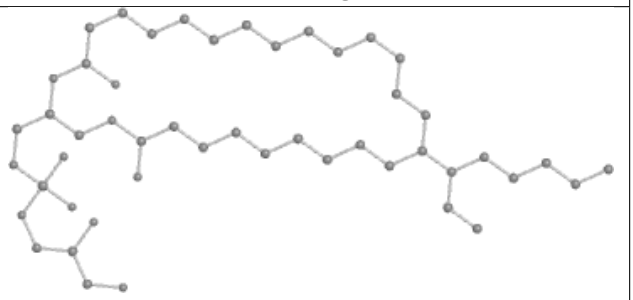


Bond angles

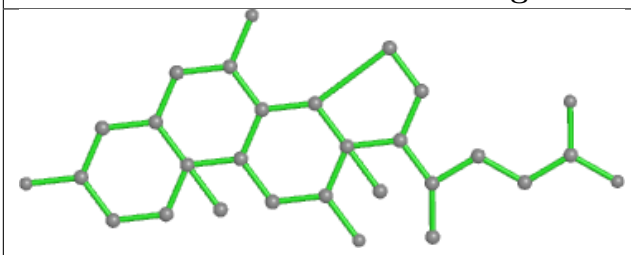


Torsions

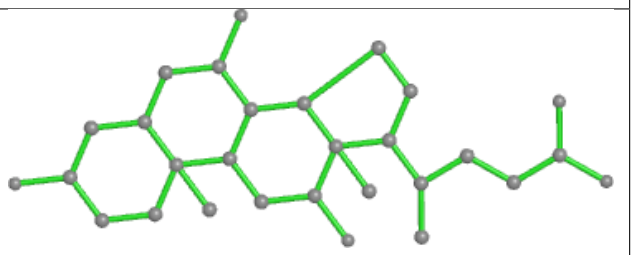


Rings

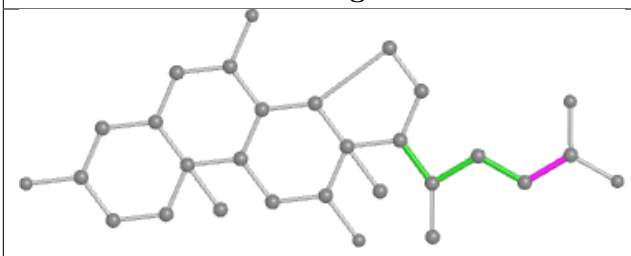
Ligand CHD G 1305



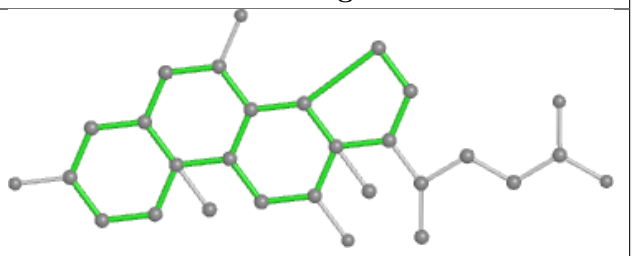
Bond lengths



Bond angles

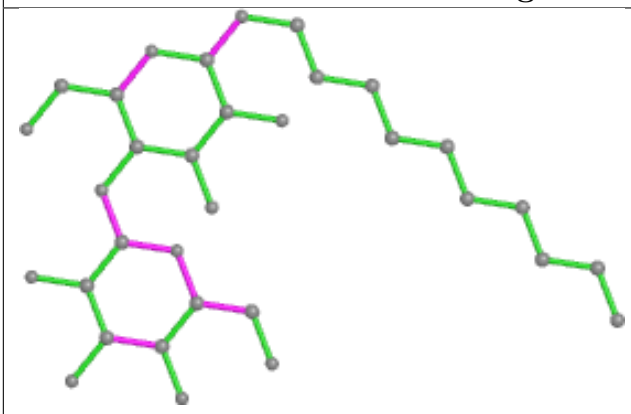


Torsions



Rings

Ligand DMU C 313



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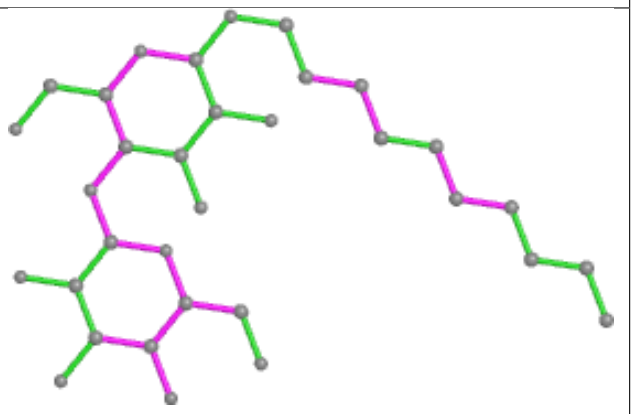
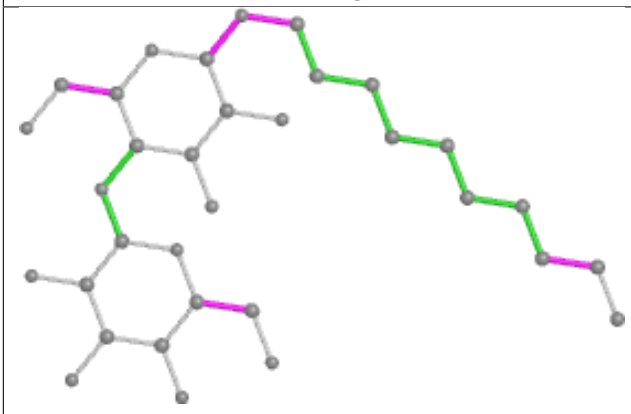
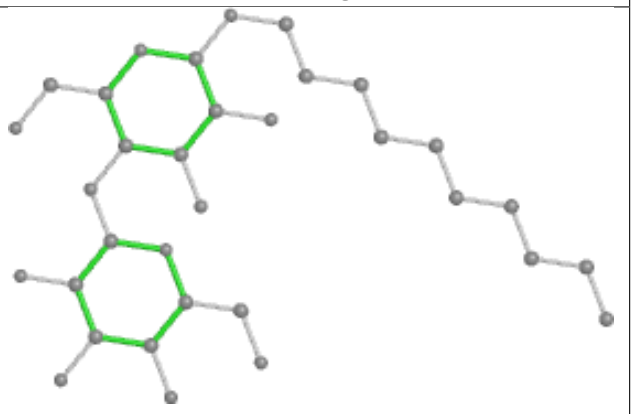


Bond angles

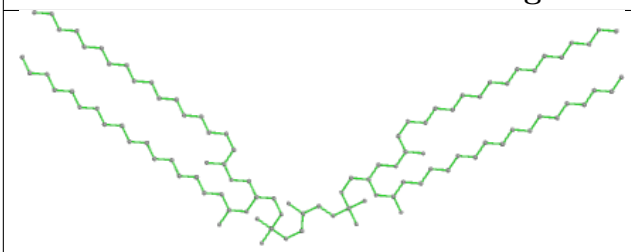


Torsions

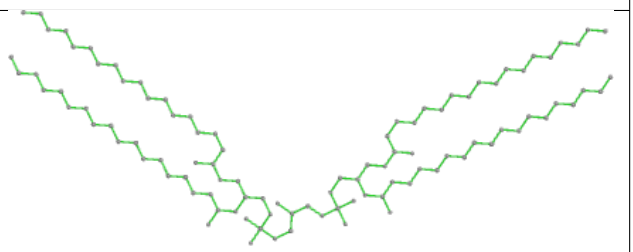


Rings

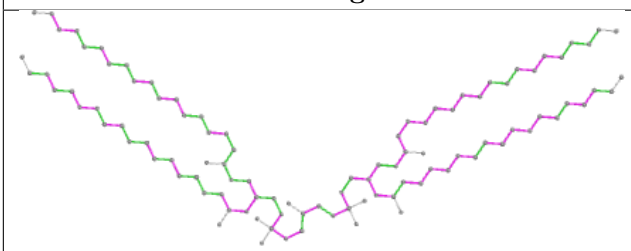
Ligand CDL C 312



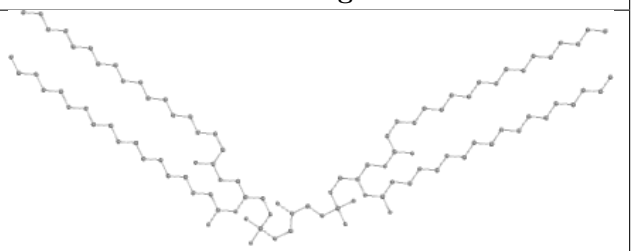
Bond lengths



Bond angles

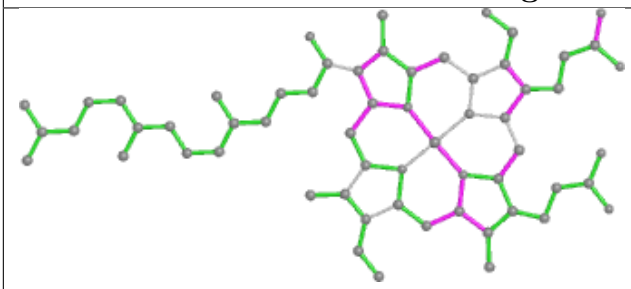


Torsions

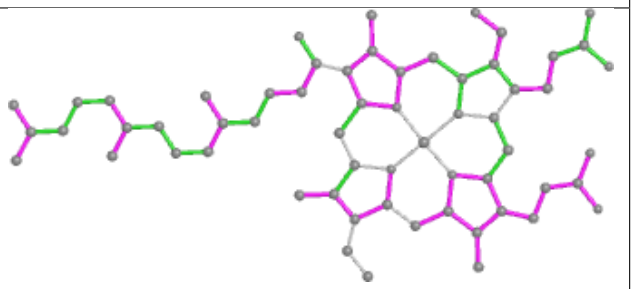


Rings

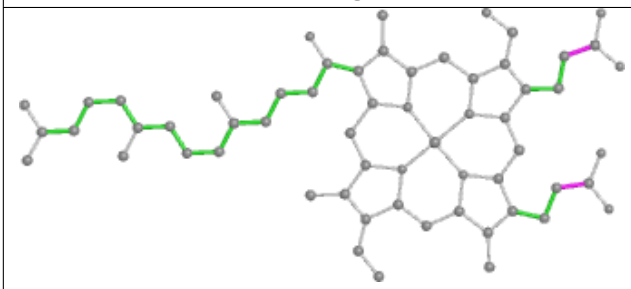
Ligand HEA N 606



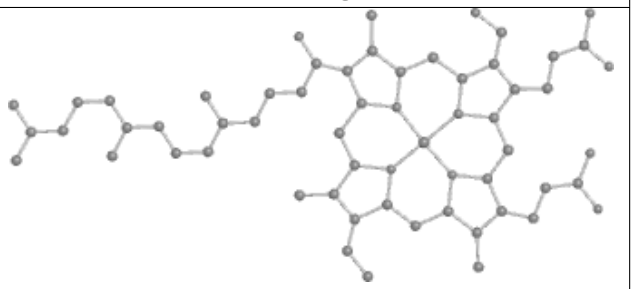
Bond lengths



Bond angles

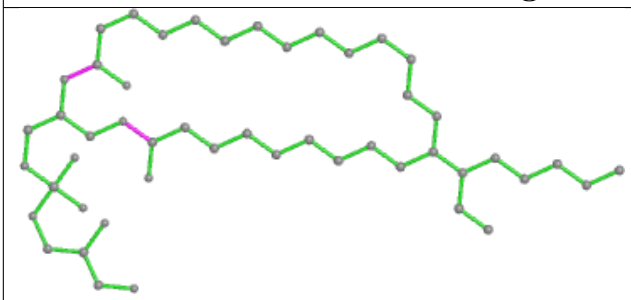


Torsions

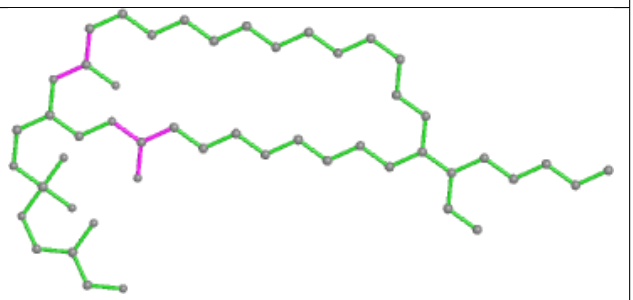


Rings

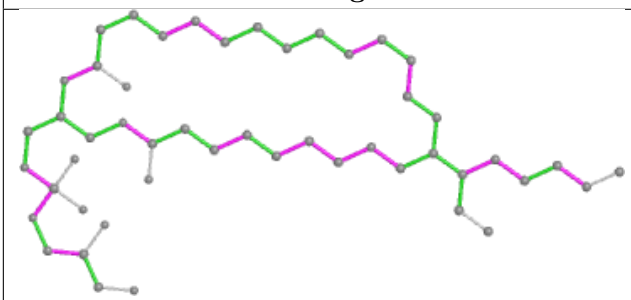
Ligand PGV N 616



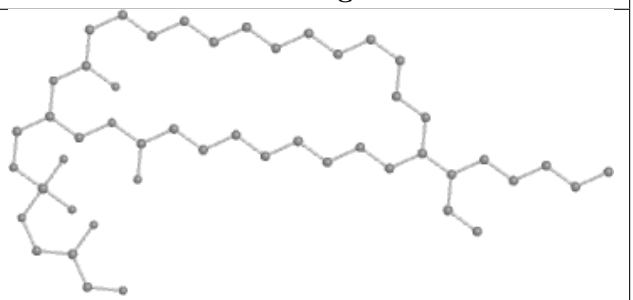
Bond lengths



Bond angles

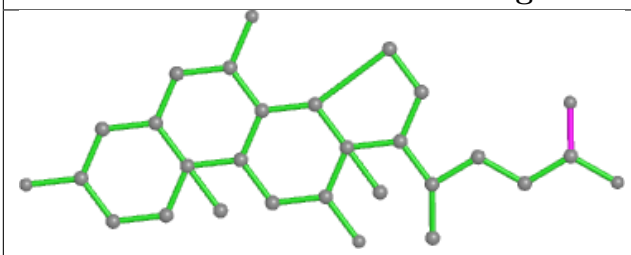


Torsions

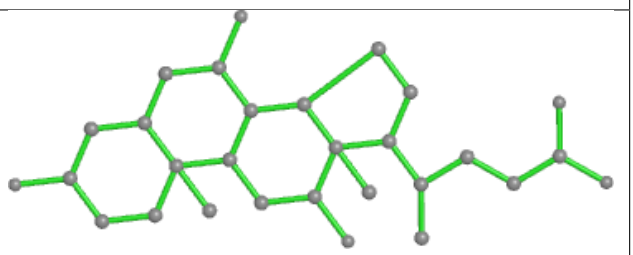


Rings

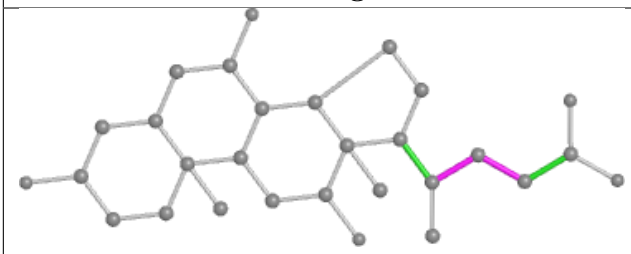
Ligand CHD J 1102



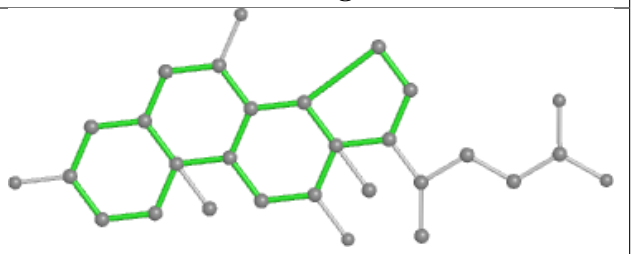
Bond lengths



Bond angles

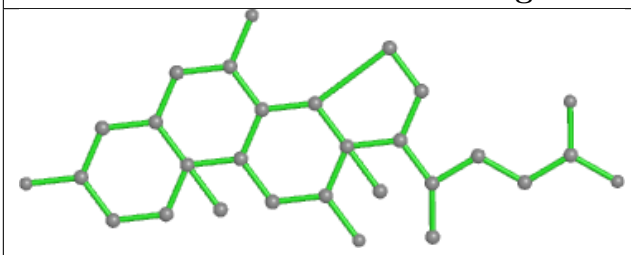


Torsions

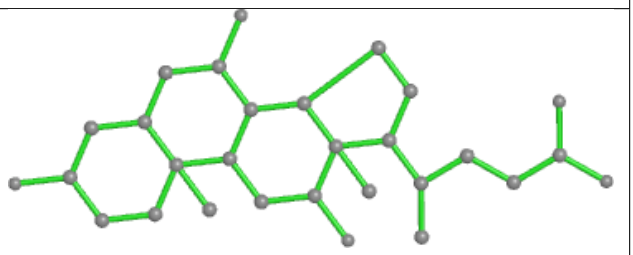


Rings

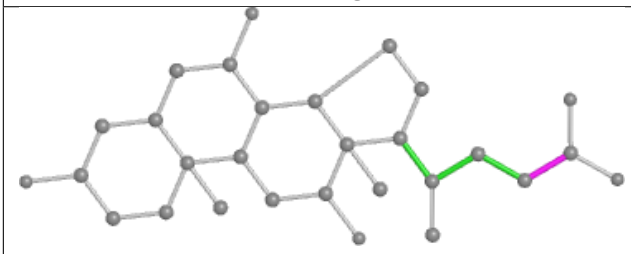
Ligand CHD W 302



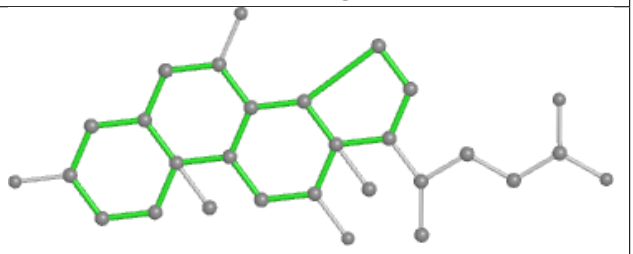
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	15.7
4	Q	4	SER	13.9
4	Q	6	VAL	13.6
5	R	109	VAL	13.0
4	Q	5	VAL	13.0
8	H	45	ALA	11.4
13	Z	42	LYS	10.4
6	F	98	HIS	10.3
6	F	97	ALA	9.3
4	Q	7	LYS	9.0
12	Y	47	LYS	8.8
8	U	48	GLY	8.2
8	U	47	GLY	8.1
7	T	10	GLY	8.0
8	U	8	ILE	7.7
6	S	96	LEU	7.7
8	U	10	ASN	7.5
11	X	55	GLU	7.4
4	Q	8	SER	7.2
13	M	43	SER	7.2
10	W	58	LYS	6.9
4	Q	3	GLY	6.9
8	U	7	LYS	6.9
6	F	96	LEU	6.8
10	W	57	HIS	6.8
9	I	37	PHE	6.7
9	V	37	PHE	6.7
8	U	45	ALA	6.7
7	G	3	ALA	6.6
8	H	48	GLY	6.6
10	J	1	PHE	6.4
4	Q	147	LYS	6.3
5	E	5	HIS	6.3
6	F	1	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
7	T	9	GLY	6.2
11	X	5	ARG	6.2
10	W	48	TYR	6.0
7	G	7	ASP	6.0
11	X	6	ALA	5.9
4	Q	2	HIS	5.9
11	X	7	PRO	5.9
5	R	5	HIS	5.8
4	Q	1	ALA	5.8
2	O	227	LEU	5.7
11	X	56	GLN	5.5
8	U	44	THR	5.5
10	J	58	LYS	5.5
7	G	2	SER	5.5
8	H	46	LYS	5.2
8	U	52	VAL	5.2
4	D	147	LYS	5.1
2	O	113	TYR	5.1
11	K	5	ARG	5.1
5	E	109	VAL	5.0
4	Q	33	LEU	4.9
8	U	43	MET	4.9
5	R	108	LYS	4.8
7	T	36	TRP	4.8
7	T	42	ARG	4.8
12	L	2	HIS	4.7
8	U	50	VAL	4.7
7	G	40	GLY	4.7
9	V	2	THR	4.6
10	J	57	HIS	4.6
8	U	49	ASP	4.6
7	G	36	TRP	4.6
7	T	40	GLY	4.6
13	Z	40	TYR	4.6
11	K	6	ALA	4.6
2	O	90	ILE	4.5
9	V	25	PHE	4.5
7	T	45	PRO	4.4
8	H	47	GLY	4.4
9	V	26	MET	4.4
6	S	97	ALA	4.4
7	T	41	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
13	Z	39	ASN	4.3
7	T	46	ALA	4.3
6	F	3	GLY	4.3
7	G	84	LYS	4.3
7	G	37	LEU	4.3
6	S	98	HIS	4.3
7	T	1	ALA	4.2
7	G	1	ALA	4.2
4	Q	51	LEU	4.0
13	Z	41	LYS	4.0
8	H	44	THR	4.0
9	I	25	PHE	4.0
11	K	7	PRO	4.0
7	T	84	LYS	4.0
6	S	22	LEU	3.9
7	G	42	ARG	3.9
8	H	8	ILE	3.9
7	G	43	GLU	3.9
7	T	39	SER	3.9
10	W	52	TRP	3.8
7	T	5	LYS	3.8
7	T	47	PHE	3.8
4	Q	46	ALA	3.8
10	J	56	PRO	3.8
8	H	10	ASN	3.8
7	G	5	LYS	3.8
6	F	95	GLN	3.8
7	G	6	GLY	3.8
11	X	13	TYR	3.7
7	T	8	HIS	3.7
6	F	2	SER	3.7
6	S	94	HIS	3.7
2	O	224	ALA	3.7
8	H	50	VAL	3.7
13	Z	35	TYR	3.7
7	T	3	ALA	3.6
11	X	19	ALA	3.5
7	T	48	ILE	3.5
8	H	43	MET	3.5
13	M	39	ASN	3.5
9	I	33	THR	3.4
1	A	70	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	3.4
8	H	51	SER	3.4
1	A	66	ILE	3.4
1	N	254	ILE	3.4
8	U	51	SER	3.3
4	Q	102	TYR	3.3
8	H	49	ASP	3.2
13	M	40	TYR	3.2
7	G	10	GLY	3.2
7	T	43	GLU	3.2
7	T	4	ALA	3.2
2	B	90	ILE	3.2
7	T	82	TYR	3.2
6	S	95	GLN	3.1
4	Q	35	ALA	3.1
6	F	22	LEU	3.1
4	Q	39	ALA	3.1
13	Z	13	LYS	3.1
9	V	34	PHE	3.1
9	V	30	GLY	3.1
4	Q	48	TRP	3.1
10	W	56	PRO	3.0
4	Q	38	LYS	3.0
7	G	8	HIS	3.0
9	I	34	PHE	3.0
7	T	2	SER	3.0
7	G	41	HIS	3.0
7	T	78	LEU	3.0
2	B	91	ASN	3.0
9	I	29	LEU	3.0
9	I	26	MET	2.9
9	V	72	ALA	2.9
2	O	221	LYS	2.8
5	R	106	LEU	2.8
9	V	33	THR	2.8
13	Z	17	ILE	2.8
8	U	11	TYR	2.8
7	G	35	SER	2.8
10	J	2	GLU	2.8
7	G	38	HIS	2.8
1	N	258	VAL	2.8
4	Q	72	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
11	X	15	ASN	2.8
1	N	203	ALA	2.7
1	A	243	VAL	2.7
1	A	245	ILE	2.7
1	A	380	VAL	2.7
8	H	85	ILE	2.7
9	V	27	VAL	2.7
9	V	31	PHE	2.6
9	V	53	ASN	2.6
1	N	381	LEU	2.6
8	U	9	LYS	2.6
1	N	389	ILE	2.6
1	N	374	VAL	2.6
10	J	52	TRP	2.6
5	E	108	LYS	2.6
1	A	73	ILE	2.6
8	H	52	VAL	2.6
11	X	18	LEU	2.6
5	R	107	ASP	2.6
1	A	374	VAL	2.6
1	N	206	ILE	2.6
3	P	38	ASN	2.6
13	M	42	LYS	2.5
6	S	93	PRO	2.5
5	R	92	THR	2.5
1	A	202	LEU	2.5
1	A	246	LEU	2.5
4	Q	49	SER	2.5
1	A	67	PHE	2.5
2	O	218	TYR	2.5
7	G	9	GLY	2.5
7	G	4	ALA	2.5
6	F	28	GLN	2.5
1	A	367	LEU	2.5
8	H	53	CYS	2.4
6	F	94	HIS	2.4
12	L	47	LYS	2.4
2	B	209	ILE	2.4
1	A	382	SER	2.4
3	P	182	TYR	2.4
8	H	42	ALA	2.4
1	A	64	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	373	VAL	2.4
1	A	386	VAL	2.4
1	N	73	ILE	2.4
2	B	165	VAL	2.4
4	Q	34	SER	2.3
2	O	222	TRP	2.3
5	E	7	THR	2.3
1	A	389	ILE	2.3
9	V	52	ARG	2.3
9	V	22	VAL	2.3
9	V	24	ALA	2.3
10	J	48	TYR	2.3
3	P	122	HIS	2.3
6	F	25	ARG	2.3
1	N	382	SER	2.3
9	V	29	LEU	2.3
3	P	3	HIS	2.3
1	A	377	PHE	2.2
7	T	49	PRO	2.2
1	N	153	ALA	2.2
4	Q	73	ARG	2.2
10	J	55	PHE	2.2
1	A	128	VAL	2.2
4	Q	78	TRP	2.2
1	A	20	LEU	2.2
5	E	94	ASN	2.2
4	Q	58	GLU	2.2
1	A	514	LYS	2.2
6	F	27	GLY	2.2
1	N	332	ILE	2.2
4	Q	40	LEU	2.2
1	A	258	VAL	2.2
5	R	94	ASN	2.2
7	G	45	PRO	2.2
1	N	24	ALA	2.2
9	I	30	GLY	2.2
9	I	38	ALA	2.2
6	F	26	LYS	2.2
5	R	105	GLY	2.1
1	N	377	PHE	2.1
9	I	19	PHE	2.1
7	G	39	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	155	VAL	2.1
1	N	380	VAL	2.1
7	T	75	VAL	2.1
1	N	385	ALA	2.1
1	A	385	ALA	2.1
12	Y	20	ARG	2.1
1	A	150	LEU	2.1
1	N	70	VAL	2.1
9	V	19	PHE	2.1
10	W	55	PHE	2.1
4	D	1	ALA	2.1
6	S	25	ARG	2.0
1	A	63	PHE	2.0
1	N	383	MET	2.0
2	O	92	ASN	2.0
1	N	386	VAL	2.0
7	T	74	ARG	2.0
9	V	23	GLY	2.0
1	A	363	LEU	2.0
1	N	195	LEU	2.0
2	O	170	LEU	2.0
2	O	60	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.72	0.24	47,87,130,139	0
7	TPO	T	11	11/12	0.84	0.32	54,119,161,165	0
2	FME	O	1	10/11	0.96	0.13	40,48,59,62	0
1	FME	A	1	10/11	0.97	0.17	45,53,79,101	0
2	FME	B	1	10/11	0.98	0.12	36,41,50,58	0
1	FME	N	1	10/11	0.98	0.21	51,59,89,92	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	P	309	4/4	0.05	0.38	81,82,85,87	0
28	SAC	V	101	9/10	0.21	0.75	129,139,152,154	0
23	DMU	C	301	33/33	0.40	0.44	87,130,143,153	0
19	EDO	Z	103	4/4	0.43	0.24	86,94,94,96	0
19	EDO	L	102	4/4	0.51	0.30	68,69,72,75	0
19	EDO	V	103	4/4	0.55	0.21	81,81,90,95	0
19	EDO	K	101	4/4	0.58	0.23	74,75,76,77	0
22	CHD	T	104	29/29	0.60	0.34	81,147,172,175	0
24	PEK	C	315	53/53	0.61	0.26	60,85,124,172	0
19	EDO	G	1306	4/4	0.61	0.15	90,90,93,95	0
20	TGL	Y	101	63/63	0.62	0.28	55,79,120,132	0
24	PEK	P	301	53/53	0.64	0.26	64,88,161,171	0
26	PSC	E	201	52/52	0.64	0.31	46,92,184,199	0
19	EDO	D	206	4/4	0.64	0.27	74,79,83,88	0
20	TGL	Q	201	63/63	0.66	0.21	67,91,111,119	0
25	CDL	C	312	100/100	0.66	0.29	68,105,138,150	0
24	PEK	P	305	53/53	0.67	0.26	59,92,159,171	0
20	TGL	N	604	63/63	0.67	0.29	65,97,118,130	0
22	CHD	Y	102	29/29	0.68	0.34	96,138,156,166	0
28	SAC	I	101	9/10	0.68	0.34	83,101,110,116	0
19	EDO	K	102	4/4	0.68	0.17	66,68,74,75	0
26	PSC	O	302	52/52	0.69	0.31	47,95,173,185	0
25	CDL	T	102	100/100	0.69	0.28	67,112,154,170	0
19	EDO	W	303	4/4	0.69	0.21	60,74,75,76	0
20	TGL	L	101	63/63	0.70	0.24	47,77,104,109	0
19	EDO	P	310	4/4	0.70	0.38	61,83,84,90	0
17	PGV	Z	102	51/51	0.71	0.36	50,90,154,168	0
25	CDL	P	307	100/100	0.72	0.23	52,96,128,136	0
24	PEK	C	304	53/53	0.72	0.25	64,89,138,146	0
19	EDO	I	102	4/4	0.73	0.15	88,88,94,94	0
17	PGV	T	101	51/51	0.74	0.24	56,90,115,134	0
20	TGL	A	615	63/63	0.74	0.26	59,87,139,151	0
23	DMU	G	1302	33/33	0.75	0.18	62,110,125,125	0
20	TGL	D	201	63/63	0.75	0.19	55,86,101,108	0
19	EDO	G	1304	4/4	0.75	0.19	75,79,80,80	0
19	EDO	C	309	4/4	0.76	0.16	75,80,83,84	0
25	CDL	C	306	100/100	0.76	0.24	48,89,122,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	S	2207	4/4	0.76	0.19	75,81,84,85	0
17	PGV	A	604	51/51	0.77	0.25	51,83,114,126	0
19	EDO	J	1103	4/4	0.78	0.12	77,77,78,85	0
19	EDO	V	102	4/4	0.78	0.17	78,79,80,83	0
19	EDO	B	304	4/4	0.78	0.21	51,59,64,72	0
19	EDO	N	613	4/4	0.79	0.22	61,65,69,80	0
19	EDO	C	310	4/4	0.81	0.15	80,89,92,100	0
17	PGV	N	616	51/51	0.81	0.21	66,87,140,156	0
23	DMU	Z	101	33/33	0.81	0.25	54,72,82,84	0
19	EDO	S	2201	4/4	0.81	0.33	58,63,63,78	0
19	EDO	O	303	4/4	0.81	0.20	53,74,76,77	0
19	EDO	F	702	4/4	0.82	0.32	70,84,89,96	0
19	EDO	N	617	4/4	0.82	0.27	87,88,92,93	0
19	EDO	B	306	4/4	0.83	0.19	70,76,78,81	0
19	EDO	G	1303	4/4	0.83	0.20	71,83,83,89	0
19	EDO	A	611	4/4	0.83	0.21	63,81,82,84	0
22	CHD	W	302	29/29	0.83	0.38	78,88,98,106	0
19	EDO	W	304	4/4	0.84	0.21	88,88,91,100	0
23	DMU	P	302	33/33	0.84	0.35	73,106,128,133	0
19	EDO	N	620	4/4	0.84	0.31	65,66,69,79	0
23	DMU	C	313	33/33	0.85	0.27	57,89,100,105	0
19	EDO	R	202	4/4	0.85	0.41	78,85,89,96	0
19	EDO	A	619	4/4	0.85	0.23	66,67,70,78	0
19	EDO	N	612	4/4	0.85	0.33	67,73,74,82	0
19	EDO	A	614	4/4	0.86	0.24	41,44,46,52	0
22	CHD	J	1102	29/29	0.86	0.34	59,74,86,97	0
19	EDO	M	102	4/4	0.87	0.41	72,75,80,83	0
19	EDO	J	1105	4/4	0.87	0.36	56,73,74,88	0
19	EDO	S	2206	4/4	0.87	0.34	55,60,63,70	0
19	EDO	A	610	4/4	0.88	0.26	38,43,46,50	0
19	EDO	S	2205	4/4	0.88	0.24	56,59,69,70	0
19	EDO	E	205	4/4	0.88	0.20	81,82,82,86	0
19	EDO	C	311	4/4	0.88	0.15	83,85,90,99	0
19	EDO	V	104	4/4	0.89	0.17	50,74,76,77	0
19	EDO	A	612	4/4	0.90	0.14	55,56,56,62	0
19	EDO	C	314	4/4	0.90	0.25	62,70,71,79	0
19	EDO	T	103	4/4	0.90	0.31	57,66,69,71	0
19	EDO	D	205	4/4	0.90	0.20	64,77,78,81	0
19	EDO	B	309	4/4	0.90	0.23	75,91,97,105	0
19	EDO	N	611	4/4	0.90	0.13	67,71,73,81	0
19	EDO	I	103	4/4	0.91	0.10	58,63,64,67	0
19	EDO	D	204	4/4	0.91	0.34	60,76,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	EDO	E	204	4/4	0.92	0.28	73,75,75,78	0
19	EDO	W	301	4/4	0.92	0.18	62,74,75,76	0
19	EDO	A	608	4/4	0.92	0.21	50,56,63,68	0
19	EDO	Q	203	4/4	0.92	0.12	73,77,82,86	0
19	EDO	R	201	4/4	0.92	0.16	54,54,55,56	0
19	EDO	U	1501	4/4	0.92	0.24	55,66,68,72	0
19	EDO	B	308	4/4	0.92	0.21	59,62,69,85	0
19	EDO	D	207	4/4	0.92	0.21	60,63,63,70	0
19	EDO	D	208	4/4	0.93	0.18	62,64,70,74	0
24	PEK	P	304	53/53	0.93	0.18	41,64,101,108	0
19	EDO	J	1104	4/4	0.93	0.12	55,55,58,62	0
19	EDO	P	311	4/4	0.93	0.12	42,51,51,60	0
19	EDO	Q	202	4/4	0.93	0.18	44,56,58,60	0
19	EDO	A	618	4/4	0.93	0.09	56,62,64,73	0
23	DMU	M	101	33/33	0.93	0.20	46,54,68,74	0
22	CHD	C	307	29/29	0.93	0.21	53,60,67,73	0
19	EDO	N	610	4/4	0.93	0.13	52,55,58,59	0
22	CHD	P	308	29/29	0.93	0.19	57,64,73,78	0
19	EDO	B	307	4/4	0.93	0.14	65,67,68,84	0
19	EDO	S	2204	4/4	0.94	0.17	50,66,66,68	0
15	MG	N	602	1/1	0.94	0.11	39,39,39,39	0
19	EDO	B	305	4/4	0.94	0.15	44,54,60,62	0
19	EDO	N	609	4/4	0.94	0.28	50,53,54,55	0
19	EDO	J	1101	4/4	0.95	0.23	52,61,64,68	0
19	EDO	N	615	4/4	0.95	0.14	55,68,73,83	0
24	PEK	C	303	53/53	0.95	0.22	37,62,93,113	0
19	EDO	F	704	4/4	0.95	0.18	61,61,69,71	0
19	EDO	N	618	4/4	0.96	0.16	54,56,62,64	0
17	PGV	A	605	51/51	0.96	0.20	28,48,85,90	0
17	PGV	C	305	51/51	0.96	0.20	32,43,94,101	0
19	EDO	A	620	4/4	0.96	0.18	45,47,52,52	0
17	PGV	N	605	51/51	0.96	0.21	34,49,85,93	0
19	EDO	D	202	4/4	0.96	0.28	62,72,77,81	0
16	NA	N	603	1/1	0.96	0.05	49,49,49,49	0
17	PGV	P	306	51/51	0.96	0.16	35,49,96,106	0
19	EDO	A	613	4/4	0.96	0.13	45,52,57,59	0
16	NA	A	603	1/1	0.96	0.09	35,35,35,35	0
19	EDO	A	616	4/4	0.96	0.12	54,66,68,68	0
19	EDO	N	614	4/4	0.96	0.28	41,45,46,47	0
19	EDO	E	202	4/4	0.96	0.17	51,52,52,54	0
19	EDO	E	203	4/4	0.96	0.20	51,52,57,59	0
15	MG	A	602	1/1	0.97	0.13	32,32,32,32	0

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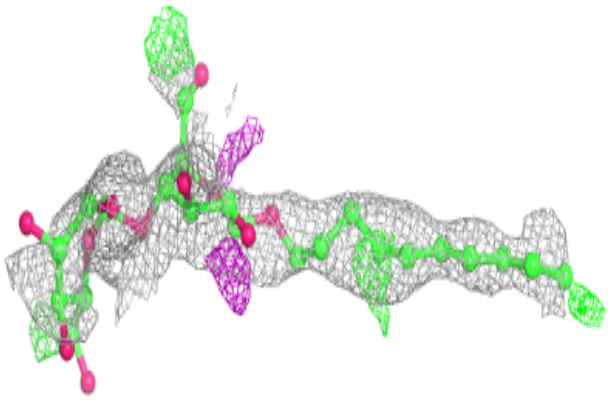
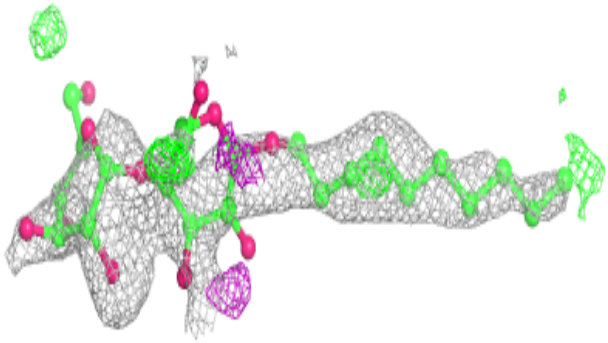
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CHD	G	1305	29/29	0.97	0.07	35,39,43,46	0
19	EDO	F	705	4/4	0.97	0.21	34,36,37,37	0
22	CHD	P	303	29/29	0.97	0.08	35,40,44,46	0
19	EDO	D	203	4/4	0.97	0.18	61,66,75,83	0
19	EDO	N	619	4/4	0.97	0.12	51,60,68,77	0
19	EDO	Q	204	4/4	0.97	0.15	73,73,75,75	0
19	EDO	T	105	4/4	0.97	0.27	44,46,47,49	0
19	EDO	C	308	4/4	0.97	0.13	43,49,53,61	0
19	EDO	A	609	4/4	0.97	0.17	33,34,35,36	0
19	EDO	N	608	4/4	0.97	0.15	42,42,45,50	0
19	EDO	S	2203	4/4	0.97	0.12	35,36,37,40	0
22	CHD	B	302	29/29	0.97	0.07	33,37,43,46	0
22	CHD	C	302	29/29	0.97	0.08	35,38,41,42	0
19	EDO	F	701	4/4	0.98	0.18	46,48,50,55	0
18	HEA	A	606	60/60	0.98	0.15	24,29,37,43	0
18	HEA	N	606	60/60	0.98	0.15	27,34,43,49	0
19	EDO	O	304	4/4	0.98	0.11	44,45,48,50	0
19	EDO	B	303	4/4	0.98	0.11	32,33,34,37	0
19	EDO	G	1301	4/4	0.98	0.15	39,40,49,51	0
19	EDO	A	617	4/4	0.98	0.26	56,61,62,69	0
18	HEA	N	607	60/60	0.98	0.16	31,36,53,61	0
27	ZN	F	703	1/1	0.99	0.06	38,38,38,38	0
27	ZN	S	2202	1/1	0.99	0.06	42,42,42,42	0
18	HEA	A	607	60/60	0.99	0.15	24,29,48,55	0
21	CUA	O	301	2/2	0.99	0.06	37,37,37,38	0
14	CU	N	601	1/1	1.00	0.13	35,35,35,35	0
14	CU	A	601	1/1	1.00	0.12	29,29,29,29	0
21	CUA	B	301	2/2	1.00	0.08	30,30,30,30	0

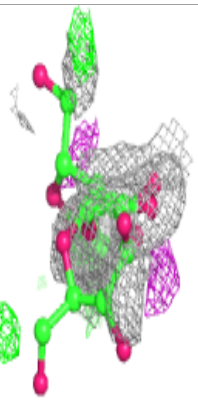
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU C 301:

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

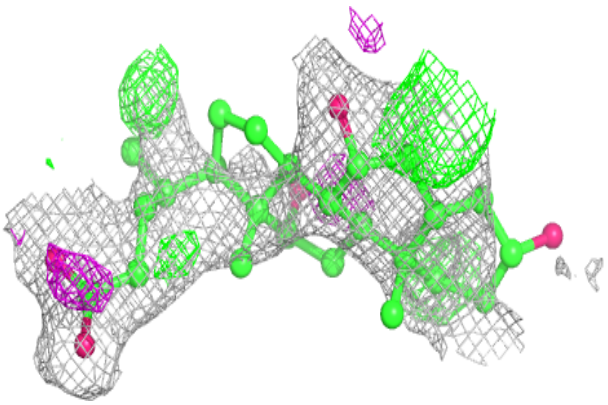


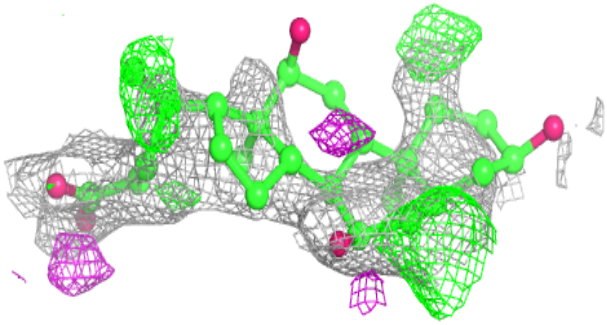


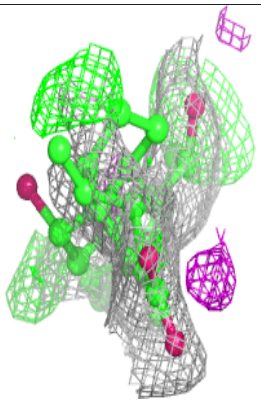


Electron density around CHD T 104:

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

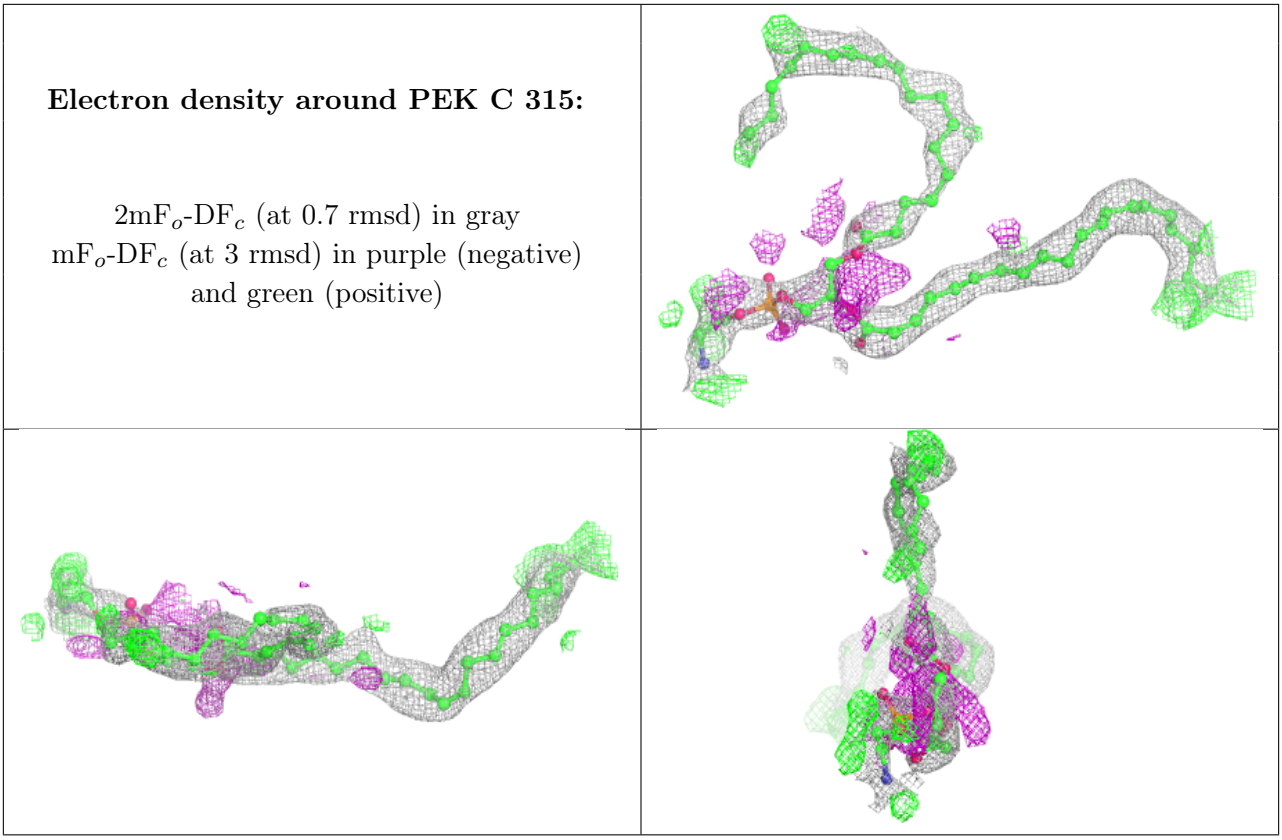






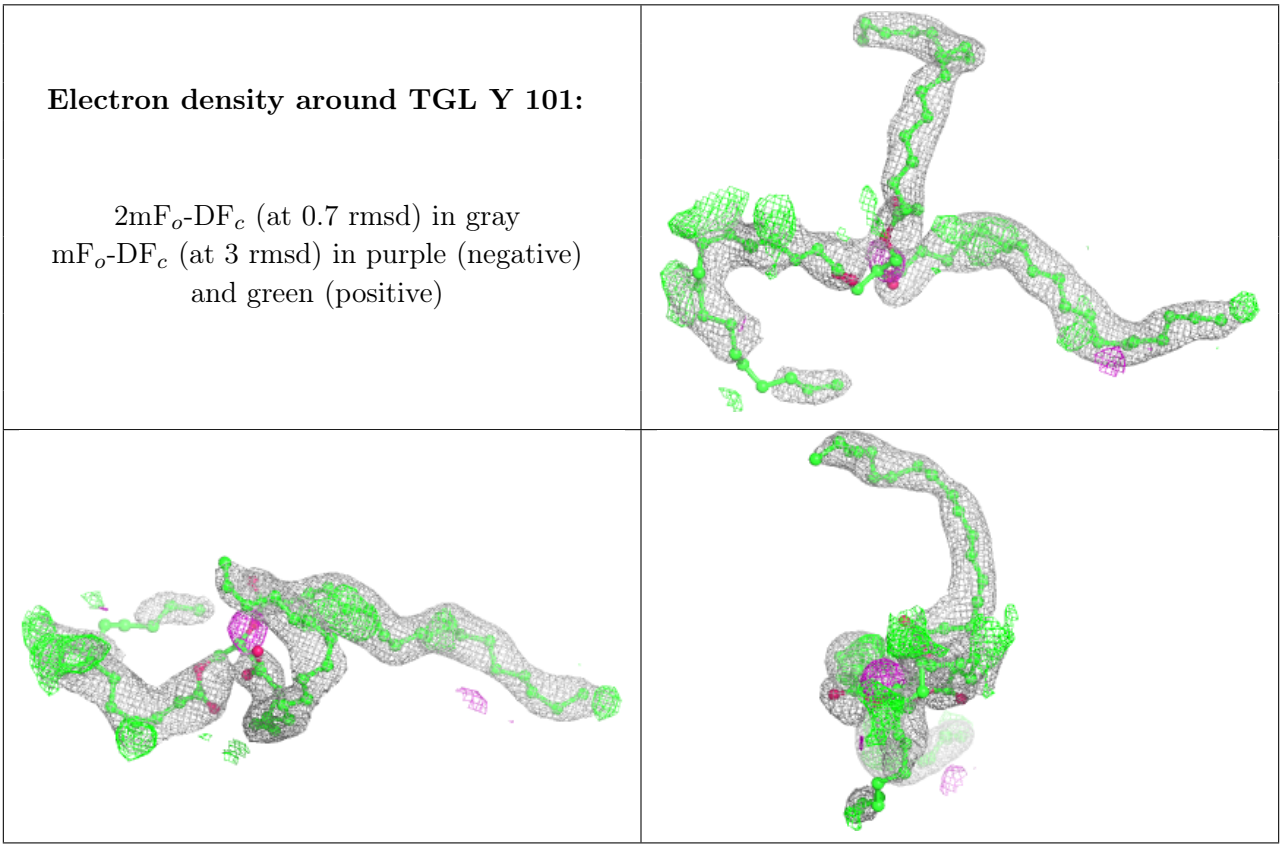
Electron density around PEK C 315:

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



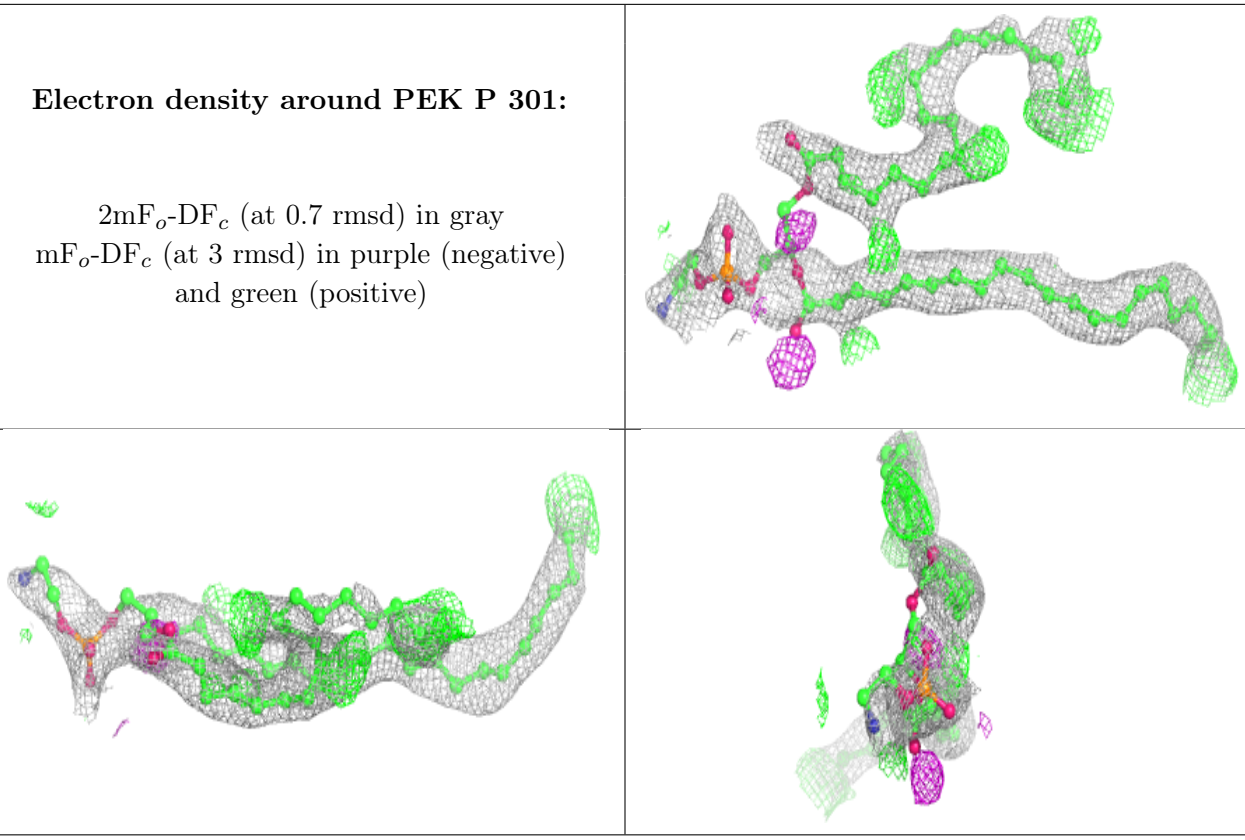
Electron density around TGL Y 101:

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



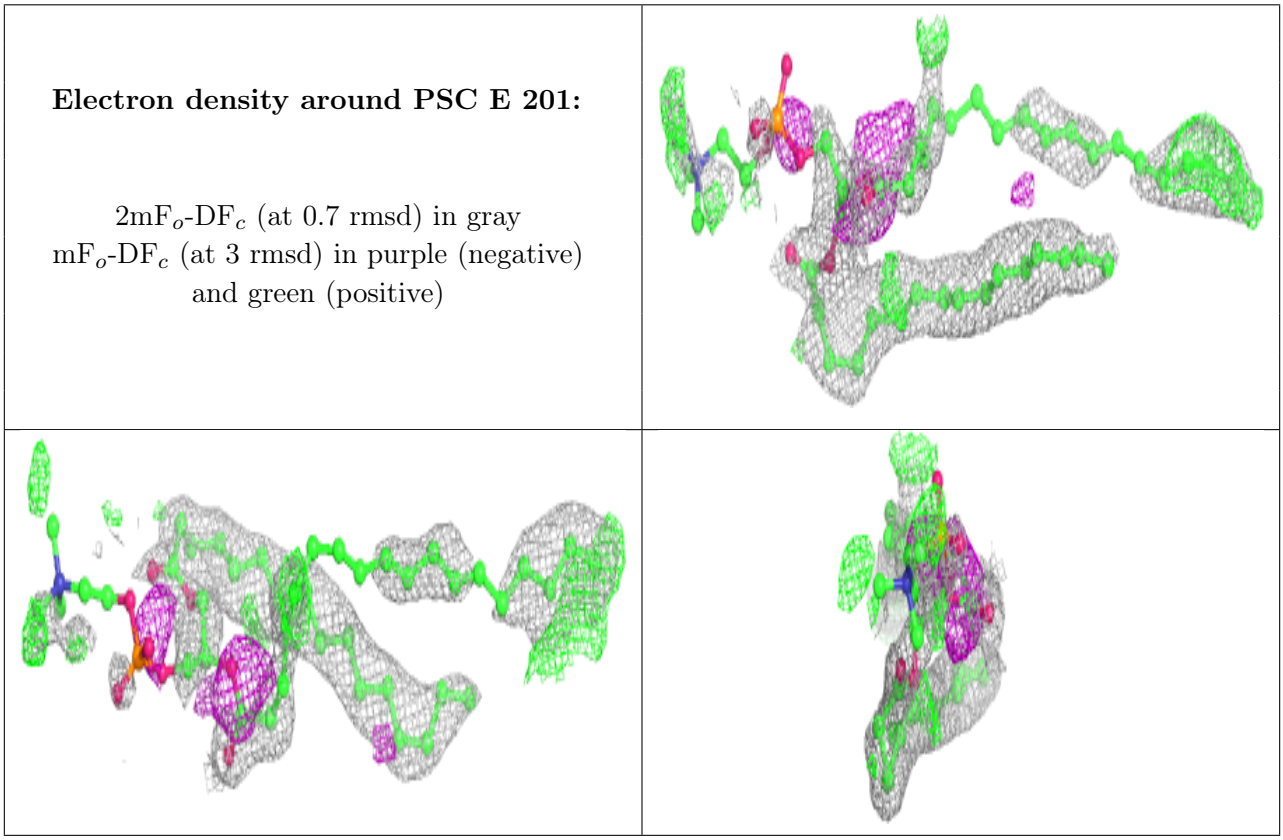
Electron density around PEK P 301:

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



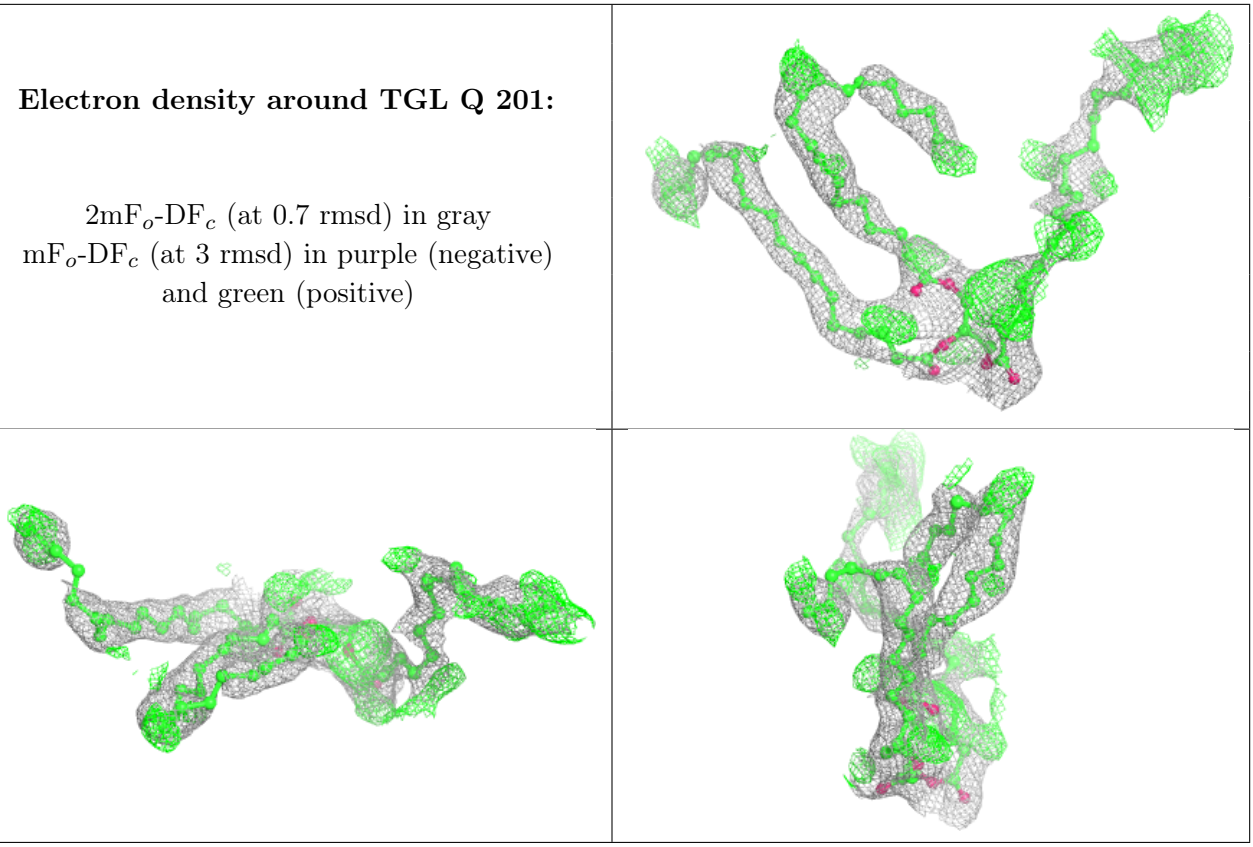
Electron density around PSC E 201:

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



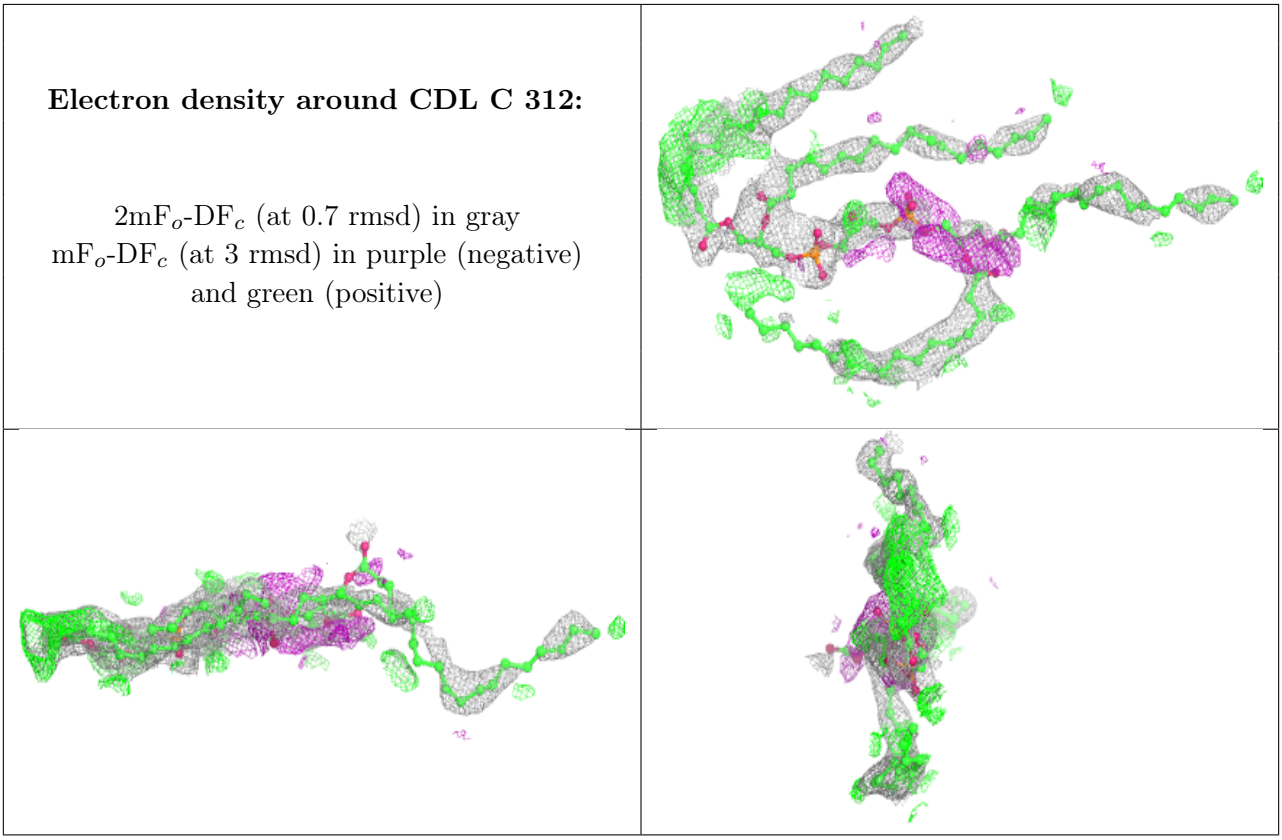
Electron density around TGL Q 201:

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



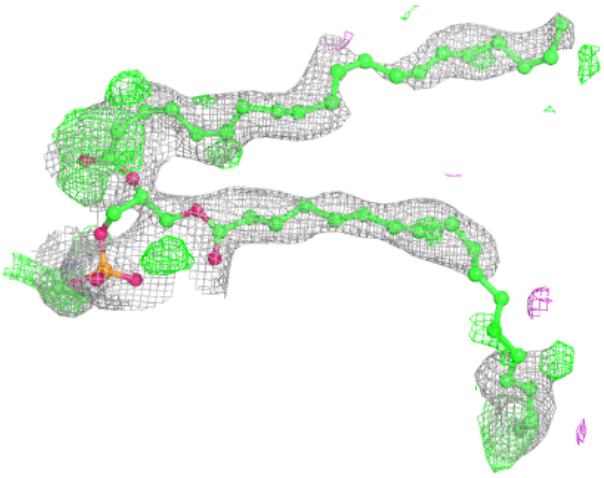
Electron density around CDL C 312:

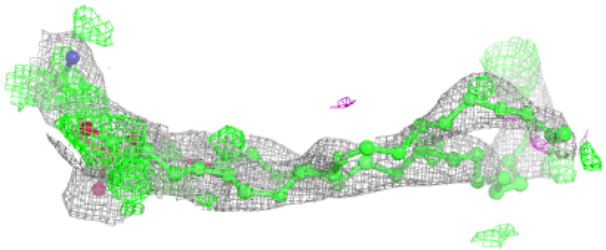
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

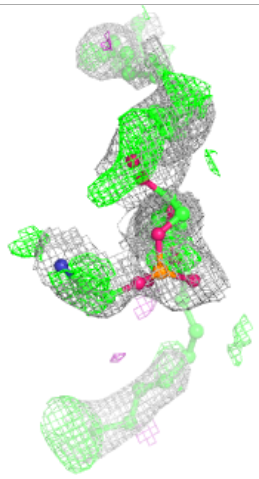


Electron density around PEK P 305:

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

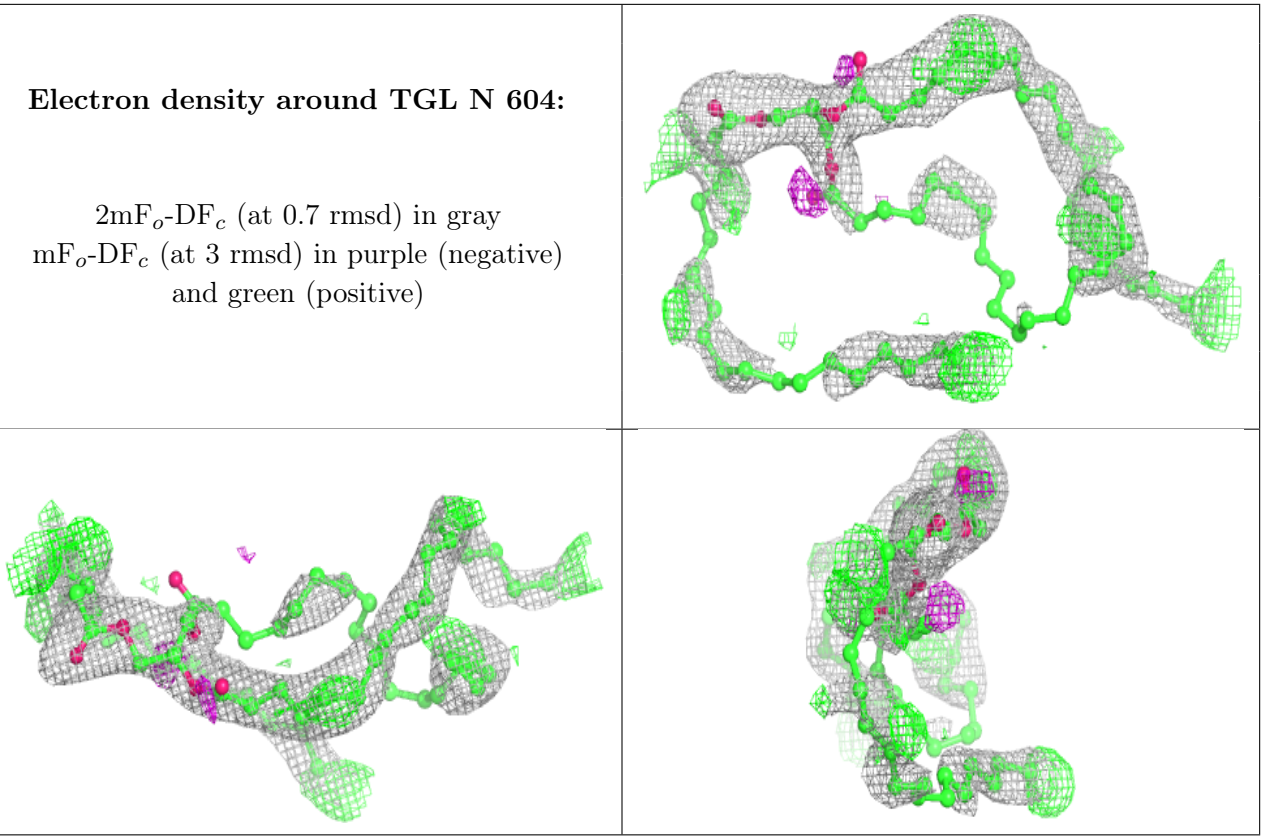






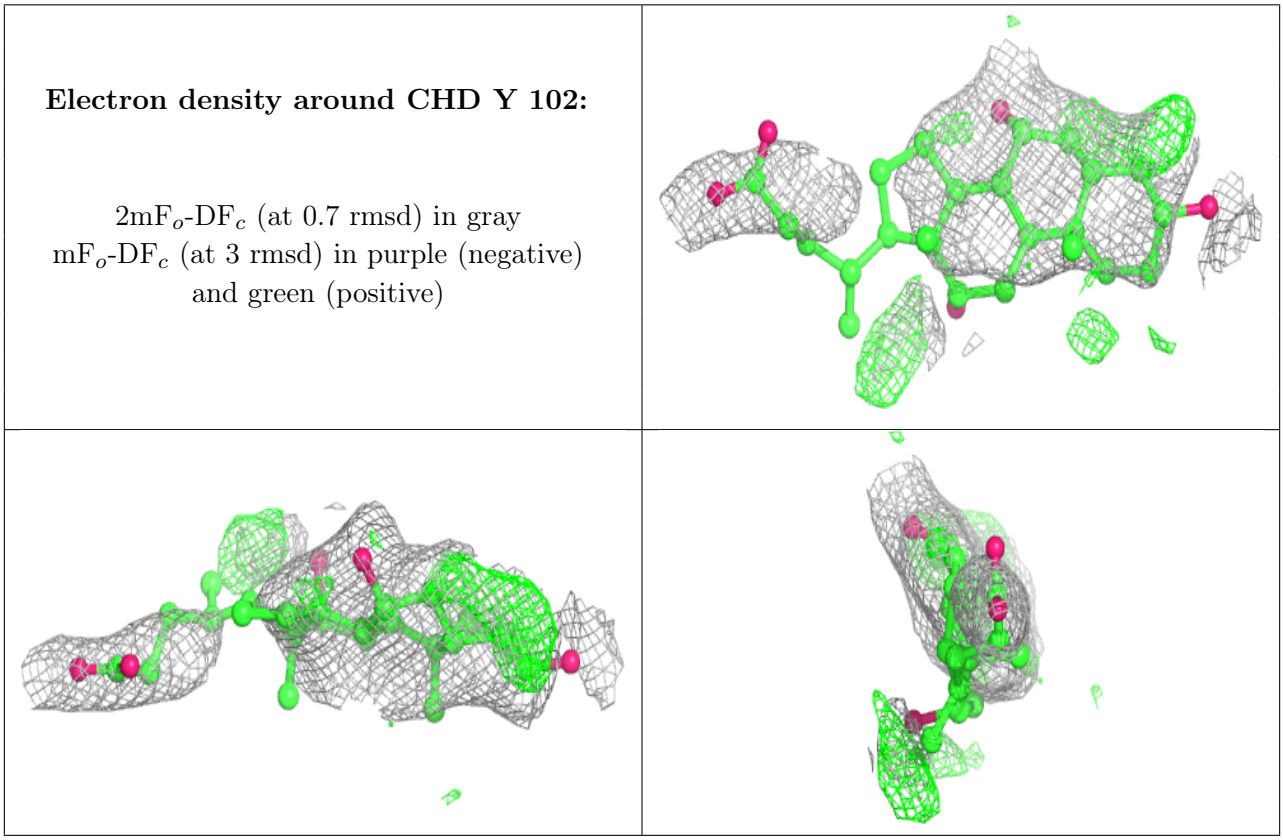
Electron density around TGL N 604:

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



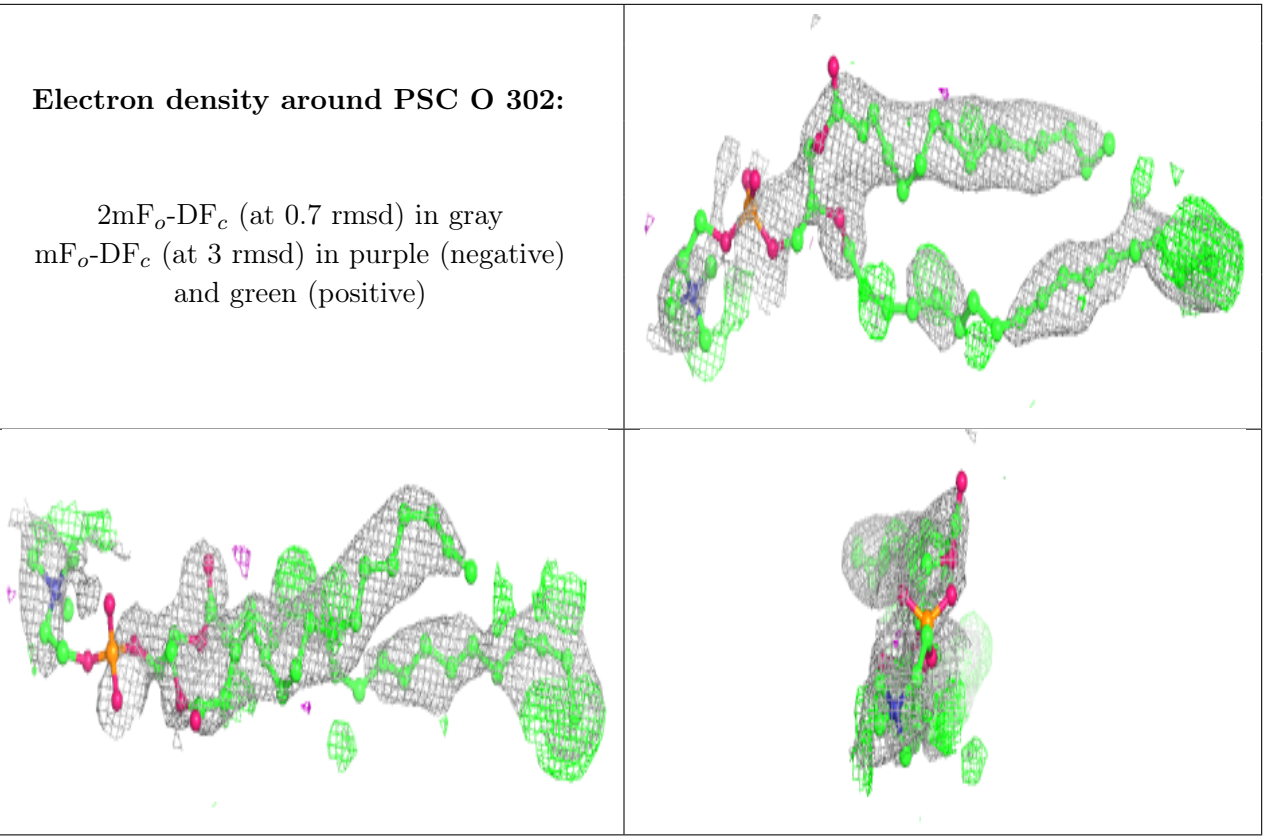
Electron density around CHD Y 102:

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



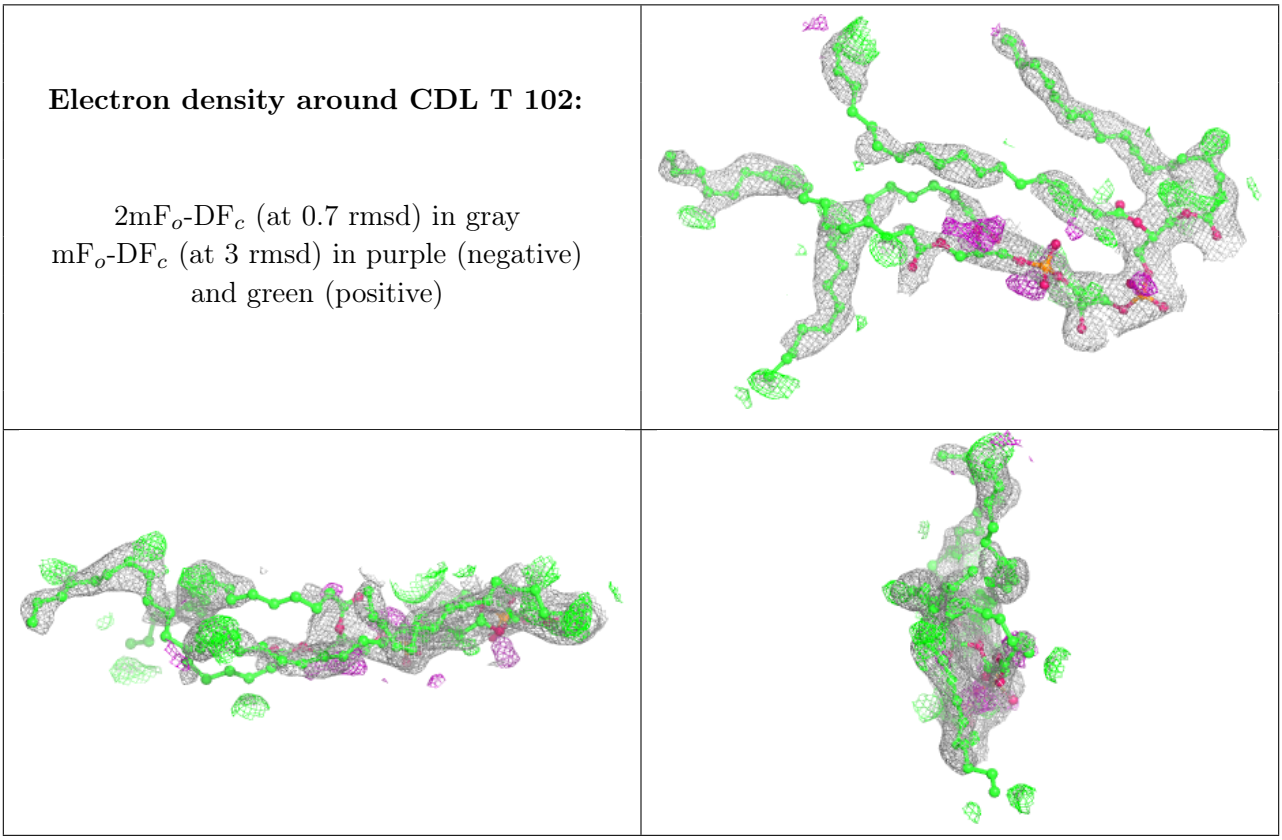
Electron density around PSC O 302:

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



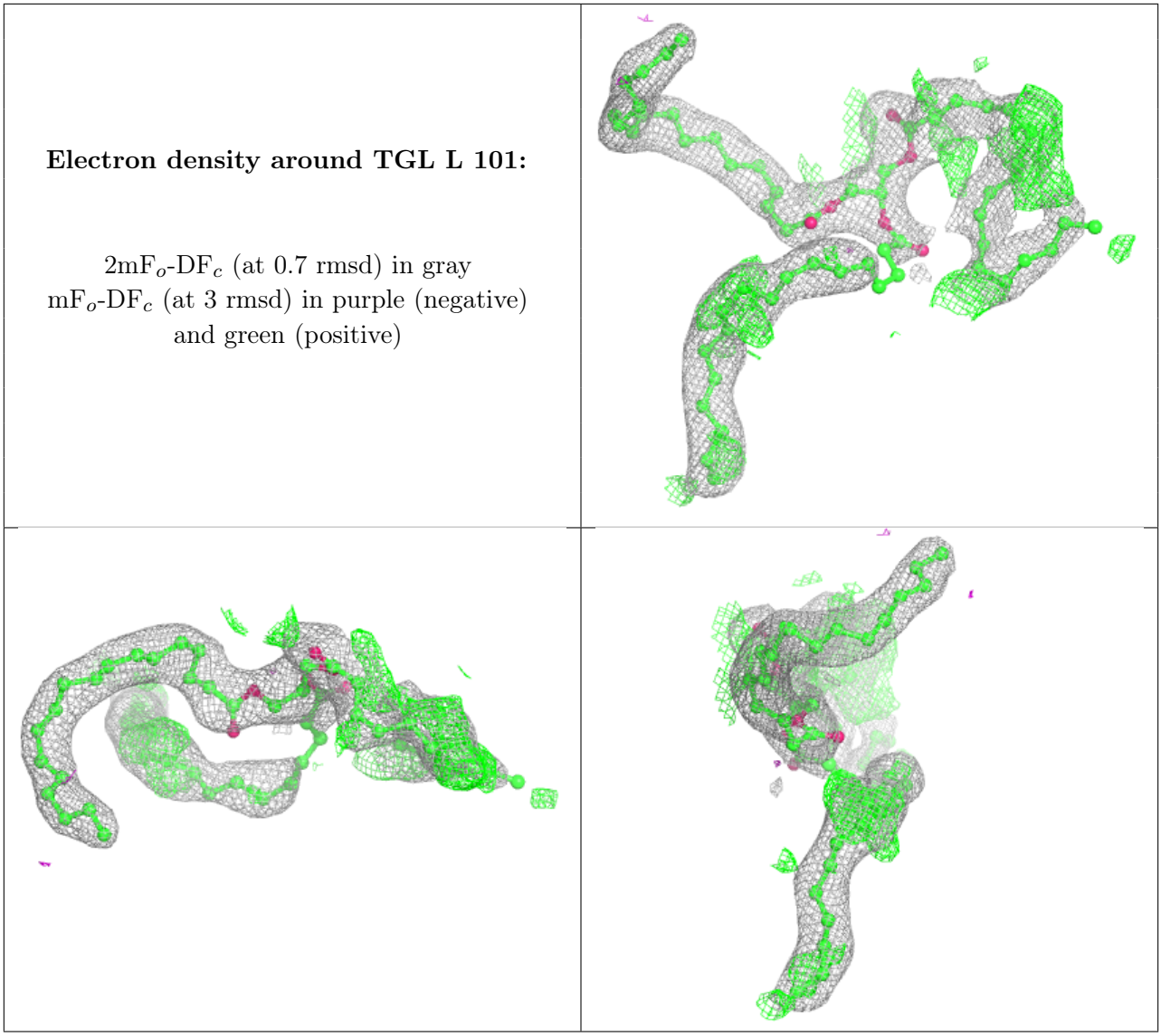
Electron density around CDL T 102:

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



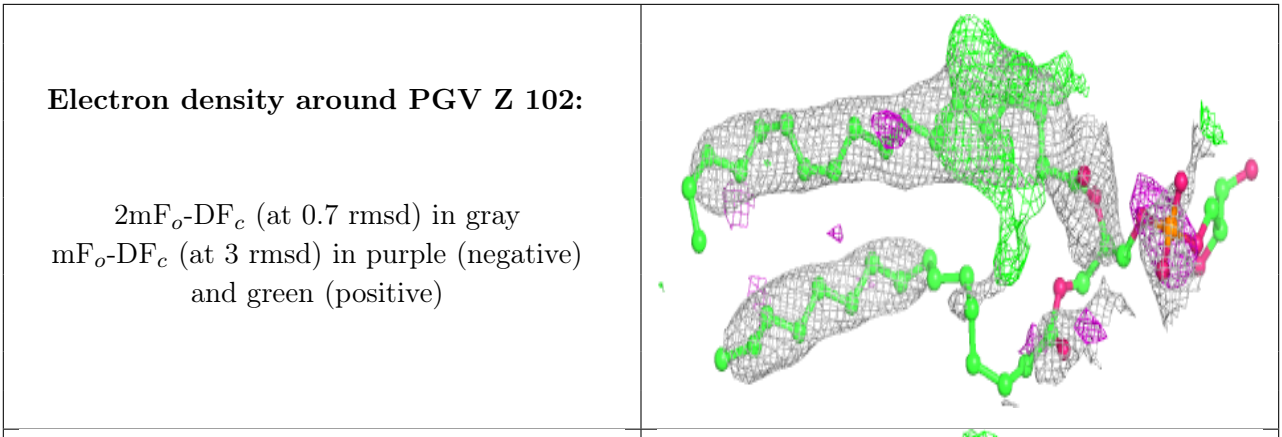
Electron density around TGL L 101:

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



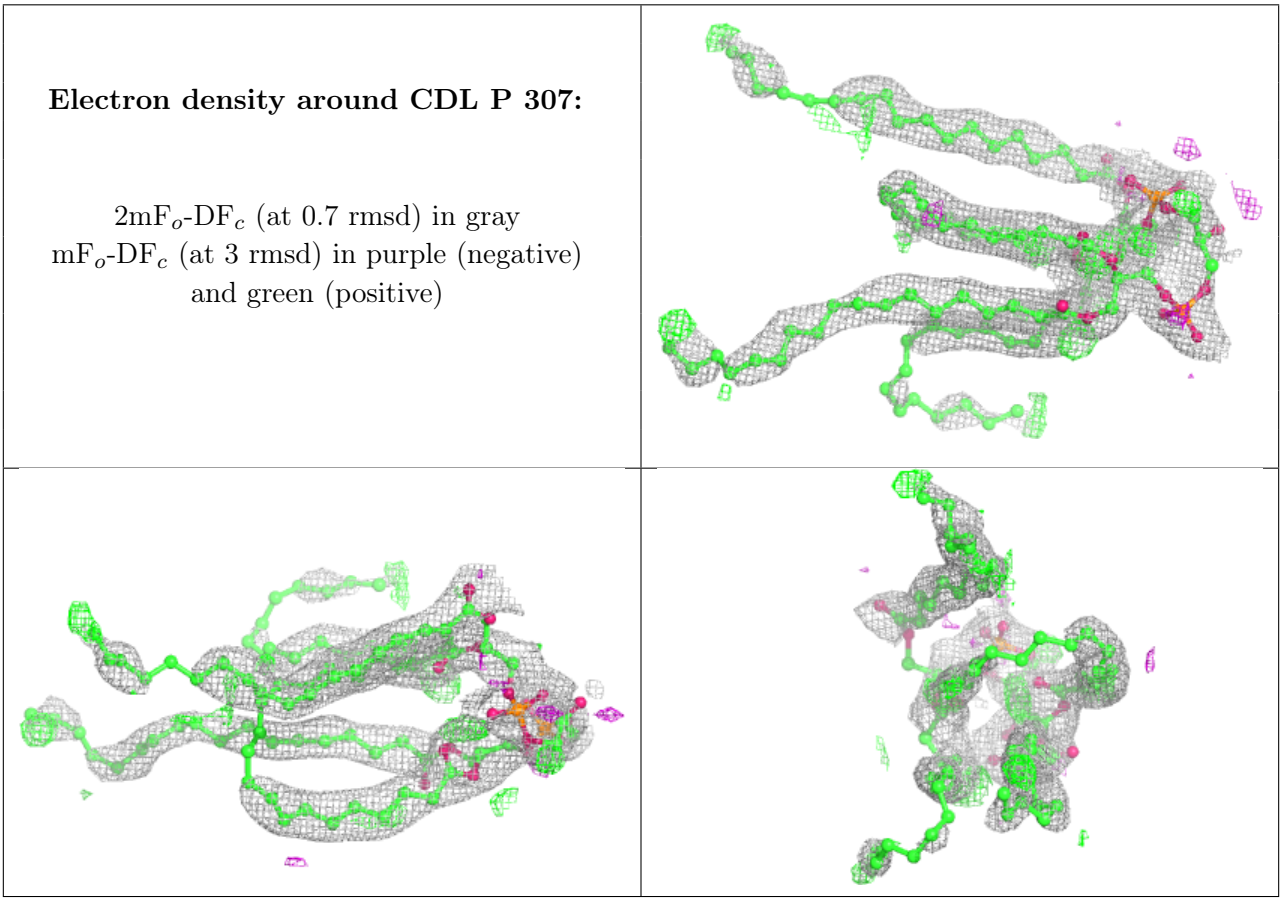
Electron density around PGV Z 102:

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



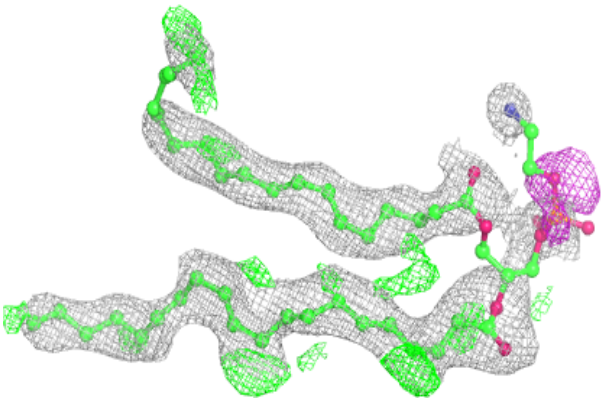
Electron density around CDL P 307:

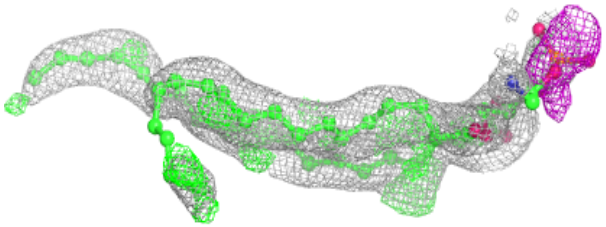
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

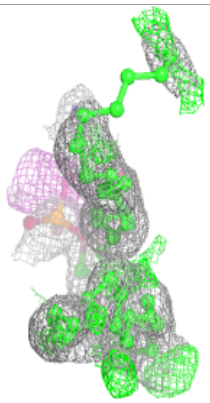


Electron density around PEK C 304:

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

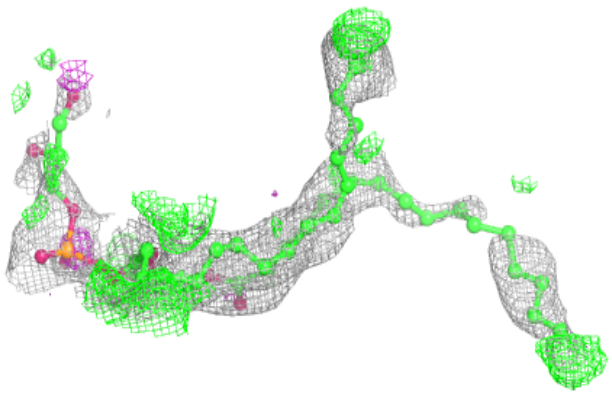


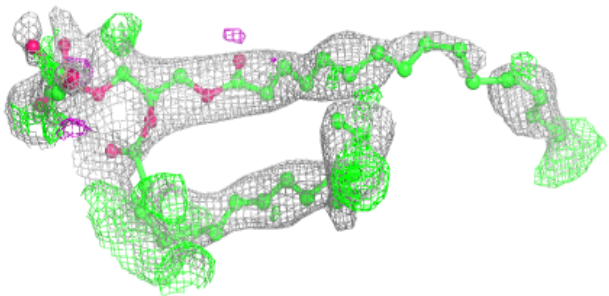


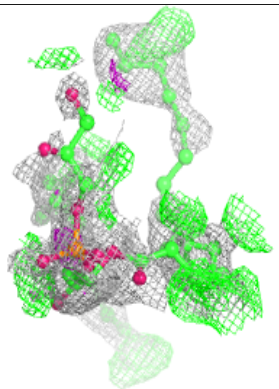


Electron density around PGV T 101:

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

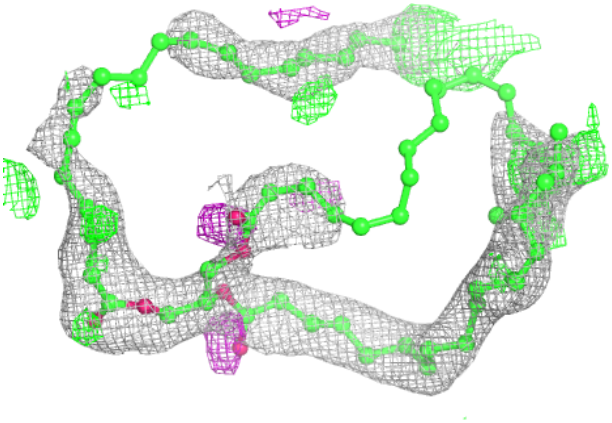


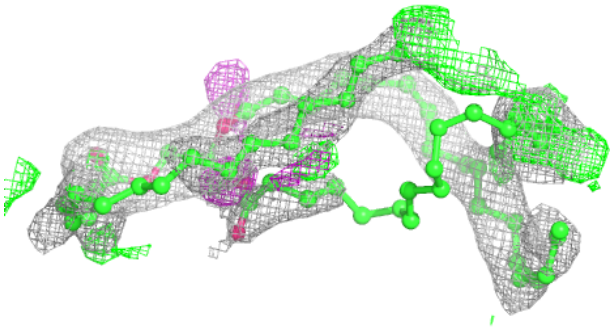


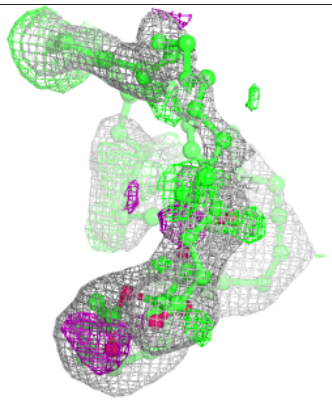


Electron density around TGL A 615:

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

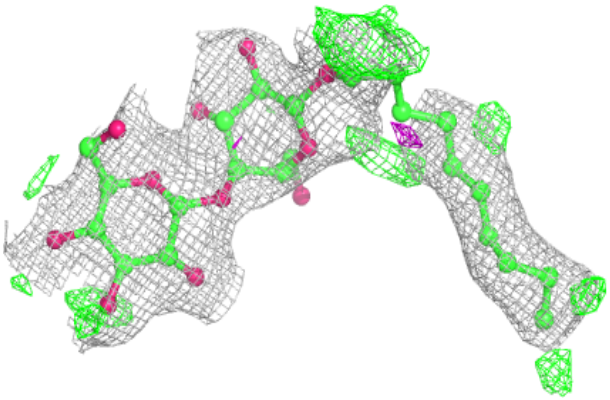


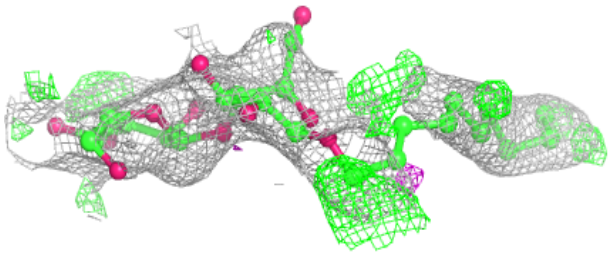


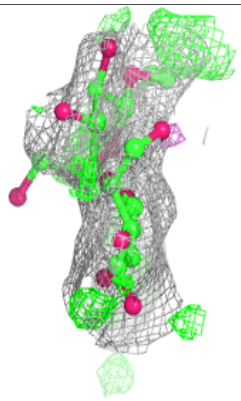


Electron density around DMU G 1302:

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

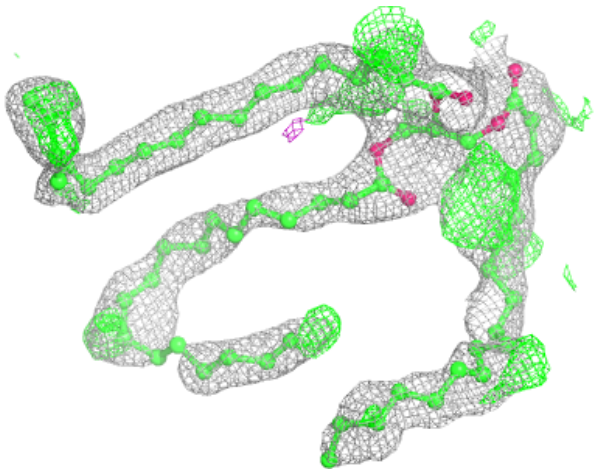


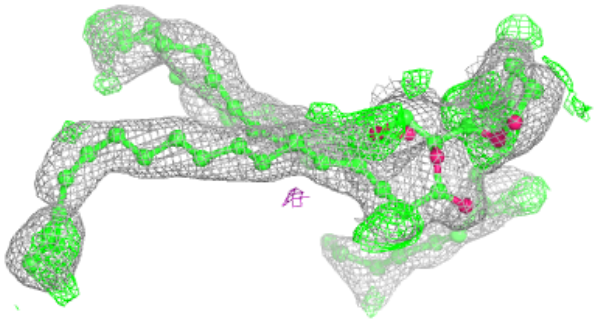


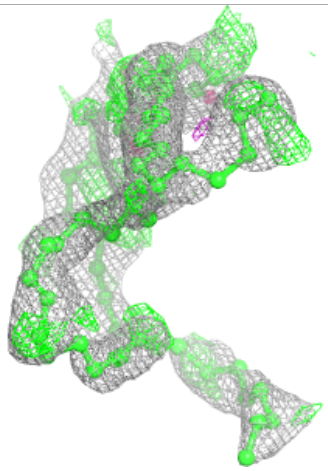


Electron density around TGL D 201:

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

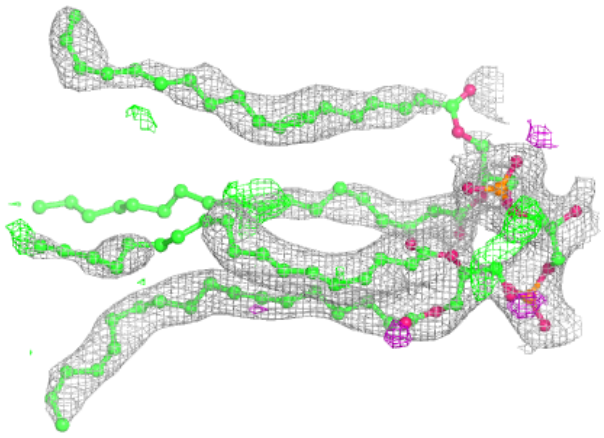


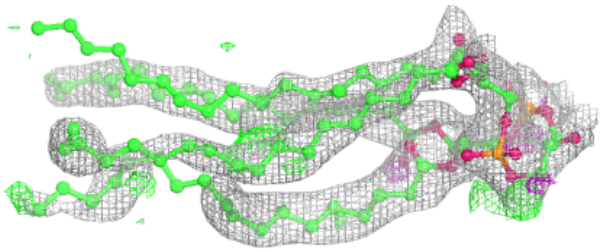


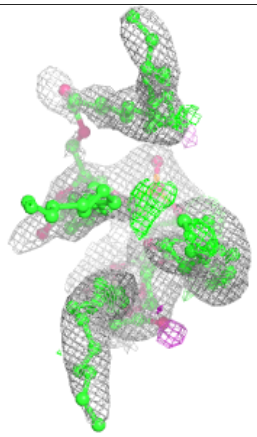


Electron density around CDL C 306:

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

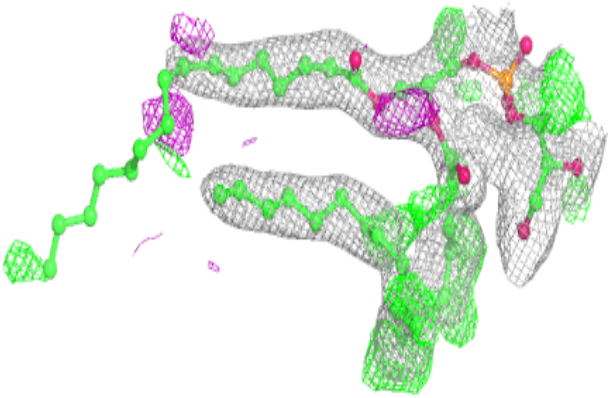


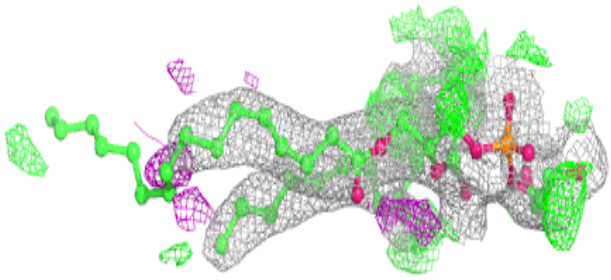


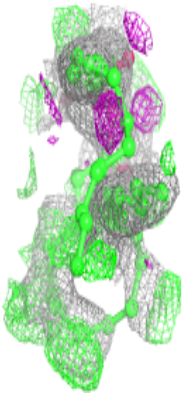


Electron density around PGV A 604:

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

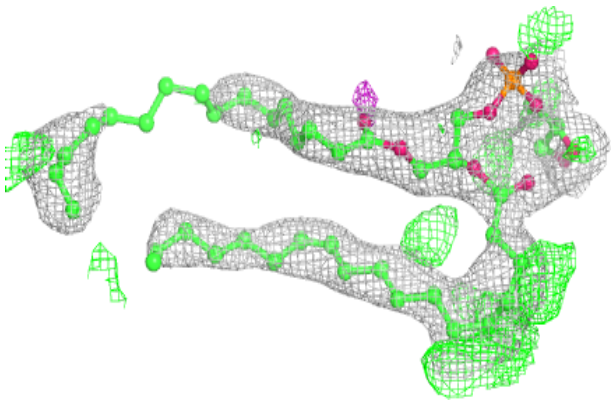


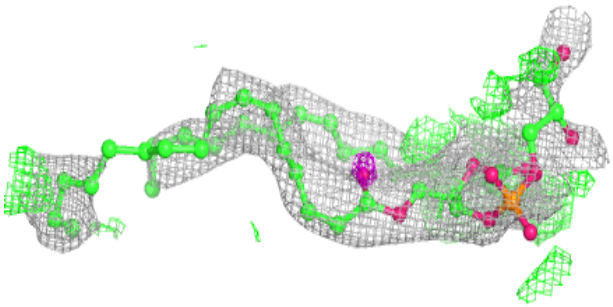


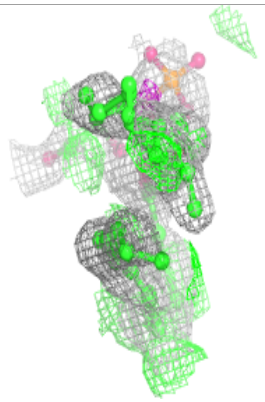


Electron density around PGV N 616:

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

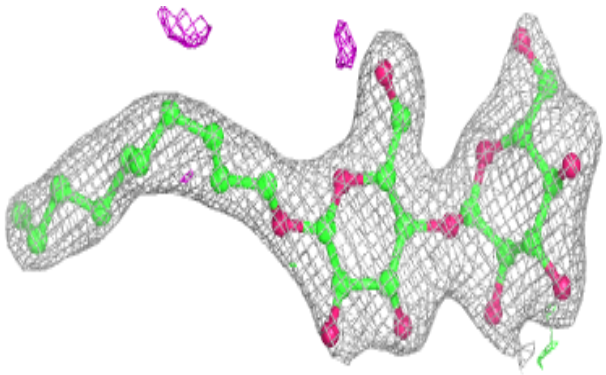


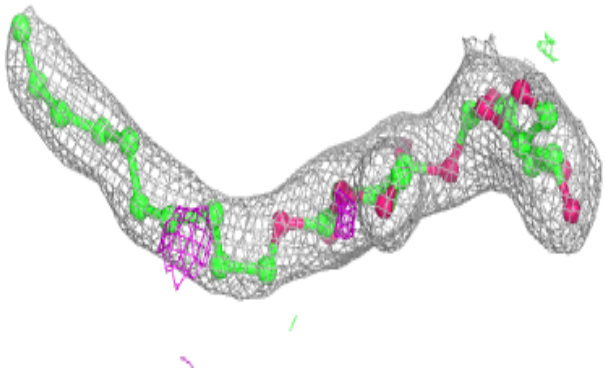


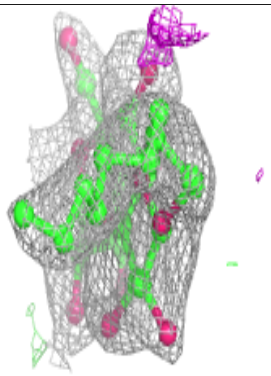


Electron density around DMU Z 101:

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

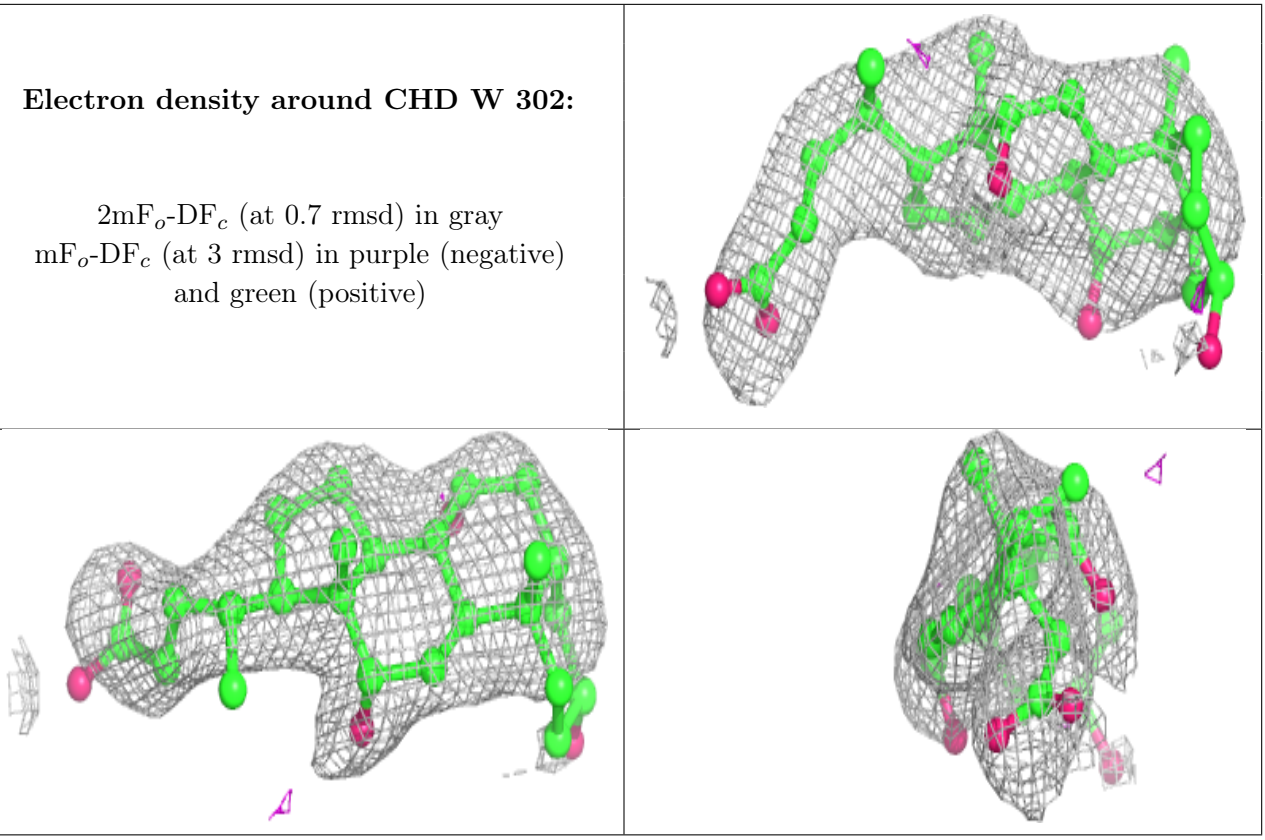






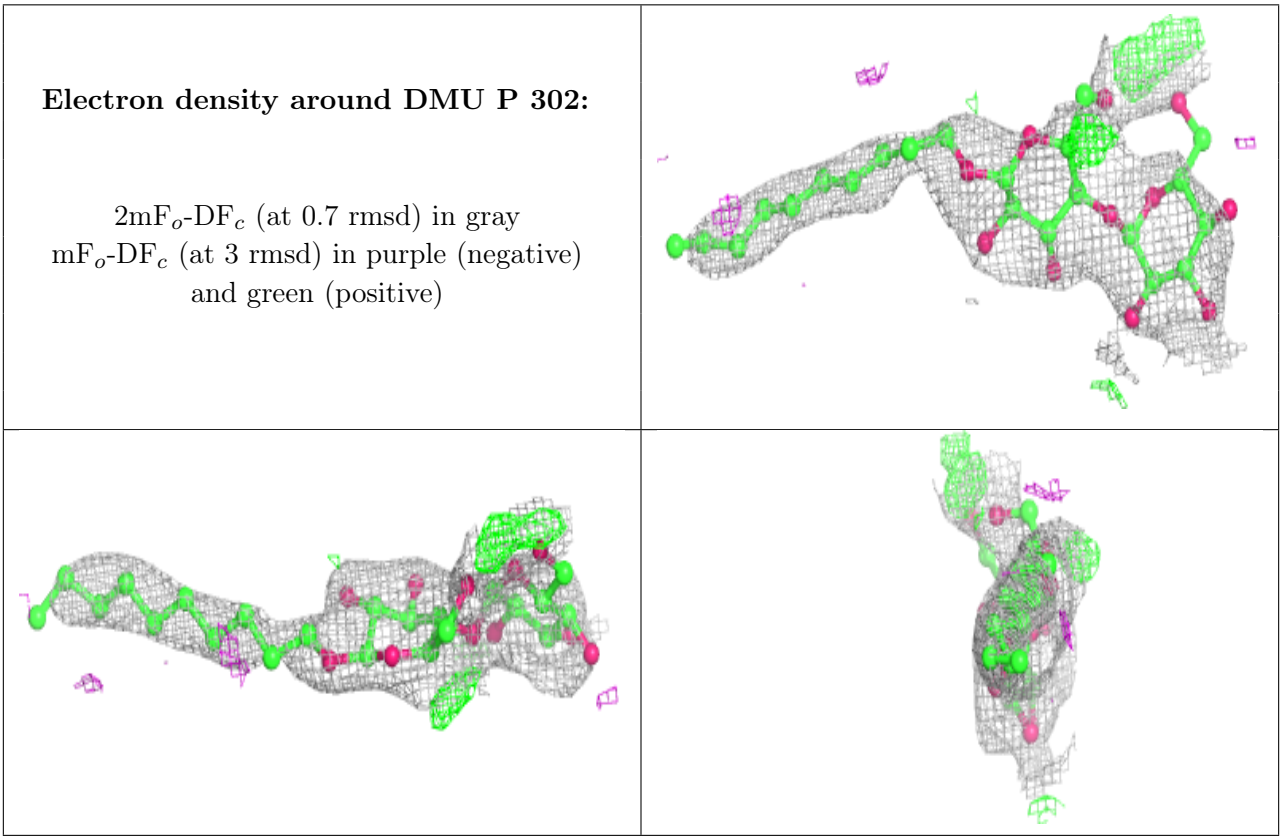
Electron density around CHD W 302:

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



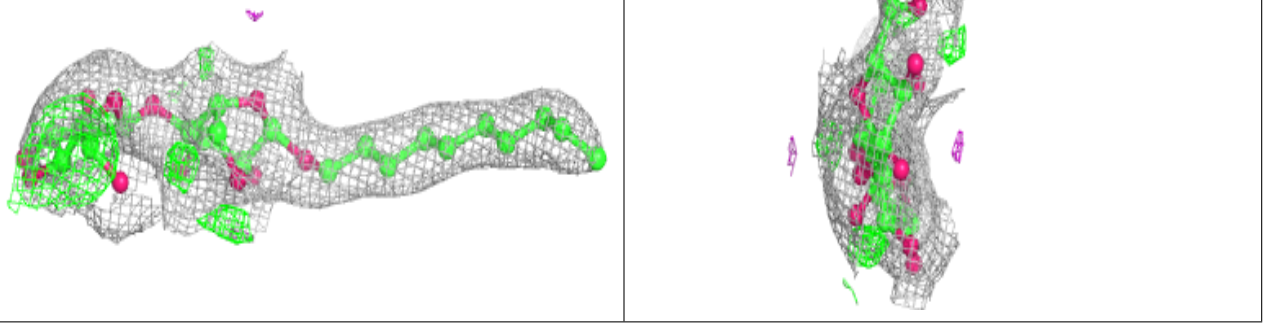
Electron density around DMU P 302:

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



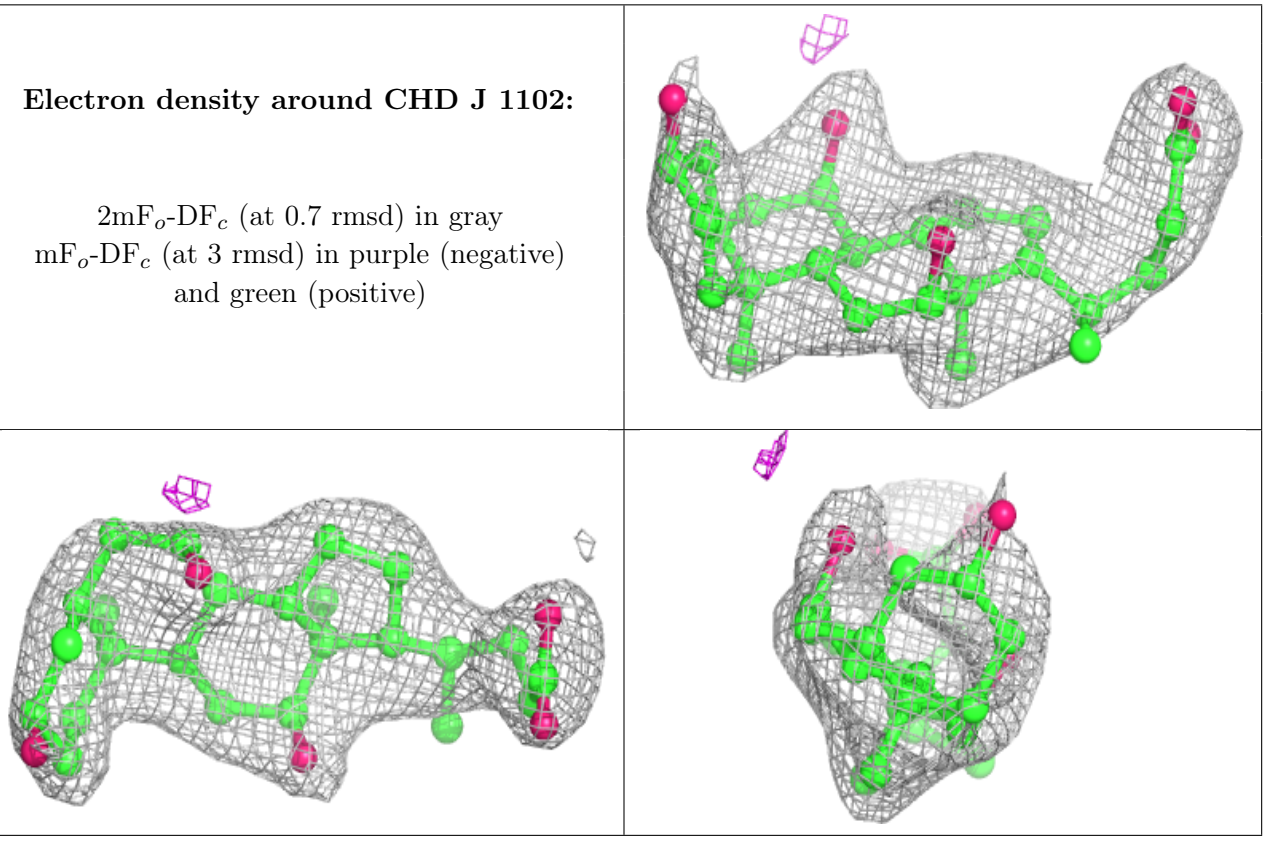
Electron density around DMU C 313:

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



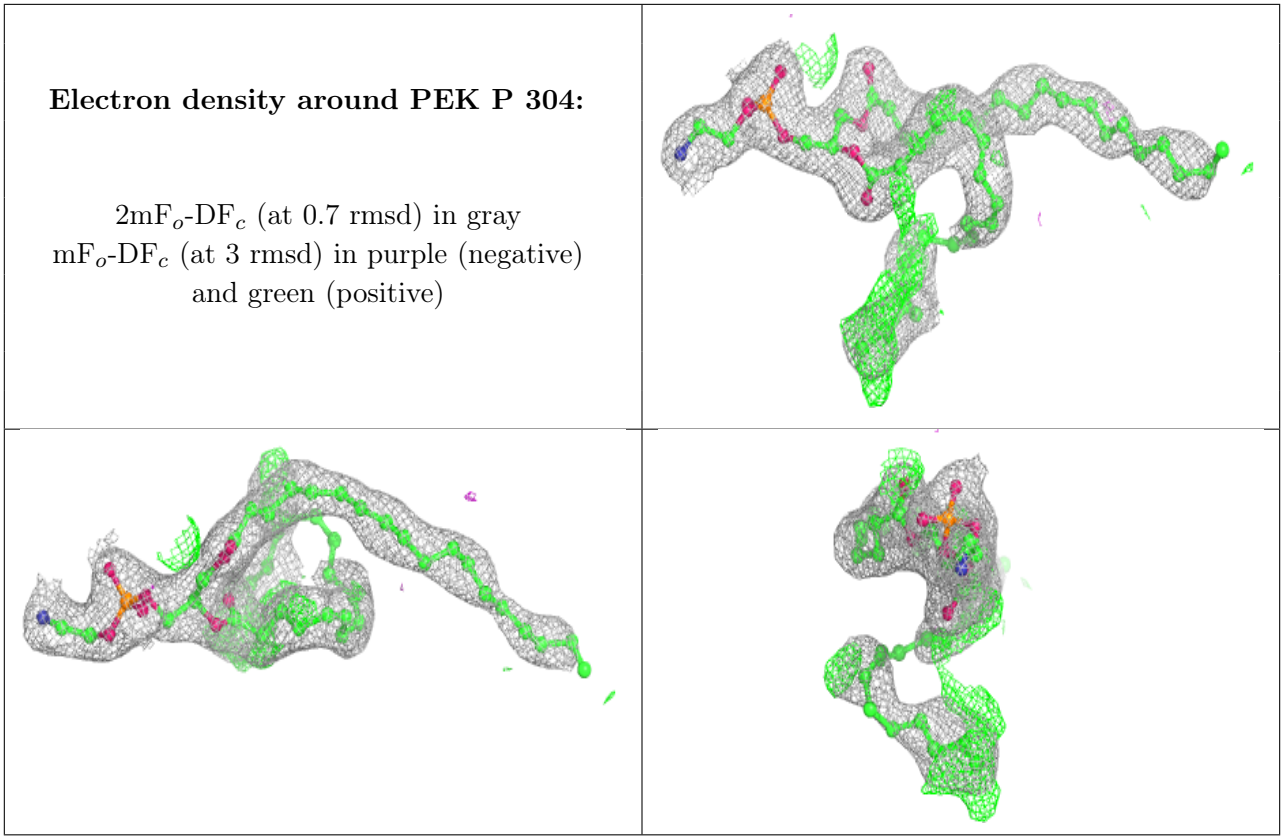
Electron density around CHD J 1102:

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



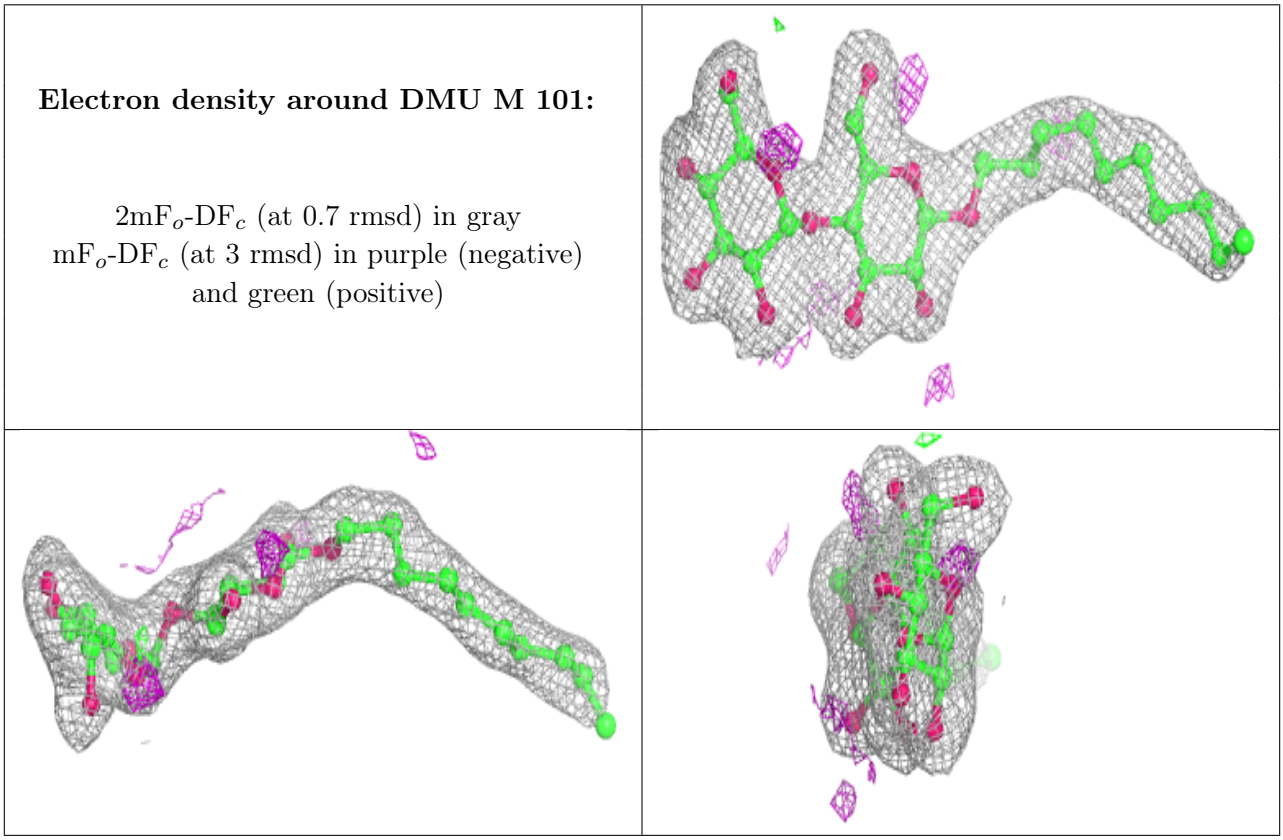
Electron density around PEK P 304:

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



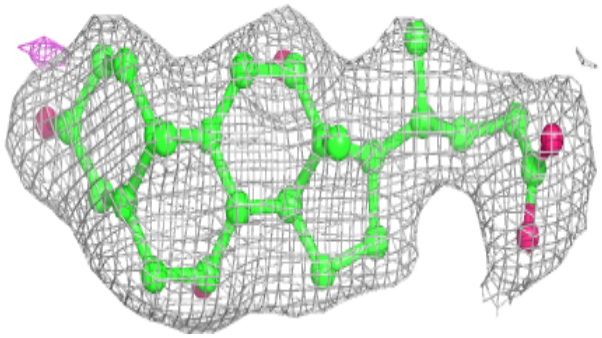
Electron density around DMU M 101:

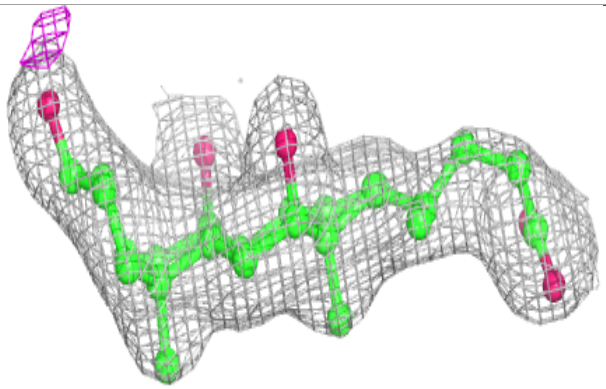
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

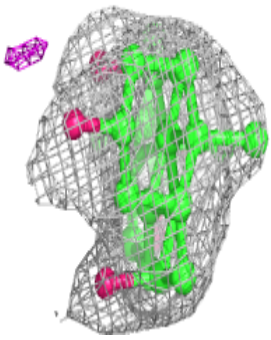


Electron density around CHD C 307:

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

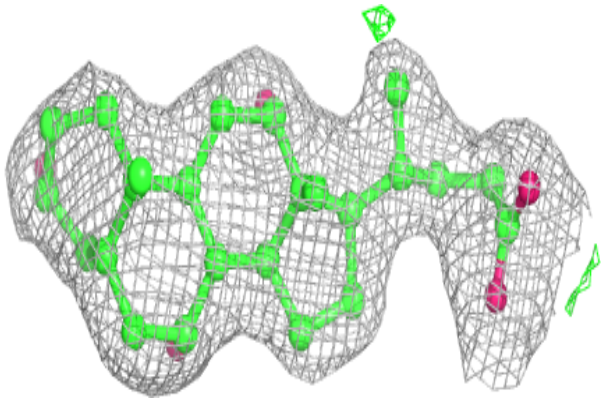


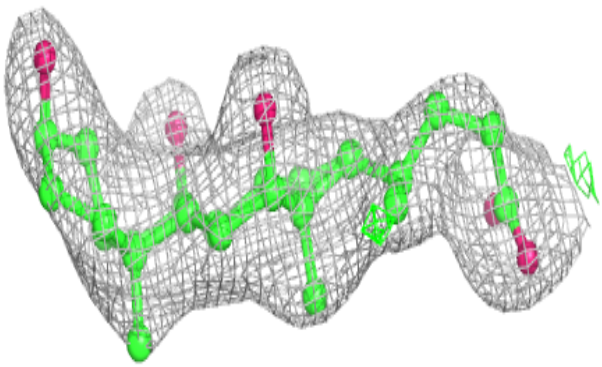


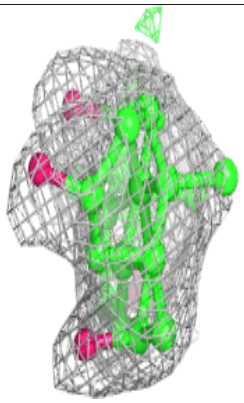


Electron density around CHD P 308:

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

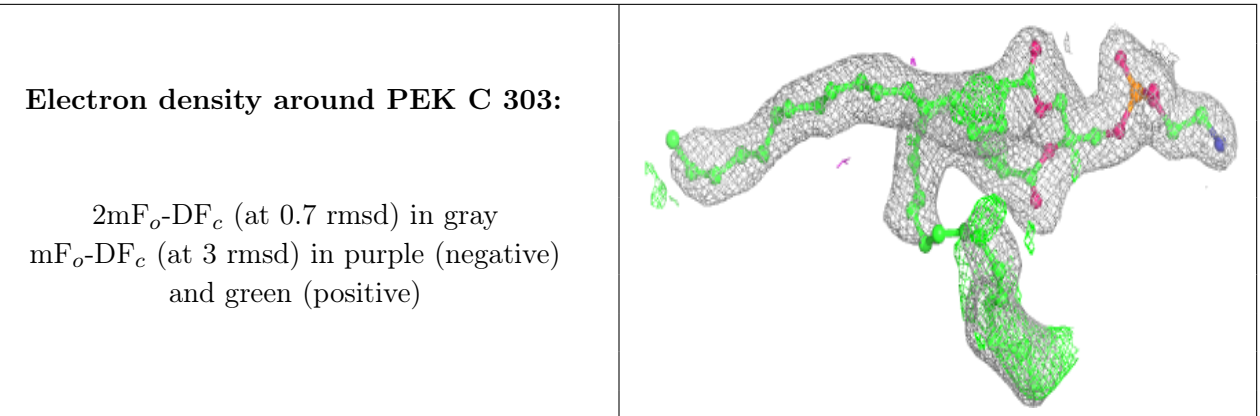


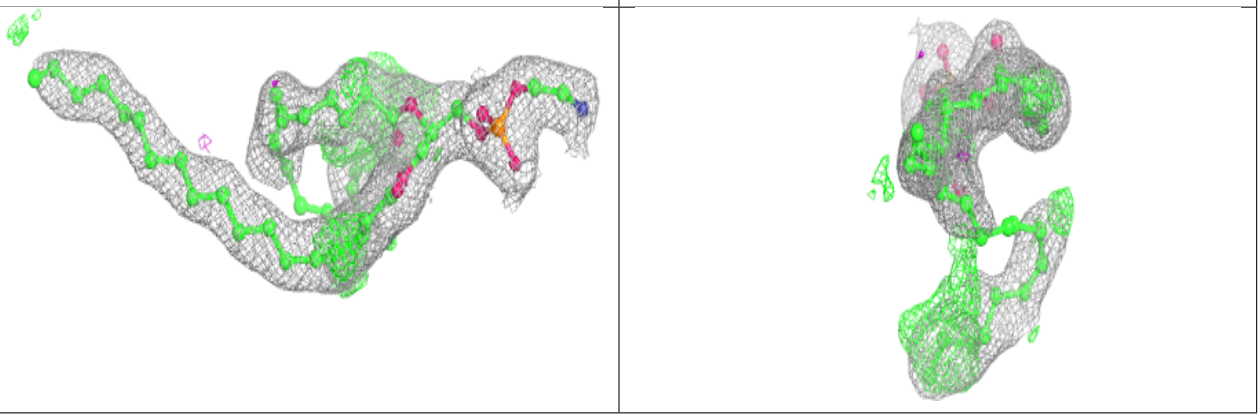




Electron density around PEK C 303:

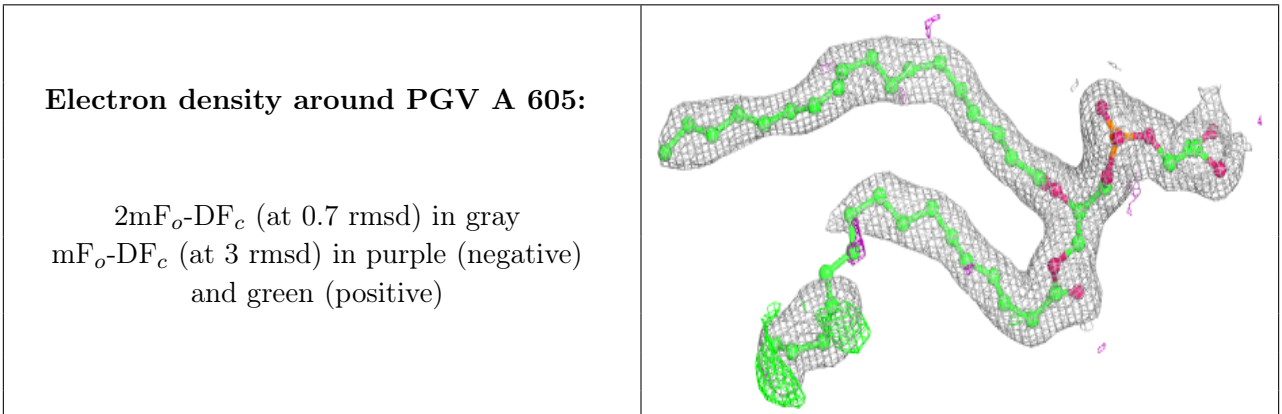
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

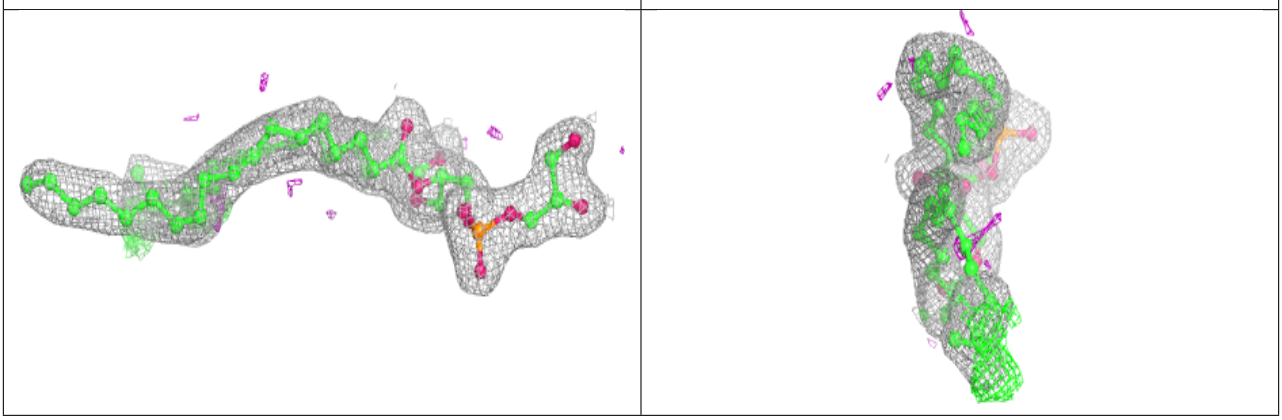




Electron density around PGV A 605:

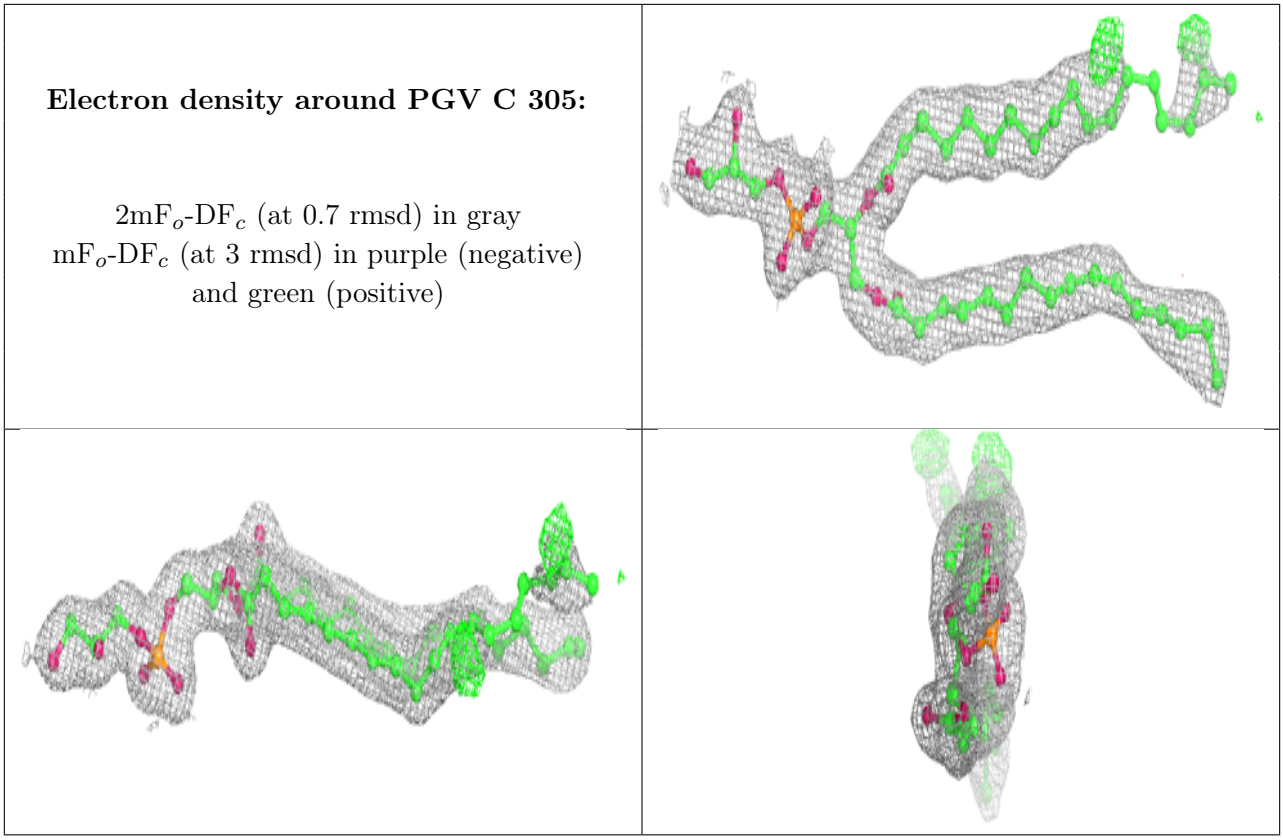
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





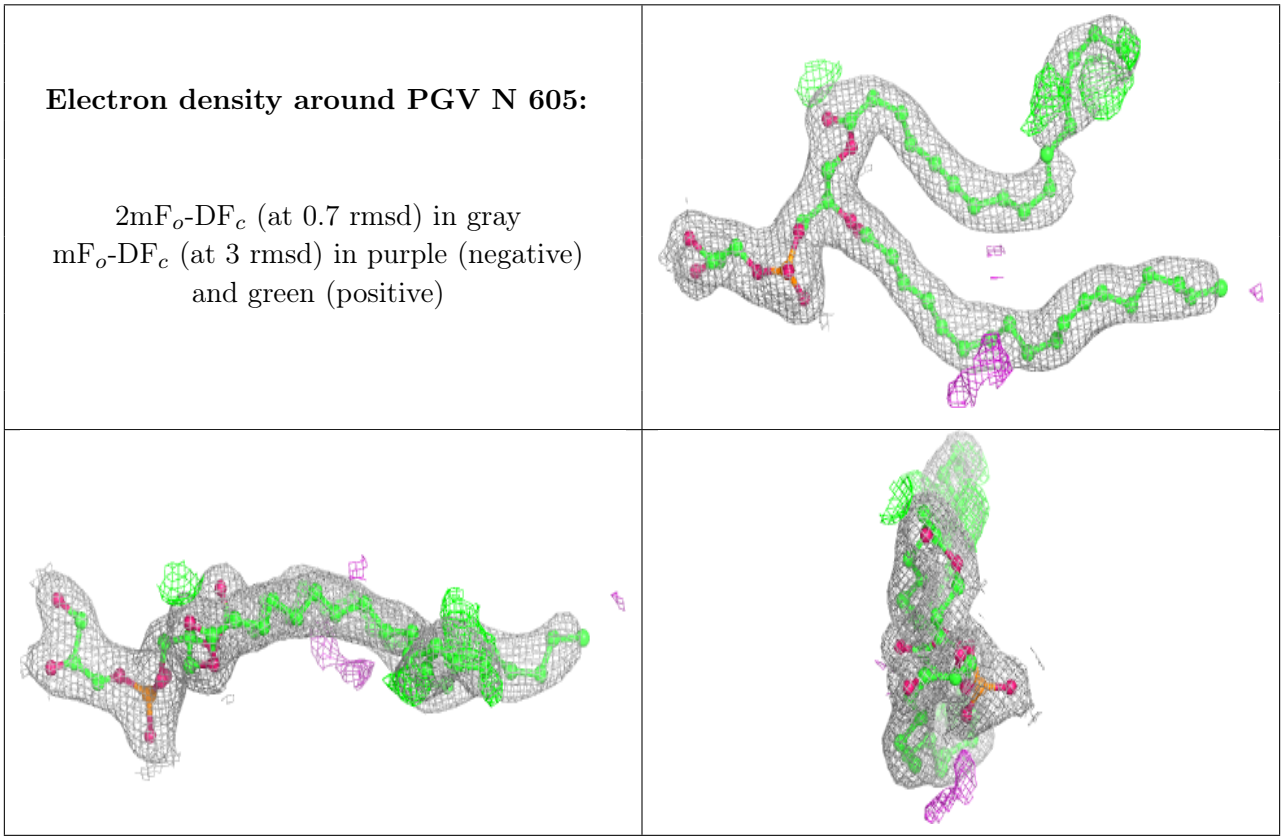
Electron density around PGV C 305:

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



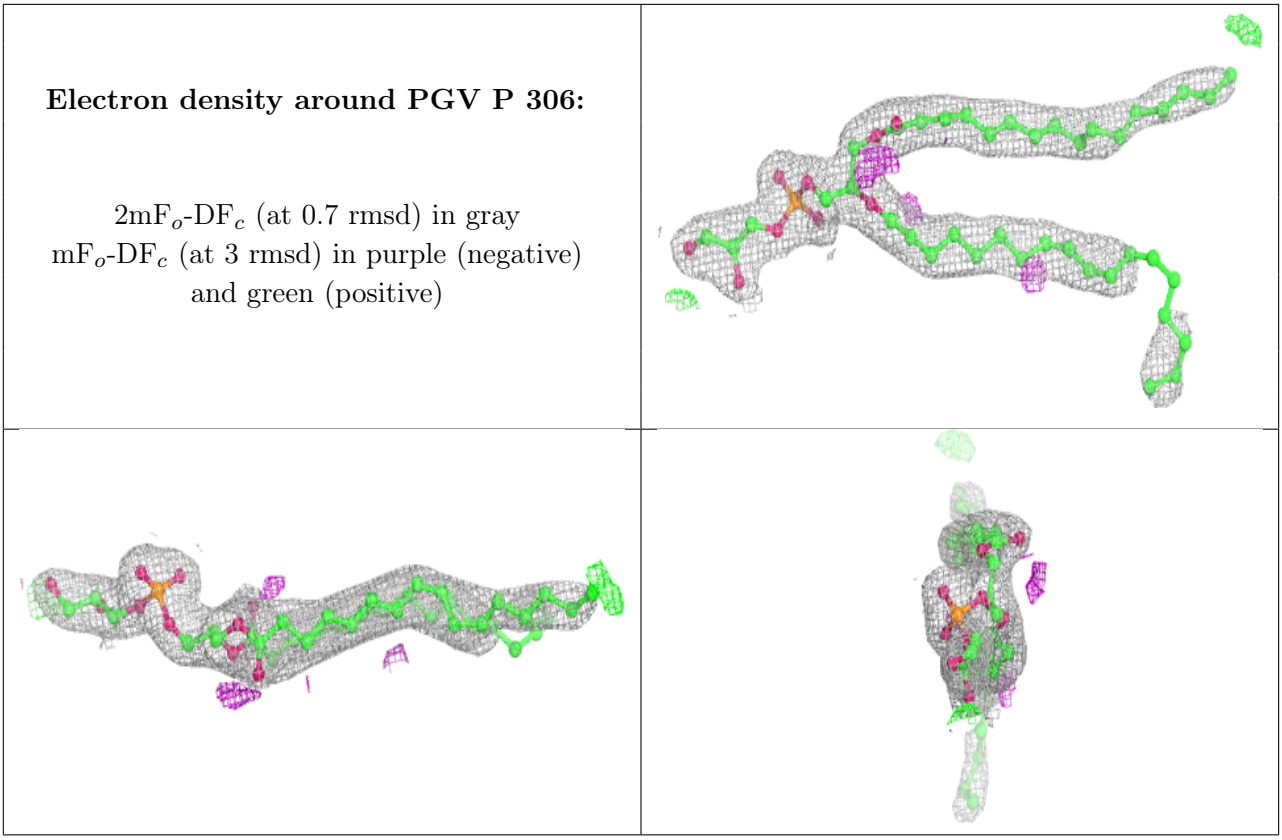
Electron density around PGV N 605:

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



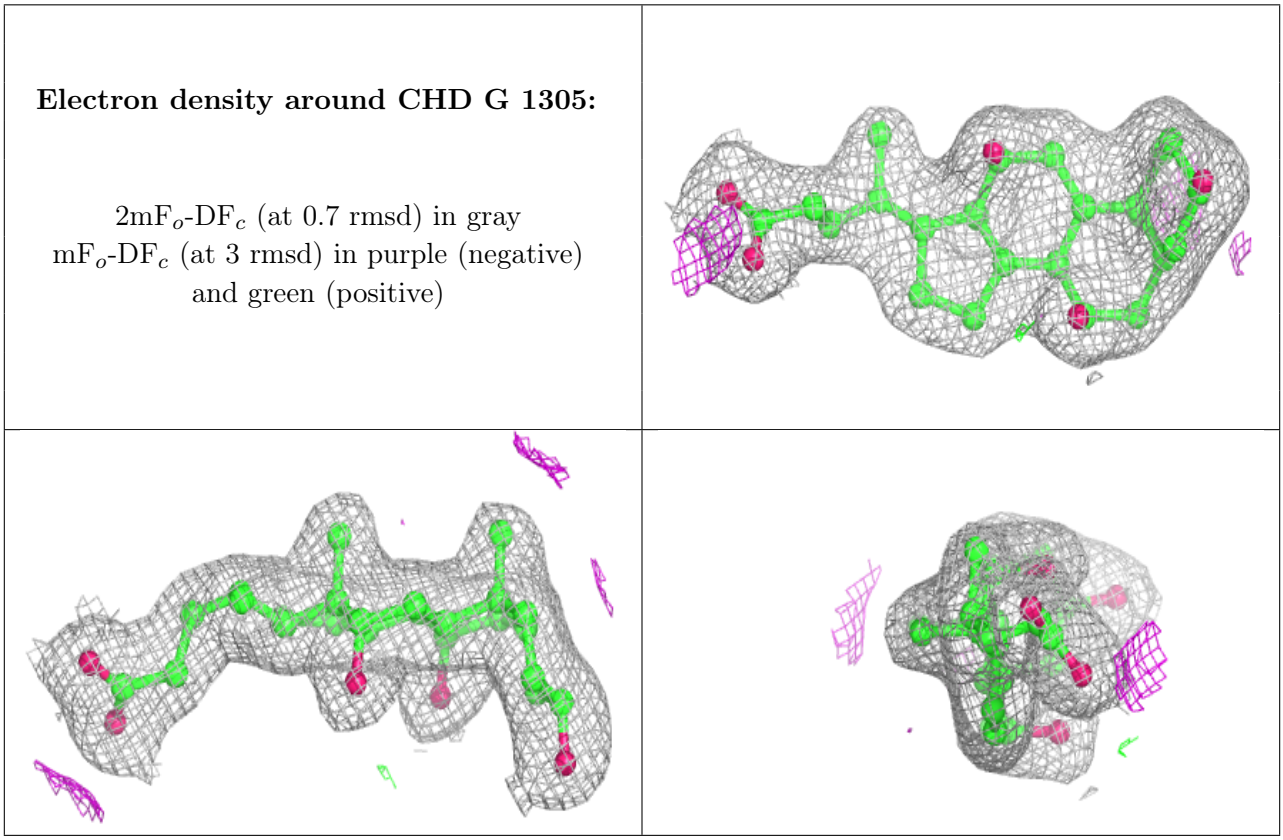
Electron density around PGV P 306:

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



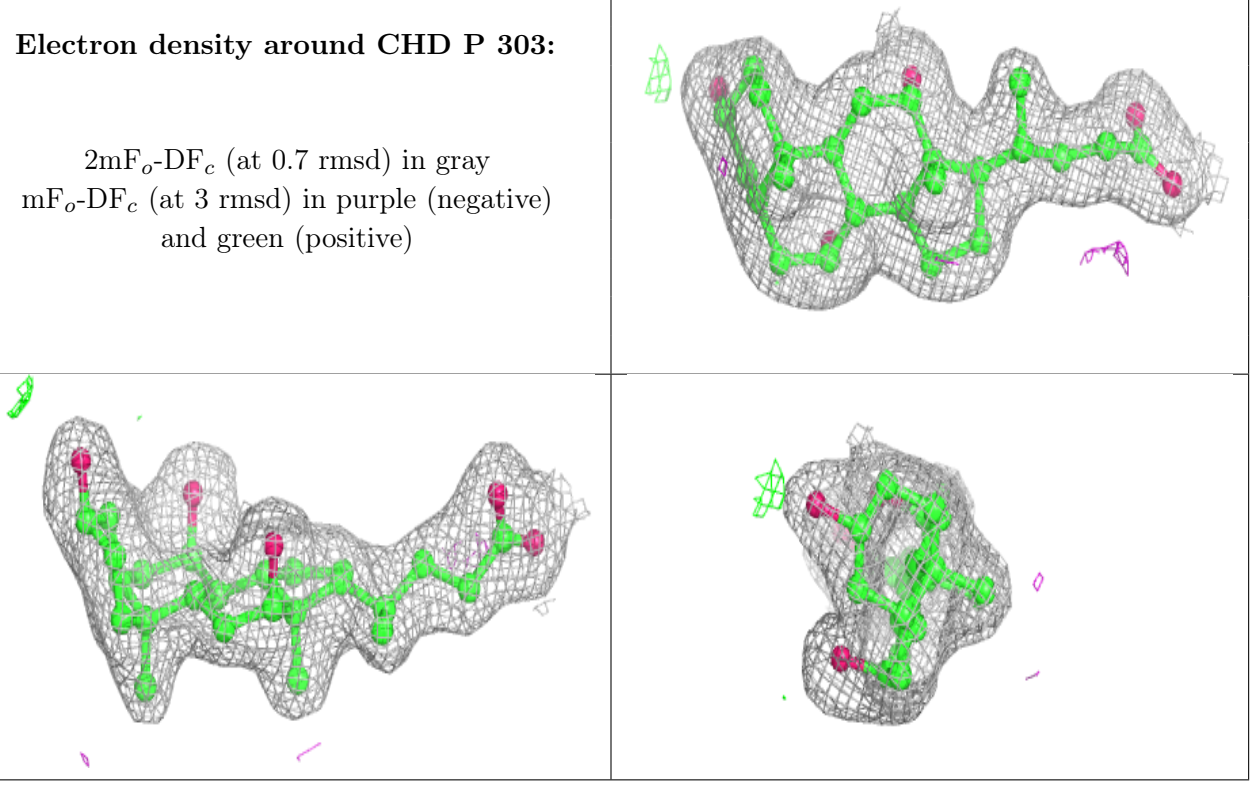
Electron density around CHD G 1305:

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



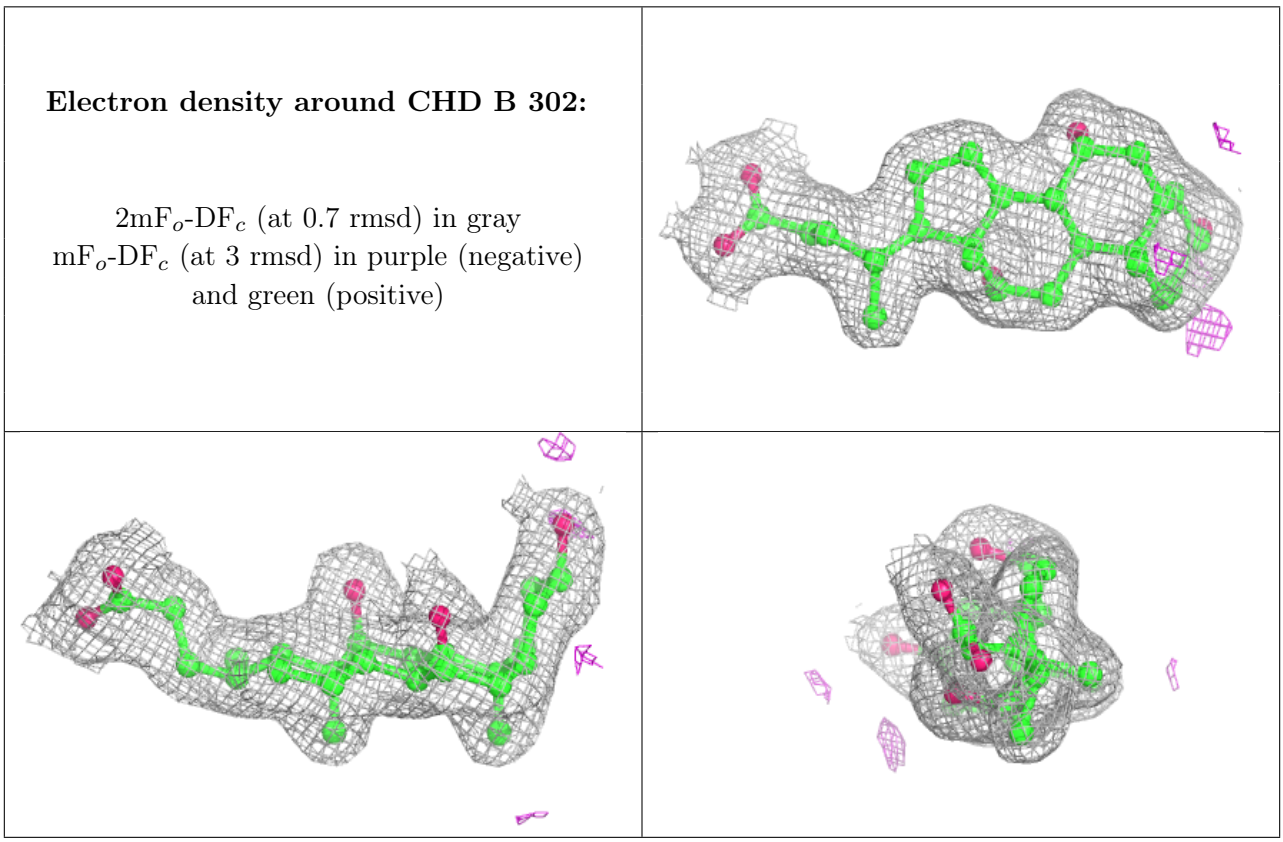
Electron density around CHD P 303:

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



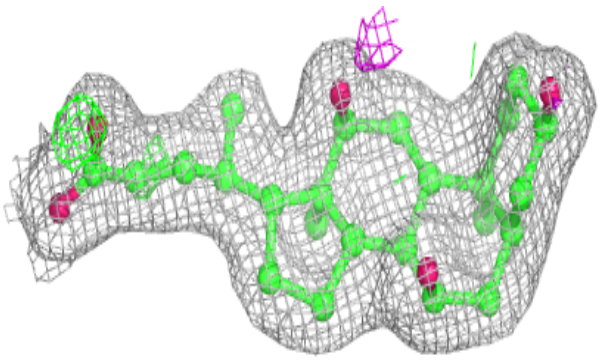
Electron density around CHD B 302:

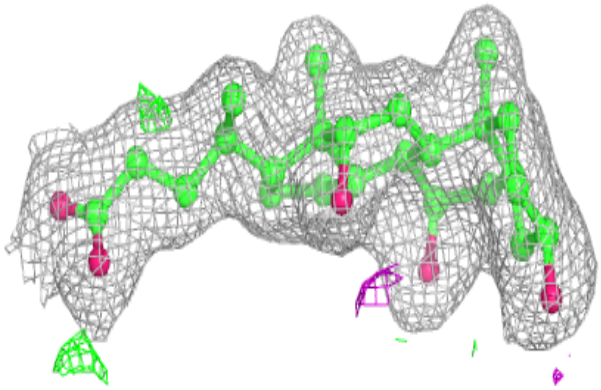
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

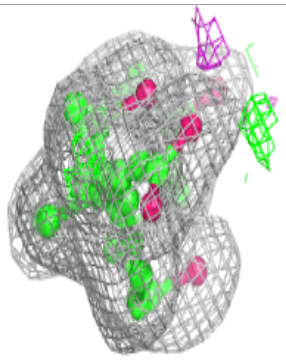


Electron density around CHD C 302:

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

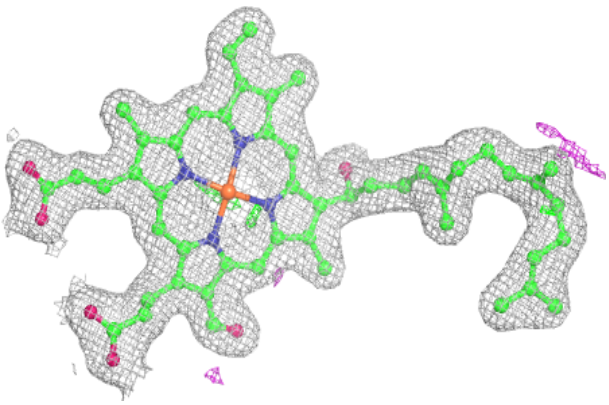


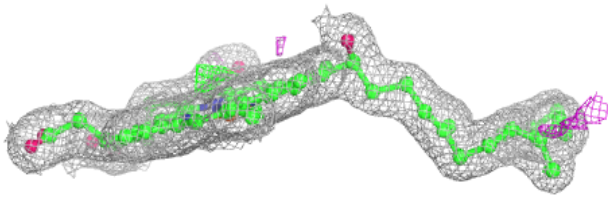


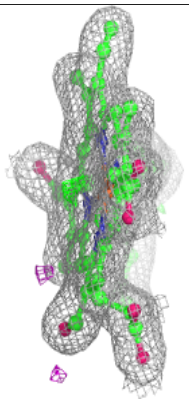


Electron density around HEA A 606:

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

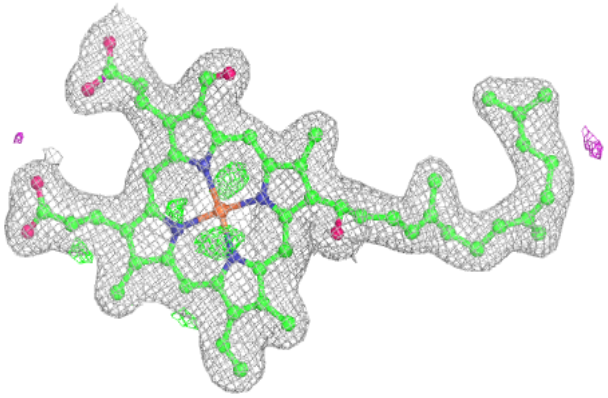


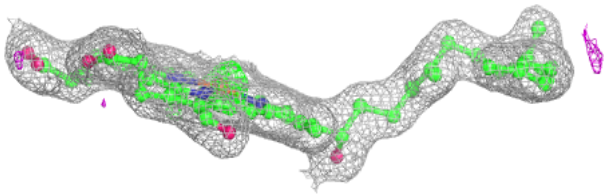


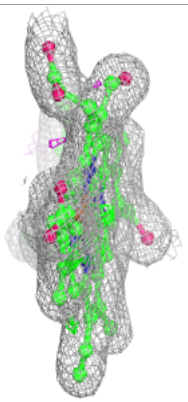


Electron density around HEA N 606:

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

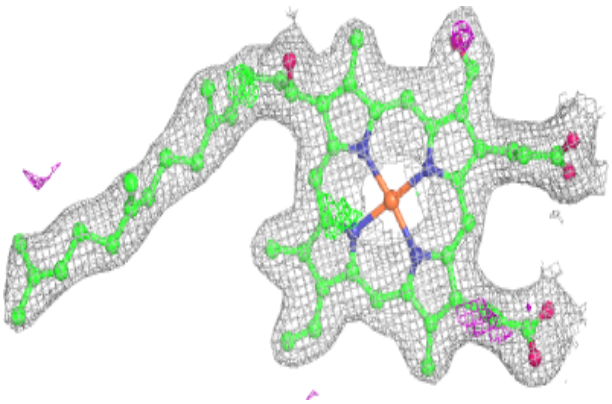


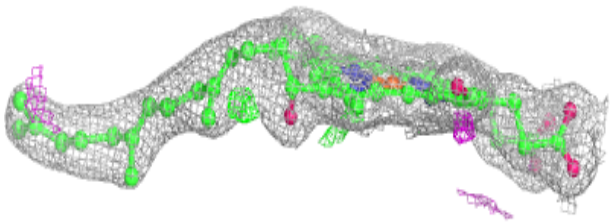


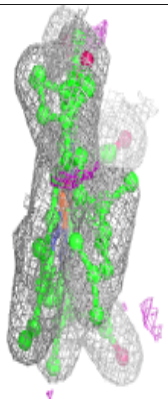


Electron density around HEA N 607:

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

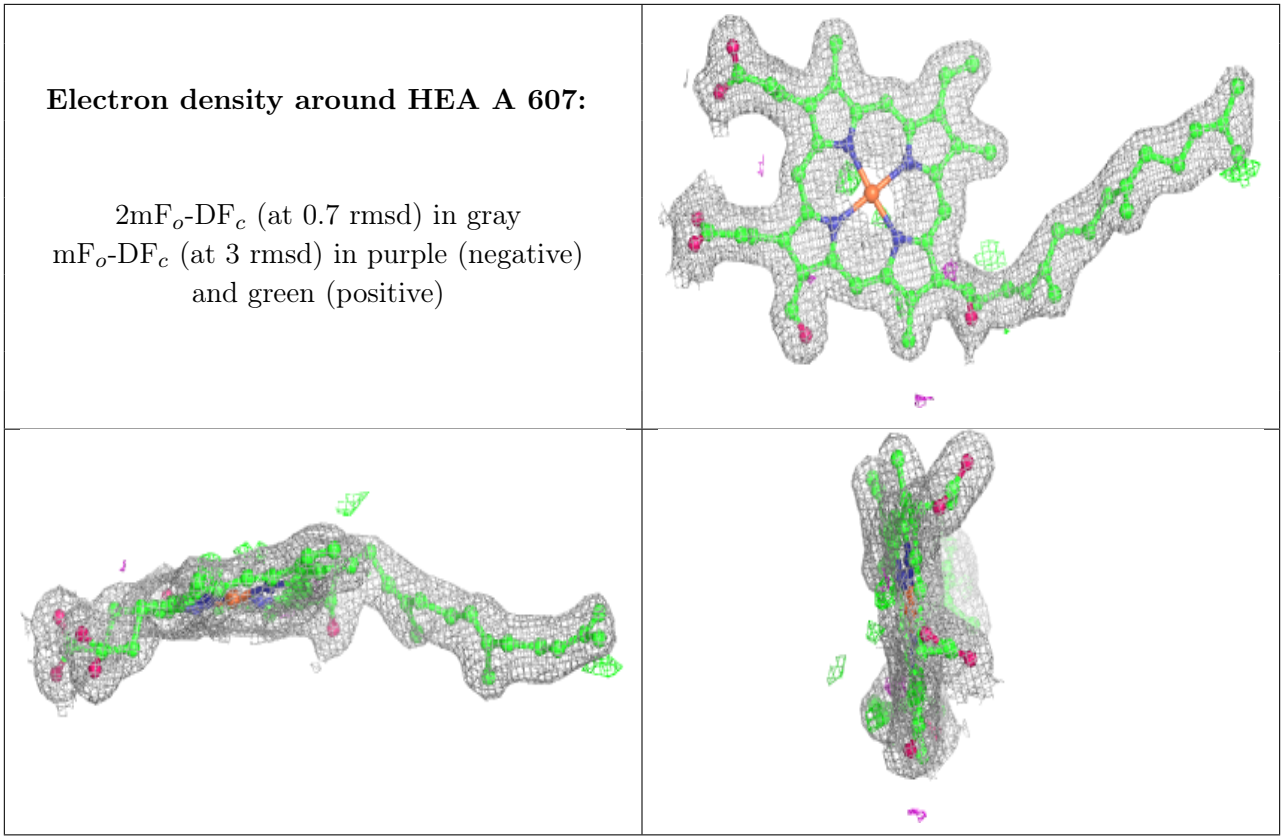






Electron density around HEA A 607:

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



6.5 Other polymers (i)

There are no such residues in this entry.