Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 12:54 PM JST

PDB ID	:	5Z86
Title	:	azide-bound cytochrome c oxidase structure determined using the crystals exposed to 20 mM azide solution for 3 days
Authors	:	Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on	:	2018-01-31
Resolution	:	1.85 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:

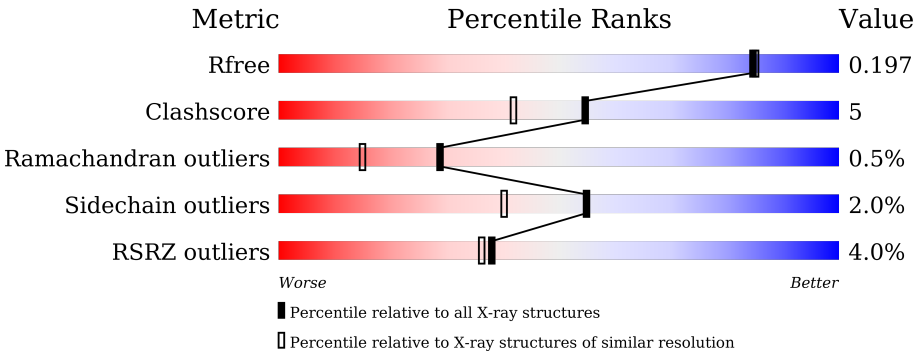
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	514	89% 11%
1	N	514	88% 12%
2	B	227	85% 14%
2	O	227	89% 11%
3	C	261	87% 11%
3	P	261	89% 10%

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Mol	Chain	Length	Quality of chain
4	D	147	3% 89% 9%
4	Q	147	8% 88% 9%
5	E	109	2% 94%
5	R	109	2% 93%
6	F	98	7% 88% 10%
6	S	98	9% 86% 10%
7	G	85	18% 78% 15% 6%
7	T	85	21% 76% 20%
8	H	85	9% 86% 5% 7%
8	U	85	9% 82% 11% 7%
9	I	73	14% 95% 5%
9	V	73	10% 92% 7%
10	J	59	3% 93% 5%
10	W	59	7% 93%
11	K	56	84% 12%
11	X	56	11% 86% 12%
12	L	47	2% 89% 9%
12	Y	47	4% 85% 13%
13	M	46	4% 78% 15% 7%
13	Z	46	15% 89% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	607	-	-	X	-
18	AZI	N	607	-	-	X	-
20	EDO	A	617	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	618	-	-	-	X
20	EDO	C	318	-	-	-	X
20	EDO	D	202	-	-	X	-
22	CHD	W	101	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33590 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	21	0
			4185	2789	648	706	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

- 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	8	0
			1891	1229	291	352	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

- 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	8	0
			2176	1452	348	360	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	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	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

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

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

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

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

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

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

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

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

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

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

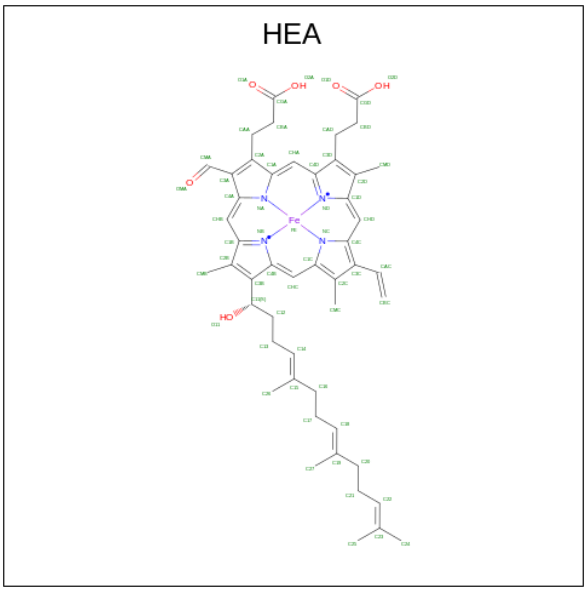
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

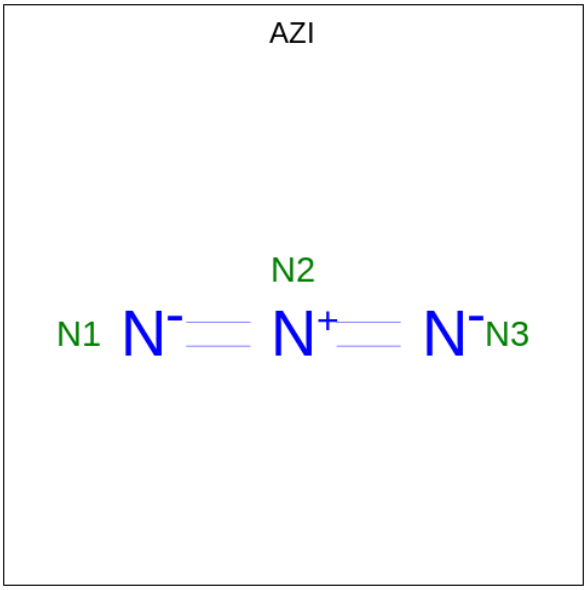
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

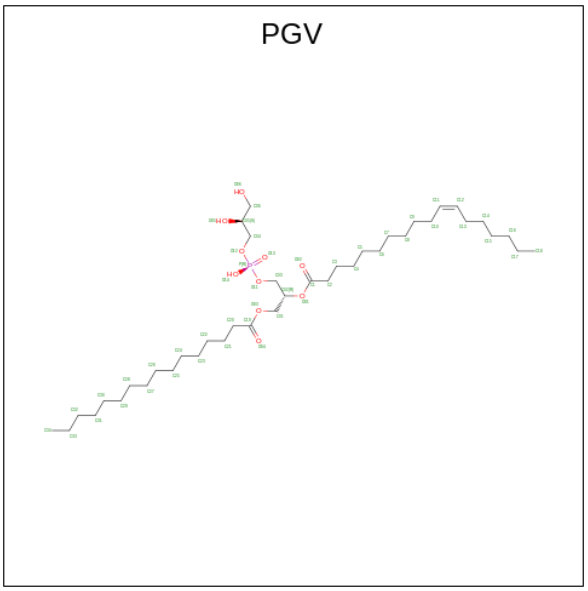
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



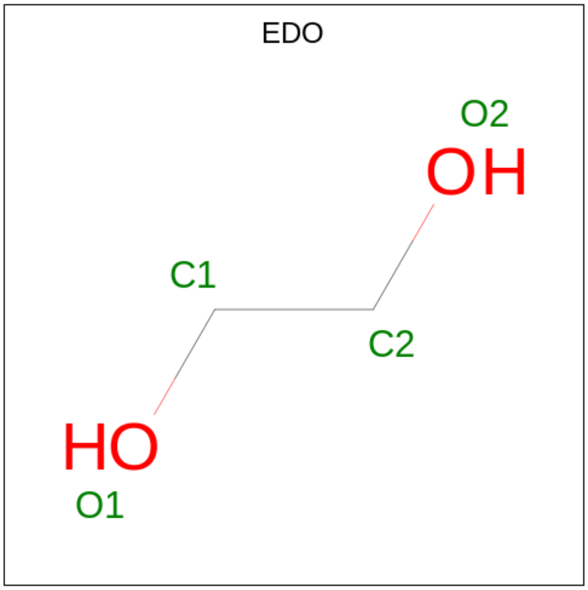
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

- Molecule 19 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
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	Z	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	D	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C O 4 2 2	0	0
20	G	1	Total C O 4 2 2	0	0
20	H	1	Total C O 4 2 2	0	0
20	J	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0

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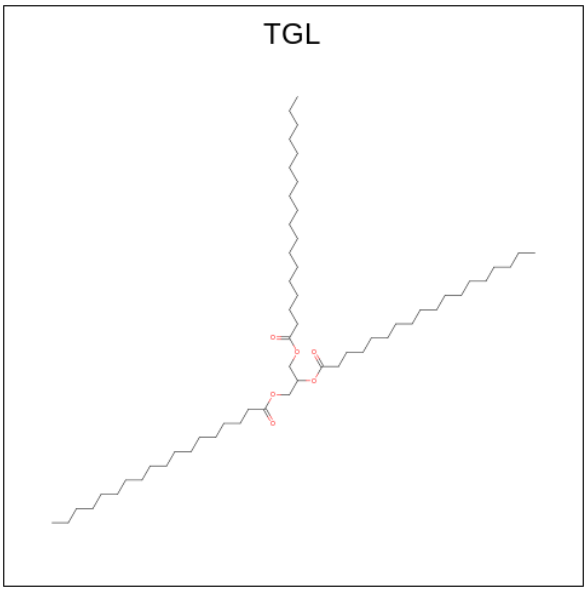
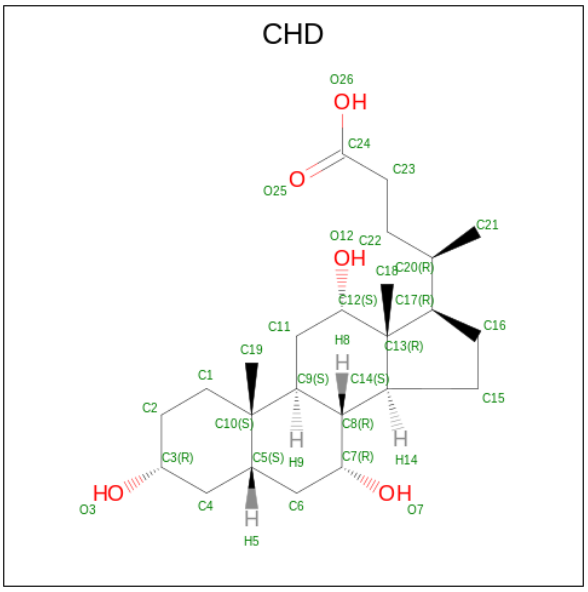
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		

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



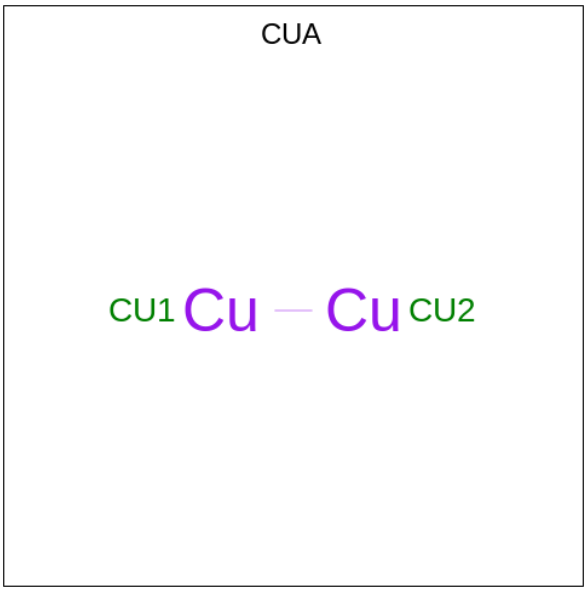
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C O 63 57 6	0	0
21	D	1	Total C O 63 57 6	0	0
21	L	1	Total C O 63 57 6	0	0
21	N	1	Total C O 63 57 6	0	0
21	Q	1	Total C O 63 57 6	0	0
21	Y	1	Total C O 63 57 6	0	0

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



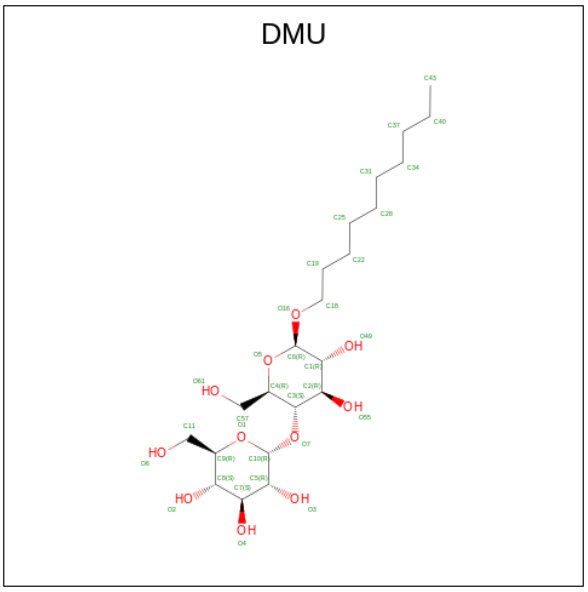
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

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



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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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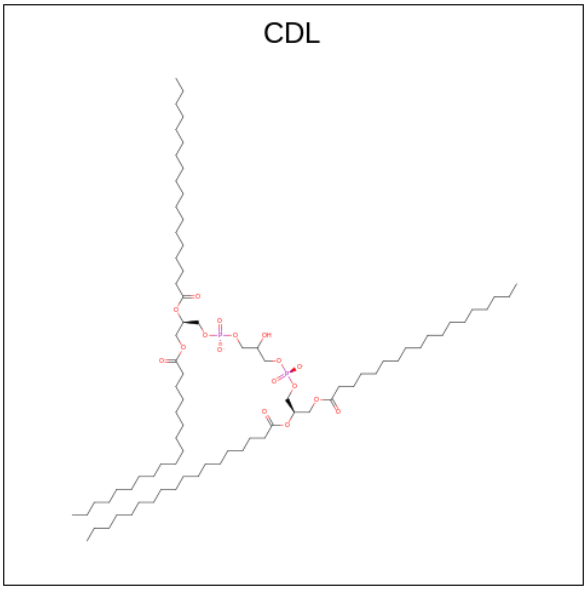
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

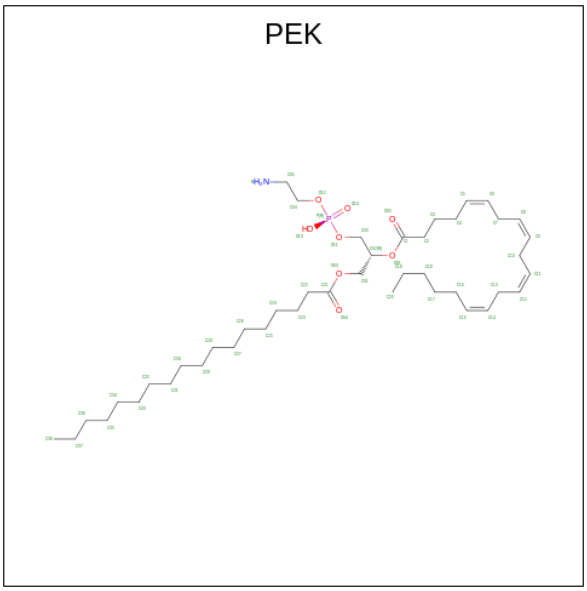
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

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



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

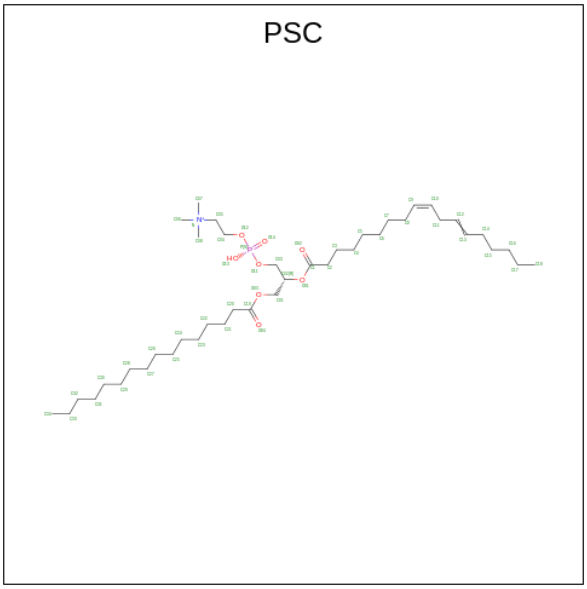
- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 28 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO

YLOXY)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
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	223	Total	O	0	0
			223	223		
30	B	140	Total	O	0	1
			141	141		
30	C	100	Total	O	0	0
			100	100		
30	D	97	Total	O	0	0
			97	97		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	E	78	Total O 78 78	0	0
30	F	86	Total O 86 86	0	0
30	G	42	Total O 42 42	0	0
30	H	35	Total O 35 35	0	0
30	I	21	Total O 21 21	0	0
30	J	21	Total O 21 21	0	0
30	K	26	Total O 26 26	0	0
30	L	29	Total O 29 29	0	0
30	M	25	Total O 25 25	0	0
30	N	204	Total O 204 204	0	0
30	O	101	Total O 102 102	0	1
30	P	102	Total O 102 102	0	0
30	Q	36	Total O 36 36	0	0
30	R	37	Total O 37 37	0	0
30	S	53	Total O 53 53	0	0
30	T	44	Total O 44 44	0	0
30	U	39	Total O 39 39	0	0
30	V	12	Total O 12 12	0	0
30	W	8	Total O 8 8	0	0
30	X	11	Total O 11 11	0	0
30	Y	14	Total O 14 14	0	0

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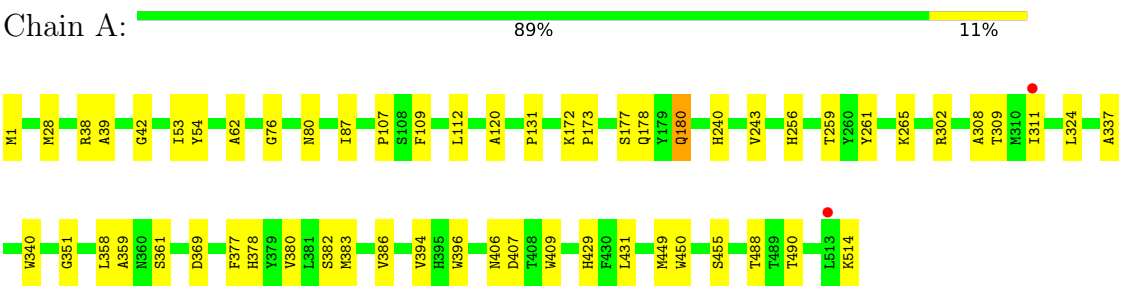
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Z	11	Total O 11 11	0	0

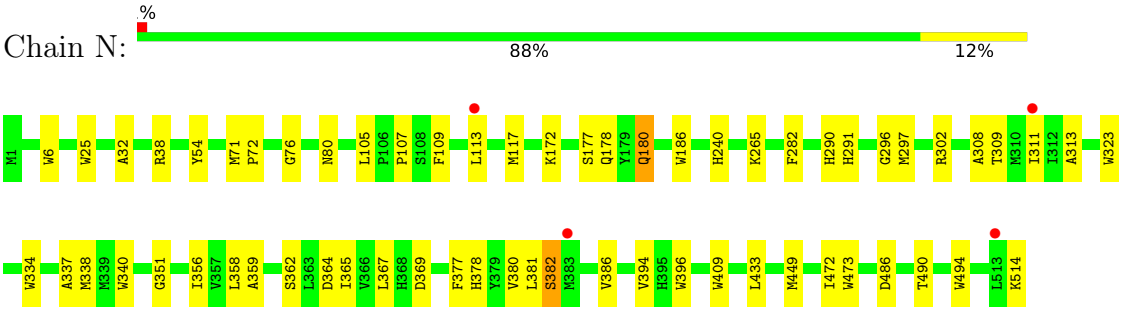
3 Residue-property plots (i)

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

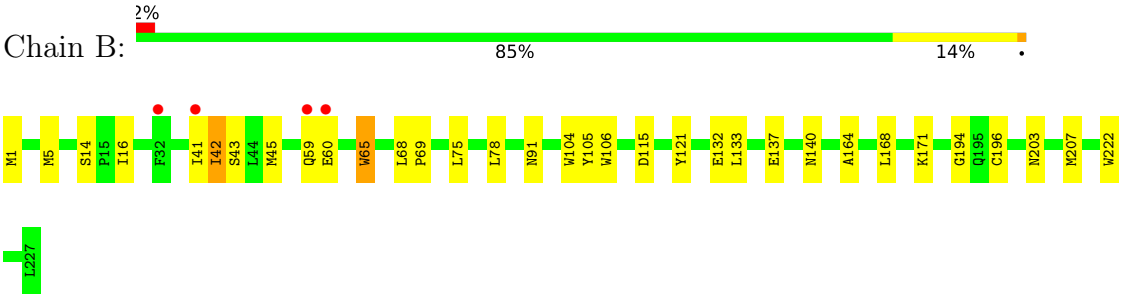
• Molecule 1: Cytochrome c oxidase subunit 1



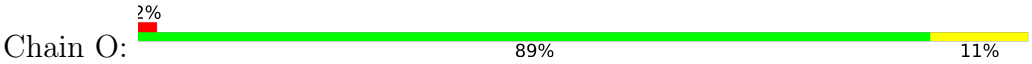
• Molecule 1: Cytochrome c oxidase subunit 1

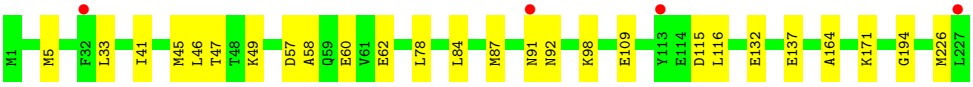


• Molecule 2: Cytochrome c oxidase subunit 2

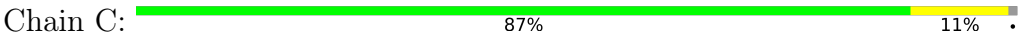


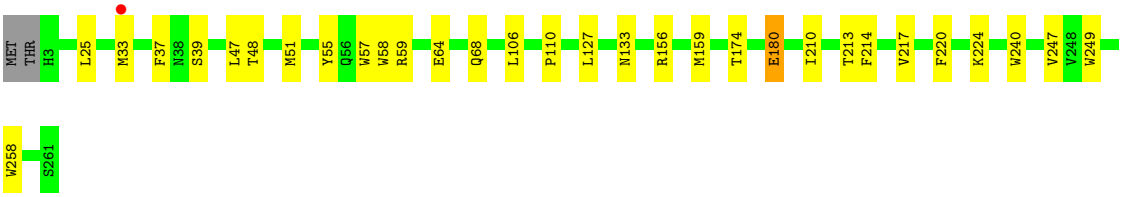
• Molecule 2: Cytochrome c oxidase subunit 2



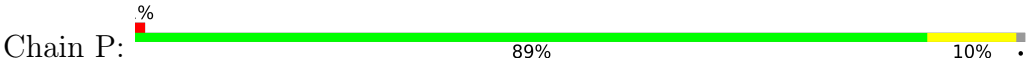


• Molecule 3: Cytochrome c oxidase subunit 3

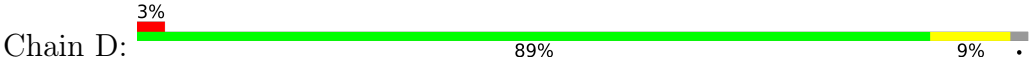


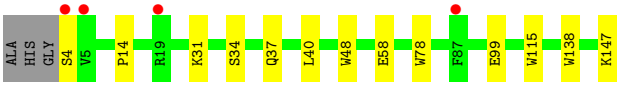


• Molecule 3: Cytochrome c oxidase subunit 3

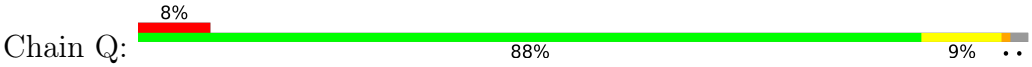


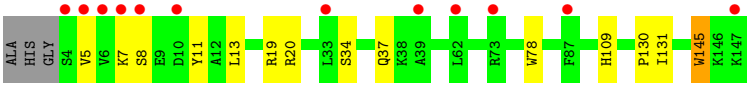
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



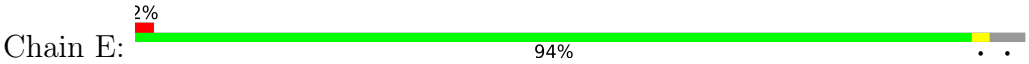


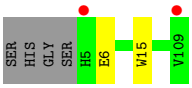
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



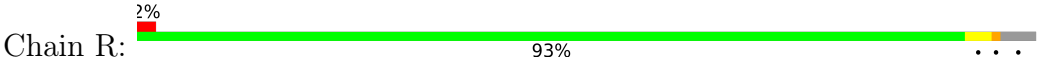


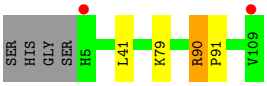
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial





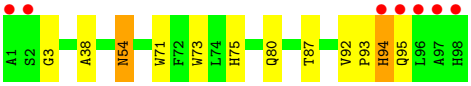
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial





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

Chain F:

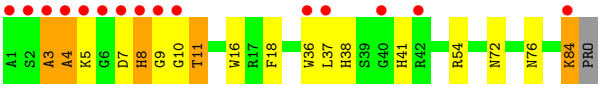


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:

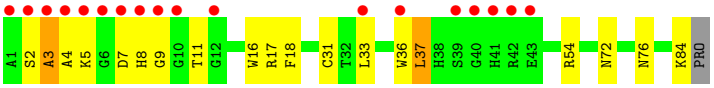
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



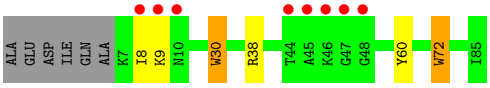
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



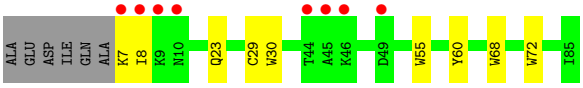
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



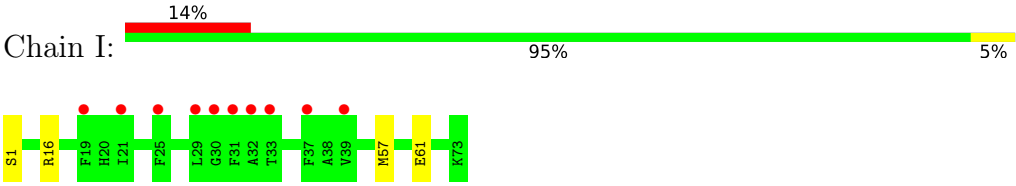
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



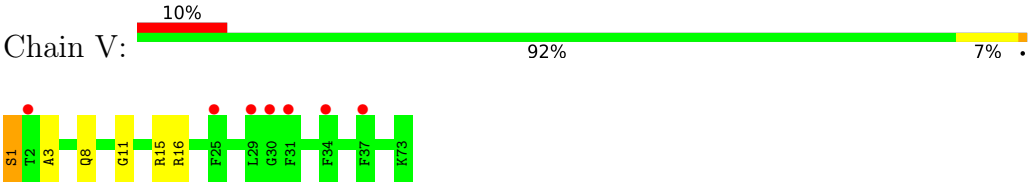
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



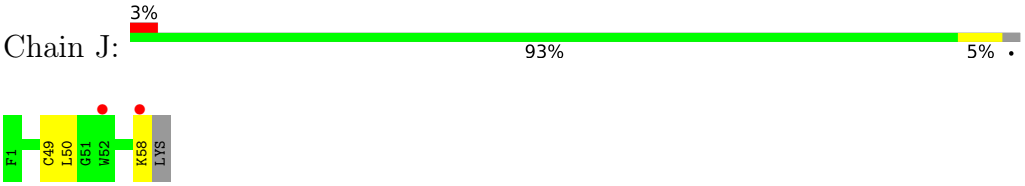
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



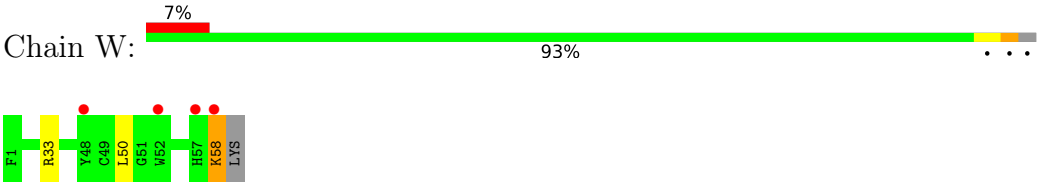
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



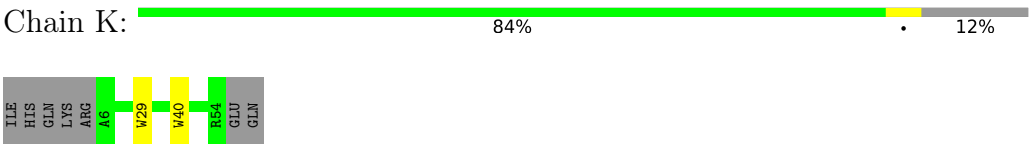
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



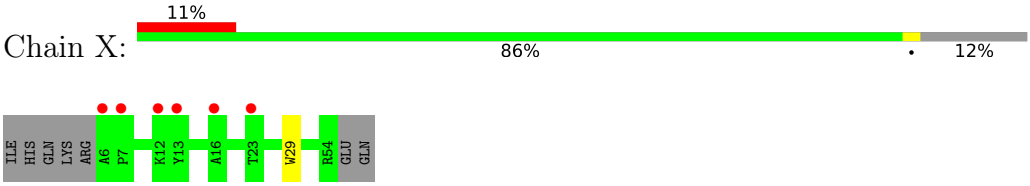
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



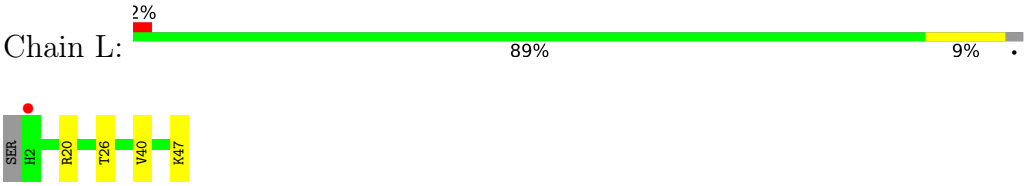
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



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

Chain L:



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

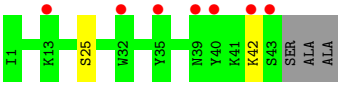
Chain Y:

• 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	183.49Å 206.29Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 108.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.5 (108.53-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.06 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.181 , 0.196 0.181 , 0.197	Depositor DCC
R_{free} test set	28473 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33590	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.62	3/4314 (0.1%)	0.58	0/5886
1	N	0.61	8/4308 (0.2%)	0.56	0/5878
2	B	0.54	3/1929 (0.2%)	0.62	0/2627
2	O	0.51	0/1908	0.57	0/2597
3	C	0.67	5/2263 (0.2%)	0.51	0/3090
3	P	0.66	2/2272 (0.1%)	0.52	0/3102
4	D	0.60	3/1259 (0.2%)	0.52	0/1698
4	Q	0.57	2/1259 (0.2%)	0.50	0/1698
5	E	0.50	1/871 (0.1%)	0.50	0/1182
5	R	0.47	0/871	0.52	0/1182
6	F	0.53	2/795 (0.3%)	0.57	0/1079
6	S	0.51	0/780	0.55	0/1058
7	G	0.65	2/702 (0.3%)	0.58	0/953
7	T	0.65	2/702 (0.3%)	0.57	0/953
8	H	0.61	2/682 (0.3%)	0.52	0/921
8	U	0.61	4/682 (0.6%)	0.51	0/921
9	I	0.38	0/605	0.48	0/802
9	V	0.37	0/605	0.47	0/802
10	J	0.50	0/471	0.45	0/636
10	W	0.50	0/480	0.49	0/648
11	K	0.68	2/398 (0.5%)	0.52	0/546
11	X	0.66	1/405 (0.2%)	0.49	0/556
12	L	0.57	0/393	0.51	0/526
12	Y	0.53	0/401	0.47	0/536
13	M	0.55	1/345 (0.3%)	0.52	0/470
13	Z	0.52	0/345	0.46	0/470
All	All	0.59	43/30045 (0.1%)	0.54	0/40817

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	115	TRP	CD2-CE2	5.31	1.47	1.41
3	C	57	TRP	CD2-CE2	5.30	1.47	1.41
1	N	323	TRP	CD2-CE2	5.28	1.47	1.41
4	D	48	TRP	CD2-CE2	5.26	1.47	1.41
1	N	409	TRP	CD2-CE2	5.26	1.47	1.41
11	K	29	TRP	CD2-CE2	5.26	1.47	1.41
3	C	58	TRP	CD2-CE2	5.25	1.47	1.41
2	B	65	TRP	CD2-CE2	5.24	1.47	1.41
7	G	36	TRP	CD2-CE2	5.21	1.47	1.41
8	H	30	TRP	CD2-CE2	5.21	1.47	1.41
6	F	71	TRP	CD2-CE2	5.19	1.47	1.41
1	A	340	TRP	CD2-CE2	5.18	1.47	1.41
8	H	72	TRP	CD2-CE2	5.18	1.47	1.41
11	X	29	TRP	CD2-CE2	5.16	1.47	1.41
8	U	72	TRP	CD2-CE2	5.16	1.47	1.41
4	Q	78	TRP	CD2-CE2	5.14	1.47	1.41
5	E	15	TRP	CD2-CE2	5.14	1.47	1.41
7	G	16	TRP	CD2-CE2	5.14	1.47	1.41
1	A	409	TRP	CD2-CE2	5.13	1.47	1.41
3	C	240	TRP	CD2-CE2	5.13	1.47	1.41
4	Q	145	TRP	CD2-CE2	5.12	1.47	1.41
4	D	138	TRP	CD2-CE2	5.11	1.47	1.41
1	N	340	TRP	CD2-CE2	5.09	1.47	1.41
1	N	473	TRP	CD2-CE2	5.09	1.47	1.41
3	P	258	TRP	CD2-CE2	5.09	1.47	1.41
1	N	6	TRP	CD2-CE2	5.07	1.47	1.41
1	N	396	TRP	CD2-CE2	5.07	1.47	1.41
1	A	396	TRP	CD2-CE2	5.06	1.47	1.41
2	B	106	TRP	CD2-CE2	5.05	1.47	1.41
7	T	16	TRP	CD2-CE2	5.05	1.47	1.41
11	K	40	TRP	CD2-CE2	5.05	1.47	1.41
7	T	36	TRP	CD2-CE2	5.04	1.47	1.41
3	C	258	TRP	CD2-CE2	5.04	1.47	1.41
13	M	32	TRP	CD2-CE2	5.04	1.47	1.41
8	U	68	TRP	CD2-CE2	5.03	1.47	1.41
6	F	73	TRP	CD2-CE2	5.03	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	25	TRP	CD2-CE2	5.03	1.47	1.41
8	U	30	TRP	CD2-CE2	5.03	1.47	1.41
3	C	249	TRP	CD2-CE2	5.03	1.47	1.41
8	U	55	TRP	CD2-CE2	5.02	1.47	1.41
1	N	494	TRP	CD2-CE2	5.01	1.47	1.41
3	P	34	TRP	CD2-CE2	5.01	1.47	1.41
2	B	222	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4185	0	4159	59	0
1	N	4179	0	4154	50	0
2	B	1891	0	1890	18	0
2	O	1870	0	1868	17	0
3	C	2176	0	2092	26	0
3	P	2185	0	2097	23	0
4	D	1224	0	1211	10	0
4	Q	1224	0	1211	9	0
5	E	852	0	845	1	0
5	R	852	0	845	2	0
6	F	778	0	754	9	0
6	S	763	0	742	11	0
7	G	686	0	652	16	0
7	T	686	0	652	9	0
8	H	662	0	623	4	0
8	U	662	0	623	1	0
9	I	601	0	613	2	0
9	V	601	0	613	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	460	0	459	2	0
10	W	469	0	464	2	0
11	K	384	0	366	0	0
11	X	391	0	374	0	0
12	L	380	0	380	6	0
12	Y	388	0	388	6	0
13	M	335	0	352	6	0
13	Z	335	0	352	1	0
14	A	180	0	162	23	0
14	N	180	0	162	19	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	4	0
18	N	6	0	0	6	0
19	A	102	0	152	6	0
19	C	102	0	152	5	0
19	N	51	0	76	0	0
19	P	102	0	152	3	0
19	Z	51	0	76	3	0
20	A	48	0	72	9	0
20	B	4	0	6	0	0
20	C	32	0	48	2	0
20	D	20	0	30	8	0
20	E	20	0	30	0	0
20	F	12	0	18	0	0
20	G	12	0	18	0	0
20	H	4	0	6	1	0
20	J	4	0	6	0	0
20	N	44	0	66	3	0
20	O	12	0	18	0	0
20	P	12	0	18	1	0
20	Q	12	0	18	1	0
20	R	20	0	30	0	0
20	S	12	0	18	1	0
20	T	4	0	6	0	0
20	U	4	0	6	0	0
20	V	4	0	6	0	0
20	W	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	63	0	110	1	0
21	D	63	0	110	7	0
21	L	63	0	110	5	0
21	N	63	0	110	2	0
21	Q	63	0	110	2	0
21	Y	63	0	110	6	0
22	B	29	0	39	0	0
22	C	58	0	78	2	0
22	G	29	0	39	1	0
22	J	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	39	4	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	99	0	126	5	0
24	M	33	0	42	0	0
24	P	99	0	126	0	0
24	Z	33	0	42	0	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	14	0
26	G	100	0	156	7	0
26	P	100	0	156	8	0
26	T	100	0	156	4	0
27	C	106	0	154	2	0
27	G	53	0	77	4	0
27	P	106	0	154	1	0
27	T	53	0	77	3	0
28	E	52	0	80	5	0
28	O	52	0	80	5	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	223	0	0	2	0
30	B	141	0	0	4	1
30	C	100	0	0	4	0
30	D	97	0	0	2	1
30	E	78	0	0	1	0
30	F	86	0	0	3	0
30	G	42	0	0	0	0
30	H	35	0	0	0	0
30	I	21	0	0	1	0
30	J	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	26	0	0	0	0
30	L	29	0	0	0	0
30	M	25	0	0	1	0
30	N	204	0	0	2	0
30	O	102	0	0	0	0
30	P	102	0	0	1	0
30	Q	36	0	0	1	0
30	R	37	0	0	0	0
30	S	53	0	0	3	0
30	T	44	0	0	0	0
30	U	39	0	0	0	0
30	V	12	0	0	1	0
30	W	8	0	0	0	0
30	X	11	0	0	0	0
30	Y	14	0	0	0	0
30	Z	11	0	0	0	0
All	All	33590	0	32691	336	1

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 (336) 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)
6:S:43:LYS:HE2	6:S:43:LYS:H	1.14	1.12
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.53	1.08
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.38	1.02
21:D:201:TGL:HG31	30:D:343:HOH:O	1.62	0.98
14:N:602[B]:HEA:HBC1	14:N:602[B]:HEA:HMC1	1.44	0.97
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	1.47	0.96
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:HBD2	1.50	0.94
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.37	0.90
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.13	0.87
7:G:84:LYS:H	7:G:84:LYS:HD2	1.38	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.25	0.85
12:L:20:ARG:HH22	21:L:101:TGL:HC32	1.43	0.82
2:O:57:ASP:H	28:O:302:PSC:H202	1.44	0.82
1:A:455:SER:HB3	20:D:202:EDO:H12	1.62	0.81
7:T:72:ASN:H	7:T:76:ASN:HD22	1.29	0.80
6:F:54[A]:ASN:C	6:F:54[A]:ASN:HD22	1.84	0.80
19:A:609:PGV:H311	13:M:19:LEU:HD23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:75:HIS:H	6:S:80:GLN:HE22	1.29	0.79
3:P:161[A]:GLN:HE22	27:P:309:PEK:H21	1.47	0.79
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.65	0.79
6:F:75:HIS:H	6:F:80:GLN:HE22	1.28	0.79
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.18	0.78
18:A:606:AZI:N1	18:A:607:AZI:N1	2.32	0.78
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.34	0.76
14:N:602[A]:HEA:HBC1	14:N:602[A]:HEA:HMC1	1.68	0.76
3:P:51[A]:MET:SD	3:P:54[A]:MET:HE1	2.25	0.76
1:A:382[B]:SER:C	1:A:383[B]:MET:HE2	2.07	0.75
6:S:43:LYS:HE2	6:S:43:LYS:N	1.98	0.75
3:P:51[A]:MET:SD	3:P:54[A]:MET:CE	2.75	0.74
1:N:309:THR:HG22	14:N:602[B]:HEA:HMB2	1.67	0.74
6:S:36:PRO:HD3	20:S:104:EDO:H11	1.69	0.74
1:A:382[B]:SER:C	1:A:383[B]:MET:CE	2.56	0.74
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.68	0.73
3:P:210:ILE:HD13	19:P:305:PGV:H301	1.70	0.73
24:C:302:DMU:H10	10:J:49:CYS:HB3	1.71	0.73
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.70	0.72
7:T:76:ASN:HD21	27:T:101:PEK:HN2	1.36	0.72
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	1.93	0.70
4:D:34:SER:H	4:D:37:GLN:HE21	1.38	0.70
12:Y:20:ARG:HH22	21:Y:101:TGL:HC52	1.56	0.70
18:N:606:AZI:N1	18:N:607:AZI:N3	2.39	0.70
7:G:38:HIS:HE1	26:G:102:CDL:H122	1.57	0.70
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.71	0.69
1:A:382[B]:SER:O	1:A:383[B]:MET:HE1	1.92	0.69
7:G:10:GLY:O	7:G:11:TPO:HB	1.92	0.68
1:A:383[B]:MET:HE2	1:A:383[B]:MET:N	2.09	0.68
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	2.08	0.68
6:S:95:GLN:HG3	6:S:96:LEU:H	1.59	0.67
6:S:43:LYS:H	6:S:43:LYS:CE	2.01	0.67
26:G:102:CDL:H622	19:P:303:PGV:H161	1.77	0.67
20:D:203:EDO:H11	30:E:354:HOH:O	1.95	0.67
3:P:67:PHE:HE2	26:P:306:CDL:H1O1	1.41	0.66
7:T:37:LEU:HD23	26:T:102:CDL:H381	1.77	0.66
10:W:33:ARG:HG2	22:W:101:CHD:H8	1.77	0.65
3:C:180:GLU:HG2	30:C:416:HOH:O	1.95	0.65
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.77	0.65
26:T:102:CDL:HB32	26:T:102:CDL:H182	1.79	0.64
10:W:58:LYS:H	10:W:58:LYS:HD2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.80	0.64
14:A:602[B]:HEA:HMD1	14:A:602[B]:HEA:CBD	2.27	0.64
20:A:617:EDO:H22	30:M:213:HOH:O	1.96	0.64
6:F:54[A]:ASN:C	6:F:54[A]:ASN:ND2	2.50	0.64
4:D:78:TRP:CA	21:D:201:TGL:HB22	2.29	0.63
1:N:297[B]:MET:HB3	30:N:780:HOH:O	1.98	0.63
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.27	0.63
4:D:99:GLU:OE2	20:D:202:EDO:H22	1.98	0.63
3:C:48:THR:HG23	26:C:305:CDL:H411	1.80	0.63
26:G:102:CDL:H371	2:O:78:LEU:HD12	1.80	0.62
4:Q:7:LYS:HE2	4:Q:13:LEU:HD22	1.81	0.62
20:C:315:EDO:H22	8:H:72:TRP:HZ2	1.66	0.61
12:L:20:ARG:NH2	21:L:101:TGL:HC32	2.15	0.60
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	2.01	0.60
1:N:240:HIS:HE1	18:N:607:AZI:N2	1.98	0.60
3:P:156:ARG:HE	22:P:307:CHD:C24	2.15	0.60
1:A:240:HIS:HE1	18:A:607:AZI:N2	2.00	0.59
14:N:602[A]:HEA:HMC1	14:N:602[A]:HEA:CBC	2.32	0.59
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.42	0.59
9:V:11:GLY:O	9:V:15:ARG:HG3	2.02	0.59
1:A:488:THR:HG21	20:A:618:EDO:H21	1.84	0.59
22:J:101:CHD:H183	22:J:101:CHD:H212	1.84	0.59
19:Z:101:PGV:H21	19:Z:101:PGV:H011	1.84	0.58
1:N:240:HIS:CE1	18:N:607:AZI:N2	2.72	0.58
3:P:224:LYS:CD	26:P:306:CDL:HB31	2.34	0.58
4:D:78:TRP:HA	21:D:201:TGL:HB22	1.86	0.58
3:C:224:LYS:CD	26:C:305:CDL:HB32	2.34	0.58
1:A:382[B]:SER:C	1:A:383[B]:MET:HE1	2.23	0.57
21:D:201:TGL:H342	9:I:16:ARG:HE	1.68	0.57
8:H:38:ARG:HH22	20:H:101:EDO:H12	1.70	0.57
1:A:240:HIS:CE1	18:A:607:AZI:N2	2.73	0.57
19:A:608:PGV:H183	27:G:101:PEK:H322	1.85	0.57
3:C:59:ARG:HA	26:C:305:CDL:H512	1.86	0.57
3:C:156:ARG:HE	22:C:306:CHD:C24	2.17	0.57
19:A:608:PGV:H322	27:G:101:PEK:H371	1.86	0.56
3:C:174:THR:HG21	26:C:305:CDL:H861	1.86	0.56
26:G:102:CDL:H591	26:G:102:CDL:H761	1.86	0.56
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.88	0.56
2:B:1:FME:HE3	2:B:133:LEU:HD22	1.87	0.56
4:Q:145:TRP:H	20:Q:204:EDO:H22	1.69	0.56
26:C:305:CDL:H811	26:C:305:CDL:H662	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:THR:HG23	26:C:305:CDL:H781	1.88	0.56
27:C:309:PEK:H351	26:T:102:CDL:H871	1.88	0.56
1:A:39:ALA:HA	20:D:202:EDO:O1	2.06	0.55
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C3C	2.35	0.55
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:CBD	2.32	0.55
7:T:3:ALA:O	7:T:4:ALA:HB3	2.07	0.55
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.37	0.54
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.90	0.54
1:A:256:HIS:HA	20:A:612:EDO:H21	1.89	0.54
1:N:358:LEU:HB3	14:N:602[A]:HEA:HMA	1.88	0.54
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:CBC	2.25	0.54
1:A:383[B]:MET:CE	1:A:383[B]:MET:N	2.69	0.54
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.90	0.54
3:C:224:LYS:HE3	26:C:305:CDL:HB32	1.89	0.54
20:N:617:EDO:H12	30:S:245:HOH:O	2.08	0.54
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.37	0.54
7:G:37:LEU:HD21	26:G:102:CDL:H381	1.90	0.54
1:N:359:ALA:HA	14:N:602[B]:HEA:OMA	2.07	0.54
3:P:51[A]:MET:HA	3:P:54[A]:MET:HE2	1.88	0.54
28:O:302:PSC:H343	28:O:302:PSC:H142	1.89	0.53
3:C:224:LYS:CE	26:C:305:CDL:HB32	2.39	0.53
1:A:131:PRO:HB3	20:A:621:EDO:H12	1.89	0.53
4:D:34:SER:H	4:D:37:GLN:NE2	2.06	0.53
3:C:33[B]:MET:HG2	3:C:39:SER:O	2.09	0.52
1:A:28:MET:CE	14:A:601:HEA:H271	2.40	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.08	0.52
3:P:67:PHE:HE2	26:P:306:CDL:O1	1.92	0.52
1:A:177:SER:H	1:A:180:GLN:HE21	1.58	0.52
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	2.94	0.52
1:N:380[A]:VAL:HG21	14:N:602[A]:HEA:C3C	2.39	0.52
2:O:41:ILE:HD13	28:O:302:PSC:H342	1.91	0.52
7:G:84:LYS:HD2	7:G:84:LYS:N	2.18	0.51
3:P:63:ARG:HE	26:P:306:CDL:HA21	1.74	0.51
6:S:43:LYS:HE3	30:S:247:HOH:O	2.10	0.51
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.92	0.51
1:N:177:SER:H	1:N:180:GLN:NE2	2.08	0.51
21:N:609:TGL:HA72	21:N:609:TGL:H131	1.92	0.51
1:N:105:LEU:HD11	20:N:611:EDO:H12	1.93	0.51
3:C:51[A]:MET:SD	26:C:305:CDL:H612	2.51	0.51
12:L:26:THR:HG23	13:M:25:SER:CB	2.41	0.50
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:601:HEA:H262	14:N:601:HEA:H122	1.93	0.50
1:A:177:SER:H	1:A:180:GLN:NE2	2.09	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.50
3:C:224:LYS:HD3	26:C:305:CDL:HB32	1.93	0.50
1:A:42:GLY:HA3	20:D:202:EDO:H21	1.93	0.50
14:A:602[B]:HEA:H122	14:A:602[B]:HEA:HHC	1.93	0.50
22:C:301:CHD:H152	19:C:308:PGV:H131	1.93	0.50
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.94	0.50
21:L:101:TGL:OC1	21:L:101:TGL:HC41	2.12	0.49
1:A:382[B]:SER:CB	1:A:383[B]:MET:HE2	2.41	0.49
12:Y:20:ARG:NH2	21:Y:101:TGL:HC52	2.27	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.93	0.49
1:A:406:ASN:HD21	19:A:609:PGV:H31	1.77	0.49
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.95	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.94	0.49
21:N:609:TGL:H352	21:N:609:TGL:H211	1.95	0.49
3:P:224:LYS:HD2	26:P:306:CDL:HB31	1.94	0.49
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.12	0.49
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.94	0.49
21:L:101:TGL:HC22	21:L:101:TGL:HC82	1.94	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
21:Y:101:TGL:HC22	21:Y:101:TGL:HC81	1.94	0.49
3:C:106:LEU:HD22	19:C:308:PGV:H41	1.95	0.49
3:C:33[B]:MET:HB2	24:C:302:DMU:H11	1.95	0.49
2:B:164:ALA:O	2:B:194:GLY:HA3	2.12	0.49
20:N:616:EDO:H21	4:Q:11:TYR:HB2	1.94	0.49
7:T:7:ASP:O	7:T:9:GLY:N	2.46	0.49
1:A:28:MET:HE1	14:A:601:HEA:H271	1.95	0.48
1:A:358:LEU:HB3	14:A:602[A]:HEA:HMA	1.95	0.48
6:F:87[B]:THR:HG21	30:F:261:HOH:O	2.13	0.48
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.94	0.48
27:T:101:PEK:H32	27:T:101:PEK:H71	1.95	0.48
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.60	0.48
1:N:380[A]:VAL:HG21	14:N:602[A]:HEA:C4C	2.43	0.48
14:N:602[A]:HEA:HBC1	14:N:602[A]:HEA:CMC	2.42	0.48
3:P:59:ARG:HA	26:P:306:CDL:H511	1.95	0.48
12:Y:12:PRO:HB2	21:Y:101:TGL:HG12	1.95	0.48
2:B:41[A]:ILE:HD13	28:E:201:PSC:H342	1.96	0.47
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.12	0.47
3:C:133:ASN:ND2	30:C:401:HOH:O	2.44	0.47
30:C:414:HOH:O	6:F:3:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.97	0.47
1:A:259:THR:HG21	20:A:612:EDO:H22	1.97	0.47
19:A:609:PGV:H312	13:M:16:ALA:HA	1.97	0.47
3:C:210:ILE:HG12	19:C:304:PGV:H132	1.96	0.47
5:E:6:GLU:HG3	28:E:201:PSC:H071	1.95	0.47
7:G:72:ASN:H	7:G:76:ASN:ND2	2.04	0.47
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.35	0.47
1:A:455:SER:HB3	20:D:202:EDO:C1	2.37	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.47
7:T:31:CYS:SG	26:T:102:CDL:H532	2.53	0.47
1:N:364:ASP:OD1	14:N:602[B]:HEA:O1A	2.33	0.47
28:E:201:PSC:H343	28:E:201:PSC:H141	1.96	0.47
21:L:101:TGL:HA92	21:L:101:TGL:H221	1.61	0.47
1:A:302[B]:ARG:NE	1:A:361[B]:SER:OG	2.45	0.46
3:C:37:PHE:CG	24:C:302:DMU:H8	2.50	0.46
1:N:351:GLY:HA3	1:N:380[B]:VAL:HB	1.97	0.46
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.46
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.13	0.46
1:N:449:MET:SD	2:O:5:MET:HG2	2.55	0.46
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.15	0.46
1:A:386:VAL:HG21	14:A:601:HEA:H261	1.97	0.46
3:C:55:TYR:HA	26:C:305:CDL:H561	1.97	0.46
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.46	0.46
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.97	0.46
6:F:93:PRO:O	6:F:94:HIS:HB2	2.15	0.46
9:V:1:SAC:H2A3	9:V:3:ALA:HB2	1.98	0.46
6:S:95:GLN:HG3	6:S:96:LEU:N	2.29	0.46
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG3	2.46	0.46
19:Z:101:PGV:H312	19:Z:101:PGV:H161	1.98	0.46
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C4C	2.46	0.46
20:D:203:EDO:H21	30:F:218:HOH:O	2.16	0.46
3:C:220:PHE:HB2	26:C:305:CDL:H711	1.98	0.45
1:A:120:ALA:HB3	20:A:611:EDO:H12	1.98	0.45
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	1.98	0.45
14:N:602[A]:HEA:C1B	18:N:607:AZI:N2	2.79	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.45
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.52	0.45
7:T:2:SER:O	7:T:3:ALA:HB3	2.17	0.45
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	1.99	0.45
2:O:47:THR:HB	21:Q:201:TGL:H181	1.97	0.45
4:D:4:SER:HB3	30:D:303:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:307:CHD:H162	22:P:307:CHD:C23	2.46	0.45
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.82	0.45
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.45
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.45
1:N:54:TYR:HB2	30:N:852:HOH:O	2.16	0.45
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.45
28:O:302:PSC:H083	28:O:302:PSC:H041	1.78	0.45
26:C:305:CDL:H232	26:C:305:CDL:H621	1.99	0.44
27:T:101:PEK:H32	27:T:101:PEK:C7	2.48	0.44
3:C:106:LEU:HB3	19:C:308:PGV:H22	1.98	0.44
19:C:308:PGV:H031	30:C:468:HOH:O	2.15	0.44
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.00	0.44
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	2.00	0.44
14:A:602[B]:HEA:HBC1	14:A:602[B]:HEA:CMC	2.24	0.44
1:N:386:VAL:HG21	14:N:601:HEA:H261	1.99	0.44
6:S:51:SER:O	6:S:94:HIS:N	2.51	0.44
1:A:76:GLY:O	1:A:80:ASN:HB2	2.18	0.44
1:A:112:LEU:C	1:A:112:LEU:HD23	2.37	0.44
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.00	0.44
22:W:101:CHD:H112	22:W:101:CHD:H12A	1.85	0.44
1:N:514:LYS:HE2	30:S:214:HOH:O	2.17	0.44
2:O:57:ASP:N	28:O:302:PSC:H202	2.22	0.44
1:A:28:MET:CE	14:A:601:HEA:C27	2.96	0.43
1:A:407:ASP:OD2	20:A:617:EDO:H11	2.18	0.43
2:B:16[B]:ILE:HG23	30:B:514:HOH:O	2.18	0.43
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.00	0.43
1:A:28:MET:HE1	14:A:601:HEA:C27	2.48	0.43
28:E:201:PSC:H51	30:I:106:HOH:O	2.16	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.01	0.43
3:P:52:LEU:HD23	26:P:306:CDL:H372	2.00	0.43
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.47	0.43
7:G:3:ALA:O	7:G:4:ALA:CB	2.66	0.43
7:G:37:LEU:HD11	26:G:102:CDL:H372	1.99	0.43
1:N:313:ALA:HB2	1:N:356:ILE:HD11	2.01	0.43
14:A:602[A]:HEA:HHA	14:A:602[A]:HEA:HAD2	1.82	0.43
1:A:383[B]:MET:CE	1:A:383[B]:MET:CA	2.96	0.43
14:A:602[A]:HEA:NB	18:A:607:AZI:N2	2.64	0.43
19:A:609:PGV:H132	19:A:609:PGV:H302	2.00	0.43
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.18	0.43
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.99	0.43
7:T:3:ALA:O	7:T:4:ALA:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:HB2	30:A:766:HOH:O	2.19	0.43
1:A:87:ILE:O	1:A:173:PRO:HD3	2.18	0.43
14:N:602[A]:HEA:C1B	18:N:607:AZI:N1	2.82	0.43
14:N:602[A]:HEA:NB	18:N:607:AZI:N2	2.63	0.43
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.84	0.43
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	2.00	0.43
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.19	0.42
1:A:351:GLY:HA3	1:A:380[B]:VAL:HB	2.00	0.42
2:B:41[A]:ILE:O	2:B:45:MET:HG2	2.19	0.42
27:G:101:PEK:H172	27:G:101:PEK:H11	2.00	0.42
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG3	2.01	0.42
2:B:42:ILE:HG22	2:B:43:SER:N	2.35	0.42
7:G:10:GLY:O	7:G:11:TPO:CB	2.66	0.42
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.84	0.42
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.19	0.42
21:D:201:TGL:HA91	21:D:201:TGL:H241	2.00	0.42
7:G:7:ASP:CG	7:G:8:HIS:H	2.21	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.01	0.42
2:B:65:TRP:O	2:B:69:PRO:HG2	2.20	0.42
20:C:315:EDO:H22	8:H:72:TRP:CZ2	2.49	0.42
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.01	0.42
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.85	0.42
3:C:217:VAL:HG22	26:C:305:CDL:H732	2.02	0.42
22:W:101:CHD:H212	22:W:101:CHD:H162	1.82	0.42
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	2.02	0.42
22:W:101:CHD:H191	22:W:101:CHD:H7	2.02	0.42
20:A:612:EDO:O2	30:A:701:HOH:O	1.64	0.42
22:G:103:CHD:H212	22:G:103:CHD:H12	2.01	0.42
13:M:34:LEU:HA	13:M:37:LEU:HG	2.01	0.42
1:A:429:HIS:HB3	21:B:301:TGL:HB31	2.01	0.41
24:C:302:DMU:H20	10:J:50:LEU:HB2	2.02	0.41
7:G:8:HIS:O	1:N:178[A]:GLN:NE2	2.53	0.41
12:L:26:THR:HG23	13:M:25:SER:HB2	2.01	0.41
3:P:226:HIS:CE1	26:P:306:CDL:HB32	2.56	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.41
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.19	0.41
5:R:41:LEU:HA	30:V:206:HOH:O	2.19	0.41
14:A:601:HEA:HHC	14:A:601:HEA:H122	2.01	0.41
1:N:472:ILE:HG21	21:Y:101:TGL:H202	2.02	0.41
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.02	0.41
1:A:449:MET:SD	2:B:5:MET:HG2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:THR:HG23	13:M:25:SER:HB3	2.02	0.41
1:N:113[A]:LEU:O	1:N:117[A]:MET:HG3	2.20	0.41
1:N:180:GLN:HE21	1:N:180:GLN:HB2	1.67	0.41
1:N:377:PHE:HB2	14:N:602[B]:HEA:HMD3	2.02	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.41
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.56	0.41
3:P:164:PHE:CD1	22:P:307:CHD:H192	2.56	0.41
12:Y:13:PHE:HB3	21:Y:101:TGL:HA41	2.03	0.41
2:B:140:ASN:HB3	30:B:504:HOH:O	2.20	0.41
9:I:57:MET:O	9:I:61:GLU:HG2	2.21	0.41
3:P:246:ASP:HB2	30:P:489:HOH:O	2.20	0.41
1:A:383[B]:MET:CE	1:A:383[B]:MET:HA	2.51	0.41
24:C:310:DMU:H32	24:C:310:DMU:H29	2.03	0.41
28:E:201:PSC:H41	28:E:201:PSC:H261	2.01	0.41
3:P:210:ILE:HG21	19:P:305:PGV:H282	2.03	0.41
20:P:312:EDO:H22	7:T:17:ARG:HD3	2.03	0.41
4:D:14:PRO:HG3	20:D:203:EDO:H22	2.03	0.41
6:F:87[A]:THR:HG21	30:F:272:HOH:O	2.21	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.56	0.41
2:B:41[B]:ILE:O	2:B:45:MET:HG2	2.20	0.40
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.02	0.40
19:Z:101:PGV:H202	19:Z:101:PGV:H42	2.03	0.40
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:N	2.69	0.40
1:A:261:TYR:OH	20:A:614:EDO:H12	2.21	0.40
2:B:105:TYR:HD1	30:B:437:HOH:O	2.03	0.40
7:G:38:HIS:CE1	26:G:102:CDL:H122	2.47	0.40
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.40
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.03	0.40
2:B:121:TYR:HE2	30:B:437:HOH:O	2.00	0.40
3:C:247:VAL:HG12	27:C:309:PEK:H132	2.03	0.40
1:N:367:LEU:HD21	1:N:433:LEU:HD23	2.03	0.40
4:Q:109:HIS:HD2	30:Q:329:HOH:O	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:437:HOH:O	30:D:335:HOH:O[2_584]	1.87	0.33

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	533/514 (104%)	517 (97%)	16 (3%)	0	100 100
1	N	532/514 (104%)	520 (98%)	12 (2%)	0	100 100
2	B	233/227 (103%)	229 (98%)	4 (2%)	0	100 100
2	O	230/227 (101%)	225 (98%)	4 (2%)	1 (0%)	34 19
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100 100
3	P	266/261 (102%)	262 (98%)	4 (2%)	0	100 100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100 100
4	Q	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22 9
5	E	103/109 (94%)	103 (100%)	0	0	100 100
5	R	103/109 (94%)	103 (100%)	0	0	100 100
6	F	100/98 (102%)	95 (95%)	3 (3%)	2 (2%)	7 1
6	S	98/98 (100%)	93 (95%)	3 (3%)	2 (2%)	7 1
7	G	82/85 (96%)	69 (84%)	7 (8%)	6 (7%)	1 0
7	T	82/85 (96%)	72 (88%)	7 (8%)	3 (4%)	3 0
8	H	77/85 (91%)	75 (97%)	1 (1%)	1 (1%)	12 3
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	12 3
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100 100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6 1
13	M	41/46 (89%)	41 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100 100
All	All	3592/3614 (99%)	3487 (97%)	87 (2%)	18 (0%)	29 15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	T	8	HIS
6	F	95	GLN
12	Y	46	LYS
7	G	3	ALA
7	G	8	HIS
8	H	8	ILE
4	Q	8	SER
6	S	94	HIS
6	S	95	GLN
7	G	5	LYS
7	G	41	HIS
7	T	3	ALA
7	T	5	LYS
7	G	9	GLY
2	O	92	ASN
8	U	8	ILE

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	446/426 (105%)	442 (99%)	4 (1%)	78 72
1	N	445/426 (104%)	438 (98%)	7 (2%)	62 49
2	B	218/210 (104%)	209 (96%)	9 (4%)	30 13
2	O	215/210 (102%)	210 (98%)	5 (2%)	50 34
3	C	232/226 (103%)	228 (98%)	4 (2%)	60 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	233/226 (103%)	230 (99%)	3 (1%)	69 58
4	D	131/129 (102%)	129 (98%)	2 (2%)	65 53
4	Q	131/129 (102%)	130 (99%)	1 (1%)	81 76
5	E	92/95 (97%)	92 (100%)	0	100 100
5	R	92/95 (97%)	90 (98%)	2 (2%)	52 36
6	F	85/81 (105%)	83 (98%)	2 (2%)	49 33
6	S	83/81 (102%)	79 (95%)	4 (5%)	25 10
7	G	68/68 (100%)	65 (96%)	3 (4%)	28 12
7	T	68/68 (100%)	63 (93%)	5 (7%)	13 3
8	H	71/75 (95%)	69 (97%)	2 (3%)	43 27
8	U	71/75 (95%)	68 (96%)	3 (4%)	30 13
9	I	57/57 (100%)	57 (100%)	0	100 100
9	V	57/57 (100%)	56 (98%)	1 (2%)	59 45
10	J	49/50 (98%)	48 (98%)	1 (2%)	55 40
10	W	50/50 (100%)	48 (96%)	2 (4%)	31 14
11	K	39/46 (85%)	39 (100%)	0	100 100
11	X	40/46 (87%)	40 (100%)	0	100 100
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 30
12	Y	40/40 (100%)	40 (100%)	0	100 100
13	M	37/38 (97%)	36 (97%)	1 (3%)	44 29
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44 29
All	All	3126/3082 (101%)	3063 (98%)	63 (2%)	55 40

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	369	ASP
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	68	LEU
2	B	75	LEU

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Mol	Chain	Res	Type
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	180	GLU
3	C	214	PHE
4	D	31	LYS
4	D	147	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
7	G	18	PHE
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	60	TYR
10	J	58	LYS
12	L	47	LYS
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	338	MET
1	N	369	ASP
1	N	382[A]	SER
1	N	382[B]	SER
2	O	33	LEU
2	O	60	GLU
2	O	91	ASN
2	O	115	ASP
2	O	171	LYS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	5	VAL
5	R	79	LYS
5	R	90	ARG
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN

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Mol	Chain	Res	Type
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	54	ARG
7	T	84	LYS
8	U	7	LYS
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
10	W	58	LYS
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	80	GLN
6	F	95	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
10	J	29	ASN
1	N	180	GLN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN

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Mol	Chain	Res	Type
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
9	V	8	GLN
10	W	29	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.15	0
2	FME	B	1	2	8,9,10	0.64	0	7,9,11	1.08	0
7	TPO	T	11	7	8,10,11	1.41	1 (12%)	10,14,16	0.79	0
7	TPO	G	11	7	8,10,11	1.38	1 (12%)	10,14,16	0.68	0
9	SAC	V	1	9	7,8,9	1.25	1 (14%)	8,9,11	0.94	0
1	FME	N	1	1	8,9,10	0.58	0	7,9,11	1.17	0
9	SAC	I	1	9	7,8,9	1.00	1 (14%)	8,9,11	0.76	0
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	1.45	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	3/9/11/13	-
9	SAC	V	1	9	-	6/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	3.14	1.50	1.46
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-O1P	2.78	1.59	1.50
9	I	1	SAC	CA-N	2.40	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	C-CA-N	2.53	114.30	109.73

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CA-CB-OG1-P
7	T	11	TPO	CB-OG1-P-O3P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	O-C-CA-CB
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
9	I	1	SAC	N-CA-CB-OG
1	A	1	FME	CB-CG-SD-CE
2	B	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
7	T	11	TPO	CB-OG1-P-O1P
9	V	1	SAC	C-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 125 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	$\#\|Z\| > 2$
20	EDO	A	619	-	3,3,3	0.49	0	2,2,2	0.29	0
20	EDO	D	202	-	3,3,3	0.34	0	2,2,2	0.53	0
18	AZI	A	606	15	0,2,2	-	-	0,1,1	-	-
27	PEK	P	309	-	52,52,52	0.95	2 (3%)	55,57,57	0.89	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	N	608	-	50,50,50	0.86	2 (4%)	53,56,56	0.88	2 (3%)
20	EDO	D	205	-	3,3,3	0.44	0	2,2,2	0.29	0
19	PGV	P	305	-	50,50,50	0.87	2 (4%)	53,56,56	0.76	0
20	EDO	J	102	-	3,3,3	0.45	0	2,2,2	0.38	0
20	EDO	F	102	-	3,3,3	0.51	0	2,2,2	0.30	0
22	CHD	G	103	-	32,32,32	0.66	0	51,51,51	0.91	1 (1%)
20	EDO	N	611	-	3,3,3	0.52	0	2,2,2	0.37	0
20	EDO	O	303	-	3,3,3	0.46	0	2,2,2	0.42	0
27	PEK	G	101	-	52,52,52	0.86	2 (3%)	55,57,57	0.81	1 (1%)
14	HEA	A	601	1	57,67,67	1.50	12 (21%)	61,103,103	1.46	10 (16%)
20	EDO	C	312	-	3,3,3	0.51	0	2,2,2	0.32	0
20	EDO	R	202	-	3,3,3	0.46	0	2,2,2	0.39	0
20	EDO	N	610	-	3,3,3	0.45	0	2,2,2	0.31	0
27	PEK	C	309	-	52,52,52	0.95	2 (3%)	55,57,57	1.00	3 (5%)
20	EDO	A	616	-	3,3,3	0.44	0	2,2,2	0.41	0
20	EDO	N	615	-	3,3,3	0.43	0	2,2,2	0.35	0
14	HEA	N	602[A]	1,18	57,67,67	1.62	11 (19%)	61,103,103	1.56	10 (16%)
22	CHD	C	306	-	32,32,32	0.58	0	51,51,51	1.17	5 (9%)
24	DMU	P	311	-	34,34,34	0.49	0	45,45,45	0.76	0
20	EDO	F	103	-	3,3,3	0.47	0	2,2,2	0.33	0
14	HEA	N	601	1	57,67,67	1.54	13 (22%)	61,103,103	1.37	8 (13%)
21	TGL	D	201	-	62,62,62	1.03	3 (4%)	65,65,65	0.90	3 (4%)
20	EDO	S	102	-	3,3,3	0.52	0	2,2,2	0.29	0
20	EDO	H	101	-	3,3,3	0.41	0	2,2,2	0.54	0
20	EDO	R	201	-	3,3,3	0.42	0	2,2,2	0.41	0
20	EDO	A	613	-	3,3,3	0.42	0	2,2,2	0.47	0
20	EDO	R	205	-	3,3,3	0.52	0	2,2,2	0.25	0
23	CUA	O	301	2	0,1,1	-	-	-		
20	EDO	E	206	-	3,3,3	0.45	0	2,2,2	0.39	0
18	AZI	N	606	15	0,2,2	-	-	0,1,1	-	-
20	EDO	A	610	-	3,3,3	0.41	0	2,2,2	0.47	0
20	EDO	A	621	-	3,3,3	0.44	0	2,2,2	0.37	0
24	DMU	C	302	-	34,34,34	0.45	0	45,45,45	0.70	1 (2%)
27	PEK	T	101	-	52,52,52	0.86	2 (3%)	55,57,57	0.86	3 (5%)
24	DMU	Z	102	-	34,34,34	0.46	0	45,45,45	0.68	1 (2%)
20	EDO	N	620	-	3,3,3	0.47	0	2,2,2	0.37	0
22	CHD	B	302	-	32,32,32	0.69	0	51,51,51	0.87	1 (1%)
20	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.30	0
22	CHD	P	301	-	32,32,32	0.66	0	51,51,51	0.88	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	C	319	-	3,3,3	0.51	0	2,2,2	0.19	0
14	HEA	N	602[B]	1,18	57,67,67	1.62	12 (21%)	61,103,103	1.43	7 (11%)
20	EDO	C	315	-	3,3,3	0.42	0	2,2,2	0.63	0
26	CDL	T	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.10	5 (4%)
20	EDO	C	314	-	3,3,3	0.46	0	2,2,2	0.37	0
20	EDO	F	104	-	3,3,3	0.43	0	2,2,2	0.33	0
21	TGL	B	301	-	62,62,62	1.03	3 (4%)	65,65,65	1.07	4 (6%)
20	EDO	N	618	-	3,3,3	0.47	0	2,2,2	0.30	0
20	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.27	0
21	TGL	Y	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.10	4 (6%)
20	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.31	0
20	EDO	N	612	-	3,3,3	0.47	0	2,2,2	0.36	0
19	PGV	A	608	-	50,50,50	0.91	2 (4%)	53,56,56	0.89	3 (5%)
20	EDO	N	613	-	3,3,3	0.40	0	2,2,2	0.47	0
20	EDO	Q	204	-	3,3,3	0.48	0	2,2,2	0.20	0
22	CHD	C	301	-	32,32,32	0.65	0	51,51,51	0.82	1 (1%)
20	EDO	A	620	-	3,3,3	0.37	0	2,2,2	0.71	0
21	TGL	L	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.08	5 (7%)
20	EDO	P	314	-	3,3,3	0.43	0	2,2,2	0.39	0
20	EDO	A	617	-	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	D	203	-	3,3,3	0.47	0	2,2,2	0.12	0
20	EDO	D	204	-	3,3,3	0.50	0	2,2,2	0.25	0
20	EDO	C	317	-	3,3,3	0.48	0	2,2,2	0.31	0
20	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.45	0
20	EDO	S	103	-	3,3,3	0.44	0	2,2,2	0.46	0
20	EDO	E	203	-	3,3,3	0.45	0	2,2,2	0.39	0
20	EDO	E	204	-	3,3,3	0.39	0	2,2,2	0.51	0
20	EDO	A	614	-	3,3,3	0.52	0	2,2,2	1.03	0
20	EDO	O	305	-	3,3,3	0.45	0	2,2,2	0.35	0
26	CDL	P	306	-	99,99,99	1.32	12 (12%)	105,111,111	1.08	5 (4%)
20	EDO	P	313	-	3,3,3	0.53	0	2,2,2	0.23	0
19	PGV	Z	101	-	50,50,50	0.96	2 (4%)	53,56,56	1.10	3 (5%)
18	AZI	N	607	14	0,2,2	-	-	0,1,1	-	-
20	EDO	A	615	-	3,3,3	0.54	0	2,2,2	0.33	0
20	EDO	Q	203	-	3,3,3	0.49	0	2,2,2	0.44	0
14	HEA	A	602[B]	1,18	57,67,67	1.61	12 (21%)	61,103,103	1.45	12 (19%)
20	EDO	Q	202	-	3,3,3	0.43	0	2,2,2	0.42	0
20	EDO	S	104	-	3,3,3	0.39	0	2,2,2	0.51	0
20	EDO	N	619	-	3,3,3	0.44	0	2,2,2	0.41	0
20	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PSC	O	302	-	51,51,51	1.10	3 (5%)	57,59,59	1.01	2 (3%)
20	EDO	E	205	-	3,3,3	0.46	0	2,2,2	0.28	0
20	EDO	U	101	-	3,3,3	0.45	0	2,2,2	0.35	0
24	DMU	P	308	-	34,34,34	0.50	0	45,45,45	0.74	0
20	EDO	V	101	-	3,3,3	0.44	0	2,2,2	0.39	0
20	EDO	G	106	-	3,3,3	0.48	0	2,2,2	0.24	0
19	PGV	P	303	-	50,50,50	0.96	2 (4%)	53,56,56	0.92	2 (3%)
14	HEA	A	602[A]	1,18	57,67,67	1.62	11 (19%)	61,103,103	1.56	14 (22%)
26	CDL	C	305	-	99,99,99	1.31	12 (12%)	105,111,111	1.11	6 (5%)
19	PGV	C	308	-	50,50,50	0.97	2 (4%)	53,56,56	0.97	3 (5%)
20	EDO	G	104	-	3,3,3	0.42	0	2,2,2	0.40	0
27	PEK	C	307	-	52,52,52	0.95	2 (3%)	55,57,57	1.00	2 (3%)
20	EDO	D	206	-	3,3,3	0.41	0	2,2,2	0.45	0
27	PEK	P	302	-	52,52,52	0.95	2 (3%)	55,57,57	0.98	3 (5%)
22	CHD	W	101	-	32,32,32	0.56	0	51,51,51	2.10	15 (29%)
20	EDO	G	105	-	3,3,3	0.53	0	2,2,2	0.21	0
22	CHD	P	307	-	32,32,32	0.59	0	51,51,51	1.36	9 (17%)
19	PGV	C	304	-	50,50,50	0.89	2 (4%)	53,56,56	0.78	3 (5%)
22	CHD	J	101	-	32,32,32	0.58	0	51,51,51	1.21	5 (9%)
20	EDO	O	304	-	3,3,3	0.43	0	2,2,2	0.44	0
24	DMU	C	311	-	34,34,34	0.61	1 (2%)	45,45,45	1.31	8 (17%)
24	DMU	M	101	-	34,34,34	0.45	0	45,45,45	0.67	1 (2%)
20	EDO	W	102	-	3,3,3	0.42	0	2,2,2	0.42	0
24	DMU	C	310	-	34,34,34	0.52	0	45,45,45	1.06	3 (6%)
24	DMU	P	310	-	34,34,34	0.52	0	45,45,45	1.09	2 (4%)
20	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.54	0
19	PGV	A	609	-	50,50,50	0.97	2 (4%)	53,56,56	1.03	2 (3%)
18	AZI	A	607	14	0,2,2	-	-	0,1,1	-	-
20	EDO	C	318	-	3,3,3	0.48	0	2,2,2	0.29	0
20	EDO	N	614	-	3,3,3	0.58	0	2,2,2	0.28	0
21	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.02	3 (4%)
20	EDO	C	316	-	3,3,3	0.47	0	2,2,2	0.32	0
21	TGL	N	609	-	62,62,62	1.02	3 (4%)	65,65,65	1.03	3 (4%)
20	EDO	N	617	-	3,3,3	0.49	0	2,2,2	0.14	0
20	EDO	C	313	-	3,3,3	0.46	0	2,2,2	0.36	0
26	CDL	G	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.07	4 (3%)
20	EDO	R	203	-	3,3,3	0.47	0	2,2,2	0.36	0
20	EDO	R	204	-	3,3,3	0.46	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	P	312	-	3,3,3	0.48	0	2,2,2	0.28	0
23	CUA	B	303	2	0,1,1	-	-	-		
28	PSC	E	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.00	2 (3%)
20	EDO	T	103	-	3,3,3	0.54	0	2,2,2	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	619	-	-	1/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
27	PEK	P	309	-	-	30/56/56/56	-
19	PGV	N	608	-	-	10/55/55/55	-
20	EDO	D	205	-	-	1/1/1/1	-
19	PGV	P	305	-	-	15/55/55/55	-
20	EDO	J	102	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
27	PEK	G	101	-	-	15/56/56/56	-
14	HEA	A	601	1	-	7/32/76/76	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
20	EDO	N	610	-	-	1/1/1/1	-
27	PEK	C	309	-	-	33/56/56/56	-
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
14	HEA	N	602[A]	1,18	-	4/32/76/76	-
22	CHD	C	306	-	-	6/9/74/74	0/4/4/4
24	DMU	P	311	-	-	13/19/59/59	0/2/2/2
20	EDO	F	103	-	-	0/1/1/1	-
14	HEA	N	601	1	-	10/32/76/76	-
21	TGL	D	201	-	-	38/65/65/65	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	R	205	-	-	1/1/1/1	-
20	EDO	E	206	-	-	0/1/1/1	-
20	EDO	A	610	-	-	1/1/1/1	-
20	EDO	A	621	-	-	1/1/1/1	-
24	DMU	C	302	-	-	11/19/59/59	0/2/2/2
27	PEK	T	101	-	-	18/56/56/56	-
24	DMU	Z	102	-	-	7/19/59/59	0/2/2/2
20	EDO	N	620	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	E	202	-	-	0/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	C	319	-	-	1/1/1/1	-
14	HEA	N	602[B]	1,18	-	5/32/76/76	-
20	EDO	C	315	-	-	0/1/1/1	-
26	CDL	T	102	-	-	70/110/110/110	-
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
21	TGL	B	301	-	-	43/65/65/65	-
20	EDO	N	618	-	-	0/1/1/1	-
20	EDO	B	304	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	38/65/65/65	-
20	EDO	A	618	-	-	1/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
19	PGV	A	608	-	-	9/55/55/55	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	Q	204	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	EDO	A	620	-	-	1/1/1/1	-
21	TGL	L	101	-	-	39/65/65/65	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
20	EDO	D	203	-	-	1/1/1/1	-
20	EDO	D	204	-	-	1/1/1/1	-
20	EDO	C	317	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	E	204	-	-	1/1/1/1	-
20	EDO	A	614	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	O	305	-	-	0/1/1/1	-
26	CDL	P	306	-	-	53/110/110/110	-
20	EDO	P	313	-	-	0/1/1/1	-
19	PGV	Z	101	-	-	30/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	-	4/32/76/76	-
20	EDO	Q	202	-	-	0/1/1/1	-
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	N	619	-	-	1/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
28	PSC	O	302	-	-	35/55/55/55	-
20	EDO	E	205	-	-	1/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
24	DMU	P	308	-	-	8/19/59/59	0/2/2/2
20	EDO	V	101	-	-	0/1/1/1	-
20	EDO	G	106	-	-	1/1/1/1	-
19	PGV	P	303	-	-	30/55/55/55	-
14	HEA	A	602[A]	1,18	-	6/32/76/76	-
26	CDL	C	305	-	-	63/110/110/110	-
19	PGV	C	308	-	-	31/55/55/55	-
20	EDO	G	104	-	-	1/1/1/1	-
27	PEK	C	307	-	-	34/56/56/56	-
20	EDO	D	206	-	-	1/1/1/1	-
27	PEK	P	302	-	-	31/56/56/56	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
20	EDO	G	105	-	-	0/1/1/1	-
22	CHD	P	307	-	-	9/9/74/74	0/4/4/4
19	PGV	C	304	-	-	20/55/55/55	-
22	CHD	J	101	-	-	9/9/74/74	0/4/4/4
20	EDO	O	304	-	-	1/1/1/1	-
24	DMU	C	311	-	-	8/19/59/59	0/2/2/2
24	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	EDO	W	102	-	-	1/1/1/1	-
24	DMU	C	310	-	-	6/19/59/59	0/2/2/2
24	DMU	P	310	-	-	9/19/59/59	0/2/2/2
20	EDO	A	612	-	-	0/1/1/1	-
19	PGV	A	609	-	-	26/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
21	TGL	Q	201	-	-	35/65/65/65	-
20	EDO	C	316	-	-	1/1/1/1	-
21	TGL	N	609	-	-	41/65/65/65	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
26	CDL	G	102	-	-	66/110/110/110	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
28	PSC	E	201	-	-	27/55/55/55	-
20	EDO	T	103	-	-	0/1/1/1	-

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	101	TGL	OG2-CB1	4.64	1.47	1.34
26	P	306	CDL	OB8-CB7	4.64	1.46	1.33
26	C	305	CDL	OB8-CB7	4.62	1.46	1.33
19	Z	101	PGV	O03-C19	4.60	1.46	1.33
21	Y	101	TGL	OG3-CC1	4.56	1.46	1.33
26	P	306	CDL	OA8-CA7	4.53	1.46	1.33
26	G	102	CDL	OB8-CB7	4.52	1.46	1.33
27	C	307	PEK	O03-C21	4.52	1.46	1.33
28	E	201	PSC	O01-C1	4.52	1.47	1.34
26	T	102	CDL	OA8-CA7	4.50	1.46	1.33
21	B	301	TGL	OG1-CA1	4.49	1.46	1.33
21	D	201	TGL	OG1-CA1	4.49	1.46	1.33
27	P	309	PEK	O03-C21	4.48	1.46	1.33
21	Y	101	TGL	OG1-CA1	4.48	1.46	1.33
27	C	309	PEK	O03-C21	4.48	1.46	1.33
21	Q	201	TGL	OG1-CA1	4.48	1.46	1.33
19	C	308	PGV	O03-C19	4.46	1.46	1.33
21	L	101	TGL	OG2-CB1	4.45	1.46	1.34
19	A	609	PGV	O03-C19	4.44	1.46	1.33
26	T	102	CDL	OB6-CB5	4.44	1.46	1.34
19	A	609	PGV	O01-C1	4.43	1.46	1.34
19	C	308	PGV	O01-C1	4.42	1.46	1.34
27	P	302	PEK	O01-C1	4.42	1.46	1.34
21	B	301	TGL	OG2-CB1	4.41	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	305	CDL	OA8-CA7	4.40	1.46	1.33
27	C	309	PEK	O01-C1	4.40	1.46	1.34
21	N	609	TGL	OG3-CC1	4.40	1.46	1.33
28	O	302	PSC	O03-C19	4.39	1.46	1.33
26	T	102	CDL	OB8-CB7	4.38	1.46	1.33
21	L	101	TGL	OG3-CC1	4.38	1.46	1.33
19	P	303	PGV	O03-C19	4.38	1.46	1.33
26	G	102	CDL	OB6-CB5	4.38	1.46	1.34
28	E	201	PSC	O03-C19	4.38	1.46	1.33
21	N	609	TGL	OG1-CA1	4.38	1.46	1.33
21	L	101	TGL	OG1-CA1	4.38	1.46	1.33
27	P	302	PEK	O03-C21	4.37	1.46	1.33
21	D	201	TGL	OG2-CB1	4.37	1.46	1.34
21	Q	201	TGL	OG2-CB1	4.36	1.46	1.34
26	G	102	CDL	OA8-CA7	4.36	1.46	1.33
21	Q	201	TGL	OG3-CC1	4.36	1.46	1.33
21	N	609	TGL	OG2-CB1	4.32	1.46	1.34
28	O	302	PSC	O01-C1	4.32	1.46	1.34
27	C	307	PEK	O01-C1	4.31	1.46	1.34
19	P	303	PGV	O01-C1	4.30	1.46	1.34
21	B	301	TGL	OG3-CC1	4.29	1.45	1.33
26	T	102	CDL	OA6-CA5	4.29	1.46	1.34
27	P	309	PEK	O01-C1	4.29	1.46	1.34
26	P	306	CDL	OA6-CA5	4.28	1.46	1.34
19	Z	101	PGV	O01-C1	4.27	1.46	1.34
26	G	102	CDL	OA6-CA5	4.25	1.46	1.34
21	D	201	TGL	OG3-CC1	4.22	1.45	1.33
26	C	305	CDL	OA6-CA5	4.18	1.46	1.34
26	P	306	CDL	OB6-CB5	4.12	1.45	1.34
14	N	602[A]	HEA	CHC-C4B	4.11	1.45	1.35
14	A	602[A]	HEA	CHD-C1D	4.08	1.45	1.35
14	A	602[B]	HEA	CHD-C1D	4.05	1.45	1.35
14	N	601	HEA	CHC-C4B	4.02	1.45	1.35
19	N	608	PGV	O03-C19	4.01	1.45	1.33
14	A	602[A]	HEA	CHC-C4B	4.01	1.45	1.35
27	T	101	PEK	O03-C21	4.00	1.45	1.33
26	C	305	CDL	OB6-CB5	3.96	1.45	1.34
19	A	608	PGV	O03-C19	3.95	1.44	1.33
14	A	601	HEA	CHC-C4B	3.93	1.45	1.35
14	A	601	HEA	CHD-C1D	3.93	1.45	1.35
14	N	602[B]	HEA	CHD-C1D	3.91	1.45	1.35
27	G	101	PEK	O01-C1	3.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[A]	HEA	CHD-C1D	3.89	1.44	1.35
27	G	101	PEK	O03-C21	3.87	1.44	1.33
19	C	304	PGV	O03-C19	3.86	1.44	1.33
14	A	602[A]	HEA	C4D-C3D	-3.85	1.38	1.45
14	A	602[B]	HEA	CHC-C4B	3.84	1.44	1.35
14	N	602[B]	HEA	CHC-C4B	3.82	1.44	1.35
19	P	305	PGV	O03-C19	3.82	1.44	1.33
19	A	608	PGV	O01-C1	3.80	1.45	1.34
14	N	601	HEA	CHD-C1D	3.72	1.44	1.35
19	C	304	PGV	O01-C1	3.70	1.44	1.34
28	E	201	PSC	C13-C12	3.69	1.53	1.31
28	O	302	PSC	C13-C12	3.69	1.53	1.31
14	N	602[A]	HEA	C4D-C3D	-3.68	1.38	1.45
19	P	305	PGV	O01-C1	3.62	1.44	1.34
27	T	101	PEK	O01-C1	3.57	1.44	1.34
14	A	602[B]	HEA	C4D-C3D	-3.54	1.38	1.45
14	N	602[B]	HEA	C4D-C3D	-3.42	1.39	1.45
14	N	602[A]	HEA	C1D-ND	-3.36	1.34	1.40
14	N	602[B]	HEA	FE-ND	3.35	2.13	1.96
19	N	608	PGV	O01-C1	3.35	1.43	1.34
14	N	602[B]	HEA	C4B-NB	-3.32	1.34	1.40
14	A	602[B]	HEA	C4B-C3B	-3.31	1.39	1.44
14	N	602[B]	HEA	C1D-ND	-3.30	1.34	1.40
14	A	602[A]	HEA	C4B-C3B	-3.30	1.39	1.44
14	N	602[A]	HEA	FE-NB	3.26	2.13	1.96
26	C	305	CDL	C62-C61	-3.23	1.33	1.51
26	C	305	CDL	C59-C58	-3.22	1.33	1.51
26	G	102	CDL	C59-C58	-3.22	1.33	1.51
14	N	601	HEA	C1D-ND	-3.22	1.34	1.40
26	P	306	CDL	C22-C21	-3.22	1.33	1.51
14	A	602[A]	HEA	C4B-NB	-3.22	1.34	1.40
26	G	102	CDL	C22-C21	-3.22	1.33	1.51
26	C	305	CDL	C19-C18	-3.21	1.33	1.51
26	G	102	CDL	C19-C18	-3.21	1.33	1.51
26	C	305	CDL	C79-C78	-3.21	1.33	1.51
26	P	306	CDL	C59-C58	-3.21	1.33	1.51
26	T	102	CDL	C22-C21	-3.21	1.33	1.51
26	C	305	CDL	C22-C21	-3.21	1.33	1.51
26	T	102	CDL	C59-C58	-3.20	1.33	1.51
26	G	102	CDL	C62-C61	-3.20	1.33	1.51
26	T	102	CDL	C19-C18	-3.20	1.33	1.51
26	G	102	CDL	C82-C81	-3.19	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[B]	HEA	C1D-ND	-3.19	1.34	1.40
14	A	602[A]	HEA	C1D-ND	-3.19	1.34	1.40
26	T	102	CDL	C82-C81	-3.18	1.33	1.51
14	N	602[B]	HEA	C4B-C3B	-3.18	1.39	1.44
26	P	306	CDL	C19-C18	-3.18	1.33	1.51
26	T	102	CDL	C79-C78	-3.18	1.33	1.51
26	P	306	CDL	C79-C78	-3.18	1.33	1.51
26	T	102	CDL	C62-C61	-3.18	1.33	1.51
26	G	102	CDL	C42-C41	-3.17	1.33	1.51
26	T	102	CDL	C42-C41	-3.17	1.33	1.51
14	N	601	HEA	C4B-NB	-3.17	1.34	1.40
26	C	305	CDL	C42-C41	-3.17	1.33	1.51
14	A	602[B]	HEA	C4B-NB	-3.17	1.34	1.40
14	N	602[B]	HEA	FE-NB	3.17	2.12	1.96
26	P	306	CDL	C42-C41	-3.16	1.33	1.51
26	G	102	CDL	C79-C78	-3.16	1.33	1.51
26	G	102	CDL	C39-C38	-3.16	1.33	1.51
26	P	306	CDL	C62-C61	-3.16	1.33	1.51
14	A	602[B]	HEA	FE-ND	3.16	2.12	1.96
26	C	305	CDL	C82-C81	-3.16	1.33	1.51
26	P	306	CDL	C82-C81	-3.15	1.33	1.51
26	T	102	CDL	C39-C38	-3.15	1.33	1.51
14	A	601	HEA	C1D-ND	-3.14	1.34	1.40
26	C	305	CDL	C39-C38	-3.13	1.34	1.51
26	P	306	CDL	C39-C38	-3.10	1.34	1.51
14	A	602[A]	HEA	FE-NB	3.10	2.12	1.96
14	N	602[A]	HEA	C4B-NB	-3.08	1.35	1.40
14	N	602[A]	HEA	C4B-C3B	-3.04	1.39	1.44
14	A	602[B]	HEA	FE-NB	3.01	2.11	1.96
14	A	601	HEA	C4D-C3D	-2.97	1.39	1.45
14	N	601	HEA	C4D-C3D	-2.93	1.40	1.45
14	N	601	HEA	C1B-C2B	-2.82	1.39	1.44
14	A	601	HEA	C4B-NB	-2.81	1.35	1.40
14	A	601	HEA	C4B-C3B	-2.74	1.40	1.44
14	N	602[A]	HEA	C1B-C2B	-2.72	1.39	1.44
14	N	602[B]	HEA	C1B-C2B	-2.71	1.39	1.44
14	N	601	HEA	C1D-C2D	-2.68	1.39	1.44
14	A	602[A]	HEA	C1D-C2D	-2.62	1.39	1.44
14	N	602[A]	HEA	C1D-C2D	-2.59	1.39	1.44
14	A	602[A]	HEA	C1B-C2B	-2.59	1.39	1.44
14	A	601	HEA	C1D-C2D	-2.56	1.39	1.44
14	N	602[A]	HEA	FE-ND	2.54	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	C1B-NB	-2.40	1.33	1.38
14	A	602[B]	HEA	C1D-C2D	-2.38	1.40	1.44
14	A	601	HEA	C1B-C2B	-2.37	1.40	1.44
14	N	601	HEA	C4B-C3B	-2.35	1.40	1.44
14	A	602[A]	HEA	C4D-ND	-2.34	1.34	1.38
14	A	602[A]	HEA	FE-ND	2.34	2.08	1.96
14	N	601	HEA	FE-NB	2.30	2.08	1.96
24	C	311	DMU	O16-C6	2.29	1.44	1.40
14	A	601	HEA	FE-ND	2.27	2.08	1.96
14	A	602[B]	HEA	C1B-C2B	-2.20	1.40	1.44
14	A	602[B]	HEA	C1B-NB	-2.20	1.34	1.38
14	A	602[B]	HEA	C4D-ND	-2.19	1.34	1.38
14	N	601	HEA	O11-C11	2.19	1.47	1.42
14	N	602[B]	HEA	C4D-ND	-2.18	1.34	1.38
14	A	601	HEA	C4D-ND	-2.17	1.34	1.38
14	A	601	HEA	C1B-NB	-2.16	1.34	1.38
14	N	601	HEA	C4D-ND	-2.16	1.34	1.38
14	N	602[A]	HEA	C4D-ND	-2.16	1.34	1.38
14	N	602[B]	HEA	C1D-C2D	-2.14	1.40	1.44
14	N	602[B]	HEA	C1B-NB	-2.11	1.34	1.38
14	A	601	HEA	FE-NB	2.10	2.07	1.96
14	N	601	HEA	FE-ND	2.09	2.07	1.96

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	101	CHD	C14-C8-C7	5.82	119.52	111.81
22	W	101	CHD	C6-C5-C4	-5.27	105.12	111.19
14	N	602[A]	HEA	CAD-CBD-CGD	-5.05	102.74	113.60
14	N	602[A]	HEA	OMA-CMA-C3A	-5.02	113.98	124.91
21	Y	101	TGL	OG2-CB1-CB2	4.79	121.83	111.50
19	Z	101	PGV	O01-C1-C2	4.78	121.80	111.50
27	P	302	PEK	O01-C1-C2	4.74	121.71	111.50
27	C	309	PEK	O01-C1-C2	4.73	121.70	111.50
21	L	101	TGL	OG2-CB1-CB2	4.67	121.56	111.50
19	A	609	PGV	O01-C1-C2	4.65	121.52	111.50
14	N	602[B]	HEA	OMA-CMA-C3A	-4.61	114.87	124.91
21	B	301	TGL	OG2-CB1-CB2	4.54	121.28	111.50
14	A	602[A]	HEA	OMA-CMA-C3A	-4.53	115.03	124.91
27	C	307	PEK	O01-C1-C2	4.40	120.99	111.50
26	T	102	CDL	OB6-CB5-C51	4.39	120.96	111.50
28	E	201	PSC	O01-C1-C2	4.33	120.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	Q	201	TGL	OG2-CB1-CB2	4.29	120.75	111.50
26	C	305	CDL	OA6-CA5-C11	4.26	120.67	111.50
21	N	609	TGL	OG2-CB1-CB2	4.23	120.62	111.50
24	C	311	DMU	C10-O1-C9	4.20	121.92	113.69
28	O	302	PSC	O01-C1-C2	4.18	120.51	111.50
22	W	101	CHD	C14-C8-C9	-4.12	104.05	109.71
19	C	308	PGV	O01-C1-C2	4.04	120.21	111.50
26	G	102	CDL	OB6-CB5-C51	4.01	120.15	111.50
26	G	102	CDL	OA6-CA5-C11	4.01	120.14	111.50
26	T	102	CDL	OA6-CA5-C11	3.98	120.08	111.50
14	N	601	HEA	C27-C19-C20	3.95	121.92	115.27
27	P	309	PEK	O01-C1-C2	3.89	119.88	111.50
26	P	306	CDL	OB6-CB5-C51	3.84	119.78	111.50
24	P	310	DMU	O7-C10-C5	3.82	118.00	108.10
22	W	101	CHD	C1-C10-C5	3.82	113.41	107.77
26	P	306	CDL	OA6-CA5-C11	3.82	119.72	111.50
14	A	602[A]	HEA	C13-C12-C11	-3.78	108.67	114.35
14	A	602[B]	HEA	C27-C19-C20	3.63	121.38	115.27
22	W	101	CHD	C11-C9-C10	3.56	117.40	113.73
14	A	601	HEA	C27-C19-C20	3.54	121.23	115.27
19	A	608	PGV	O03-C19-C20	3.43	122.67	111.91
22	W	101	CHD	C13-C17-C20	3.42	123.58	119.50
19	N	608	PGV	O03-C19-C20	3.40	122.59	111.91
14	A	602[B]	HEA	CMB-C2B-C3B	-3.32	124.02	130.34
19	P	303	PGV	O01-C1-C2	3.31	118.63	111.50
14	A	602[A]	HEA	CAD-CBD-CGD	-3.30	106.50	113.60
14	A	602[B]	HEA	OMA-CMA-C3A	-3.29	117.73	124.91
24	C	310	DMU	O7-C10-C5	3.29	116.61	108.10
24	C	311	DMU	O1-C9-C8	3.28	115.65	109.69
26	C	305	CDL	CB4-OB6-CB5	-3.23	109.85	117.79
14	A	601	HEA	C13-C12-C11	-3.20	109.55	114.35
19	Z	101	PGV	O03-C19-C20	3.18	121.88	111.91
14	N	602[A]	HEA	CAA-CBA-CGA	-3.16	104.91	113.76
19	P	303	PGV	O03-C19-C20	3.14	121.77	111.91
14	A	601	HEA	C4A-CHB-C1B	3.12	126.68	122.56
21	Y	101	TGL	OG1-CA1-CA2	3.10	121.64	111.91
14	N	601	HEA	CBA-CAA-C2A	3.10	117.83	112.60
26	T	102	CDL	OA8-CA7-C31	3.08	121.57	111.91
22	W	101	CHD	C4-C5-C10	3.08	115.92	112.66
22	J	101	CHD	C21-C20-C22	-3.07	105.55	110.36
22	W	101	CHD	C10-C9-C8	3.07	115.12	111.82
27	T	101	PEK	O03-C21-C22	3.07	121.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	301	TGL	OG3-CC1-CC2	3.06	121.51	111.91
21	D	201	TGL	OG2-CB1-CB2	3.04	118.05	111.50
19	A	608	PGV	O03-C19-O04	-3.00	116.03	123.59
26	C	305	CDL	OB6-CB5-C51	2.98	117.93	111.50
14	A	602[A]	HEA	CHA-C4D-ND	2.97	127.65	124.43
21	N	609	TGL	OG3-CC1-CC2	2.96	121.19	111.91
24	C	310	DMU	O16-C6-C1	2.95	112.91	108.30
19	A	609	PGV	O03-C19-C20	2.95	121.16	111.91
14	N	601	HEA	C4A-CHB-C1B	2.95	126.45	122.56
14	N	602[B]	HEA	CAA-CBA-CGA	-2.92	105.58	113.76
14	N	602[B]	HEA	C27-C19-C20	2.90	120.15	115.27
26	P	306	CDL	OB8-CB7-C71	2.90	121.01	111.91
21	N	609	TGL	OG1-CA1-CA2	2.90	121.01	111.91
19	C	308	PGV	O03-C19-C20	2.89	120.98	111.91
28	E	201	PSC	O03-C19-C20	2.86	120.89	111.91
24	C	311	DMU	C6-C1-C2	2.85	115.93	110.00
28	O	302	PSC	O03-C19-C20	2.84	120.81	111.91
21	Q	201	TGL	OG3-CC1-CC2	2.81	120.72	111.91
22	P	307	CHD	C17-C13-C12	-2.81	115.11	117.67
14	A	602[A]	HEA	C26-C15-C16	2.78	119.94	115.27
21	Q	201	TGL	OG1-CA1-CA2	2.77	120.60	111.91
19	N	608	PGV	O03-C19-O04	-2.77	116.60	123.59
21	L	101	TGL	OG1-CA1-CA2	2.77	120.58	111.91
14	N	602[B]	HEA	CMB-C2B-C3B	-2.76	125.08	130.34
14	A	601	HEA	CBA-CAA-C2A	2.73	117.21	112.60
22	W	101	CHD	C22-C20-C17	2.71	115.88	110.28
26	P	306	CDL	OA8-CA7-C31	2.70	120.39	111.91
27	G	101	PEK	O01-C1-C2	2.70	117.32	111.50
21	L	101	TGL	OG3-CC1-CC2	2.67	120.28	111.91
24	P	310	DMU	O16-C6-C1	2.66	112.46	108.30
22	W	101	CHD	C23-C22-C20	-2.66	109.66	114.52
22	W	101	CHD	C19-C10-C1	-2.66	103.98	108.26
22	P	307	CHD	C23-C22-C20	-2.65	109.68	114.52
27	C	307	PEK	O03-C21-C22	2.65	120.22	111.91
26	C	305	CDL	OB8-CB7-C71	2.65	120.21	111.91
14	A	602[B]	HEA	CMB-C2B-C1B	2.64	129.06	125.04
14	A	601	HEA	O2A-CGA-CBA	2.63	122.49	114.03
14	A	601	HEA	O1A-CGA-CBA	-2.63	114.63	123.08
26	G	102	CDL	OA8-CA7-C31	2.62	120.14	111.91
22	P	307	CHD	C13-C17-C20	-2.59	116.40	119.50
22	W	101	CHD	C16-C17-C13	2.59	106.10	103.55
26	G	102	CDL	OB8-CB7-C71	2.59	120.03	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[A]	HEA	C26-C15-C16	2.59	119.62	115.27
22	W	101	CHD	C15-C14-C8	2.58	121.94	118.33
27	C	309	PEK	O03-C21-C22	2.58	119.99	111.91
21	L	101	TGL	OG2-CB1-OB1	-2.57	117.50	123.70
26	C	305	CDL	OA8-CA7-C31	2.55	119.91	111.91
14	A	602[A]	HEA	CAA-CBA-CGA	-2.55	106.62	113.76
14	A	602[A]	HEA	CAD-C3D-C2D	2.53	132.59	127.88
24	C	311	DMU	O16-C6-C1	2.53	112.25	108.30
14	N	602[A]	HEA	C4B-NB-C1B	2.51	107.66	105.07
14	N	601	HEA	O2A-CGA-CBA	2.49	122.05	114.03
26	T	102	CDL	OB8-CB7-C71	2.47	119.67	111.91
27	P	302	PEK	O03-C21-C22	2.47	119.66	111.91
22	G	103	CHD	C11-C9-C8	2.47	114.49	110.88
21	B	301	TGL	OG1-CA1-CA2	2.46	119.64	111.91
21	Y	101	TGL	OG3-CC1-CC2	2.46	119.63	111.91
22	W	101	CHD	C18-C13-C12	-2.45	106.57	109.07
27	T	101	PEK	O01-C1-C2	2.45	116.78	111.50
22	J	101	CHD	C1-C10-C5	2.45	111.39	107.77
22	P	307	CHD	C6-C7-C8	2.45	114.09	111.48
14	A	602[B]	HEA	C4A-CHB-C1B	2.44	125.78	122.56
21	D	201	TGL	OG1-CA1-CA2	2.42	119.51	111.91
14	A	602[B]	HEA	CAD-CBD-CGD	-2.42	108.39	113.60
14	A	602[B]	HEA	C26-C15-C16	2.39	119.29	115.27
19	C	304	PGV	O03-C19-O04	-2.39	117.56	123.59
22	P	307	CHD	C14-C13-C12	2.36	109.60	107.40
27	P	309	PEK	O03-C21-C22	2.36	119.30	111.91
24	C	311	DMU	C1-C2-C3	2.35	115.06	109.68
21	Y	101	TGL	OG2-CB1-OB1	-2.35	118.02	123.70
14	N	602[A]	HEA	C13-C12-C11	-2.35	110.81	114.35
14	A	602[A]	HEA	CMB-C2B-C3B	-2.35	125.86	130.34
22	J	101	CHD	C21-C20-C17	2.34	116.51	112.92
24	C	311	DMU	C7-C8-C9	2.34	114.41	110.24
14	A	602[B]	HEA	C13-C12-C11	-2.32	110.86	114.35
21	D	201	TGL	OG3-CC1-CC2	2.32	119.18	111.91
14	N	601	HEA	C13-C12-C11	-2.30	110.89	114.35
22	P	307	CHD	C15-C14-C8	2.28	121.52	118.33
21	B	301	TGL	OG3-CC1-OC1	-2.28	117.85	123.59
14	A	602[A]	HEA	CMB-C2B-C1B	2.27	128.50	125.04
14	A	601	HEA	CAA-CBA-CGA	-2.27	107.41	113.76
14	N	601	HEA	CAA-CBA-CGA	-2.26	107.41	113.76
24	M	101	DMU	C18-O16-C6	-2.25	110.12	113.84
14	A	601	HEA	CMC-C2C-C1C	-2.24	125.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	602[B]	HEA	C17-C18-C19	-2.24	122.26	127.66
19	C	304	PGV	O01-C1-C2	2.24	116.32	111.50
26	P	306	CDL	CB4-OB6-CB5	-2.24	112.28	117.79
14	A	601	HEA	OMA-CMA-C3A	-2.23	120.04	124.91
19	A	608	PGV	O01-C1-C2	2.23	116.32	111.50
22	J	101	CHD	C15-C14-C13	2.23	105.74	103.55
14	N	602[B]	HEA	CMB-C2B-C1B	2.23	128.43	125.04
24	C	311	DMU	O1-C9-C11	2.23	111.97	106.44
22	C	306	CHD	C23-C22-C20	-2.22	110.46	114.52
19	C	304	PGV	O03-C19-C20	2.21	118.83	111.91
24	C	311	DMU	O5-C4-C57	2.20	111.89	106.44
14	A	602[A]	HEA	C1D-ND-C4D	2.19	107.34	105.07
14	A	602[B]	HEA	CAA-CBA-CGA	-2.19	107.62	113.76
14	A	602[A]	HEA	C27-C19-C20	2.19	118.95	115.27
22	C	306	CHD	C15-C14-C13	2.19	105.70	103.55
14	A	601	HEA	CMC-C2C-C3C	2.18	128.76	124.68
27	T	101	PEK	O01-C1-O02	-2.18	118.44	123.70
22	P	307	CHD	C15-C14-C13	2.18	105.69	103.55
14	N	602[A]	HEA	C27-C19-C20	2.18	118.93	115.27
27	C	309	PEK	O01-C1-O02	-2.16	118.47	123.70
21	L	101	TGL	OG3-CC1-OC1	-2.16	118.14	123.59
26	C	305	CDL	OA6-CA5-OA7	-2.16	118.49	123.70
22	B	302	CHD	C15-C14-C13	2.15	105.66	103.55
24	Z	102	DMU	C10-O7-C3	-2.15	112.64	117.96
22	P	307	CHD	C19-C10-C1	-2.15	104.80	108.26
14	A	602[B]	HEA	C4B-NB-C1B	2.12	107.26	105.07
22	C	306	CHD	C6-C7-C8	2.11	113.74	111.48
14	A	602[B]	HEA	CAD-C3D-C2D	2.11	131.80	127.88
14	N	602[B]	HEA	CAD-CBD-CGD	-2.11	109.07	113.60
14	N	602[A]	HEA	CBD-CAD-C3D	2.10	118.46	112.63
14	N	602[B]	HEA	C26-C15-C16	2.09	118.79	115.27
14	N	602[A]	HEA	C25-C23-C24	2.08	119.20	114.60
22	C	306	CHD	C4-C5-C10	2.07	114.86	112.66
26	T	102	CDL	OA8-CA7-OA9	-2.07	118.38	123.59
14	N	602[A]	HEA	C13-C14-C15	-2.07	122.69	127.66
24	C	310	DMU	C18-O16-C6	-2.06	110.42	113.84
14	N	601	HEA	O1A-CGA-CBA	-2.06	116.46	123.08
22	P	307	CHD	C16-C17-C20	2.06	115.33	112.15
22	P	301	CHD	C19-C10-C1	-2.06	104.95	108.26
14	A	602[A]	HEA	CAD-C3D-C4D	-2.04	121.09	124.66
19	C	308	PGV	O03-C19-O04	-2.04	118.44	123.59
14	A	602[A]	HEA	CHA-C4D-C3D	-2.03	121.86	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3C-C4C-NC	2.03	111.83	109.21
19	Z	101	PGV	O01-C1-O02	-2.02	118.82	123.70
22	C	306	CHD	C19-C10-C1	-2.01	105.02	108.26
24	C	302	DMU	C18-O16-C6	-2.01	110.50	113.84
22	J	101	CHD	C6-C5-C4	-2.01	108.88	111.19
14	A	602[A]	HEA	C25-C23-C24	2.01	119.04	114.60
27	P	302	PEK	O01-C1-O02	-2.01	118.85	123.70
22	C	301	CHD	C15-C14-C13	2.01	105.52	103.55
22	W	101	CHD	C14-C13-C12	2.01	109.27	107.40

There are no chirality outliers.

All (1052) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	602[B]	HEA	C2D-C3D-CAD-CBD
19	A	609	PGV	C03-O11-P-O12
19	A	609	PGV	C03-O11-P-O13
19	A	609	PGV	C03-O11-P-O14
19	A	609	PGV	C04-C05-C06-O06
19	A	609	PGV	C2-C1-O01-C02
19	C	304	PGV	C10-C11-C12-C13
19	C	308	PGV	C03-O11-P-O13
19	C	308	PGV	C2-C1-O01-C02
19	P	303	PGV	C02-C03-O11-P
19	Z	101	PGV	C03-O11-P-O12
19	Z	101	PGV	C04-C05-C06-O06
19	Z	101	PGV	O02-C1-O01-C02
21	B	301	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	CB2-CB1-OG2-CG2
21	Y	101	TGL	OB1-CB1-OG2-CG2
22	J	101	CHD	C13-C17-C20-C21
22	P	307	CHD	C20-C22-C23-C24
24	C	302	DMU	C19-C18-O16-C6
24	C	311	DMU	O5-C6-O16-C18
24	P	310	DMU	C5-C10-O7-C3
24	P	311	DMU	C1-C6-O16-C18
24	P	311	DMU	O5-C6-O16-C18
26	C	305	CDL	O1-C1-CB2-OB2
26	C	305	CDL	C1-CA2-OA2-PA1
26	C	305	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	CB3-OB5-PB2-OB3
26	C	305	CDL	CB3-OB5-PB2-OB4
26	C	305	CDL	OB7-CB5-OB6-CB4
26	C	305	CDL	C51-CB5-OB6-CB4
26	G	102	CDL	CA3-OA5-PA1-OA2
26	G	102	CDL	C11-CA5-OA6-CA4
26	G	102	CDL	CB2-OB2-PB2-OB3
26	G	102	CDL	CB3-OB5-PB2-OB3
26	G	102	CDL	OB6-CB4-CB6-OB8
26	P	306	CDL	CA3-OA5-PA1-OA3
26	T	102	CDL	CA2-OA2-PA1-OA3
26	T	102	CDL	CA3-OA5-PA1-OA4
26	T	102	CDL	CB2-OB2-PB2-OB3
26	T	102	CDL	CB2-OB2-PB2-OB5
26	T	102	CDL	CB3-OB5-PB2-OB2
26	T	102	CDL	CB3-OB5-PB2-OB3
27	C	307	PEK	C03-O11-P-O12
27	C	307	PEK	C03-O11-P-O13
27	C	307	PEK	C03-O11-P-O14
27	C	307	PEK	O12-C04-C05-N
27	C	307	PEK	C2-C1-O01-C02
27	C	307	PEK	C4-C5-C6-C7
27	C	307	PEK	C12-C13-C14-C15
27	C	309	PEK	O12-C04-C05-N
27	C	309	PEK	O02-C1-O01-C02
27	C	309	PEK	C2-C1-O01-C02
27	C	309	PEK	C9-C10-C11-C12
27	C	309	PEK	C12-C13-C14-C15
27	P	302	PEK	C03-O11-P-O13
27	P	302	PEK	C04-O12-P-O13
27	P	302	PEK	C2-C1-O01-C02
27	P	309	PEK	C03-O11-P-O14
27	P	309	PEK	C2-C1-O01-C02
27	P	309	PEK	C4-C5-C6-C7
27	P	309	PEK	C7-C8-C9-C10
27	T	101	PEK	C11-C10-C9-C8
27	T	101	PEK	C11-C12-C13-C14
28	E	201	PSC	C03-O11-P-O13
28	E	201	PSC	O12-C04-C05-N
28	E	201	PSC	C2-C1-O01-C02
28	O	302	PSC	C03-O11-P-O12
28	O	302	PSC	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
28	O	302	PSC	C04-O12-P-O14
28	O	302	PSC	O12-C04-C05-N
28	O	302	PSC	C2-C1-O01-C02
28	O	302	PSC	C11-C12-C13-C14
19	Z	101	PGV	O04-C19-O03-C01
21	Y	101	TGL	CG2-CG1-OG1-CA1
24	C	310	DMU	C5-C10-O7-C3
19	Z	101	PGV	C20-C19-O03-C01
21	B	301	TGL	OC1-CC1-OG3-CG3
21	D	201	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	OC1-CC1-OG3-CG3
21	Y	101	TGL	OA1-CA1-OG1-CG1
26	T	102	CDL	OA9-CA7-OA8-CA6
28	E	201	PSC	O04-C19-O03-C01
28	O	302	PSC	O04-C19-O03-C01
19	A	609	PGV	O02-C1-O01-C02
19	C	308	PGV	O02-C1-O01-C02
21	B	301	TGL	OB1-CB1-OG2-CG2
26	C	305	CDL	OA7-CA5-OA6-CA4
27	C	307	PEK	O02-C1-O01-C02
27	P	302	PEK	O02-C1-O01-C02
27	P	309	PEK	O02-C1-O01-C02
28	O	302	PSC	O02-C1-O01-C02
21	N	609	TGL	OC1-CC1-OG3-CG3
19	A	609	PGV	C20-C19-O03-C01
21	B	301	TGL	CC2-CC1-OG3-CG3
21	N	609	TGL	CA2-CA1-OG1-CG1
21	Q	201	TGL	CC2-CC1-OG3-CG3
21	Y	101	TGL	CA2-CA1-OG1-CG1
26	T	102	CDL	C31-CA7-OA8-CA6
28	E	201	PSC	C20-C19-O03-C01
28	O	302	PSC	C20-C19-O03-C01
19	Z	101	PGV	C2-C1-O01-C02
21	L	101	TGL	CB2-CB1-OG2-CG2
22	J	101	CHD	C16-C17-C20-C22
22	J	101	CHD	C13-C17-C20-C22
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	N	601	HEA	C27-C19-C20-C21
22	J	101	CHD	C20-C22-C23-C24
21	D	201	TGL	CC2-CC1-OG3-CG3
21	L	101	TGL	CA2-CA1-OG1-CG1
21	N	609	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
26	G	102	CDL	C31-CA7-OA8-CA6
26	T	102	CDL	C71-CB7-OB8-CB6
27	P	302	PEK	C22-C21-O03-C01
24	P	311	DMU	O5-C4-C57-O61
19	C	308	PGV	C10-C11-C12-C13
27	C	307	PEK	C7-C8-C9-C10
27	G	101	PEK	C10-C11-C12-C13
27	G	101	PEK	C13-C14-C15-C16
27	T	101	PEK	C4-C5-C6-C7
27	T	101	PEK	C13-C14-C15-C16
14	N	602[B]	HEA	C4D-C3D-CAD-CBD
26	G	102	CDL	OA7-CA5-OA6-CA4
28	E	201	PSC	O02-C1-O01-C02
19	A	609	PGV	O04-C19-O03-C01
21	L	101	TGL	OA1-CA1-OG1-CG1
26	T	102	CDL	OB9-CB7-OB8-CB6
21	D	201	TGL	CG2-CG1-OG1-CA1
21	N	609	TGL	OA1-CA1-OG1-CG1
21	N	609	TGL	CB2-CB1-OG2-CG2
27	P	302	PEK	O04-C21-O03-C01
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
24	P	310	DMU	O6-C11-C9-O1
24	P	311	DMU	O6-C11-C9-O1
24	P	311	DMU	C3-C4-C57-O61
19	A	609	PGV	C02-C03-O11-P
26	G	102	CDL	OA9-CA7-OA8-CA6
24	C	302	DMU	O6-C11-C9-O1
24	C	311	DMU	O5-C4-C57-O61
22	C	306	CHD	C17-C20-C22-C23
22	J	101	CHD	C17-C20-C22-C23
22	P	307	CHD	C17-C20-C22-C23
27	C	309	PEK	C13-C14-C15-C16
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
26	P	306	CDL	C51-CB5-OB6-CB4
26	G	102	CDL	CB2-C1-CA2-OA2
21	N	609	TGL	OB1-CB1-OG2-CG2
22	P	307	CHD	C21-C20-C22-C23
19	C	308	PGV	C20-C19-O03-C01
21	B	301	TGL	CA2-CA1-OG1-CG1
24	C	302	DMU	O6-C11-C9-C8
24	C	311	DMU	C3-C4-C57-O61
22	W	101	CHD	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
21	N	609	TGL	CA1-CA2-CA3-CA4
22	J	101	CHD	C21-C20-C22-C23
24	C	311	DMU	C1-C6-O16-C18
19	P	303	PGV	O03-C01-C02-O01
21	B	301	TGL	OA1-CA1-OG1-CG1
14	N	601	HEA	C18-C19-C20-C21
21	Q	201	TGL	CB2-CB1-OG2-CG2
26	T	102	CDL	CB7-C71-C72-C73
19	C	308	PGV	O04-C19-O03-C01
24	P	310	DMU	O6-C11-C9-C8
24	P	311	DMU	O6-C11-C9-C8
26	C	305	CDL	C31-CA7-OA8-CA6
26	P	306	CDL	C71-CB7-OB8-CB6
21	B	301	TGL	CA1-CA2-CA3-CA4
21	D	201	TGL	CB1-CB2-CB3-CB4
21	N	609	TGL	CC1-CC2-CC3-CC4
27	P	309	PEK	C1-C2-C3-C4
27	C	307	PEK	C10-C11-C12-C13
27	G	101	PEK	C7-C8-C9-C10
27	T	101	PEK	C7-C8-C9-C10
28	E	201	PSC	C11-C10-C9-C8
19	C	308	PGV	O05-C05-C06-O06
19	Z	101	PGV	O05-C05-C06-O06
19	C	304	PGV	C19-C20-C21-C22
19	Z	101	PGV	C19-C20-C21-C22
21	B	301	TGL	CB1-CB2-CB3-CB4
21	D	201	TGL	CA1-CA2-CA3-CA4
21	Q	201	TGL	CB1-CB2-CB3-CB4
21	Q	201	TGL	CC1-CC2-CC3-CC4
21	Y	101	TGL	CB1-CB2-CB3-CB4
26	C	305	CDL	CA7-C31-C32-C33
26	C	305	CDL	CB5-C51-C52-C53
26	G	102	CDL	CA5-C11-C12-C13
26	P	306	CDL	OB7-CB5-OB6-CB4
22	C	306	CHD	C21-C20-C22-C23
20	A	621	EDO	O1-C1-C2-O2
20	C	319	EDO	O1-C1-C2-O2
20	U	101	EDO	O1-C1-C2-O2
22	W	101	CHD	C16-C17-C20-C22
24	C	311	DMU	O16-C18-C19-C22
28	E	201	PSC	C1-C2-C3-C4
24	Z	102	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
26	G	102	CDL	O1-C1-CA2-OA2
19	P	305	PGV	C10-C11-C12-C13
19	Z	101	PGV	C10-C11-C12-C13
27	C	309	PEK	C10-C11-C12-C13
27	P	302	PEK	C10-C11-C12-C13
24	Z	102	DMU	O6-C11-C9-C8
26	P	306	CDL	OB9-CB7-OB8-CB6
19	C	308	PGV	C03-O11-P-O12
19	P	303	PGV	C03-O11-P-O12
26	C	305	CDL	CA3-OA5-PA1-OA2
26	C	305	CDL	CB3-OB5-PB2-OB2
26	T	102	CDL	CA2-OA2-PA1-OA5
27	C	309	PEK	C03-O11-P-O12
27	P	302	PEK	C03-O11-P-O12
27	P	302	PEK	C04-O12-P-O11
27	P	309	PEK	C04-O12-P-O11
28	E	201	PSC	C03-O11-P-O12
22	W	101	CHD	C16-C17-C20-C21
26	C	305	CDL	CA2-C1-CB2-OB2
21	Q	201	TGL	OB1-CB1-OG2-CG2
24	P	308	DMU	O16-C18-C19-C22
28	O	302	PSC	C29-C30-C31-C32
22	C	306	CHD	C20-C22-C23-C24
27	C	309	PEK	C22-C21-O03-C01
27	C	307	PEK	C2-C3-C4-C5
27	T	101	PEK	C1-C2-C3-C4
21	D	201	TGL	C11-C10-CB9-CB8
21	N	609	TGL	CB7-CB8-CB9-C10
21	Q	201	TGL	C10-C11-C12-C13
26	G	102	CDL	C42-C43-C44-C45
27	G	101	PEK	C24-C25-C26-C27
19	N	608	PGV	C23-C24-C25-C26
21	D	201	TGL	C24-C25-C26-C27
21	L	101	TGL	C21-C20-CA9-CA8
21	L	101	TGL	C21-C22-C23-C24
21	N	609	TGL	C11-C10-CB9-CB8
21	N	609	TGL	CB9-C10-C11-C12
21	N	609	TGL	C14-C29-C30-C31
21	Q	201	TGL	C12-C13-C14-C29
24	M	101	DMU	C19-C22-C25-C28
26	C	305	CDL	C11-C12-C13-C14
26	C	305	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C63-C64-C65-C66
26	C	305	CDL	C72-C73-C74-C75
26	G	102	CDL	C20-C21-C22-C23
26	G	102	CDL	C72-C73-C74-C75
26	P	306	CDL	C19-C20-C21-C22
26	P	306	CDL	C40-C41-C42-C43
28	E	201	PSC	C22-C23-C24-C25
19	P	303	PGV	C6-C7-C8-C9
19	Z	101	PGV	C24-C25-C26-C27
21	B	301	TGL	CA4-CA5-CA6-CA7
21	B	301	TGL	C13-C14-C29-C30
21	L	101	TGL	C12-C13-C14-C29
21	Y	101	TGL	C21-C20-CA9-CA8
21	Y	101	TGL	CB2-CB3-CB4-CB5
21	Y	101	TGL	CB6-CB7-CB8-CB9
21	Y	101	TGL	CC7-CC8-CC9-C15
26	C	305	CDL	C77-C78-C79-C80
27	C	309	PEK	C24-C25-C26-C27
28	E	201	PSC	C23-C24-C25-C26
21	D	201	TGL	C19-C33-C34-C35
21	L	101	TGL	C22-C23-C24-C25
21	N	609	TGL	C10-C11-C12-C13
21	Y	101	TGL	CC3-CC4-CC5-CC6
24	P	310	DMU	C25-C28-C31-C34
26	T	102	CDL	C52-C53-C54-C55
27	C	309	PEK	C23-C24-C25-C26
19	C	304	PGV	C14-C15-C16-C17
19	C	308	PGV	C26-C27-C28-C29
21	L	101	TGL	C18-C19-C33-C34
21	N	609	TGL	CA5-CA6-CA7-CA8
21	Q	201	TGL	CA6-CA7-CA8-CA9
21	Q	201	TGL	C13-C14-C29-C30
21	Y	101	TGL	C23-C24-C25-C26
26	C	305	CDL	C21-C22-C23-C24
26	G	102	CDL	C63-C64-C65-C66
28	O	302	PSC	C2-C3-C4-C5
26	P	306	CDL	C73-C74-C75-C76
28	O	302	PSC	C1-C2-C3-C4
26	P	306	CDL	C31-CA7-OA8-CA6
19	A	608	PGV	C30-C31-C32-C33
19	P	303	PGV	C24-C25-C26-C27
21	L	101	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CC9-C15-C16-C17
21	Q	201	TGL	C19-C33-C34-C35
21	Y	101	TGL	CA9-C20-C21-C22
24	C	302	DMU	C31-C34-C37-C40
26	C	305	CDL	C53-C54-C55-C56
26	C	305	CDL	C73-C74-C75-C76
26	T	102	CDL	C61-C62-C63-C64
26	C	305	CDL	OA9-CA7-OA8-CA6
27	C	309	PEK	O04-C21-O03-C01
19	A	608	PGV	C28-C29-C30-C31
19	C	304	PGV	C13-C14-C15-C16
19	C	304	PGV	C22-C23-C24-C25
19	P	303	PGV	C2-C3-C4-C5
19	P	305	PGV	C24-C25-C26-C27
21	B	301	TGL	C21-C20-CA9-CA8
21	D	201	TGL	C10-C11-C12-C13
21	D	201	TGL	CC9-C15-C16-C17
21	L	101	TGL	CB5-CB6-CB7-CB8
21	N	609	TGL	C22-C23-C24-C25
21	Q	201	TGL	CB9-C10-C11-C12
21	Y	101	TGL	C24-C25-C26-C27
24	P	311	DMU	C28-C31-C34-C37
26	P	306	CDL	C61-C62-C63-C64
27	P	302	PEK	C25-C26-C27-C28
27	C	309	PEK	C21-C22-C23-C24
19	A	609	PGV	C2-C3-C4-C5
19	C	308	PGV	C4-C5-C6-C7
19	P	303	PGV	C5-C6-C7-C8
21	Q	201	TGL	CA2-CA3-CA4-CA5
21	Y	101	TGL	CB5-CB6-CB7-CB8
24	C	302	DMU	C28-C31-C34-C37
24	P	311	DMU	C19-C22-C25-C28
26	C	305	CDL	C12-C13-C14-C15
26	G	102	CDL	C34-C35-C36-C37
26	P	306	CDL	C12-C13-C14-C15
26	T	102	CDL	C19-C20-C21-C22
26	T	102	CDL	C41-C42-C43-C44
27	G	101	PEK	C16-C17-C18-C19
28	E	201	PSC	C2-C3-C4-C5
24	P	310	DMU	C22-C25-C28-C31
26	G	102	CDL	C43-C44-C45-C46
26	G	102	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C53-C54-C55-C56
26	T	102	CDL	C77-C78-C79-C80
27	G	101	PEK	C25-C26-C27-C28
28	O	302	PSC	C24-C25-C26-C27
19	C	308	PGV	C04-C05-C06-O06
19	P	303	PGV	C04-C05-C06-O06
26	T	102	CDL	C11-CA5-OA6-CA4
19	C	304	PGV	C27-C28-C29-C30
21	Y	101	TGL	C12-C13-C14-C29
19	P	305	PGV	C12-C13-C14-C15
19	A	609	PGV	C14-C15-C16-C17
19	C	308	PGV	C2-C3-C4-C5
21	B	301	TGL	CA2-CA3-CA4-CA5
21	B	301	TGL	CA3-CA4-CA5-CA6
21	B	301	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	CA6-CA7-CA8-CA9
21	B	301	TGL	C16-C17-C18-C19
21	B	301	TGL	C23-C24-C25-C26
21	D	201	TGL	C21-C20-CA9-CA8
21	D	201	TGL	C20-C21-C22-C23
21	N	609	TGL	C21-C20-CA9-CA8
21	N	609	TGL	CB6-CB7-CB8-CB9
21	Y	101	TGL	CC5-CC6-CC7-CC8
24	Z	102	DMU	C28-C31-C34-C37
26	C	305	CDL	C74-C75-C76-C77
26	G	102	CDL	C13-C14-C15-C16
26	P	306	CDL	C21-C22-C23-C24
26	T	102	CDL	C12-C13-C14-C15
26	T	102	CDL	C33-C34-C35-C36
26	T	102	CDL	C59-C60-C61-C62
27	P	302	PEK	C33-C34-C35-C36
19	P	303	PGV	C3-C4-C5-C6
19	Z	101	PGV	C26-C27-C28-C29
21	D	201	TGL	CA7-CA8-CA9-C20
21	D	201	TGL	CB9-C10-C11-C12
21	L	101	TGL	CB2-CB3-CB4-CB5
21	L	101	TGL	CC6-CC7-CC8-CC9
21	L	101	TGL	C16-C15-CC9-CC8
21	L	101	TGL	C14-C29-C30-C31
21	Y	101	TGL	C10-C11-C12-C13
21	Y	101	TGL	C20-C21-C22-C23
26	C	305	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C80-C81-C82-C83
26	T	102	CDL	C14-C15-C16-C17
26	T	102	CDL	C34-C35-C36-C37
26	T	102	CDL	C73-C74-C75-C76
27	P	309	PEK	O12-C04-C05-N
19	C	308	PGV	C23-C24-C25-C26
19	P	303	PGV	C4-C5-C6-C7
21	Q	201	TGL	CA5-CA6-CA7-CA8
24	C	311	DMU	C31-C34-C37-C40
26	C	305	CDL	C17-C18-C19-C20
26	P	306	CDL	C78-C79-C80-C81
27	C	309	PEK	C30-C31-C32-C33
27	P	309	PEK	C32-C33-C34-C35
28	O	302	PSC	C26-C27-C28-C29
19	C	304	PGV	C28-C29-C30-C31
21	L	101	TGL	C17-C18-C19-C33
21	Q	201	TGL	CB5-CB6-CB7-CB8
26	G	102	CDL	C11-C12-C13-C14
27	C	309	PEK	C33-C34-C35-C36
21	L	101	TGL	CC3-CC4-CC5-CC6
21	N	609	TGL	CC5-CC6-CC7-CC8
21	N	609	TGL	C24-C25-C26-C27
21	Q	201	TGL	C11-C10-CB9-CB8
26	P	306	CDL	C43-C44-C45-C46
26	T	102	CDL	C13-C14-C15-C16
27	P	302	PEK	C34-C35-C36-C37
28	O	302	PSC	C25-C26-C27-C28
19	C	304	PGV	C7-C8-C9-C10
19	C	308	PGV	C20-C21-C22-C23
21	B	301	TGL	CB4-CB5-CB6-CB7
21	D	201	TGL	C13-C14-C29-C30
21	Y	101	TGL	C11-C12-C13-C14
24	P	308	DMU	C22-C25-C28-C31
24	P	311	DMU	C22-C25-C28-C31
26	C	305	CDL	C51-C52-C53-C54
26	P	306	CDL	C31-C32-C33-C34
26	T	102	CDL	C75-C76-C77-C78
27	C	309	PEK	C34-C35-C36-C37
26	T	102	CDL	CA7-C31-C32-C33
21	B	301	TGL	C24-C25-C26-C27
21	N	609	TGL	CA4-CA5-CA6-CA7
21	N	609	TGL	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
21	N	609	TGL	CC7-CC8-CC9-C15
21	Y	101	TGL	C15-C16-C17-C18
24	Z	102	DMU	C25-C28-C31-C34
26	T	102	CDL	C80-C81-C82-C83
28	E	201	PSC	C24-C25-C26-C27
26	T	102	CDL	OA7-CA5-OA6-CA4
19	A	609	PGV	C10-C11-C12-C13
26	P	306	CDL	C35-C36-C37-C38
26	G	102	CDL	C62-C63-C64-C65
26	G	102	CDL	C79-C80-C81-C82
27	C	307	PEK	C16-C17-C18-C19
19	A	609	PGV	O05-C05-C06-O06
19	C	304	PGV	C21-C22-C23-C24
19	P	303	PGV	C28-C29-C30-C31
19	Z	101	PGV	C3-C4-C5-C6
21	L	101	TGL	CA2-CA3-CA4-CA5
21	N	609	TGL	CC6-CC7-CC8-CC9
27	G	101	PEK	C27-C28-C29-C30
27	P	302	PEK	C29-C30-C31-C32
28	O	302	PSC	C22-C23-C24-C25
27	T	101	PEK	C2-C3-C4-C5
27	G	101	PEK	C23-C24-C25-C26
27	T	101	PEK	C26-C27-C28-C29
21	D	201	TGL	CA2-CA1-OG1-CG1
21	N	609	TGL	C13-C14-C29-C30
26	G	102	CDL	C12-C13-C14-C15
27	P	302	PEK	C26-C27-C28-C29
21	B	301	TGL	CA7-CA8-CA9-C20
21	L	101	TGL	CA9-C20-C21-C22
24	M	101	DMU	C31-C34-C37-C40
24	P	310	DMU	C19-C22-C25-C28
28	O	302	PSC	C4-C5-C6-C7
22	J	101	CHD	C16-C17-C20-C21
24	P	310	DMU	C28-C31-C34-C37
26	P	306	CDL	C42-C43-C44-C45
27	P	302	PEK	C27-C28-C29-C30
28	E	201	PSC	C4-C5-C6-C7
24	P	311	DMU	C18-C19-C22-C25
19	P	305	PGV	C30-C31-C32-C33
21	B	301	TGL	C22-C23-C24-C25
20	A	610	EDO	O1-C1-C2-O2
20	A	618	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	D	202	EDO	O1-C1-C2-O2
20	D	206	EDO	O1-C1-C2-O2
20	E	204	EDO	O1-C1-C2-O2
20	G	104	EDO	O1-C1-C2-O2
20	O	304	EDO	O1-C1-C2-O2
20	S	104	EDO	O1-C1-C2-O2
19	N	608	PGV	C26-C27-C28-C29
21	B	301	TGL	C21-C22-C23-C24
19	P	305	PGV	C7-C8-C9-C10
21	B	301	TGL	C16-C15-CC9-CC8
21	B	301	TGL	CA9-C20-C21-C22
21	D	201	TGL	CC2-CC3-CC4-CC5
21	Q	201	TGL	C22-C23-C24-C25
27	P	302	PEK	C32-C33-C34-C35
26	P	306	CDL	OA9-CA7-OA8-CA6
19	A	609	PGV	C1-C2-C3-C4
26	P	306	CDL	CA5-C11-C12-C13
28	O	302	PSC	C19-C20-C21-C22
19	P	305	PGV	C22-C23-C24-C25
21	Q	201	TGL	C23-C24-C25-C26
26	G	102	CDL	C41-C42-C43-C44
26	P	306	CDL	C41-C42-C43-C44
22	P	307	CHD	C16-C17-C20-C21
19	C	308	PGV	C30-C31-C32-C33
21	L	101	TGL	C20-C21-C22-C23
27	P	302	PEK	C13-C14-C15-C16
19	C	308	PGV	C12-C13-C14-C15
28	O	302	PSC	C6-C7-C8-C9
19	A	608	PGV	C23-C24-C25-C26
21	Y	101	TGL	C16-C15-CC9-CC8
26	T	102	CDL	C60-C61-C62-C63
24	P	310	DMU	C18-C19-C22-C25
26	C	305	CDL	C14-C15-C16-C17
26	C	305	CDL	C59-C60-C61-C62
26	G	102	CDL	C14-C15-C16-C17
26	G	102	CDL	C35-C36-C37-C38
26	P	306	CDL	C57-C58-C59-C60
26	P	306	CDL	C82-C83-C84-C85
26	T	102	CDL	C72-C73-C74-C75
27	C	307	PEK	C25-C26-C27-C28
21	L	101	TGL	C19-C33-C34-C35
26	C	305	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C56-C57-C58-C59
27	C	307	PEK	C32-C33-C34-C35
21	D	201	TGL	CC1-CC2-CC3-CC4
21	B	301	TGL	C12-C13-C14-C29
21	D	201	TGL	OA1-CA1-OG1-CG1
26	P	306	CDL	C20-C21-C22-C23
26	T	102	CDL	C57-C58-C59-C60
27	P	309	PEK	C30-C31-C32-C33
26	T	102	CDL	C51-CB5-OB6-CB4
21	Y	101	TGL	C16-C17-C18-C19
26	T	102	CDL	OB7-CB5-OB6-CB4
24	P	308	DMU	O6-C11-C9-C8
26	P	306	CDL	C53-C54-C55-C56
21	L	101	TGL	C11-C12-C13-C14
21	Y	101	TGL	CC4-CC5-CC6-CC7
26	C	305	CDL	C31-C32-C33-C34
28	O	302	PSC	C23-C24-C25-C26
19	N	608	PGV	C11-C10-C9-C8
27	C	309	PEK	C2-C3-C4-C5
28	O	302	PSC	C13-C14-C15-C16
21	N	609	TGL	C16-C17-C18-C19
26	C	305	CDL	C58-C59-C60-C61
26	P	306	CDL	C22-C23-C24-C25
21	B	301	TGL	CB5-CB6-CB7-CB8
27	G	101	PEK	C4-C5-C6-C7
21	L	101	TGL	C23-C24-C25-C26
21	N	609	TGL	C15-C16-C17-C18
21	D	201	TGL	CC5-CC6-CC7-CC8
26	T	102	CDL	C31-C32-C33-C34
26	T	102	CDL	C82-C83-C84-C85
19	P	303	PGV	C13-C14-C15-C16
19	P	303	PGV	C20-C21-C22-C23
26	C	305	CDL	C33-C34-C35-C36
22	P	307	CHD	C13-C17-C20-C22
21	Y	101	TGL	CA3-CA4-CA5-CA6
24	P	308	DMU	C31-C34-C37-C40
26	P	306	CDL	C56-C57-C58-C59
26	T	102	CDL	C62-C63-C64-C65
19	P	303	PGV	C01-C02-C03-O11
19	Z	101	PGV	C01-C02-C03-O11
26	P	306	CDL	OA5-CA3-CA4-CA6
27	P	309	PEK	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C35-C36-C37-C38
26	C	305	CDL	C41-C42-C43-C44
26	T	102	CDL	C17-C18-C19-C20
26	T	102	CDL	C23-C24-C25-C26
24	C	311	DMU	C18-C19-C22-C25
22	P	307	CHD	C16-C17-C20-C22
21	N	609	TGL	C23-C24-C25-C26
26	C	305	CDL	C39-C40-C41-C42
27	T	101	PEK	C33-C34-C35-C36
19	P	303	PGV	O12-C04-C05-C06
19	C	308	PGV	C6-C7-C8-C9
19	P	305	PGV	C28-C29-C30-C31
21	Y	101	TGL	C18-C19-C33-C34
21	Y	101	TGL	C14-C29-C30-C31
19	C	308	PGV	C3-C4-C5-C6
21	D	201	TGL	C21-C22-C23-C24
21	L	101	TGL	C10-C11-C12-C13
19	P	303	PGV	O03-C01-C02-C03
21	L	101	TGL	OG1-CG1-CG2-CG3
21	N	609	TGL	OG1-CG1-CG2-CG3
26	P	306	CDL	CB3-CB4-CB6-OB8
27	C	309	PEK	O03-C01-C02-C03
24	C	310	DMU	C18-C19-C22-C25
21	Y	101	TGL	C29-C30-C31-C32
24	Z	102	DMU	O16-C18-C19-C22
26	T	102	CDL	C16-C17-C18-C19
27	C	309	PEK	C17-C18-C19-C20
19	A	608	PGV	C31-C32-C33-C34
19	Z	101	PGV	C31-C32-C33-C34
21	L	101	TGL	CA6-CA7-CA8-CA9
21	Q	201	TGL	CA7-CA8-CA9-C20
24	P	311	DMU	C34-C37-C40-C43
26	C	305	CDL	C24-C25-C26-C27
26	C	305	CDL	C43-C44-C45-C46
21	Y	101	TGL	CA1-CA2-CA3-CA4
19	Z	101	PGV	C30-C31-C32-C33
21	B	301	TGL	C25-C26-C27-C28
28	O	302	PSC	C3-C4-C5-C6
14	N	601	HEA	C15-C16-C17-C18
27	C	307	PEK	C35-C36-C37-C38
19	P	303	PGV	C31-C32-C33-C34
19	Z	101	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C84-C85-C86-C87
21	D	201	TGL	C18-C19-C33-C34
21	L	101	TGL	C29-C30-C31-C32
26	P	306	CDL	C44-C45-C46-C47
26	P	306	CDL	C11-CA5-OA6-CA4
24	Z	102	DMU	C19-C22-C25-C28
19	Z	101	PGV	C1-C2-C3-C4
24	C	302	DMU	C22-C25-C28-C31
26	P	306	CDL	C74-C75-C76-C77
26	G	102	CDL	C59-C60-C61-C62
21	Y	101	TGL	CG1-CG2-OG2-CB1
24	C	311	DMU	C34-C37-C40-C43
26	G	102	CDL	C16-C17-C18-C19
19	N	608	PGV	C31-C32-C33-C34
26	P	306	CDL	C11-C12-C13-C14
26	T	102	CDL	C18-C19-C20-C21
27	C	309	PEK	C26-C27-C28-C29
21	N	609	TGL	CB2-CB3-CB4-CB5
21	Y	101	TGL	CA6-CA7-CA8-CA9
28	E	201	PSC	C26-C27-C28-C29
26	T	102	CDL	OB5-CB3-CB4-OB6
27	P	302	PEK	C4-C5-C6-C7
21	B	301	TGL	CC6-CC7-CC8-CC9
21	N	609	TGL	CC9-C15-C16-C17
21	Q	201	TGL	CC7-CC8-CC9-C15
22	P	307	CHD	C13-C17-C20-C21
20	N	620	EDO	O1-C1-C2-O2
26	G	102	CDL	C53-C54-C55-C56
26	T	102	CDL	OA6-CA4-CA6-OA8
28	E	201	PSC	O03-C01-C02-O01
19	N	608	PGV	C27-C28-C29-C30
26	C	305	CDL	C44-C45-C46-C47
26	G	102	CDL	C82-C83-C84-C85
26	C	305	CDL	C83-C84-C85-C86
27	C	309	PEK	C29-C30-C31-C32
27	P	302	PEK	C21-C22-C23-C24
19	C	308	PGV	C15-C16-C17-C18
26	G	102	CDL	C56-C57-C58-C59
26	C	305	CDL	C71-CB7-OB8-CB6
19	C	308	PGV	C31-C32-C33-C34
27	C	307	PEK	C24-C25-C26-C27
21	D	201	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	Z	101	PGV	C2-C3-C4-C5
21	B	301	TGL	CB9-C10-C11-C12
26	T	102	CDL	C55-C56-C57-C58
26	P	306	CDL	C60-C61-C62-C63
27	C	309	PEK	C15-C16-C17-C18
19	A	608	PGV	C10-C11-C12-C13
19	N	608	PGV	C10-C11-C12-C13
21	D	201	TGL	C12-C13-C14-C29
26	C	305	CDL	C15-C16-C17-C18
26	G	102	CDL	C64-C65-C66-C67
26	C	305	CDL	OA5-CA3-CA4-CA6
26	G	102	CDL	OB5-CB3-CB4-CB6
21	Q	201	TGL	C17-C18-C19-C33
21	D	201	TGL	C11-C12-C13-C14
26	C	305	CDL	CB4-CB6-OB8-CB7
21	N	609	TGL	CB4-CB5-CB6-CB7
28	E	201	PSC	C5-C6-C7-C8
14	N	601	HEA	C12-C13-C14-C15
28	O	302	PSC	C28-C29-C30-C31
19	Z	101	PGV	C05-C04-O12-P
24	P	311	DMU	C31-C34-C37-C40
19	P	303	PGV	C22-C23-C24-C25
27	G	101	PEK	C17-C18-C19-C20
28	E	201	PSC	C30-C31-C32-C33
21	Q	201	TGL	C16-C15-CC9-CC8
27	C	309	PEK	C25-C26-C27-C28
21	Q	201	TGL	OG1-CG1-CG2-CG3
26	C	305	CDL	CB3-CB4-CB6-OB8
26	G	102	CDL	CA3-CA4-CA6-OA8
26	P	306	CDL	OA7-CA5-OA6-CA4
21	B	301	TGL	CC5-CC6-CC7-CC8
21	N	609	TGL	C19-C33-C34-C35
27	T	101	PEK	C23-C24-C25-C26
19	A	609	PGV	C31-C32-C33-C34
26	P	306	CDL	C24-C25-C26-C27
26	P	306	CDL	C72-C73-C74-C75
26	G	102	CDL	C31-C32-C33-C34
21	Q	201	TGL	CC2-CC3-CC4-CC5
26	G	102	CDL	C22-C23-C24-C25
19	A	609	PGV	C22-C23-C24-C25
26	T	102	CDL	C44-C45-C46-C47
26	T	102	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	CA3-OA5-PA1-OA2
27	C	307	PEK	C5-C6-C7-C8
27	C	309	PEK	C11-C10-C9-C8
27	P	302	PEK	C9-C10-C11-C12
27	P	302	PEK	C12-C13-C14-C15
27	P	309	PEK	C03-O11-P-O12
27	P	309	PEK	C5-C6-C7-C8
27	P	309	PEK	C11-C10-C9-C8
28	E	201	PSC	C9-C10-C11-C12
28	E	201	PSC	C10-C11-C12-C13
28	O	302	PSC	C9-C10-C11-C12
26	P	306	CDL	CB5-C51-C52-C53
19	Z	101	PGV	O01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-OA6
26	G	102	CDL	OB5-CB3-CB4-OB6
27	P	309	PEK	O01-C02-C03-O11
27	P	309	PEK	C22-C21-O03-C01
26	T	102	CDL	C74-C75-C76-C77
19	C	304	PGV	C12-C13-C14-C15
26	C	305	CDL	OB9-CB7-OB8-CB6
21	B	301	TGL	C15-C16-C17-C18
21	N	609	TGL	CA9-C20-C21-C22
26	C	305	CDL	C56-C57-C58-C59
26	T	102	CDL	C24-C25-C26-C27
22	W	101	CHD	C17-C20-C22-C23
19	C	304	PGV	C15-C16-C17-C18
27	T	101	PEK	C34-C35-C36-C37
21	N	609	TGL	CA7-CA8-CA9-C20
21	N	609	TGL	C25-C26-C27-C28
26	P	306	CDL	C84-C85-C86-C87
21	L	101	TGL	OG1-CG1-CG2-OG2
21	L	101	TGL	OG2-CG2-CG3-OG3
26	P	306	CDL	OB6-CB4-CB6-OB8
27	C	309	PEK	O03-C01-C02-O01
26	C	305	CDL	C20-C21-C22-C23
14	A	601	HEA	C15-C16-C17-C18
26	G	102	CDL	C84-C85-C86-C87
26	T	102	CDL	C79-C80-C81-C82
27	T	101	PEK	C17-C18-C19-C20
21	B	301	TGL	C17-C18-C19-C33
26	T	102	CDL	C21-C22-C23-C24
19	A	609	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	CB3-CB4-CB5-CB6
27	P	309	PEK	C23-C24-C25-C26
20	A	614	EDO	O1-C1-C2-O2
20	A	620	EDO	O1-C1-C2-O2
20	C	316	EDO	O1-C1-C2-O2
26	P	306	CDL	C38-C39-C40-C41
27	C	307	PEK	C29-C30-C31-C32
26	G	102	CDL	OB7-CB5-OB6-CB4
26	G	102	CDL	C51-CB5-OB6-CB4
21	D	201	TGL	CA3-CA4-CA5-CA6
19	C	308	PGV	C14-C15-C16-C17
26	G	102	CDL	C23-C24-C25-C26
14	A	601	HEA	C27-C19-C20-C21
19	P	303	PGV	O12-C04-C05-O05
26	T	102	CDL	C54-C55-C56-C57
19	C	308	PGV	C7-C8-C9-C10
19	C	308	PGV	C21-C22-C23-C24
21	B	301	TGL	CB2-CB3-CB4-CB5
19	A	609	PGV	C20-C21-C22-C23
26	T	102	CDL	C39-C40-C41-C42
21	L	101	TGL	C25-C26-C27-C28
26	G	102	CDL	C75-C76-C77-C78
21	D	201	TGL	C17-C18-C19-C33
28	E	201	PSC	C29-C30-C31-C32
19	N	608	PGV	C13-C14-C15-C16
19	P	303	PGV	C7-C8-C9-C10
21	Q	201	TGL	CC5-CC6-CC7-CC8
21	L	101	TGL	C11-C10-CB9-CB8
27	C	307	PEK	C22-C21-O03-C01
24	C	302	DMU	O5-C6-O16-C18
19	P	305	PGV	C1-C2-C3-C4
21	L	101	TGL	CG1-CG2-CG3-OG3
19	P	303	PGV	O01-C02-C03-O11
26	G	102	CDL	OA5-CA3-CA4-OA6
26	P	306	CDL	OA5-CA3-CA4-OA6
28	O	302	PSC	O01-C02-C03-O11
22	W	101	CHD	C13-C17-C20-C21
26	C	305	CDL	C82-C83-C84-C85
27	P	302	PEK	C28-C29-C30-C31
24	C	302	DMU	C1-C6-O16-C18
19	A	608	PGV	C26-C27-C28-C29
21	B	301	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	OG1-CG1-CG2-OG2
21	N	609	TGL	OG1-CG1-CG2-OG2
26	C	305	CDL	OA6-CA4-CA6-OA8
26	C	305	CDL	OB6-CB4-CB6-OB8
26	G	102	CDL	C71-CB7-OB8-CB6
19	C	304	PGV	C25-C26-C27-C28
19	C	308	PGV	C24-C25-C26-C27
21	Y	101	TGL	C19-C33-C34-C35
19	P	303	PGV	O05-C05-C06-O06
26	C	305	CDL	C52-C53-C54-C55
27	C	307	PEK	C17-C18-C19-C20
27	P	309	PEK	O04-C21-O03-C01
27	C	307	PEK	C34-C35-C36-C37
19	P	305	PGV	C11-C12-C13-C14
27	C	307	PEK	O04-C21-O03-C01
26	P	306	CDL	C13-C14-C15-C16
19	C	308	PGV	C29-C30-C31-C32
19	P	303	PGV	C29-C30-C31-C32
21	Y	101	TGL	C22-C23-C24-C25
27	P	309	PEK	C29-C30-C31-C32
26	T	102	CDL	CA4-CA6-OA8-CA7
24	C	302	DMU	C19-C22-C25-C28
26	G	102	CDL	CB2-OB2-PB2-OB5
27	C	307	PEK	C04-O12-P-O11
28	E	201	PSC	C04-O12-P-O11
19	C	304	PGV	C02-C03-O11-P
19	P	305	PGV	C02-C03-O11-P
19	Z	101	PGV	C02-C03-O11-P
19	C	308	PGV	C03-O11-P-O14
19	P	303	PGV	C03-O11-P-O13
19	Z	101	PGV	C03-O11-P-O14
26	C	305	CDL	CA3-OA5-PA1-OA3
26	G	102	CDL	CA3-OA5-PA1-OA4
26	T	102	CDL	CA2-OA2-PA1-OA4
27	C	309	PEK	C03-O11-P-O14
27	P	302	PEK	C03-O11-P-O14
27	P	309	PEK	C03-O11-P-O13
27	P	309	PEK	C04-O12-P-O14
28	O	302	PSC	C03-O11-P-O13
26	T	102	CDL	OB5-CB3-CB4-CB6
27	P	309	PEK	C01-C02-C03-O11
28	O	302	PSC	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
20	D	203	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
20	R	204	EDO	O1-C1-C2-O2
27	T	101	PEK	C3-C4-C5-C6
27	P	309	PEK	C26-C27-C28-C29
27	C	309	PEK	C35-C36-C37-C38
19	C	304	PGV	C1-C2-C3-C4
26	P	306	CDL	C32-C33-C34-C35
21	L	101	TGL	CB3-CB4-CB5-CB6
19	Z	101	PGV	C5-C6-C7-C8
26	G	102	CDL	OB9-CB7-OB8-CB6
24	P	308	DMU	O6-C11-C9-O1
19	P	305	PGV	C31-C32-C33-C34
21	L	101	TGL	CC4-CC5-CC6-CC7
21	B	301	TGL	OG1-CG1-CG2-CG3
26	C	305	CDL	CA3-CA4-CA6-OA8
26	G	102	CDL	CB3-CB4-CB6-OB8
26	T	102	CDL	CA3-CA4-CA6-OA8
26	T	102	CDL	C22-C23-C24-C25
27	P	309	PEK	C33-C34-C35-C36
27	T	101	PEK	C25-C26-C27-C28
28	E	201	PSC	O03-C01-C02-C03
26	G	102	CDL	OA6-CA4-CA6-OA8
21	B	301	TGL	C11-C12-C13-C14
21	D	201	TGL	C14-C29-C30-C31
26	T	102	CDL	C20-C21-C22-C23
28	E	201	PSC	C21-C22-C23-C24
21	D	201	TGL	CA2-CA3-CA4-CA5
26	C	305	CDL	C81-C82-C83-C84
26	G	102	CDL	C17-C18-C19-C20
28	O	302	PSC	C31-C32-C33-C34
19	N	608	PGV	C30-C31-C32-C33
24	C	302	DMU	C18-C19-C22-C25
21	L	101	TGL	C13-C14-C29-C30
28	E	201	PSC	C11-C12-C13-C14
21	Q	201	TGL	C21-C20-CA9-CA8
26	G	102	CDL	C80-C81-C82-C83
19	A	609	PGV	C15-C16-C17-C18
21	B	301	TGL	CC2-CC3-CC4-CC5
21	B	301	TGL	CC4-CC5-CC6-CC7
27	C	309	PEK	C28-C29-C30-C31
26	G	102	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C11-C12-C13-C14
14	N	601	HEA	C11-C12-C13-C14
21	D	201	TGL	C16-C15-CC9-CC8
28	O	302	PSC	C27-C28-C29-C30
21	N	609	TGL	CC4-CC5-CC6-CC7
27	P	302	PEK	C35-C36-C37-C38
27	C	307	PEK	C26-C27-C28-C29
21	B	301	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	C13-C14-C29-C30
19	C	304	PGV	C23-C24-C25-C26
20	D	204	EDO	O1-C1-C2-O2
20	P	312	EDO	O1-C1-C2-O2
20	R	202	EDO	O1-C1-C2-O2
19	C	308	PGV	C13-C14-C15-C16
14	N	601	HEA	C19-C20-C21-C22
21	D	201	TGL	OG2-CG2-CG3-OG3
19	A	609	PGV	C04-O12-P-O11
19	C	308	PGV	C04-O12-P-O11
19	P	303	PGV	C04-O12-P-O11
26	G	102	CDL	CA2-OA2-PA1-OA5
26	G	102	CDL	CB3-OB5-PB2-OB2
26	P	306	CDL	CB3-OB5-PB2-OB2
26	T	102	CDL	CA3-OA5-PA1-OA2
27	C	309	PEK	C04-O12-P-O11
21	D	201	TGL	CG1-CG2-CG3-OG3
21	N	609	TGL	CC2-CC3-CC4-CC5
14	A	601	HEA	C18-C19-C20-C21
19	C	304	PGV	C9-C10-C11-C12
21	Y	101	TGL	CB4-CB5-CB6-CB7
21	D	201	TGL	CA9-C20-C21-C22
19	Z	101	PGV	C14-C15-C16-C17
28	O	302	PSC	C02-C03-O11-P
21	B	301	TGL	C10-C11-C12-C13
21	L	101	TGL	C15-C16-C17-C18
26	T	102	CDL	C11-C12-C13-C14
19	P	303	PGV	C11-C10-C9-C8
27	P	309	PEK	C15-C16-C17-C18
21	N	609	TGL	CB1-CB2-CB3-CB4
21	Q	201	TGL	CA3-CA4-CA5-CA6
19	Z	101	PGV	C28-C29-C30-C31
14	N	601	HEA	CAD-CBD-CGD-O1D
26	P	306	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
24	P	308	DMU	C25-C28-C31-C34
27	C	307	PEK	C33-C34-C35-C36
19	C	308	PGV	C5-C6-C7-C8
21	Q	201	TGL	CB7-CB8-CB9-C10
24	C	302	DMU	C25-C28-C31-C34
22	B	302	CHD	C22-C23-C24-O25
22	G	103	CHD	C22-C23-C24-O26
19	N	608	PGV	C15-C16-C17-C18
26	P	306	CDL	C33-C34-C35-C36
26	T	102	CDL	C1-CB2-OB2-PB2
21	D	201	TGL	CC7-CC8-CC9-C15
26	G	102	CDL	C81-C82-C83-C84
19	P	303	PGV	C12-C13-C14-C15
20	W	102	EDO	O1-C1-C2-O2
19	A	608	PGV	C19-C20-C21-C22
26	G	102	CDL	C15-C16-C17-C18
26	G	102	CDL	C77-C78-C79-C80
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
19	C	304	PGV	C26-C27-C28-C29
21	N	609	TGL	C11-C12-C13-C14
24	P	311	DMU	C25-C28-C31-C34
27	C	307	PEK	C23-C24-C25-C26
21	D	201	TGL	CB7-CB8-CB9-C10
21	Q	201	TGL	CB4-CB5-CB6-CB7
22	G	103	CHD	C22-C23-C24-O25
27	P	309	PEK	C22-C23-C24-C25
28	O	302	PSC	C14-C15-C16-C17
19	A	609	PGV	C12-C13-C14-C15
14	A	601	HEA	CAD-CBD-CGD-O1D
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
22	B	302	CHD	C22-C23-C24-O26
22	C	306	CHD	C22-C23-C24-O25
24	C	310	DMU	O16-C18-C19-C22
21	Q	201	TGL	C14-C29-C30-C31
27	C	307	PEK	C6-C7-C8-C9
27	C	307	PEK	C11-C10-C9-C8
27	G	101	PEK	C11-C10-C9-C8
27	P	302	PEK	C5-C6-C7-C8
27	P	302	PEK	C11-C10-C9-C8
27	T	101	PEK	C5-C6-C7-C8
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
14	N	602[B]	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	C	306	CHD	C22-C23-C24-O26
26	C	305	CDL	C79-C80-C81-C82
26	G	102	CDL	C24-C25-C26-C27
26	T	102	CDL	C64-C65-C66-C67
26	G	102	CDL	OA5-CA3-CA4-CA6
14	N	601	HEA	CAD-CBD-CGD-O2D
22	P	307	CHD	C22-C23-C24-O26
22	P	307	CHD	C22-C23-C24-O25
21	Q	201	TGL	C29-C30-C31-C32
27	G	101	PEK	C26-C27-C28-C29
27	P	309	PEK	C25-C26-C27-C28
27	G	101	PEK	C22-C23-C24-C25
19	Z	101	PGV	O03-C01-C02-O01
19	P	303	PGV	C9-C10-C11-C12
14	N	602[B]	HEA	CAA-CBA-CGA-O2A
21	Q	201	TGL	C16-C17-C18-C19
26	T	102	CDL	C63-C64-C65-C66
21	Y	101	TGL	C25-C26-C27-C28
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
19	A	609	PGV	C29-C30-C31-C32
21	Q	201	TGL	CA9-C20-C21-C22
27	G	101	PEK	C34-C35-C36-C37
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
24	C	310	DMU	O1-C10-O7-C3
27	P	309	PEK	C35-C36-C37-C38
19	P	305	PGV	C05-C04-O12-P
26	C	305	CDL	C32-C33-C34-C35
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
19	A	608	PGV	O03-C19-C20-C21
24	Z	102	DMU	C31-C34-C37-C40
27	P	302	PEK	C7-C8-C9-C10
19	A	608	PGV	C24-C25-C26-C27
24	P	308	DMU	C28-C31-C34-C37
26	T	102	CDL	C42-C43-C44-C45
21	N	609	TGL	C21-C22-C23-C24
19	C	304	PGV	C11-C12-C13-C14
27	P	309	PEK	C3-C4-C5-C6
19	P	305	PGV	C15-C16-C17-C18
19	N	608	PGV	O03-C19-C20-C21
26	P	306	CDL	O1-C1-CA2-OA2
14	A	601	HEA	C12-C13-C14-C15
27	P	302	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
19	P	303	PGV	C19-C20-C21-C22
26	P	306	CDL	C58-C59-C60-C61
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
27	C	307	PEK	O01-C1-C2-C3
19	Z	101	PGV	O01-C1-C2-C3
22	J	101	CHD	C22-C23-C24-O26
21	D	201	TGL	C29-C30-C31-C32
26	P	306	CDL	C79-C80-C81-C82
14	A	601	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
21	D	201	TGL	OG2-CB1-CB2-CB3
21	D	201	TGL	OB1-CB1-OG2-CG2
19	A	609	PGV	O01-C1-C2-C3
21	L	101	TGL	OG1-CA1-CA2-CA3
22	W	101	CHD	C22-C23-C24-O26
21	B	301	TGL	OG3-CC1-CC2-CC3
27	C	309	PEK	O01-C1-C2-C3
27	P	302	PEK	C1-C2-C3-C4
19	Z	101	PGV	O03-C01-C02-C03
27	P	302	PEK	C02-C03-O11-P
19	A	609	PGV	C28-C29-C30-C31
27	C	307	PEK	C13-C14-C15-C16
19	C	304	PGV	C31-C32-C33-C34
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
22	P	301	CHD	C22-C23-C24-O26
26	C	305	CDL	C57-C58-C59-C60
27	C	307	PEK	C1-C2-C3-C4
20	A	619	EDO	O1-C1-C2-O2
20	C	314	EDO	O1-C1-C2-O2
20	E	205	EDO	O1-C1-C2-O2
20	J	102	EDO	O1-C1-C2-O2
20	N	613	EDO	O1-C1-C2-O2
20	N	619	EDO	O1-C1-C2-O2
19	A	609	PGV	C21-C22-C23-C24
19	A	609	PGV	C11-C10-C9-C8
22	C	301	CHD	C22-C23-C24-O26
22	P	301	CHD	C22-C23-C24-O25
28	O	302	PSC	O03-C01-C02-O01
21	Y	101	TGL	C11-C10-CB9-CB8
22	W	101	CHD	C22-C23-C24-O25
14	N	601	HEA	CAA-CBA-CGA-O1A
21	L	101	TGL	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C32-C31-CA7-OA8
26	C	305	CDL	C54-C55-C56-C57
19	C	308	PGV	C19-C20-C21-C22
14	N	602[B]	HEA	C15-C16-C17-C18
19	Z	101	PGV	C27-C28-C29-C30
27	P	302	PEK	O01-C1-C2-C3
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
22	C	301	CHD	C22-C23-C24-O25
27	C	309	PEK	O02-C1-C2-C3
22	C	306	CHD	C16-C17-C20-C22
19	P	305	PGV	C29-C30-C31-C32
27	C	309	PEK	C3-C4-C5-C6
22	J	101	CHD	C22-C23-C24-O25
19	Z	101	PGV	O02-C1-C2-C3
24	M	101	DMU	O6-C11-C9-C8
24	P	308	DMU	C34-C37-C40-C43
21	B	301	TGL	OC1-CC1-CC2-CC3
26	P	306	CDL	C12-C11-CA5-OA6
28	O	302	PSC	C15-C16-C17-C18
27	C	307	PEK	O02-C1-C2-C3
26	G	102	CDL	C32-C31-CA7-OA8
27	T	101	PEK	O01-C1-C2-C3
26	T	102	CDL	C32-C31-CA7-OA9
19	C	308	PGV	C04-O12-P-O13
26	T	102	CDL	CA3-OA5-PA1-OA3
28	O	302	PSC	C04-C05-N-C08
20	D	205	EDO	O1-C1-C2-O2
20	G	106	EDO	O1-C1-C2-O2
20	N	610	EDO	O1-C1-C2-O2
20	R	205	EDO	O1-C1-C2-O2
24	C	310	DMU	C19-C22-C25-C28
27	P	309	PEK	C2-C3-C4-C5
26	G	102	CDL	C32-C33-C34-C35
26	G	102	CDL	C36-C37-C38-C39
27	C	307	PEK	C3-C4-C5-C6
19	P	303	PGV	C30-C31-C32-C33
21	L	101	TGL	CA7-CA8-CA9-C20
21	Q	201	TGL	CB2-CB3-CB4-CB5
14	N	601	HEA	CAA-CBA-CGA-O2A
19	C	304	PGV	C20-C21-C22-C23
26	G	102	CDL	C19-C20-C21-C22
28	E	201	PSC	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	O	302	PSC	C04-C05-N-C06
26	T	102	CDL	C12-C11-CA5-OA6
27	C	307	PEK	C28-C29-C30-C31
26	C	305	CDL	OB5-CB3-CB4-OB6
26	G	102	CDL	C32-C31-CA7-OA9
26	P	306	CDL	C12-C11-CA5-OA7
27	G	101	PEK	O03-C21-C22-C23
27	T	101	PEK	O02-C1-C2-C3
24	C	310	DMU	C19-C18-O16-C6
24	P	310	DMU	C19-C18-O16-C6
28	E	201	PSC	O03-C19-C20-C21
27	T	101	PEK	C15-C16-C17-C18
19	P	305	PGV	C23-C24-C25-C26
26	G	102	CDL	O1-C1-CB2-OB2
27	C	309	PEK	C14-C15-C16-C17
26	G	102	CDL	C60-C61-C62-C63

There are no ring outliers.

57 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	202	EDO	5	0
18	A	606	AZI	1	0
27	P	309	PEK	1	0
19	P	305	PGV	2	0
22	G	103	CHD	1	0
20	N	611	EDO	1	0
27	G	101	PEK	4	0
14	A	601	HEA	8	0
27	C	309	PEK	2	0
14	N	602[A]	HEA	9	0
22	C	306	CHD	1	0
14	N	601	HEA	3	0
21	D	201	TGL	7	0
20	H	101	EDO	1	0
18	N	606	AZI	1	0
20	A	621	EDO	1	0
24	C	302	DMU	4	0
27	T	101	PEK	3	0
14	N	602[B]	HEA	7	0
20	C	315	EDO	2	0
26	T	102	CDL	4	0

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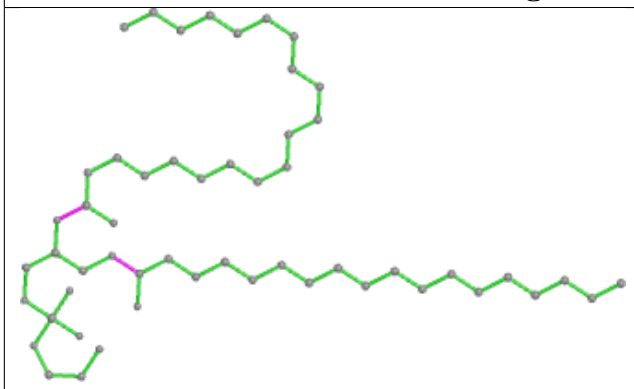
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	301	TGL	1	0
21	Y	101	TGL	6	0
20	A	618	EDO	1	0
19	A	608	PGV	2	0
20	Q	204	EDO	1	0
22	C	301	CHD	1	0
21	L	101	TGL	5	0
20	A	617	EDO	2	0
20	D	203	EDO	3	0
20	A	611	EDO	1	0
20	A	614	EDO	1	0
26	P	306	CDL	8	0
19	Z	101	PGV	3	0
18	N	607	AZI	6	0
14	A	602[B]	HEA	9	0
20	S	104	EDO	1	0
20	N	616	EDO	1	0
28	O	302	PSC	5	0
19	P	303	PGV	1	0
14	A	602[A]	HEA	6	0
26	C	305	CDL	14	0
19	C	308	PGV	4	0
22	W	101	CHD	4	0
22	P	307	CHD	3	0
19	C	304	PGV	1	0
22	J	101	CHD	1	0
24	C	310	DMU	1	0
20	A	612	EDO	3	0
19	A	609	PGV	4	0
18	A	607	AZI	4	0
21	Q	201	TGL	2	0
21	N	609	TGL	2	0
20	N	617	EDO	1	0
26	G	102	CDL	7	0
20	P	312	EDO	1	0
28	E	201	PSC	5	0

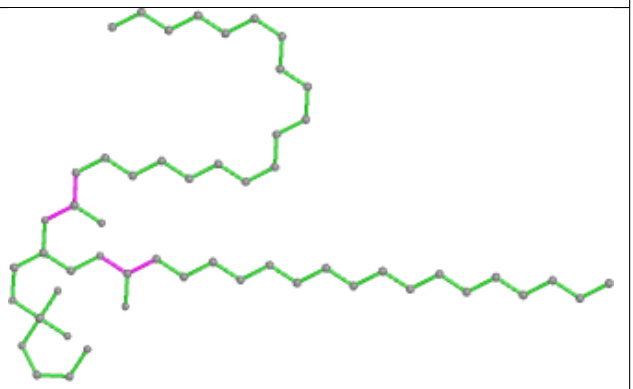
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

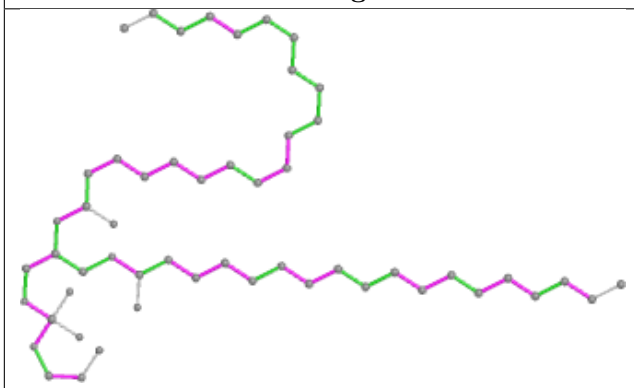
Ligand PEK P 309



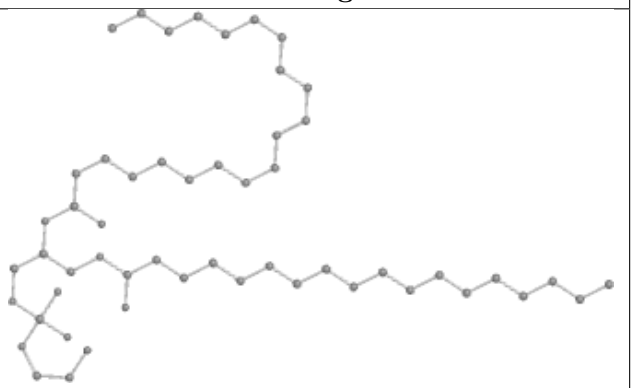
Bond lengths



Bond angles

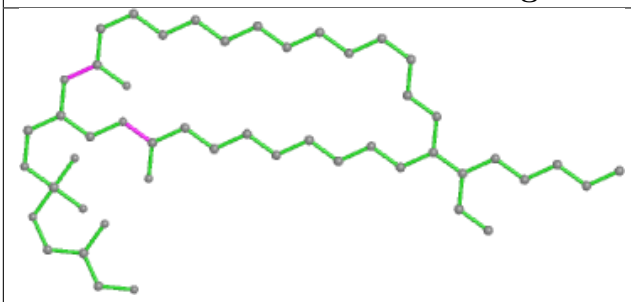


Torsions

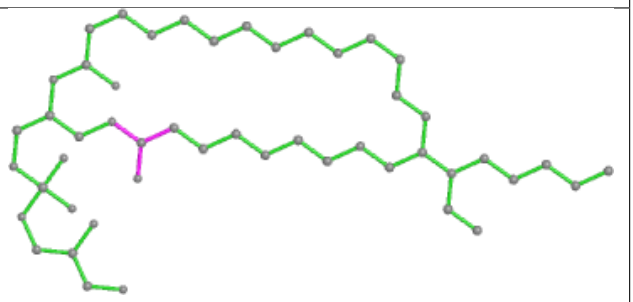


Rings

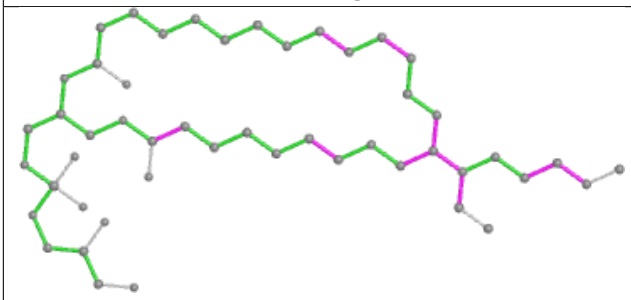
Ligand PGV N 608



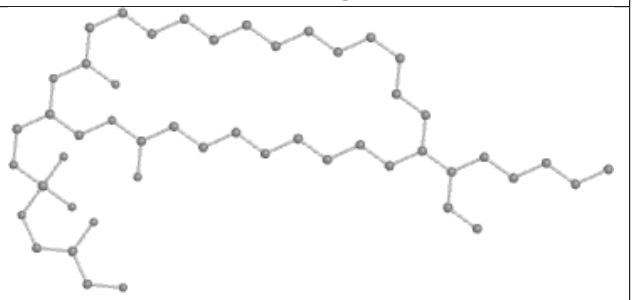
Bond lengths



Bond angles

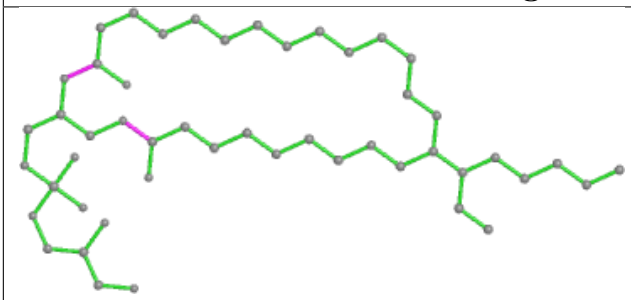


Torsions

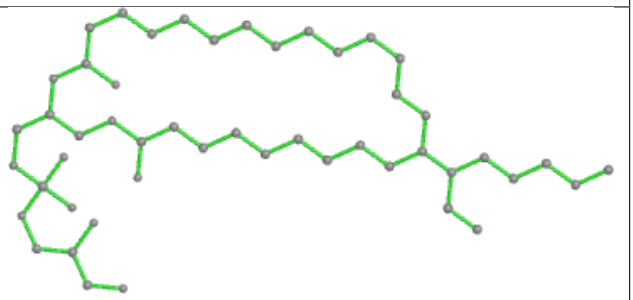


Rings

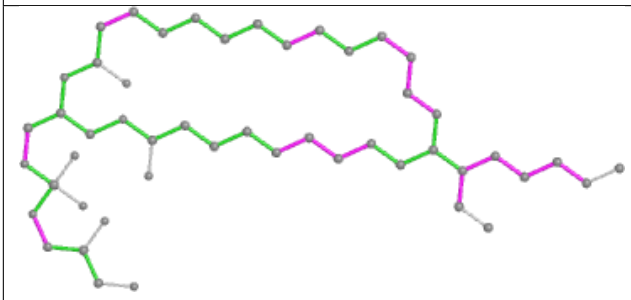
Ligand PGV P 305



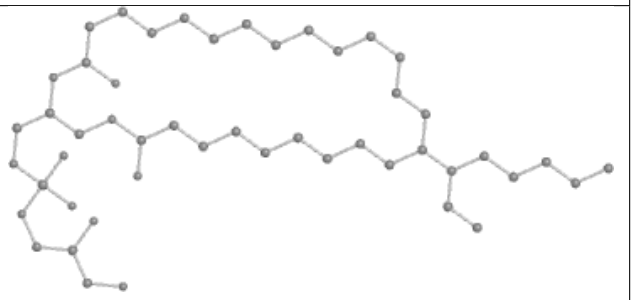
Bond lengths



Bond angles

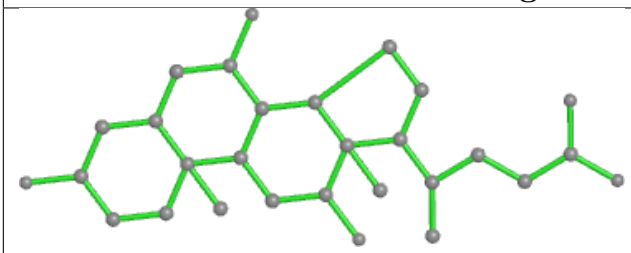


Torsions

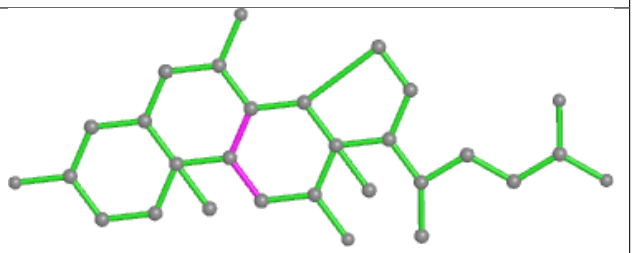


Rings

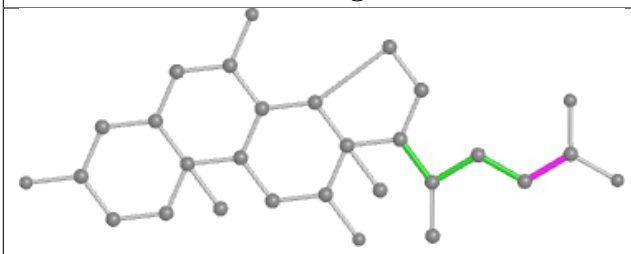
Ligand CHD G 103



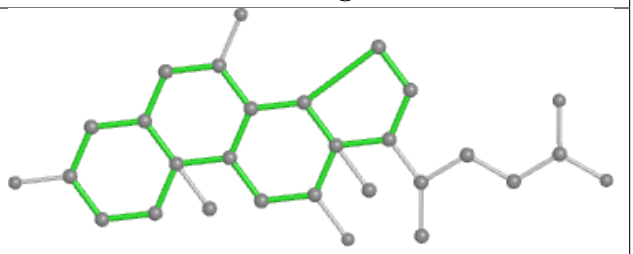
Bond lengths



Bond angles

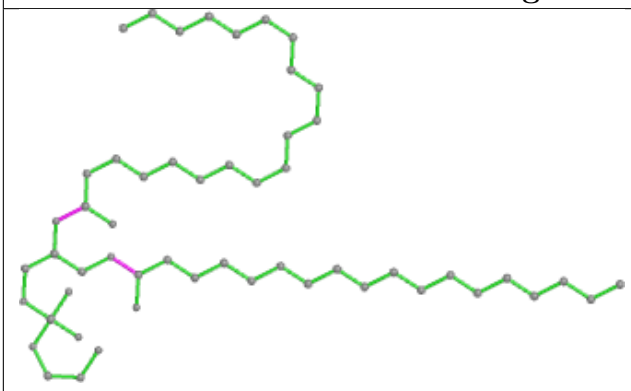


Torsions

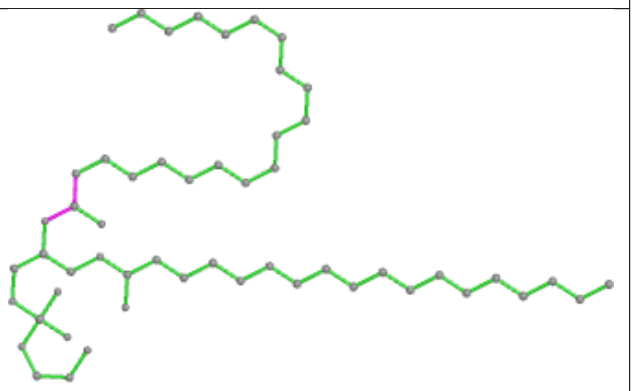


Rings

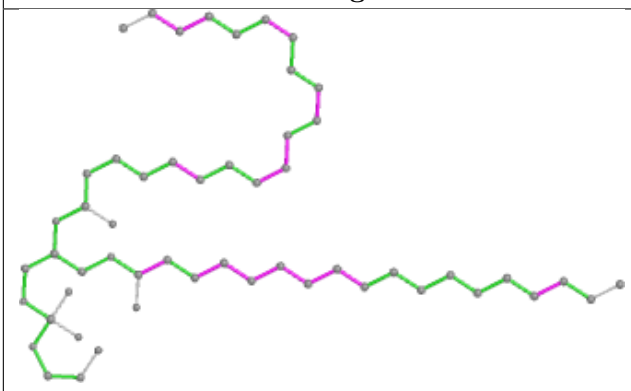
Ligand PEK G 101



Bond lengths



Bond angles



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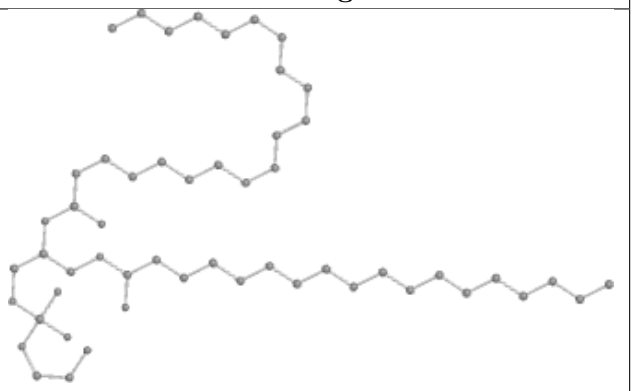
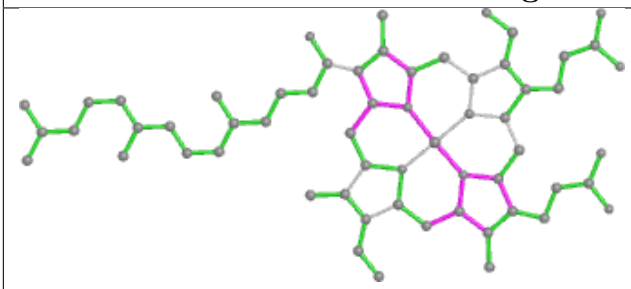


Rings

Ligand HEA A 601



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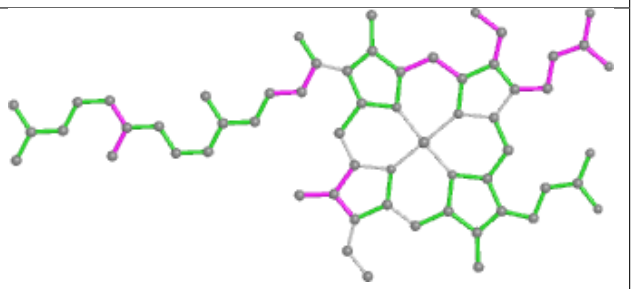
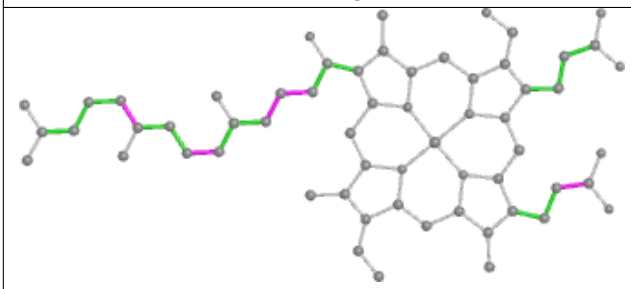
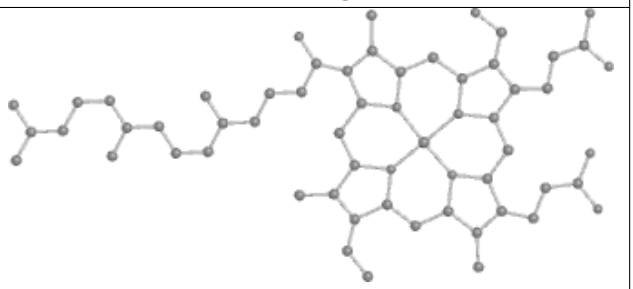


Bond angles

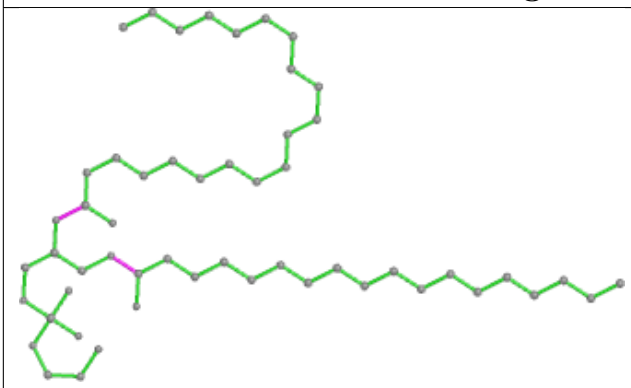


Torsions



Rings

Ligand PEK C 309



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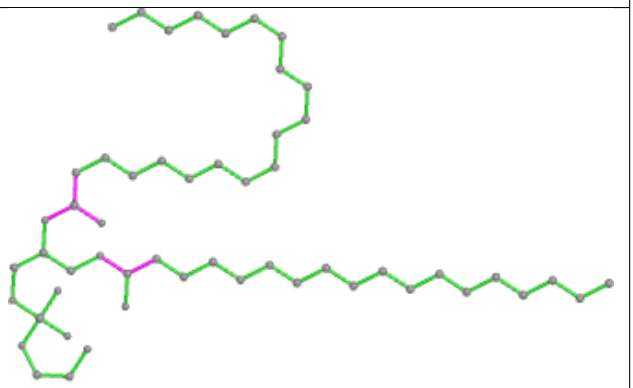
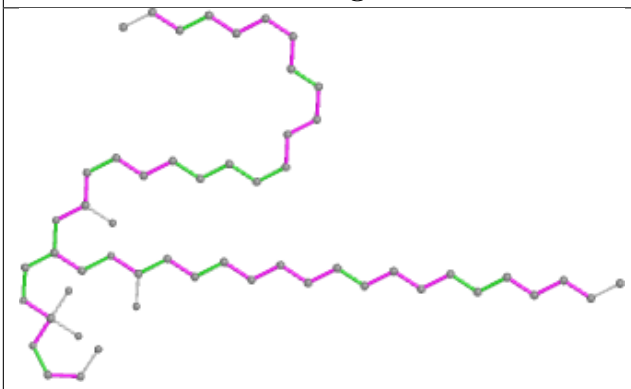
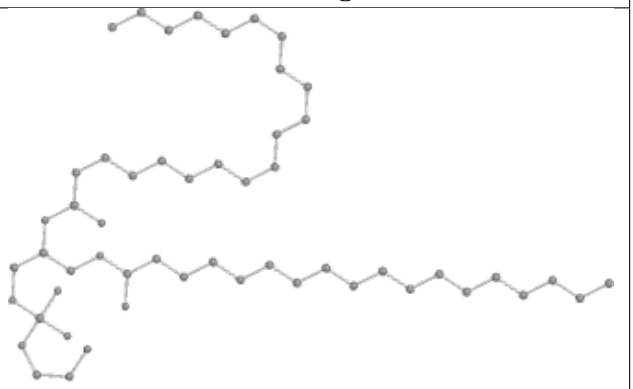


Bond angles

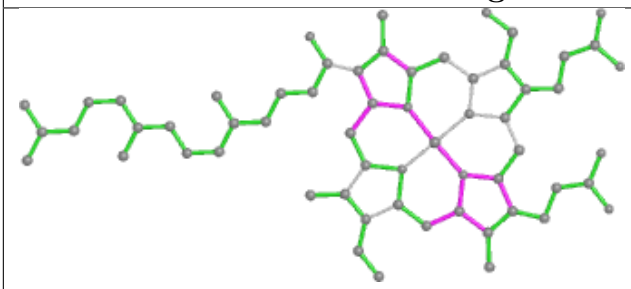


Torsions



Rings

Ligand HEA N 602 (A)



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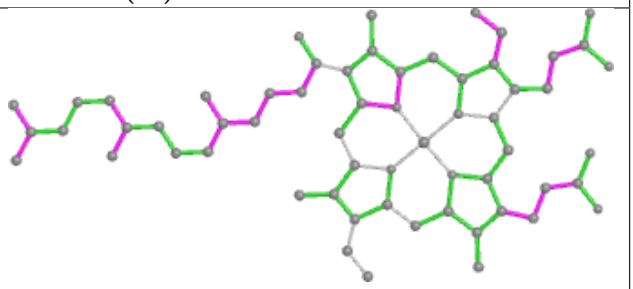
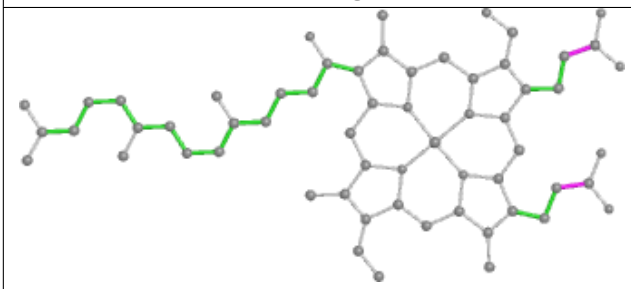


Bond angles



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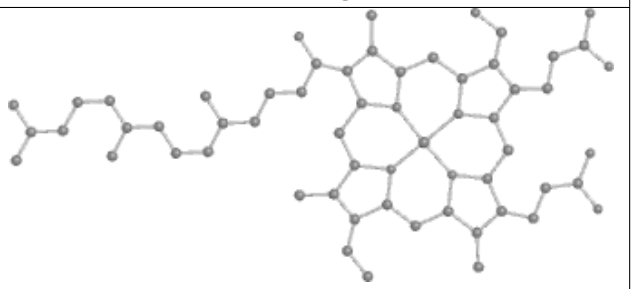
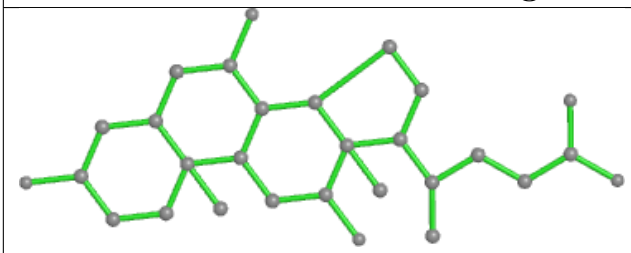


Rings

Ligand CHD C 306



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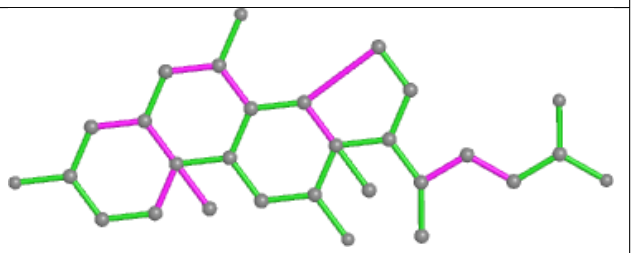
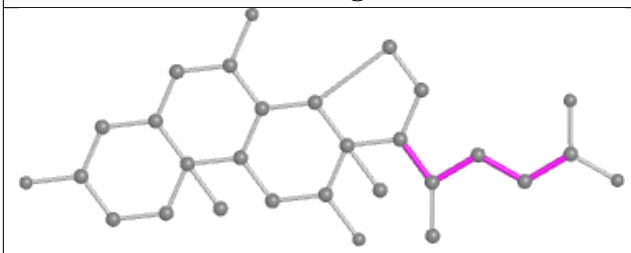
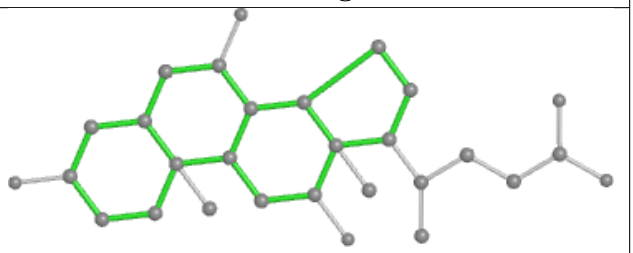


Bond angles

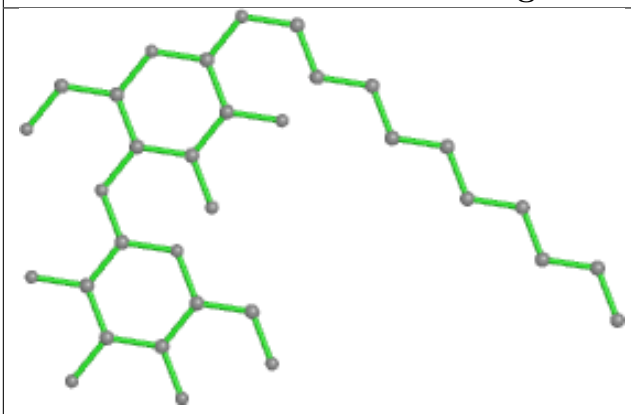


Torsions



Rings

Ligand DMU P 311



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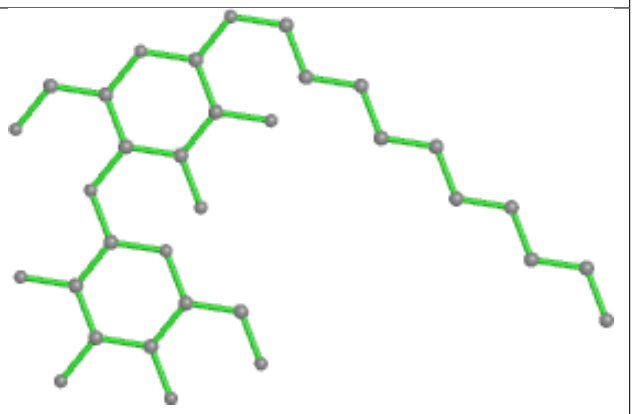
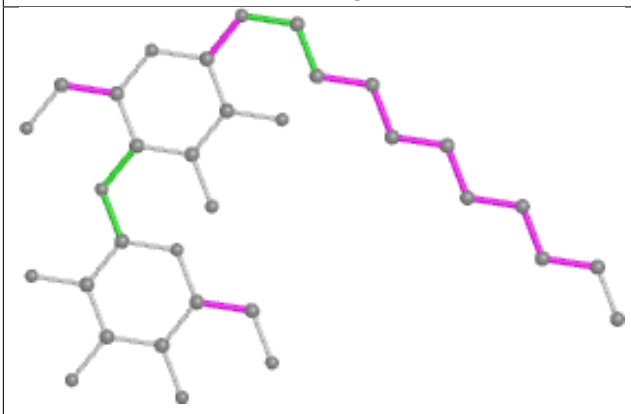
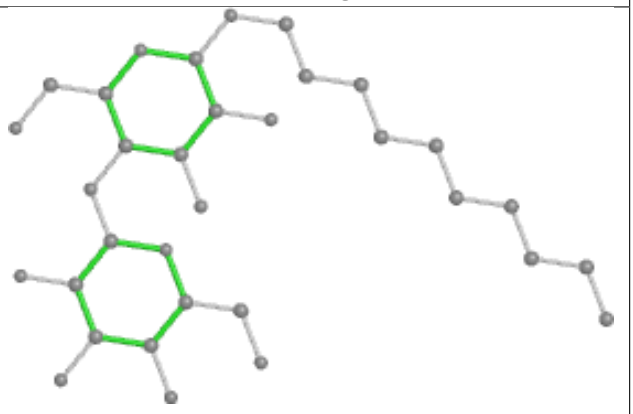


Bond angles

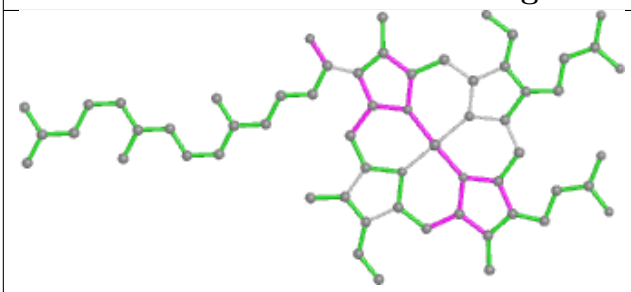


Torsions

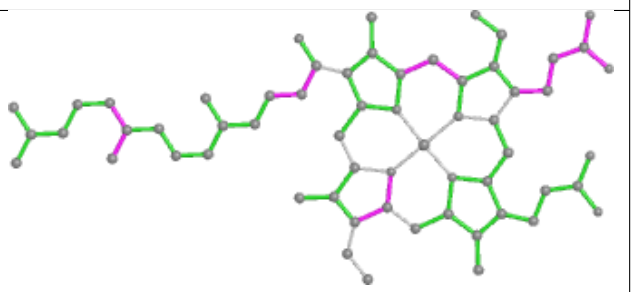


Rings

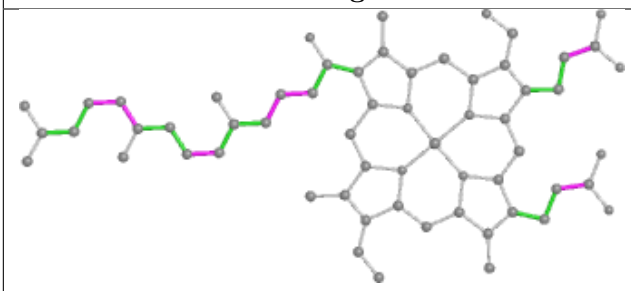
Ligand HEA N 601



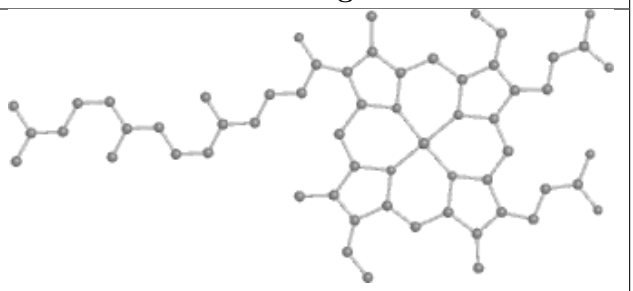
Bond lengths



Bond angles

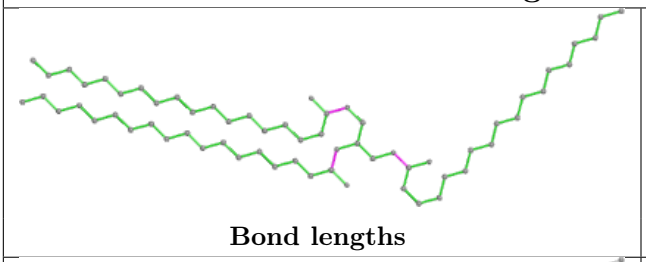


Torsions



Rings

Ligand TGL D 201



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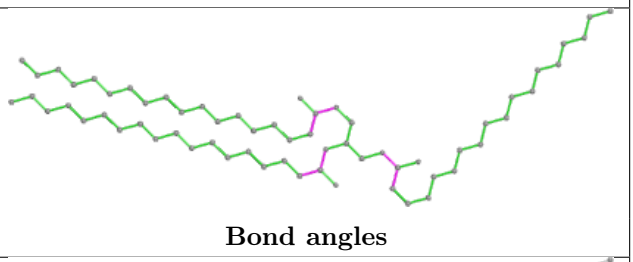
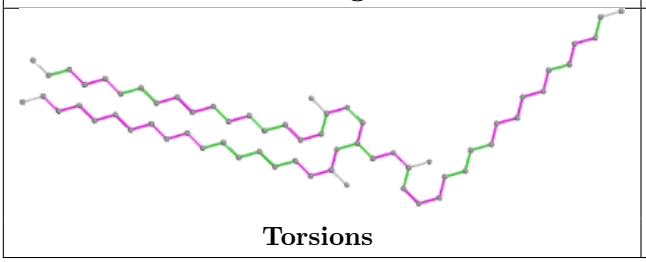
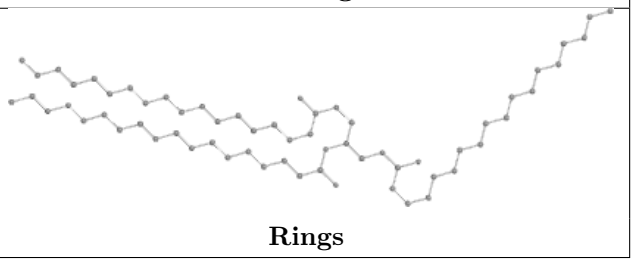


Bond angles

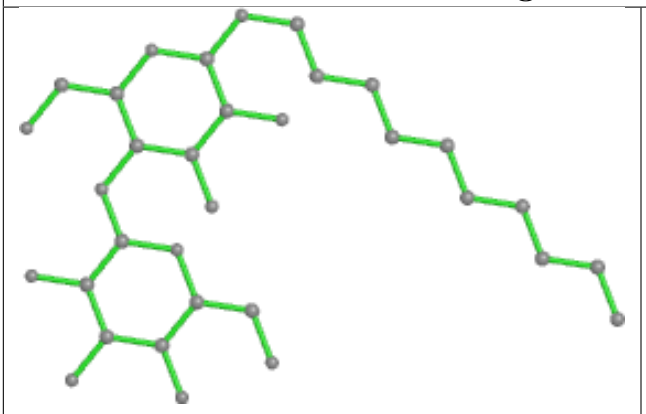


Torsions



Rings

Ligand DMU C 302



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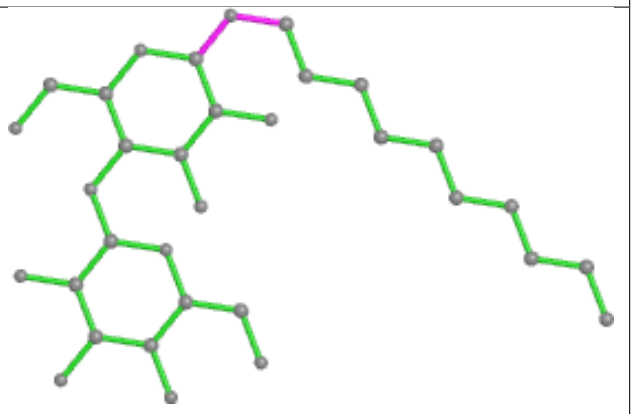
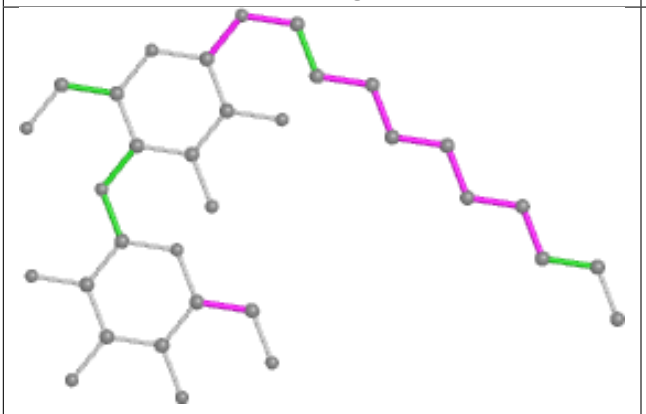
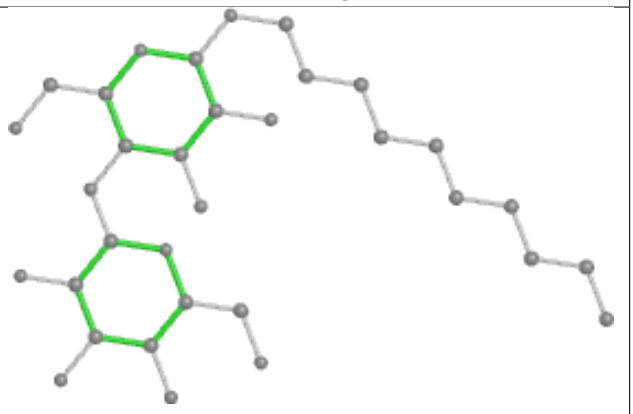


Bond angles

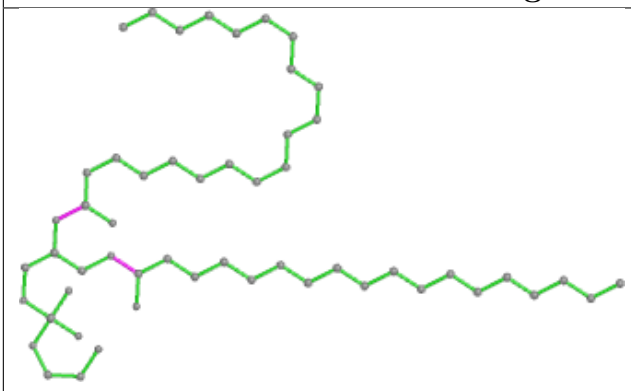


Torsions



Rings

Ligand PEK T 101



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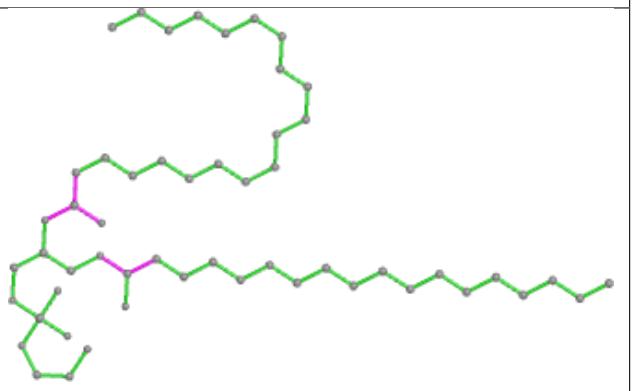
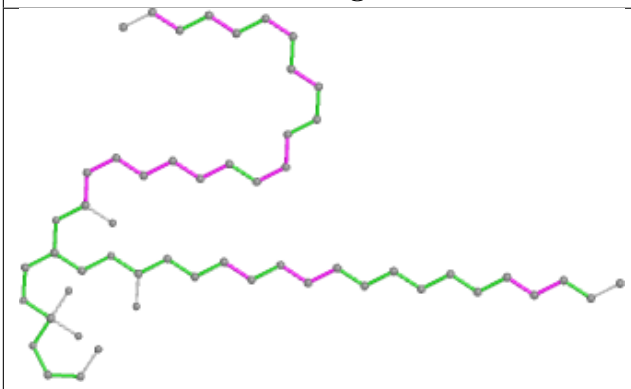
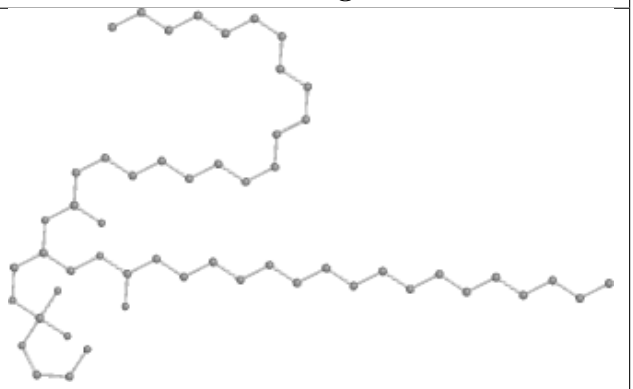


Bond angles

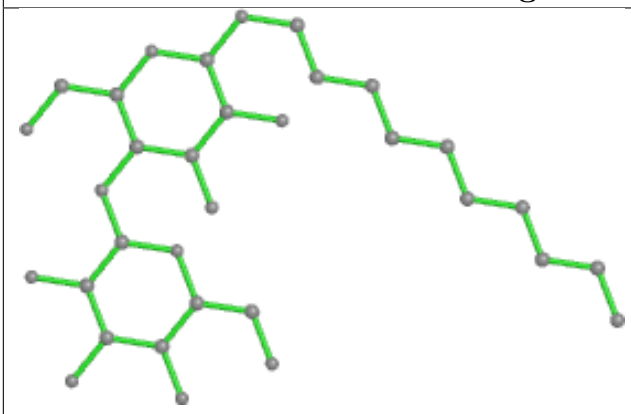


Torsions

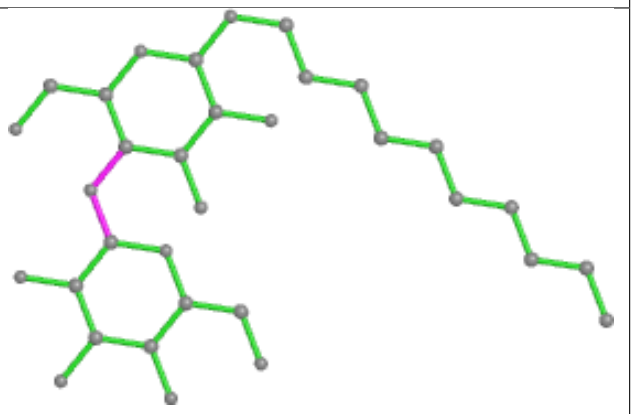


Rings

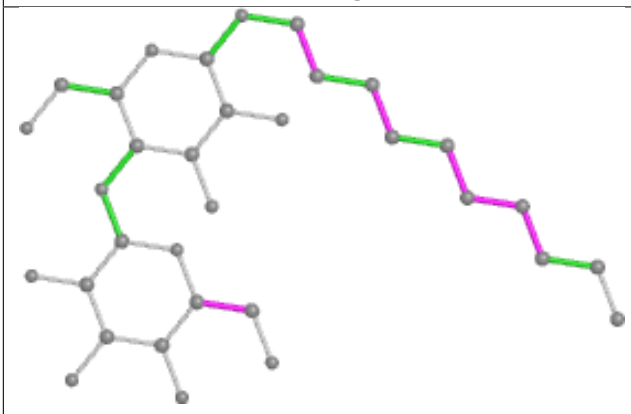
Ligand DMU Z 102



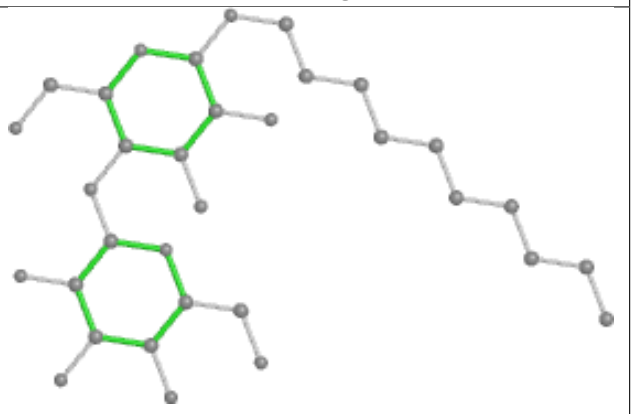
Bond lengths



Bond angles

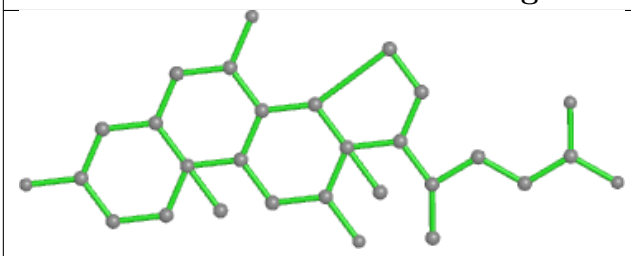


Torsions

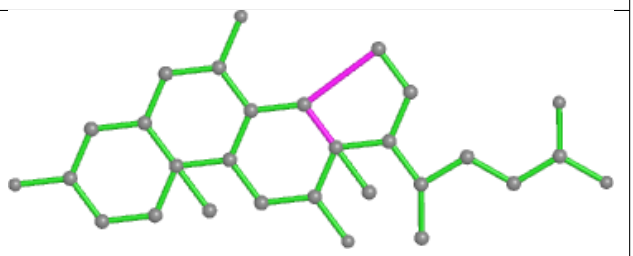


Rings

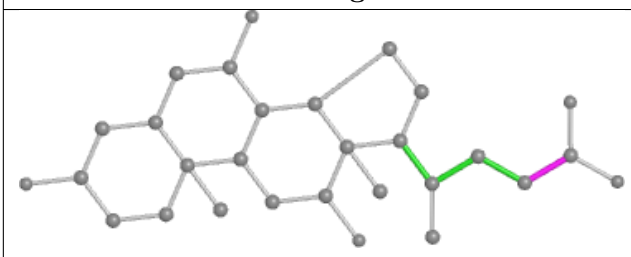
Ligand CHD B 302



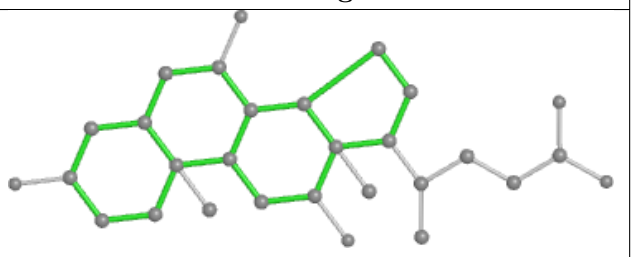
Bond lengths



Bond angles

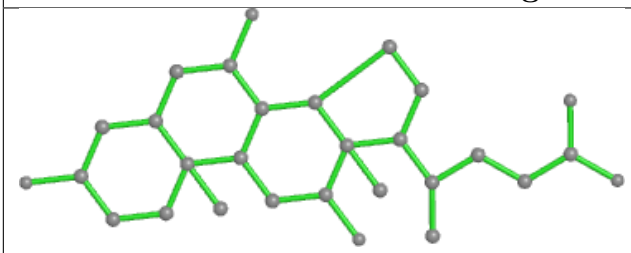


Torsions

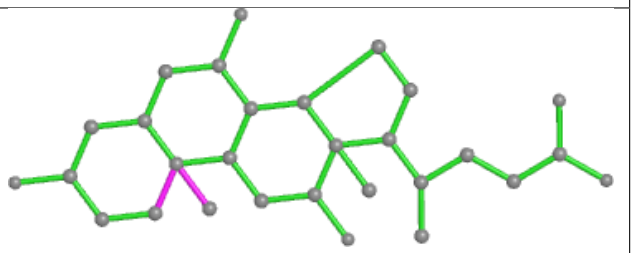


Rings

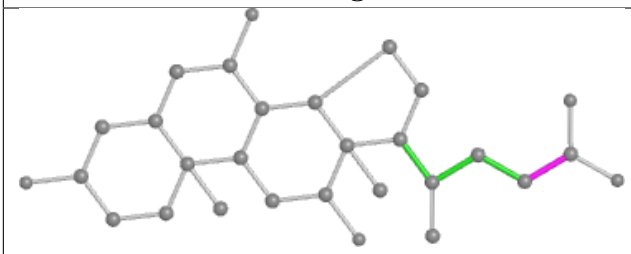
Ligand CHD P 301



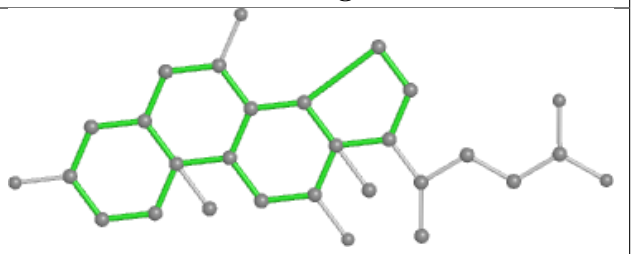
Bond lengths



Bond angles

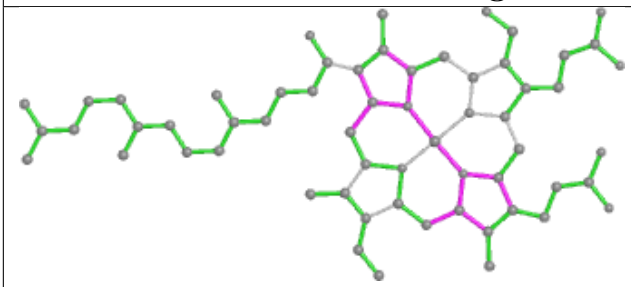


Torsions

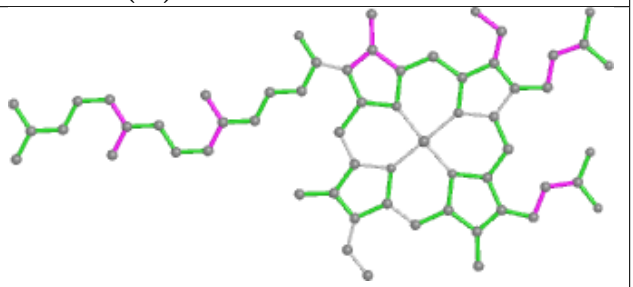


Rings

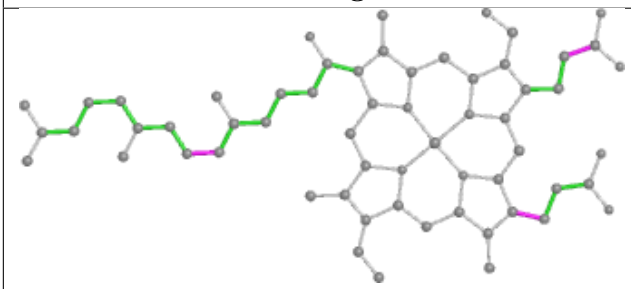
Ligand HEA N 602 (B)



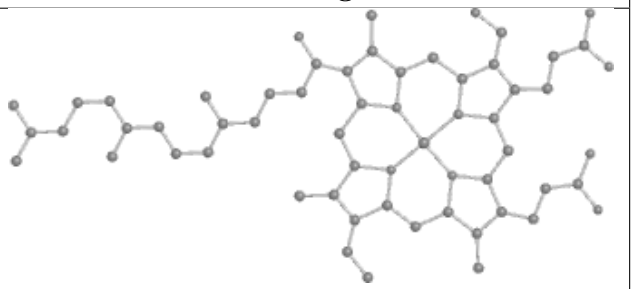
Bond lengths



Bond angles

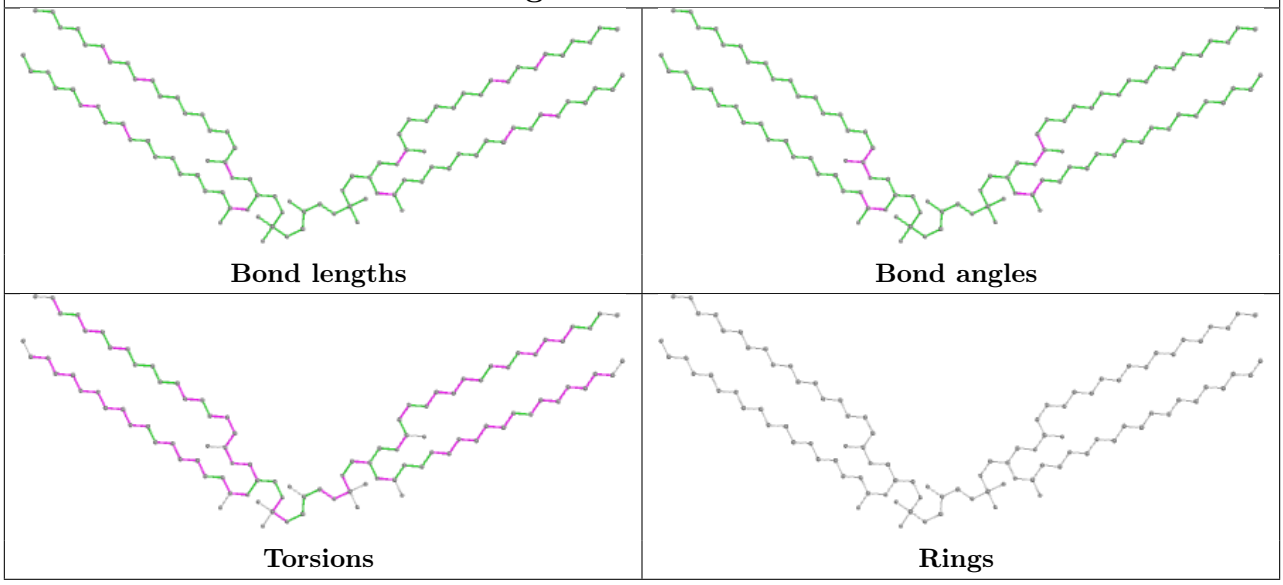


Torsions

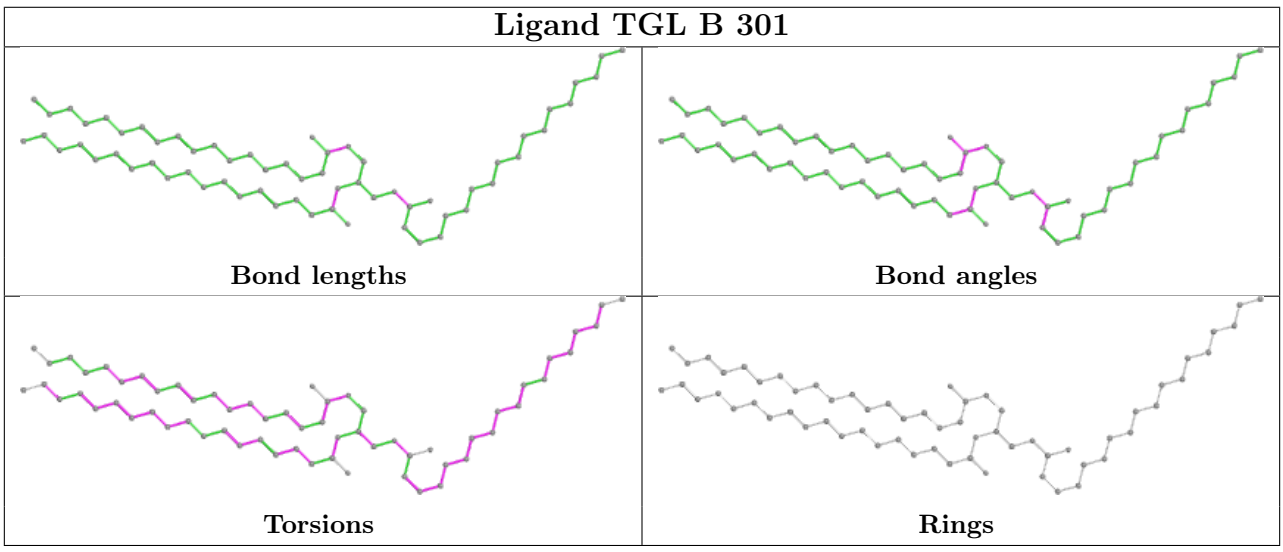


Rings

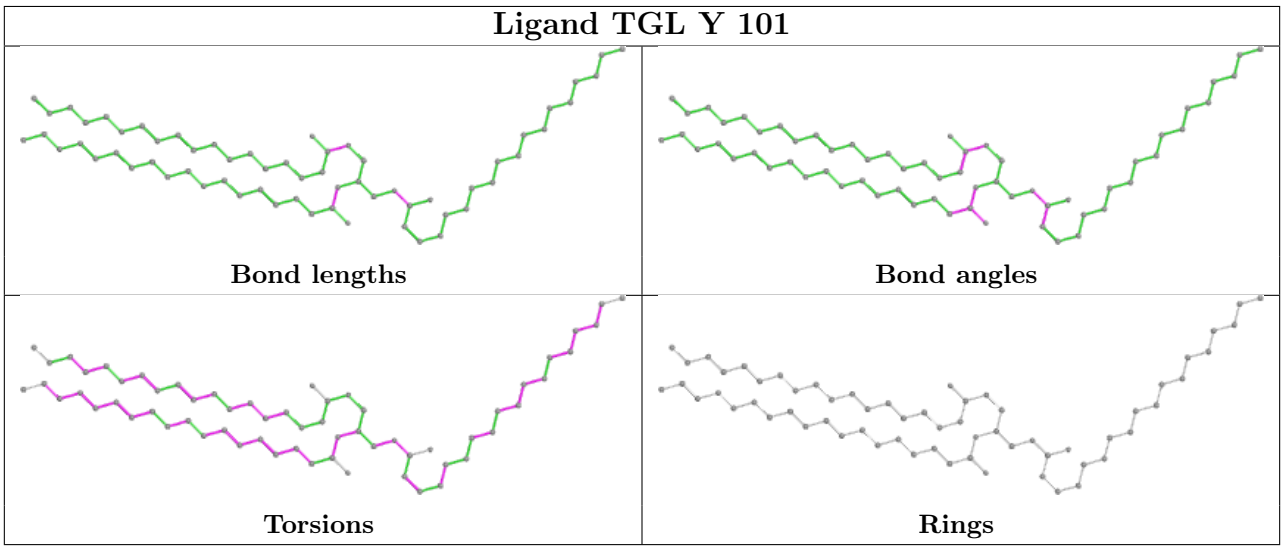
Ligand CDL T 102



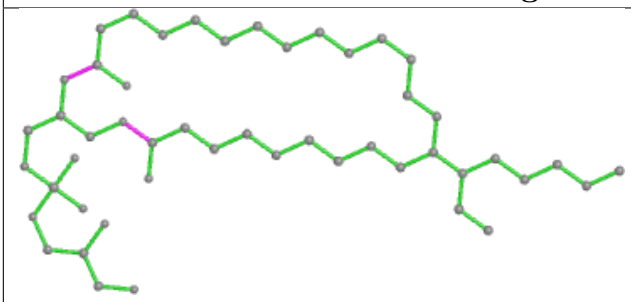
Ligand TGL B 301



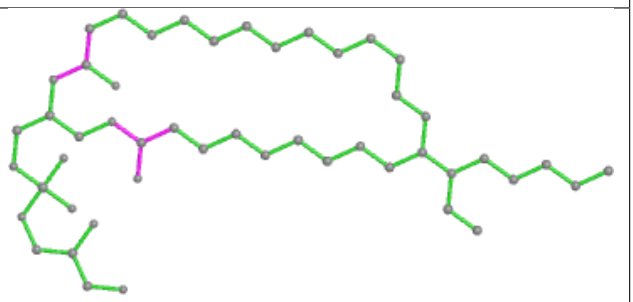
Ligand TGL Y 101



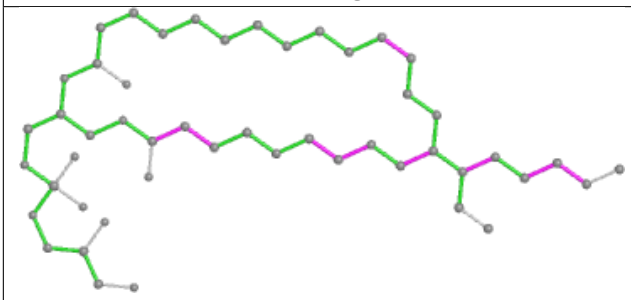
Ligand PGV A 608



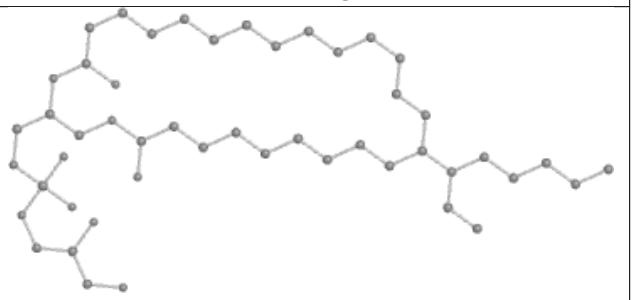
Bond lengths



Bond angles

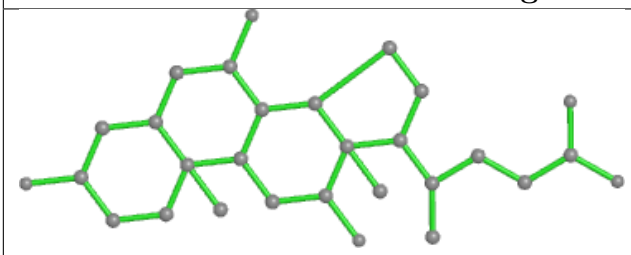


Torsions

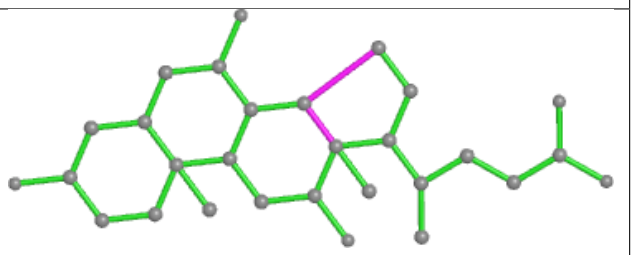


Rings

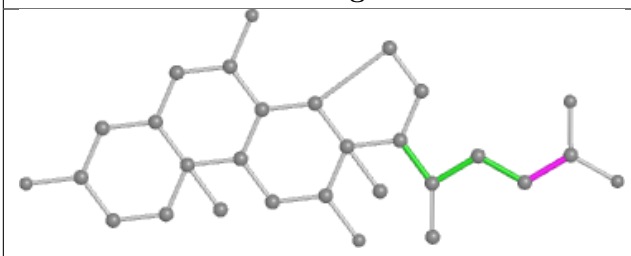
Ligand CHD C 301



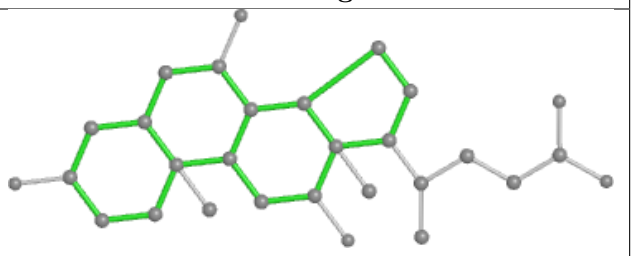
Bond lengths



Bond angles

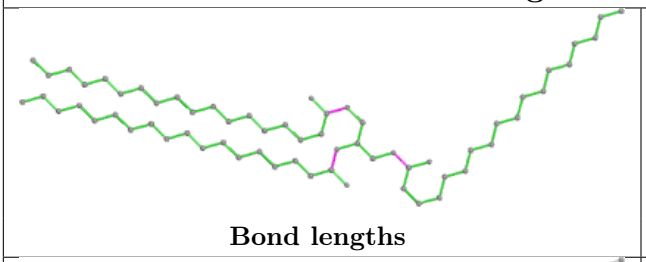


Torsions

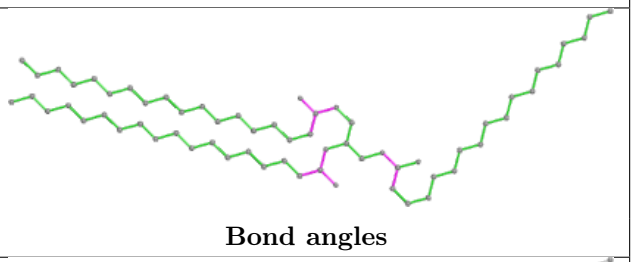


Rings

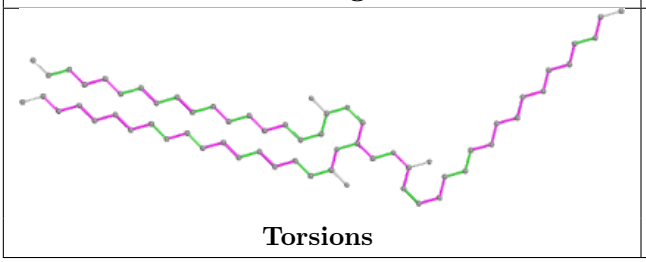
Ligand TGL L 101



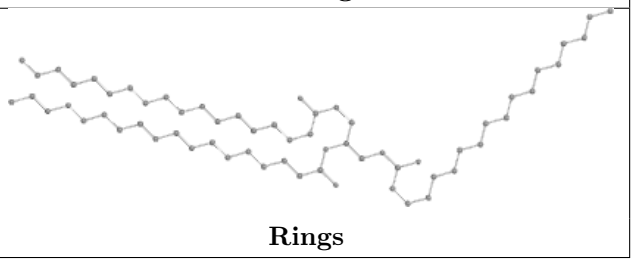
Bond lengths



Bond angles

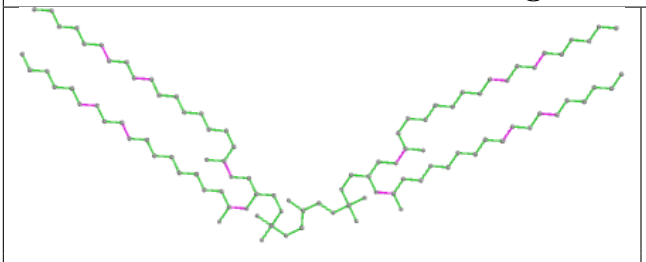


Torsions

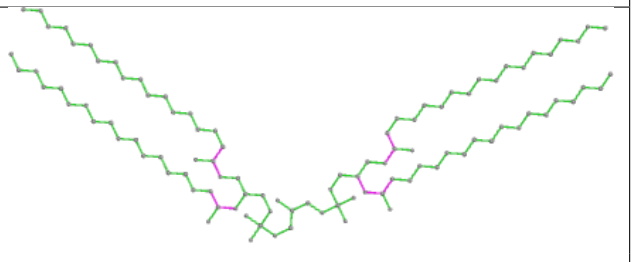


Rings

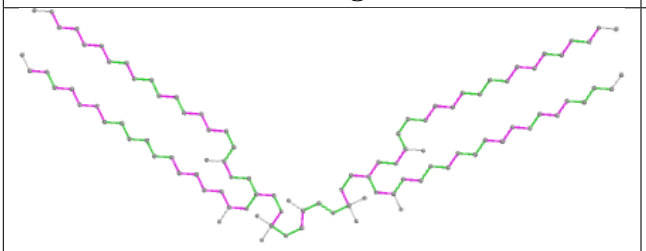
Ligand CDL P 306



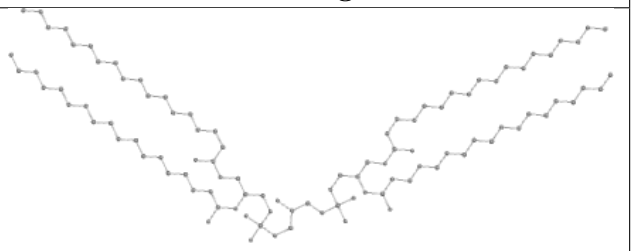
Bond lengths



Bond angles

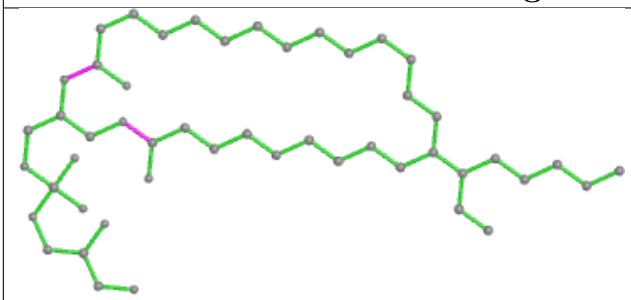


Torsions

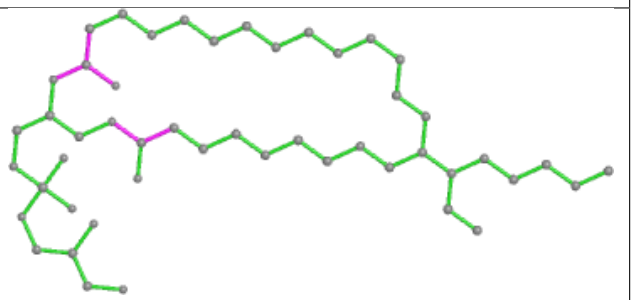


Rings

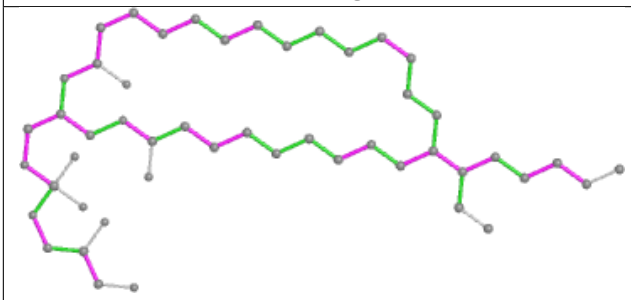
Ligand PGV Z 101



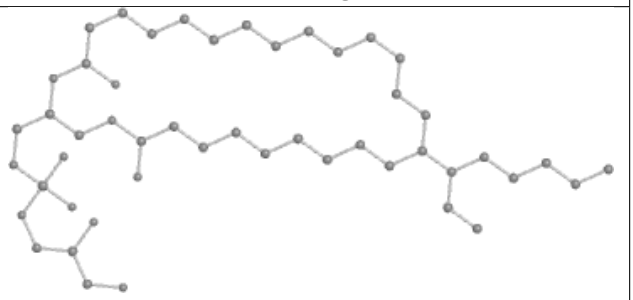
Bond lengths



Bond angles

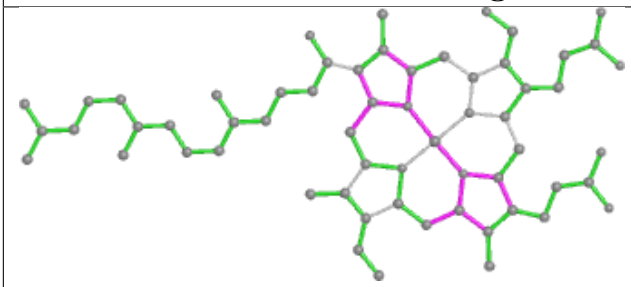


Torsions

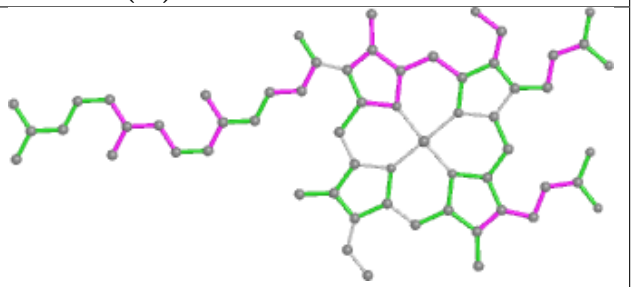


Rings

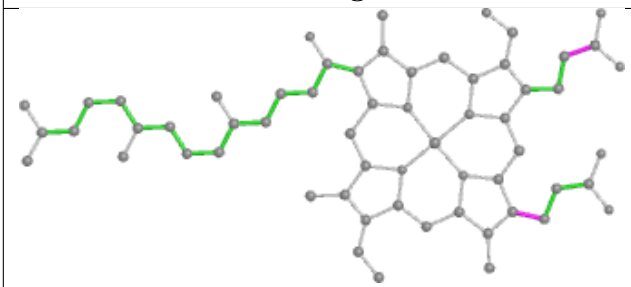
Ligand HEA A 602 (B)



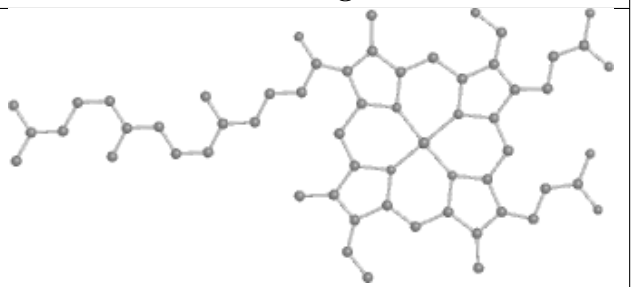
Bond lengths



Bond angles

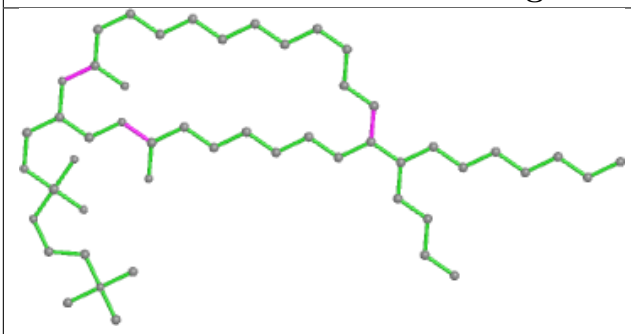


Torsions

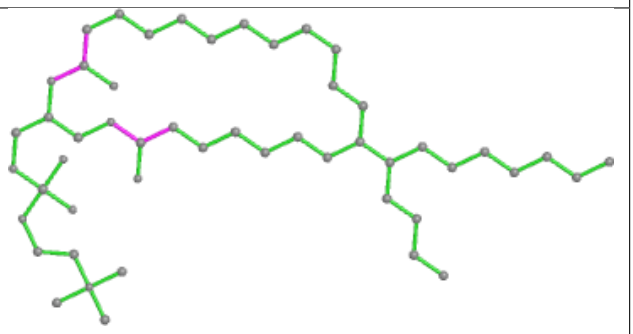


Rings

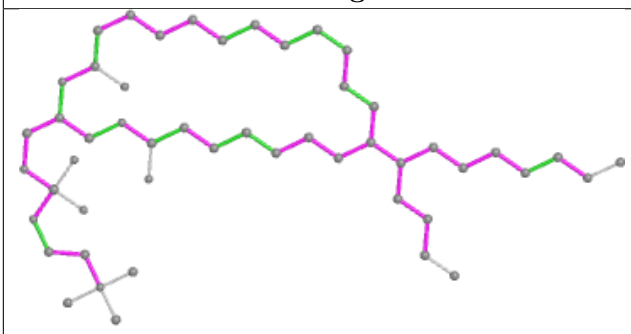
Ligand PSC O 302



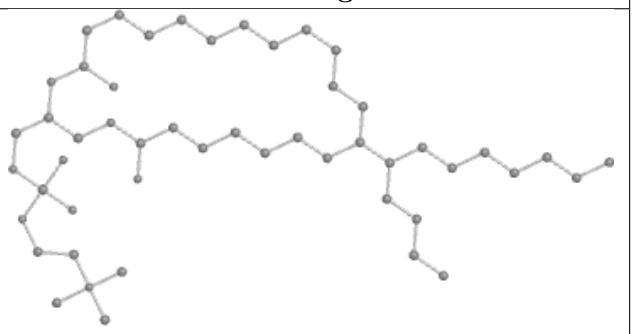
Bond lengths



Bond angles

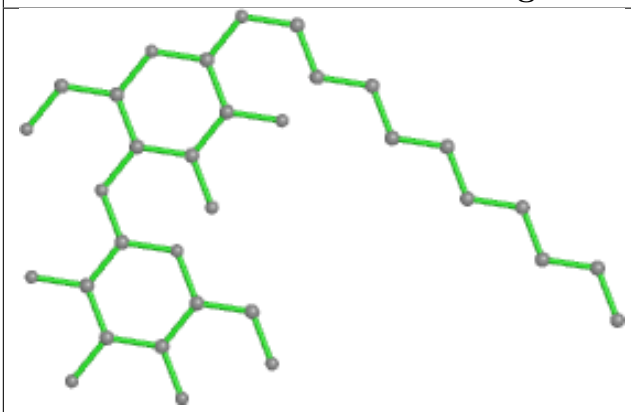


Torsions

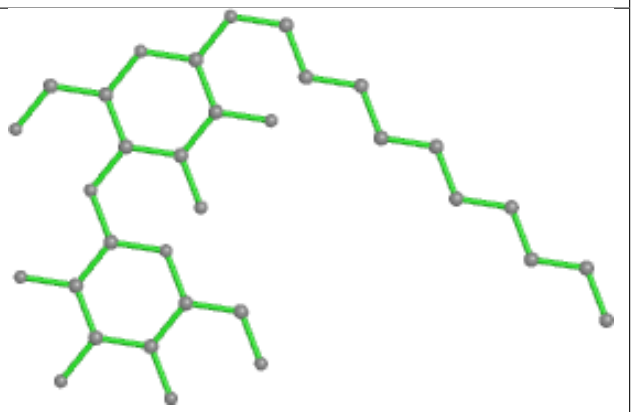


Rings

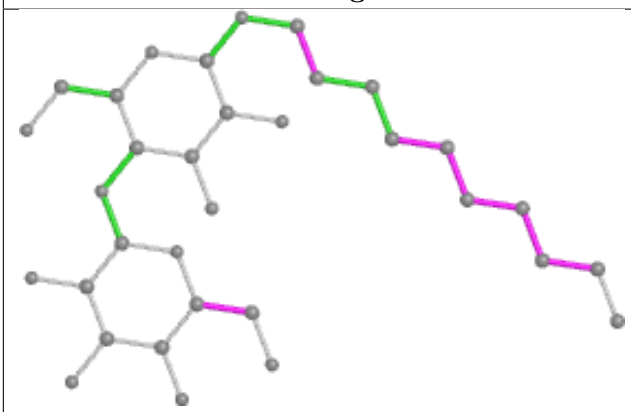
Ligand DMU P 308



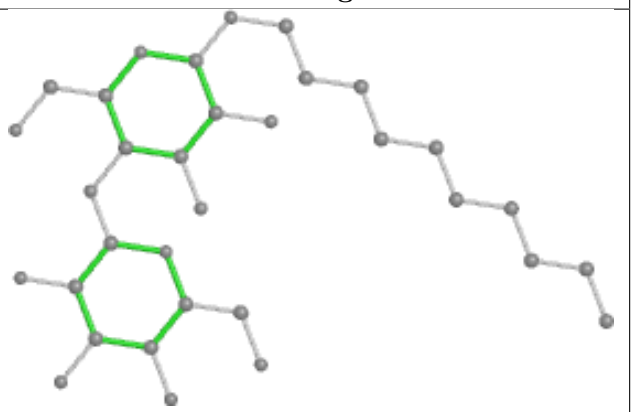
Bond lengths



Bond angles

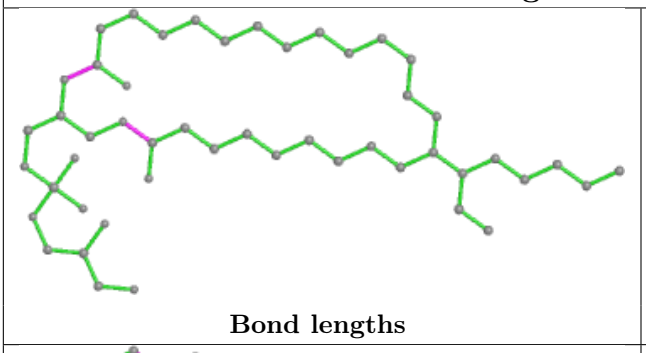


Torsions

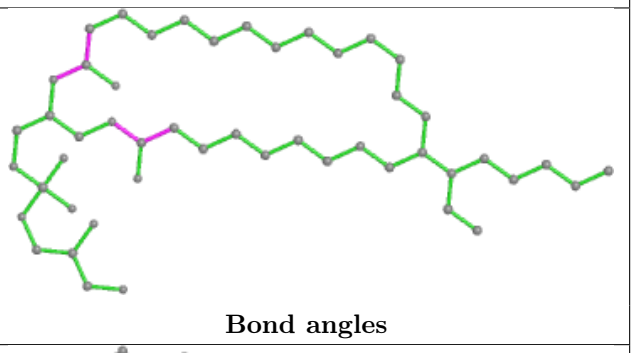


Rings

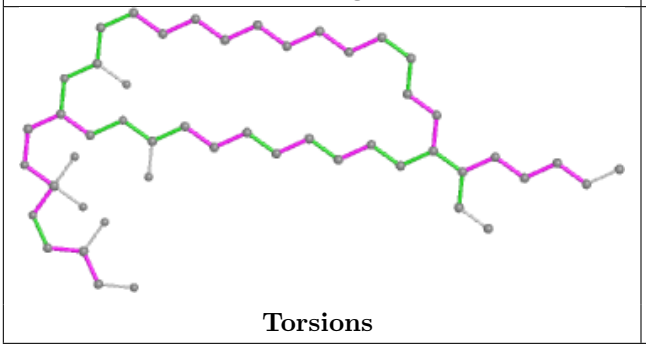
Ligand PGV P 303



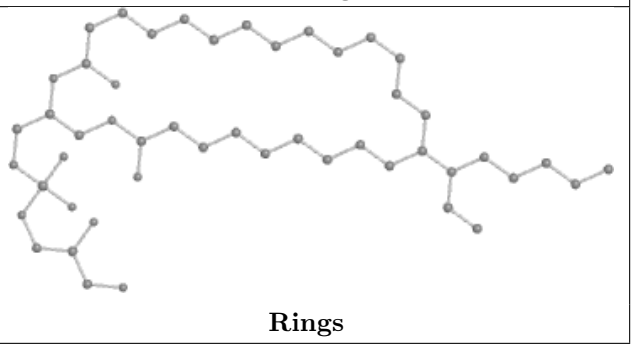
Bond lengths



Bond angles

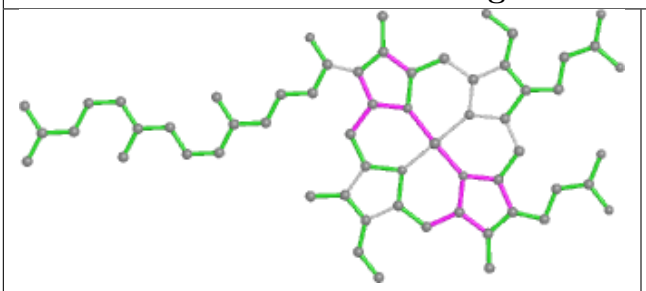


Torsions

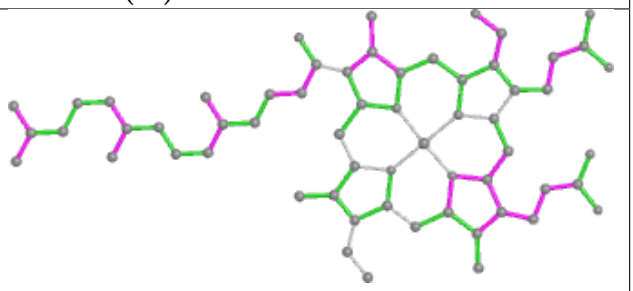


Rings

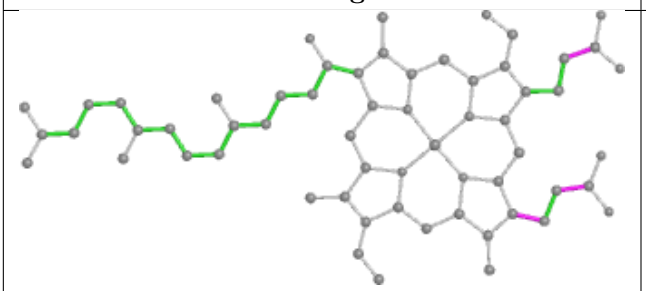
Ligand HEA A 602 (A)



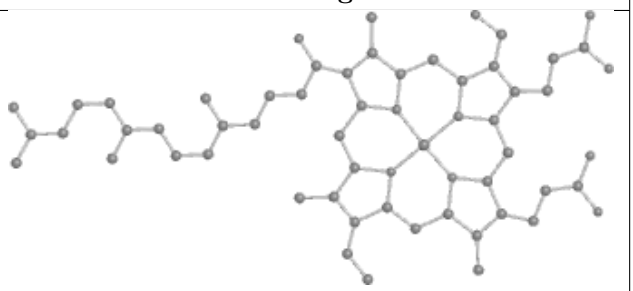
Bond lengths



Bond angles

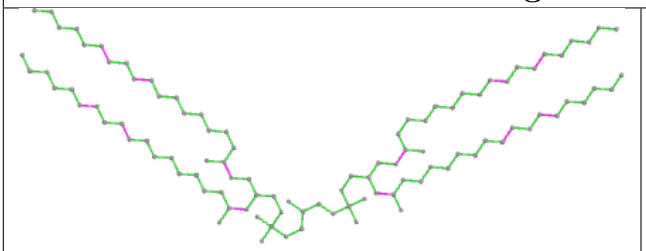


Torsions

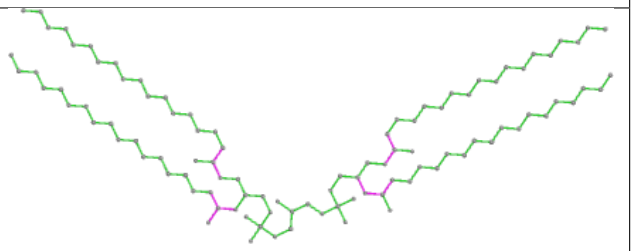


Rings

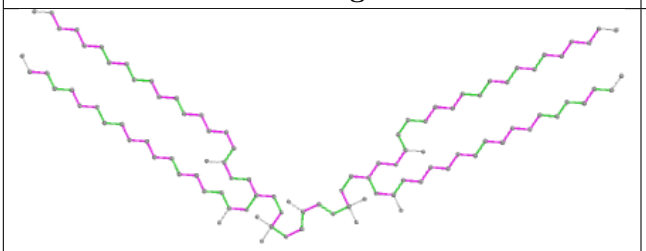
Ligand CDL C 305



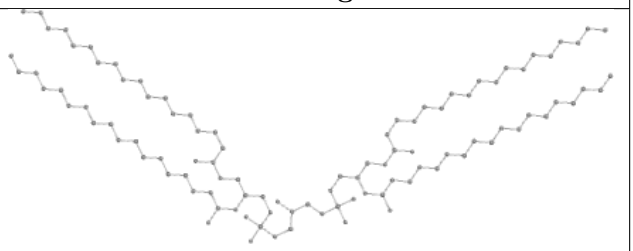
Bond lengths



Bond angles

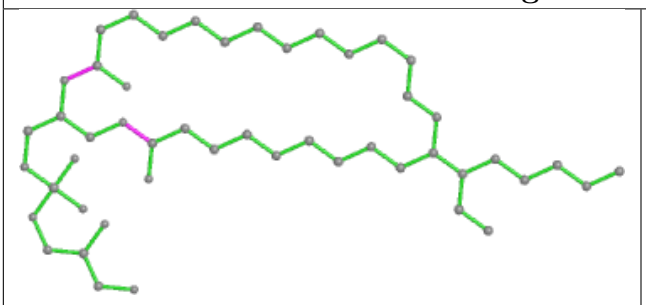


Torsions

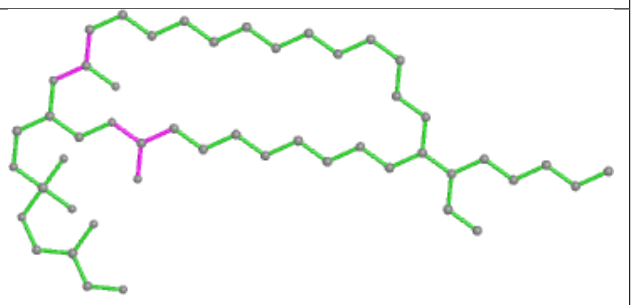


Rings

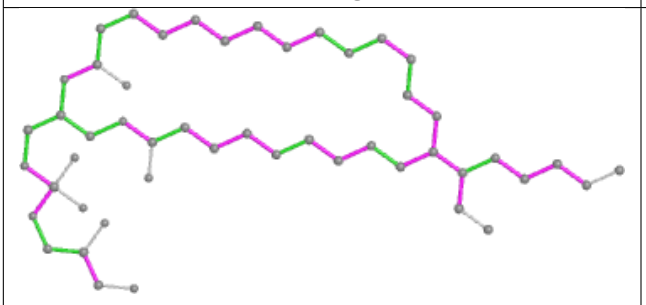
Ligand PGV C 308



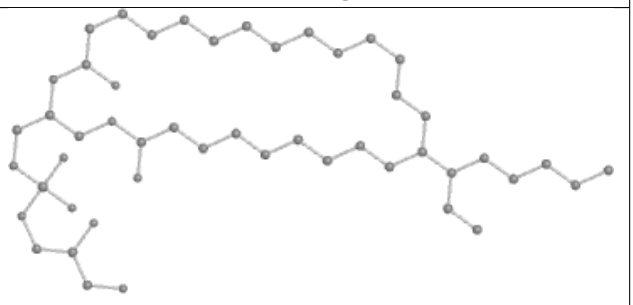
Bond lengths



Bond angles

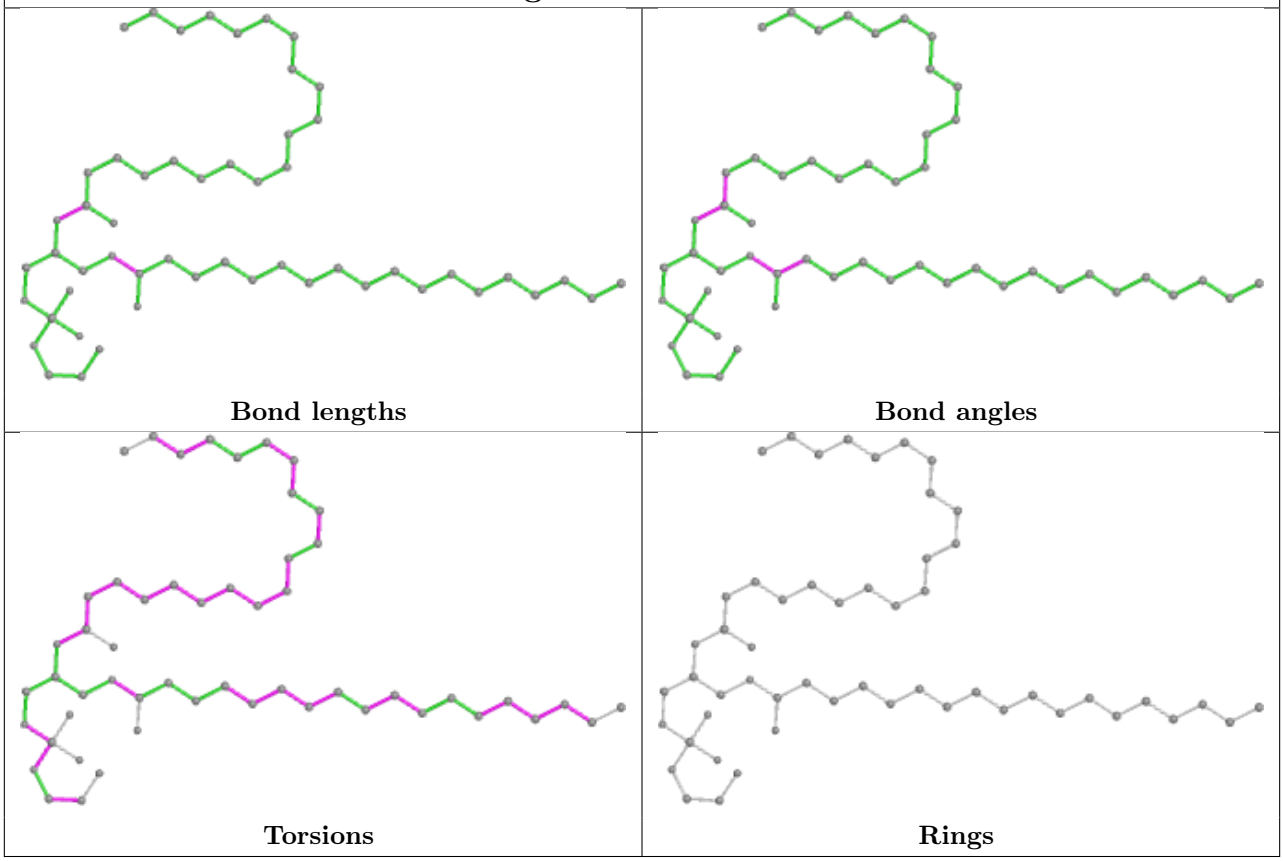


Torsions

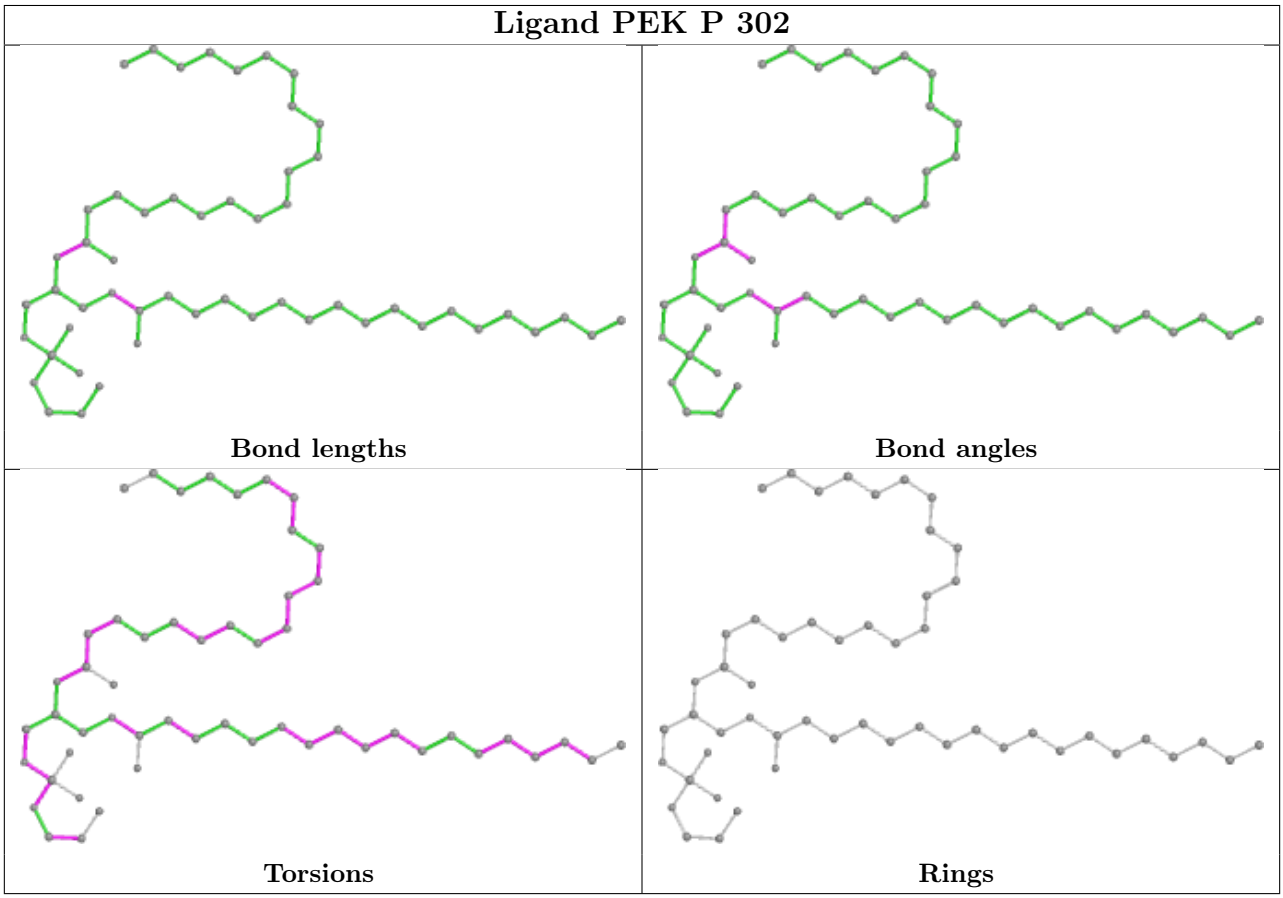


Rings

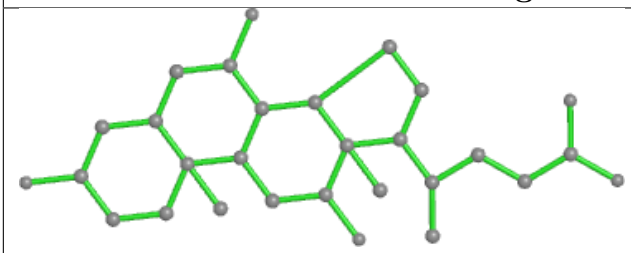
Ligand PEK C 307



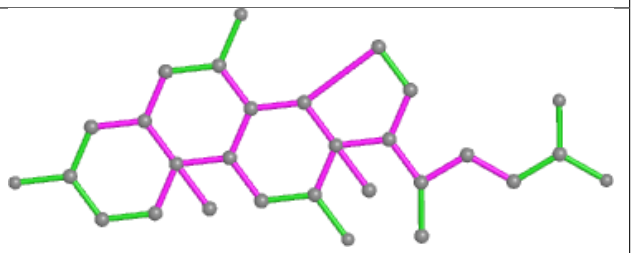
Ligand PEK P 302



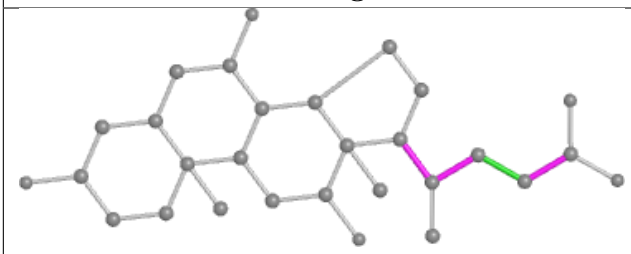
Ligand CHD W 101



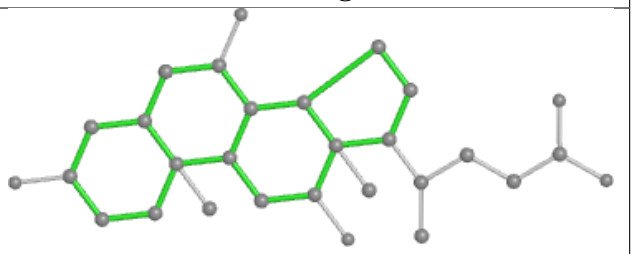
Bond lengths



Bond angles

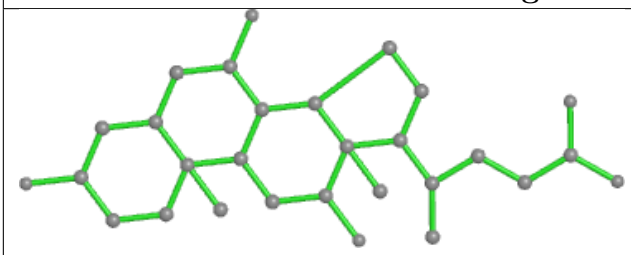


Torsions

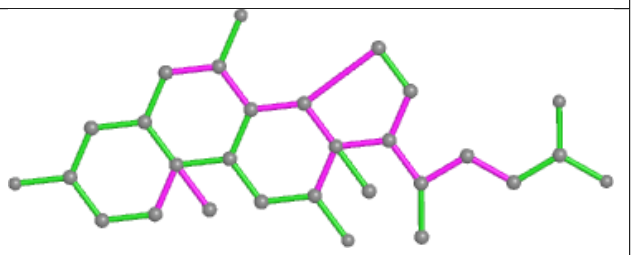


Rings

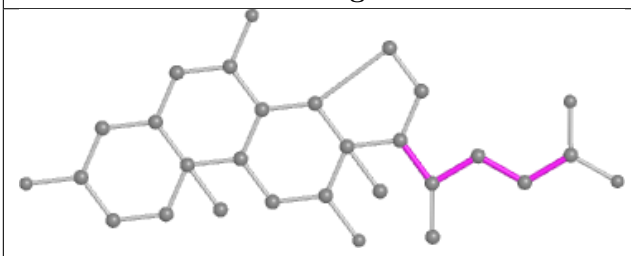
Ligand CHD P 307



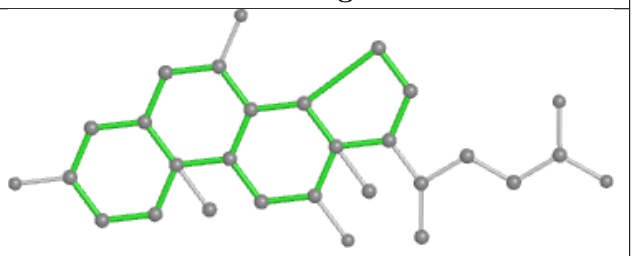
Bond lengths



Bond angles

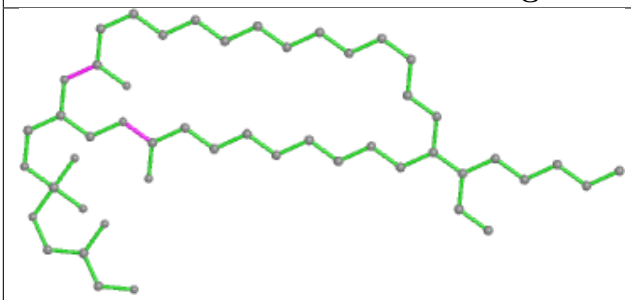


Torsions

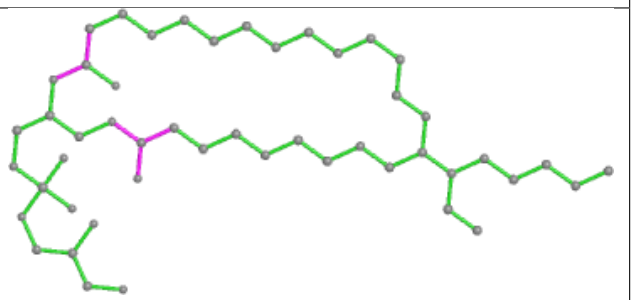


Rings

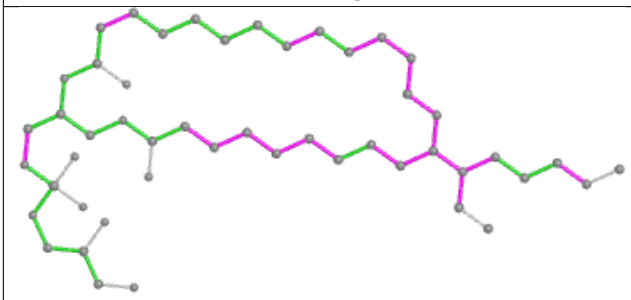
Ligand PGV C 304



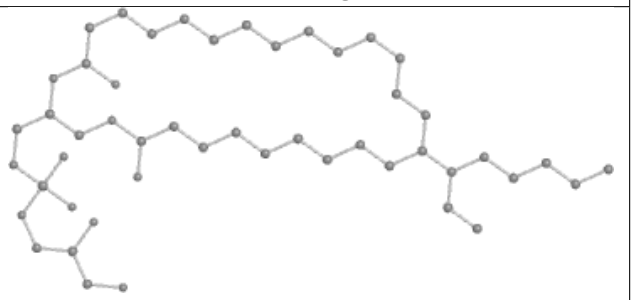
Bond lengths



Bond angles

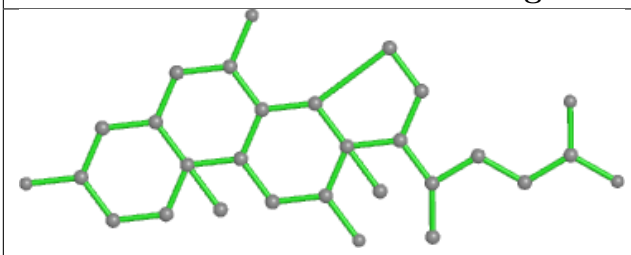


Torsions

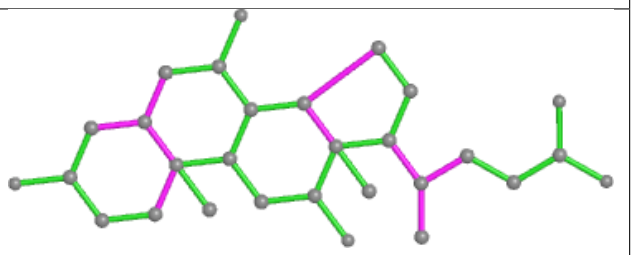


Rings

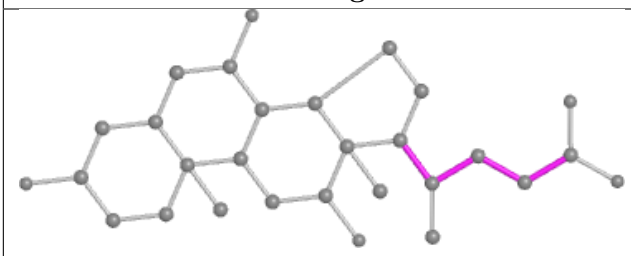
Ligand CHD J 101



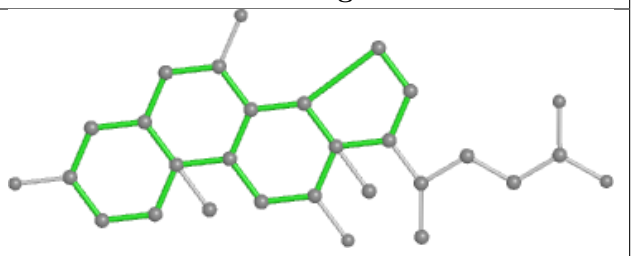
Bond lengths



Bond angles

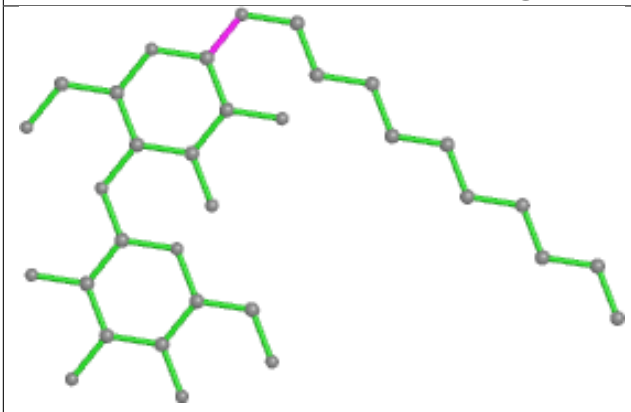


Torsions

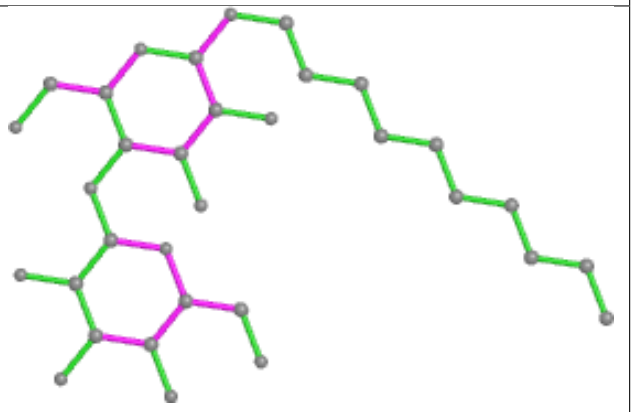


Rings

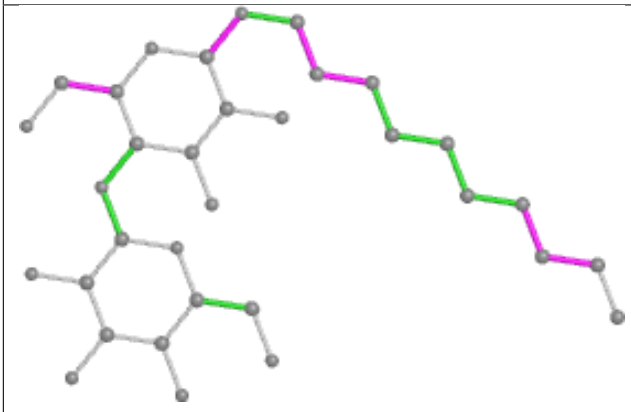
Ligand DMU C 311



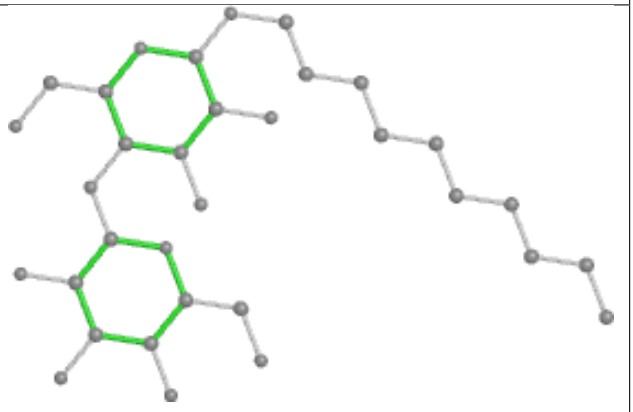
Bond lengths



Bond angles

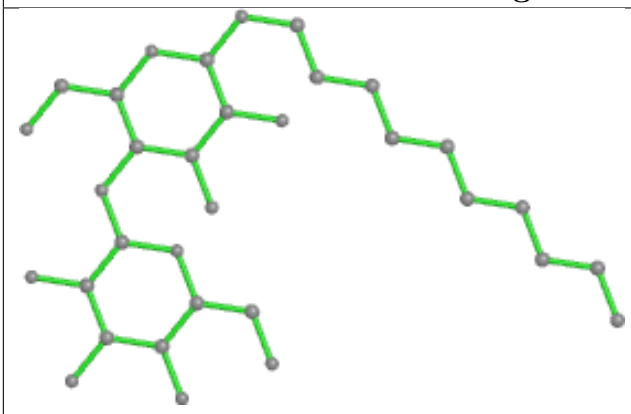


Torsions

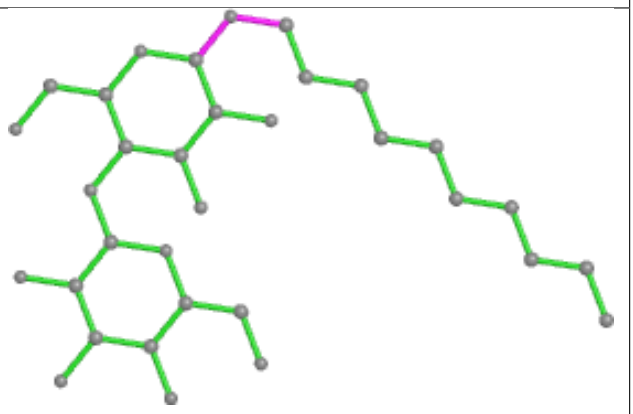


Rings

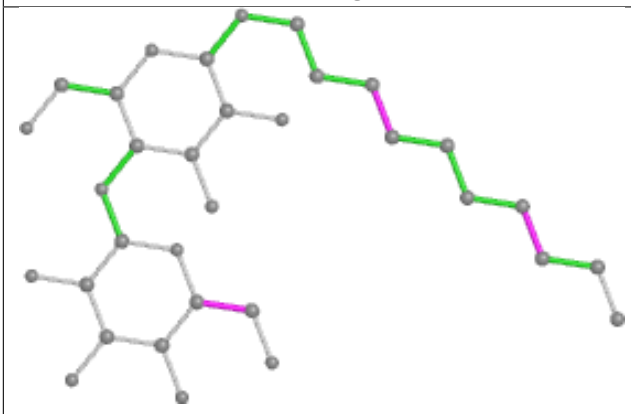
Ligand DMU M 101



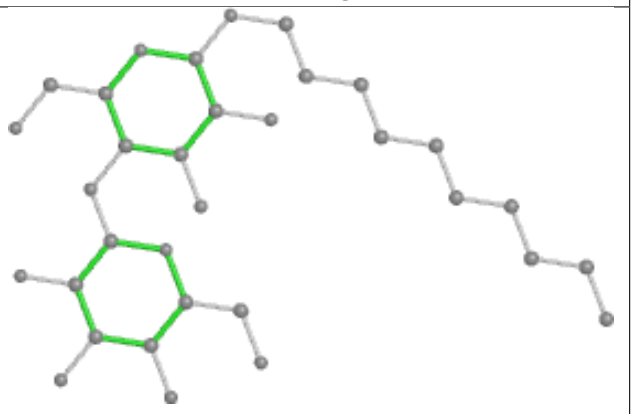
Bond lengths



Bond angles

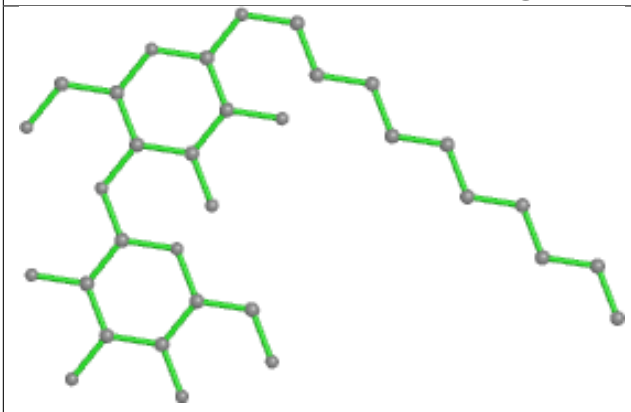


Torsions

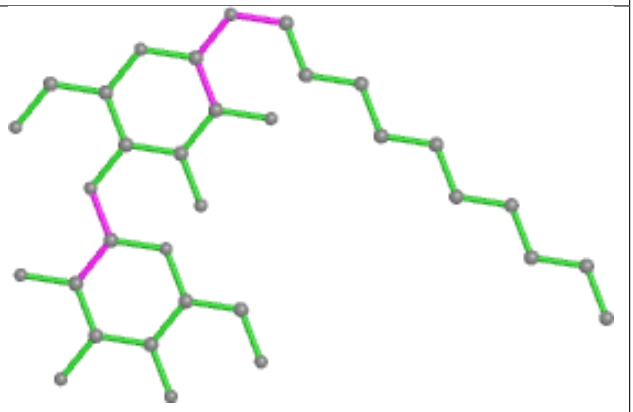


Rings

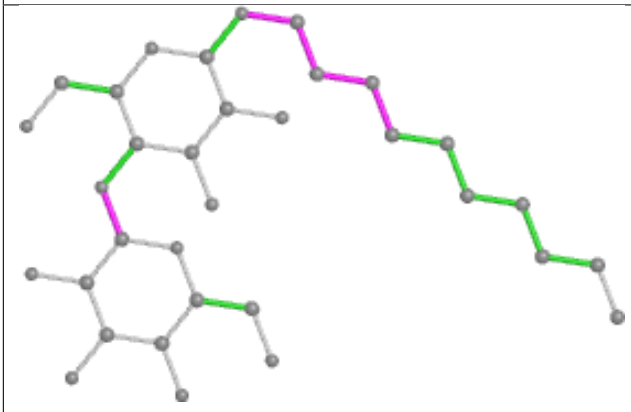
Ligand DMU C 310



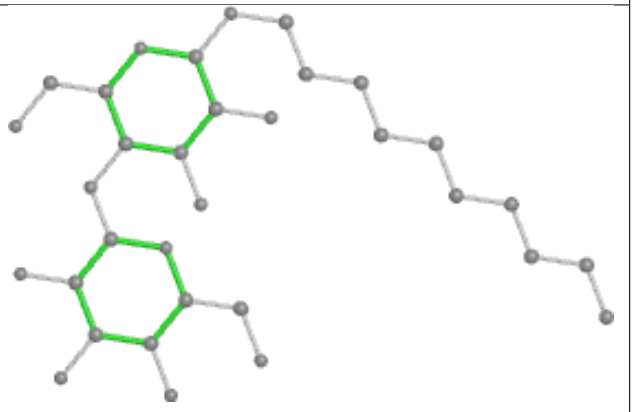
Bond lengths



Bond angles

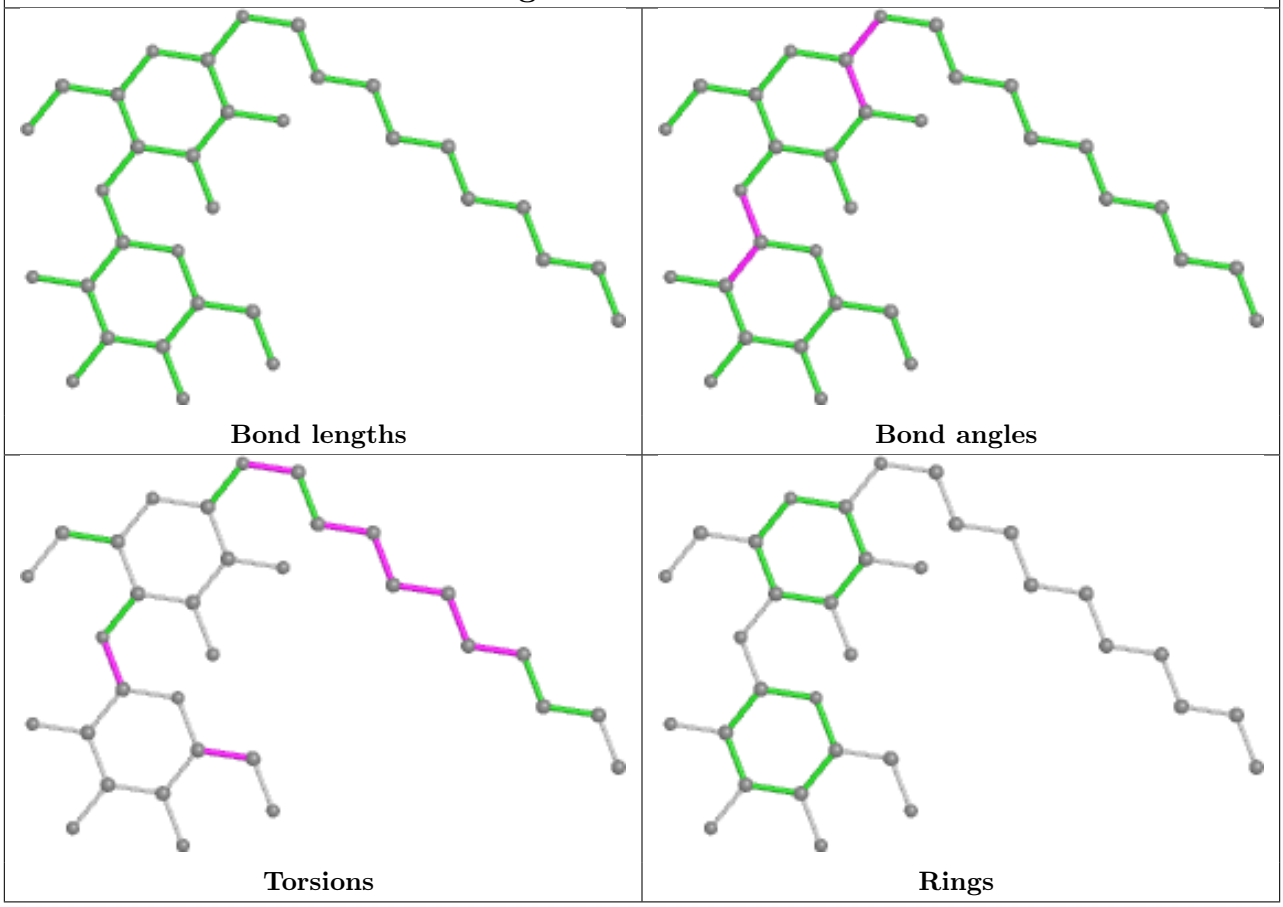


Torsions

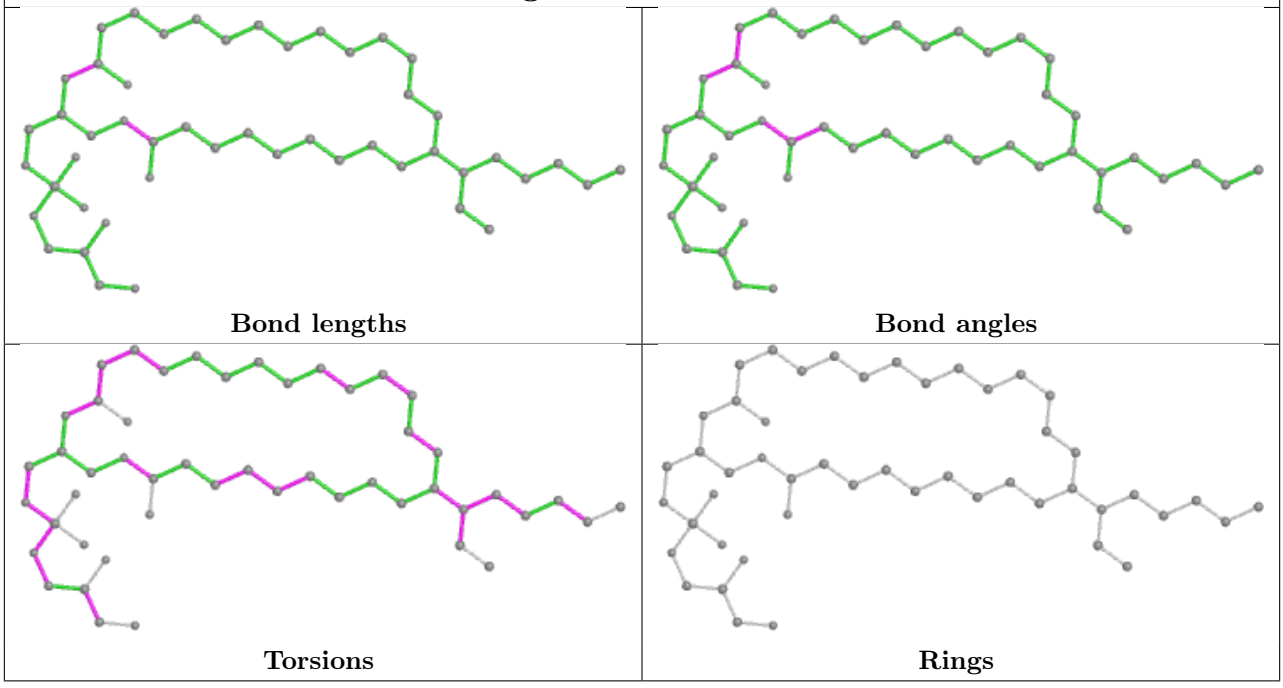


Rings

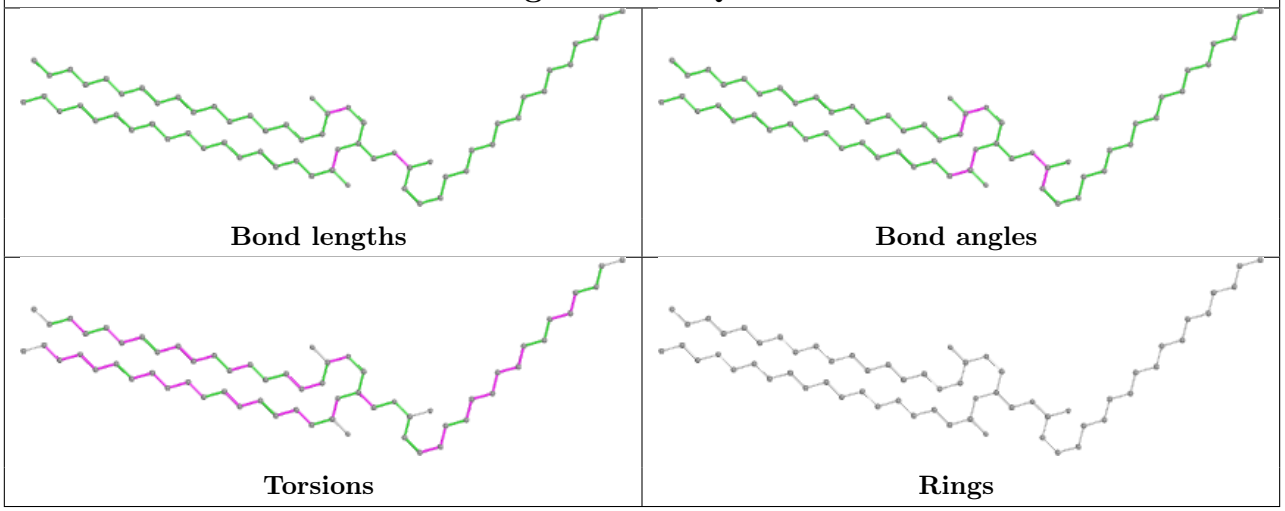
Ligand DMU P 310



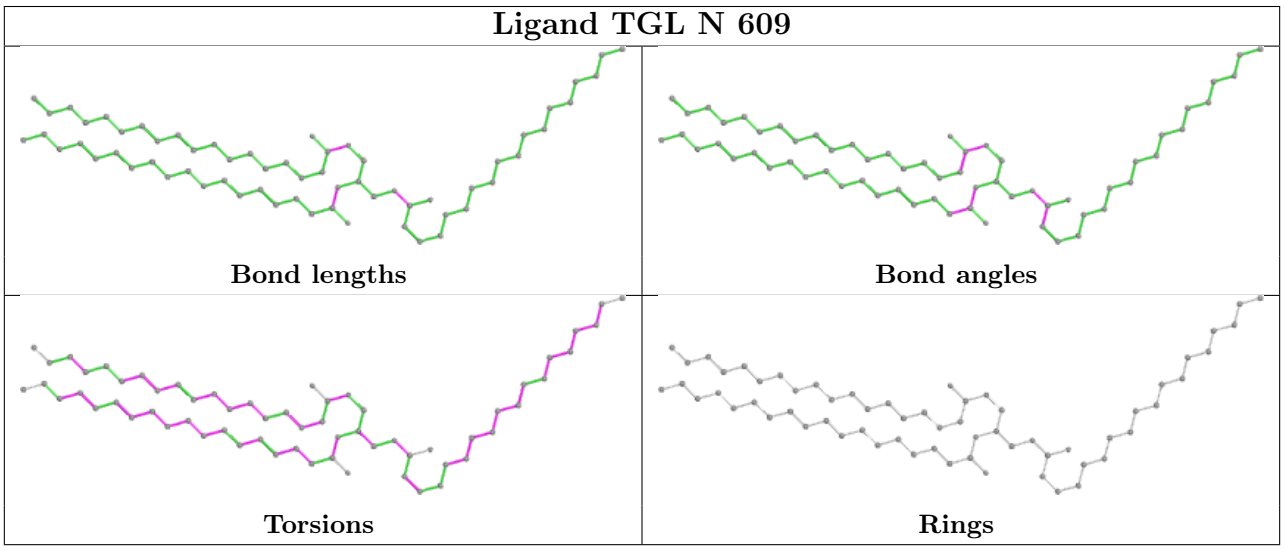
Ligand PGV A 609



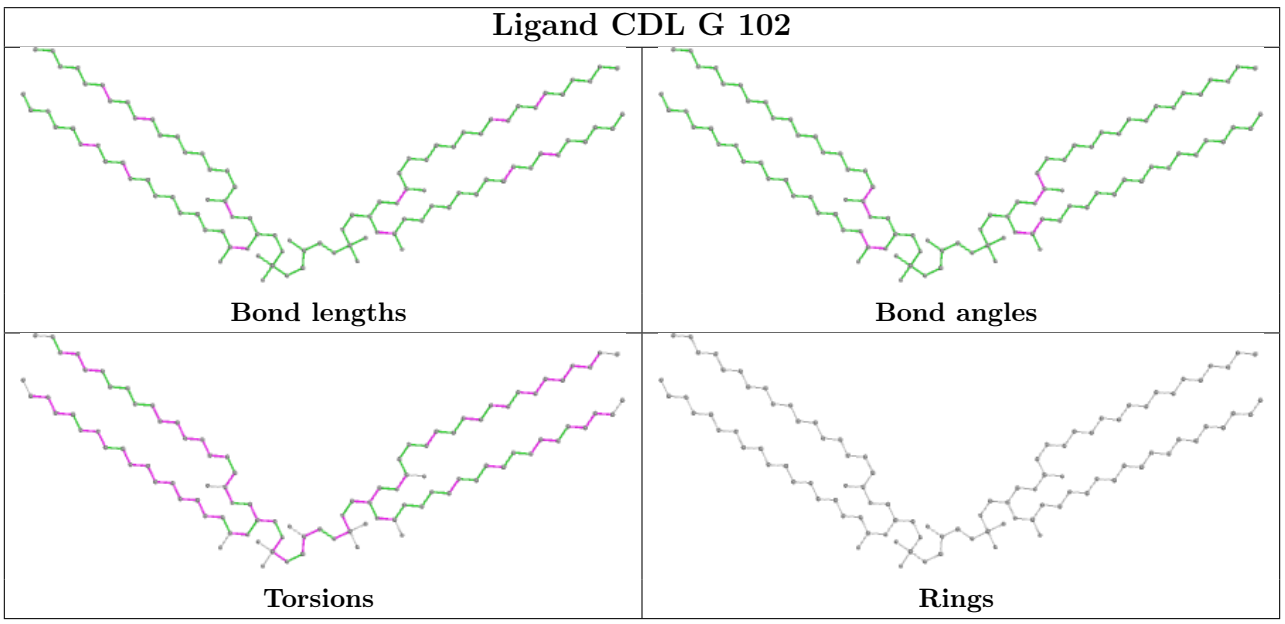
Ligand TGL Q 201



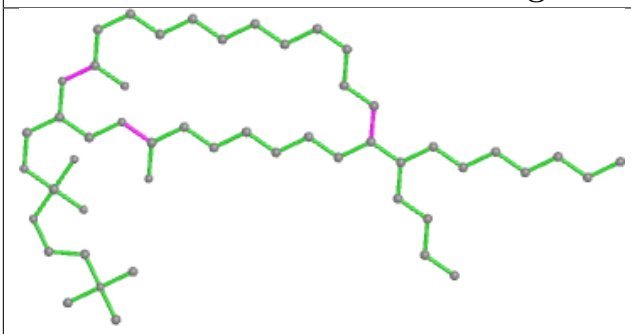
Ligand TGL N 609



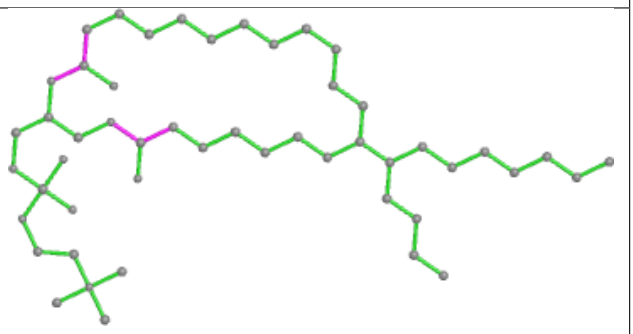
Ligand CDL G 102



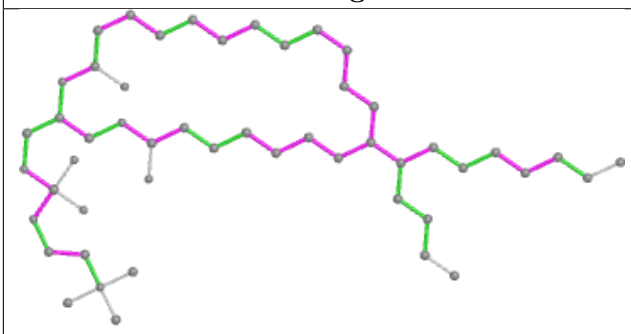
Ligand PSC E 201



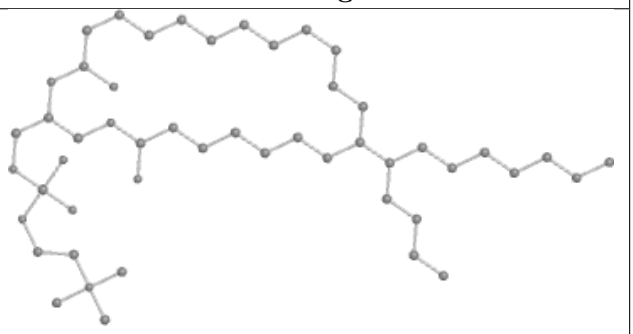
Bond lengths



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%)	0.05	2 (0%) 92 92	23, 28, 36, 71	0
1	N	513/514 (99%)	-0.01	4 (0%) 86 86	26, 33, 42, 72	0
2	B	226/227 (99%)	0.06	4 (1%) 68 68	27, 36, 55, 71	0
2	O	226/227 (99%)	0.15	4 (1%) 68 68	32, 43, 65, 84	0
3	C	259/261 (99%)	0.19	1 (0%) 92 92	25, 32, 42, 71	0
3	P	259/261 (99%)	0.03	2 (0%) 86 86	27, 33, 43, 65	0
4	D	144/147 (97%)	-0.07	4 (2%) 53 52	29, 38, 59, 74	0
4	Q	144/147 (97%)	0.79	12 (8%) 11 11	40, 51, 74, 130	0
5	E	105/109 (96%)	-0.10	2 (1%) 66 66	30, 37, 57, 108	0
5	R	105/109 (96%)	0.06	2 (1%) 66 66	36, 45, 64, 117	0
6	F	98/98 (100%)	0.63	7 (7%) 16 15	29, 39, 96, 147	0
6	S	98/98 (100%)	1.04	9 (9%) 9 8	30, 42, 104, 130	0
7	G	83/85 (97%)	1.27	15 (18%) 1 1	31, 40, 102, 145	0
7	T	83/85 (97%)	1.15	18 (21%) 0 0	30, 42, 96, 133	0
8	H	79/85 (92%)	0.38	8 (10%) 7 6	34, 43, 90, 100	0
8	U	79/85 (92%)	0.43	8 (10%) 7 6	38, 48, 95, 119	0
9	I	72/73 (98%)	0.72	10 (13%) 2 3	35, 48, 81, 93	0
9	V	72/73 (98%)	0.61	7 (9%) 7 7	34, 58, 79, 93	0
10	J	58/59 (98%)	0.47	2 (3%) 45 42	33, 42, 64, 110	0
10	W	58/59 (98%)	0.52	4 (6%) 16 16	37, 47, 68, 123	0
11	K	49/56 (87%)	0.03	0 100 100	35, 42, 56, 62	0
11	X	49/56 (87%)	0.62	6 (12%) 4 4	45, 53, 68, 77	0
12	L	46/47 (97%)	0.09	1 (2%) 62 61	30, 34, 53, 88	0
12	Y	46/47 (97%)	0.32	2 (4%) 35 33	37, 44, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.20	2 (4%) 31 30	31, 35, 68, 107	0
13	Z	43/46 (93%)	0.72	7 (16%) 1 2	41, 48, 78, 130	0
All	All	3550/3614 (98%)	0.25	143 (4%) 38 36	23, 37, 68, 147	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	30.4
4	Q	5	VAL	17.7
4	Q	6	VAL	17.1
6	F	1	ALA	15.9
4	Q	7	LYS	14.3
4	Q	4	SER	13.7
13	Z	43	SER	13.6
7	G	3	ALA	13.0
6	S	96	LEU	12.9
7	T	3	ALA	12.7
7	G	10	GLY	11.9
6	F	97	ALA	11.7
6	S	98	HIS	10.7
4	Q	8	SER	10.3
6	S	1	ALA	10.1
5	R	109	VAL	9.6
10	J	58	LYS	9.1
7	G	9	GLY	8.8
6	S	94	HIS	8.7
10	W	58	LYS	8.7
7	T	8	HIS	8.5
6	F	96	LEU	8.3
7	G	6	GLY	8.1
7	G	5	LYS	7.7
6	S	95	GLN	7.7
6	F	98	HIS	7.6
7	G	2	SER	7.5
9	I	30	GLY	7.5
6	F	2	SER	7.3
5	R	5	HIS	6.9
6	S	2	SER	6.9
7	T	10	GLY	6.7
6	S	93	PRO	6.6
8	U	8	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	6.0
7	T	5	LYS	5.9
7	T	4	ALA	5.7
7	T	2	SER	5.7
12	Y	47	LYS	5.7
7	T	1	ALA	5.6
9	I	29	LEU	5.5
9	I	37	PHE	5.5
9	V	25	PHE	5.4
7	T	6	GLY	5.1
6	F	94	HIS	5.1
9	I	25	PHE	4.9
11	X	13	TYR	4.9
7	G	40	GLY	4.9
7	T	36	TRP	4.9
9	V	29	LEU	4.8
8	H	46	LYS	4.8
7	G	4	ALA	4.8
8	U	7	LYS	4.7
7	T	39	SER	4.6
7	G	42	ARG	4.5
8	H	45	ALA	4.5
7	G	36	TRP	4.5
8	H	47	GLY	4.4
13	M	43	SER	4.4
5	E	109	VAL	4.4
11	X	7	PRO	4.3
7	G	7	ASP	4.2
4	Q	87[A]	PHE	4.2
3	P	3	HIS	4.2
13	M	42	LYS	4.1
9	V	37	PHE	4.0
6	F	95	GLN	4.0
7	T	42	ARG	4.0
2	O	227	LEU	4.0
2	O	113	TYR	3.9
11	X	6	ALA	3.9
8	H	44	THR	3.9
2	O	32[A]	PHE	3.8
7	T	41	HIS	3.7
7	T	7	ASP	3.6
13	Z	42	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	33	THR	3.4
9	V	30	GLY	3.3
8	U	44	THR	3.3
7	T	40	GLY	3.3
7	G	84	LYS	3.2
10	W	57	HIS	3.2
7	G	8	HIS	3.1
1	N	311[A]	ILE	3.1
2	B	59	GLN	3.1
8	U	10	ASN	3.0
11	X	12	LYS	3.0
1	N	113[A]	LEU	3.0
8	H	10	ASN	2.9
11	X	23	THR	2.9
11	X	16	ALA	2.9
3	C	33[A]	MET	2.8
2	O	91	ASN	2.8
6	S	3	GLY	2.8
4	Q	147	LYS	2.8
8	H	9	LYS	2.8
7	T	33	LEU	2.8
9	V	2	THR	2.8
4	D	4	SER	2.8
3	P	33[A]	MET	2.7
10	W	48	TYR	2.7
8	U	49	ASP	2.7
10	J	52	TRP	2.7
8	U	9	LYS	2.6
9	V	34	PHE	2.6
12	L	2	HIS	2.6
8	H	8	ILE	2.6
9	I	31	PHE	2.6
13	Z	40	TYR	2.6
12	Y	45	LEU	2.6
8	U	45	ALA	2.6
9	I	19	PHE	2.5
9	I	32	ALA	2.5
13	Z	32	TRP	2.5
2	B	32[A]	PHE	2.5
2	B	60	GLU	2.5
9	I	21	ILE	2.5
10	W	52	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
7	T	12	GLY	2.5
9	V	31	PHE	2.5
4	D	5	VAL	2.4
7	G	37	LEU	2.4
1	A	311[A]	ILE	2.4
8	H	48	GLY	2.4
7	T	9	GLY	2.4
5	E	5	HIS	2.4
13	Z	39	ASN	2.4
1	N	513	LEU	2.4
4	Q	33	LEU	2.4
13	Z	35	TYR	2.4
13	Z	13	LYS	2.3
8	U	46	LYS	2.3
1	A	513	LEU	2.3
4	D	19[A]	ARG	2.3
7	T	43	GLU	2.2
1	N	383[A]	MET	2.1
4	Q	10	ASP	2.1
4	Q	73	ARG	2.1
9	I	39	VAL	2.1
2	B	41[A]	ILE	2.1
4	Q	39	ALA	2.0
4	D	87[A]	PHE	2.0
4	Q	62	LEU	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
9	SAC	V	1	9/10	0.07	0.56	110,113,117,121	0
7	TPO	G	11	11/12	0.31	0.39	93,113,122,123	0
7	TPO	T	11	11/12	0.50	0.29	95,116,126,126	0
9	SAC	I	1	9/10	0.81	0.25	67,72,74,75	0
1	FME	A	1	10/11	0.91	0.13	42,46,67,74	0
1	FME	N	1	10/11	0.93	0.14	48,52,70,72	0
2	FME	O	1	10/11	0.95	0.14	41,42,50,52	0
2	FME	B	1	10/11	0.96	0.14	34,35,42,47	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
22	CHD	W	101	29/29	0.19	0.52	101,119,127,128	0
20	EDO	C	318	4/4	0.24	0.92	92,94,95,96	0
20	EDO	C	317	4/4	0.50	0.39	72,80,80,81	0
26	CDL	T	102	100/100	0.52	0.34	63,89,130,135	0
20	EDO	Q	204	4/4	0.53	0.22	76,76,78,79	0
20	EDO	D	203	4/4	0.54	0.38	68,72,72,77	0
27	PEK	C	309	53/53	0.54	0.40	56,100,141,149	0
27	PEK	C	307	53/53	0.55	0.29	56,84,135,140	0
21	TGL	Y	101	63/63	0.56	0.37	55,85,115,134	0
20	EDO	A	619	4/4	0.58	0.22	66,67,67,70	0
27	PEK	P	309	53/53	0.59	0.31	50,75,113,116	0
28	PSC	E	201	52/52	0.59	0.35	55,80,147,151	0
20	EDO	D	204	4/4	0.61	0.33	75,77,80,80	0
27	PEK	P	302	53/53	0.61	0.28	53,90,138,147	0
26	CDL	G	102	100/100	0.63	0.37	62,94,124,132	0
20	EDO	C	316	4/4	0.65	0.20	73,75,77,80	0
26	CDL	P	306	100/100	0.65	0.32	51,84,110,116	0
28	PSC	O	302	52/52	0.65	0.32	53,91,144,152	0
21	TGL	Q	201	63/63	0.66	0.26	66,80,94,97	0
19	PGV	C	308	51/51	0.66	0.24	60,78,106,113	0
21	TGL	L	101	63/63	0.67	0.30	43,74,92,95	0
24	DMU	C	302	33/33	0.68	0.38	51,80,99,103	0
19	PGV	P	303	51/51	0.68	0.31	62,85,114,123	0
20	EDO	O	305	4/4	0.70	0.17	76,77,78,78	0
20	EDO	G	106	4/4	0.71	0.23	72,73,74,74	0
19	PGV	Z	101	51/51	0.71	0.36	58,80,101,104	0
24	DMU	P	308	33/33	0.71	0.36	53,81,112,114	0
20	EDO	J	102	4/4	0.72	0.15	85,86,86,88	0
24	DMU	P	310	33/33	0.73	0.23	70,78,88,92	0
24	DMU	C	310	33/33	0.74	0.27	65,78,99,100	0
21	TGL	D	201	63/63	0.74	0.24	51,67,90,94	0
19	PGV	A	609	51/51	0.74	0.32	43,78,96,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CDL	C	305	100/100	0.75	0.28	55,78,108,113	0
20	EDO	C	314	4/4	0.75	0.26	67,70,71,73	0
20	EDO	A	618	4/4	0.76	0.53	55,59,61,62	0
24	DMU	C	311	33/33	0.76	0.19	61,82,101,103	0
20	EDO	C	313	4/4	0.77	0.19	67,67,70,74	0
22	CHD	J	101	29/29	0.77	0.26	82,86,100,102	0
20	EDO	N	611	4/4	0.77	0.37	41,42,46,53	0
20	EDO	H	101	4/4	0.77	0.17	62,65,66,69	0
21	TGL	N	609	63/63	0.77	0.27	60,82,100,104	0
20	EDO	Q	203	4/4	0.77	0.35	63,64,66,67	0
20	EDO	G	104	4/4	0.78	0.20	70,70,72,74	0
20	EDO	A	617	4/4	0.80	0.42	64,67,69,72	0
20	EDO	U	101	4/4	0.80	0.17	70,70,70,73	0
20	EDO	A	614	4/4	0.81	0.19	28,30,32,45	0
21	TGL	B	301	63/63	0.81	0.26	50,78,104,107	0
20	EDO	D	202	4/4	0.81	0.70	51,54,55,56	0
20	EDO	R	204	4/4	0.82	0.42	62,63,66,67	0
20	EDO	N	620	4/4	0.83	0.34	46,55,55,56	0
22	CHD	C	306	29/29	0.84	0.17	59,61,63,67	0
22	CHD	P	307	29/29	0.84	0.19	57,59,62,64	0
20	EDO	A	616	4/4	0.85	0.23	53,54,54,61	0
24	DMU	P	311	33/33	0.85	0.23	72,89,98,99	0
20	EDO	E	204	4/4	0.85	0.25	55,58,59,60	0
20	EDO	N	610	4/4	0.85	0.15	74,74,74,75	0
20	EDO	N	617	4/4	0.86	0.32	47,50,52,53	0
24	DMU	Z	102	33/33	0.86	0.20	52,58,70,70	0
20	EDO	C	315	4/4	0.86	0.26	44,54,56,60	0
20	EDO	N	616	4/4	0.87	0.15	50,50,51,53	0
20	EDO	S	103	4/4	0.87	0.31	61,63,67,69	0
20	EDO	A	615	4/4	0.87	0.19	45,46,46,47	0
20	EDO	F	104	4/4	0.88	0.28	53,53,55,57	0
20	EDO	R	201	4/4	0.88	0.21	67,68,68,71	0
20	EDO	R	205	4/4	0.89	0.25	49,52,54,55	0
20	EDO	P	312	4/4	0.89	0.21	37,42,43,49	0
20	EDO	A	613	4/4	0.90	0.22	67,70,71,73	0
20	EDO	N	619	4/4	0.90	0.25	54,60,62,72	0
20	EDO	V	101	4/4	0.90	0.18	63,64,64,64	0
20	EDO	C	319	4/4	0.91	0.22	39,45,46,53	0
20	EDO	A	612	4/4	0.91	0.20	39,45,47,53	0
20	EDO	W	102	4/4	0.91	0.31	55,60,60,67	0
20	EDO	A	611	4/4	0.91	0.21	52,56,58,61	0
20	EDO	A	620	4/4	0.91	0.47	49,50,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	D	206	4/4	0.91	0.19	59,60,61,64	0
20	EDO	N	613	4/4	0.92	0.20	60,62,65,68	0
20	EDO	O	304	4/4	0.92	0.16	66,67,67,70	0
20	EDO	R	202	4/4	0.92	0.21	58,61,62,64	0
18	AZI	N	607	3/3	0.92	0.13	35,35,36,36	0
20	EDO	E	206	4/4	0.92	0.26	65,65,66,68	0
16	MG	N	604	1/1	0.92	0.12	33,33,33,33	0
20	EDO	N	618	4/4	0.93	0.25	53,56,58,58	0
24	DMU	M	101	33/33	0.93	0.14	43,49,55,58	0
20	EDO	R	203	4/4	0.94	0.12	45,46,46,46	0
18	AZI	A	607	3/3	0.94	0.17	32,32,33,33	0
20	EDO	F	103	4/4	0.94	0.12	38,39,39,41	0
16	MG	A	604	1/1	0.94	0.10	27,27,27,27	0
27	PEK	T	101	53/53	0.94	0.17	34,52,79,81	0
20	EDO	S	104	4/4	0.94	0.21	49,50,50,52	0
20	EDO	Q	202	4/4	0.94	0.22	69,69,70,71	0
27	PEK	G	101	53/53	0.95	0.17	33,50,79,81	0
20	EDO	D	205	4/4	0.95	0.20	43,45,49,53	0
20	EDO	N	614	4/4	0.95	0.11	37,38,40,40	0
20	EDO	P	314	4/4	0.95	0.29	61,62,65,66	0
20	EDO	E	202	4/4	0.95	0.13	45,46,50,52	0
20	EDO	N	612	4/4	0.95	0.19	42,45,46,47	0
22	CHD	B	302	29/29	0.96	0.12	30,31,34,39	0
22	CHD	C	301	29/29	0.96	0.09	30,32,34,35	0
25	UNX	C	303	1/1	0.96	0.24	32,32,32,32	0
20	EDO	T	103	4/4	0.96	0.18	40,42,43,44	0
20	EDO	E	205	4/4	0.96	0.12	41,41,43,45	0
25	UNX	P	304	1/1	0.97	0.20	28,28,28,28	0
19	PGV	P	305	51/51	0.97	0.15	31,39,73,77	0
14	HEA	N	602[A]	60/60	0.97	0.15	28,30,33,33	60
23	CUA	O	301	2/2	0.97	0.15	34,34,34,35	0
20	EDO	A	610	4/4	0.97	0.21	40,43,44,44	0
19	PGV	C	304	51/51	0.97	0.16	30,38,76,84	0
14	HEA	N	602[B]	60/60	0.97	0.15	26,28,39,40	60
19	PGV	N	608	51/51	0.97	0.14	31,39,63,67	0
20	EDO	A	621	4/4	0.97	0.20	37,43,43,44	0
20	EDO	O	303	4/4	0.97	0.22	40,40,41,41	0
22	CHD	G	103	29/29	0.97	0.13	31,33,36,40	0
19	PGV	A	608	51/51	0.97	0.16	28,37,58,63	0
22	CHD	P	301	29/29	0.97	0.08	31,34,36,39	0
14	HEA	A	602[A]	60/60	0.98	0.14	22,25,29,31	60
20	EDO	N	615	4/4	0.98	0.12	33,36,37,37	0

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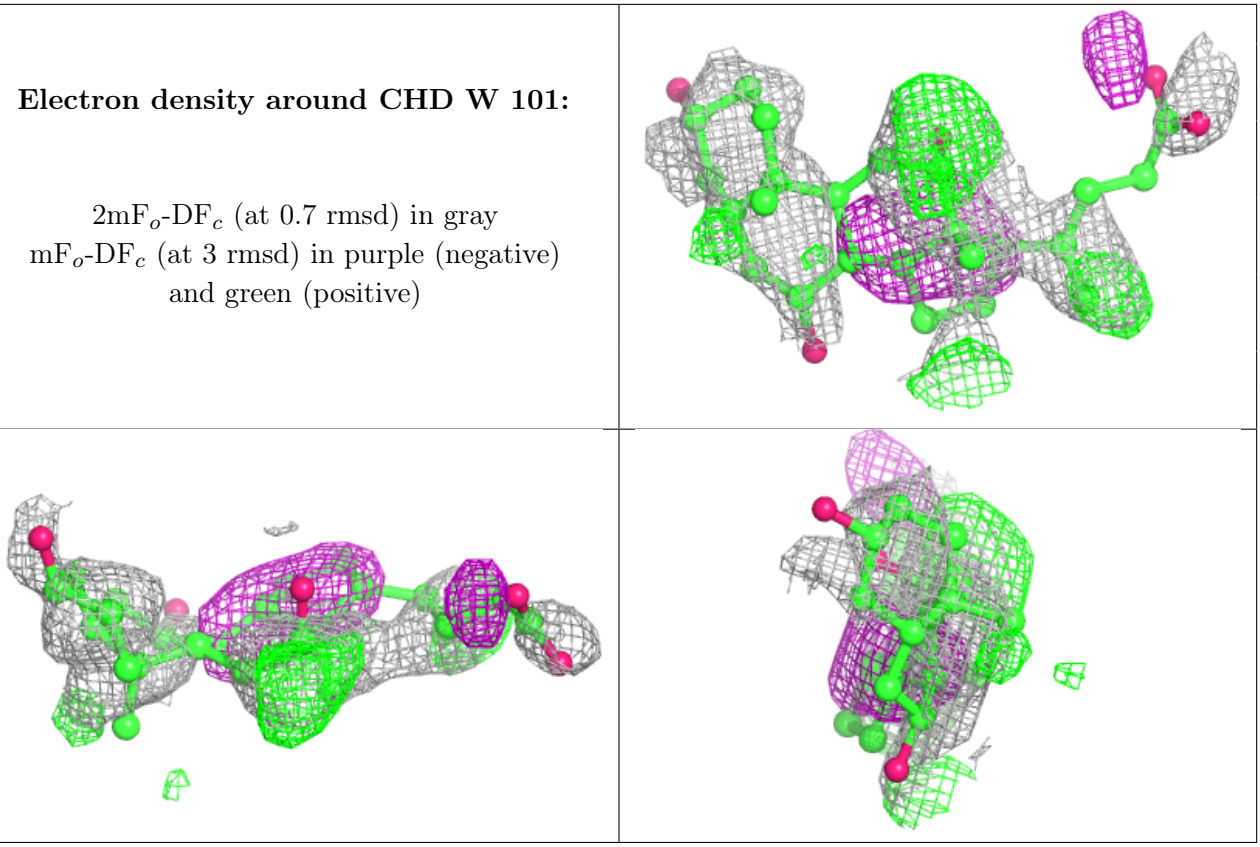
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	B	304	4/4	0.98	0.14	31,33,36,36	0
20	EDO	P	313	4/4	0.98	0.24	43,43,43,45	0
14	HEA	A	602[B]	60/60	0.98	0.14	24,26,30,31	60
14	HEA	N	601	60/60	0.98	0.13	29,32,51,53	0
23	CUA	B	303	2/2	0.98	0.17	28,28,28,29	0
14	HEA	A	601	60/60	0.98	0.12	23,26,45,47	0
20	EDO	E	203	4/4	0.98	0.11	43,43,45,46	0
20	EDO	G	105	4/4	0.98	0.10	34,36,39,40	0
18	AZI	N	606	3/3	0.99	0.12	36,36,36,37	0
20	EDO	F	102	4/4	0.99	0.12	28,28,29,30	0
17	NA	N	605	1/1	0.99	0.05	38,38,38,38	0
18	AZI	A	606	3/3	0.99	0.15	30,30,31,32	0
20	EDO	S	102	4/4	0.99	0.10	32,33,33,33	0
20	EDO	C	312	4/4	0.99	0.09	40,41,41,42	0
17	NA	A	605	1/1	0.99	0.07	30,30,30,30	0
15	CU	N	603	1/1	1.00	0.18	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.16	28,28,28,28	0
29	ZN	F	101	1/1	1.00	0.15	34,34,34,34	0
29	ZN	S	101	1/1	1.00	0.14	37,37,37,37	0

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

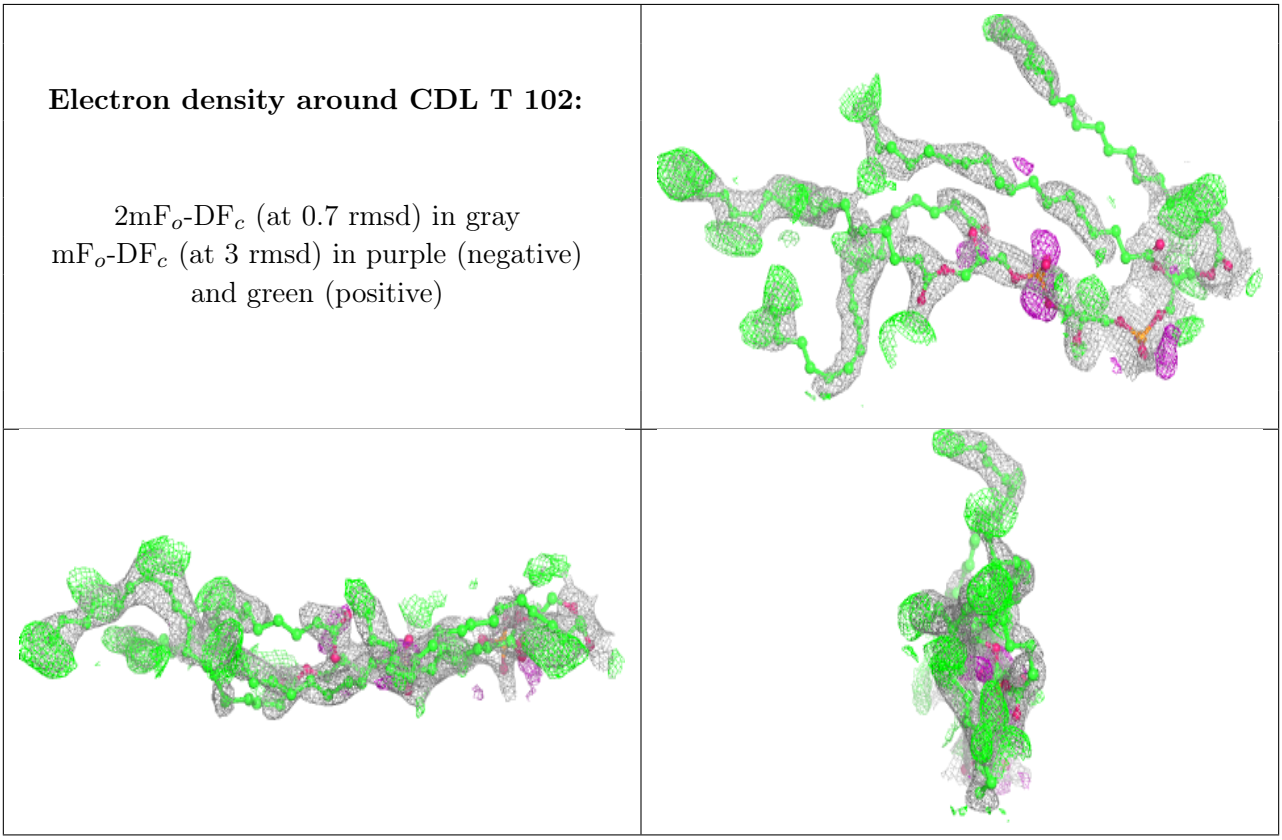
Electron density around CHD W 101:

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



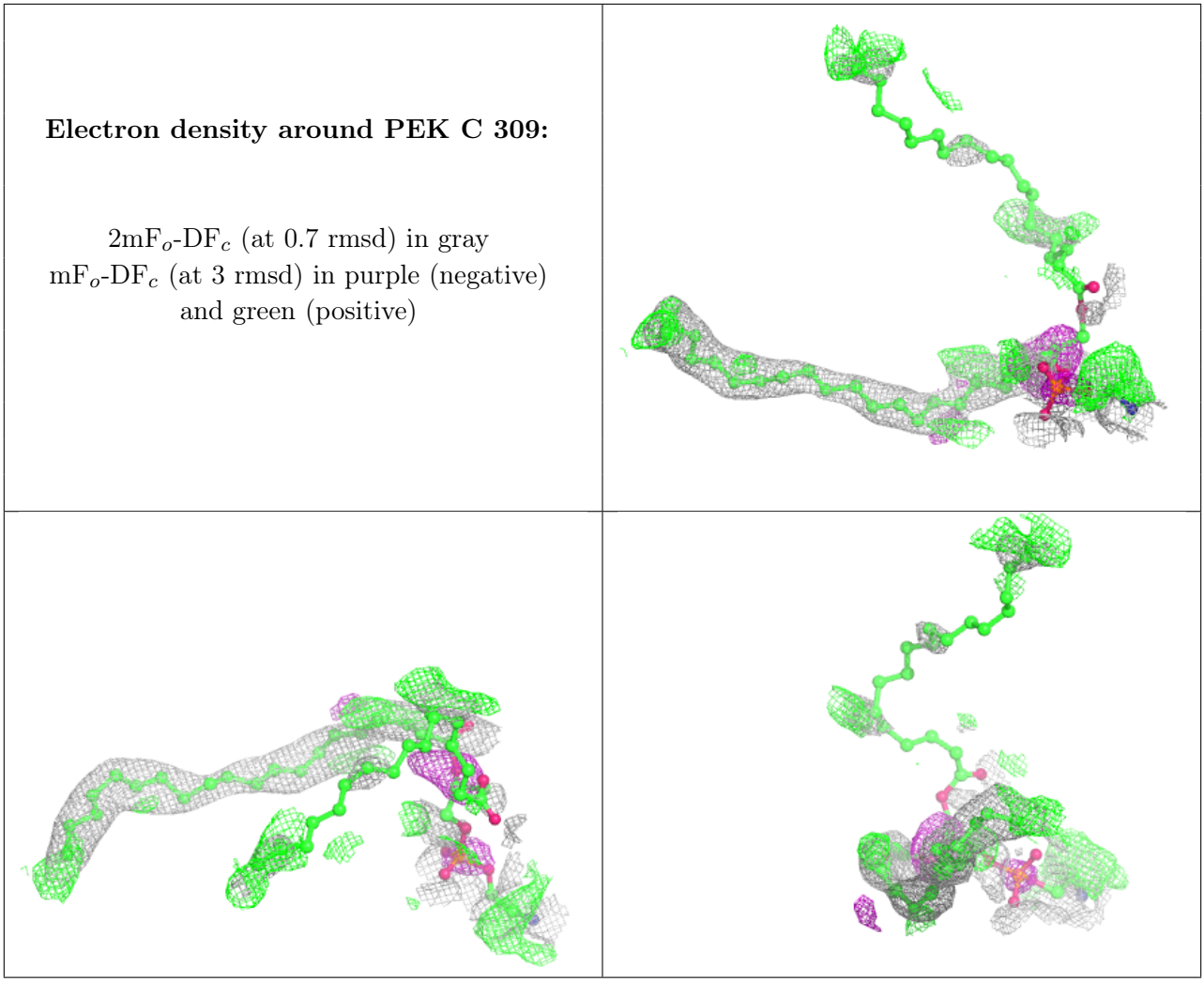
Electron density around CDL T 102:

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



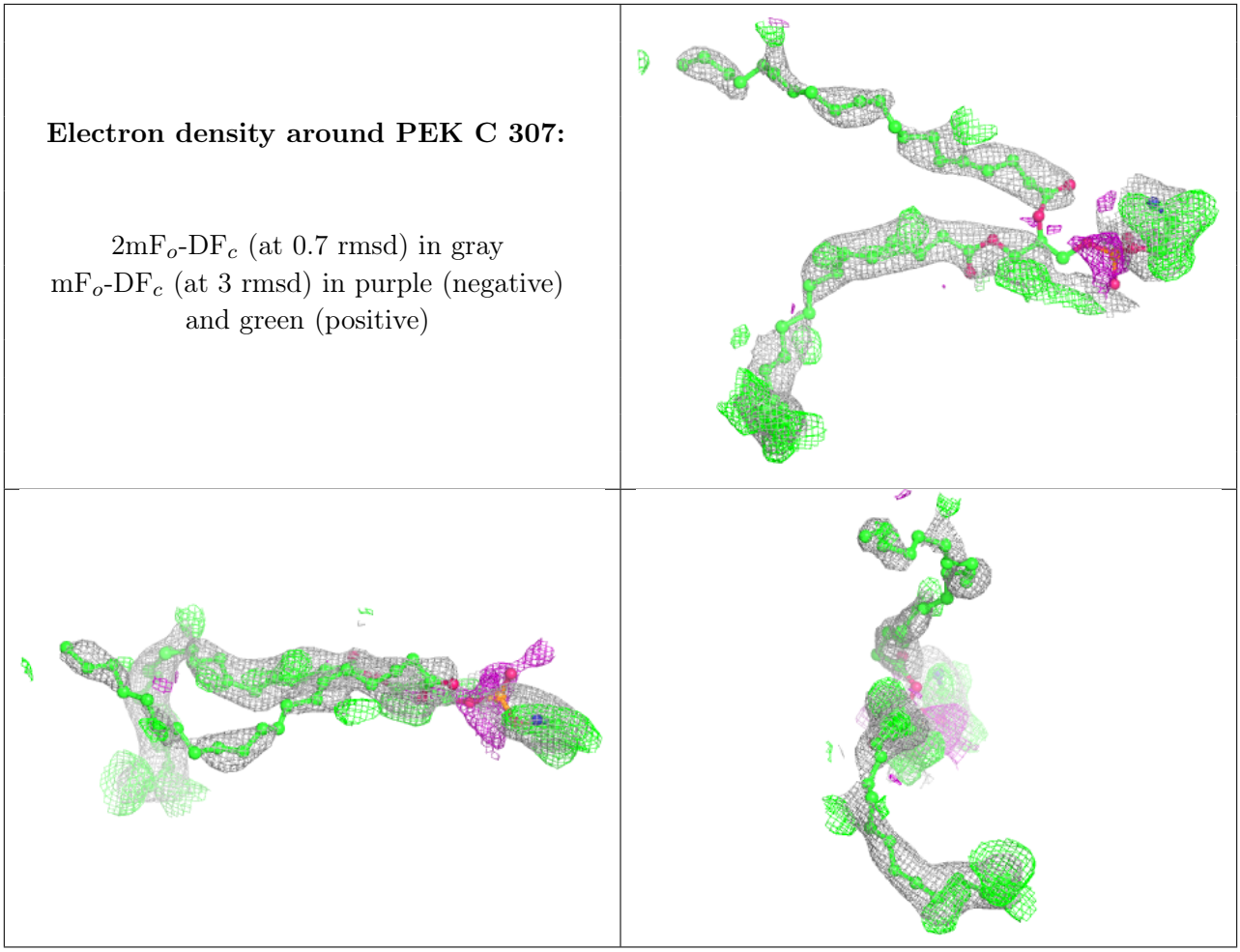
Electron density around PEK C 309:

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



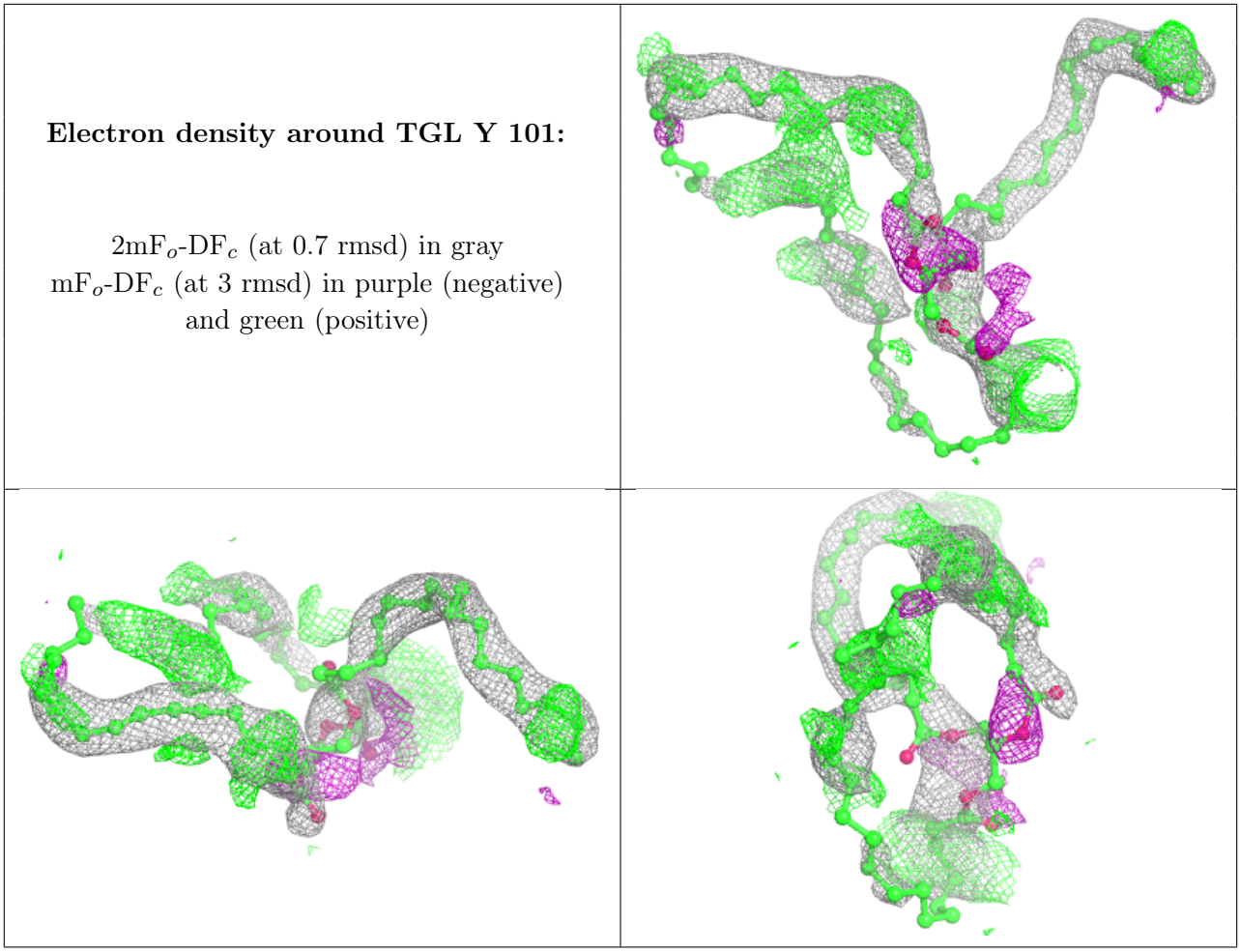
Electron density around PEK C 307:

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



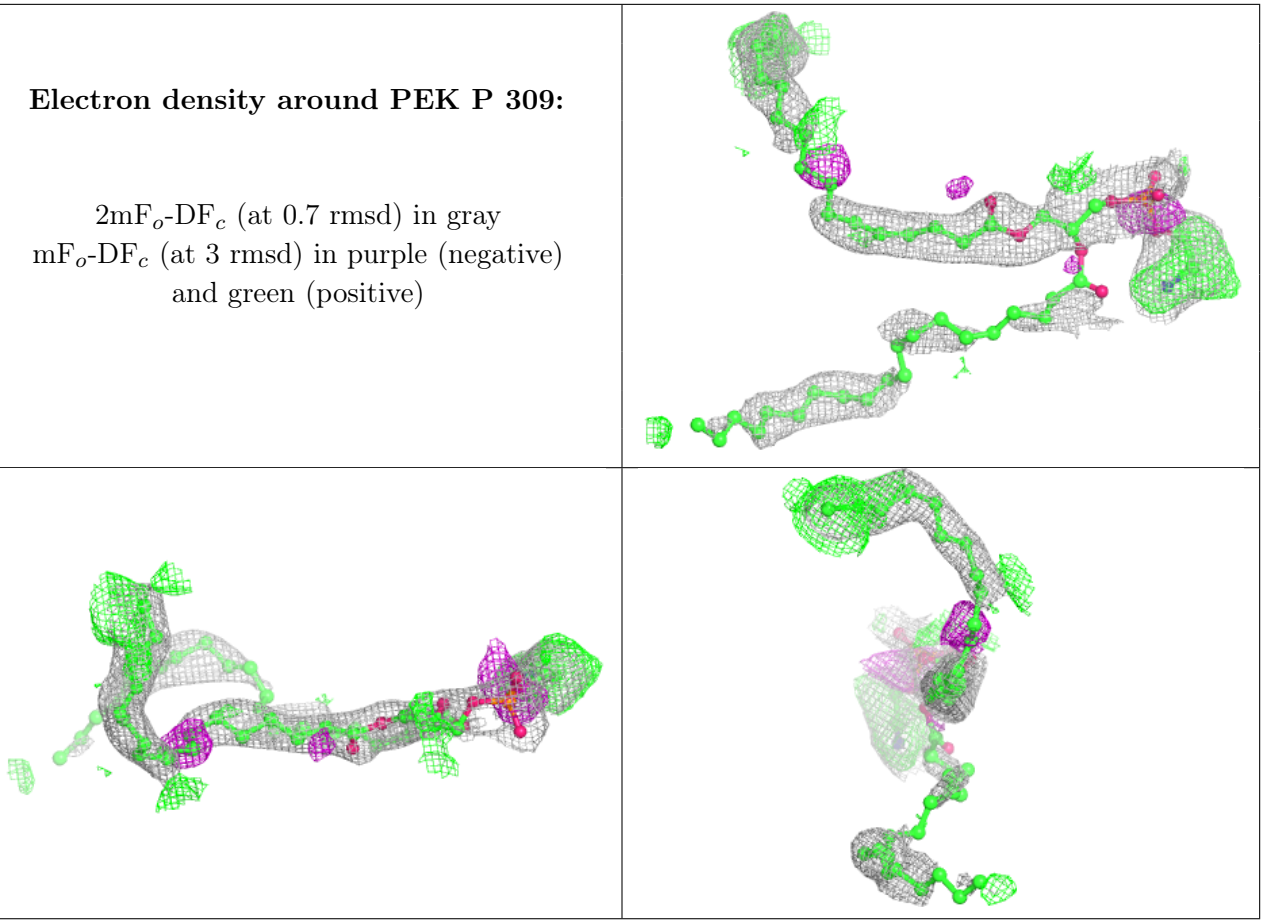
Electron density around TGL Y 101:

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



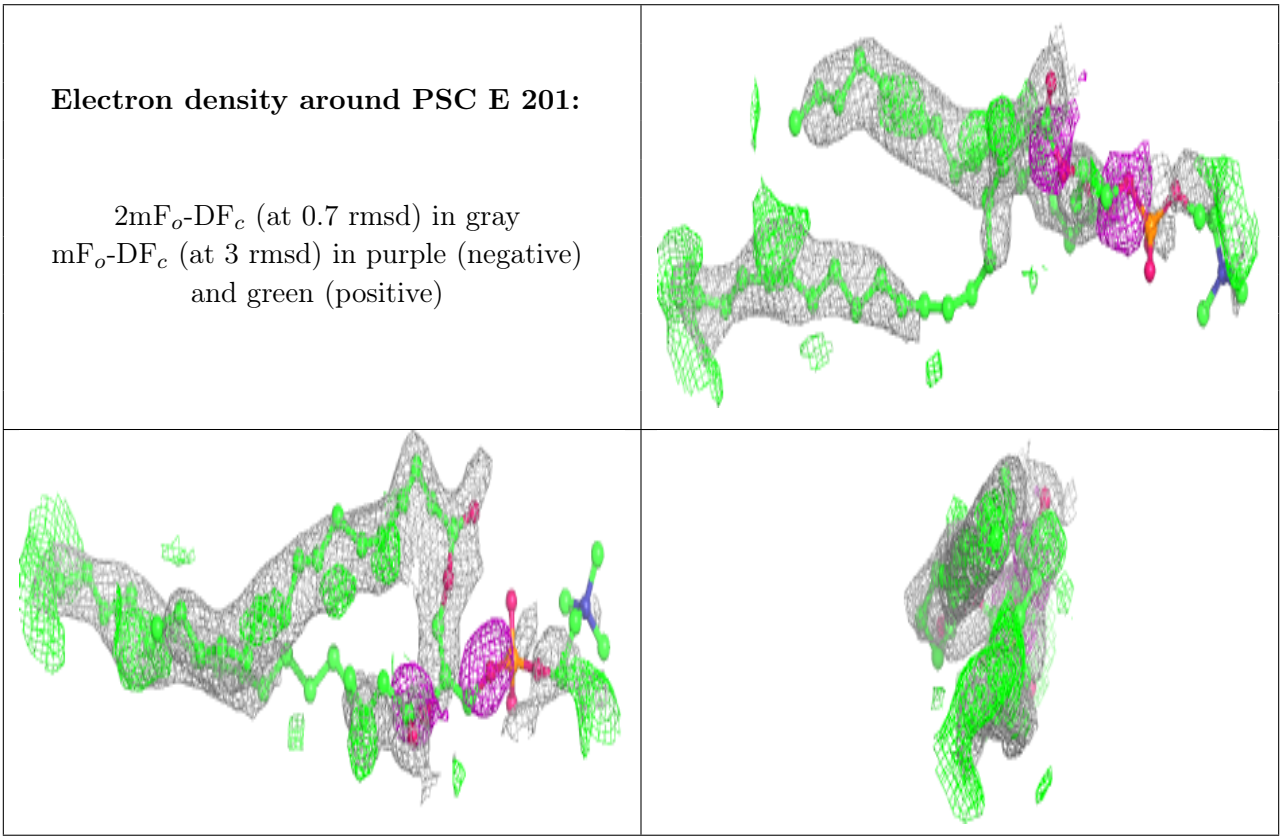
Electron density around PEK P 309:

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



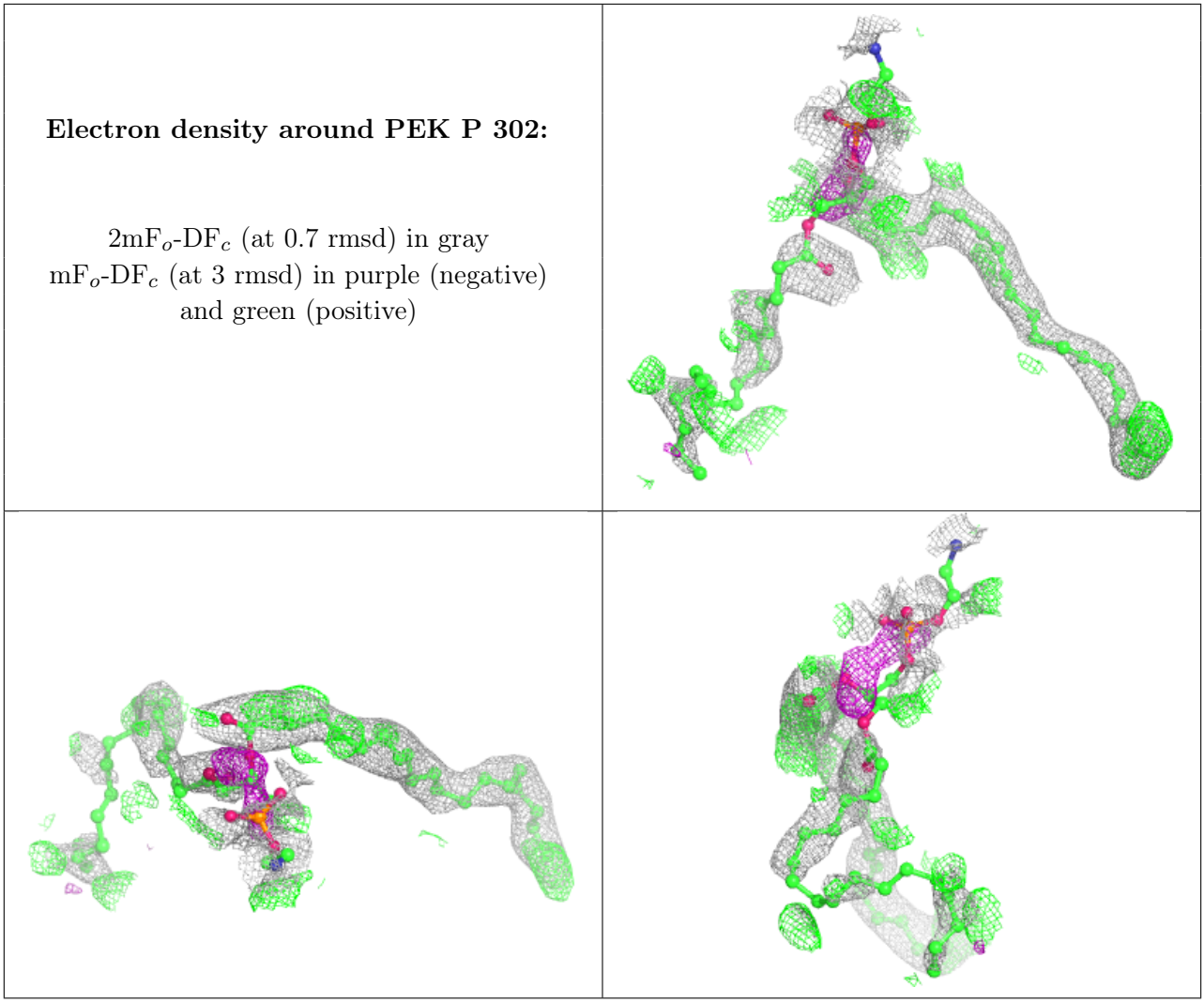
Electron density around PSC E 201:

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



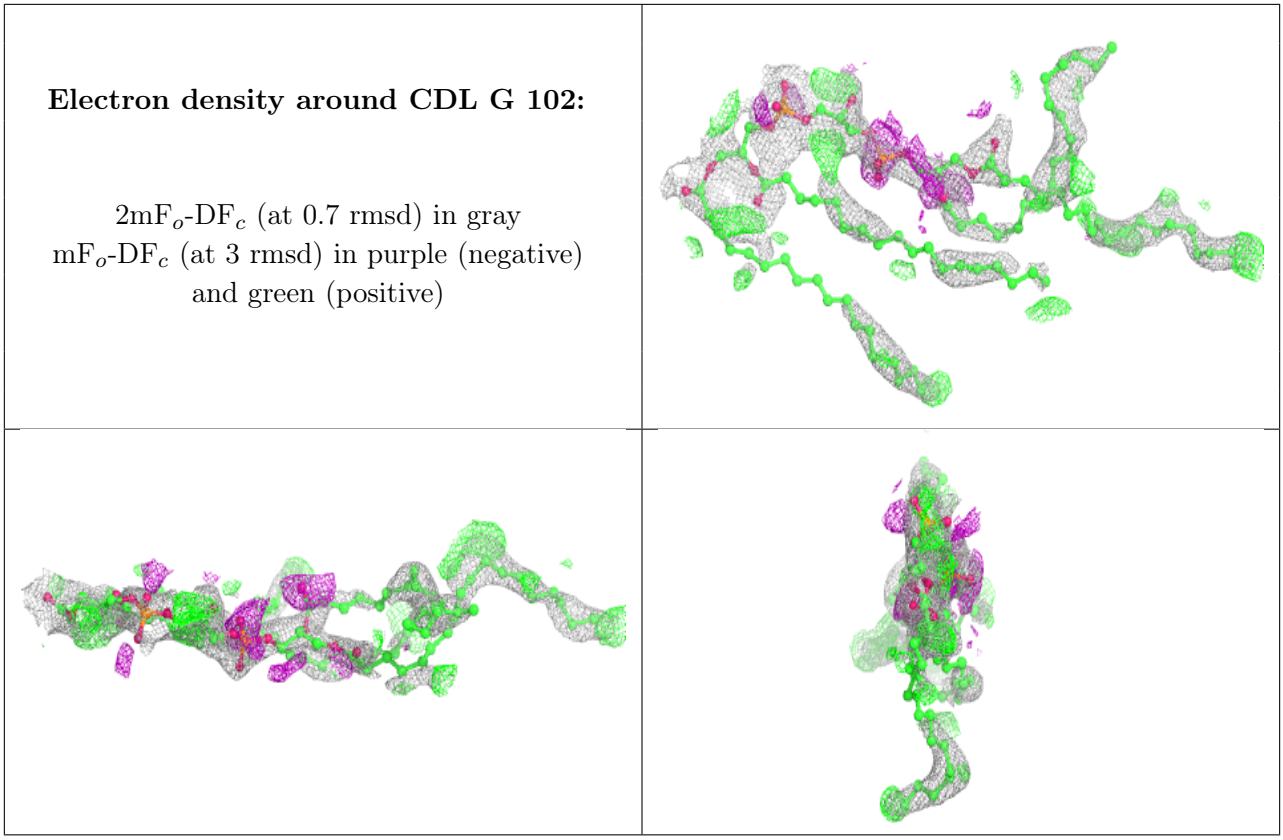
Electron density around PEK P 302:

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



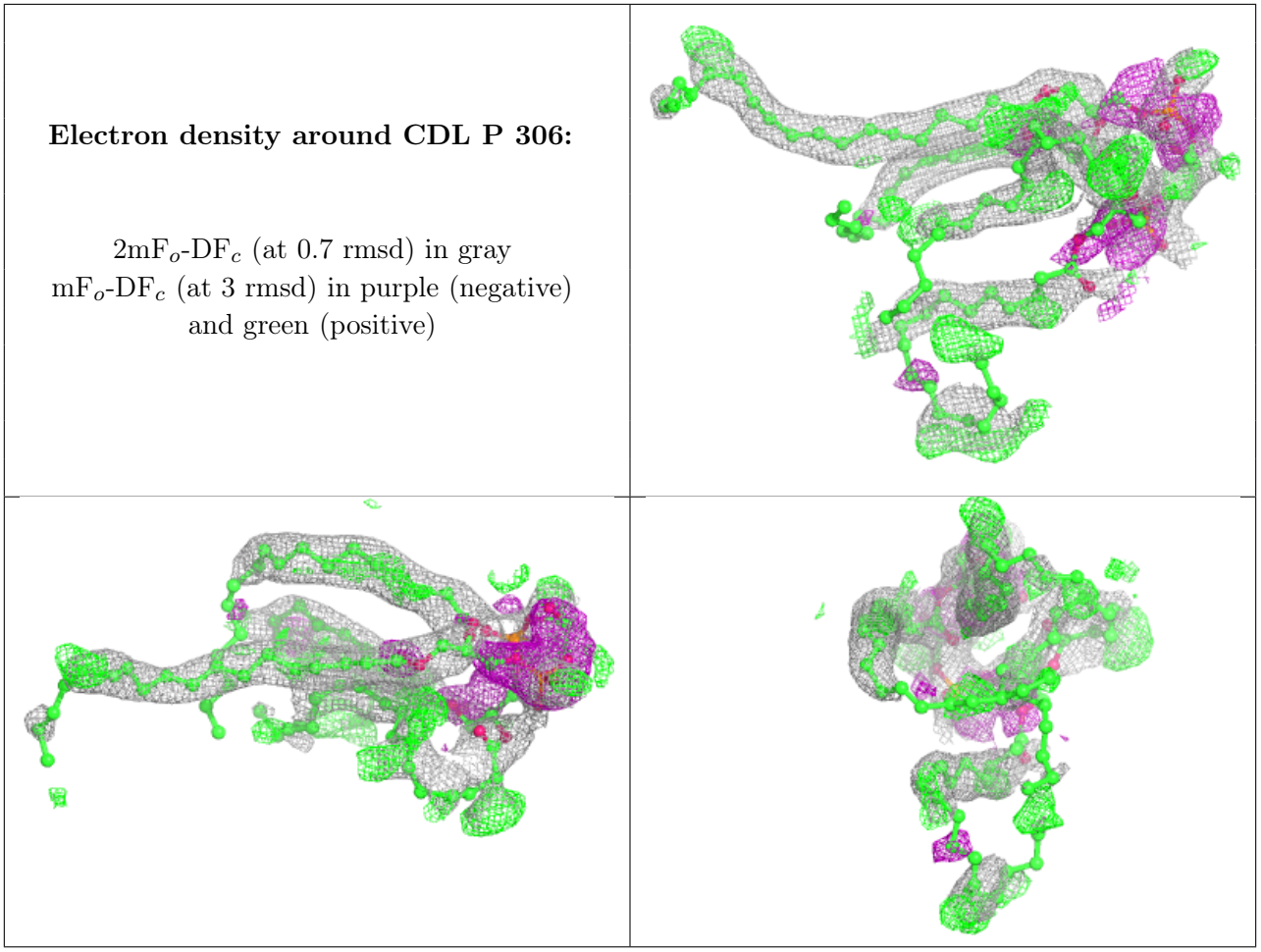
Electron density around CDL G 102:

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



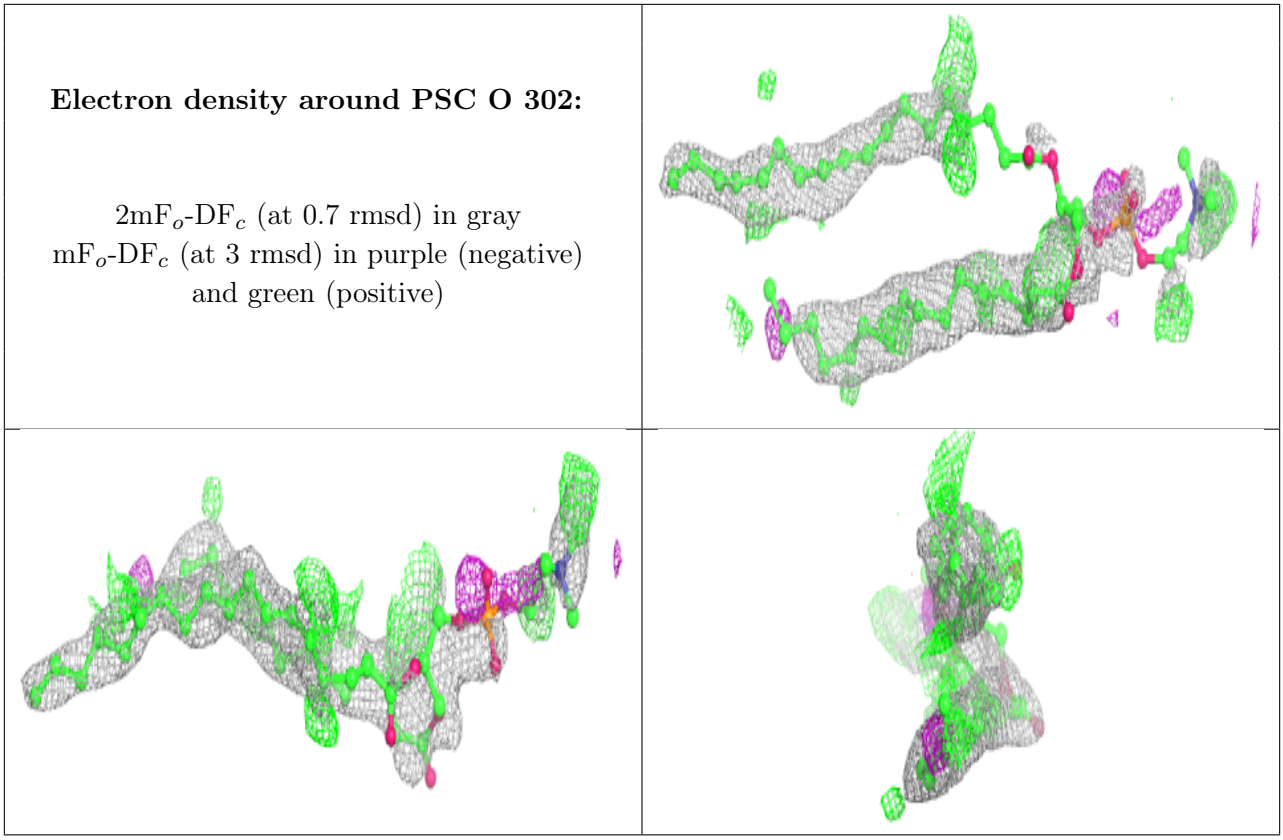
Electron density around CDL P 306:

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



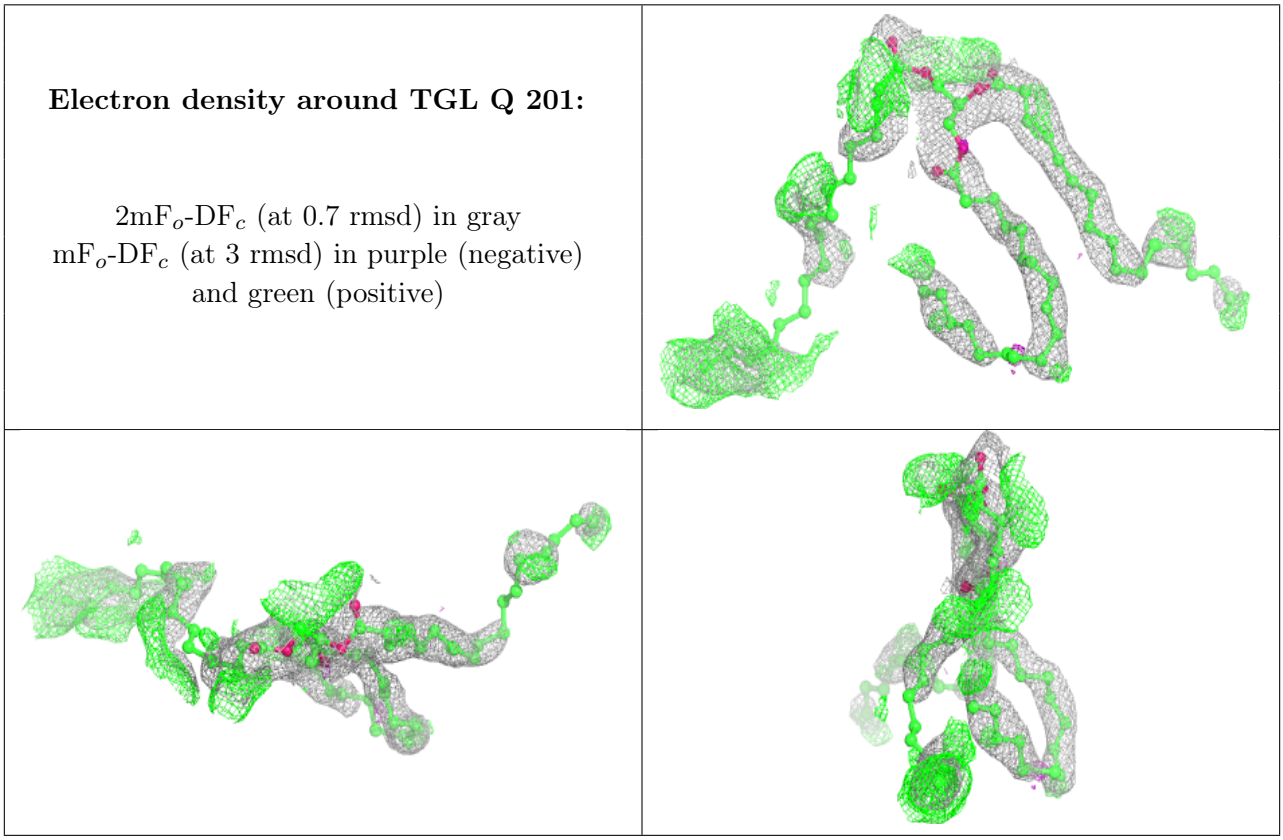
Electron density around PSC O 302:

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



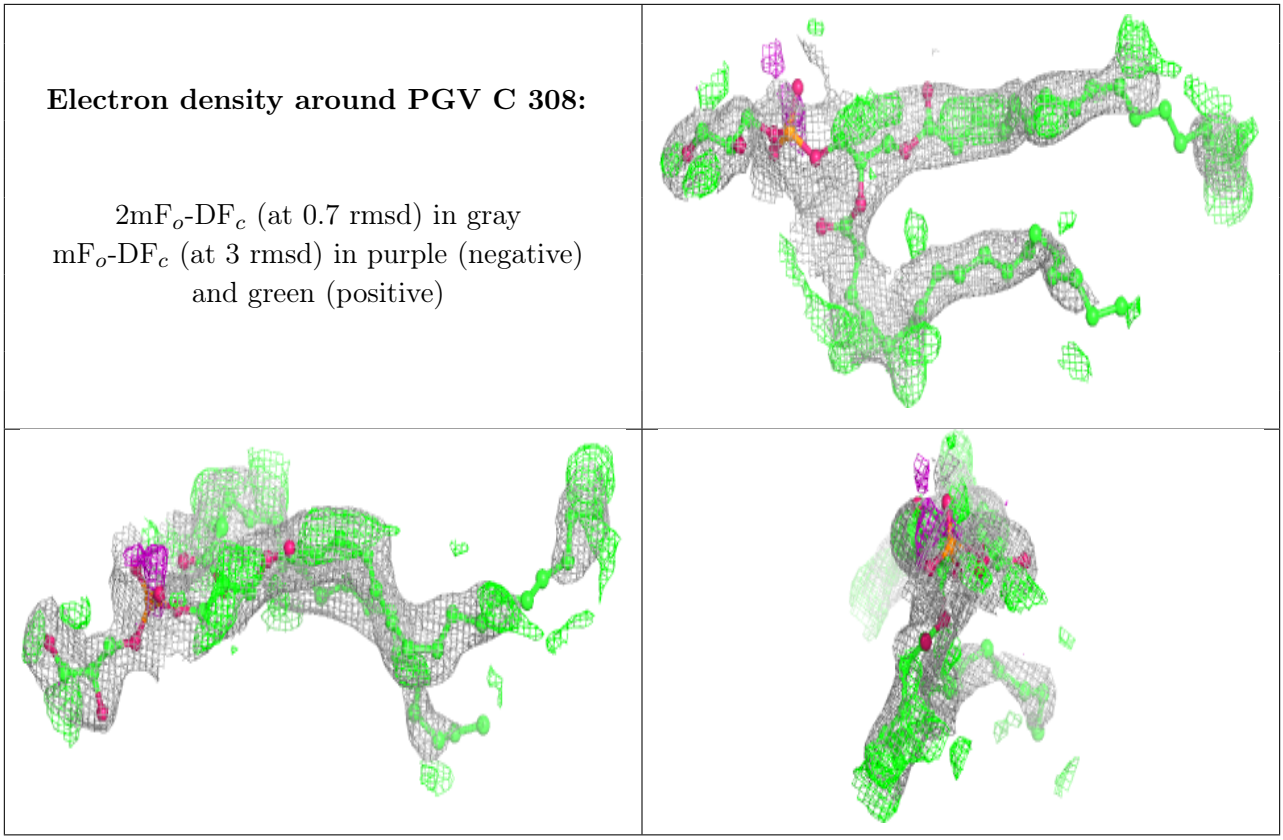
Electron density around TGL Q 201:

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



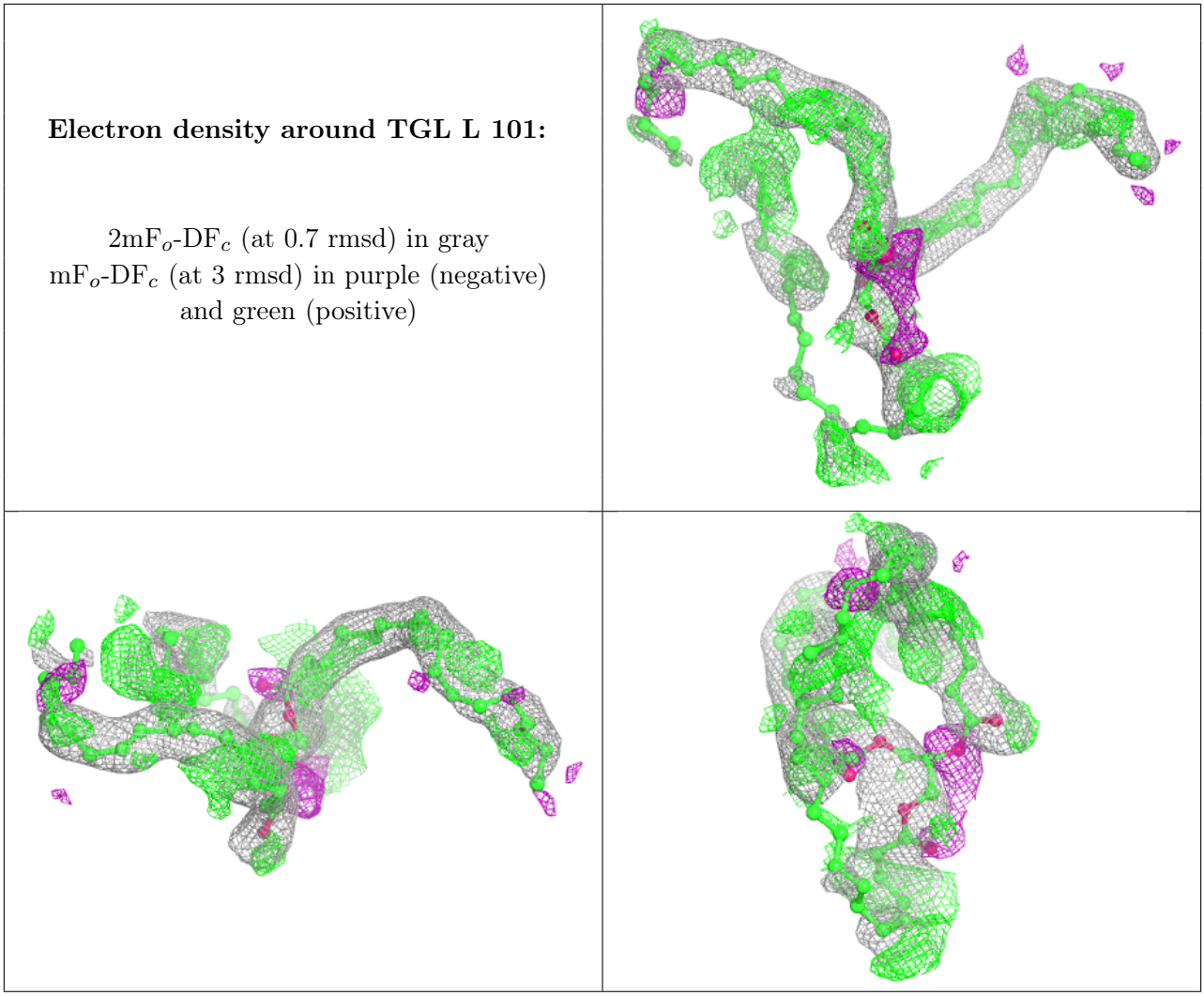
Electron density around PGV C 308:

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



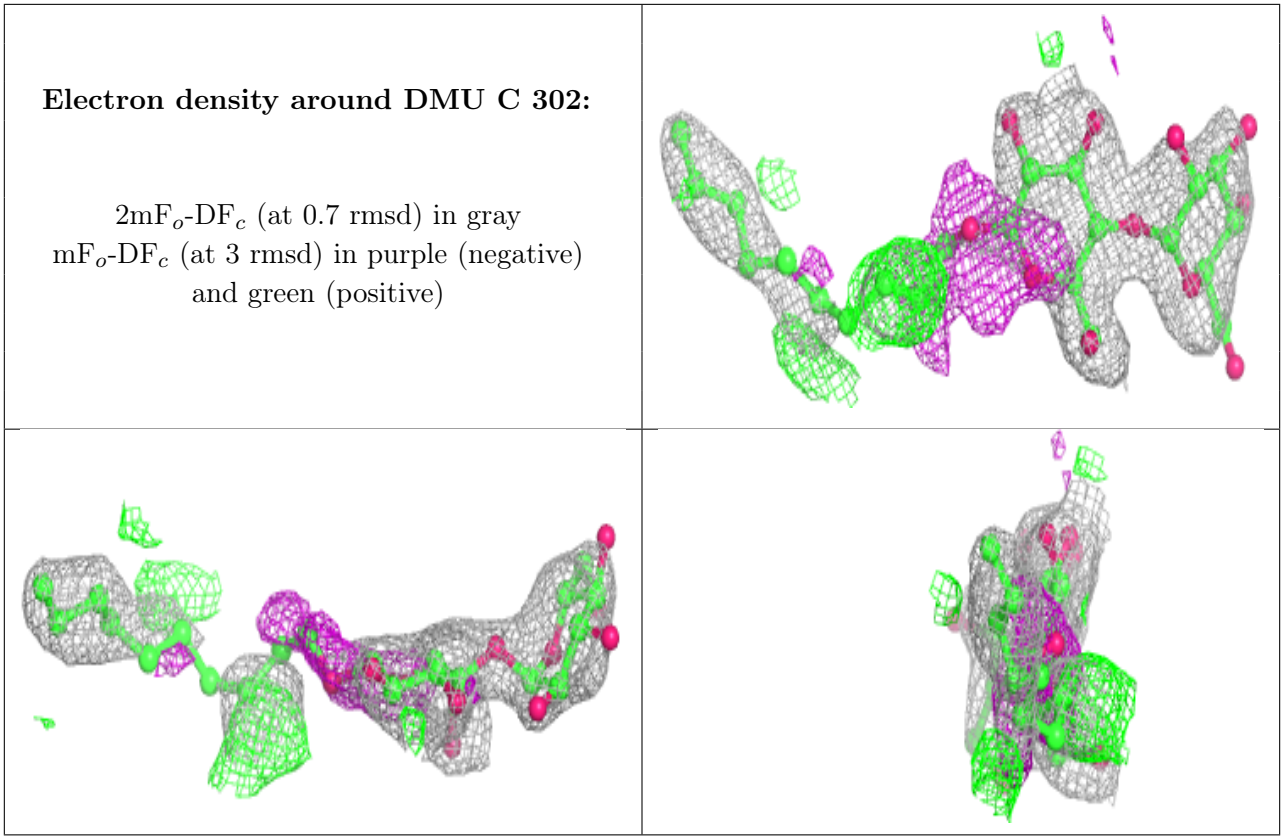
Electron density around TGL L 101:

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



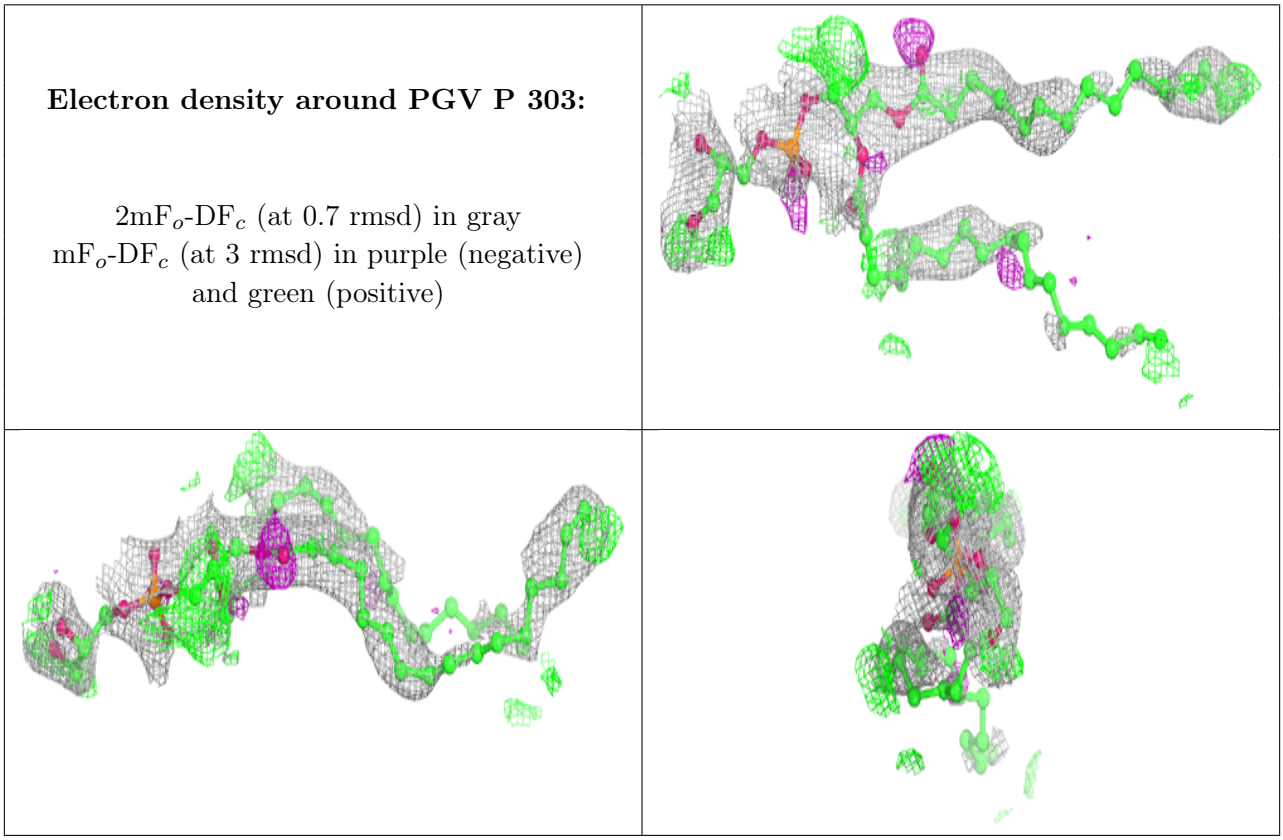
Electron density around DMU C 302:

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



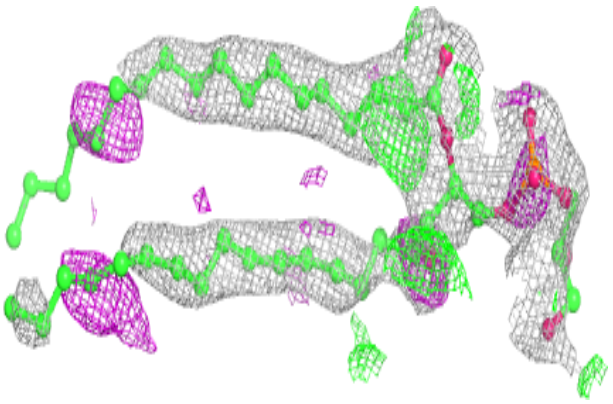
Electron density around PGV P 303:

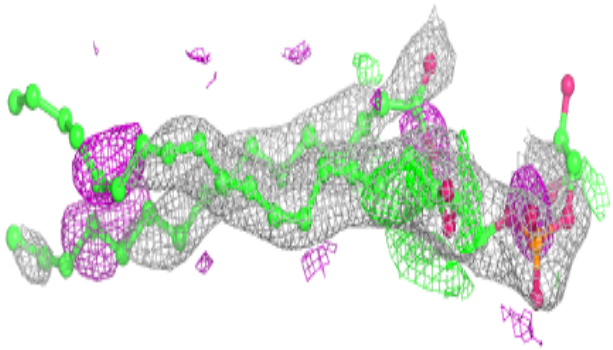
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

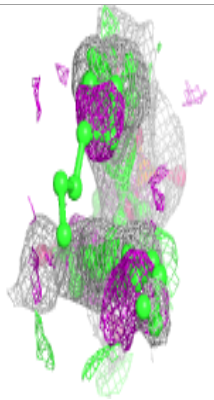


Electron density around PGV Z 101:

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

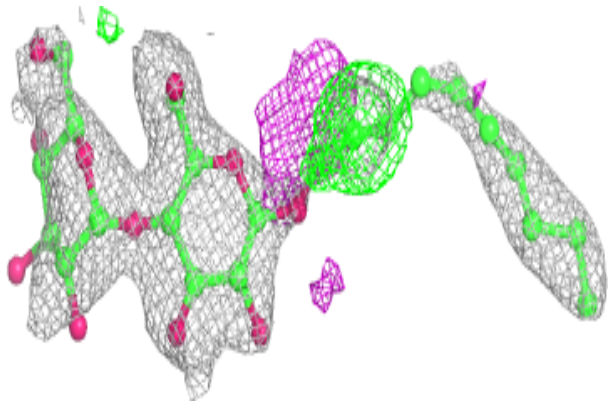


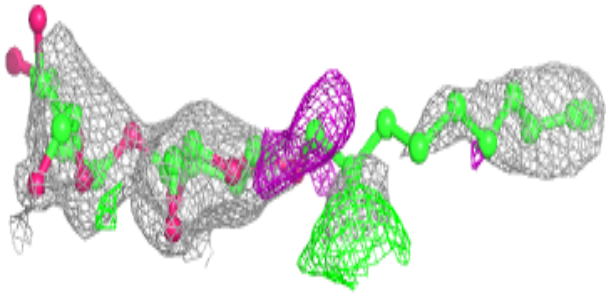


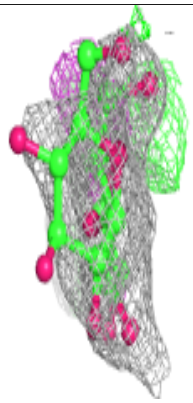


Electron density around DMU P 308:

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

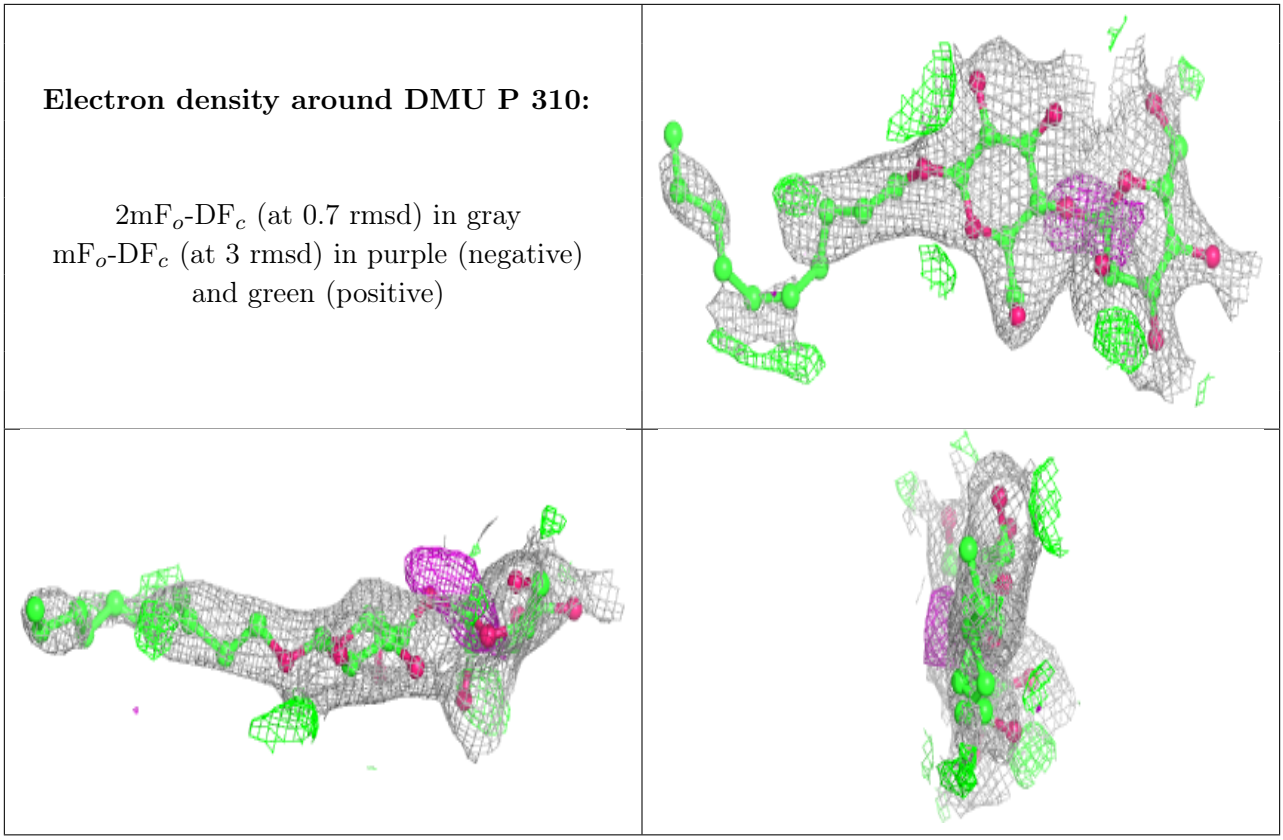






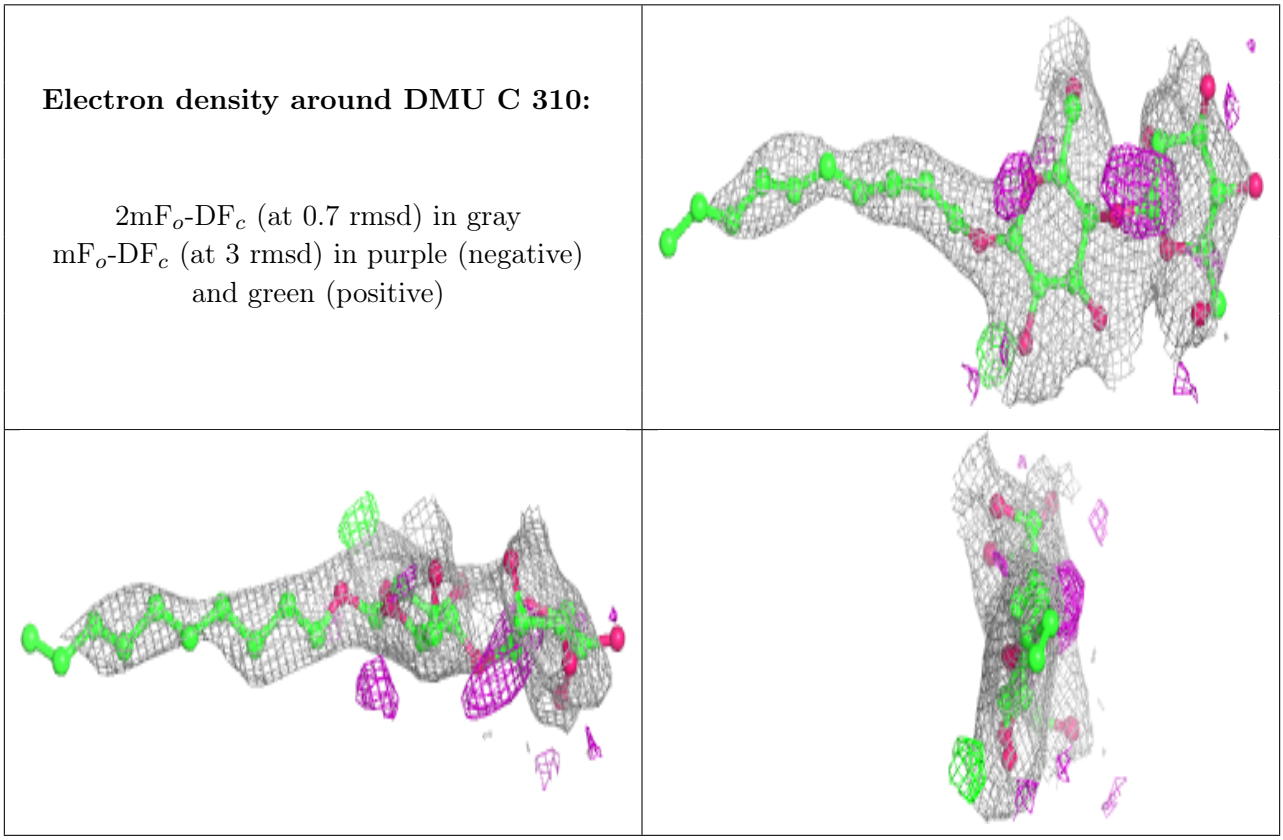
Electron density around DMU P 310:

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



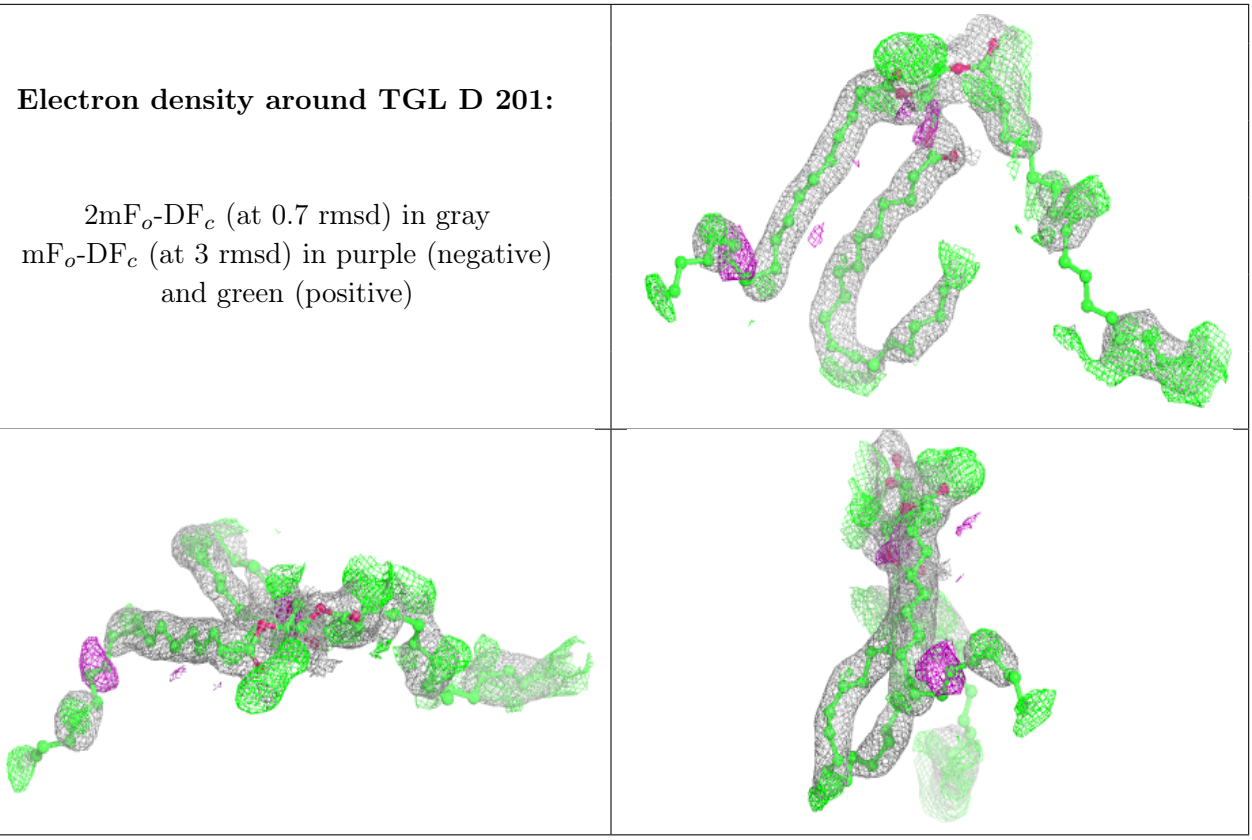
Electron density around DMU C 310:

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



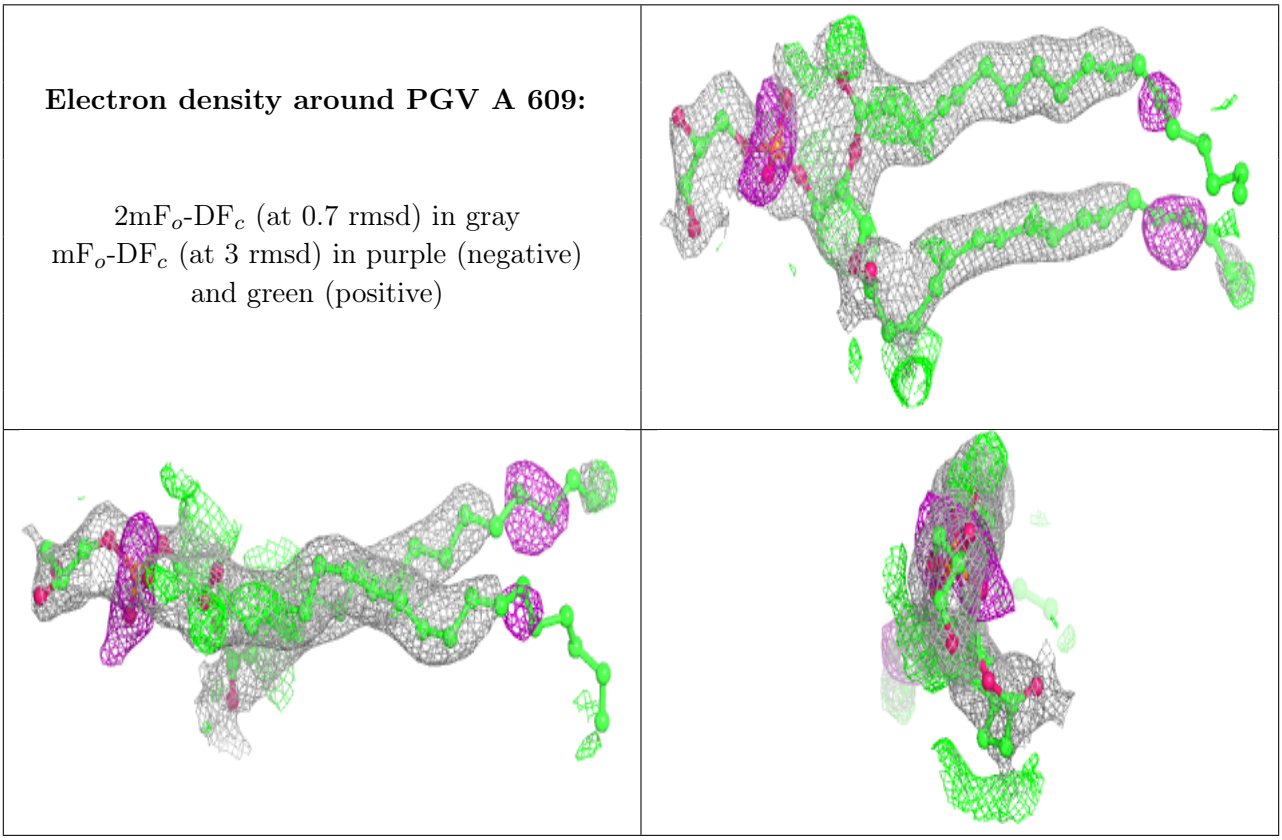
Electron density around TGL D 201:

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



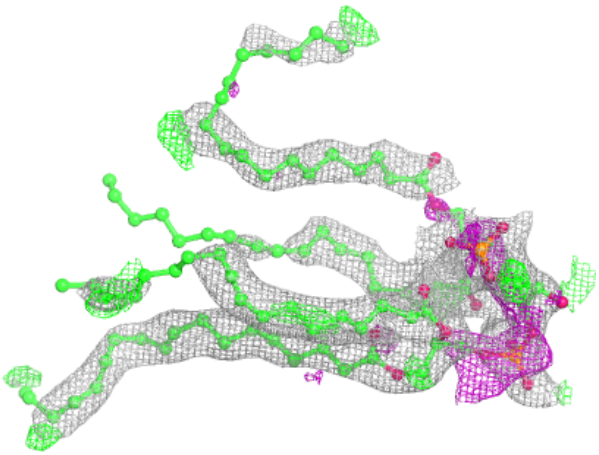
Electron density around PGV A 609:

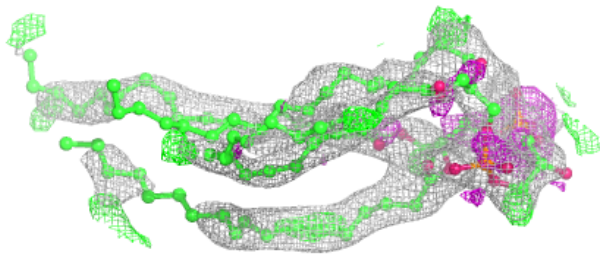
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

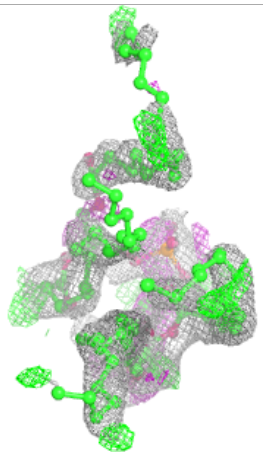


Electron density around CDL C 305:

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

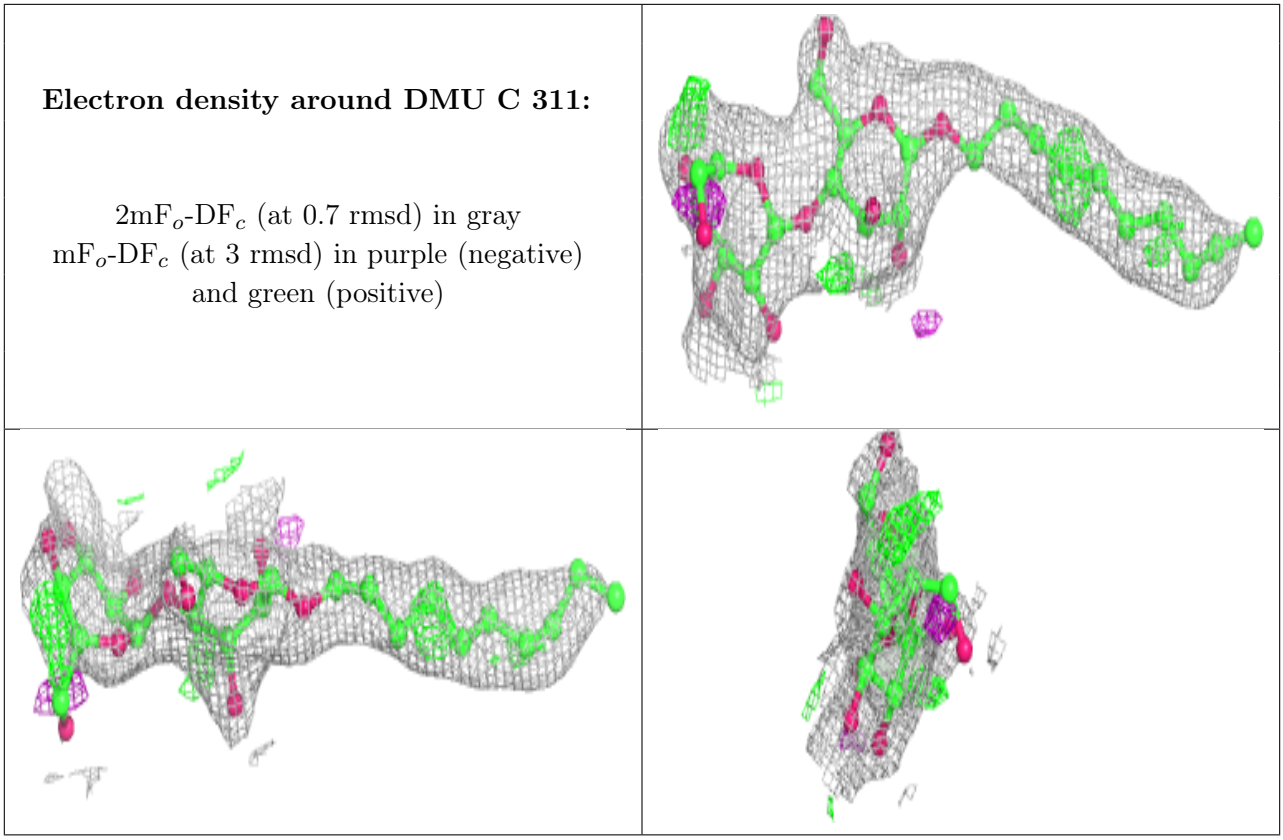






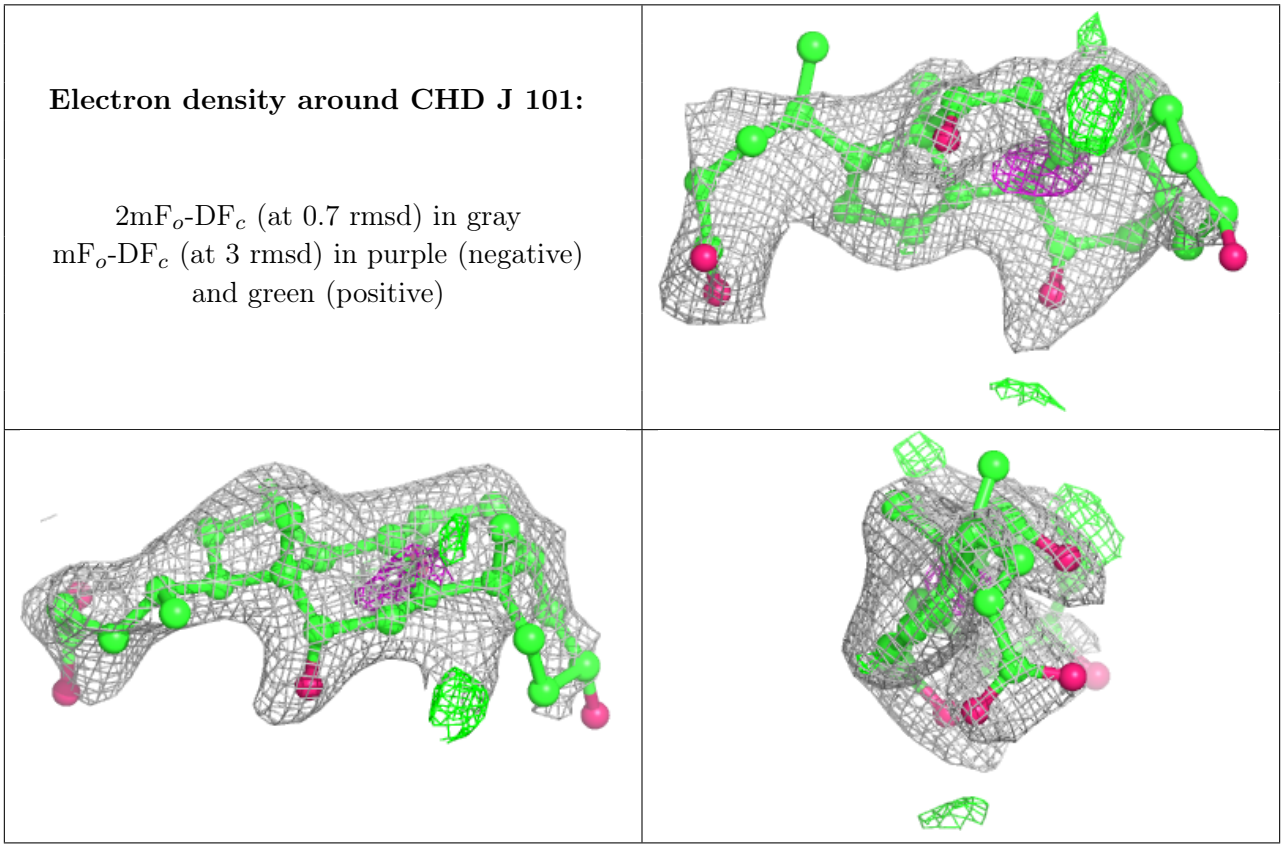
Electron density around DMU C 311:

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



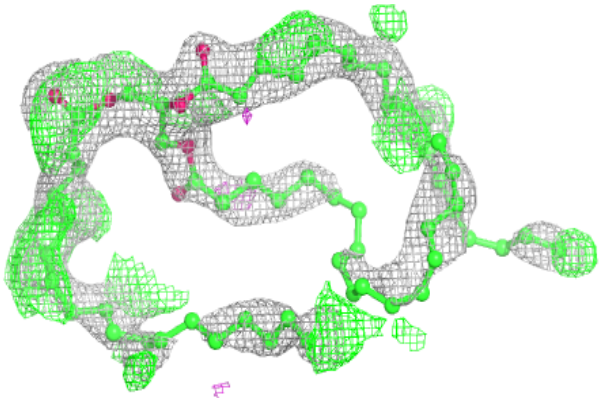
Electron density around CHD J 101:

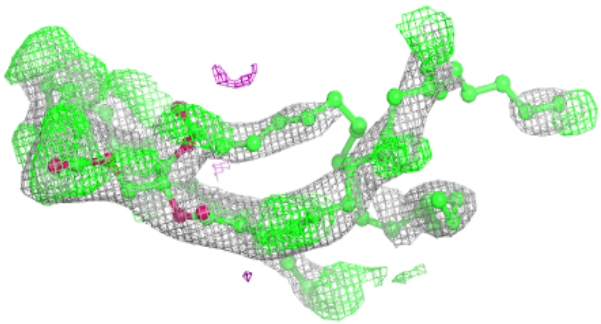
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

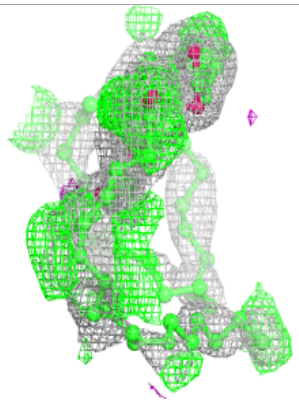


Electron density around TGL N 609:

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

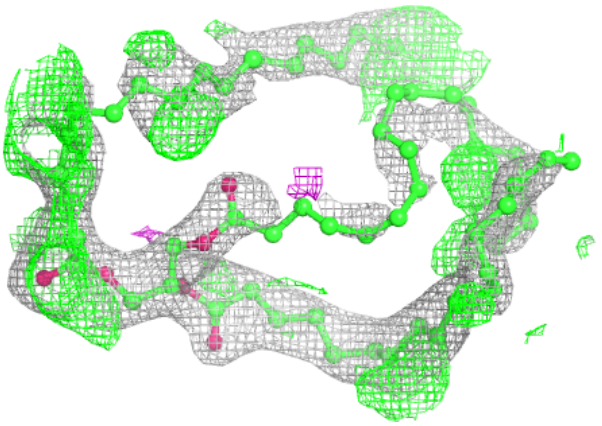


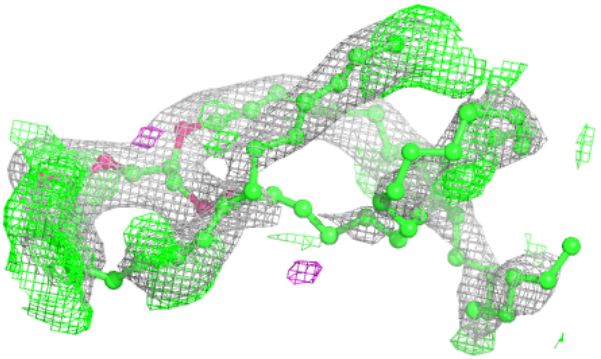


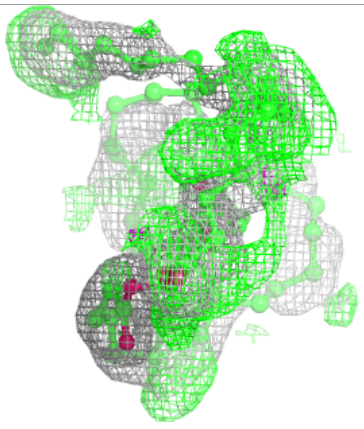


Electron density around TGL B 301:

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

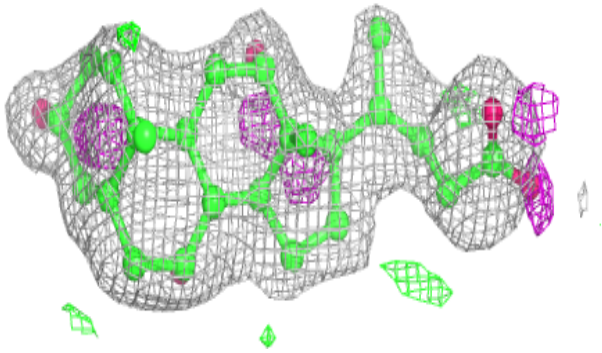


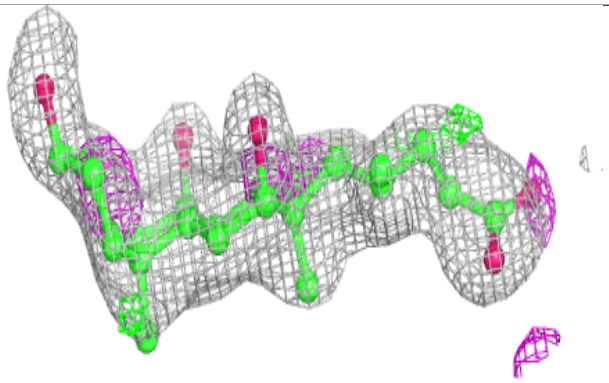


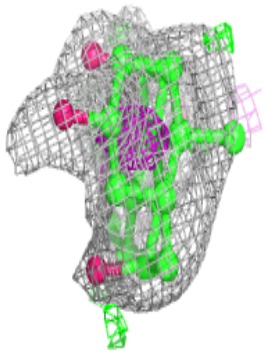


Electron density around CHD C 306:

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

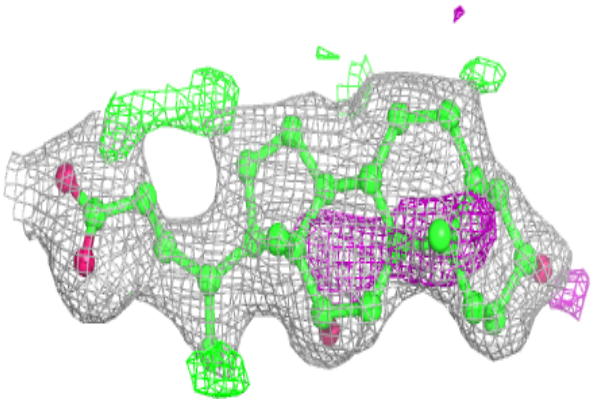


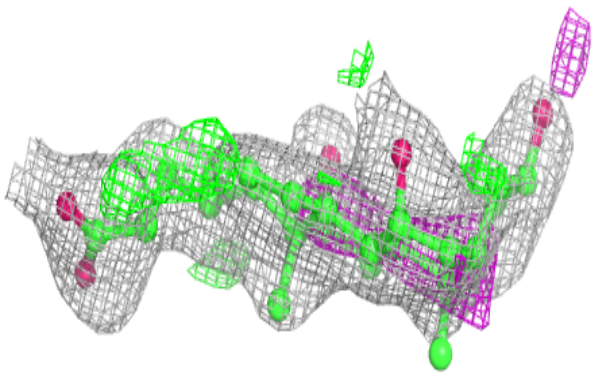


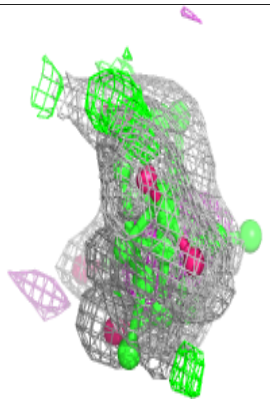


Electron density around CHD P 307:

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

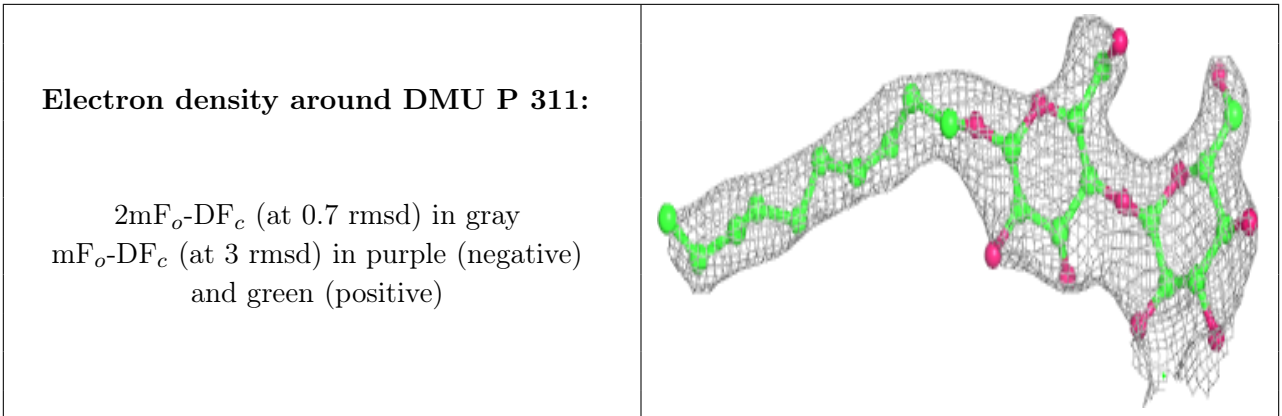


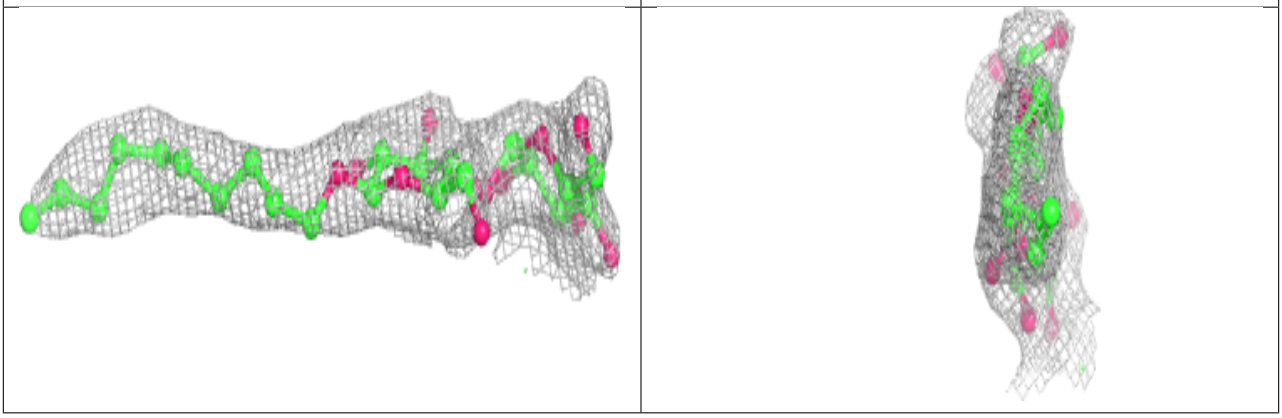




Electron density around DMU P 311:

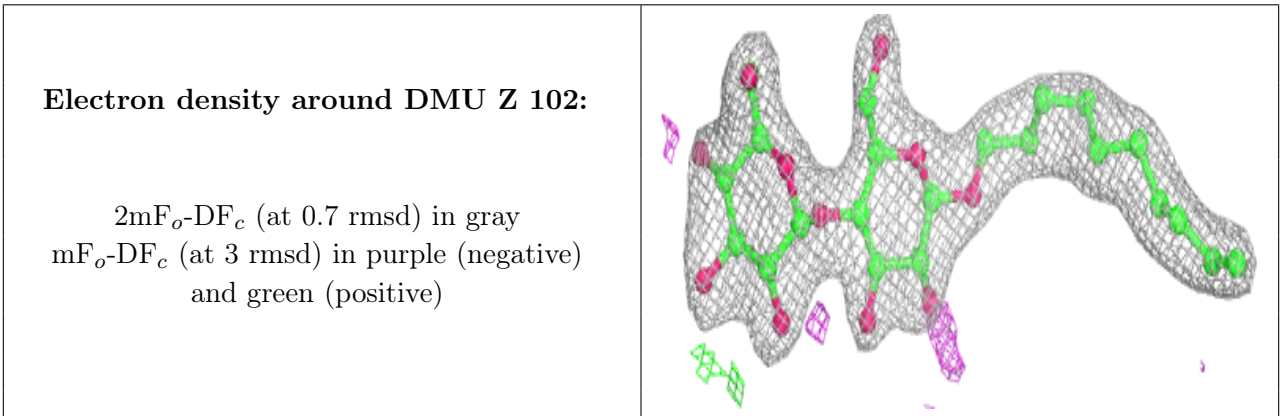
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

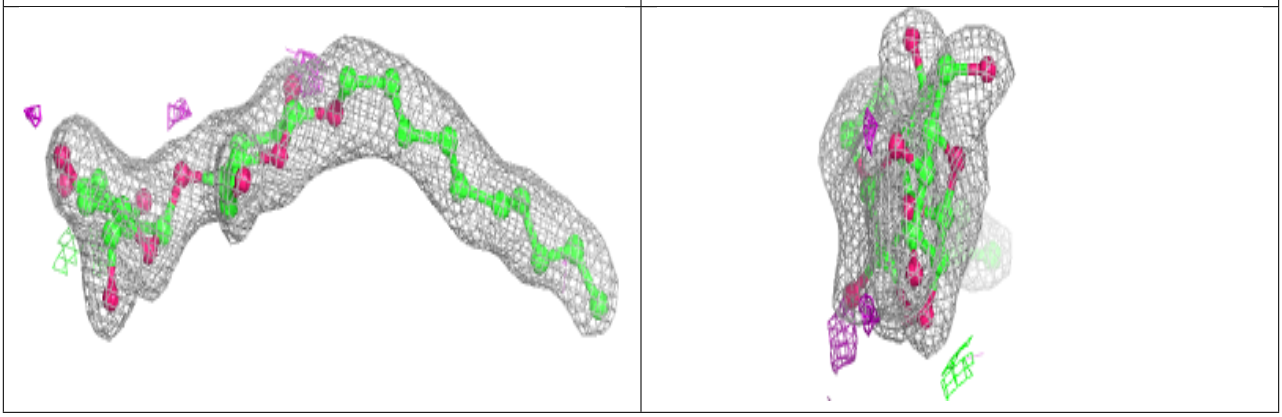




Electron density around DMU Z 102:

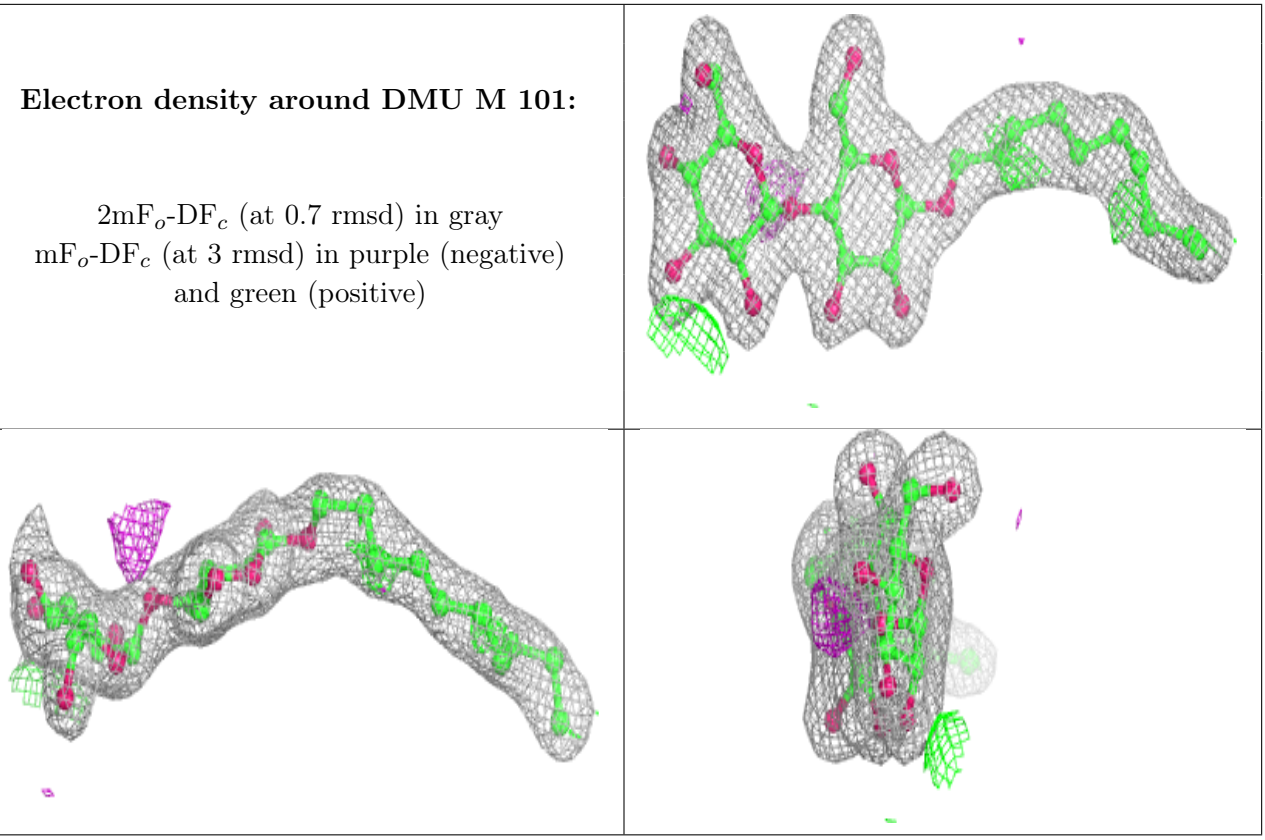
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





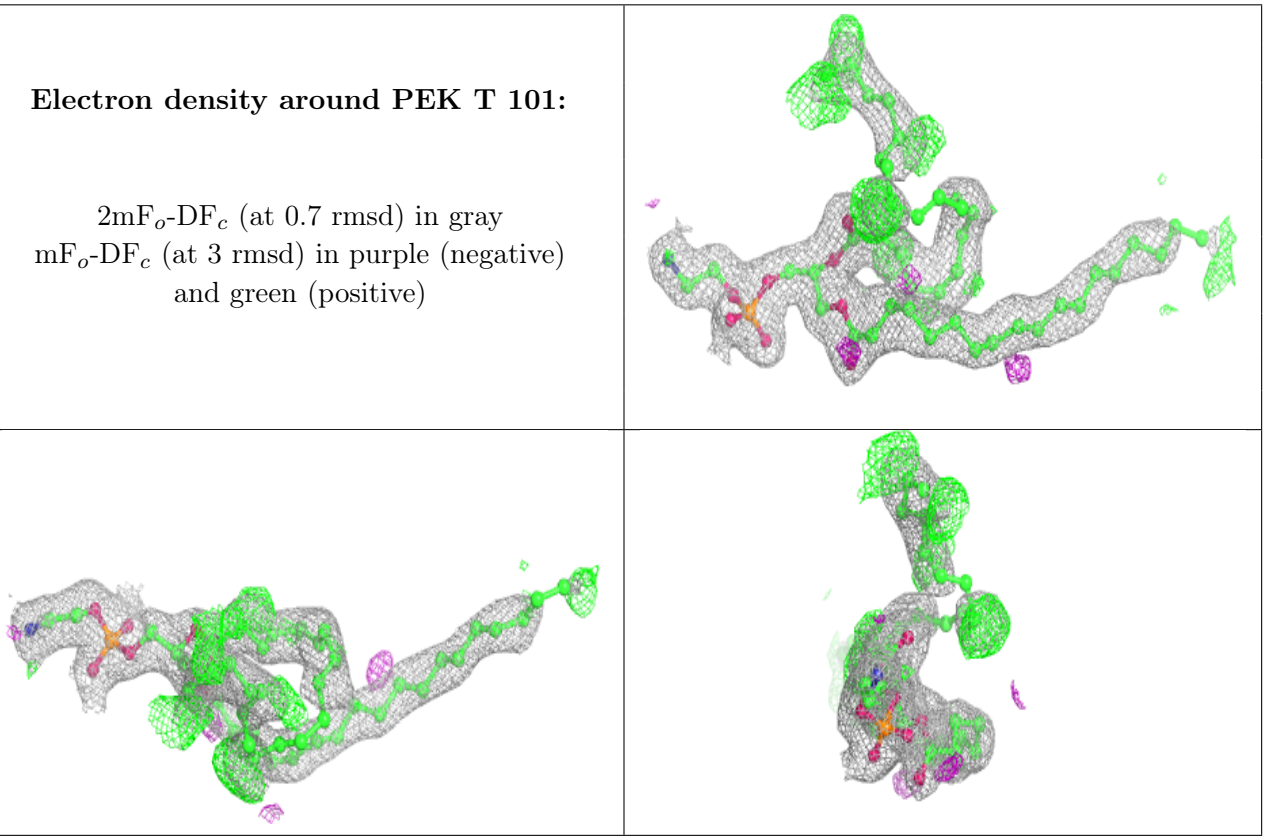
Electron density around DMU M 101:

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



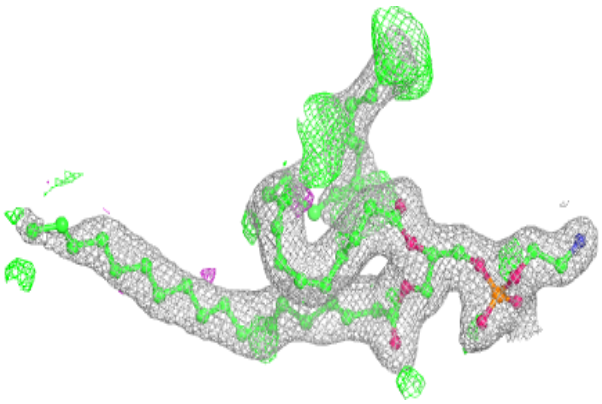
Electron density around PEK T 101:

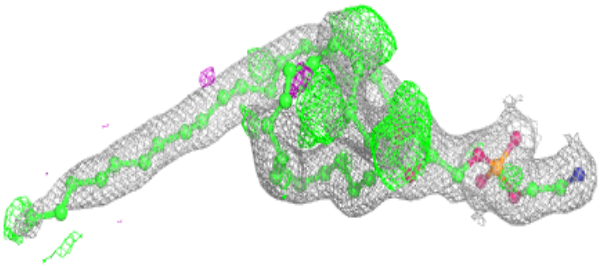
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

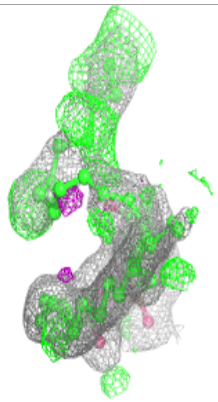


Electron density around PEK G 101:

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

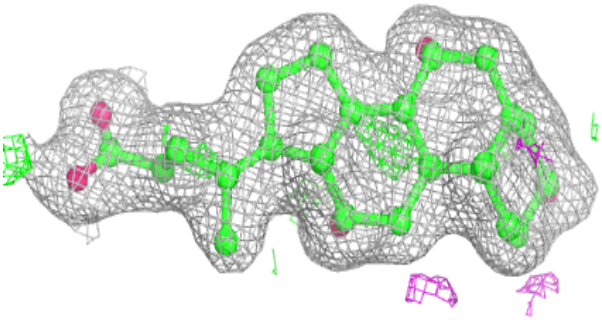


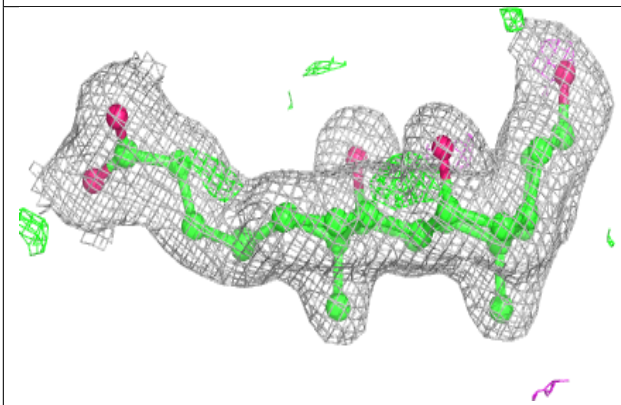


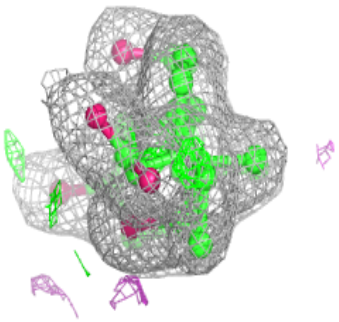


Electron density around CHD B 302:

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

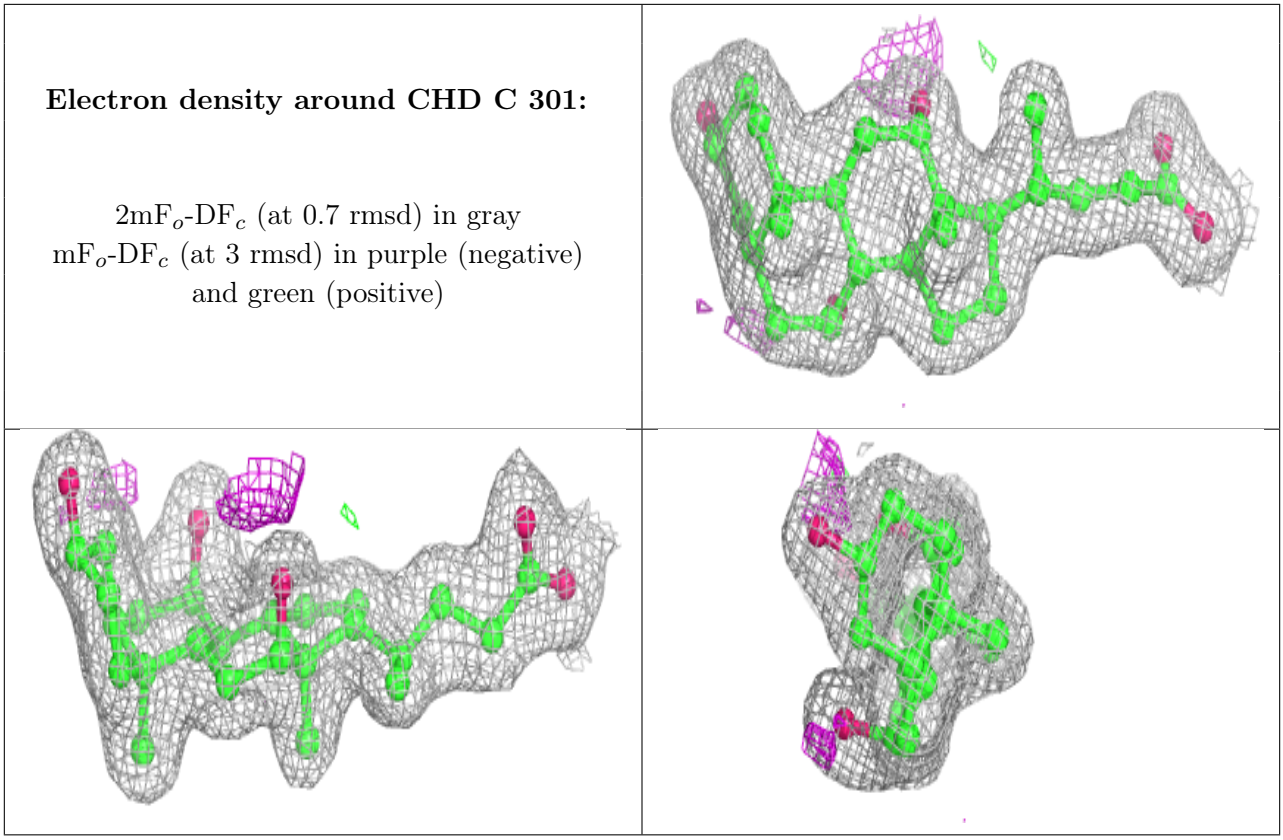






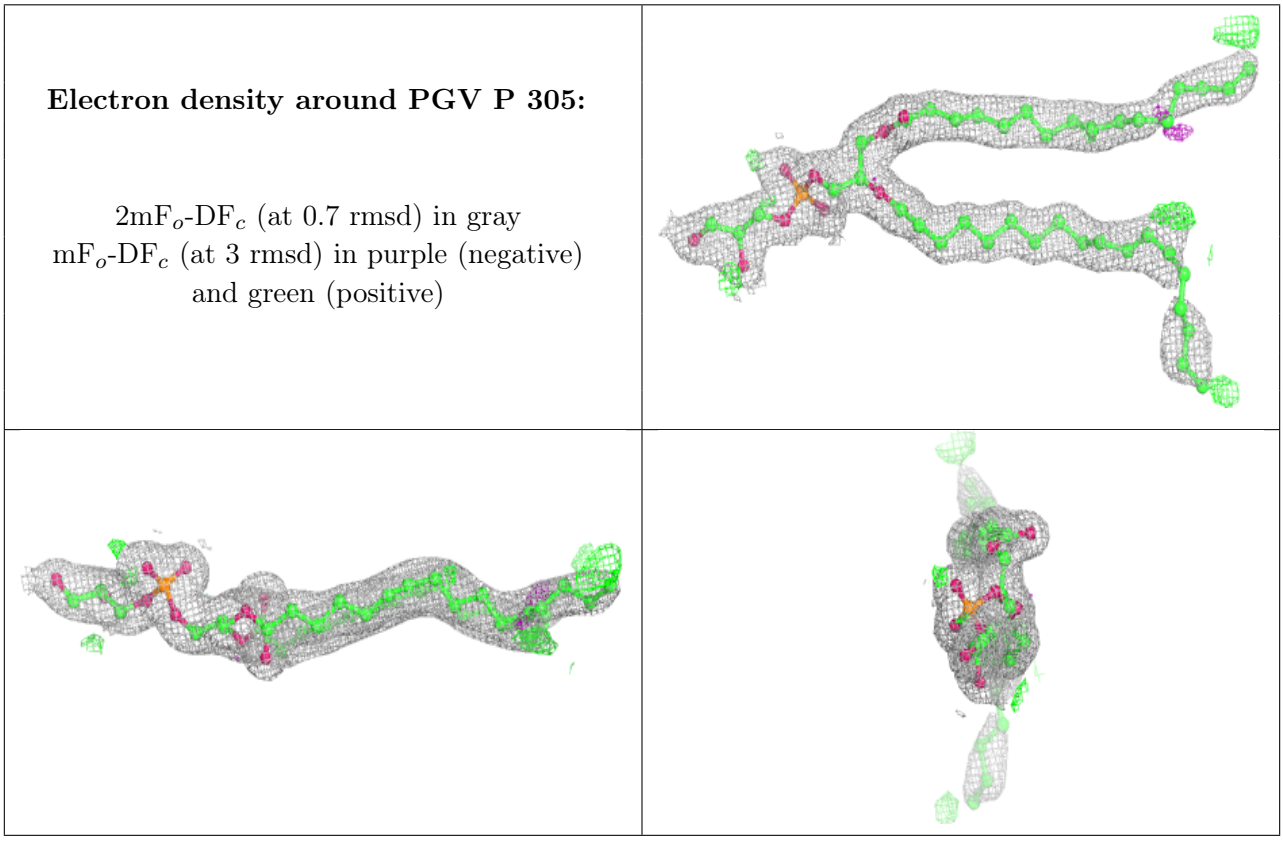
Electron density around CHD C 301:

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



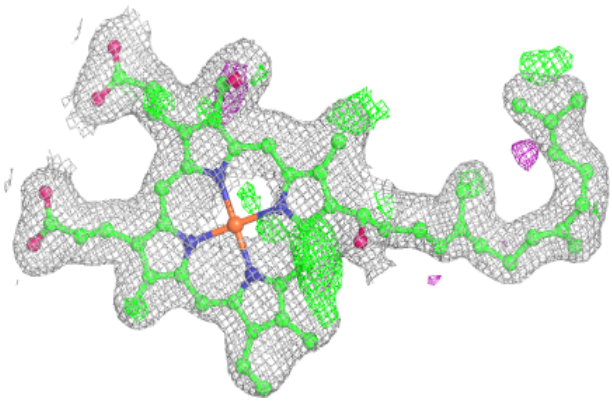
Electron density around PGV P 305:

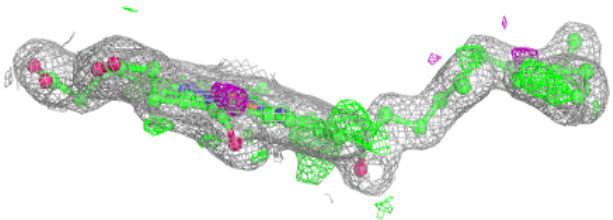
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

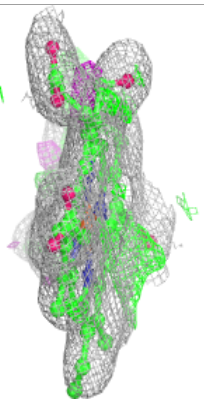


Electron density around HEA N 602 (A):

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

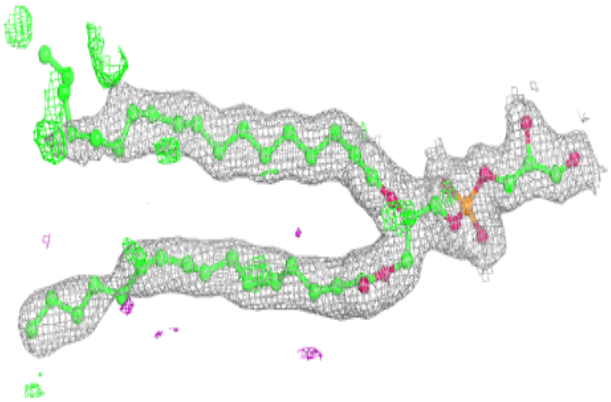


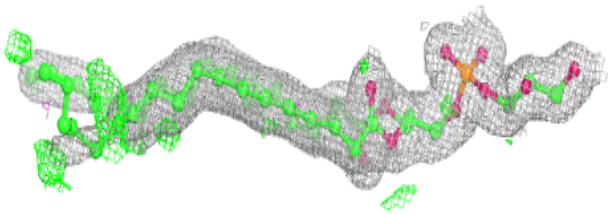


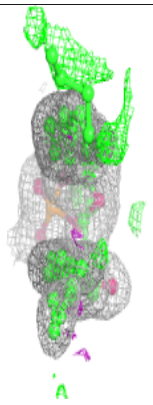


Electron density around PGV C 304:

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

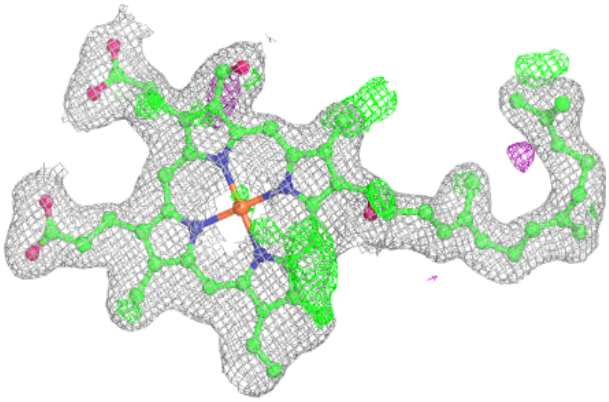


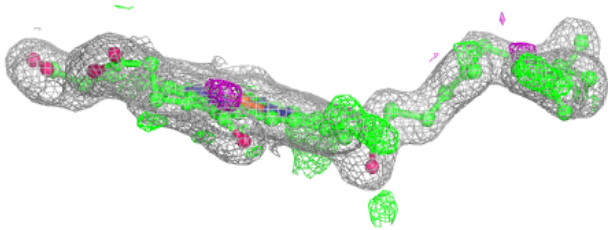


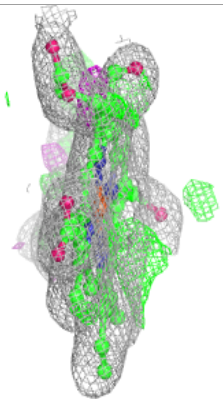


Electron density around HEA N 602 (B):

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

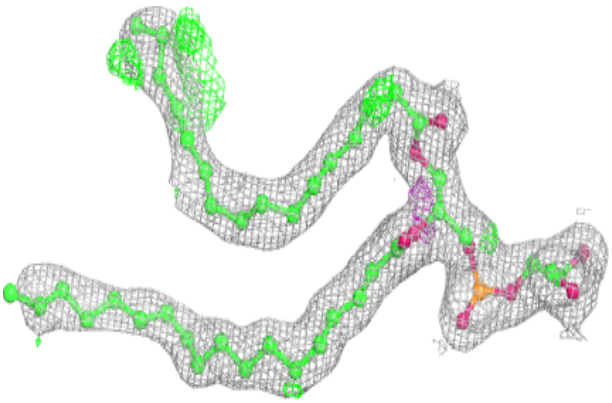


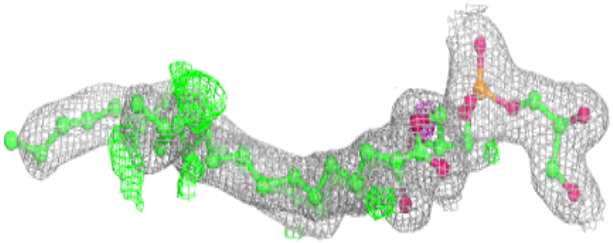




Electron density around PGV N 608:

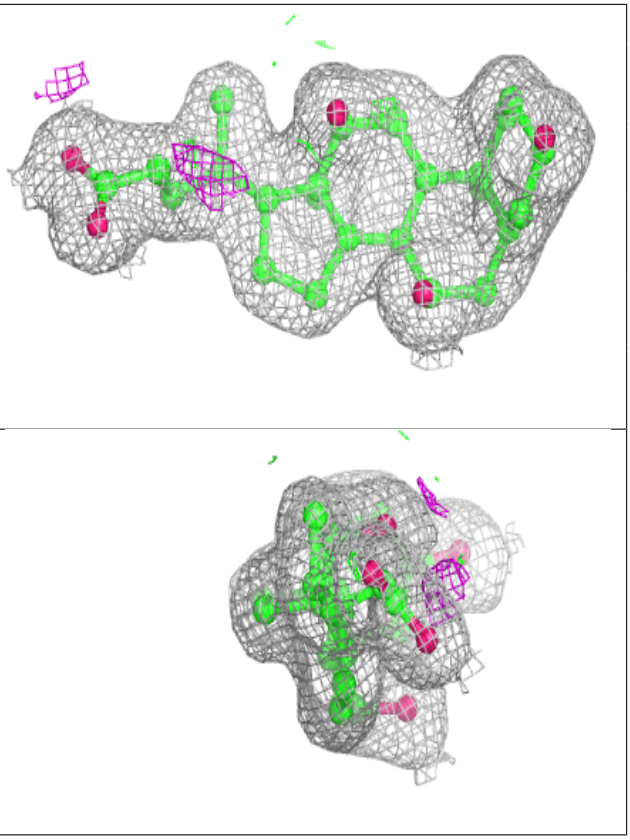
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





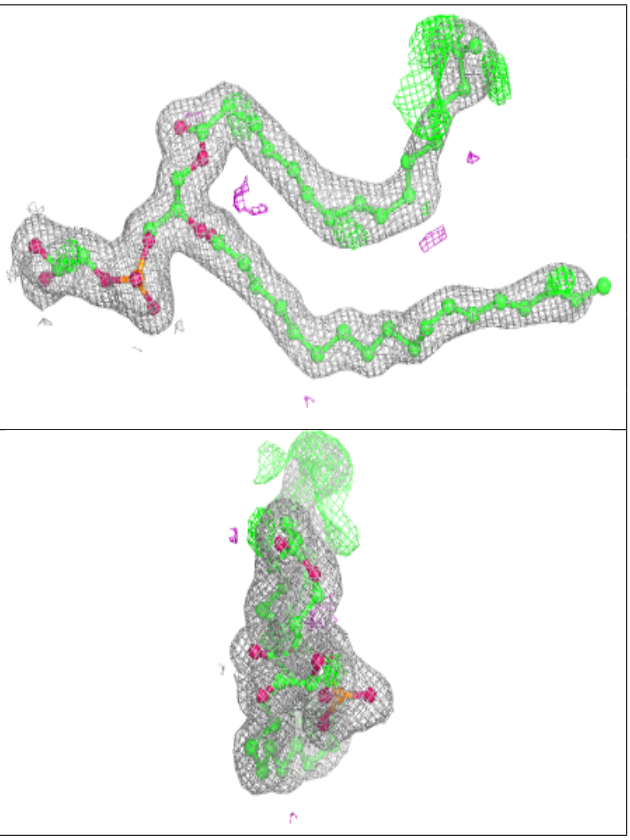
Electron density around CHD G 103:

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



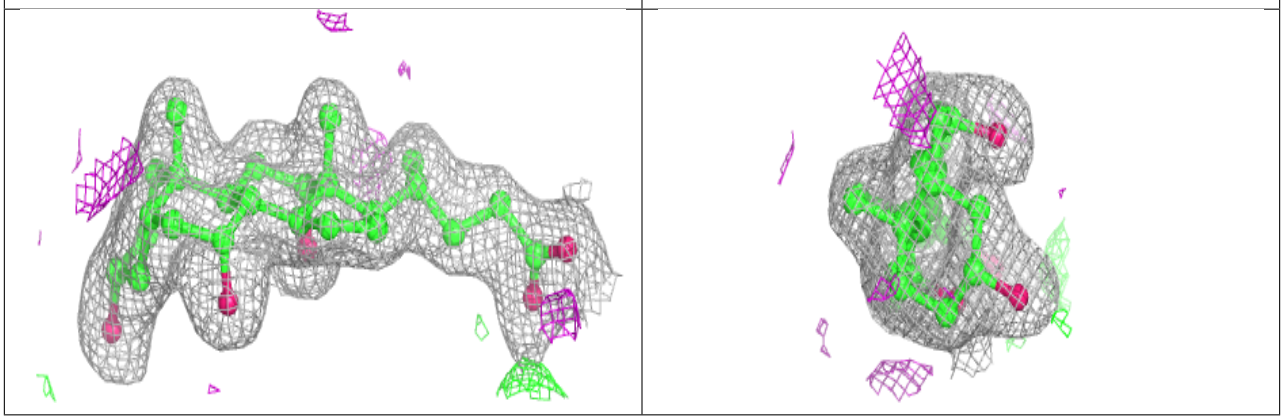
Electron density around PGV A 608:

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



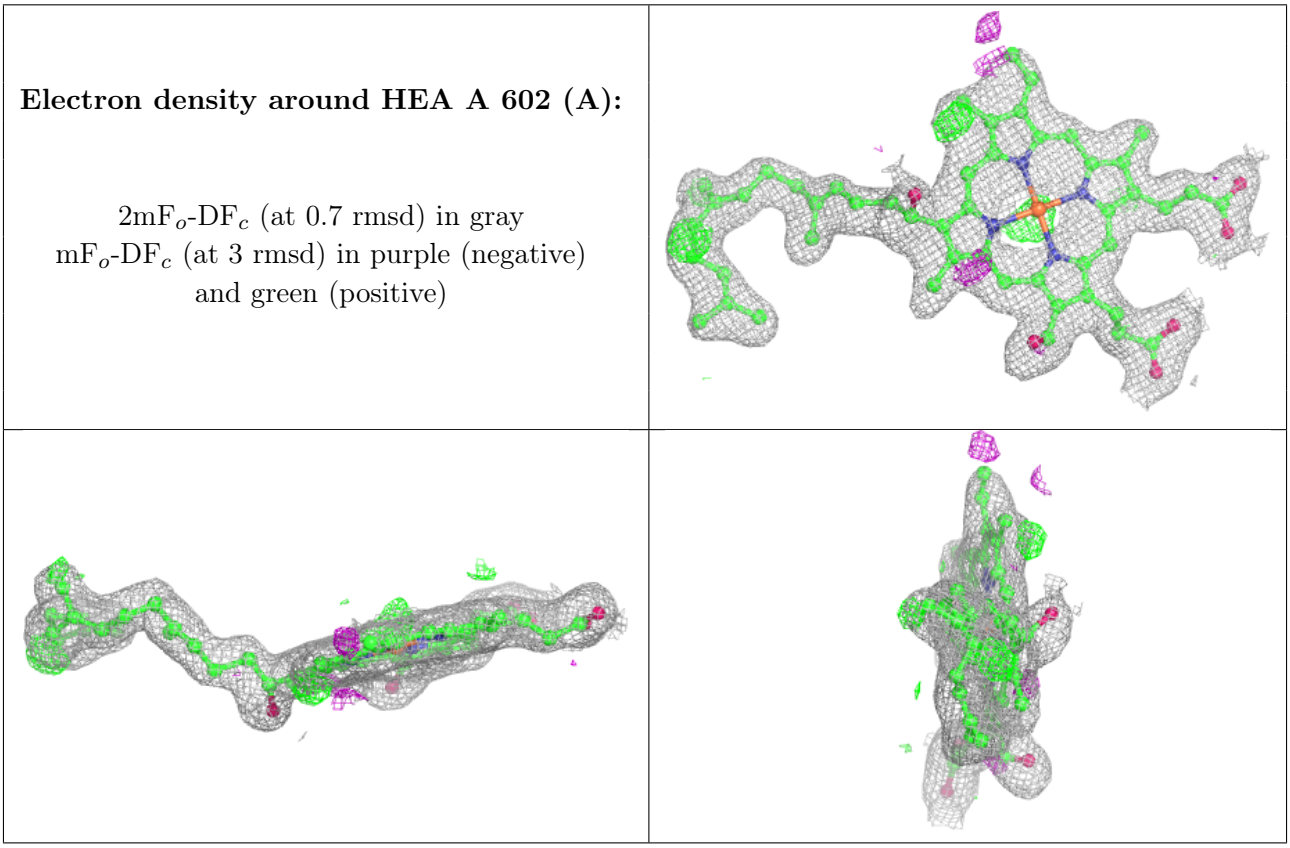
Electron density around CHD P 301:

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



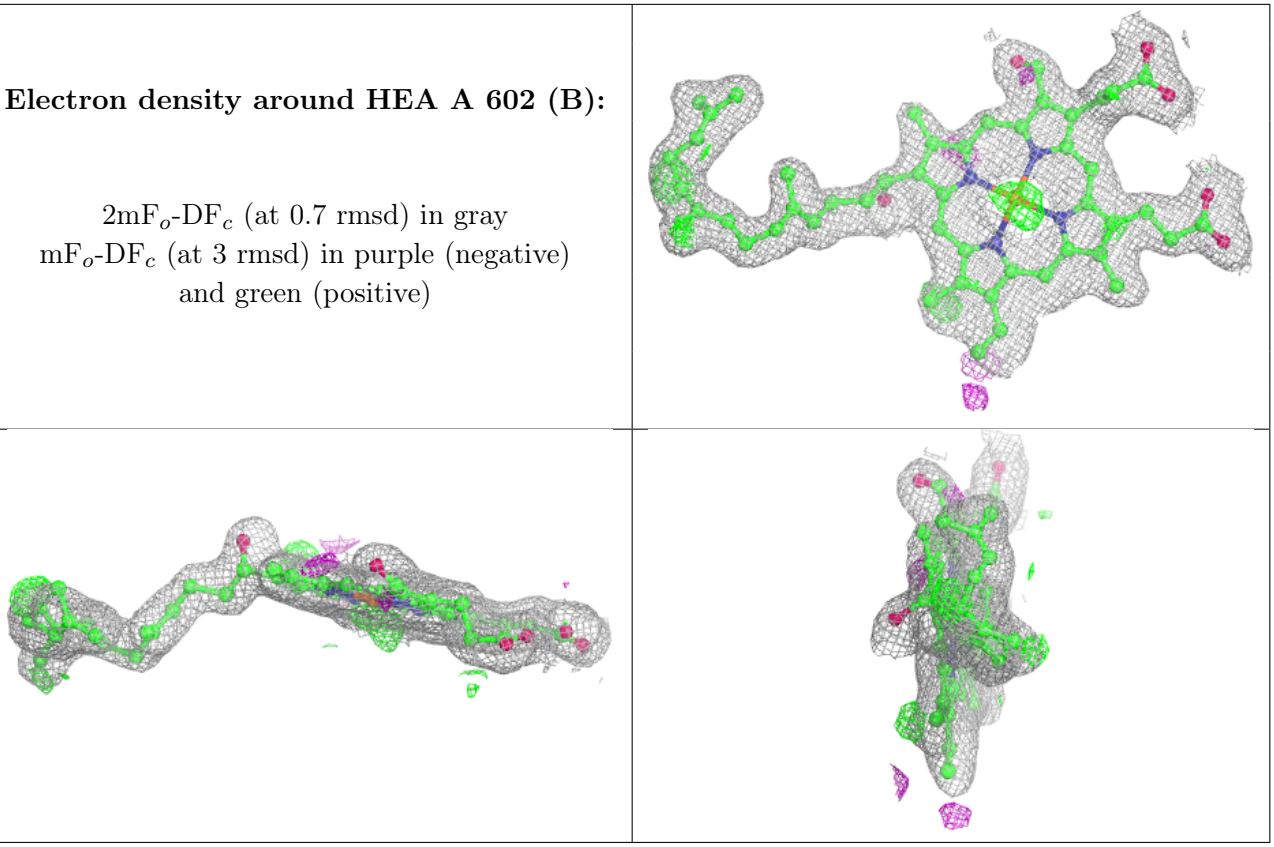
Electron density around HEA A 602 (A):

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



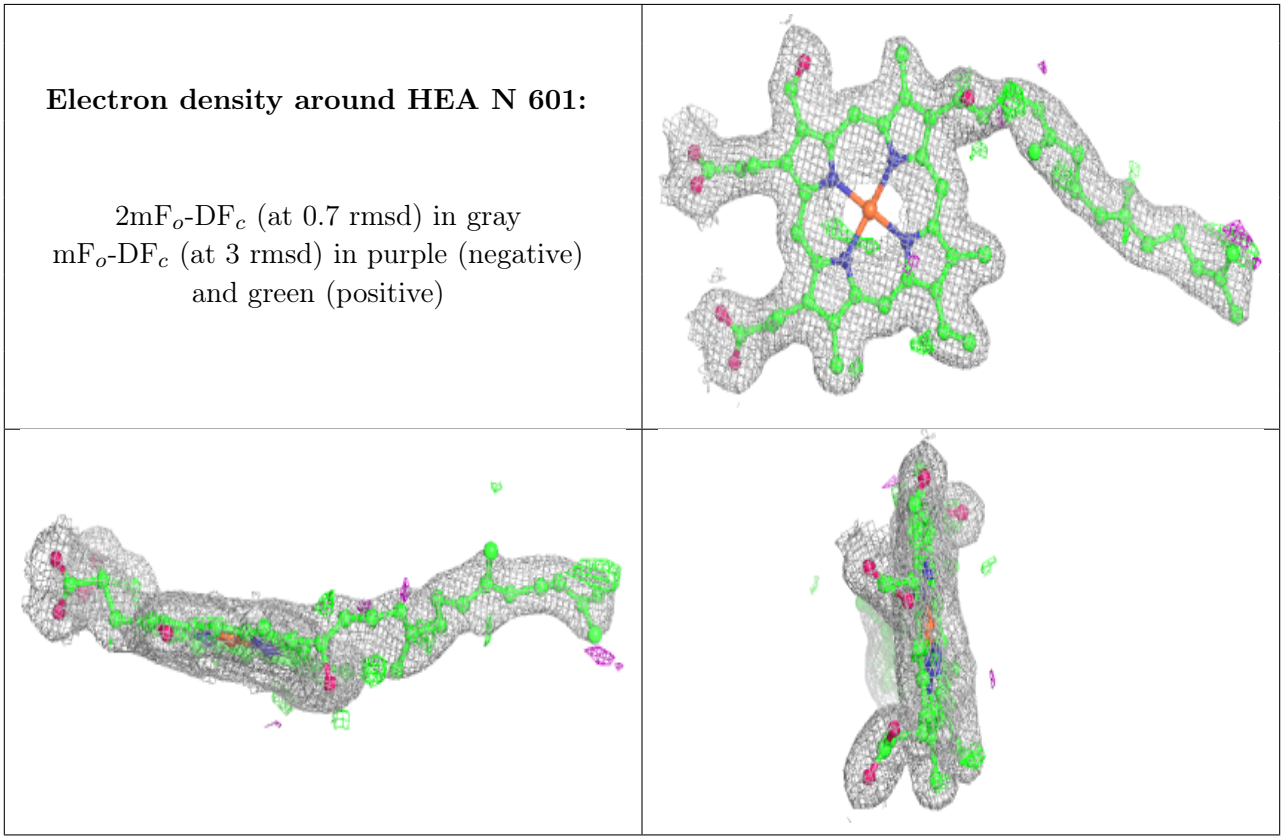
Electron density around HEA A 602 (B):

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



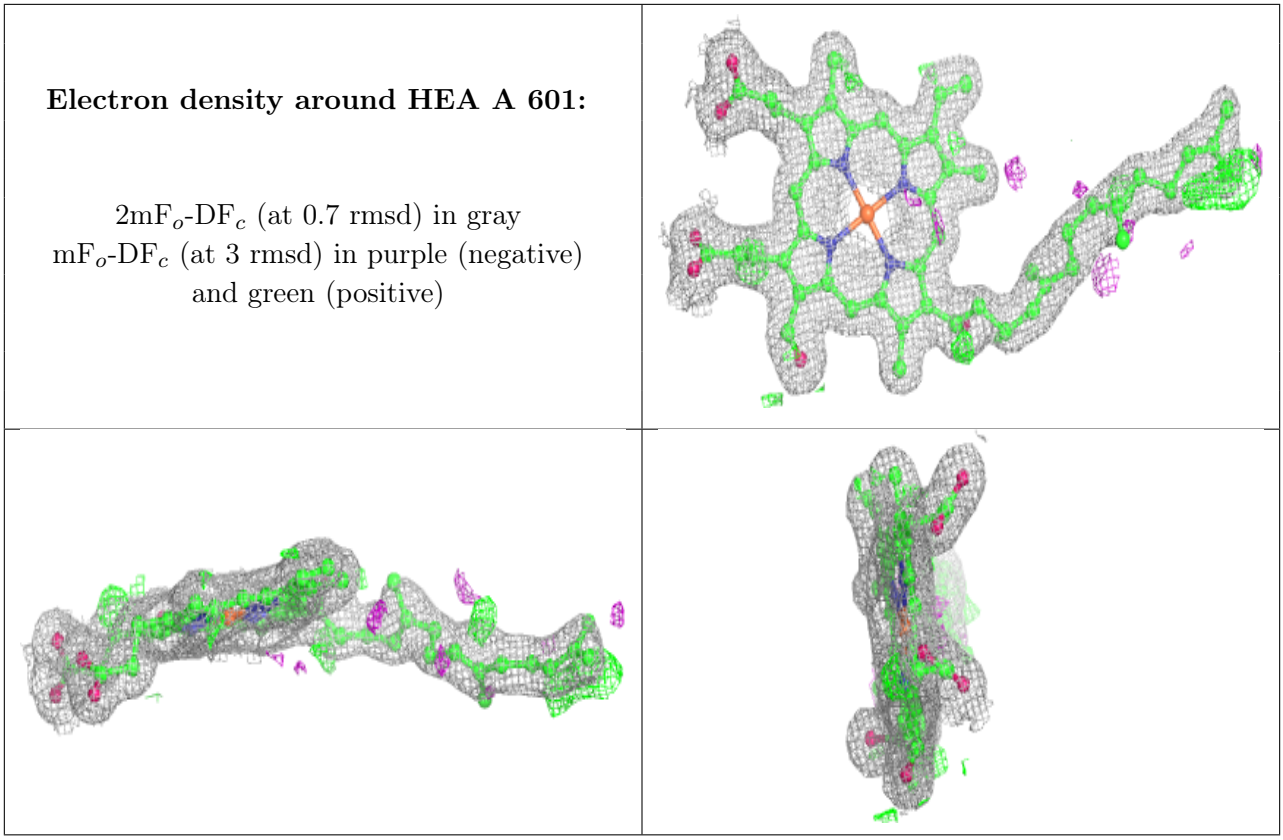
Electron density around HEA N 601:

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



Electron density around HEA A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.