Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:57 PM JST

PDB ID	:	5Z85
Title	:	The structure of azide-bound cytochrome c oxidase determined using the another batch crystals exposed to 20 mM azide solution for 2 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:

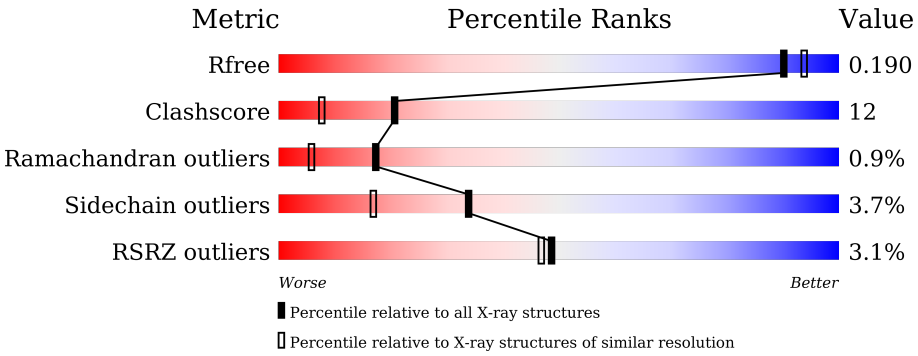
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	82% 16% •
1	N	514	82% 16% •
2	B	227	% 73% 24% •
2	O	227	% 75% 23% •
3	C	261	82% 17% ••
3	P	261	% 80% 19% ••

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Mol	Chain	Length	Quality of chain
4	D	147	79% 17%
4	Q	147	6% 74% 18% 5%
5	E	109	2% 83% 12%
5	R	109	2% 84% 10%
6	F	98	7% 78% 20%
6	S	98	8% 79% 13% 5%
7	G	85	16% 56% 28% 11%
7	T	85	19% 68% 19% 11%
8	H	85	8% 73% 13% 5% 7%
8	U	85	7% 75% 13% 5% 7%
9	I	73	7% 70% 25% 5%
9	V	73	7% 73% 23%
10	J	59	7% 85% 12%
10	W	59	3% 86% 10%
11	K	56	79% 9% 12%
11	X	56	7% 71% 16% 12%
12	L	47	2% 77% 19%
12	Y	47	2% 81% 17%
13	M	46	2% 74% 17% 7%
13	Z	46	9% 76% 17% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	607	-	-	X	-
18	AZI	N	607	-	-	X	-
21	EDO	A	612	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	A	614	-	X	X	-
21	EDO	A	618	-	-	X	-
21	EDO	C	318	-	-	-	X
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	-
21	EDO	D	204	-	-	-	X
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	Q	204	-	-	X	-
27	CDL	C	305	-	-	X	-
27	CDL	G	102	-	-	X	-
27	CDL	P	306	-	-	X	-
27	CDL	T	103	-	-	X	-
7	TPO	T	11	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33411 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	18	0
			4165	2777	645	703	40			
1	N	514	Total	C	N	O	S	0	18	0
			4160	2774	642	702	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	4	0
			1859	1211	285	344	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	7	0
			2171	1449	347	360	15			
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	1	0
			1204	783	198	219	4			
4	Q	144	Total	C	N	O	S	0	2	0
			1213	791	198	220	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	3	0
			771	477	138	150	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	0	0
			675	431	129	113	1	1			

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

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

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

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

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

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

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

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

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

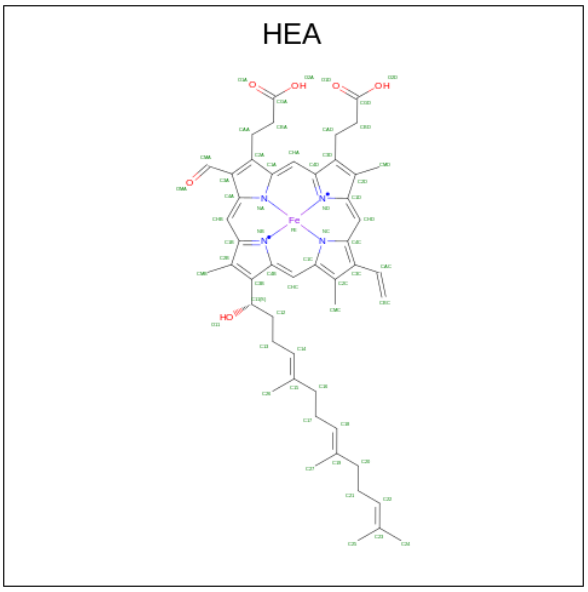
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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		

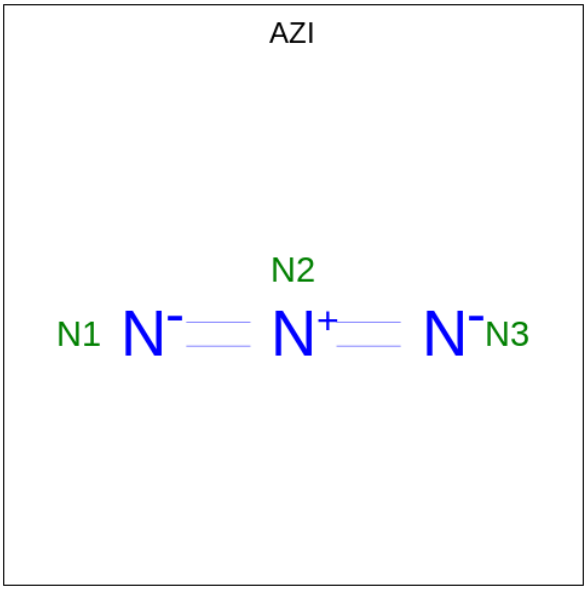
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

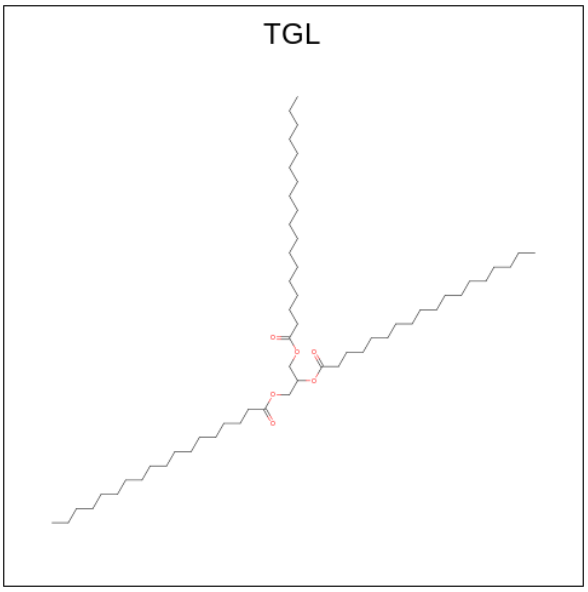
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



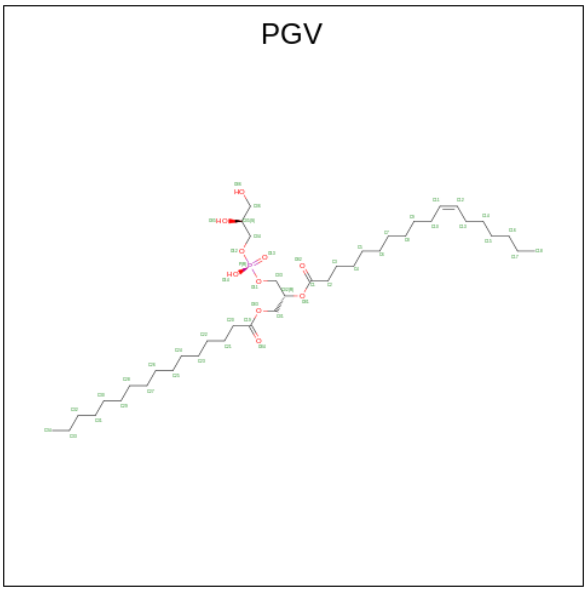
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

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



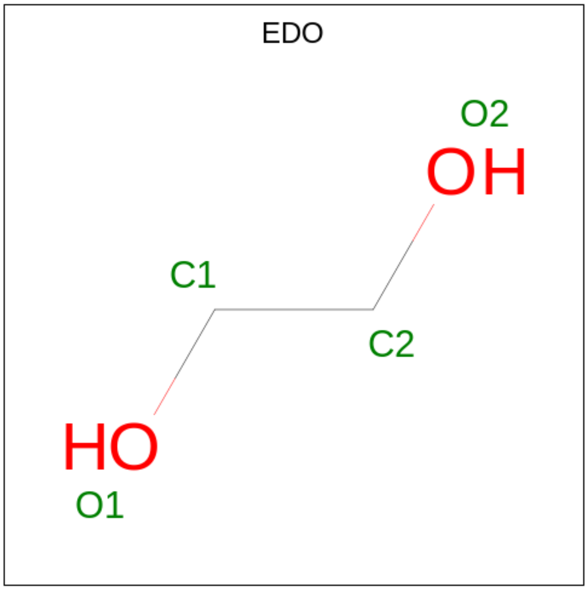
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0
19	Y	1	Total C O 63 57 6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

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



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

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

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

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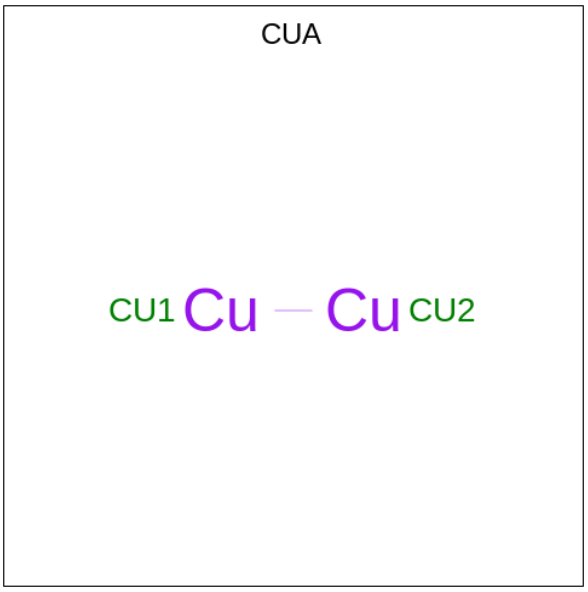
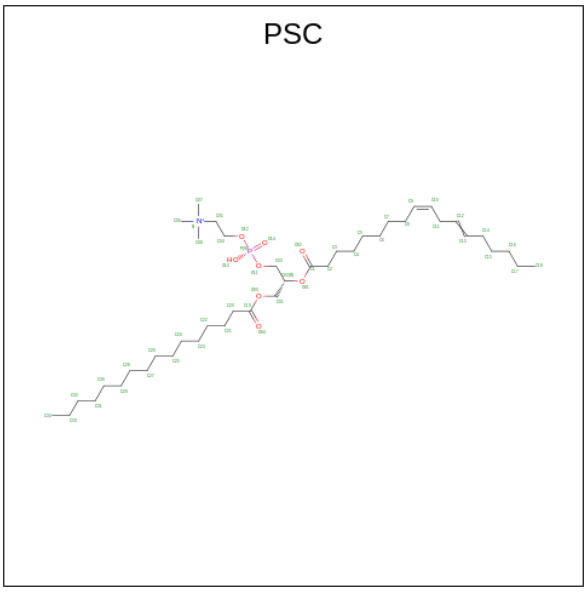
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	Q	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21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

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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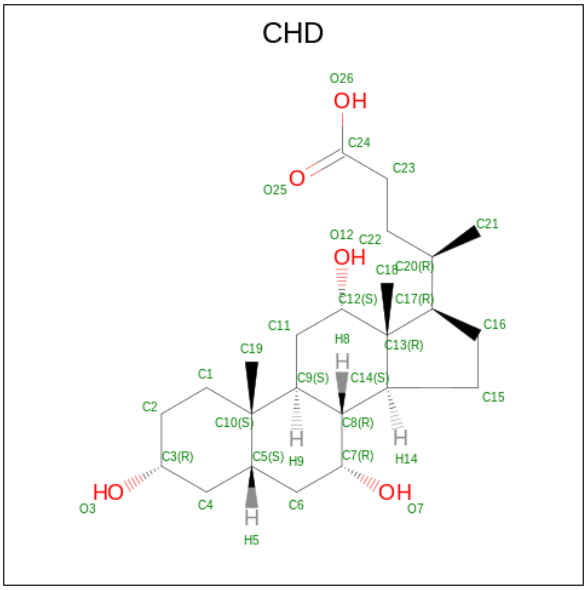
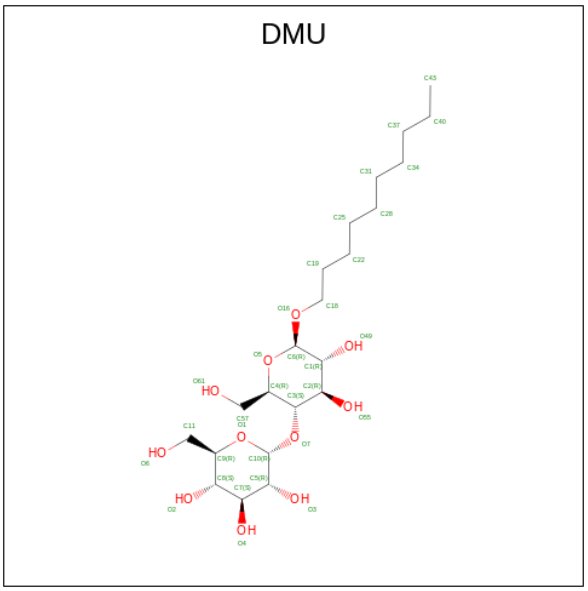
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



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

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

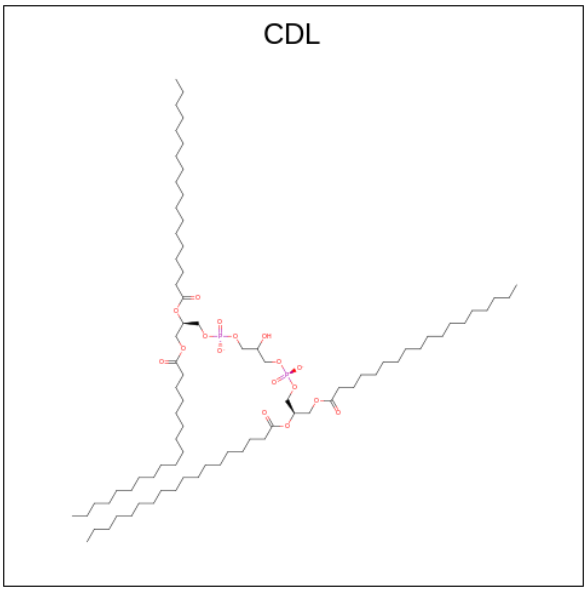


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 33 22 11	0	0
25	C	1	Total C O 33 22 11	0	0
25	C	1	Total C O 33 22 11	0	0
25	M	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	Z	1	Total C O 33 22 11	0	0

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

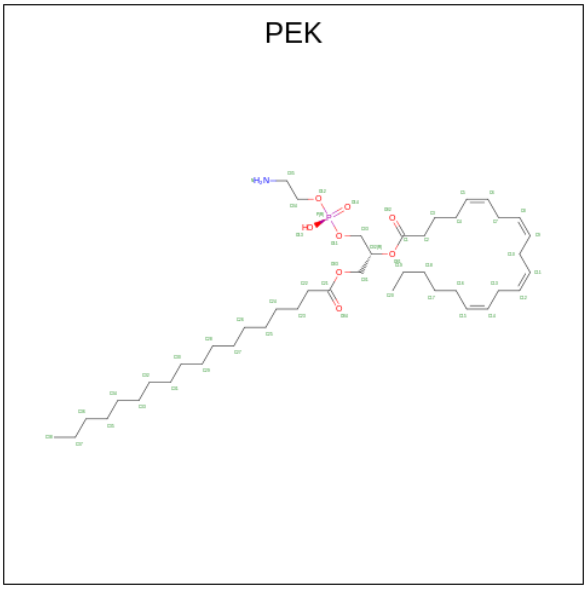
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total X 1 1	0	0
26	P	1	Total X 1 1	0	0

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



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

- Molecule 28 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	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	219	Total	O	0	0
			219	219		
30	B	131	Total	O	0	1
			132	132		
30	C	96	Total	O	0	0
			96	96		
30	D	93	Total	O	0	0
			93	93		
30	E	85	Total	O	0	0
			85	85		
30	F	78	Total	O	0	0
			78	78		
30	G	37	Total	O	0	0
			37	37		
30	H	30	Total	O	0	0
			30	30		
30	I	20	Total	O	0	0
			20	20		
30	J	22	Total	O	0	0
			22	22		

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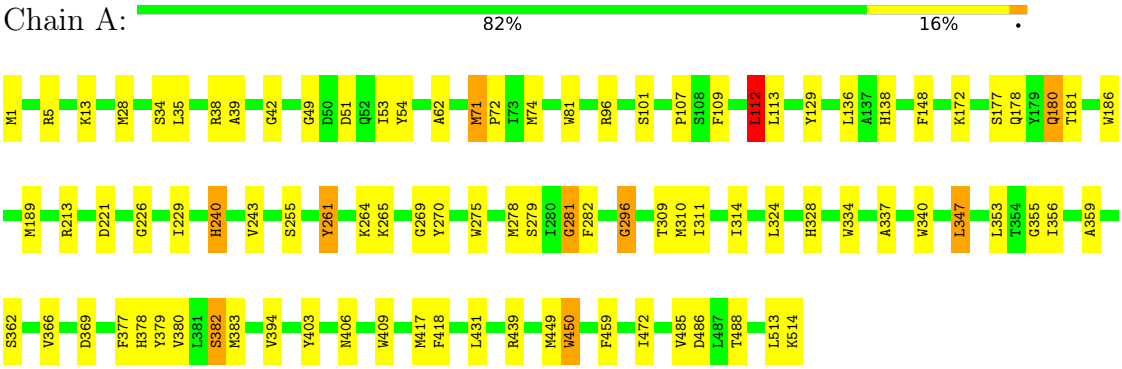
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	17	Total O 17 17	0	0
30	L	21	Total O 21 21	0	0
30	M	22	Total O 22 22	0	0
30	N	217	Total O 217 217	0	0
30	O	114	Total O 115 115	0	1
30	P	95	Total O 95 95	0	0
30	Q	57	Total O 57 57	0	0
30	R	56	Total O 56 56	0	0
30	S	65	Total O 65 65	0	0
30	T	33	Total O 33 33	0	0
30	U	38	Total O 38 38	0	0
30	V	16	Total O 16 16	0	0
30	W	13	Total O 13 13	0	0
30	X	15	Total O 15 15	0	0
30	Y	14	Total O 14 14	0	0
30	Z	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

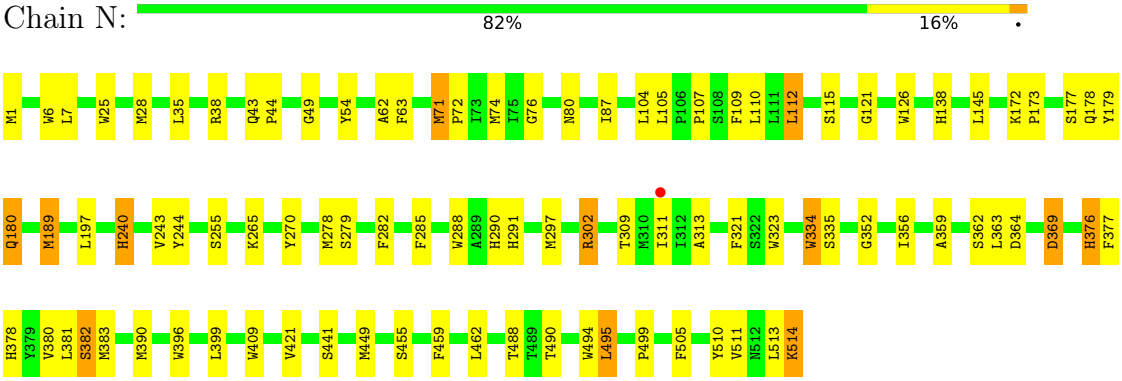
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



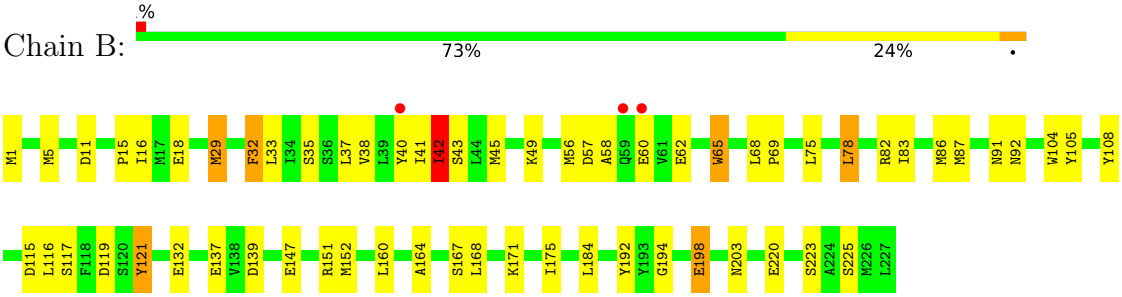
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



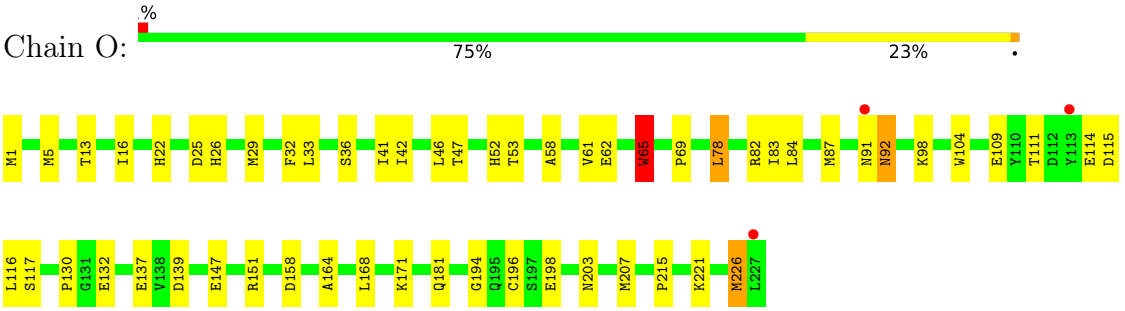
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



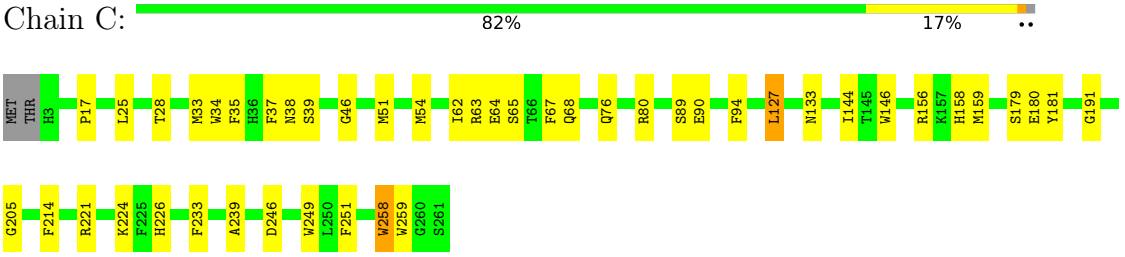
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



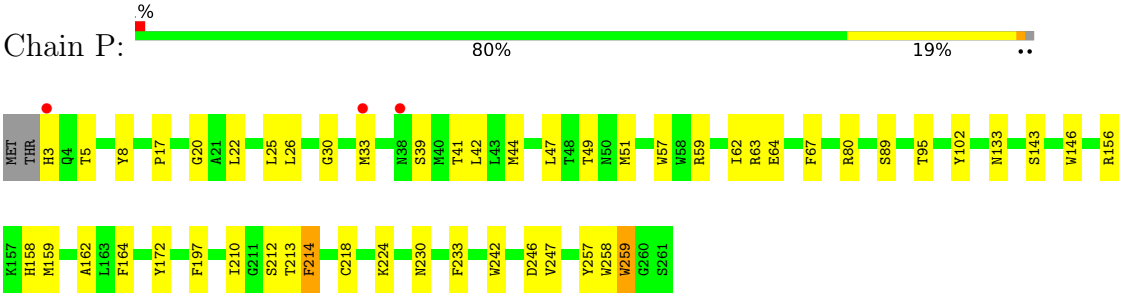
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



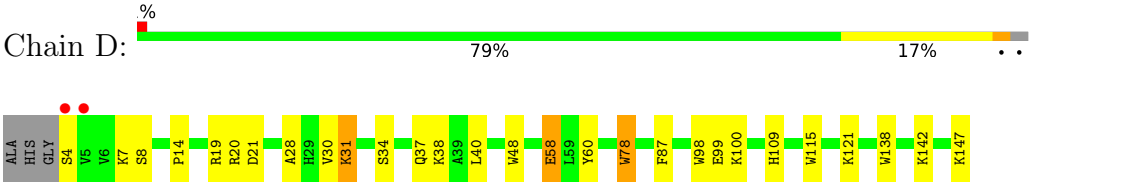
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



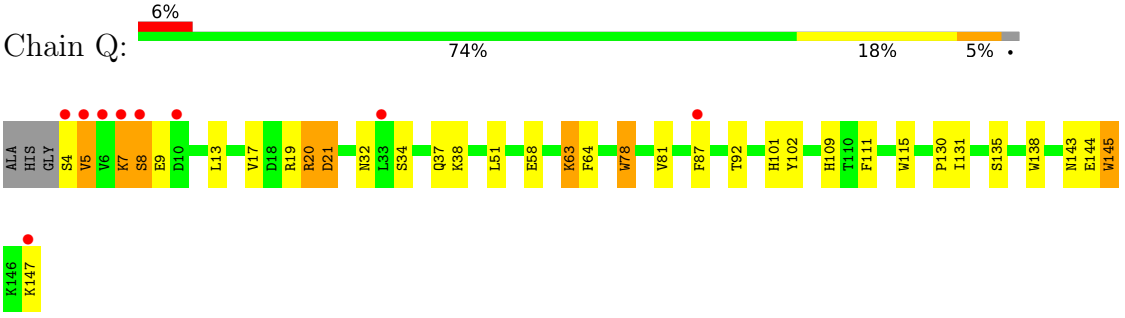
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



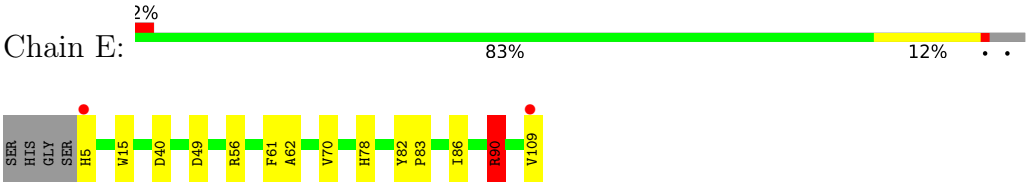
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



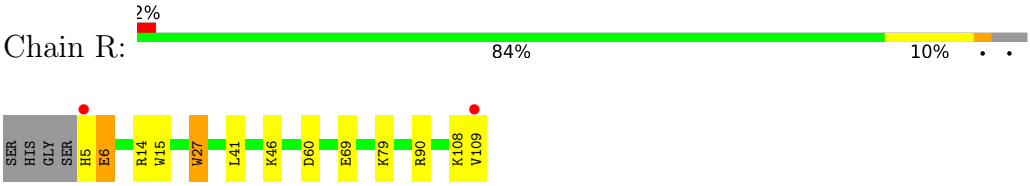
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



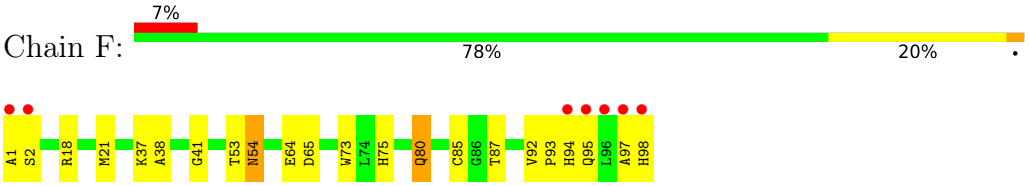
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



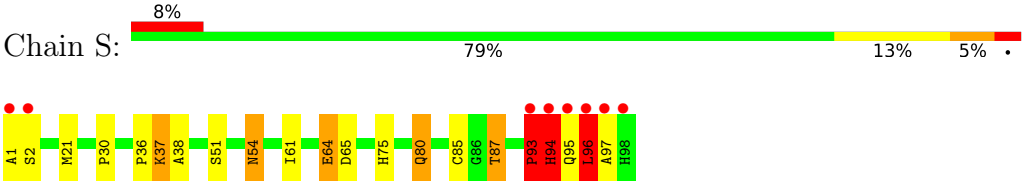
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



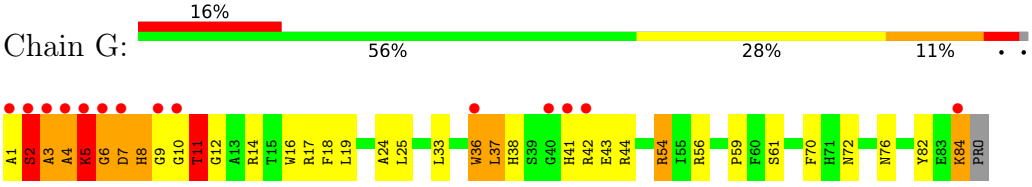
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



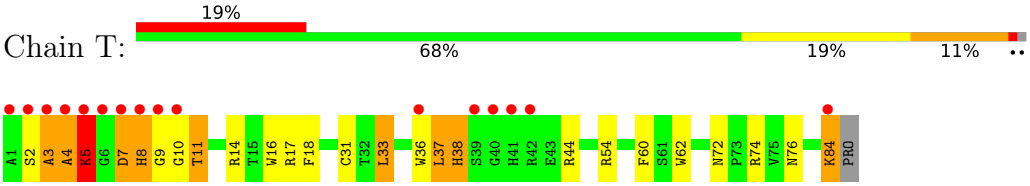
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



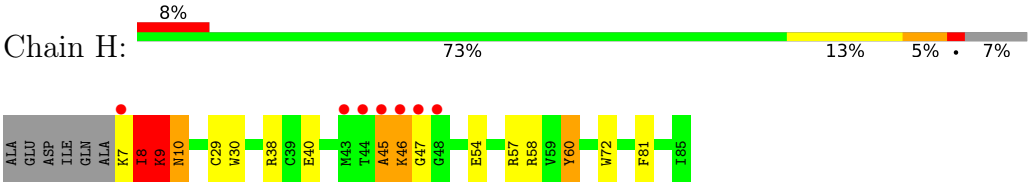
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



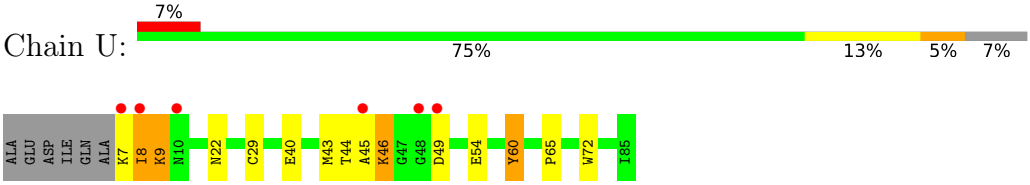
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



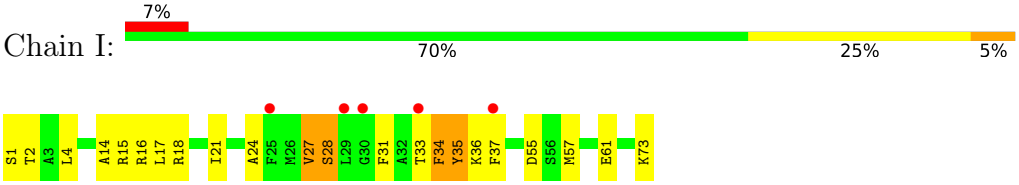
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



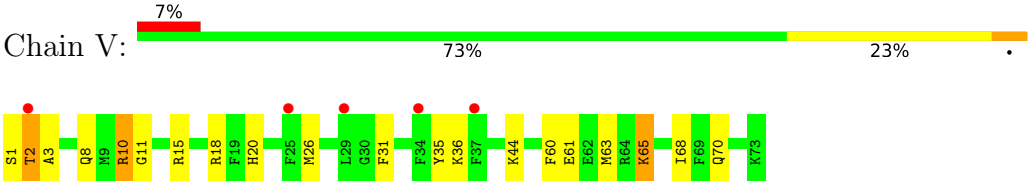
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



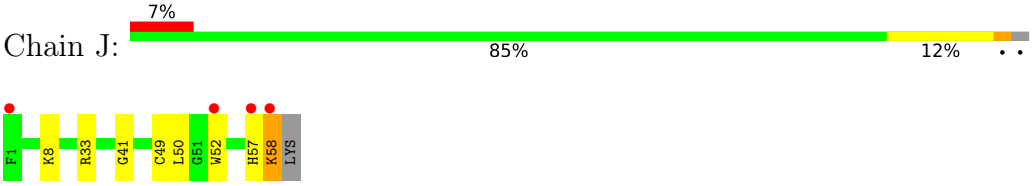
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



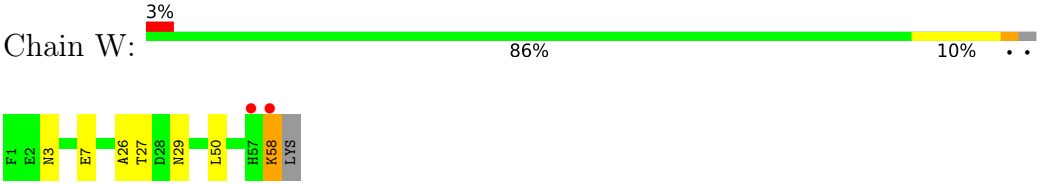
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



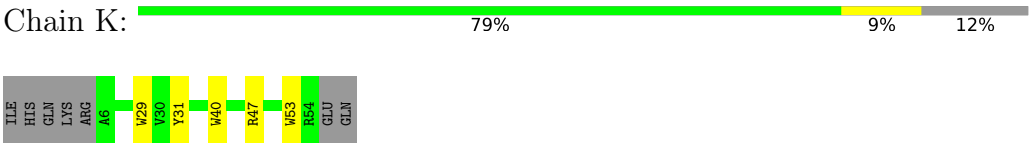
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



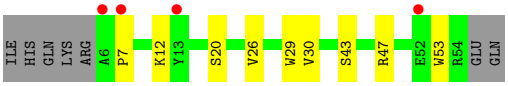
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:

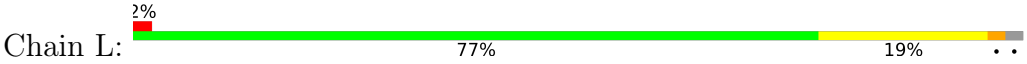


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

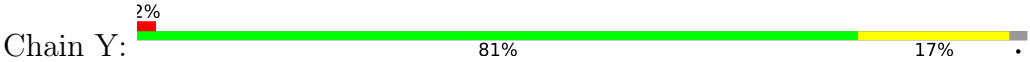
Chain X:

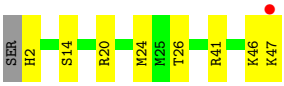


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

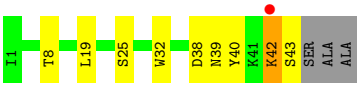


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

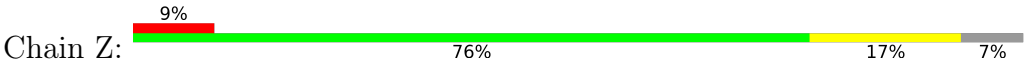


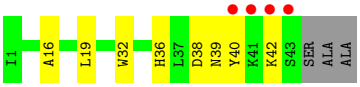


• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.13Å 205.89Å 177.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 136.83 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-1.85) 99.4 (136.83-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.13 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.163 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	28242 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33411	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.63	25/4294 (0.6%)	1.33	26/5861 (0.4%)
1	N	1.55	25/4289 (0.6%)	1.22	14/5853 (0.2%)
2	B	1.49	9/1896 (0.5%)	1.28	16/2582 (0.6%)
2	O	1.25	5/1908 (0.3%)	1.16	5/2597 (0.2%)
3	C	1.57	15/2258 (0.7%)	1.13	2/3084 (0.1%)
3	P	1.56	15/2272 (0.7%)	1.14	5/3102 (0.2%)
4	D	1.52	8/1238 (0.6%)	1.23	6/1669 (0.4%)
4	Q	1.13	3/1248 (0.2%)	1.13	5/1684 (0.3%)
5	E	1.51	6/871 (0.7%)	1.46	6/1182 (0.5%)
5	R	1.26	3/871 (0.3%)	1.08	2/1182 (0.2%)
6	F	1.36	3/788 (0.4%)	1.16	2/1069 (0.2%)
6	S	1.29	0/780	1.18	4/1058 (0.4%)
7	G	1.51	5/702 (0.7%)	1.20	7/953 (0.7%)
7	T	1.47	4/690 (0.6%)	1.16	5/937 (0.5%)
8	H	1.34	5/682 (0.7%)	0.99	0/921
8	U	1.14	1/682 (0.1%)	0.93	0/921
9	I	1.27	2/605 (0.3%)	1.22	4/802 (0.5%)
9	V	1.06	0/605	1.11	2/802 (0.2%)
10	J	1.26	1/471 (0.2%)	1.10	1/636 (0.2%)
10	W	1.21	1/471 (0.2%)	1.03	0/636
11	K	1.40	4/398 (1.0%)	1.12	1/546 (0.2%)
11	X	1.09	2/405 (0.5%)	0.86	0/556
12	L	1.46	3/393 (0.8%)	1.25	2/526 (0.4%)
12	Y	1.22	0/401	1.03	0/536
13	M	1.39	2/345 (0.6%)	1.06	0/470
13	Z	1.20	0/345	0.95	0/470
All	All	1.45	147/29908 (0.5%)	1.19	115/40635 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
4	Q	0	1
5	R	0	1
6	F	0	1
6	S	0	1
7	G	0	1
8	H	0	2
8	U	0	1
9	V	0	1
12	Y	0	1
All	All	0	13

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	SER	CB-OG	11.28	1.56	1.42
2	O	65	TRP	NE1-CE2	-10.74	1.23	1.37
2	B	198	GLU	CD-OE2	-10.28	1.14	1.25
2	B	65	TRP	CD2-CE2	9.24	1.52	1.41
2	O	65	TRP	CD2-CE2	9.08	1.52	1.41
1	A	96	ARG	CZ-NH1	8.32	1.43	1.33
1	N	279	SER	CA-CB	8.23	1.65	1.52
1	A	49	GLY	C-O	7.92	1.36	1.23
1	N	49	GLY	C-O	7.92	1.36	1.23
3	P	89	SER	CB-OG	7.34	1.51	1.42
4	D	58	GLU	CD-OE1	7.33	1.33	1.25
7	G	16	TRP	CD2-CE2	7.25	1.50	1.41
2	O	36	SER	CB-OG	7.11	1.51	1.42
1	A	409	TRP	CD2-CE2	7.11	1.49	1.41
8	H	72	TRP	CD2-CE2	7.04	1.49	1.41
7	G	36	TRP	CD2-CE2	6.99	1.49	1.41
1	N	335	SER	CB-OG	6.97	1.51	1.42
5	E	78	HIS	N-CA	6.75	1.59	1.46
11	K	29	TRP	CD2-CE2	6.74	1.49	1.41
7	T	16	TRP	CD2-CE2	6.73	1.49	1.41
1	N	270	TYR	CE1-CZ	-6.72	1.29	1.38
1	A	34	SER	CB-OG	-6.69	1.33	1.42
1	N	25	TRP	CD2-CE2	6.64	1.49	1.41
1	A	279	SER	CA-CB	6.53	1.62	1.52
4	Q	138	TRP	CD2-CE2	6.51	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	179	TYR	CE1-CZ	6.50	1.47	1.38
3	P	259	TRP	CD2-CE2	6.45	1.49	1.41
3	P	64	GLU	CD-OE2	6.41	1.32	1.25
12	L	19	TRP	CD2-CE2	6.29	1.49	1.41
11	K	40	TRP	CD2-CE2	6.28	1.48	1.41
1	N	409	TRP	CD2-CE2	6.26	1.48	1.41
1	A	74	MET	CB-CG	6.24	1.71	1.51
1	A	81	TRP	CG-CD1	6.18	1.45	1.36
3	P	172	TYR	CG-CD1	6.18	1.47	1.39
2	O	198	GLU	CD-OE2	-6.16	1.18	1.25
3	C	249	TRP	CD2-CE2	6.15	1.48	1.41
1	N	352	GLY	N-CA	6.09	1.55	1.46
1	A	379	TYR	CE2-CZ	6.09	1.46	1.38
3	C	35	PHE	CG-CD2	6.09	1.47	1.38
2	B	220	GLU	CD-OE1	-6.08	1.19	1.25
7	T	36	TRP	CD2-CE2	6.05	1.48	1.41
4	D	78	TRP	CD2-CE2	6.05	1.48	1.41
13	M	32	TRP	CD2-CE2	6.01	1.48	1.41
11	K	53	TRP	CD2-CE2	6.01	1.48	1.41
4	Q	78	TRP	CD2-CE2	6.00	1.48	1.41
3	C	258	TRP	CD2-CE2	5.97	1.48	1.41
6	F	18	ARG	CZ-NH1	5.97	1.40	1.33
5	R	69	GLU	CD-OE2	-5.95	1.19	1.25
3	C	181	TYR	CE1-CZ	5.95	1.46	1.38
1	N	126	TRP	CD2-CE2	5.94	1.48	1.41
3	P	258	TRP	CD2-CE2	5.94	1.48	1.41
3	C	251	PHE	CG-CD2	5.93	1.47	1.38
5	R	27	TRP	CD2-CE2	5.92	1.48	1.41
1	A	362	SER	CA-CB	5.92	1.61	1.52
3	P	143	SER	CA-CB	5.91	1.61	1.52
10	W	26	ALA	CA-CB	5.89	1.64	1.52
2	B	225	SER	CA-CB	5.89	1.61	1.52
3	P	242	TRP	CD2-CE2	5.88	1.48	1.41
1	N	288	TRP	CE3-CZ3	5.87	1.48	1.38
1	N	396	TRP	CG-CD1	5.85	1.45	1.36
2	B	223	SER	CA-CB	5.84	1.61	1.52
5	E	15	TRP	CD2-CE2	5.83	1.48	1.41
3	P	30	GLY	N-CA	5.83	1.54	1.46
8	H	30	TRP	CD2-CE2	5.82	1.48	1.41
11	X	29	TRP	CD2-CE2	5.82	1.48	1.41
4	D	87	PHE	CG-CD1	5.78	1.47	1.38
3	C	259	TRP	CD2-CE2	5.78	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	115	TRP	CD2-CE2	5.72	1.48	1.41
3	C	34	TRP	CD2-CE2	5.70	1.48	1.41
1	A	129	TYR	CD1-CE1	5.69	1.47	1.39
1	A	281	GLY	N-CA	5.69	1.54	1.46
7	G	61	SER	CA-CB	5.68	1.61	1.52
4	Q	145	TRP	CD2-CE2	5.68	1.48	1.41
1	A	101	SER	CB-OG	5.67	1.49	1.42
8	H	40	GLU	CD-OE2	5.66	1.31	1.25
7	T	60	PHE	CG-CD1	5.63	1.47	1.38
2	B	192	TYR	CB-CG	5.62	1.60	1.51
3	C	65	SER	CB-OG	5.62	1.49	1.42
1	A	340	TRP	CD2-CE2	5.61	1.48	1.41
7	G	36	TRP	CG-CD2	5.61	1.53	1.43
1	A	275	TRP	CD2-CE2	5.60	1.48	1.41
1	A	264	LYS	CD-CE	5.59	1.65	1.51
1	N	334	TRP	CD2-CE2	5.57	1.48	1.41
1	A	226	GLY	N-CA	5.56	1.54	1.46
9	I	28	SER	CB-OG	5.54	1.49	1.42
3	C	205	GLY	N-CA	5.53	1.54	1.46
1	A	74	MET	CG-SD	-5.52	1.66	1.81
11	X	53	TRP	CD2-CE2	5.50	1.48	1.41
1	N	63	PHE	CE1-CZ	5.50	1.47	1.37
8	U	72	TRP	CD2-CE2	5.47	1.48	1.41
3	C	65	SER	CA-CB	5.46	1.61	1.52
1	N	494	TRP	CD2-CE2	5.45	1.47	1.41
1	A	261	TYR	CE2-CZ	5.44	1.45	1.38
6	F	73	TRP	CD2-CE2	5.42	1.47	1.41
4	D	98	TRP	CD2-CE2	5.39	1.47	1.41
3	P	57	TRP	CD2-CE2	5.38	1.47	1.41
1	A	269	GLY	N-CA	5.38	1.54	1.46
1	A	51	ASP	CB-CG	5.38	1.63	1.51
11	K	31	TYR	CG-CD1	5.37	1.46	1.39
2	B	121	TYR	CE1-CZ	5.37	1.45	1.38
3	P	212	SER	CA-CB	5.36	1.60	1.52
5	E	62	ALA	CA-CB	5.34	1.63	1.52
4	D	138	TRP	CD2-CE2	5.34	1.47	1.41
1	N	323	TRP	CD2-CE2	5.33	1.47	1.41
1	A	255	SER	CA-CB	5.32	1.60	1.52
1	N	6	TRP	CD2-CE2	5.30	1.47	1.41
4	D	48	TRP	CD2-CE2	5.29	1.47	1.41
6	F	73	TRP	CE3-CZ3	5.29	1.47	1.38
3	P	102	TYR	CD2-CE2	5.28	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	74	MET	CB-CG	5.25	1.68	1.51
5	E	56	ARG	CZ-NH2	5.23	1.39	1.33
4	D	60	TYR	CG-CD1	5.22	1.46	1.39
5	E	90	ARG	CZ-NH1	5.21	1.39	1.33
2	B	167	SER	CB-OG	-5.21	1.35	1.42
1	N	288	TRP	CD2-CE2	5.21	1.47	1.41
3	C	46	GLY	N-CA	5.20	1.53	1.46
3	P	20	GLY	N-CA	5.20	1.53	1.46
3	C	94	PHE	CD2-CE2	5.20	1.49	1.39
1	N	376	HIS	CG-CD2	5.20	1.44	1.35
5	R	15	TRP	CD2-CE2	5.20	1.47	1.41
3	P	218	CYS	CB-SG	5.20	1.91	1.82
8	H	81	PHE	CE2-CZ	5.18	1.47	1.37
7	T	62	TRP	CD2-CE2	5.17	1.47	1.41
1	A	450	TRP	CD2-CE2	5.16	1.47	1.41
7	G	56	ARG	CZ-NH1	5.16	1.39	1.33
1	A	186	TRP	CD2-CE2	5.15	1.47	1.41
1	N	270	TYR	CB-CG	5.15	1.59	1.51
1	A	275	TRP	CD2-CE3	5.15	1.48	1.40
1	N	63	PHE	CG-CD1	5.15	1.46	1.38
2	B	198	GLU	CD-OE1	-5.14	1.20	1.25
3	P	8	TYR	CG-CD1	5.14	1.45	1.39
10	J	33	ARG	CA-CB	5.13	1.65	1.53
2	O	147	GLU	CD-OE1	-5.09	1.20	1.25
1	N	455	SER	CB-OG	5.08	1.48	1.42
12	L	33	PHE	CG-CD2	5.07	1.46	1.38
1	A	403	TYR	CG-CD1	5.06	1.45	1.39
5	E	61	PHE	CG-CD1	5.06	1.46	1.38
9	I	4	LEU	CA-CB	5.06	1.65	1.53
3	C	221	ARG	CZ-NH1	5.06	1.39	1.33
12	L	28	PHE	CB-CG	5.04	1.59	1.51
1	N	441	SER	CB-OG	5.04	1.48	1.42
1	N	179	TYR	CB-CG	5.03	1.59	1.51
3	C	146	TRP	CE3-CZ3	5.03	1.47	1.38
8	H	58	ARG	CZ-NH1	5.02	1.39	1.33
3	P	197	PHE	CE1-CZ	5.02	1.46	1.37
1	N	255	SER	CA-CB	5.00	1.60	1.52
13	M	40	TYR	CG-CD1	5.00	1.45	1.39

All (115) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	90	ARG	NE-CZ-NH1	22.36	131.48	120.30
5	E	90	ARG	NE-CZ-NH2	-16.92	111.84	120.30
1	A	278	MET	CG-SD-CE	-16.40	73.96	100.20
4	Q	20	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	71	MET	CG-SD-CE	-15.80	74.93	100.20
1	N	71	MET	CG-SD-CE	-15.18	75.92	100.20
4	Q	20	ARG	NE-CZ-NH1	14.35	127.48	120.30
2	O	65	TRP	CA-CB-CG	12.82	138.06	113.70
1	N	302	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	96	ARG	NE-CZ-NH2	-11.97	114.31	120.30
2	O	65	TRP	CB-CA-C	-9.58	91.24	110.40
1	A	189	MET	CG-SD-CE	-9.10	85.64	100.20
11	K	47	ARG	NE-CZ-NH1	8.96	124.78	120.30
9	I	16	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	5	ARG	NE-CZ-NH1	-8.03	116.28	120.30
7	T	7	ASP	N-CA-C	8.01	132.63	111.00
12	L	20	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	B	82	ARG	NE-CZ-NH2	-7.98	116.31	120.30
6	F	18	ARG	NE-CZ-NH2	-7.93	116.34	120.30
9	V	10	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	347	LEU	CA-CB-CG	-7.65	97.70	115.30
1	A	278	MET	CA-CB-CG	-7.54	100.48	113.30
2	O	82	ARG	NE-CZ-NH2	-7.54	116.53	120.30
4	Q	21	ASP	CB-CG-OD2	7.45	125.01	118.30
1	A	112	LEU	CD1-CG-CD2	-7.43	88.22	110.50
1	A	96	ARG	NE-CZ-NH1	7.33	123.97	120.30
12	L	20	ARG	CG-CD-NE	-7.28	96.51	111.80
7	G	54	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	N	302	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	35	LEU	CB-CG-CD2	7.05	122.99	111.00
5	E	49	ASP	CB-CG-OD1	6.91	124.52	118.30
1	N	369	ASP	CB-CG-OD1	6.81	124.43	118.30
2	B	139	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	310	MET	CA-CB-CG	-6.74	101.84	113.30
1	A	213	ARG	NE-CZ-NH2	-6.62	116.99	120.30
5	R	60	ASP	CB-CG-OD1	6.54	124.18	118.30
4	D	21	ASP	CB-CG-OD2	6.52	124.17	118.30
5	E	90	ARG	CD-NE-CZ	6.45	132.63	123.60
4	D	20	ARG	NE-CZ-NH1	-6.44	117.08	120.30
2	O	139	ASP	CB-CG-OD1	6.42	124.08	118.30
7	G	54	ARG	NE-CZ-NH2	-6.39	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	ARG	NE-CZ-NH1	6.38	123.49	120.30
5	E	90	ARG	CB-CG-CD	6.37	128.17	111.60
1	A	347	LEU	CB-CG-CD2	6.35	121.80	111.00
4	Q	20	ARG	CG-CD-NE	-6.34	98.48	111.80
1	A	49	GLY	N-CA-C	-6.31	97.32	113.10
3	C	90	GLU	OE1-CD-OE2	6.25	130.81	123.30
2	B	151	ARG	NE-CZ-NH1	6.22	123.41	120.30
7	G	14	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	353	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	A	38	ARG	NE-CZ-NH2	-6.06	117.27	120.30
7	T	33	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	112	LEU	CB-CG-CD2	-6.00	100.81	111.00
7	G	5	LYS	CB-CA-C	5.97	122.34	110.40
9	I	27	VAL	CB-CA-C	-5.96	100.07	111.40
2	B	42	ILE	CG1-CB-CG2	-5.95	98.30	111.40
2	B	29	MET	CG-SD-CE	5.93	109.69	100.20
2	B	198	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	A	439	ARG	NE-CZ-NH2	-5.90	117.35	120.30
4	Q	63	LYS	CD-CE-NZ	-5.83	98.30	111.70
1	N	7	LEU	CB-CG-CD1	5.82	120.89	111.00
2	B	32[A]	PHE	CB-CG-CD1	-5.81	116.73	120.80
2	B	32[B]	PHE	CB-CG-CD1	-5.81	116.73	120.80
2	B	151	ARG	NE-CZ-NH2	-5.77	117.42	120.30
6	F	18	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	366	VAL	CA-CB-CG2	-5.74	102.29	110.90
3	C	127	LEU	CB-CG-CD1	5.74	120.75	111.00
7	G	25	LEU	CB-CG-CD2	5.71	120.70	111.00
3	P	214	PHE	CB-CG-CD1	5.69	124.78	120.80
2	B	152	MET	CG-SD-CE	5.66	109.26	100.20
2	B	18	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	N	74	MET	CB-CG-SD	-5.63	95.50	112.40
1	A	129	TYR	CB-CG-CD2	-5.62	117.62	121.00
9	I	55	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	270	TYR	CD1-CE1-CZ	-5.61	114.75	119.80
1	N	112	LEU	CD1-CG-CD2	-5.60	93.70	110.50
9	V	10	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	119	ASP	CB-CG-OD2	-5.58	113.28	118.30
9	I	16	ARG	NE-CZ-NH1	5.52	123.06	120.30
7	T	74	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	N	104	LEU	CB-CG-CD1	-5.49	101.67	111.00
4	D	7	LYS	CD-CE-NZ	5.49	124.32	111.70
7	T	5	LYS	CB-CA-C	5.48	121.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	214	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	38	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	N	244	TYR	CA-CB-CG	-5.47	103.01	113.40
1	A	74	MET	CB-CG-SD	-5.46	96.01	112.40
3	P	233	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	B	45	MET	CG-SD-CE	5.44	108.90	100.20
6	S	21[A]	MET	CG-SD-CE	5.44	108.90	100.20
6	S	21[B]	MET	CG-SD-CE	5.44	108.90	100.20
2	B	11	ASP	CB-CG-OD1	5.40	123.16	118.30
1	N	145	LEU	CB-CG-CD1	-5.37	101.86	111.00
3	P	49	THR	CA-CB-CG2	-5.36	104.89	112.40
4	D	38	LYS	CB-CG-CD	-5.35	97.70	111.60
1	N	189	MET	CB-CG-SD	-5.34	96.38	112.40
2	B	147	GLU	OE1-CD-OE2	-5.33	116.90	123.30
6	S	94	HIS	N-CA-C	5.31	125.33	111.00
1	N	244	TYR	CZ-CE2-CD2	-5.31	115.03	119.80
4	D	58	GLU	CA-CB-CG	-5.29	101.77	113.40
1	N	390	MET	CG-SD-CE	5.28	108.65	100.20
6	S	61	ILE	N-CA-C	-5.28	96.75	111.00
1	A	296	GLY	O-C-N	-5.28	114.26	122.70
1	A	310	MET	CG-SD-CE	-5.25	91.80	100.20
7	T	14	ARG	NE-CZ-NH1	-5.25	117.67	120.30
7	G	7	ASP	N-CA-C	5.22	125.09	111.00
5	R	14	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	198	GLU	CA-C-N	-5.14	105.89	117.20
10	J	33	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	D	142	LYS	CD-CE-NZ	-5.09	100.00	111.70
5	E	40	ASP	CB-CG-OD1	5.09	122.88	118.30
2	O	158	ASP	CB-CG-OD1	5.07	122.86	118.30
7	G	19	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	N	363	LEU	CB-CG-CD1	-5.02	102.47	111.00
3	P	257	TYR	CD1-CE1-CZ	-5.01	115.29	119.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
6	F	93	PRO	Peptide
7	G	11	TPO	Peptide
8	H	8	ILE	Peptide

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Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
4	Q	9	GLU	Peptide
5	R	108	LYS	Peptide
6	S	93	PRO	Peptide
8	U	9	LYS	Peptide
9	V	2	THR	Peptide
12	Y	46	LYS	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	4165	0	4137	80	0
1	N	4160	0	4132	89	0
2	B	1859	0	1869	44	0
2	O	1870	0	1868	41	0
3	C	2171	0	2085	43	0
3	P	2185	0	2097	52	0
4	D	1204	0	1195	23	0
4	Q	1213	0	1199	34	0
5	E	852	0	845	4	0
5	R	852	0	845	4	0
6	F	771	0	747	26	0
6	S	763	0	742	17	0
7	G	686	0	652	51	0
7	T	675	0	643	37	0
8	H	662	0	623	12	0
8	U	662	0	623	11	0
9	I	601	0	613	18	0
9	V	601	0	613	17	0
10	J	460	0	459	6	0
10	W	460	0	459	7	0
11	K	384	0	366	0	0
11	X	391	0	374	11	0
12	L	380	0	380	11	0
12	Y	388	0	388	11	0
13	M	335	0	352	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	Z	335	0	352	8	0
14	A	180	0	162	25	0
14	N	180	0	162	26	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	6	0
18	N	6	0	0	6	0
19	A	63	0	110	4	0
19	D	63	0	110	13	0
19	L	63	0	110	17	0
19	N	63	0	110	4	0
19	Q	63	0	110	12	0
19	Y	63	0	110	16	0
20	A	51	0	76	4	0
20	C	102	0	152	4	0
20	M	51	0	76	3	0
20	N	102	0	152	14	0
20	P	102	0	152	12	0
21	A	44	0	66	21	0
21	B	4	0	6	0	0
21	C	36	0	54	3	0
21	D	20	0	30	12	0
21	E	20	0	30	0	0
21	F	12	0	18	1	0
21	G	8	0	12	1	0
21	H	4	0	6	3	0
21	N	44	0	66	15	0
21	O	12	0	18	0	0
21	P	16	0	24	1	0
21	Q	12	0	18	6	0
21	R	20	0	30	3	0
21	S	12	0	18	3	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	O	52	0	80	16	0
24	C	58	0	78	5	0
24	G	29	0	39	1	0
24	P	58	0	77	6	0
24	T	29	0	39	0	0
25	C	99	0	126	18	0
25	M	33	0	42	0	0
25	P	99	0	126	14	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	0	0
27	C	100	0	156	26	0
27	G	100	0	156	24	0
27	P	100	0	156	22	0
27	T	100	0	156	25	0
28	C	53	0	77	12	0
28	G	106	0	154	23	0
28	P	106	0	154	5	0
28	T	53	0	77	10	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	219	0	0	13	0
30	B	132	0	0	15	1
30	C	96	0	0	5	0
30	D	93	0	0	8	1
30	E	85	0	0	1	0
30	F	78	0	0	3	0
30	G	37	0	0	4	0
30	H	30	0	0	0	0
30	I	20	0	0	2	0
30	J	22	0	0	0	0
30	K	17	0	0	0	0
30	L	21	0	0	0	0
30	M	22	0	0	3	0
30	N	217	0	0	14	0
30	O	115	0	0	4	0
30	P	95	0	0	3	0
30	Q	57	0	0	10	0
30	R	56	0	0	4	0
30	S	65	0	0	1	0
30	T	33	0	0	0	0
30	U	38	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	16	0	0	3	0
30	W	13	0	0	1	0
30	X	15	0	0	2	0
30	Y	14	0	0	0	0
30	Z	12	0	0	2	0
All	All	33411	0	32479	789	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 12.

All (789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:614:EDO:C1	21:A:614:EDO:C2	1.83	1.54
20:N:608:PGV:C2	20:N:608:PGV:H011	1.28	1.46
19:L:101:TGL:HC62	19:L:101:TGL:CC2	1.34	1.38
21:A:614:EDO:C2	21:A:614:EDO:O1	1.74	1.29
1:N:297[B]:MET:HB2	30:N:782:HOH:O	1.36	1.25
1:A:112:LEU:HG	30:A:903:HOH:O	1.32	1.22
8:H:9:LYS:HD3	8:H:10:ASN:N	1.53	1.22
20:N:608:PGV:C2	20:N:608:PGV:C01	2.16	1.22
20:N:608:PGV:C01	20:N:608:PGV:H21	1.71	1.21
4:Q:7:LYS:HE2	30:Q:301:HOH:O	1.40	1.18
21:A:612:EDO:C2	30:A:701:HOH:O	1.91	1.16
19:D:201:TGL:HG31	30:D:357:HOH:O	1.42	1.16
21:A:617:EDO:H12	30:A:756:HOH:O	1.41	1.15
21:A:618:EDO:H21	30:A:715:HOH:O	1.42	1.15
2:B:160:LEU:HB2	30:B:453:HOH:O	1.44	1.15
19:L:101:TGL:HC22	19:L:101:TGL:CC6	1.73	1.15
19:Q:201:TGL:HG32	30:Q:316:HOH:O	1.49	1.12
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.11	1.11
7:G:8:HIS:CD2	7:G:9:GLY:H	1.69	1.10
3:P:67:PHE:HE2	27:P:306:CDL:H1	1.17	1.09
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.32	1.09
20:C:308:PGV:H22	20:C:308:PGV:H72	1.14	1.08
20:N:608:PGV:H011	20:N:608:PGV:H22	1.10	1.04
2:B:49:LYS:HE2	30:B:515:HOH:O	1.54	1.04
1:A:39:ALA:HA	21:D:202:EDO:O1	1.56	1.03
1:A:513:LEU:O	1:A:514:LYS:HB2	1.51	1.03
7:G:10:GLY:O	7:G:11:TPO:HB	1.54	1.02
20:N:608:PGV:H011	20:N:608:PGV:H21	1.06	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:101:TGL:HC41	19:Y:101:TGL:OC1	1.22	1.01
1:N:513:LEU:O	1:N:514:LYS:HB2	1.59	1.01
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.01	1.00
3:C:67:PHE:HE2	27:C:305:CDL:H1	1.24	0.99
1:A:282:PHE:HA	7:T:4:ALA:CB	1.93	0.99
27:T:103:CDL:H361	27:T:103:CDL:H112	1.45	0.99
21:A:614:EDO:O1	21:A:614:EDO:H21	1.60	0.98
8:H:9:LYS:HD3	8:H:10:ASN:H	0.82	0.98
19:Y:101:TGL:OC1	19:Y:101:TGL:CC4	2.12	0.98
19:Y:101:TGL:CG1	19:Y:101:TGL:HA31	1.93	0.97
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.04	0.96
4:Q:7:LYS:CE	30:Q:301:HOH:O	2.02	0.96
2:O:116:LEU:CD1	2:O:226:MET:HG2	1.96	0.96
3:P:33[A]:MET:HB2	25:P:308:DMU:C19	1.95	0.96
8:H:9:LYS:CD	8:H:10:ASN:H	1.77	0.95
1:A:486[B]:ASP:OD2	4:D:19:ARG:HD2	1.64	0.94
7:G:84:LYS:H	7:G:84:LYS:HZ3	1.15	0.94
3:P:67:PHE:CE2	27:P:306:CDL:H1	2.01	0.94
23:O:302:PSC:C07	9:V:10:ARG:HH21	1.80	0.94
3:C:224:LYS:CD	27:C:305:CDL:HB31	1.97	0.94
19:L:101:TGL:CC2	19:L:101:TGL:CC6	2.23	0.93
12:L:20:ARG:NH2	19:L:101:TGL:HC51	1.83	0.93
24:C:306:CHD:H162	24:C:306:CHD:H231	1.49	0.93
5:E:90:ARG:HD2	30:E:369:HOH:O	1.67	0.93
21:D:203:EDO:H11	30:D:306:HOH:O	1.69	0.93
1:A:221:ASP:OD1	21:A:620:EDO:H11	1.69	0.93
2:B:87[B]:MET:HG2	30:B:481:HOH:O	1.67	0.92
9:V:11:GLY:O	9:V:15:ARG:HG3	1.69	0.91
20:C:304:PGV:H12	20:C:304:PGV:H171	1.52	0.91
21:N:621:EDO:H22	30:N:830:HOH:O	1.69	0.91
1:N:297[B]:MET:CB	30:N:782:HOH:O	1.98	0.91
23:B:302:PSC:O01	9:I:14:ALA:HB2	1.71	0.91
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.53	0.90
27:T:103:CDL:H131	27:T:103:CDL:H372	1.53	0.90
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.54	0.90
1:A:112:LEU:C	1:A:112:LEU:HD23	1.92	0.90
13:M:19:LEU:HD23	20:M:101:PGV:H311	1.52	0.90
7:G:8:HIS:HD2	7:G:9:GLY:H	0.98	0.89
28:G:104:PEK:H032	3:P:80[B]:ARG:NH2	1.87	0.89
28:C:307:PEK:H051	6:F:1:ALA:H2	1.36	0.88
3:C:67:PHE:CE2	27:C:305:CDL:H1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:609:PGV:H183	28:G:101:PEK:H322	1.56	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.22	0.87
3:P:33[A]:MET:HB2	25:P:308:DMU:H8	1.55	0.86
7:G:84:LYS:H	7:G:84:LYS:NZ	1.73	0.86
1:N:511:VAL:H	21:N:621:EDO:H21	1.38	0.85
3:C:224:LYS:HD2	27:C:305:CDL:HB31	1.56	0.85
27:G:102:CDL:H161	27:G:102:CDL:OB3	1.75	0.85
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	1.75	0.85
28:G:101:PEK:H162	28:G:101:PEK:C12	2.07	0.85
30:A:867:HOH:O	2:B:87[B]:MET:HE1	1.77	0.85
7:G:59:PRO:O	21:G:105:EDO:H22	1.76	0.84
12:L:20:ARG:HH22	19:L:101:TGL:HC51	1.41	0.84
30:B:527:HOH:O	19:D:201:TGL:C28	2.25	0.84
19:Y:101:TGL:HA31	19:Y:101:TGL:HG11	1.57	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.24	0.84
11:X:47:ARG:HB3	11:X:47:ARG:NH1	1.92	0.84
3:P:33[A]:MET:HB2	25:P:308:DMU:H9	1.60	0.84
30:N:772:HOH:O	2:O:87[A]:MET:SD	2.36	0.83
19:L:101:TGL:HC62	19:L:101:TGL:HC22	0.84	0.83
30:A:867:HOH:O	2:B:87[B]:MET:CE	2.27	0.82
1:N:112:LEU:HG	30:N:901:HOH:O	1.80	0.82
14:N:602[A]:HEA:HBC1	14:N:602[A]:HEA:HMC1	1.61	0.82
2:O:92:ASN:HB3	30:U:213:HOH:O	1.79	0.82
11:X:47:ARG:HH11	11:X:47:ARG:CB	1.93	0.82
3:C:33:MET:HB2	25:C:302:DMU:C19	2.10	0.82
13:M:8:THR:HG23	30:M:221:HOH:O	1.79	0.82
28:C:307:PEK:H051	6:F:1:ALA:N	1.95	0.81
9:I:15:ARG:NH2	30:I:101:HOH:O	2.13	0.81
12:L:20:ARG:HH22	19:L:101:TGL:CC5	1.92	0.81
3:P:33[B]:MET:SD	25:P:308:DMU:H8	2.21	0.81
1:A:136[B]:LEU:HD11	30:A:913:HOH:O	1.79	0.81
8:U:9:LYS:HG3	8:U:9:LYS:O	1.79	0.81
7:T:2:SER:OG	28:T:102:PEK:H281	1.80	0.81
7:G:76:ASN:HD21	28:G:101:PEK:HN2	1.29	0.80
27:G:102:CDL:C65	27:G:102:CDL:H611	2.11	0.80
3:C:33:MET:HB2	25:C:302:DMU:H8	1.63	0.80
12:Y:20:ARG:HH22	19:Y:101:TGL:HC52	1.45	0.80
18:A:606:AZI:N1	18:A:607:AZI:N1	2.30	0.80
6:F:1:ALA:CB	21:S:103:EDO:O1	2.30	0.80
7:T:72:ASN:H	7:T:76:ASN:HD22	1.29	0.79
23:O:302:PSC:H342	23:O:302:PSC:H12	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:614:EDO:H11	30:M:216:HOH:O	1.80	0.79
7:G:8:HIS:O	1:N:178[A]:GLN:NE2	2.15	0.79
27:C:305:CDL:H821	27:C:305:CDL:H782	1.64	0.79
6:S:75:HIS:H	6:S:80:GLN:HE22	1.28	0.79
24:P:307:CHD:H231	24:P:307:CHD:H162	1.66	0.78
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.47	0.78
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.83	0.78
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.64	0.78
1:N:178[A]:GLN:CG	30:N:715:HOH:O	2.32	0.78
1:N:505:PHE:H	21:N:618:EDO:H22	1.49	0.78
3:P:33[A]:MET:HE1	3:P:42:LEU:N	1.95	0.77
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.72	0.77
7:T:5:LYS:HB2	28:T:102:PEK:H331	1.65	0.77
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.85	0.77
28:C:307:PEK:H292	30:O:445:HOH:O	1.84	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.76
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.33	0.76
30:B:527:HOH:O	19:D:201:TGL:H281	1.83	0.76
21:R:204:EDO:H11	30:R:348:HOH:O	1.84	0.76
7:T:5:LYS:HG3	28:T:102:PEK:H352	1.68	0.76
1:N:359:ALA:HA	14:N:602[B]:HEA:OMA	1.84	0.76
3:P:63:ARG:HE	27:P:306:CDL:CA2	1.99	0.76
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.66	0.76
3:C:63:ARG:HE	27:C:305:CDL:HA21	1.50	0.75
20:N:608:PGV:H312	13:Z:19:LEU:HD23	1.68	0.75
7:T:5:LYS:HG3	28:T:102:PEK:C35	2.17	0.75
4:D:4:SER:OG	30:D:302:HOH:O	2.04	0.75
3:C:63:ARG:HE	27:C:305:CDL:CA2	2.00	0.74
20:P:302:PGV:H061	8:U:22:ASN:HD22	1.52	0.74
1:A:221:ASP:OD1	21:A:620:EDO:C1	2.35	0.74
19:Q:201:TGL:CG3	30:Q:316:HOH:O	2.20	0.74
25:C:302:DMU:O61	25:C:310:DMU:H41	1.87	0.74
25:C:302:DMU:O61	25:C:310:DMU:C11	2.36	0.74
21:R:204:EDO:C1	30:R:348:HOH:O	2.35	0.74
20:N:608:PGV:C01	20:N:608:PGV:H22	1.99	0.73
27:T:103:CDL:H112	27:T:103:CDL:C36	2.18	0.73
1:A:513:LEU:O	1:A:514:LYS:CB	2.26	0.73
9:V:18:ARG:HD3	30:V:214:HOH:O	1.86	0.73
8:U:7:LYS:O	8:U:8:ILE:HB	1.88	0.73
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.18	0.73
8:H:38:ARG:HH22	21:H:101:EDO:H12	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:HIS:HD2	10:J:58:LYS:HD2	1.53	0.73
1:N:362[B]:SER:OG	30:N:702:HOH:O	2.06	0.73
25:C:310:DMU:H29	25:C:310:DMU:O1	1.88	0.73
23:O:302:PSC:H342	23:O:302:PSC:C12	2.19	0.73
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.69	0.73
6:F:75:HIS:H	6:F:80:GLN:HE22	1.33	0.73
19:Y:101:TGL:OG1	19:Y:101:TGL:OG3	2.07	0.73
3:C:158:HIS:HE1	6:F:1:ALA:HA	1.55	0.72
7:T:8:HIS:CD2	7:T:8:HIS:O	2.42	0.72
19:A:608:TGL:H102	19:A:608:TGL:H281	1.71	0.72
21:A:614:EDO:C2	21:A:614:EDO:HO1	2.03	0.72
23:B:302:PSC:C1	9:I:14:ALA:HB2	2.18	0.72
1:N:105:LEU:HD11	21:N:612:EDO:H12	1.69	0.72
3:P:63:ARG:HE	27:P:306:CDL:HA21	1.55	0.72
6:F:64:GLU:O	6:F:65:ASP:HB2	1.90	0.72
20:C:308:PGV:H72	20:C:308:PGV:C2	2.07	0.72
7:G:7:ASP:OD1	1:N:178[B]:GLN:HG3	1.89	0.72
2:O:116:LEU:HD13	2:O:226:MET:CG	2.16	0.72
27:C:305:CDL:H671	27:C:305:CDL:H811	1.71	0.72
7:G:8:HIS:CD2	7:G:9:GLY:N	2.53	0.72
2:O:47:THR:HB	19:Q:201:TGL:H181	1.70	0.71
1:N:177:SER:H	1:N:180:GLN:HE21	1.38	0.71
10:W:27:THR:HB	30:W:110:HOH:O	1.89	0.71
27:G:102:CDL:H611	27:G:102:CDL:H661	1.71	0.71
27:G:102:CDL:H751	27:G:102:CDL:H561	1.73	0.71
12:L:20:ARG:HH22	19:L:101:TGL:CC6	2.03	0.71
27:T:103:CDL:H361	27:T:103:CDL:C11	2.20	0.70
3:C:51[B]:MET:HE3	27:C:305:CDL:H392	1.71	0.70
23:O:302:PSC:O01	23:O:302:PSC:H201	1.91	0.70
27:G:102:CDL:H632	20:P:302:PGV:H152	1.73	0.70
23:O:302:PSC:H201	23:O:302:PSC:C02	2.21	0.70
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.07	0.70
23:B:302:PSC:H31	9:I:17:LEU:HD23	1.72	0.70
1:N:505:PHE:H	21:N:618:EDO:C2	2.03	0.70
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.73	0.70
20:A:609:PGV:H343	28:G:101:PEK:H382	1.74	0.70
2:B:41[B]:ILE:HD12	9:I:21:ILE:CD1	2.22	0.69
24:C:306:CHD:H162	24:C:306:CHD:C23	2.21	0.69
21:D:203:EDO:C1	30:D:306:HOH:O	2.32	0.69
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.74	0.69
14:N:602[B]:HEA:HBC1	14:N:602[B]:HEA:HMC1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486[B]:ASP:OD2	4:D:19:ARG:CD	2.41	0.69
1:N:505:PHE:N	21:N:618:EDO:H22	2.07	0.69
11:X:47:ARG:NH1	11:X:47:ARG:CB	2.52	0.69
2:B:41[A]:ILE:HD13	23:B:302:PSC:H342	1.73	0.69
27:G:102:CDL:H611	27:G:102:CDL:C66	2.21	0.69
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	1.75	0.68
11:X:47:ARG:HD2	30:X:113:HOH:O	1.92	0.68
1:A:459:PHE:CE1	21:D:202:EDO:H11	2.28	0.68
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.34	0.68
13:Z:32:TRP:CH2	30:Z:212:HOH:O	2.46	0.68
7:G:2:SER:OG	28:G:104:PEK:H291	1.95	0.67
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.76	0.67
21:N:621:EDO:O2	30:N:703:HOH:O	2.12	0.67
27:P:306:CDL:H312	27:P:306:CDL:H191	1.75	0.67
1:A:334:TRP:CZ3	19:D:201:TGL:HA52	2.30	0.67
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.77	0.67
1:N:511:VAL:N	21:N:621:EDO:H21	2.09	0.67
19:A:608:TGL:H122	19:A:608:TGL:HA61	1.77	0.66
4:D:28:ALA:H	4:D:31[B]:LYS:NZ	1.93	0.66
6:F:1:ALA:HB3	21:S:103:EDO:O1	1.95	0.66
20:P:302:PGV:C06	8:U:22:ASN:HD22	2.08	0.66
25:C:302:DMU:H11	10:J:49:CYS:HB3	1.76	0.66
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.92	0.66
20:N:609:PGV:H343	28:P:304:PEK:H381	1.78	0.66
7:G:7:ASP:CG	1:N:178[B]:GLN:HE21	1.98	0.66
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.36	0.66
11:X:47:ARG:HH11	11:X:47:ARG:HB2	1.59	0.66
25:C:302:DMU:H20	10:J:50:LEU:HB2	1.77	0.66
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.25	0.66
6:F:87[B]:THR:HG21	30:F:256:HOH:O	1.96	0.65
27:T:103:CDL:H652	27:T:103:CDL:H612	1.78	0.65
9:V:18:ARG:HG3	30:V:213:HOH:O	1.96	0.65
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.78	0.65
28:C:307:PEK:H6	28:C:307:PEK:H222	1.78	0.65
4:Q:145:TRP:H	21:Q:204:EDO:H22	1.60	0.65
7:G:8:HIS:HD2	7:G:9:GLY:N	1.84	0.65
28:T:102:PEK:H361	27:T:103:CDL:H852	1.76	0.65
28:P:304:PEK:HN2	7:T:76:ASN:HD21	1.43	0.65
4:Q:7:LYS:O	4:Q:7:LYS:HD3	1.95	0.65
7:G:84:LYS:NZ	7:G:84:LYS:N	2.44	0.65
9:I:34:PHE:O	9:I:36:LYS:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:304:PGV:H181	27:C:305:CDL:H652	1.79	0.65
7:T:7:ASP:O	7:T:9:GLY:N	2.27	0.65
1:A:406:ASN:HD21	20:M:101:PGV:H22	1.61	0.64
1:N:177:SER:H	1:N:180:GLN:NE2	1.95	0.64
7:G:38:HIS:CE1	27:G:102:CDL:H141	2.33	0.64
1:N:309:THR:HG22	14:N:602[B]:HEA:HMB2	1.80	0.64
3:C:51[B]:MET:CE	27:C:305:CDL:H392	2.26	0.64
9:I:27:VAL:HG12	9:I:28:SER:N	2.12	0.64
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.33	0.64
20:A:609:PGV:C18	28:G:101:PEK:H322	2.27	0.64
23:B:302:PSC:H32	9:I:14:ALA:HA	1.80	0.64
7:G:2:SER:O	28:G:104:PEK:H341	1.98	0.64
27:G:102:CDL:H611	27:G:102:CDL:H652	1.78	0.64
19:A:608:TGL:HA61	19:A:608:TGL:H101	1.79	0.64
28:C:307:PEK:H041	7:G:17:ARG:HH22	1.63	0.64
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.81	0.63
2:O:53:THR:HG21	30:Q:311:HOH:O	1.96	0.63
12:Y:20:ARG:NH2	19:Y:101:TGL:HC52	2.12	0.63
3:C:180[B]:GLU:HG2	30:C:417:HOH:O	1.97	0.63
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.64	0.63
2:B:16[B]:ILE:HG23	30:B:505:HOH:O	1.98	0.63
27:G:102:CDL:H232	1:N:311[B]:ILE:CD1	2.29	0.63
3:P:246:ASP:HB2	30:P:487:HOH:O	1.98	0.63
3:C:33:MET:HB2	25:C:302:DMU:H9	1.80	0.62
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	1.96	0.62
4:D:30:VAL:HG13	30:D:302:HOH:O	1.98	0.62
28:G:104:PEK:H032	3:P:80[B]:ARG:HH21	1.62	0.62
9:I:31:PHE:CD1	9:I:31:PHE:C	2.72	0.62
11:X:7:PRO:HB2	11:X:12:LYS:HZ2	1.63	0.62
4:Q:8:SER:HB3	4:Q:13:LEU:HD11	1.81	0.62
3:P:33[B]:MET:CE	25:P:308:DMU:H6	2.30	0.62
27:T:103:CDL:H782	27:T:103:CDL:H571	1.82	0.62
21:N:621:EDO:H12	6:S:36:PRO:HD3	1.82	0.62
3:P:210:ILE:HD13	20:P:305:PGV:H301	1.80	0.62
7:G:3:ALA:HB3	28:G:104:PEK:H362	1.81	0.62
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.81	0.61
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.15	0.61
1:A:178[B]:GLN:HE22	7:T:10:GLY:HA3	1.65	0.61
2:B:37:LEU:O	2:B:41[B]:ILE:HG12	1.99	0.61
3:P:259:TRP:CD1	25:P:310:DMU:H30	2.36	0.61
27:P:306:CDL:H182	27:P:306:CDL:OA8	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:61:GLU:OE1	9:V:65:LYS:NZ	2.33	0.61
3:C:158:HIS:CE1	6:F:1:ALA:HA	2.35	0.61
3:C:133:ASN:ND2	30:C:401:HOH:O	2.22	0.61
2:B:105:TYR:HD1	30:B:468:HOH:O	1.82	0.61
1:N:364:ASP:OD1	14:N:602[B]:HEA:O1A	2.19	0.61
19:D:201:TGL:CG3	30:D:357:HOH:O	2.20	0.61
7:G:12:GLY:N	30:G:202:HOH:O	2.34	0.61
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:HG23	2.01	0.61
1:A:261:TYR:OH	21:A:614:EDO:H12	2.00	0.60
7:T:8:HIS:O	7:T:8:HIS:HD2	1.83	0.60
7:G:37:LEU:HD23	27:G:102:CDL:H381	1.83	0.60
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.47	0.60
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE3	2.37	0.60
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.83	0.60
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.60
1:A:282:PHE:CA	7:T:4:ALA:HB1	2.30	0.60
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.84	0.60
21:C:312:EDO:H12	21:C:313:EDO:H21	1.83	0.60
4:Q:5:VAL:HB	30:Q:357:HOH:O	2.01	0.60
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	2.90	0.60
3:C:62:ILE:HD12	27:C:305:CDL:H522	1.84	0.59
1:A:328:HIS:NE2	23:B:302:PSC:H22	2.17	0.59
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.83	0.59
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.59
19:N:610:TGL:HB92	19:N:610:TGL:C28	2.31	0.59
3:C:156:ARG:HE	24:C:306:CHD:C24	2.15	0.59
1:N:243:VAL:HB	14:N:602[B]:HEA:HAC	1.85	0.59
2:B:198:GLU:CG	30:B:453:HOH:O	2.50	0.59
7:G:5:LYS:HB2	28:G:104:PEK:H342	1.84	0.59
28:G:104:PEK:C03	3:P:80[B]:ARG:HH22	2.14	0.59
1:N:505:PHE:HA	21:N:618:EDO:H22	1.85	0.59
14:N:601:HEA:H262	14:N:601:HEA:H122	1.84	0.59
2:O:29[B]:MET:HG3	9:V:35:TYR:CD1	2.38	0.59
19:Y:101:TGL:HG11	19:Y:101:TGL:CA3	2.32	0.59
3:C:224:LYS:CE	27:C:305:CDL:HB31	2.31	0.59
4:D:78:TRP:N	19:D:201:TGL:HB21	2.18	0.58
27:G:102:CDL:H232	1:N:311[B]:ILE:HD11	1.85	0.58
28:G:104:PEK:C03	3:P:80[B]:ARG:NH2	2.62	0.58
1:N:178[A]:GLN:CD	30:N:715:HOH:O	2.41	0.58
1:N:28:MET:CE	14:N:601:HEA:H271	2.34	0.58
3:P:133:ASN:ND2	30:P:401:HOH:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:505:PHE:CA	21:N:618:EDO:H22	2.33	0.58
21:N:612:EDO:H21	30:N:796:HOH:O	2.03	0.58
1:A:282:PHE:CA	7:T:4:ALA:CB	2.77	0.58
28:G:104:PEK:H032	3:P:80[B]:ARG:HH22	1.64	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.84	0.58
19:L:101:TGL:OA1	19:L:101:TGL:OG3	2.22	0.58
1:A:177:SER:H	1:A:180:GLN:HE21	1.50	0.57
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.86	0.57
19:Q:201:TGL:H232	19:Q:201:TGL:HA91	1.86	0.57
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.01	0.57
14:N:602[A]:HEA:C1B	18:N:607:AZI:N2	2.66	0.57
2:B:32[B]:PHE:HE2	30:B:531:HOH:O	1.87	0.57
1:N:356:ILE:HA	14:N:602[B]:HEA:HMB3	1.86	0.57
1:A:28:MET:CE	14:A:601:HEA:H271	2.35	0.57
1:A:178[B]:GLN:H	1:A:178[B]:GLN:NE2	2.02	0.57
4:D:100:LYS:NZ	30:D:301:HOH:O	1.96	0.57
9:V:8:GLN:HG2	9:V:15:ARG:CZ	2.34	0.57
3:C:33:MET:CB	25:C:302:DMU:H9	2.34	0.57
4:Q:7:LYS:O	4:Q:8:SER:HB2	2.05	0.57
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.88	0.57
2:B:65:TRP:CD1	23:B:302:PSC:H142	2.40	0.56
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:HBD2	1.87	0.56
3:C:54[A]:MET:HE3	27:C:305:CDL:H611	1.87	0.56
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.40	0.56
3:P:158:HIS:CE1	6:S:1:ALA:O	2.58	0.56
4:Q:144:GLU:HB2	21:Q:204:EDO:H21	1.86	0.56
8:H:8:ILE:O	8:H:8:ILE:HG22	2.04	0.56
27:G:102:CDL:H531	27:G:102:CDL:H241	1.88	0.56
19:Y:101:TGL:HA31	19:Y:101:TGL:HG12	1.86	0.56
27:C:305:CDL:H821	27:C:305:CDL:C78	2.28	0.56
9:I:35:TYR:CD1	9:I:35:TYR:C	2.80	0.56
3:P:33[A]:MET:CB	25:P:308:DMU:H9	2.35	0.56
7:T:31:CYS:SG	27:T:103:CDL:H542	2.46	0.56
1:A:281:GLY:C	7:T:4:ALA:HB1	2.27	0.55
23:B:302:PSC:H52	23:B:302:PSC:H262	1.87	0.55
9:I:33:THR:C	9:I:34:PHE:O	2.42	0.55
20:P:302:PGV:H061	8:U:22:ASN:ND2	2.20	0.55
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.32	0.55
7:G:4:ALA:CB	1:N:282:PHE:HA	2.35	0.55
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.72	0.55
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:608:PGV:H21	20:N:608:PGV:H012	1.79	0.55
7:T:5:LYS:HG3	28:T:102:PEK:H351	1.88	0.55
13:Z:32:TRP:CZ2	30:Z:212:HOH:O	2.60	0.55
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	1.87	0.55
10:W:29:ASN:HD22	10:W:29:ASN:H	1.54	0.55
1:A:178[B]:GLN:H	1:A:178[B]:GLN:HE21	1.54	0.55
1:A:39:ALA:CA	21:D:202:EDO:O1	2.42	0.55
20:A:609:PGV:H343	28:G:101:PEK:C38	2.37	0.55
3:C:258:TRP:CH2	25:C:309:DMU:H12	2.41	0.55
7:T:3:ALA:O	7:T:4:ALA:CB	2.55	0.55
23:O:302:PSC:H072	9:V:10:ARG:HH21	1.69	0.55
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.89	0.55
3:P:33[B]:MET:HE3	25:P:308:DMU:H6	1.88	0.55
2:B:92:ASN:N	30:B:401:HOH:O	1.92	0.55
20:N:608:PGV:H291	13:Z:16:ALA:HA	1.89	0.55
1:A:28:MET:HE2	14:A:601:HEA:C27	2.37	0.54
24:P:301:CHD:H151	20:P:302:PGV:H52	1.87	0.54
3:P:63:ARG:HE	27:P:306:CDL:HA22	1.69	0.54
3:P:33[B]:MET:SD	25:P:308:DMU:C19	2.95	0.54
7:T:31:CYS:SG	27:T:103:CDL:H522	2.47	0.54
24:C:306:CHD:C23	24:C:306:CHD:C16	2.84	0.54
1:A:112:LEU:HD23	1:A:113[A]:LEU:N	2.22	0.54
2:B:198:GLU:HG3	30:B:453:HOH:O	2.06	0.54
7:G:10:GLY:O	7:G:11:TPO:CB	2.43	0.54
12:L:29:PHE:HZ	19:L:101:TGL:HA91	1.72	0.54
27:P:306:CDL:H521	27:P:306:CDL:OB9	2.07	0.54
14:N:602[A]:HEA:HMC1	14:N:602[A]:HEA:CBC	2.35	0.54
27:P:306:CDL:H132	27:P:306:CDL:OA7	2.08	0.54
25:C:310:DMU:H23	10:J:41:GLY:HA3	1.89	0.54
20:M:101:PGV:O02	20:M:101:PGV:H032	2.08	0.54
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.53	0.54
7:T:44:ARG:HH22	7:T:84:LYS:HZ1	1.56	0.54
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.42	0.54
28:C:307:PEK:C05	6:F:1:ALA:N	2.68	0.54
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.07	0.53
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.39	0.53
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.38	0.53
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.08	0.53
1:A:112:LEU:CG	30:A:903:HOH:O	2.16	0.53
1:N:178[A]:GLN:HG2	30:N:715:HOH:O	2.02	0.53
13:Z:36:HIS:CD2	13:Z:39:ASN:ND2	2.75	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.53
27:C:305:CDL:HB21	27:C:305:CDL:OB6	2.08	0.53
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	1.91	0.53
28:C:307:PEK:C38	27:G:102:CDL:H273	2.38	0.53
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.53
3:C:62:ILE:CD1	27:C:305:CDL:H522	2.38	0.53
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.38	0.53
3:P:95:THR:HG21	20:P:302:PGV:H292	1.90	0.53
24:C:306:CHD:H231	24:C:306:CHD:C16	2.30	0.53
3:P:33[B]:MET:SD	25:P:308:DMU:H6	2.49	0.53
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.37	0.53
2:O:13:THR:HB	2:O:168:LEU:HD23	1.90	0.53
28:P:304:PEK:C11	28:P:304:PEK:C15	2.87	0.53
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.43	0.53
1:A:311[B]:ILE:HG13	1:A:314:ILE:HD12	1.89	0.52
3:C:224:LYS:HE3	27:C:305:CDL:HB31	1.90	0.52
11:X:47:ARG:CD	30:X:113:HOH:O	2.53	0.52
21:A:617:EDO:H22	30:M:216:HOH:O	2.10	0.52
1:N:54:TYR:HB2	30:N:834:HOH:O	2.08	0.52
1:N:112:LEU:HD23	1:N:112:LEU:C	2.29	0.52
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.57	0.52
28:P:309:PEK:H041	7:T:17:ARG:HH22	1.74	0.52
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.90	0.52
1:N:380[A]:VAL:HG21	14:N:602[A]:HEA:C3C	2.39	0.52
7:T:38:HIS:CE1	27:T:103:CDL:H132	2.43	0.52
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.91	0.52
2:B:56:MET:HB3	23:B:302:PSC:H231	1.90	0.52
3:C:258:TRP:CZ3	27:G:102:CDL:H642	2.45	0.52
2:O:25:ASP:O	2:O:29[B]:MET:HB2	2.09	0.52
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.91	0.52
1:A:311[A]:ILE:HD12	27:T:103:CDL:H221	1.91	0.52
3:P:213:THR:HG23	27:P:306:CDL:H771	1.92	0.52
9:V:8:GLN:HG2	9:V:15:ARG:NH2	2.24	0.52
1:A:355:GLY:C	14:A:602[B]:HEA:HMB3	2.30	0.52
30:O:490:HOH:O	19:Q:201:TGL:HC61	2.10	0.52
3:P:59:ARG:HA	27:P:306:CDL:H511	1.93	0.51
1:A:485:VAL:HB	21:A:618:EDO:H22	1.92	0.51
12:L:26:THR:HG23	13:M:25:SER:CB	2.40	0.51
12:L:26:THR:HG23	13:M:25:SER:HB3	1.92	0.51
7:T:84:LYS:HA	7:T:84:LYS:HE3	1.92	0.51
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.51
28:C:307:PEK:C04	6:F:1:ALA:H1	2.24	0.51
14:A:602[A]:HEA:NB	18:A:607:AZI:N2	2.55	0.51
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.93	0.51
27:C:305:CDL:H811	27:C:305:CDL:C67	2.40	0.51
18:N:606:AZI:N1	18:N:607:AZI:N1	2.59	0.51
19:N:610:TGL:HB92	19:N:610:TGL:H281	1.92	0.51
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.50
14:N:602[A]:HEA:NB	18:N:607:AZI:N2	2.55	0.50
9:V:31:PHE:C	9:V:31:PHE:CD1	2.84	0.50
21:A:612:EDO:H22	30:A:701:HOH:O	1.84	0.50
3:C:38:ASN:HA	30:C:437:HOH:O	2.11	0.50
28:C:307:PEK:O02	28:C:307:PEK:H42	2.11	0.50
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.46	0.50
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.11	0.50
23:O:302:PSC:H142	23:O:302:PSC:C34	2.41	0.50
3:P:62:ILE:HD12	27:P:306:CDL:H522	1.94	0.50
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C3C	2.41	0.50
4:D:28:ALA:H	4:D:31[B]:LYS:HZ3	1.59	0.50
1:N:309:THR:HG22	14:N:602[A]:HEA:HMB2	1.93	0.50
1:A:282:PHE:HZ	27:T:103:CDL:H751	1.76	0.50
27:G:102:CDL:H372	2:O:78:LEU:HD12	1.93	0.50
19:N:610:TGL:HA61	2:O:32[B]:PHE:CE1	2.46	0.50
2:O:69:PRO:HG3	23:O:302:PSC:H182	1.93	0.50
3:C:224:LYS:CD	27:C:305:CDL:CB3	2.81	0.50
3:P:224:LYS:HE3	27:P:306:CDL:HB32	1.94	0.50
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.94	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.50
10:W:58:LYS:N	10:W:58:LYS:HD2	2.27	0.50
1:A:28:MET:CE	14:A:601:HEA:C27	2.89	0.50
14:A:602[A]:HEA:C1B	18:A:607:AZI:N3	2.75	0.50
19:A:608:TGL:CA8	19:A:608:TGL:H221	2.41	0.50
21:A:612:EDO:C1	30:A:701:HOH:O	2.41	0.50
4:Q:4:SER:HA	4:Q:32:ASN:HB2	1.94	0.50
1:A:472:ILE:HG21	19:L:101:TGL:HA92	1.94	0.49
4:Q:145:TRP:CD1	21:Q:204:EDO:H22	2.47	0.49
8:H:38:ARG:HH12	21:H:101:EDO:C2	2.25	0.49
2:O:41:ILE:HG21	23:O:302:PSC:H332	1.94	0.49
1:A:54:TYR:HB2	30:A:740:HOH:O	2.13	0.49
1:N:514:LYS:HE2	30:S:219:HOH:O	2.12	0.49
3:C:63:ARG:HE	27:C:305:CDL:HA22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.94	0.49
8:U:44:THR:C	8:U:46:LYS:H	2.15	0.49
14:N:602[A]:HEA:C1B	18:N:607:AZI:N3	2.76	0.49
2:O:53:THR:CG2	30:Q:311:HOH:O	2.59	0.49
9:I:18:ARG:HG3	30:I:110:HOH:O	2.13	0.49
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.95	0.49
25:C:302:DMU:O61	25:C:310:DMU:H40	2.13	0.49
4:Q:7:LYS:NZ	30:Q:301:HOH:O	2.35	0.49
7:T:44:ARG:HH22	7:T:84:LYS:NZ	2.10	0.49
1:A:265:LYS:NZ	21:A:616:EDO:H22	2.28	0.48
28:T:102:PEK:H341	27:T:103:CDL:H872	1.94	0.48
1:A:282:PHE:N	7:T:4:ALA:HB1	2.28	0.48
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC3	3.01	0.48
3:C:33:MET:HA	25:C:302:DMU:H9	1.94	0.48
3:P:33[B]:MET:HA	25:P:308:DMU:H9	1.95	0.48
27:P:306:CDL:H411	27:P:306:CDL:H452	1.94	0.48
2:B:57:ASP:H	23:B:302:PSC:H221	1.78	0.48
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.96	0.48
23:O:302:PSC:H073	9:V:10:ARG:HH21	1.69	0.48
3:C:33:MET:CB	25:C:302:DMU:C19	2.85	0.48
1:N:511:VAL:H	21:N:621:EDO:C2	2.19	0.48
1:N:243:VAL:HG11	14:N:602[B]:HEA:HMD2	1.95	0.48
5:E:86:ILE:O	5:E:90:ARG:HG2	2.14	0.48
28:G:104:PEK:H132	3:P:247:VAL:HG12	1.95	0.48
1:N:28:MET:CE	14:N:601:HEA:C27	2.91	0.48
19:N:610:TGL:C28	19:N:610:TGL:CB9	2.92	0.48
2:B:78:LEU:CD1	27:T:103:CDL:H382	2.44	0.48
5:R:46:LYS:NZ	30:R:303:HOH:O	2.46	0.48
7:G:70[B]:PHE:HB2	28:G:101:PEK:H041	1.96	0.48
23:O:302:PSC:C07	9:V:10:ARG:NH2	2.63	0.48
3:P:156:ARG:HE	24:P:307:CHD:C24	2.27	0.48
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.43	0.48
1:A:178[B]:GLN:NE2	7:T:10:GLY:HA3	2.27	0.47
6:S:54:ASN:HD22	6:S:54:ASN:C	2.16	0.47
6:F:1:ALA:HB1	21:S:103:EDO:O1	2.14	0.47
27:T:103:CDL:OB3	27:T:103:CDL:H141	2.14	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.47
7:G:5:LYS:HG3	28:G:104:PEK:H351	1.96	0.47
27:T:103:CDL:OA5	27:T:103:CDL:H121	2.15	0.47
1:A:355:GLY:O	14:A:602[B]:HEA:HMB3	2.14	0.47
1:A:148:PHE:HB3	3:C:28:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:618:EDO:C2	30:A:715:HOH:O	2.23	0.47
2:B:121:TYR:CE2	30:B:468:HOH:O	2.56	0.47
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.47
3:C:179:SER:HB2	21:C:317:EDO:H11	1.96	0.47
1:N:189:MET:HE2	30:N:715:HOH:O	2.15	0.47
28:P:309:PEK:H41	28:P:309:PEK:H221	1.97	0.47
1:A:514:LYS:HG3	6:F:38:ALA:CB	2.45	0.47
3:C:144[A]:ILE:CD1	3:C:239:ALA:HA	2.44	0.47
1:N:28:MET:HE1	14:N:601:HEA:H271	1.97	0.47
2:O:26:HIS:O	2:O:29[B]:MET:HB3	2.14	0.47
24:P:307:CHD:H231	24:P:307:CHD:C16	2.37	0.47
27:G:102:CDL:CB5	27:G:102:CDL:H201	2.45	0.47
10:W:58:LYS:HE2	10:W:58:LYS:HA	1.97	0.47
28:G:104:PEK:H132	3:P:247:VAL:CG1	2.45	0.47
8:U:43:MET:HE3	8:U:49:ASP:N	2.30	0.47
12:L:29:PHE:CZ	19:L:101:TGL:HA91	2.50	0.46
2:O:87[B]:MET:CE	30:O:478:HOH:O	2.62	0.46
3:P:158:HIS:HE1	6:S:1:ALA:O	1.98	0.46
21:P:312:EDO:O1	6:S:1:ALA:HB1	2.14	0.46
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.97	0.46
6:F:21[B]:MET:HB2	6:F:21[B]:MET:HE2	1.59	0.46
1:N:240:HIS:HE1	18:N:607:AZI:N2	2.13	0.46
27:T:103:CDL:H612	27:T:103:CDL:C65	2.44	0.46
1:A:356:ILE:HA	14:A:602[B]:HEA:HMB3	1.98	0.46
14:A:602[B]:HEA:H122	14:A:602[B]:HEA:HHC	1.98	0.46
19:L:101:TGL:H212	19:L:101:TGL:HA81	1.46	0.46
25:C:309:DMU:H36	25:C:309:DMU:H34	1.14	0.46
7:G:37:LEU:CD2	27:G:102:CDL:H381	2.45	0.46
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.34	0.46
9:V:2:THR:HG22	9:V:3:ALA:O	2.15	0.46
14:A:602[A]:HEA:HMD1	14:A:602[A]:HEA:HBD2	1.97	0.46
2:B:65:TRP:O	2:B:69:PRO:HG2	2.15	0.46
19:D:201:TGL:H242	19:D:201:TGL:HA91	1.98	0.46
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.51	0.46
7:G:24:ALA:HA	27:G:102:CDL:H801	1.98	0.46
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.50	0.46
28:C:307:PEK:H382	27:G:102:CDL:H273	1.98	0.46
7:G:84:LYS:N	7:G:84:LYS:HZ2	2.13	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.51	0.46
27:T:103:CDL:H202	27:T:103:CDL:C51	2.45	0.46
21:C:314:EDO:H12	30:C:467:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:621:EDO:H12	6:S:36:PRO:CD	2.46	0.46
4:Q:109:HIS:HD2	30:Q:342:HOH:O	1.98	0.46
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.56	0.46
2:B:38:VAL:O	2:B:42:ILE:HB	2.16	0.46
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.96	0.46
6:S:51:SER:O	6:S:94:HIS:HA	2.16	0.46
4:D:78:TRP:CA	19:D:201:TGL:CB2	2.94	0.45
6:F:75:HIS:H	6:F:80:GLN:NE2	2.09	0.45
19:Y:101:TGL:HA22	19:Y:101:TGL:HA51	1.43	0.45
1:A:378:HIS:O	1:A:383[B]:MET:HG2	2.17	0.45
21:D:203:EDO:H21	30:F:201:HOH:O	2.16	0.45
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.98	0.45
8:H:60:TYR:CD1	8:H:60:TYR:C	2.89	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.82	0.45
4:Q:87[B]:PHE:HZ	11:X:20:SER:HB3	1.82	0.45
8:U:44:THR:O	8:U:46:LYS:N	2.39	0.45
7:G:3:ALA:O	7:G:4:ALA:CB	2.64	0.45
12:L:2:HIS:CG	12:L:3:TYR:H	2.34	0.45
1:A:13:LYS:HB3	21:A:610:EDO:H12	1.98	0.45
4:Q:145:TRP:H	21:Q:204:EDO:C2	2.29	0.45
14:A:601:HEA:HHC	14:A:601:HEA:H122	1.98	0.45
14:N:602[B]:HEA:HMC1	14:N:602[B]:HEA:CBC	2.46	0.45
27:T:103:CDL:H451	27:T:103:CDL:H422	1.76	0.45
21:A:614:EDO:H21	21:A:614:EDO:HO1	1.68	0.45
7:G:1:ALA:CB	20:P:302:PGV:C32	2.95	0.45
7:G:1:ALA:HB2	20:P:302:PGV:C32	2.46	0.45
3:P:246:ASP:HB2	30:P:484:HOH:O	2.16	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.90	0.45
1:A:311[A]:ILE:HD12	27:T:103:CDL:C22	2.47	0.45
21:A:612:EDO:O2	30:A:701:HOH:O	1.68	0.45
3:C:39:SER:OG	25:C:310:DMU:H2	2.15	0.45
28:G:101:PEK:C12	28:G:101:PEK:C16	2.83	0.45
2:B:198:GLU:HG2	30:B:453:HOH:O	2.15	0.45
7:G:3:ALA:HB3	28:G:104:PEK:H341	1.99	0.45
27:T:103:CDL:H532	27:T:103:CDL:H251	1.98	0.45
7:G:7:ASP:OD2	1:N:178[B]:GLN:NE2	2.50	0.45
1:N:383[B]:MET:SD	1:N:421:VAL:HG11	2.57	0.45
2:O:116:LEU:HG	2:O:117:SER:N	2.29	0.45
23:O:302:PSC:H012	23:O:302:PSC:O13	2.16	0.45
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.99	0.45
6:S:30:PRO:HB2	6:S:96:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:TYR:HE2	30:B:468:HOH:O	1.94	0.44
27:G:102:CDL:C23	1:N:311[B]:ILE:HD11	2.47	0.44
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.55	0.44
24:P:301:CHD:H12	24:P:301:CHD:H212	1.99	0.44
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:CG2	2.64	0.44
4:Q:81:VAL:HG11	19:Q:201:TGL:HB52	1.98	0.44
7:T:37:LEU:HD23	27:T:103:CDL:H391	1.99	0.44
1:N:377:PHE:HB2	14:N:602[B]:HEA:HMD3	1.99	0.44
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.53	0.44
7:T:2:SER:O	28:T:102:PEK:H322	2.18	0.44
8:H:7:LYS:O	8:H:8:ILE:HG13	2.17	0.44
12:L:20:ARG:NH2	19:L:101:TGL:CC5	2.58	0.44
7:T:11:TPO:O3P	28:T:102:PEK:H051	2.18	0.44
2:B:56:MET:CB	23:B:302:PSC:H231	2.48	0.44
3:C:226:HIS:CE1	27:C:305:CDL:HB32	2.52	0.44
27:C:305:CDL:HB62	27:C:305:CDL:H521	1.99	0.44
10:J:8:LYS:HD3	10:J:8:LYS:HA	1.72	0.44
11:X:26:VAL:O	11:X:30:VAL:HG23	2.17	0.44
2:B:83:ILE:O	2:B:87[B]:MET:HB3	2.17	0.44
2:B:108:TYR:O	2:B:117:SER:HA	2.17	0.44
7:G:44:ARG:HD2	7:G:82:TYR:CZ	2.52	0.44
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.17	0.44
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.35	0.44
7:G:1:ALA:O	7:G:3:ALA:N	2.50	0.44
20:N:608:PGV:H343	20:N:608:PGV:H182	1.98	0.44
21:Q:204:EDO:H12	30:Q:314:HOH:O	2.16	0.44
2:B:92:ASN:HA	30:B:401:HOH:O	2.18	0.44
2:B:42:ILE:HG22	2:B:43:SER:N	2.33	0.44
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.44
9:I:57:MET:O	9:I:61:GLU:HG2	2.18	0.44
1:N:399:LEU:O	1:N:499:PRO:HA	2.18	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
7:T:8:HIS:C	7:T:10:GLY:H	2.20	0.44
1:N:449:MET:SD	2:O:5:MET:HG2	2.58	0.43
27:T:103:CDL:H571	27:T:103:CDL:H762	2.00	0.43
3:C:246:ASP:HB2	30:C:486:HOH:O	2.17	0.43
8:H:9:LYS:HZ2	8:H:9:LYS:HA	1.83	0.43
2:O:87[B]:MET:HE3	30:O:478:HOH:O	2.18	0.43
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.48	0.43
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	2.00	0.43
12:Y:20:ARG:NH1	12:Y:24[B]:MET:SD	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:HE2	14:A:601:HEA:H273	1.99	0.43
6:F:54[A]:ASN:C	6:F:54[A]:ASN:HD22	2.20	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.00	0.43
1:N:510:TYR:HA	21:N:621:EDO:H21	2.00	0.43
19:Q:201:TGL:HG32	19:Q:201:TGL:OB1	2.17	0.43
8:H:45:ALA:O	8:H:47:GLY:N	2.50	0.43
1:N:488:THR:HB	1:N:495:LEU:HD13	2.00	0.43
3:P:164:PHE:CD1	24:P:307:CHD:H192	2.53	0.43
5:R:5:HIS:O	5:R:6:GLU:HB3	2.18	0.43
8:U:43:MET:HE3	8:U:49:ASP:H	1.83	0.43
7:G:3:ALA:CB	28:G:104:PEK:H362	2.46	0.43
10:J:52:TRP:O	10:J:57:HIS:CE1	2.71	0.43
23:O:302:PSC:H231	23:O:302:PSC:H202	1.67	0.43
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.19	0.43
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.00	0.43
7:G:1:ALA:HB2	20:P:302:PGV:H322	2.00	0.43
21:R:204:EDO:H12	30:R:348:HOH:O	2.08	0.43
3:C:37:PHE:CB	25:C:302:DMU:H7	2.48	0.43
4:D:121:LYS:HZ3	21:D:206:EDO:H22	1.84	0.43
19:L:101:TGL:HC71	19:L:101:TGL:HC31	2.00	0.43
1:N:87:ILE:O	1:N:173:PRO:HD3	2.18	0.43
2:O:87[B]:MET:HE1	30:U:234:HOH:O	2.18	0.43
23:O:302:PSC:C12	23:O:302:PSC:C34	2.95	0.43
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.53	0.43
3:C:191:GLY:HA3	30:G:213:HOH:O	2.17	0.43
4:D:14:PRO:HB3	21:D:203:EDO:H22	1.99	0.43
7:G:2:SER:HB2	1:N:197:LEU:HD21	2.01	0.43
28:G:101:PEK:H101	28:G:101:PEK:H42	2.00	0.43
1:N:313:ALA:HB2	1:N:356:ILE:HD11	2.01	0.43
1:N:321:PHE:CZ	23:O:302:PSC:H162	2.53	0.43
1:A:42:GLY:HA3	21:D:202:EDO:H21	2.01	0.43
1:A:240:HIS:HE1	18:A:607:AZI:N2	2.17	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.00	0.43
1:N:110:LEU:HG	25:P:308:DMU:H24	2.01	0.43
4:Q:5:VAL:O	4:Q:5:VAL:HG23	2.18	0.43
7:T:72:ASN:N	7:T:76:ASN:HD22	2.08	0.43
2:B:16[A]:ILE:CD1	2:B:87[A]:MET:HG2	2.48	0.42
3:P:59:ARG:HB2	27:P:306:CDL:H512	2.01	0.42
21:Q:203:EDO:H11	5:R:27:TRP:NE1	2.34	0.42
1:A:417:MET:CE	14:A:601:HEA:H263	2.49	0.42
19:L:101:TGL:HC71	19:L:101:TGL:CC3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.07	0.42
3:P:62:ILE:CD1	27:P:306:CDL:H522	2.48	0.42
1:A:488:THR:HG21	21:A:618:EDO:H11	2.02	0.42
27:C:305:CDL:OA3	27:C:305:CDL:OB7	2.37	0.42
2:O:52:HIS:CE1	23:O:302:PSC:H212	2.55	0.42
1:A:172:LYS:HD2	1:A:181:THR:CG2	2.50	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.56	0.42
14:N:602[B]:HEA:H11	14:N:602[B]:HEA:HMB1	1.76	0.42
14:A:602[A]:HEA:C1B	18:A:607:AZI:N2	2.83	0.42
28:C:307:PEK:C05	6:F:1:ALA:H1	2.32	0.42
7:G:6:GLY:H	1:N:278[B]:MET:HE1	1.84	0.42
19:L:101:TGL:HC71	19:L:101:TGL:HC41	1.71	0.42
3:P:22:LEU:O	3:P:26:LEU:HG	2.20	0.42
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.55	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.42
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.42
27:P:306:CDL:H191	27:P:306:CDL:C31	2.48	0.42
25:P:310:DMU:H36	25:P:310:DMU:H34	1.44	0.42
1:A:449:MET:SD	2:B:5:MET:HG2	2.59	0.42
4:D:121:LYS:NZ	21:D:206:EDO:H22	2.34	0.42
5:E:86:ILE:HD13	5:E:86:ILE:HA	1.89	0.42
27:G:102:CDL:H661	27:G:102:CDL:C61	2.45	0.42
1:N:240:HIS:CE1	18:N:607:AZI:N2	2.87	0.42
3:P:41:THR:HA	3:P:44[B]:MET:CE	2.50	0.42
1:A:514:LYS:HA	6:F:38:ALA:CB	2.47	0.42
9:I:27:VAL:HG12	9:I:28:SER:CA	2.50	0.42
1:N:378:HIS:HA	1:N:382[B]:SER:CB	2.48	0.42
2:O:111:THR:HA	2:O:114:GLU:O	2.20	0.42
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	2.02	0.42
1:A:240:HIS:CE1	18:A:607:AZI:N2	2.88	0.42
2:B:65:TRP:HD1	23:B:302:PSC:H142	1.84	0.42
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	2.02	0.42
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	2.01	0.42
4:Q:130:PRO:HA	4:Q:135:SER:HB2	2.02	0.42
2:O:61:VAL:HG22	2:O:65:TRP:CZ3	2.55	0.42
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.49	0.41
1:A:377:PHE:HB2	14:A:602[B]:HEA:HMD3	2.02	0.41
10:W:29:ASN:H	10:W:29:ASN:ND2	2.18	0.41
25:C:310:DMU:H6	25:C:310:DMU:H1	1.91	0.41
7:G:11:TPO:C	30:G:202:HOH:O	2.66	0.41
1:N:297[B]:MET:HB3	30:N:782:HOH:O	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:459:PHE:HB3	4:Q:92:THR:CG2	2.50	0.41
20:N:608:PGV:C31	13:Z:19:LEU:HD23	2.44	0.41
3:P:33[A]:MET:HA	25:P:308:DMU:H9	2.01	0.41
3:P:224:LYS:HZ1	27:P:306:CDL:H112	1.84	0.41
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:CBC	2.50	0.41
27:G:102:CDL:H362	27:G:102:CDL:H121	2.02	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.20	0.41
27:P:306:CDL:H132	27:P:306:CDL:H162	1.62	0.41
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:CBD	2.49	0.41
27:T:103:CDL:OB3	27:T:103:CDL:H162	2.21	0.41
20:N:609:PGV:H262	20:P:305:PGV:H292	2.03	0.41
3:C:51[A]:MET:HB3	27:C:305:CDL:H381	2.02	0.41
3:C:76:GLN:NE2	3:C:80[A]:ARG:HH21	2.18	0.41
28:C:307:PEK:O02	28:C:307:PEK:C4	2.68	0.41
27:P:306:CDL:H273	27:P:306:CDL:H472	2.02	0.41
7:T:38:HIS:ND1	7:T:38:HIS:N	2.67	0.41
1:N:514:LYS:HA	6:S:38:ALA:CB	2.46	0.41
6:S:37:LYS:HD2	6:S:37:LYS:HA	1.79	0.41
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.02	0.41
1:A:347:LEU:HD11	1:A:418:PHE:CE1	2.55	0.41
3:C:224:LYS:HE3	27:C:305:CDL:CB3	2.50	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.41
2:O:87[B]:MET:CE	30:U:234:HOH:O	2.69	0.41
27:P:306:CDL:H812	27:P:306:CDL:H842	1.69	0.41
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.56	0.41
4:D:109:HIS:HD2	30:D:360:HOH:O	2.04	0.41
7:G:37:LEU:HG	27:G:102:CDL:H361	2.02	0.41
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.55	0.41
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.21	0.41
20:N:608:PGV:H42	20:N:608:PGV:H202	2.02	0.41
3:P:224:LYS:CE	27:P:306:CDL:HB32	2.50	0.41
11:X:43:SER:O	11:X:47:ARG:HD3	2.21	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
1:N:378:HIS:O	1:N:383[B]:MET:HG2	2.22	0.41
9:I:73:LYS:HD3	9:I:73:LYS:HA	1.84	0.40
1:N:28:MET:HE1	14:N:601:HEA:C27	2.51	0.40
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.40
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	2.03	0.40
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.55	0.40
20:P:302:PGV:H231	20:P:302:PGV:H202	1.82	0.40
2:B:57:ASP:N	23:B:302:PSC:H221	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:104:EDO:H22	30:F:271:HOH:O	2.20	0.40
7:G:12:GLY:N	30:G:201:HOH:O	2.32	0.40
2:O:41:ILE:O	2:O:42:ILE:C	2.57	0.40
8:U:54:GLU:OE1	8:U:54:GLU:HA	2.22	0.40
24:G:103:CHD:H12	24:G:103:CHD:H212	2.04	0.40
8:H:38:ARG:HH12	21:H:101:EDO:H21	1.86	0.40
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.21	0.40
7:T:84:LYS:HA	7:T:84:LYS:CE	2.52	0.40
10:W:3:ASN:OD1	10:W:3:ASN:C	2.58	0.40
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.88	0.40
13:M:39:ASN:O	13:M:43:SER:HB3	2.22	0.40
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.03	0.40
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.40
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.86	0.40
7:G:38:HIS:NE2	27:G:102:CDL:H141	2.36	0.40
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.02	0.40
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.57	0.40
5:R:41:LEU:HA	30:V:211:HOH:O	2.21	0.40
7:T:7:ASP:H	28:T:102:PEK:H292	1.86	0.40
27:T:103:CDL:H791	27:T:103:CDL:H821	1.51	0.40
10:W:58:LYS:NZ	12:Y:47:LYS:HD2	2.37	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:468:HOH:O	30:D:353:HOH:O[2_584]	1.99	0.21

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	530/514 (103%)	514 (97%)	16 (3%)	0	100 100
1	N	530/514 (103%)	516 (97%)	14 (3%)	0	100 100
2	B	229/227 (101%)	223 (97%)	6 (3%)	0	100 100
2	O	230/227 (101%)	224 (97%)	5 (2%)	1 (0%)	34 19
3	C	264/261 (101%)	260 (98%)	4 (2%)	0	100 100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100 100
4	D	143/147 (97%)	139 (97%)	4 (3%)	0	100 100
4	Q	144/147 (98%)	138 (96%)	4 (3%)	2 (1%)	11 3
5	E	103/109 (94%)	103 (100%)	0	0	100 100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15 5
6	F	99/98 (101%)	93 (94%)	2 (2%)	4 (4%)	3 0
6	S	98/98 (100%)	89 (91%)	4 (4%)	5 (5%)	2 0
7	G	82/85 (96%)	69 (84%)	6 (7%)	7 (8%)	1 0
7	T	81/85 (95%)	70 (86%)	7 (9%)	4 (5%)	2 0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3 0
8	U	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	3 0
9	I	71/73 (97%)	68 (96%)	1 (1%)	2 (3%)	5 0
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	56/59 (95%)	56 (100%)	0	0	100 100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100 100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100 100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6 1
13	Z	41/46 (89%)	41 (100%)	0	0	100 100
All	All	3576/3614 (99%)	3444 (96%)	99 (3%)	33 (1%)	17 6

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	94	HIS
6	F	95	GLN

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Mol	Chain	Res	Type
7	G	2	SER
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS
8	H	8	ILE
9	I	34	PHE
9	I	35	TYR
5	R	6	GLU
6	S	94	HIS
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
7	G	3	ALA
8	H	46	LYS
13	M	42	LYS
4	Q	5	VAL
6	S	95	GLN
7	T	4	ALA
8	U	46	LYS
7	G	6	GLY
7	G	41	HIS
8	H	45	ALA
6	S	97	ALA
8	U	45	ALA
6	F	97	ALA
4	Q	8	SER
6	S	96	LEU
2	O	92	ASN
6	S	93	PRO

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	443/426 (104%)	436 (98%)	7 (2%)	62 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	443/426 (104%)	434 (98%)	9 (2%)	55 40
2	B	214/210 (102%)	201 (94%)	13 (6%)	18 5
2	O	215/210 (102%)	207 (96%)	8 (4%)	34 17
3	C	231/226 (102%)	227 (98%)	4 (2%)	60 47
3	P	233/226 (103%)	228 (98%)	5 (2%)	53 38
4	D	129/129 (100%)	125 (97%)	4 (3%)	40 23
4	Q	130/129 (101%)	124 (95%)	6 (5%)	27 11
5	E	92/95 (97%)	88 (96%)	4 (4%)	29 12
5	R	92/95 (97%)	89 (97%)	3 (3%)	38 21
6	F	84/81 (104%)	80 (95%)	4 (5%)	25 10
6	S	83/81 (102%)	74 (89%)	9 (11%)	6 1
7	G	68/68 (100%)	59 (87%)	9 (13%)	4 0
7	T	67/68 (98%)	61 (91%)	6 (9%)	9 1
8	H	71/75 (95%)	66 (93%)	5 (7%)	15 3
8	U	71/75 (95%)	67 (94%)	4 (6%)	21 7
9	I	57/57 (100%)	55 (96%)	2 (4%)	36 18
9	V	57/57 (100%)	53 (93%)	4 (7%)	15 3
10	J	49/50 (98%)	48 (98%)	1 (2%)	55 40
10	W	49/50 (98%)	46 (94%)	3 (6%)	18 5
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%)	38 (95%)	2 (5%)	24 9
13	M	37/38 (97%)	35 (95%)	2 (5%)	22 8
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22 8
All	All	3110/3082 (101%)	2993 (96%)	117 (4%)	34 16

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	112	LEU
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
2	B	15	PRO
2	B	29	MET
2	B	35	SER
2	B	42	ILE
2	B	60	GLU
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	115	ASP
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	8	SER
4	D	31[A]	LYS
4	D	31[B]	LYS
4	D	147	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
6	F	98	HIS
7	G	2	SER
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS

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Mol	Chain	Res	Type
8	H	9	LYS
8	H	10	ASN
8	H	29	CYS
8	H	46	LYS
8	H	60	TYR
9	I	2	THR
9	I	37	PHE
10	J	58	LYS
12	L	47	LYS
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	369	ASP
1	N	382[A]	SER
1	N	382[B]	SER
1	N	495	LEU
1	N	514	LYS
2	O	33	LEU
2	O	65	TRP
2	O	78	LEU
2	O	91	ASN
2	O	115	ASP
2	O	171	LYS
2	O	221	LYS
2	O	226	MET
3	P	3	HIS
3	P	17	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
4	Q	143	ASN
4	Q	147	LYS
5	R	79	LYS
5	R	90	ARG
5	R	109	VAL

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Mol	Chain	Res	Type
6	S	2	SER
6	S	37	LYS
6	S	54	ASN
6	S	64	GLU
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	93	PRO
6	S	96	LEU
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
8	U	65	PRO
9	V	26	MET
9	V	36	LYS
9	V	65	LYS
9	V	70	GLN
10	W	7	GLU
10	W	50	LEU
10	W	58	LYS
12	Y	2	HIS
12	Y	26	THR
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	109	HIS

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Mol	Chain	Res	Type
4	D	143	ASN
5	E	94	ASN
6	F	80	GLN
6	F	95	GLN
7	G	8	HIS
7	G	34	ASN
7	G	76	ASN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	180	GLN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	122	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	8	HIS
7	T	76	ASN
8	U	22	ASN
8	U	37	HIS
9	V	53	ASN
10	W	29	ASN
10	W	57	HIS
13	Z	36	HIS
13	Z	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	1.71	1 (14%)	8,9,11	1.29	1 (12%)
1	FME	A	1	1	8,9,10	1.24	0	7,9,11	2.13	4 (57%)
9	SAC	I	1	9	7,8,9	1.37	1 (14%)	8,9,11	1.71	1 (12%)
7	TPO	G	11	7	8,10,11	2.12	2 (25%)	10,14,16	1.61	2 (20%)
1	FME	N	1	1	8,9,10	1.19	1 (12%)	7,9,11	1.36	0
7	TPO	T	11	7	8,10,11	1.70	1 (12%)	10,14,16	0.99	1 (10%)
2	FME	O	1	2	8,9,10	1.48	1 (12%)	7,9,11	1.73	2 (28%)
2	FME	B	1	2	8,9,10	1.85	2 (25%)	7,9,11	1.97	2 (28%)

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.51	1.61	1.50
7	G	11	TPO	P-OG1	3.20	1.65	1.59
7	G	11	TPO	P-O1P	3.19	1.60	1.50
9	I	1	SAC	CA-N	3.19	1.50	1.46
1	N	1	FME	CA-N	2.91	1.50	1.46
2	B	1	FME	CB-CG	2.91	1.62	1.51
2	B	1	FME	CA-N	2.90	1.50	1.46
2	O	1	FME	CA-N	2.90	1.50	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	OG-CB-CA	-4.02	100.70	110.97
2	B	1	FME	C-CA-N	-3.44	103.53	109.73
2	B	1	FME	CG-CB-CA	-3.34	103.67	112.95
2	O	1	FME	CG-CB-CA	-3.09	104.35	112.95
1	A	1	FME	CE-SD-CG	3.08	110.99	100.40
9	V	1	SAC	C-CA-N	2.88	114.92	109.73
2	O	1	FME	CA-N-CN	2.58	126.80	122.82
7	G	11	TPO	O2P-P-OG1	2.57	117.50	105.99
7	G	11	TPO	CG2-CB-CA	2.52	118.14	113.16
1	A	1	FME	C-CA-N	2.40	114.06	109.73
1	A	1	FME	CA-N-CN	2.39	126.50	122.82
7	T	11	TPO	O-C-CA	-2.06	119.37	124.78
1	A	1	FME	O1-CN-N	-2.05	119.87	125.27

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	3	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 131 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 121 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	$\#\|Z\| > 2$
21	EDO	C	314	-	3,3,3	0.71	0	2,2,2	0.60	0
19	TGL	D	201	-	62,62,62	1.84	5 (8%)	65,65,65	2.30	12 (18%)
14	HEA	N	602[A]	18,1	57,67,67	1.64	12 (21%)	61,103,103	2.09	23 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	TGL	Q	201	-	62,62,62	1.55	4 (6%)	65,65,65	1.45	9 (13%)
21	EDO	O	304	-	3,3,3	0.39	0	2,2,2	1.00	0
25	DMU	P	308	-	34,34,34	1.10	1 (2%)	45,45,45	1.52	4 (8%)
21	EDO	G	105	-	3,3,3	0.59	0	2,2,2	0.55	0
21	EDO	C	318	-	3,3,3	0.48	0	2,2,2	0.35	0
18	AZI	N	607	14	0,2,2	-	-	0,1,1	-	-
19	TGL	L	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.76	15 (23%)
21	EDO	G	106	-	3,3,3	0.99	0	2,2,2	0.58	0
25	DMU	C	310	-	34,34,34	0.97	1 (2%)	45,45,45	2.20	12 (26%)
24	CHD	C	306	-	32,32,32	1.24	4 (12%)	51,51,51	3.07	18 (35%)
27	CDL	G	102	-	99,99,99	1.52	15 (15%)	105,111,111	1.51	19 (18%)
21	EDO	S	102	-	3,3,3	1.03	0	2,2,2	0.34	0
21	EDO	D	203	-	3,3,3	0.29	0	2,2,2	0.69	0
21	EDO	F	104	-	3,3,3	0.34	0	2,2,2	0.33	0
21	EDO	T	104	-	3,3,3	1.14	0	2,2,2	0.54	0
21	EDO	E	203	-	3,3,3	0.35	0	2,2,2	1.55	0
14	HEA	N	601	1	57,67,67	1.77	16 (28%)	61,103,103	2.61	30 (49%)
23	PSC	B	302	-	51,51,51	1.44	4 (7%)	57,59,59	1.50	5 (8%)
21	EDO	N	617	-	3,3,3	0.96	0	2,2,2	0.16	0
21	EDO	C	315	-	3,3,3	1.08	0	2,2,2	1.12	0
20	PGV	C	304	-	50,50,50	0.95	2 (4%)	53,56,56	1.53	10 (18%)
20	PGV	N	609	-	50,50,50	1.07	4 (8%)	53,56,56	1.30	4 (7%)
21	EDO	Q	204	-	3,3,3	0.72	0	2,2,2	0.24	0
24	CHD	T	101	-	32,32,32	2.17	13 (40%)	51,51,51	1.96	18 (35%)
24	CHD	P	301	-	32,32,32	1.68	8 (25%)	51,51,51	2.07	18 (35%)
21	EDO	A	616	-	3,3,3	0.61	0	2,2,2	1.13	0
21	EDO	E	204	-	3,3,3	0.65	0	2,2,2	0.36	0
21	EDO	A	615	-	3,3,3	1.27	0	2,2,2	0.24	0
21	EDO	N	615	-	3,3,3	1.72	1 (33%)	2,2,2	0.26	0
21	EDO	P	314	-	3,3,3	0.55	0	2,2,2	0.65	0
14	HEA	A	601	1	57,67,67	1.77	15 (26%)	61,103,103	2.75	36 (59%)
21	EDO	R	201	-	3,3,3	0.36	0	2,2,2	0.92	0
21	EDO	A	611	-	3,3,3	0.57	0	2,2,2	1.01	0
21	EDO	P	312	-	3,3,3	0.82	0	2,2,2	1.90	1 (50%)
21	EDO	V	101	-	3,3,3	0.41	0	2,2,2	0.43	0
25	DMU	Z	101	-	34,34,34	0.82	1 (2%)	45,45,45	1.26	5 (11%)
25	DMU	P	311	-	34,34,34	0.85	1 (2%)	45,45,45	1.60	8 (17%)
21	EDO	D	205	-	3,3,3	0.46	0	2,2,2	1.14	0
21	EDO	C	316	-	3,3,3	0.57	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	N	611	-	3,3,3	0.48	0	2,2,2	1.43	0
21	EDO	A	612	-	3,3,3	0.95	0	2,2,2	1.36	0
14	HEA	A	602[A]	18,1	57,67,67	1.64	10 (17%)	61,103,103	2.13	20 (32%)
20	PGV	P	302	-	50,50,50	1.16	2 (4%)	53,56,56	1.40	8 (15%)
21	EDO	R	202	-	3,3,3	0.48	0	2,2,2	1.00	0
19	TGL	N	610	-	62,62,62	1.22	4 (6%)	65,65,65	1.72	11 (16%)
21	EDO	S	104	-	3,3,3	0.75	0	2,2,2	1.58	1 (50%)
21	EDO	C	313	-	3,3,3	0.56	0	2,2,2	0.57	0
21	EDO	C	319	-	3,3,3	0.92	0	2,2,2	1.51	0
21	EDO	O	305	-	3,3,3	0.45	0	2,2,2	0.37	0
24	CHD	C	301	-	32,32,32	1.81	9 (28%)	51,51,51	2.44	16 (31%)
21	EDO	A	613	-	3,3,3	0.30	0	2,2,2	1.38	0
21	EDO	A	619	-	3,3,3	0.59	0	2,2,2	0.97	0
21	EDO	D	206	-	3,3,3	0.32	0	2,2,2	1.19	0
21	EDO	N	613	-	3,3,3	0.66	0	2,2,2	0.48	0
21	EDO	N	619	-	3,3,3	0.54	0	2,2,2	0.21	0
21	EDO	C	311	-	3,3,3	1.08	0	2,2,2	0.32	0
21	EDO	S	103	-	3,3,3	0.80	0	2,2,2	0.44	0
21	EDO	N	620	-	3,3,3	0.45	0	2,2,2	1.44	0
21	EDO	D	202	-	3,3,3	0.46	0	2,2,2	0.46	0
21	EDO	U	101	-	3,3,3	0.44	0	2,2,2	0.49	0
21	EDO	N	616	-	3,3,3	0.57	0	2,2,2	1.31	0
21	EDO	A	614	-	3,3,3	3.04	1 (33%)	2,2,2	4.76	1 (50%)
21	EDO	N	614	-	3,3,3	0.53	0	2,2,2	0.94	0
21	EDO	N	621	-	3,3,3	0.78	0	2,2,2	0.25	0
28	PEK	G	104	-	52,52,52	1.32	5 (9%)	55,57,57	1.53	6 (10%)
24	CHD	G	103	-	32,32,32	1.58	7 (21%)	51,51,51	1.77	16 (31%)
14	HEA	N	602[B]	18,1	57,67,67	1.57	12 (21%)	61,103,103	1.84	16 (26%)
20	PGV	A	609	-	50,50,50	1.09	2 (4%)	53,56,56	1.16	5 (9%)
21	EDO	E	205	-	3,3,3	0.55	0	2,2,2	0.77	0
21	EDO	N	612	-	3,3,3	1.23	0	2,2,2	1.79	1 (50%)
19	TGL	A	608	-	62,62,62	1.32	5 (8%)	65,65,65	2.26	11 (16%)
22	CUA	B	301	2	0,1,1	-	-	-		
25	DMU	C	302	-	34,34,34	1.16	2 (5%)	45,45,45	1.80	7 (15%)
21	EDO	R	203	-	3,3,3	0.87	0	2,2,2	0.48	0
21	EDO	A	618	-	3,3,3	0.41	0	2,2,2	1.36	0
22	CUA	O	301	2	0,1,1	-	-	-		
20	PGV	P	305	-	50,50,50	1.04	4 (8%)	53,56,56	1.39	7 (13%)
24	CHD	P	307	-	32,32,32	1.40	4 (12%)	51,51,51	2.96	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	P	315	-	3,3,3	0.45	0	2,2,2	0.70	0
23	PSC	O	302	-	51,51,51	1.28	3 (5%)	57,59,59	1.29	5 (8%)
21	EDO	A	620	-	3,3,3	0.33	0	2,2,2	1.09	0
21	EDO	A	617	-	3,3,3	0.27	0	2,2,2	1.71	1 (50%)
27	CDL	P	306	-	99,99,99	1.66	19 (19%)	105,111,111	1.55	18 (17%)
21	EDO	P	313	-	3,3,3	0.96	0	2,2,2	0.36	0
28	PEK	P	309	-	52,52,52	1.24	2 (3%)	55,57,57	1.43	6 (10%)
20	PGV	M	101	-	50,50,50	1.41	4 (8%)	53,56,56	1.61	8 (15%)
21	EDO	H	101	-	3,3,3	0.29	0	2,2,2	2.25	2 (100%)
28	PEK	P	304	-	52,52,52	1.00	4 (7%)	55,57,57	1.23	5 (9%)
21	EDO	A	610	-	3,3,3	0.33	0	2,2,2	1.48	0
20	PGV	C	308	-	50,50,50	1.24	2 (4%)	53,56,56	1.35	5 (9%)
25	DMU	P	310	-	34,34,34	0.78	1 (2%)	45,45,45	2.38	11 (24%)
18	AZI	A	606	15	0,2,2	-	-	0,1,1	-	-
18	AZI	N	606	15	0,2,2	-	-	0,1,1	-	-
21	EDO	E	201	-	3,3,3	0.64	0	2,2,2	0.45	0
21	EDO	O	303	-	3,3,3	0.80	0	2,2,2	0.92	0
21	EDO	F	102	-	3,3,3	1.10	0	2,2,2	0.25	0
21	EDO	D	204	-	3,3,3	0.76	0	2,2,2	0.71	0
25	DMU	C	309	-	34,34,34	0.88	2 (5%)	45,45,45	2.62	12 (26%)
21	EDO	F	103	-	3,3,3	0.80	0	2,2,2	0.68	0
21	EDO	N	618	-	3,3,3	0.78	0	2,2,2	0.85	0
28	PEK	G	101	-	52,52,52	1.05	5 (9%)	55,57,57	1.33	10 (18%)
25	DMU	M	102	-	34,34,34	0.60	0	45,45,45	1.42	5 (11%)
21	EDO	Q	202	-	3,3,3	0.29	0	2,2,2	1.13	0
18	AZI	A	607	14	0,2,2	-	-	0,1,1	-	-
21	EDO	C	312	-	3,3,3	0.36	0	2,2,2	0.60	0
19	TGL	Y	101	-	62,62,62	1.47	4 (6%)	65,65,65	1.55	11 (16%)
21	EDO	R	205	-	3,3,3	1.16	0	2,2,2	0.36	0
21	EDO	Q	203	-	3,3,3	1.23	0	2,2,2	1.03	0
28	PEK	C	307	-	52,52,52	1.21	4 (7%)	55,57,57	1.33	7 (12%)
21	EDO	B	303	-	3,3,3	0.80	0	2,2,2	0.32	0
27	CDL	T	103	-	99,99,99	1.44	12 (12%)	105,111,111	1.47	19 (18%)
20	PGV	N	608	-	50,50,50	1.21	2 (4%)	53,56,56	1.34	6 (11%)
21	EDO	E	202	-	3,3,3	0.54	0	2,2,2	0.89	0
14	HEA	A	602[B]	18,1	57,67,67	1.52	10 (17%)	61,103,103	2.16	20 (32%)
28	PEK	T	102	-	52,52,52	1.28	2 (3%)	55,57,57	1.49	7 (12%)
21	EDO	R	204	-	3,3,3	0.26	0	2,2,2	0.45	0
21	EDO	C	317	-	3,3,3	0.73	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CDL	C	305	-	99,99,99	1.55	17 (17%)	105,111,111	1.58	19 (18%)

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
21	EDO	C	314	-	-	1/1/1/1	-
19	TGL	D	201	-	-	41/65/65/65	-
14	HEA	N	602[A]	18,1	-	4/32/76/76	-
19	TGL	Q	201	-	-	39/65/65/65	-
21	EDO	O	304	-	-	1/1/1/1	-
25	DMU	P	308	-	-	6/19/59/59	0/2/2/2
21	EDO	G	105	-	-	1/1/1/1	-
21	EDO	C	318	-	-	1/1/1/1	-
19	TGL	L	101	-	-	43/65/65/65	-
21	EDO	G	106	-	-	0/1/1/1	-
25	DMU	C	310	-	-	10/19/59/59	0/2/2/2
24	CHD	C	306	-	-	6/9/74/74	0/4/4/4
27	CDL	G	102	-	-	58/110/110/110	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
14	HEA	N	601	1	-	6/32/76/76	-
23	PSC	B	302	-	-	30/55/55/55	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	C	315	-	-	0/1/1/1	-
20	PGV	C	304	-	-	18/55/55/55	-
20	PGV	N	609	-	-	9/55/55/55	-
21	EDO	Q	204	-	-	0/1/1/1	-
24	CHD	T	101	-	-	2/9/74/74	0/4/4/4
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	A	616	-	-	1/1/1/1	-
21	EDO	E	204	-	-	1/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	P	314	-	-	0/1/1/1	-
14	HEA	A	601	1	-	6/32/76/76	-
21	EDO	R	201	-	-	1/1/1/1	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	V	101	-	-	1/1/1/1	-
25	DMU	Z	101	-	-	3/19/59/59	0/2/2/2
25	DMU	P	311	-	-	13/19/59/59	0/2/2/2
21	EDO	D	205	-	-	0/1/1/1	-
21	EDO	C	316	-	-	1/1/1/1	-
21	EDO	N	611	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
14	HEA	A	602[A]	18,1	-	6/32/76/76	-
20	PGV	P	302	-	-	25/55/55/55	-
21	EDO	R	202	-	-	1/1/1/1	-
19	TGL	N	610	-	-	37/65/65/65	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	C	319	-	-	1/1/1/1	-
21	EDO	O	305	-	-	1/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	N	613	-	-	1/1/1/1	-
21	EDO	N	619	-	-	1/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	D	202	-	-	0/1/1/1	-
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
28	PEK	G	104	-	-	36/56/56/56	-
24	CHD	G	103	-	-	2/9/74/74	0/4/4/4
14	HEA	N	602[B]	18,1	-	6/32/76/76	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	E	205	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	612	-	-	1/1/1/1	-
19	TGL	A	608	-	-	39/65/65/65	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
21	EDO	R	203	-	-	0/1/1/1	-
21	EDO	A	618	-	-	0/1/1/1	-
20	PGV	P	305	-	-	9/55/55/55	-
24	CHD	P	307	-	-	7/9/74/74	0/4/4/4
21	EDO	P	315	-	-	0/1/1/1	-
23	PSC	O	302	-	-	32/55/55/55	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
27	CDL	P	306	-	-	62/110/110/110	-
21	EDO	P	313	-	-	0/1/1/1	-
28	PEK	P	309	-	-	28/56/56/56	-
20	PGV	M	101	-	-	23/55/55/55	-
21	EDO	H	101	-	-	0/1/1/1	-
28	PEK	P	304	-	-	16/56/56/56	-
21	EDO	A	610	-	-	1/1/1/1	-
20	PGV	C	308	-	-	27/55/55/55	-
25	DMU	P	310	-	-	7/19/59/59	0/2/2/2
21	EDO	O	303	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
25	DMU	C	309	-	-	6/19/59/59	0/2/2/2
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
28	PEK	G	101	-	-	18/56/56/56	-
25	DMU	M	102	-	-	5/19/59/59	0/2/2/2
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	C	312	-	-	1/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
21	EDO	R	205	-	-	1/1/1/1	-
21	EDO	Q	203	-	-	0/1/1/1	-
28	PEK	C	307	-	-	32/56/56/56	-
21	EDO	B	303	-	-	0/1/1/1	-
27	CDL	T	103	-	-	53/110/110/110	-
20	PGV	N	608	-	-	27/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	E	202	-	-	0/1/1/1	-
14	HEA	A	602[B]	18,1	-	5/32/76/76	-
28	PEK	T	102	-	-	22/56/56/56	-
21	EDO	R	204	-	-	1/1/1/1	-
21	EDO	C	317	-	-	1/1/1/1	-
27	CDL	C	305	-	-	66/110/110/110	-

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	8.49	1.47	1.22
19	Q	201	TGL	OB1-CB1	7.18	1.43	1.22
19	Y	101	TGL	OG2-CB1	6.54	1.52	1.34
19	D	201	TGL	OG1-CA1	6.47	1.52	1.33
19	D	201	TGL	OG2-CB1	6.35	1.52	1.34
28	T	102	PEK	O01-C1	6.21	1.51	1.34
19	Y	101	TGL	OG3-CC1	6.18	1.51	1.33
23	B	302	PSC	O01-C1	6.13	1.51	1.34
20	N	608	PGV	O03-C19	6.06	1.51	1.33
27	P	306	CDL	OA8-CA7	6.05	1.51	1.33
28	G	104	PEK	O03-C21	6.05	1.51	1.33
27	G	102	CDL	OB6-CB5	6.04	1.51	1.34
19	A	608	TGL	OG1-CA1	5.89	1.50	1.33
27	P	306	CDL	OB8-CB7	5.88	1.50	1.33
27	C	305	CDL	OB8-CB7	5.72	1.50	1.33
19	Q	201	TGL	OG2-CB1	5.69	1.50	1.34
27	G	102	CDL	OB8-CB7	5.67	1.49	1.33
20	M	101	PGV	O03-C19	5.62	1.49	1.33
28	C	307	PEK	O01-C1	5.56	1.50	1.34
27	T	103	CDL	OB8-CB7	5.43	1.49	1.33
20	C	308	PGV	O01-C1	5.43	1.49	1.34
27	T	103	CDL	OB6-CB5	5.38	1.49	1.34
28	P	309	PEK	O01-C1	5.37	1.49	1.34
24	C	301	CHD	C11-C9	5.29	1.62	1.53
27	T	103	CDL	OA8-CA7	5.25	1.48	1.33
27	C	305	CDL	OA8-CA7	5.24	1.48	1.33
27	P	306	CDL	OA6-CA5	5.13	1.48	1.34
25	C	302	DMU	O16-C6	5.11	1.48	1.40
23	O	302	PSC	O01-C1	5.08	1.48	1.34
28	T	102	PEK	O03-C21	5.04	1.48	1.33
21	A	614	EDO	C2-C1	5.04	1.83	1.48
20	C	308	PGV	O03-C19	5.02	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	O	302	PSC	O03-C19	4.95	1.47	1.33
19	Y	101	TGL	OG1-CA1	4.90	1.47	1.33
19	N	610	TGL	OG1-CA1	4.88	1.47	1.33
28	G	104	PEK	O01-C1	4.84	1.48	1.34
25	P	308	DMU	O16-C6	4.82	1.48	1.40
20	M	101	PGV	O01-C1	4.78	1.47	1.34
27	G	102	CDL	OA8-CA7	4.77	1.47	1.33
28	P	309	PEK	O03-C21	4.77	1.47	1.33
19	N	610	TGL	OG2-CB1	4.70	1.47	1.34
20	P	302	PGV	O01-C1	4.63	1.47	1.34
19	L	101	TGL	OG1-CA1	4.57	1.46	1.33
19	Q	201	TGL	OG1-CA1	4.54	1.46	1.33
20	N	608	PGV	O01-C1	4.53	1.47	1.34
19	N	610	TGL	OG3-CC1	4.52	1.46	1.33
14	A	602[B]	HEA	CHC-C4B	4.52	1.46	1.35
28	C	307	PEK	O03-C21	4.48	1.46	1.33
27	C	305	CDL	OA6-CA5	4.44	1.46	1.34
20	P	302	PGV	O03-C19	4.36	1.46	1.33
27	T	103	CDL	OA6-CA5	4.33	1.46	1.34
19	L	101	TGL	OG2-CB1	4.31	1.46	1.34
19	Q	201	TGL	OG3-CC1	4.31	1.45	1.33
24	T	101	CHD	C8-C7	4.30	1.60	1.53
25	C	310	DMU	O16-C6	4.23	1.47	1.40
23	B	302	PSC	O03-C19	4.18	1.45	1.33
14	A	602[A]	HEA	C4D-C3D	-4.15	1.37	1.45
27	C	305	CDL	PB2-OB3	4.14	1.65	1.50
27	C	305	CDL	OB6-CB5	4.12	1.45	1.34
27	P	306	CDL	OB6-CB5	4.12	1.45	1.34
27	G	102	CDL	OA6-CA5	4.10	1.45	1.34
19	L	101	TGL	OG3-CC1	4.08	1.45	1.33
14	N	602[B]	HEA	C1D-ND	-4.03	1.33	1.40
23	B	302	PSC	C13-C12	4.03	1.55	1.31
24	T	101	CHD	C19-C10	3.97	1.61	1.54
20	M	101	PGV	O02-C1	3.96	1.34	1.22
23	O	302	PSC	C13-C12	3.94	1.54	1.31
14	N	602[A]	HEA	CHC-C4B	3.93	1.45	1.35
19	A	608	TGL	OG2-CB1	3.91	1.45	1.34
24	G	103	CHD	C4-C5	3.88	1.60	1.53
14	N	601	HEA	O11-C11	3.79	1.51	1.42
14	A	602[A]	HEA	CHC-C4B	3.78	1.44	1.35
14	N	602[A]	HEA	O11-C11	3.78	1.51	1.42
14	N	601	HEA	CHD-C1D	3.75	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	306	CDL	PB2-OB3	3.69	1.64	1.50
14	A	602[B]	HEA	CHD-C1D	3.68	1.44	1.35
14	A	602[A]	HEA	CHD-C1D	3.64	1.44	1.35
14	A	601	HEA	CHD-C1D	3.63	1.44	1.35
14	N	602[B]	HEA	CHC-C4B	3.60	1.44	1.35
28	P	304	PEK	P-O14	3.56	1.63	1.50
24	P	301	CHD	C8-C7	3.50	1.59	1.53
28	G	101	PEK	O03-C21	3.47	1.43	1.33
23	B	302	PSC	C2-C1	3.46	1.60	1.50
19	D	201	TGL	OG3-CC1	3.44	1.43	1.33
14	A	601	HEA	C3A-C2A	-3.44	1.35	1.40
14	N	601	HEA	C3C-C2C	-3.43	1.35	1.40
19	A	608	TGL	OG2-CG2	3.42	1.55	1.46
14	N	601	HEA	CMD-C2D	3.39	1.58	1.50
27	C	305	CDL	C59-C58	-3.36	1.32	1.51
14	A	601	HEA	C12-C11	-3.36	1.47	1.52
25	P	311	DMU	O16-C6	3.36	1.45	1.40
14	A	601	HEA	CHC-C4B	3.31	1.43	1.35
14	N	602[A]	HEA	C4D-C3D	-3.31	1.39	1.45
19	A	608	TGL	OC1-CC1	-3.31	1.12	1.22
14	N	601	HEA	CHC-C4B	3.27	1.43	1.35
24	T	101	CHD	C1-C2	3.26	1.60	1.53
14	N	602[B]	HEA	FE-NB	3.24	2.12	1.96
20	P	305	PGV	C01-C02	3.24	1.60	1.50
28	G	101	PEK	O01-C1	3.23	1.43	1.34
14	N	602[B]	HEA	FE-ND	3.23	2.12	1.96
25	Z	101	DMU	O16-C6	3.22	1.45	1.40
27	C	305	CDL	C79-C78	-3.21	1.33	1.51
14	A	601	HEA	C4B-C3B	-3.18	1.39	1.44
27	P	306	CDL	PA1-OA5	3.17	1.72	1.59
24	P	307	CHD	C20-C17	3.17	1.59	1.54
27	G	102	CDL	C59-C58	-3.15	1.33	1.51
14	N	602[A]	HEA	CHD-C1D	3.15	1.43	1.35
27	T	103	CDL	C59-C58	-3.14	1.34	1.51
20	N	609	PGV	O03-C01	3.13	1.52	1.45
14	N	601	HEA	CMC-C2C	3.10	1.58	1.51
27	P	306	CDL	C22-C21	-3.09	1.34	1.51
19	A	608	TGL	OG3-CC1	3.09	1.42	1.33
24	C	301	CHD	C8-C7	3.07	1.58	1.53
14	N	601	HEA	C12-C11	-3.05	1.47	1.52
24	T	101	CHD	C4-C3	3.04	1.57	1.51
24	T	101	CHD	C18-C13	3.04	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C12-C13	3.03	1.63	1.53
24	P	301	CHD	C23-C24	3.02	1.57	1.50
14	N	602[A]	HEA	C4B-NB	-3.00	1.35	1.40
27	P	306	CDL	C19-C18	-2.99	1.34	1.51
27	C	305	CDL	C82-C81	-2.97	1.34	1.51
27	T	103	CDL	C62-C61	-2.94	1.35	1.51
27	C	305	CDL	C62-C61	-2.93	1.35	1.51
14	A	601	HEA	CBD-CAD	2.91	1.61	1.52
14	A	601	HEA	O11-C11	2.91	1.49	1.42
27	G	102	CDL	C22-C21	-2.90	1.35	1.51
27	C	305	CDL	C22-C21	-2.90	1.35	1.51
27	T	103	CDL	C79-C78	-2.88	1.35	1.51
27	G	102	CDL	C62-C61	-2.88	1.35	1.51
24	G	103	CHD	C8-C7	2.87	1.58	1.53
27	C	305	CDL	C19-C18	-2.87	1.35	1.51
24	T	101	CHD	C20-C17	2.86	1.59	1.54
25	C	309	DMU	O16-C6	2.86	1.45	1.40
27	P	306	CDL	C39-C38	-2.85	1.35	1.51
24	T	101	CHD	C11-C9	2.85	1.58	1.53
14	A	601	HEA	C1D-ND	-2.84	1.35	1.40
14	N	602[A]	HEA	C4B-C3B	-2.84	1.39	1.44
14	N	602[B]	HEA	C4B-C3B	-2.84	1.39	1.44
27	P	306	CDL	C59-C58	-2.84	1.35	1.51
24	P	301	CHD	C11-C9	2.83	1.58	1.53
24	G	103	CHD	O7-C7	2.82	1.49	1.43
27	P	306	CDL	C79-C78	-2.82	1.35	1.51
14	A	602[A]	HEA	C4B-C3B	-2.82	1.39	1.44
14	N	601	HEA	C1B-C2B	-2.81	1.39	1.44
27	P	306	CDL	C62-C61	-2.80	1.35	1.51
20	A	609	PGV	O01-C1	2.80	1.42	1.34
27	G	102	CDL	C82-C81	-2.79	1.35	1.51
14	A	602[B]	HEA	C1B-NB	-2.77	1.33	1.38
24	P	307	CHD	C8-C9	2.77	1.59	1.53
14	N	602[B]	HEA	CHD-C1D	2.77	1.42	1.35
27	P	306	CDL	O1-C1	2.77	1.51	1.43
14	N	602[B]	HEA	C4B-NB	-2.76	1.35	1.40
27	G	102	CDL	C42-C41	-2.75	1.36	1.51
20	P	305	PGV	O05-C05	2.75	1.51	1.43
14	A	602[B]	HEA	FE-ND	2.75	2.10	1.96
27	G	102	CDL	C19-C18	-2.75	1.36	1.51
27	C	305	CDL	O1-C1	2.73	1.51	1.43
20	P	305	PGV	O01-C02	-2.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	102	CDL	C79-C78	-2.71	1.36	1.51
14	N	602[B]	HEA	C1B-C2B	-2.71	1.39	1.44
27	T	103	CDL	C39-C38	-2.69	1.36	1.51
27	P	306	CDL	CB2-C1	2.68	1.60	1.51
27	G	102	CDL	C39-C38	-2.68	1.36	1.51
14	A	602[A]	HEA	C1D-C2D	-2.67	1.39	1.44
24	P	301	CHD	C11-C12	2.66	1.57	1.53
27	P	306	CDL	C42-C41	-2.66	1.36	1.51
14	A	602[B]	HEA	C4D-ND	-2.66	1.33	1.38
27	T	103	CDL	C22-C21	-2.65	1.36	1.51
27	C	305	CDL	C39-C38	-2.65	1.36	1.51
21	N	615	EDO	O2-C2	2.64	1.55	1.42
24	T	101	CHD	O7-C7	2.61	1.48	1.43
14	N	601	HEA	C4B-C3B	-2.59	1.40	1.44
24	T	101	CHD	C2-C3	2.59	1.57	1.51
24	C	301	CHD	C1-C2	2.59	1.58	1.53
27	T	103	CDL	C42-C41	-2.59	1.37	1.51
28	P	304	PEK	O03-C21	2.58	1.40	1.33
27	G	102	CDL	CB3-CB4	2.57	1.58	1.50
27	P	306	CDL	C82-C81	-2.57	1.37	1.51
20	A	609	PGV	C3-C2	2.57	1.61	1.52
24	T	101	CHD	C4-C5	2.57	1.58	1.53
24	C	306	CHD	C4-C3	2.55	1.56	1.51
20	P	305	PGV	O03-C19	2.55	1.40	1.33
27	T	103	CDL	C19-C18	-2.54	1.37	1.51
24	T	101	CHD	C21-C20	2.53	1.59	1.53
24	P	301	CHD	C16-C15	2.53	1.60	1.54
24	C	306	CHD	C20-C17	2.52	1.58	1.54
24	C	301	CHD	C16-C17	2.52	1.59	1.54
14	N	602[B]	HEA	C4D-ND	-2.52	1.33	1.38
27	C	305	CDL	C42-C41	-2.52	1.37	1.51
19	D	201	TGL	OC1-CC1	2.51	1.30	1.22
25	P	310	DMU	O16-C6	2.51	1.44	1.40
28	G	101	PEK	P-O14	2.50	1.59	1.50
27	P	306	CDL	PB2-OB2	2.49	1.69	1.59
27	T	103	CDL	C82-C81	-2.48	1.37	1.51
27	C	305	CDL	CB2-C1	2.48	1.59	1.51
27	P	306	CDL	CA3-CA4	2.47	1.58	1.50
24	P	301	CHD	C6-C7	2.47	1.57	1.52
14	N	601	HEA	CBD-CGD	2.46	1.56	1.50
24	G	103	CHD	C2-C3	2.45	1.57	1.51
24	P	307	CHD	C11-C9	2.45	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[A]	HEA	O11-C11	2.44	1.48	1.42
24	C	301	CHD	C23-C24	2.42	1.56	1.50
20	N	609	PGV	O03-C19	2.42	1.40	1.33
14	A	602[A]	HEA	C18-C19	2.41	1.38	1.33
14	N	601	HEA	C1D-C2D	-2.41	1.39	1.44
24	C	301	CHD	C4-C3	2.40	1.56	1.51
14	A	602[B]	HEA	C4B-C3B	-2.40	1.40	1.44
14	A	602[B]	HEA	C4D-C3D	-2.38	1.40	1.45
14	A	602[B]	HEA	C3A-CMA	2.37	1.51	1.46
14	A	602[A]	HEA	O1D-CGD	2.37	1.30	1.22
14	N	601	HEA	CBA-CGA	2.33	1.56	1.50
24	C	301	CHD	C11-C12	2.33	1.57	1.53
28	P	304	PEK	O01-C1	2.32	1.40	1.34
14	A	601	HEA	CMD-C2D	2.32	1.55	1.50
19	Y	101	TGL	CG3-CG2	2.31	1.57	1.50
24	P	307	CHD	C16-C17	2.29	1.59	1.54
14	A	601	HEA	C16-C17	-2.29	1.46	1.53
14	N	602[A]	HEA	C1B-NB	-2.28	1.34	1.38
14	A	601	HEA	O1A-CGA	2.27	1.29	1.22
24	P	301	CHD	C8-C14	2.27	1.58	1.53
14	A	601	HEA	CMB-C2B	2.26	1.55	1.50
14	A	601	HEA	CMC-C2C	2.26	1.56	1.51
24	C	301	CHD	C2-C3	2.25	1.57	1.51
20	N	609	PGV	C01-C02	2.24	1.57	1.50
24	G	103	CHD	C13-C14	2.24	1.59	1.55
25	C	309	DMU	C8-C9	2.23	1.57	1.53
19	N	610	TGL	OC1-CC1	-2.22	1.15	1.22
14	N	601	HEA	OMA-CMA	2.22	1.29	1.21
14	N	601	HEA	C1C-CHC	2.21	1.47	1.41
14	N	602[A]	HEA	C1C-CHC	2.20	1.47	1.41
28	G	104	PEK	P-O11	2.20	1.68	1.59
14	N	601	HEA	C4D-C3D	-2.19	1.41	1.45
20	C	304	PGV	O03-C19	2.18	1.39	1.33
28	G	104	PEK	C03-C02	2.17	1.57	1.50
28	G	101	PEK	O01-C02	2.16	1.52	1.46
20	N	609	PGV	O06-C06	2.16	1.51	1.42
14	N	602[B]	HEA	O1D-CGD	2.16	1.29	1.22
24	C	306	CHD	C8-C9	2.16	1.58	1.53
24	C	306	CHD	C16-C17	2.15	1.58	1.54
28	C	307	PEK	P-O12	2.14	1.68	1.59
27	G	102	CDL	PB2-OB5	2.13	1.67	1.59
24	G	103	CHD	C18-C13	2.12	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[A]	HEA	C1D-C2D	-2.12	1.40	1.44
27	C	305	CDL	OB6-CB4	-2.12	1.41	1.46
24	P	301	CHD	O26-C24	-2.12	1.23	1.30
28	P	304	PEK	C6-C5	2.11	1.44	1.31
20	C	304	PGV	C03-C02	2.11	1.57	1.50
14	N	602[A]	HEA	C1B-C2B	-2.10	1.40	1.44
27	P	306	CDL	PA1-OA2	2.10	1.67	1.59
24	C	301	CHD	C21-C20	2.10	1.58	1.53
14	N	602[A]	HEA	FE-NB	2.10	2.07	1.96
14	A	602[A]	HEA	C20-C19	2.09	1.55	1.51
27	C	305	CDL	PB2-OB2	2.09	1.67	1.59
27	G	102	CDL	CB6-CB4	2.09	1.57	1.50
14	N	602[A]	HEA	C18-C19	2.09	1.38	1.33
20	M	101	PGV	C01-C02	2.08	1.57	1.50
24	T	101	CHD	C15-C14	2.08	1.58	1.54
14	A	602[A]	HEA	C4B-NB	-2.08	1.36	1.40
24	G	103	CHD	C19-C10	2.08	1.58	1.54
14	N	602[B]	HEA	C18-C19	2.06	1.37	1.33
14	A	601	HEA	CAD-C3D	2.05	1.56	1.51
14	A	602[B]	HEA	FE-NB	2.04	2.06	1.96
14	N	602[B]	HEA	C3D-C2D	2.03	1.41	1.36
28	G	104	PEK	C01-C02	2.03	1.56	1.50
28	G	101	PEK	C05-C04	2.03	1.58	1.50
14	N	601	HEA	C16-C17	-2.02	1.46	1.53
25	C	302	DMU	O5-C6	2.02	1.47	1.41
14	A	602[B]	HEA	C1D-ND	-2.00	1.36	1.40
24	T	101	CHD	O25-C24	2.00	1.28	1.22
28	C	307	PEK	C03-C02	2.00	1.56	1.50

All (575) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	306	CHD	C23-C22-C20	-12.06	92.49	114.52
19	D	201	TGL	OG2-CB1-CB2	-10.38	89.13	111.50
25	C	310	DMU	O16-C6-C1	9.57	123.24	108.30
25	C	309	DMU	C10-O1-C9	-9.15	95.73	113.69
19	D	201	TGL	OG2-CB1-OB1	8.62	144.53	123.70
19	A	608	TGL	OG3-CC1-OC1	-8.61	101.87	123.59
19	A	608	TGL	OG2-CB1-CB2	8.23	129.23	111.50
24	P	307	CHD	C16-C17-C20	8.17	124.79	112.15
24	P	307	CHD	C23-C22-C20	-8.02	99.88	114.52
19	N	610	TGL	OG2-CB1-CB2	7.54	127.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C13-C14-C15	-6.94	110.94	127.66
14	N	601	HEA	C13-C14-C15	-6.92	111.00	127.66
24	P	307	CHD	C6-C7-C8	6.88	118.82	111.48
28	T	102	PEK	O01-C1-C2	6.87	126.31	111.50
25	P	310	DMU	O16-C6-C1	6.82	118.96	108.30
21	A	614	EDO	O1-C1-C2	-6.71	63.62	111.91
25	C	302	DMU	O16-C6-C1	6.65	118.68	108.30
25	C	309	DMU	C10-C5-C7	-6.63	96.20	110.00
25	C	309	DMU	O16-C6-C1	6.59	118.59	108.30
28	G	104	PEK	O01-C1-C2	6.48	125.46	111.50
23	B	302	PSC	O01-C1-C2	6.42	125.34	111.50
24	C	301	CHD	C23-C22-C20	-6.28	103.05	114.52
25	C	309	DMU	O7-C10-C5	6.20	124.17	108.10
25	P	308	DMU	O16-C6-C1	6.15	117.90	108.30
20	P	302	PGV	O03-C19-C20	6.08	131.00	111.91
19	A	608	TGL	OG2-CG2-CG3	5.96	129.98	108.40
24	C	306	CHD	C21-C20-C17	5.95	122.03	112.92
14	A	601	HEA	C13-C12-C11	-5.93	105.44	114.35
14	A	602[A]	HEA	CHA-C4D-ND	5.92	130.86	124.43
27	G	102	CDL	OB6-CB5-C51	5.88	124.18	111.50
25	P	310	DMU	C18-O16-C6	-5.85	104.14	113.84
19	L	101	TGL	CC6-CC5-CC4	-5.82	84.90	114.42
19	Q	201	TGL	OG2-CB1-CB2	-5.81	98.97	111.50
27	C	305	CDL	OA2-PA1-OA3	5.77	131.61	109.07
14	N	602[A]	HEA	CAD-CBD-CGD	-5.74	101.25	113.60
14	A	601	HEA	C3D-C4D-ND	5.74	115.91	110.36
25	P	310	DMU	O7-C10-C5	5.74	122.96	108.10
25	P	310	DMU	O49-C1-C2	-5.74	97.09	110.35
24	C	306	CHD	C6-C7-C8	5.69	117.56	111.48
23	O	302	PSC	O01-C1-C2	5.65	123.68	111.50
24	P	307	CHD	C15-C14-C8	5.64	126.22	118.33
14	A	602[B]	HEA	C27-C19-C20	5.57	124.64	115.27
27	C	305	CDL	OA6-CA5-C11	5.56	123.48	111.50
28	P	309	PEK	O01-C1-C2	5.55	123.47	111.50
24	C	306	CHD	C17-C13-C12	-5.45	112.69	117.67
25	C	310	DMU	C18-O16-C6	5.44	122.86	113.84
20	C	304	PGV	O03-C19-O04	-5.42	109.92	123.59
24	C	301	CHD	C5-C4-C3	-5.39	104.84	112.76
14	N	602[A]	HEA	OMA-CMA-C3A	-5.39	113.17	124.91
14	A	601	HEA	C3C-C4C-NC	5.35	116.13	109.21
20	M	101	PGV	O01-C1-O02	5.34	136.61	123.70
24	C	306	CHD	C16-C17-C20	5.30	120.35	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	101	TGL	OG2-CB1-CB2	5.25	122.82	111.50
19	D	201	TGL	CB3-CB2-CB1	5.24	132.68	113.62
24	P	307	CHD	C14-C13-C12	5.21	112.25	107.40
14	A	601	HEA	CHA-C4D-C3D	-5.19	117.20	124.84
14	A	602[A]	HEA	C13-C12-C11	-5.11	106.68	114.35
24	C	301	CHD	C22-C20-C17	-5.10	99.75	110.28
23	B	302	PSC	O01-C1-O02	-5.10	111.38	123.70
14	N	601	HEA	C4D-CHA-C1A	-5.05	115.90	122.56
24	P	301	CHD	C1-C10-C5	5.04	115.22	107.77
14	N	601	HEA	C2B-C1B-NB	5.01	115.89	109.88
24	P	301	CHD	C22-C20-C17	-5.00	99.95	110.28
27	T	103	CDL	OA6-CA5-C11	5.00	122.27	111.50
25	P	311	DMU	C6-O5-C4	4.99	123.49	113.69
27	P	306	CDL	OA6-CA5-C11	4.99	122.25	111.50
25	C	302	DMU	C10-O1-C9	-4.98	103.91	113.69
14	N	601	HEA	C1D-ND-C4D	-4.96	99.95	105.07
24	C	301	CHD	C5-C6-C7	4.91	119.88	114.46
24	P	301	CHD	C23-C22-C20	-4.91	105.54	114.52
24	C	306	CHD	C15-C14-C8	4.90	125.19	118.33
24	C	301	CHD	C1-C2-C3	-4.81	104.30	110.47
25	P	310	DMU	C10-O1-C9	-4.78	104.31	113.69
24	P	307	CHD	O7-C7-C6	-4.70	98.27	109.94
24	C	306	CHD	C14-C13-C12	4.67	111.75	107.40
19	D	201	TGL	CG1-OG1-CA1	4.60	134.16	117.12
19	A	608	TGL	OG3-CC1-CC2	4.57	126.26	111.91
19	A	608	TGL	CG3-CG2-CG1	-4.57	100.99	111.79
19	Y	101	TGL	CG2-OG2-CB1	4.56	129.02	117.79
14	N	601	HEA	CHA-C4D-C3D	-4.54	118.17	124.84
27	P	306	CDL	OB8-CB7-C71	4.50	126.02	111.91
14	A	602[B]	HEA	CAD-C3D-C2D	4.43	136.12	127.88
24	C	306	CHD	C15-C14-C13	4.42	107.89	103.55
14	N	602[B]	HEA	CMB-C2B-C3B	-4.41	121.93	130.34
20	M	101	PGV	O01-C1-C2	-4.38	102.06	111.50
14	A	601	HEA	C1B-C2B-C3B	-4.38	101.56	106.80
14	A	601	HEA	C2B-C1B-NB	4.38	115.13	109.88
28	P	309	PEK	O03-C21-O04	-4.37	112.55	123.59
19	L	101	TGL	C22-C21-C20	-4.36	92.27	114.42
19	D	201	TGL	OG1-CA1-CA2	4.35	125.57	111.91
20	C	308	PGV	O01-C1-C2	4.35	120.88	111.50
19	N	610	TGL	OG3-CC1-CC2	4.35	125.56	111.91
19	A	608	TGL	CC3-CC2-CC1	4.35	129.43	113.62
14	N	601	HEA	C2D-C1D-ND	4.34	114.98	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	104	PEK	O03-C21-C22	4.33	125.48	111.91
19	A	608	TGL	CG3-OG3-CC1	4.32	133.12	117.12
14	N	602[B]	HEA	CMB-C2B-C1B	4.32	131.62	125.04
20	M	101	PGV	C4-C3-C2	-4.30	97.72	113.19
14	A	602[A]	HEA	C27-C19-C20	4.30	122.50	115.27
20	C	308	PGV	O03-C19-C20	4.27	125.32	111.91
24	P	301	CHD	C21-C20-C22	-4.25	103.70	110.36
28	P	304	PEK	O03-C21-C22	4.24	125.20	111.91
25	P	310	DMU	C10-C5-C7	-4.23	101.18	110.00
28	T	102	PEK	C02-O01-C1	4.23	128.21	117.79
24	C	301	CHD	O3-C3-C2	-4.21	99.45	110.16
14	N	602[A]	HEA	C13-C12-C11	-4.20	108.04	114.35
27	P	306	CDL	OA8-CA6-CA4	4.20	120.65	108.43
14	A	602[B]	HEA	C13-C12-C11	-4.19	108.05	114.35
24	T	101	CHD	C11-C12-C13	4.19	115.54	111.24
19	A	608	TGL	OG2-CB1-OB1	-4.15	113.67	123.70
14	A	602[A]	HEA	CHA-C4D-C3D	-4.15	118.74	124.84
28	C	307	PEK	O01-C1-C2	4.14	120.43	111.50
14	N	601	HEA	OMA-CMA-C3A	-4.14	115.90	124.91
14	N	601	HEA	C3D-C4D-ND	4.10	114.32	110.36
19	N	610	TGL	OG1-CA1-CA2	4.04	124.57	111.91
14	N	602[A]	HEA	CBA-CAA-C2A	-4.03	105.81	112.60
19	D	201	TGL	CG3-OG3-CC1	4.01	131.99	117.12
14	A	602[B]	HEA	CMC-C2C-C1C	-4.01	122.30	128.46
25	C	302	DMU	O16-C18-C19	4.00	123.58	109.56
27	G	102	CDL	OA6-CA5-C11	4.00	120.11	111.50
14	N	601	HEA	C12-C13-C14	3.96	122.70	112.23
20	N	608	PGV	O03-C19-C20	3.96	124.33	111.91
14	N	601	HEA	C25-C23-C24	-3.96	105.87	114.60
14	N	602[A]	HEA	C26-C15-C16	3.95	121.92	115.27
20	M	101	PGV	C3-C2-C1	3.95	128.00	113.62
14	N	601	HEA	C1B-C2B-C3B	-3.95	102.08	106.80
27	T	103	CDL	C83-C82-C81	3.94	134.45	114.42
24	C	301	CHD	C11-C9-C10	-3.93	109.68	113.73
27	T	103	CDL	OA8-CA7-C31	3.92	124.22	111.91
14	A	602[B]	HEA	O11-C11-C12	-3.92	98.47	109.42
27	G	102	CDL	OA8-CA7-C31	3.91	124.19	111.91
20	C	304	PGV	C30-C29-C28	-3.91	94.60	114.42
20	C	308	PGV	O03-C19-O04	-3.90	113.74	123.59
20	N	609	PGV	O03-C19-O04	-3.90	113.74	123.59
27	G	102	CDL	CB4-OB6-CB5	3.90	127.40	117.79
24	C	301	CHD	C11-C12-C13	3.90	115.24	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	610	TGL	CG3-OG3-CC1	3.89	131.53	117.12
25	P	311	DMU	C18-O16-C6	3.88	120.27	113.84
19	N	610	TGL	OG2-CB1-OB1	-3.86	114.37	123.70
24	G	103	CHD	C4-C3-C2	-3.85	105.96	110.55
14	A	602[A]	HEA	CMB-C2B-C1B	3.83	130.87	125.04
24	P	307	CHD	C19-C10-C9	-3.83	105.91	111.18
27	G	102	CDL	CB6-OB8-CB7	3.82	131.28	117.12
19	L	101	TGL	OG3-CC1-OC1	-3.82	113.96	123.59
24	T	101	CHD	O12-C12-C13	-3.81	104.58	111.03
24	C	306	CHD	C5-C6-C7	3.80	118.66	114.46
14	A	601	HEA	CAD-CBD-CGD	-3.76	105.52	113.60
14	N	602[B]	HEA	C3D-C4D-ND	3.75	113.99	110.36
25	P	311	DMU	O16-C6-C1	3.75	114.15	108.30
27	T	103	CDL	OB6-CB5-C51	3.74	119.57	111.50
27	P	306	CDL	OA8-CA7-C31	3.73	123.60	111.91
14	A	602[B]	HEA	CMD-C2D-C1D	-3.72	119.38	125.04
19	Q	201	TGL	CB3-CB2-CB1	3.69	127.02	113.62
25	M	102	DMU	C18-O16-C6	-3.67	107.75	113.84
24	C	306	CHD	C4-C5-C10	3.66	116.55	112.66
28	C	307	PEK	O03-C21-C22	3.66	123.39	111.91
14	A	602[B]	HEA	C3D-C4D-ND	3.65	113.89	110.36
14	N	601	HEA	C16-C15-C14	3.64	128.49	121.12
28	G	101	PEK	C2-C3-C4	-3.64	106.75	113.23
14	N	602[B]	HEA	C4D-CHA-C1A	3.63	127.36	122.56
25	P	308	DMU	O16-C18-C19	3.63	122.29	109.56
20	N	608	PGV	C01-O03-C19	3.62	130.53	117.12
20	N	609	PGV	O03-C19-C20	3.61	123.25	111.91
28	C	307	PEK	O03-C21-O04	-3.61	114.48	123.59
27	C	305	CDL	OB8-CB7-C71	3.60	123.21	111.91
14	A	602[A]	HEA	OMA-CMA-C3A	-3.60	117.06	124.91
14	N	602[B]	HEA	CAA-CBA-CGA	-3.59	103.70	113.76
24	C	306	CHD	C1-C10-C5	3.57	113.05	107.77
24	T	101	CHD	C19-C10-C1	-3.54	102.56	108.26
24	P	307	CHD	C11-C9-C8	3.52	116.03	110.88
14	A	602[B]	HEA	C26-C15-C16	3.52	121.19	115.27
14	A	601	HEA	C4A-CHB-C1B	3.49	127.17	122.56
25	C	310	DMU	O5-C4-C57	3.49	115.11	106.44
14	N	601	HEA	C20-C21-C22	-3.48	100.43	111.88
25	C	302	DMU	C11-C9-C8	3.48	121.16	113.00
24	C	301	CHD	C6-C7-C8	-3.48	107.77	111.48
24	C	301	CHD	C19-C10-C9	-3.48	106.39	111.18
14	A	602[A]	HEA	CAD-C3D-C4D	-3.46	118.62	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C4B-NB-C1B	-3.45	101.51	105.07
14	A	601	HEA	C20-C19-C18	3.44	128.07	121.12
14	A	601	HEA	O2A-CGA-CBA	3.43	125.06	114.03
28	P	304	PEK	C2-C3-C4	3.43	119.35	113.23
20	P	305	PGV	O01-C1-O02	-3.43	115.42	123.70
19	Y	101	TGL	OG3-CG3-CG2	3.42	118.40	108.43
14	N	601	HEA	CHD-C1D-C2D	-3.41	117.28	126.72
24	P	307	CHD	C5-C4-C3	-3.40	107.77	112.76
24	T	101	CHD	C15-C14-C13	-3.37	100.25	103.55
24	C	306	CHD	C13-C17-C20	-3.37	115.48	119.50
24	P	301	CHD	C6-C5-C10	3.36	116.23	112.66
25	M	102	DMU	C22-C19-C18	-3.36	98.58	113.49
14	A	601	HEA	C1D-ND-C4D	-3.34	101.63	105.07
28	P	309	PEK	O03-C21-C22	3.32	122.33	111.91
14	A	602[A]	HEA	CAD-CBD-CGD	-3.32	106.45	113.60
14	N	602[A]	HEA	O2A-CGA-CBA	3.32	124.69	114.03
19	Y	101	TGL	CC4-CC3-CC2	-3.31	101.29	113.19
14	A	602[A]	HEA	C1B-C2B-C3B	-3.31	102.85	106.80
28	C	307	PEK	C02-O01-C1	3.29	125.89	117.79
19	L	101	TGL	C26-C25-C24	-3.28	97.77	114.42
27	T	103	CDL	CB4-OB6-CB5	3.28	125.86	117.79
14	A	602[B]	HEA	CHD-C1D-ND	3.26	128.41	124.38
14	A	602[B]	HEA	C17-C18-C19	-3.26	119.80	127.66
20	P	302	PGV	O01-C1-C2	3.26	118.52	111.50
24	C	306	CHD	C19-C10-C1	-3.26	103.01	108.26
24	C	306	CHD	C11-C9-C8	3.25	115.64	110.88
14	A	602[A]	HEA	C12-C13-C14	-3.25	103.65	112.23
20	N	609	PGV	O01-C1-O02	-3.24	115.86	123.70
14	A	601	HEA	C17-C18-C19	-3.24	119.85	127.66
14	N	602[A]	HEA	C12-C13-C14	-3.24	103.68	112.23
28	G	104	PEK	C01-O03-C21	3.24	129.11	117.12
19	Y	101	TGL	OG3-CC1-CC2	3.22	122.03	111.91
14	A	602[A]	HEA	CAA-CBA-CGA	-3.22	104.73	113.76
27	P	306	CDL	PA1-OA2-CA2	3.22	140.55	121.68
27	C	305	CDL	PA1-OA2-CA2	3.22	140.54	121.68
25	P	310	DMU	O3-C5-C10	3.21	117.86	110.05
20	P	305	PGV	O03-C01-C02	-3.21	99.08	108.43
14	A	602[B]	HEA	CMD-C2D-C3D	3.20	134.80	126.12
24	C	306	CHD	C22-C23-C24	-3.20	104.02	112.51
14	N	602[B]	HEA	CAD-C3D-C2D	3.20	133.83	127.88
20	A	609	PGV	O03-C19-O04	-3.19	115.53	123.59
27	P	306	CDL	OA2-PA1-OA3	3.19	121.53	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	602[A]	HEA	CAD-C3D-C2D	3.19	133.82	127.88
24	P	307	CHD	C22-C23-C24	-3.19	104.05	112.51
14	A	602[B]	HEA	CMC-C2C-C3C	3.18	130.63	124.68
19	Q	201	TGL	CG2-OG2-CB1	-3.18	109.97	117.79
24	G	103	CHD	C1-C2-C3	-3.17	106.40	110.47
14	N	601	HEA	C4B-NB-C1B	-3.16	101.81	105.07
19	L	101	TGL	CG2-OG2-CB1	3.16	125.56	117.79
14	N	602[B]	HEA	O11-C11-C12	-3.15	100.61	109.42
23	B	302	PSC	O03-C19-C20	3.13	121.74	111.91
19	N	610	TGL	CG3-CG2-CG1	-3.13	104.38	111.79
28	G	101	PEK	C25-C24-C23	-3.12	98.59	114.42
24	C	301	CHD	C9-C11-C12	-3.12	110.18	114.30
28	G	104	PEK	O03-C01-C02	3.10	117.46	108.43
24	T	101	CHD	C16-C17-C20	-3.09	107.37	112.15
14	A	602[A]	HEA	C2B-C1B-NB	3.09	113.58	109.88
24	T	101	CHD	O26-C24-O25	-3.08	115.61	123.30
24	P	307	CHD	C21-C20-C17	3.07	117.62	112.92
28	G	101	PEK	C24-C23-C22	-3.07	102.16	113.19
25	Z	101	DMU	C10-O7-C3	-3.06	110.38	117.96
19	Q	201	TGL	OG2-CB1-OB1	3.06	131.10	123.70
24	P	301	CHD	C14-C13-C12	3.06	110.25	107.40
14	A	601	HEA	C4D-C3D-C2D	-3.05	102.45	106.90
14	A	601	HEA	CMC-C2C-C3C	3.04	130.37	124.68
14	N	602[A]	HEA	C27-C19-C20	3.03	120.38	115.27
24	P	307	CHD	C14-C8-C9	-3.03	105.55	109.71
14	N	602[B]	HEA	C21-C22-C23	-3.03	117.40	127.75
19	D	201	TGL	OG1-CA1-OA1	-3.02	115.97	123.59
25	C	309	DMU	O5-C4-C57	3.02	113.94	106.44
24	P	307	CHD	O25-C24-C23	-3.02	113.39	123.08
14	A	601	HEA	CAA-CBA-CGA	-3.01	105.33	113.76
14	N	602[A]	HEA	C20-C21-C22	-3.00	102.03	111.88
19	N	610	TGL	CB4-CB3-CB2	2.99	123.94	113.19
19	Q	201	TGL	OG1-CA1-CA2	2.99	121.28	111.91
14	A	602[B]	HEA	CMB-C2B-C3B	-2.98	124.66	130.34
20	C	304	PGV	O03-C19-C20	2.97	121.24	111.91
20	M	101	PGV	O03-C19-C20	2.97	121.23	111.91
19	N	610	TGL	OG3-CC1-OC1	-2.97	116.10	123.59
28	T	102	PEK	O03-C21-C22	2.97	121.22	111.91
20	P	302	PGV	O04-C19-C20	-2.97	112.16	123.73
24	P	307	CHD	O3-C3-C4	-2.96	103.95	109.85
27	G	102	CDL	OA8-CA7-OA9	-2.95	116.14	123.59
27	P	306	CDL	CB4-OB6-CB5	-2.95	110.52	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	310	DMU	O49-C1-C6	-2.95	102.88	110.05
25	C	310	DMU	O7-C10-C5	2.94	115.73	108.10
27	C	305	CDL	OA8-CA7-C31	2.94	121.14	111.91
19	Y	101	TGL	CG3-OG3-CC1	2.94	128.00	117.12
24	P	307	CHD	C6-C5-C10	2.93	115.77	112.66
24	C	306	CHD	O7-C7-C6	-2.93	102.67	109.94
25	C	310	DMU	C10-O7-C3	-2.93	110.72	117.96
19	Y	101	TGL	CG1-OG1-CA1	2.93	127.97	117.12
27	C	305	CDL	OA5-PA1-OA3	-2.93	97.64	109.07
14	A	601	HEA	C2D-C1D-ND	2.92	113.30	109.84
24	T	101	CHD	O26-C24-C23	2.92	123.41	114.03
24	G	103	CHD	C16-C17-C13	-2.92	100.69	103.55
23	B	302	PSC	O03-C19-O04	-2.92	116.23	123.59
14	A	601	HEA	CAD-C3D-C4D	2.92	129.76	124.66
19	A	608	TGL	OG3-CG3-CG2	2.92	116.92	108.43
14	A	602[B]	HEA	CAD-C3D-C4D	-2.92	119.56	124.66
24	G	103	CHD	C11-C12-C13	2.91	114.24	111.24
25	C	309	DMU	O55-C2-C1	2.91	117.08	110.35
24	C	301	CHD	C16-C17-C20	-2.91	107.64	112.15
25	C	309	DMU	C7-C8-C9	2.90	115.41	110.24
19	L	101	TGL	OG3-CC1-CC2	2.90	121.00	111.91
24	P	307	CHD	C15-C14-C13	2.89	106.39	103.55
24	G	103	CHD	C19-C10-C1	-2.89	103.61	108.26
24	G	103	CHD	C6-C5-C4	-2.88	107.88	111.19
19	Q	201	TGL	OG3-CC1-CC2	2.87	120.92	111.91
14	N	602[B]	HEA	OMA-CMA-C3A	-2.87	118.66	124.91
24	T	101	CHD	C22-C23-C24	-2.86	104.91	112.51
27	P	306	CDL	OB8-CB7-OB9	-2.86	116.37	123.59
24	G	103	CHD	C23-C22-C20	-2.86	109.29	114.52
20	P	302	PGV	O03-C01-C02	2.86	116.76	108.43
14	A	601	HEA	OMA-CMA-C3A	-2.86	118.69	124.91
14	N	602[A]	HEA	C17-C18-C19	2.85	134.53	127.66
24	P	307	CHD	C18-C13-C12	-2.84	106.17	109.07
24	T	101	CHD	C5-C4-C3	-2.84	108.59	112.76
24	P	301	CHD	C4-C5-C10	-2.83	109.65	112.66
25	Z	101	DMU	O49-C1-C2	-2.83	103.80	110.35
19	Q	201	TGL	OG3-CC1-OC1	-2.82	116.46	123.59
24	P	307	CHD	C10-C9-C8	2.81	114.84	111.82
25	P	310	DMU	O5-C6-O16	-2.81	103.33	109.97
20	P	305	PGV	C03-C02-C01	-2.80	105.16	111.79
27	G	102	CDL	C23-C22-C21	2.79	128.57	114.42
14	N	601	HEA	O2A-CGA-CBA	2.79	122.98	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	101	CHD	O3-C3-C4	-2.79	104.31	109.85
24	C	306	CHD	O26-C24-O25	2.78	130.24	123.30
27	T	103	CDL	CB6-OB8-CB7	2.77	127.38	117.12
24	G	103	CHD	C9-C11-C12	2.76	117.95	114.30
28	P	304	PEK	O03-C21-O04	-2.76	116.63	123.59
24	P	301	CHD	C5-C6-C7	2.76	117.50	114.46
24	G	103	CHD	O12-C12-C11	-2.76	103.51	109.12
24	P	307	CHD	C17-C13-C12	-2.74	115.17	117.67
14	N	602[B]	HEA	C25-C23-C24	2.73	120.64	114.60
20	P	305	PGV	C27-C26-C25	-2.73	100.58	114.42
20	N	608	PGV	O01-C02-C01	2.73	118.28	108.40
27	P	306	CDL	C56-C55-C54	2.73	128.27	114.42
14	A	601	HEA	C4D-CHA-C1A	-2.73	118.96	122.56
24	T	101	CHD	O7-C7-C6	2.73	116.70	109.94
27	C	305	CDL	C42-C41-C40	2.73	128.26	114.42
28	G	104	PEK	O01-C1-O02	-2.71	117.15	123.70
27	P	306	CDL	C83-C82-C81	2.70	128.13	114.42
24	P	307	CHD	C1-C10-C5	2.69	111.75	107.77
28	P	304	PEK	C24-C23-C22	-2.69	103.51	113.19
14	A	602[B]	HEA	CHB-C1B-NB	2.69	127.35	124.43
14	A	601	HEA	CHD-C1D-C2D	-2.68	119.30	126.72
25	M	102	DMU	C6-C1-C2	-2.68	104.41	110.00
20	P	302	PGV	O03-C19-O04	-2.68	116.83	123.59
14	A	602[A]	HEA	C26-C15-C16	2.67	119.76	115.27
27	C	305	CDL	CB6-CB4-CB3	-2.67	105.48	111.79
27	T	103	CDL	OB8-CB7-C71	2.67	120.27	111.91
14	A	601	HEA	CMC-C2C-C1C	-2.66	124.37	128.46
19	Q	201	TGL	OG1-CA1-OA1	-2.66	116.88	123.59
28	T	102	PEK	C01-O03-C21	2.66	126.96	117.12
20	A	609	PGV	O03-C19-C20	2.65	120.23	111.91
14	N	601	HEA	CHD-C1D-ND	2.65	127.66	124.38
14	N	602[A]	HEA	CHA-C4D-C3D	-2.64	120.96	124.84
14	N	601	HEA	CHA-C4D-ND	2.64	127.30	124.43
14	N	602[B]	HEA	C17-C16-C15	-2.63	104.31	112.98
27	C	305	CDL	C78-C77-C76	-2.63	101.07	114.42
19	Y	101	TGL	OG1-CA1-CA2	2.62	120.14	111.91
20	A	609	PGV	C30-C29-C28	2.62	127.73	114.42
24	P	301	CHD	C6-C5-C4	-2.62	108.17	111.19
27	C	305	CDL	OB2-PB2-OB3	2.61	119.28	109.07
27	T	103	CDL	C43-C42-C41	2.61	127.68	114.42
19	A	608	TGL	OG1-CA1-CA2	2.61	120.09	111.91
23	O	302	PSC	O01-C1-O02	-2.61	117.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	310	DMU	C6-C1-C2	2.60	115.41	110.00
27	G	102	CDL	OB7-CB5-C51	-2.59	113.61	123.73
27	G	102	CDL	O1-C1-CA2	-2.59	100.47	109.56
27	T	103	CDL	OB8-CB6-CB4	2.59	115.97	108.43
24	T	101	CHD	C2-C1-C10	-2.59	108.34	112.78
25	C	309	DMU	O7-C10-O1	2.59	117.90	110.67
25	C	309	DMU	O5-C6-O16	-2.58	103.85	109.97
20	C	304	PGV	C4-C3-C2	-2.58	103.92	113.19
20	P	305	PGV	C22-C21-C20	-2.58	103.92	113.19
19	L	101	TGL	CA4-CA3-CA2	-2.58	103.93	113.19
19	L	101	TGL	CA7-CA6-CA5	-2.58	101.35	114.42
14	N	602[B]	HEA	CBA-CAA-C2A	-2.57	108.27	112.60
19	Y	101	TGL	OG2-CB1-OB1	-2.57	117.49	123.70
20	N	608	PGV	C6-C5-C4	-2.57	101.40	114.42
24	G	103	CHD	C18-C13-C12	2.55	111.67	109.07
27	P	306	CDL	OA6-CA5-OA7	-2.55	117.53	123.70
27	C	305	CDL	C39-C38-C37	2.55	127.36	114.42
14	N	601	HEA	CAD-C3D-C4D	2.55	129.11	124.66
24	G	103	CHD	C22-C20-C17	2.54	115.54	110.28
19	Q	201	TGL	OG3-CG3-CG2	2.54	115.83	108.43
14	N	601	HEA	C17-C18-C19	-2.54	121.55	127.66
25	P	311	DMU	O1-C9-C11	2.54	112.75	106.44
19	N	610	TGL	OG2-CG2-CG3	2.54	117.59	108.40
27	C	305	CDL	CA6-OA8-CA7	2.53	126.50	117.12
19	D	201	TGL	CG3-CG2-CG1	2.53	117.76	111.79
24	P	301	CHD	O26-C24-O25	-2.53	117.00	123.30
14	N	601	HEA	C24-C23-C22	2.53	129.95	122.65
24	C	306	CHD	C4-C3-C2	2.52	113.57	110.55
27	P	306	CDL	OB6-CB5-C51	2.52	116.94	111.50
19	D	201	TGL	CA3-CA2-CA1	2.52	122.79	113.62
27	P	306	CDL	OB2-PB2-OB3	2.52	118.90	109.07
25	C	310	DMU	O1-C9-C11	2.52	112.69	106.44
25	P	310	DMU	O5-C4-C57	2.52	112.69	106.44
28	G	101	PEK	C02-O01-C1	-2.51	111.60	117.79
24	P	307	CHD	C19-C10-C1	-2.51	104.22	108.26
14	A	601	HEA	CBD-CAD-C3D	-2.51	105.67	112.63
24	T	101	CHD	C6-C5-C10	-2.50	110.00	112.66
23	B	302	PSC	C4-C3-C2	2.50	122.17	113.19
20	C	308	PGV	O03-C01-C02	2.50	115.71	108.43
14	N	602[B]	HEA	C24-C23-C22	-2.49	115.44	122.65
25	Z	101	DMU	C6-O5-C4	2.48	118.56	113.69
25	P	311	DMU	O5-C4-C3	2.48	114.98	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C27-C19-C18	-2.47	117.35	123.68
27	G	102	CDL	OB8-CB7-C71	2.47	119.65	111.91
25	Z	101	DMU	C11-C9-C8	2.46	118.77	113.00
20	C	304	PGV	C28-C27-C26	-2.46	101.94	114.42
14	N	602[B]	HEA	C4D-C3D-C2D	-2.45	103.32	106.90
14	A	602[B]	HEA	O2A-CGA-CBA	2.45	121.92	114.03
19	D	201	TGL	CC3-CC2-CC1	-2.45	104.71	113.62
19	D	201	TGL	OG3-CC1-OC1	-2.45	117.42	123.59
19	N	610	TGL	OG1-CA1-OA1	-2.44	117.42	123.59
24	P	301	CHD	C14-C8-C7	-2.44	108.57	111.81
25	Z	101	DMU	C18-O16-C6	-2.44	109.80	113.84
14	N	601	HEA	O1A-CGA-CBA	-2.43	115.26	123.08
24	T	101	CHD	C23-C22-C20	-2.43	110.08	114.52
27	T	103	CDL	OA8-CA7-OA9	-2.43	117.46	123.59
27	C	305	CDL	OB4-PB2-OB5	-2.42	96.49	107.75
20	M	101	PGV	O03-C01-C02	2.42	115.48	108.43
14	N	601	HEA	CHB-C1B-C2B	-2.42	121.20	124.98
21	H	101	EDO	O1-C1-C2	-2.42	94.53	111.91
28	P	309	PEK	O01-C1-O02	-2.41	117.87	123.70
27	T	103	CDL	C80-C79-C78	2.41	126.67	114.42
28	G	101	PEK	O04-C21-C22	2.41	133.13	123.73
28	G	101	PEK	C33-C32-C31	-2.41	102.21	114.42
14	A	602[A]	HEA	CMD-C2D-C1D	2.40	128.70	125.04
28	C	307	PEK	O01-C02-C03	2.40	117.10	108.40
25	M	102	DMU	O49-C1-C6	-2.40	104.22	110.05
14	A	602[B]	HEA	O1A-CGA-CBA	-2.40	115.38	123.08
20	N	609	PGV	O02-C1-C2	2.40	133.09	123.73
14	N	601	HEA	C26-C15-C16	-2.39	111.25	115.27
14	N	602[A]	HEA	CHB-C1B-C2B	-2.39	121.25	124.98
25	M	102	DMU	C28-C25-C22	-2.38	102.32	114.42
14	N	601	HEA	O2D-CGD-CBD	2.38	121.69	114.03
28	P	304	PEK	O01-C02-C03	-2.38	99.78	108.40
14	N	602[A]	HEA	CHD-C1D-ND	2.38	127.32	124.38
20	C	304	PGV	O14-P-O13	2.38	123.99	112.24
27	T	103	CDL	OA6-CA5-OA7	-2.38	117.96	123.70
20	P	305	PGV	O01-C1-C2	2.37	116.61	111.50
20	P	302	PGV	C21-C20-C19	-2.37	105.00	113.62
20	C	308	PGV	C25-C24-C23	2.37	126.46	114.42
24	P	301	CHD	C16-C17-C20	-2.37	108.48	112.15
27	P	306	CDL	C57-C56-C55	-2.36	102.42	114.42
25	P	310	DMU	O7-C3-C4	-2.36	102.99	109.45
14	A	602[B]	HEA	C20-C19-C18	-2.36	116.35	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T	102	PEK	O01-C1-O02	-2.35	118.02	123.70
14	A	602[A]	HEA	C13-C14-C15	-2.35	122.01	127.66
14	A	601	HEA	C20-C21-C22	-2.35	104.17	111.88
27	T	103	CDL	C19-C18-C17	2.35	126.33	114.42
14	N	602[A]	HEA	CAA-CBA-CGA	-2.34	107.19	113.76
14	N	601	HEA	C27-C19-C18	-2.33	117.71	123.68
19	L	101	TGL	CB7-CB6-CB5	-2.32	102.63	114.42
14	A	601	HEA	C4B-C3B-C2B	2.32	111.37	107.41
20	A	609	PGV	C34-C33-C32	-2.32	95.84	113.42
19	A	608	TGL	CG1-OG1-CA1	2.31	125.69	117.12
25	C	302	DMU	O1-C9-C11	2.31	112.18	106.44
24	G	103	CHD	C5-C6-C7	2.31	117.01	114.46
27	G	102	CDL	C82-C81-C80	2.31	126.15	114.42
14	N	602[A]	HEA	C25-C23-C24	2.30	119.69	114.60
14	N	602[A]	HEA	O1A-CGA-CBA	-2.30	115.69	123.08
21	P	312	EDO	O2-C2-C1	2.30	128.45	111.91
19	L	101	TGL	CG3-CG2-CG1	-2.30	106.35	111.79
25	P	311	DMU	C11-C9-C8	-2.29	107.64	113.00
24	C	301	CHD	C4-C5-C10	-2.29	110.23	112.66
24	G	103	CHD	C15-C16-C17	2.29	109.66	105.13
14	N	602[A]	HEA	C3D-C4D-ND	2.28	112.57	110.36
27	G	102	CDL	C80-C79-C78	2.28	126.00	114.42
24	T	101	CHD	C1-C2-C3	-2.27	107.55	110.47
24	P	301	CHD	C10-C9-C8	-2.27	109.39	111.82
20	P	302	PGV	O06-C06-C05	2.26	121.04	110.20
14	N	602[A]	HEA	C1B-C2B-C3B	-2.26	104.10	106.80
20	M	101	PGV	C21-C20-C19	2.26	121.82	113.62
27	G	102	CDL	C39-C38-C37	2.26	125.88	114.42
24	T	101	CHD	C13-C14-C8	-2.25	111.86	114.74
19	L	101	TGL	OG2-CB1-CB2	2.25	116.36	111.50
14	A	601	HEA	C16-C15-C14	2.25	125.67	121.12
19	L	101	TGL	C23-C22-C21	-2.25	103.00	114.42
28	T	102	PEK	O03-C01-C02	2.25	114.98	108.43
20	C	304	PGV	C23-C22-C21	2.25	125.84	114.42
27	P	306	CDL	C54-C53-C52	-2.24	103.08	114.42
14	A	601	HEA	C16-C17-C18	-2.23	104.54	111.88
24	C	301	CHD	C1-C10-C5	2.23	111.06	107.77
14	N	602[B]	HEA	C17-C18-C19	2.22	133.00	127.66
24	P	307	CHD	C5-C6-C7	2.22	116.91	114.46
20	N	608	PGV	C4-C3-C2	-2.21	105.23	113.19
24	P	307	CHD	C13-C17-C20	-2.21	116.85	119.50
20	A	609	PGV	O01-C1-C2	2.21	116.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	305	CDL	C62-C61-C60	2.20	125.62	114.42
27	C	305	CDL	OA6-CA5-OA7	-2.20	118.38	123.70
24	P	307	CHD	C21-C20-C22	-2.20	106.91	110.36
25	P	308	DMU	C6-C1-C2	-2.20	105.41	110.00
27	T	103	CDL	CA6-CA4-CA3	-2.20	106.58	111.79
14	N	601	HEA	C3C-C4C-NC	2.20	112.06	109.21
24	C	301	CHD	C2-C1-C10	2.19	116.54	112.78
27	G	102	CDL	OA6-CA5-OA7	-2.19	118.40	123.70
24	G	103	CHD	C1-C10-C9	2.19	114.80	111.35
28	P	309	PEK	C02-O01-C1	2.19	123.18	117.79
14	A	602[B]	HEA	CHD-C1D-C2D	-2.19	120.67	126.72
14	A	601	HEA	CMB-C2B-C3B	2.19	134.51	130.34
28	P	309	PEK	C03-C02-C01	-2.18	106.62	111.79
14	A	601	HEA	C26-C15-C16	-2.18	111.60	115.27
14	N	602[A]	HEA	C21-C20-C19	2.18	120.15	112.98
27	C	305	CDL	C43-C42-C41	2.17	125.46	114.42
14	A	602[A]	HEA	CMC-C2C-C3C	2.17	128.74	124.68
28	G	101	PEK	O11-P-O14	-2.17	100.58	109.07
24	P	301	CHD	C9-C11-C12	-2.17	111.44	114.30
25	C	309	DMU	O3-C5-C10	2.17	115.32	110.05
27	T	103	CDL	C59-C58-C57	2.17	125.44	114.42
24	P	301	CHD	C17-C13-C12	-2.17	115.69	117.67
19	D	201	TGL	OC1-CC1-CC2	2.16	132.18	123.73
14	N	601	HEA	C21-C22-C23	2.16	135.14	127.75
14	A	602[A]	HEA	C16-C15-C14	-2.16	116.74	121.12
14	A	601	HEA	CHA-C4D-ND	2.16	126.78	124.43
25	C	310	DMU	O2-C8-C9	-2.16	103.94	109.30
14	A	602[A]	HEA	C17-C18-C19	2.15	132.84	127.66
20	P	305	PGV	C3-C2-C1	-2.15	105.81	113.62
25	P	310	DMU	O4-C7-C8	2.15	115.31	110.35
19	N	610	TGL	OG1-CG1-CG2	2.14	114.67	108.43
27	T	103	CDL	C40-C39-C38	2.14	125.29	114.42
24	P	301	CHD	C1-C10-C9	-2.14	107.99	111.35
14	N	602[A]	HEA	C17-C16-C15	2.14	120.01	112.98
24	T	101	CHD	C1-C10-C5	2.14	110.92	107.77
14	A	602[A]	HEA	CMB-C2B-C3B	-2.13	126.27	130.34
24	G	103	CHD	C16-C17-C20	-2.13	108.85	112.15
27	P	306	CDL	C39-C38-C37	2.13	125.23	114.42
14	N	601	HEA	C27-C19-C20	2.13	118.85	115.27
21	S	104	EDO	O1-C1-C2	-2.13	96.61	111.91
14	N	601	HEA	O2D-CGD-O1D	-2.12	118.00	123.30
24	P	307	CHD	O26-C24-O25	2.12	128.59	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[A]	HEA	CAD-C3D-C4D	2.12	128.36	124.66
27	G	102	CDL	CA6-OA8-CA7	2.12	124.96	117.12
19	L	101	TGL	C25-C24-C23	-2.12	103.68	114.42
25	C	310	DMU	O5-C6-O16	2.11	114.98	109.97
21	A	617	EDO	O2-C2-C1	-2.11	96.73	111.91
24	T	101	CHD	C18-C13-C12	-2.11	106.92	109.07
25	C	310	DMU	O16-C18-C19	2.10	116.93	109.56
27	C	305	CDL	C54-C53-C52	-2.10	103.75	114.42
25	C	310	DMU	O6-C11-C9	2.09	118.48	111.29
27	G	102	CDL	C83-C82-C81	2.09	125.04	114.42
27	T	103	CDL	C22-C21-C20	2.09	125.04	114.42
20	C	304	PGV	O01-C1-O02	-2.09	118.65	123.70
19	Y	101	TGL	OC1-CC1-CC2	-2.09	115.59	123.73
20	M	101	PGV	O05-C05-C06	-2.09	99.93	109.12
28	T	102	PEK	O02-C1-C2	-2.08	115.60	123.73
28	C	307	PEK	O01-C02-C01	2.08	115.94	108.40
27	T	103	CDL	CA6-OA8-CA7	2.08	124.83	117.12
28	G	104	PEK	O04-C21-C22	-2.08	115.61	123.73
27	P	306	CDL	C43-C42-C41	2.08	124.98	114.42
20	C	304	PGV	C25-C24-C23	2.08	124.96	114.42
25	C	302	DMU	O49-C1-C2	-2.07	105.55	110.35
28	G	101	PEK	O01-C02-C01	-2.07	100.89	108.40
19	L	101	TGL	CB9-CB8-CB7	-2.07	103.90	114.42
28	G	101	PEK	O03-C01-C02	-2.07	102.40	108.43
24	G	103	CHD	C19-C10-C9	2.07	114.03	111.18
24	P	301	CHD	O3-C3-C2	-2.07	104.90	110.16
21	H	101	EDO	O2-C2-C1	-2.07	97.04	111.91
20	P	302	PGV	O01-C1-O02	-2.06	118.71	123.70
14	A	601	HEA	CHD-C1D-ND	2.06	126.92	124.38
14	A	601	HEA	O2A-CGA-O1A	-2.06	118.17	123.30
27	G	102	CDL	C19-C18-C17	2.06	124.86	114.42
14	N	602[A]	HEA	C4A-CHB-C1B	2.05	125.27	122.56
27	G	102	CDL	C43-C42-C41	2.05	124.85	114.42
20	N	608	PGV	C02-O01-C1	-2.05	112.74	117.79
25	C	302	DMU	O5-C6-O16	2.05	114.83	109.97
23	O	302	PSC	C28-C27-C26	-2.05	104.02	114.42
28	G	101	PEK	O03-C21-O04	-2.04	118.44	123.59
19	L	101	TGL	C20-CA9-CA8	-2.04	104.09	114.42
20	C	304	PGV	C32-C31-C30	-2.04	104.09	114.42
28	C	307	PEK	P-O12-C04	2.03	131.61	121.59
23	O	302	PSC	O03-C01-C02	2.03	114.35	108.43
25	C	309	DMU	O7-C3-C4	-2.02	103.90	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	P	306	CDL	OA5-PA1-OA3	-2.02	101.16	109.07
25	P	311	DMU	C2-C3-C4	2.02	115.57	110.93
27	G	102	CDL	OA2-PA1-OA3	-2.02	101.16	109.07
14	N	602[B]	HEA	C21-C20-C19	2.02	119.63	112.98
24	C	301	CHD	C16-C15-C14	-2.02	101.13	105.13
14	A	602[B]	HEA	CAD-CBD-CGD	-2.02	109.25	113.60
27	C	305	CDL	OA4-PA1-OA3	2.02	122.22	112.24
24	P	301	CHD	C16-C17-C13	2.02	105.53	103.55
14	N	602[A]	HEA	C2B-C1B-NB	2.02	112.30	109.88
21	N	612	EDO	O2-C2-C1	-2.02	97.41	111.91
27	C	305	CDL	C13-C12-C11	-2.01	105.96	113.19
14	A	601	HEA	O1A-CGA-CBA	-2.01	116.62	123.08
19	Y	101	TGL	C26-C25-C24	-2.01	104.22	114.42
23	O	302	PSC	C25-C24-C23	-2.01	104.22	114.42
25	C	309	DMU	O4-C7-C8	2.01	114.99	110.35
25	P	311	DMU	C57-C4-C3	-2.01	107.48	113.33
27	T	103	CDL	C23-C22-C21	2.00	124.60	114.42
25	P	308	DMU	O1-C9-C11	2.00	111.42	106.44
14	A	601	HEA	C3A-C4A-NA	2.00	114.73	110.94

There are no chirality outliers.

All (979) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
19	D	201	TGL	CG2-CG1-OG1-CA1
19	L	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	OA1-CA1-OG1-CG1
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	C	308	PGV	C03-O11-P-O14
20	C	308	PGV	C04-O12-P-O14
20	C	308	PGV	C02-C03-O11-P
20	C	308	PGV	C04-C05-C06-O06
20	M	101	PGV	C04-O12-P-O13
20	M	101	PGV	C02-C01-O03-C19
20	M	101	PGV	C03-C02-O01-C1
20	N	608	PGV	C04-C05-C06-O06
20	N	608	PGV	O02-C1-O01-C02
20	N	608	PGV	C2-C1-O01-C02
20	P	302	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
23	B	302	PSC	C03-O11-P-O13
23	B	302	PSC	O12-C04-C05-N
23	O	302	PSC	C03-O11-P-O12
23	O	302	PSC	C2-C1-O01-C02
23	O	302	PSC	O04-C19-O03-C01
23	O	302	PSC	C20-C19-O03-C01
23	O	302	PSC	C11-C12-C13-C14
24	P	307	CHD	C16-C17-C20-C22
25	C	302	DMU	C1-C6-O16-C18
25	C	302	DMU	O5-C6-O16-C18
25	C	310	DMU	C1-C6-O16-C18
25	C	310	DMU	O5-C6-O16-C18
25	C	310	DMU	C19-C18-O16-C6
25	P	308	DMU	C1-C6-O16-C18
25	P	308	DMU	O5-C6-O16-C18
25	P	311	DMU	O5-C6-O16-C18
27	C	305	CDL	CA2-OA2-PA1-OA4
27	C	305	CDL	CA3-OA5-PA1-OA2
27	C	305	CDL	OA7-CA5-OA6-CA4
27	C	305	CDL	C11-CA5-OA6-CA4
27	C	305	CDL	CB2-OB2-PB2-OB4
27	G	102	CDL	CA3-OA5-PA1-OA3
27	G	102	CDL	C11-CA5-OA6-CA4
27	G	102	CDL	CB2-OB2-PB2-OB3
27	G	102	CDL	OB6-CB4-CB6-OB8
27	P	306	CDL	CB2-C1-CA2-OA2
27	P	306	CDL	CA2-OA2-PA1-OA4
27	P	306	CDL	CB2-OB2-PB2-OB3
27	P	306	CDL	CB2-OB2-PB2-OB4
27	P	306	CDL	CB2-OB2-PB2-OB5
27	P	306	CDL	CB3-OB5-PB2-OB4
27	T	103	CDL	CA2-OA2-PA1-OA5
27	T	103	CDL	CA3-OA5-PA1-OA4
27	T	103	CDL	OA7-CA5-OA6-CA4
27	T	103	CDL	CB3-OB5-PB2-OB2
28	C	307	PEK	C04-O12-P-O11
28	C	307	PEK	C04-O12-P-O13
28	C	307	PEK	C04-O12-P-O14
28	C	307	PEK	C2-C1-O01-C02
28	C	307	PEK	C4-C5-C6-C7
28	C	307	PEK	C10-C11-C12-C13
28	G	104	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
28	G	104	PEK	C03-O11-P-O14
28	G	104	PEK	C04-O12-P-O14
28	G	104	PEK	C05-C04-O12-P
28	G	104	PEK	C4-C5-C6-C7
28	G	104	PEK	C9-C10-C11-C12
28	P	304	PEK	C11-C12-C13-C14
28	P	309	PEK	C03-O11-P-O13
28	P	309	PEK	C2-C1-O01-C02
28	T	102	PEK	C03-O11-P-O13
28	T	102	PEK	C04-O12-P-O14
28	T	102	PEK	O12-C04-C05-N
28	T	102	PEK	O02-C1-O01-C02
28	T	102	PEK	C2-C1-O01-C02
23	B	302	PSC	O04-C19-O03-C01
27	G	102	CDL	OA9-CA7-OA8-CA6
25	P	310	DMU	C5-C10-O7-C3
19	D	201	TGL	CC2-CC1-OG3-CG3
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OC1-CC1-OG3-CG3
19	Q	201	TGL	OC1-CC1-OG3-CG3
20	N	608	PGV	O04-C19-O03-C01
24	P	307	CHD	C16-C17-C20-C21
24	P	307	CHD	C13-C17-C20-C21
25	C	309	DMU	C5-C10-O7-C3
19	L	101	TGL	OB1-CB1-OG2-CG2
23	O	302	PSC	O02-C1-O01-C02
27	C	305	CDL	OB7-CB5-OB6-CB4
27	G	102	CDL	OA7-CA5-OA6-CA4
28	P	309	PEK	O02-C1-O01-C02
25	C	310	DMU	O6-C11-C9-C8
19	A	608	TGL	CC2-CC1-OG3-CG3
19	Q	201	TGL	CC2-CC1-OG3-CG3
20	M	101	PGV	C20-C19-O03-C01
20	N	608	PGV	C20-C19-O03-C01
23	B	302	PSC	C20-C19-O03-C01
27	G	102	CDL	C31-CA7-OA8-CA6
27	T	103	CDL	C11-CA5-OA6-CA4
24	P	307	CHD	C13-C17-C20-C22
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	N	602[B]	HEA	C2D-C3D-CAD-CBD
27	P	306	CDL	C13-C14-C15-C16
28	G	104	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
20	M	101	PGV	C10-C11-C12-C13
28	G	101	PEK	C7-C8-C9-C10
28	G	101	PEK	C10-C11-C12-C13
19	L	101	TGL	CC2-CC3-CC4-CC5
14	N	602[B]	HEA	C4D-C3D-CAD-CBD
28	C	307	PEK	O02-C1-O01-C02
19	D	201	TGL	OA1-CA1-OG1-CG1
28	G	104	PEK	O04-C21-O03-C01
25	C	310	DMU	O5-C4-C57-O61
27	T	103	CDL	C79-C80-C81-C82
19	L	101	TGL	CA2-CA1-OG1-CG1
20	M	101	PGV	O04-C19-O03-C01
25	P	308	DMU	O6-C11-C9-C8
25	P	311	DMU	O6-C11-C9-C8
27	C	305	CDL	C51-CB5-OB6-CB4
27	P	306	CDL	C51-CB5-OB6-CB4
23	B	302	PSC	C19-C20-C21-C22
25	P	308	DMU	O6-C11-C9-O1
27	C	305	CDL	C79-C80-C81-C82
19	N	610	TGL	C22-C23-C24-C25
19	Q	201	TGL	CA9-C20-C21-C22
19	Y	101	TGL	CA2-CA3-CA4-CA5
20	C	304	PGV	C24-C25-C26-C27
20	M	101	PGV	C20-C21-C22-C23
23	B	302	PSC	C21-C22-C23-C24
25	P	310	DMU	C28-C31-C34-C37
25	P	311	DMU	O6-C11-C9-O1
28	C	307	PEK	C1-C2-C3-C4
19	D	201	TGL	C21-C22-C23-C24
23	O	302	PSC	C22-C23-C24-C25
19	D	201	TGL	CA2-CA1-OG1-CG1
25	C	310	DMU	O6-C11-C9-O1
25	P	310	DMU	O6-C11-C9-O1
27	P	306	CDL	OB7-CB5-OB6-CB4
27	P	306	CDL	C81-C82-C83-C84
19	L	101	TGL	OA1-CA1-OG1-CG1
19	A	608	TGL	CA9-C20-C21-C22
28	G	104	PEK	C1-C2-C3-C4
27	T	103	CDL	OA9-CA7-OA8-CA6
19	A	608	TGL	CA2-CA1-OG1-CG1
19	N	610	TGL	CA2-CA1-OG1-CG1
27	T	103	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
25	C	310	DMU	C3-C4-C57-O61
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
25	C	310	DMU	O1-C10-O7-C3
20	C	308	PGV	O12-C04-C05-C06
20	N	608	PGV	O12-C04-C05-C06
27	C	305	CDL	CB2-C1-CA2-OA2
19	A	608	TGL	OB1-CB1-OG2-CG2
19	N	610	TGL	OC1-CC1-OG3-CG3
19	N	610	TGL	CC2-CC1-OG3-CG3
19	Y	101	TGL	CB1-CB2-CB3-CB4
24	C	306	CHD	C17-C20-C22-C23
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
27	G	102	CDL	C58-C59-C60-C61
28	P	309	PEK	C33-C34-C35-C36
25	P	310	DMU	O6-C11-C9-C8
27	P	306	CDL	O1-C1-CB2-OB2
24	C	306	CHD	C21-C20-C22-C23
25	P	311	DMU	C1-C6-O16-C18
25	P	311	DMU	C3-C4-C57-O61
20	N	608	PGV	C19-C20-C21-C22
19	L	101	TGL	C21-C20-CA9-CA8
19	A	608	TGL	CB1-CB2-CB3-CB4
23	O	302	PSC	C11-C10-C9-C8
28	C	307	PEK	C7-C8-C9-C10
20	N	608	PGV	O05-C05-C06-O06
19	A	608	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	CB1-CB2-CB3-CB4
19	N	610	TGL	CA1-CA2-CA3-CA4
28	P	309	PEK	C21-C22-C23-C24
20	N	608	PGV	C02-C03-O11-P
27	C	305	CDL	CA7-C31-C32-C33
27	C	305	CDL	CB5-C51-C52-C53
27	P	306	CDL	CB5-C51-C52-C53
28	G	104	PEK	C21-C22-C23-C24
21	C	319	EDO	O1-C1-C2-O2
27	G	102	CDL	C61-C62-C63-C64
19	Y	101	TGL	CC1-CC2-CC3-CC4
19	A	608	TGL	OA1-CA1-OG1-CG1
25	P	311	DMU	O16-C18-C19-C22
20	N	608	PGV	O12-C04-C05-O05
27	C	305	CDL	O1-C1-CA2-OA2
27	C	305	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
27	P	306	CDL	O1-C1-CA2-OA2
19	N	610	TGL	OA1-CA1-OG1-CG1
20	P	305	PGV	C10-C11-C12-C13
28	P	304	PEK	C7-C8-C9-C10
28	P	304	PEK	C13-C14-C15-C16
28	P	309	PEK	C10-C11-C12-C13
19	A	608	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CA9-C20-C21-C22
27	P	306	CDL	C53-C54-C55-C56
20	C	308	PGV	C03-O11-P-O12
20	C	308	PGV	C04-O12-P-O11
20	M	101	PGV	C03-O11-P-O12
23	B	302	PSC	C03-O11-P-O12
27	C	305	CDL	CA2-OA2-PA1-OA5
27	C	305	CDL	CB2-OB2-PB2-OB5
27	P	306	CDL	CA2-OA2-PA1-OA5
27	T	103	CDL	CA3-OA5-PA1-OA2
28	C	307	PEK	C03-O11-P-O12
28	G	104	PEK	C03-O11-P-O12
28	P	309	PEK	C03-O11-P-O12
28	P	309	PEK	C04-O12-P-O11
28	T	102	PEK	C03-O11-P-O12
27	G	102	CDL	CA5-C11-C12-C13
28	T	102	PEK	C2-C3-C4-C5
20	C	304	PGV	C13-C14-C15-C16
20	C	308	PGV	C23-C24-C25-C26
19	A	608	TGL	CA2-CA3-CA4-CA5
19	A	608	TGL	CB4-CB5-CB6-CB7
19	L	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	C10-C11-C12-C13
20	C	308	PGV	C20-C21-C22-C23
20	C	308	PGV	C28-C29-C30-C31
20	N	608	PGV	C14-C15-C16-C17
20	P	302	PGV	C22-C23-C24-C25
27	C	305	CDL	C63-C64-C65-C66
27	G	102	CDL	C63-C64-C65-C66
27	T	103	CDL	C31-C32-C33-C34
28	G	101	PEK	C26-C27-C28-C29
28	T	102	PEK	C26-C27-C28-C29
19	A	608	TGL	C14-C29-C30-C31
19	N	610	TGL	CA6-CA7-CA8-CA9
19	Q	201	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	C12-C13-C14-C29
19	Q	201	TGL	CC9-C15-C16-C17
23	B	302	PSC	C23-C24-C25-C26
27	C	305	CDL	C40-C41-C42-C43
27	G	102	CDL	C77-C78-C79-C80
27	P	306	CDL	C12-C13-C14-C15
27	P	306	CDL	C16-C17-C18-C19
27	T	103	CDL	C13-C14-C15-C16
20	N	608	PGV	C01-C02-O01-C1
23	B	302	PSC	O02-C1-O01-C02
19	Y	101	TGL	CA1-CA2-CA3-CA4
19	N	610	TGL	CB4-CB5-CB6-CB7
19	N	610	TGL	CB9-C10-C11-C12
20	C	308	PGV	C6-C7-C8-C9
23	B	302	PSC	C2-C3-C4-C5
28	G	104	PEK	C24-C25-C26-C27
28	T	102	PEK	C10-C11-C12-C13
19	L	101	TGL	CA5-CA6-CA7-CA8
19	L	101	TGL	CC7-CC8-CC9-C15
19	N	610	TGL	CC5-CC6-CC7-CC8
20	C	304	PGV	C22-C23-C24-C25
27	P	306	CDL	C82-C83-C84-C85
27	T	103	CDL	C14-C15-C16-C17
27	T	103	CDL	C74-C75-C76-C77
28	G	104	PEK	C33-C34-C35-C36
19	A	608	TGL	C16-C17-C18-C19
19	N	610	TGL	C11-C10-CB9-CB8
20	C	304	PGV	C7-C8-C9-C10
23	O	302	PSC	C5-C6-C7-C8
23	O	302	PSC	C24-C25-C26-C27
27	P	306	CDL	C56-C57-C58-C59
27	T	103	CDL	C20-C21-C22-C23
19	D	201	TGL	CA1-CA2-CA3-CA4
27	T	103	CDL	CA7-C31-C32-C33
19	A	608	TGL	CA4-CA5-CA6-CA7
19	A	608	TGL	C12-C13-C14-C29
19	D	201	TGL	C19-C33-C34-C35
20	C	308	PGV	C13-C14-C15-C16
20	P	302	PGV	C2-C3-C4-C5
27	C	305	CDL	C57-C58-C59-C60
27	C	305	CDL	C75-C76-C77-C78
27	T	103	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	G	104	PEK	C34-C35-C36-C37
19	N	610	TGL	CB7-CB8-CB9-C10
19	N	610	TGL	C13-C14-C29-C30
19	Q	201	TGL	C13-C14-C29-C30
20	M	101	PGV	C14-C15-C16-C17
20	N	608	PGV	C27-C28-C29-C30
27	T	103	CDL	C80-C81-C82-C83
27	P	306	CDL	CB4-CB6-OB8-CB7
19	A	608	TGL	C10-C11-C12-C13
19	D	201	TGL	CC5-CC6-CC7-CC8
19	L	101	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	CA9-C20-C21-C22
20	C	304	PGV	C23-C24-C25-C26
20	M	101	PGV	C13-C14-C15-C16
27	C	305	CDL	C43-C44-C45-C46
27	C	305	CDL	C73-C74-C75-C76
27	G	102	CDL	C11-C12-C13-C14
27	G	102	CDL	C14-C15-C16-C17
27	P	306	CDL	C22-C23-C24-C25
27	T	103	CDL	C81-C82-C83-C84
28	G	101	PEK	C23-C24-C25-C26
19	A	608	TGL	C13-C14-C29-C30
20	C	308	PGV	C14-C15-C16-C17
20	P	302	PGV	C24-C25-C26-C27
27	C	305	CDL	C38-C39-C40-C41
20	M	101	PGV	C04-C05-C06-O06
20	P	302	PGV	C04-C05-C06-O06
19	N	610	TGL	OB1-CB1-OG2-CG2
23	B	302	PSC	C2-C1-O01-C02
19	Y	101	TGL	CC3-CC4-CC5-CC6
25	M	102	DMU	C19-C22-C25-C28
25	P	310	DMU	C19-C22-C25-C28
27	P	306	CDL	C73-C74-C75-C76
28	G	101	PEK	C16-C17-C18-C19
19	Q	201	TGL	C22-C23-C24-C25
19	Y	101	TGL	C11-C12-C13-C14
23	B	302	PSC	C5-C6-C7-C8
27	C	305	CDL	C12-C13-C14-C15
27	C	305	CDL	C58-C59-C60-C61
27	G	102	CDL	C60-C61-C62-C63
27	P	306	CDL	C31-C32-C33-C34
28	C	307	PEK	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	C16-C15-CC9-CC8
19	A	608	TGL	C20-C21-C22-C23
19	D	201	TGL	CC6-CC7-CC8-CC9
19	L	101	TGL	C12-C13-C14-C29
19	Q	201	TGL	CA4-CA5-CA6-CA7
20	N	608	PGV	C3-C4-C5-C6
20	P	305	PGV	C7-C8-C9-C10
27	T	103	CDL	C52-C53-C54-C55
27	T	103	CDL	C73-C74-C75-C76
19	Q	201	TGL	CA2-CA3-CA4-CA5
19	Q	201	TGL	CC5-CC6-CC7-CC8
19	Y	101	TGL	CB4-CB5-CB6-CB7
20	C	308	PGV	C21-C22-C23-C24
27	G	102	CDL	C55-C56-C57-C58
19	N	610	TGL	CB1-CB2-CB3-CB4
19	Y	101	TGL	C23-C24-C25-C26
27	C	305	CDL	C23-C24-C25-C26
27	G	102	CDL	C13-C14-C15-C16
27	T	103	CDL	C11-C12-C13-C14
19	Q	201	TGL	C23-C24-C25-C26
27	T	103	CDL	C33-C34-C35-C36
27	T	103	CDL	C71-C72-C73-C74
19	N	610	TGL	CC6-CC7-CC8-CC9
19	L	101	TGL	C11-C12-C13-C14
19	N	610	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	CA6-CA7-CA8-CA9
23	B	302	PSC	C3-C4-C5-C6
27	T	103	CDL	CB3-CB4-CB6-OB8
23	B	302	PSC	C11-C10-C9-C8
19	A	608	TGL	CA6-CA7-CA8-CA9
19	N	610	TGL	CA7-CA8-CA9-C20
27	T	103	CDL	C59-C60-C61-C62
20	C	304	PGV	C19-C20-C21-C22
19	A	608	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CC4-CC5-CC6-CC7
20	C	308	PGV	C3-C4-C5-C6
19	Q	201	TGL	C11-C10-CB9-CB8
23	O	302	PSC	C23-C24-C25-C26
19	Y	101	TGL	CB2-CB3-CB4-CB5
23	O	302	PSC	C3-C4-C5-C6
27	P	306	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
28	C	307	PEK	C26-C27-C28-C29
28	G	101	PEK	C15-C16-C17-C18
28	P	309	PEK	C15-C16-C17-C18
20	C	308	PGV	O12-C04-C05-O05
23	O	302	PSC	C2-C3-C4-C5
27	G	102	CDL	C81-C82-C83-C84
19	Y	101	TGL	C20-C21-C22-C23
27	P	306	CDL	C80-C81-C82-C83
19	Y	101	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	C21-C22-C23-C24
19	L	101	TGL	C18-C19-C33-C34
25	C	309	DMU	O16-C18-C19-C22
19	Q	201	TGL	CB1-CB2-CB3-CB4
21	A	610	EDO	O1-C1-C2-O2
21	A	614	EDO	O1-C1-C2-O2
21	A	616	EDO	O1-C1-C2-O2
21	A	619	EDO	O1-C1-C2-O2
21	C	317	EDO	O1-C1-C2-O2
21	C	318	EDO	O1-C1-C2-O2
21	D	203	EDO	O1-C1-C2-O2
21	D	206	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
21	G	105	EDO	O1-C1-C2-O2
21	N	611	EDO	O1-C1-C2-O2
21	O	304	EDO	O1-C1-C2-O2
21	P	312	EDO	O1-C1-C2-O2
21	R	201	EDO	O1-C1-C2-O2
21	V	101	EDO	O1-C1-C2-O2
25	P	311	DMU	O5-C4-C57-O61
19	A	608	TGL	C23-C24-C25-C26
19	D	201	TGL	C11-C10-CB9-CB8
27	G	102	CDL	C59-C60-C61-C62
27	P	306	CDL	C21-C22-C23-C24
27	P	306	CDL	C38-C39-C40-C41
20	C	308	PGV	C20-C19-O03-C01
27	C	305	CDL	C31-CA7-OA8-CA6
20	C	308	PGV	C5-C6-C7-C8
27	G	102	CDL	C21-C22-C23-C24
27	G	102	CDL	C31-C32-C33-C34
19	N	610	TGL	CC1-CC2-CC3-CC4
28	G	104	PEK	C31-C32-C33-C34
28	G	104	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	P	302	PGV	C6-C7-C8-C9
27	G	102	CDL	C73-C74-C75-C76
28	T	102	PEK	C24-C25-C26-C27
20	N	608	PGV	C11-C10-C9-C8
20	P	305	PGV	C12-C13-C14-C15
19	Q	201	TGL	OB1-CB1-OG2-CG2
27	T	103	CDL	C71-CB7-OB8-CB6
28	P	304	PEK	C34-C35-C36-C37
27	C	305	CDL	OA9-CA7-OA8-CA6
20	A	609	PGV	C28-C29-C30-C31
19	Q	201	TGL	C19-C33-C34-C35
25	P	311	DMU	C22-C25-C28-C31
25	C	310	DMU	C18-C19-C22-C25
19	L	101	TGL	C11-C10-CB9-CB8
19	N	610	TGL	CA3-CA4-CA5-CA6
23	O	302	PSC	C29-C30-C31-C32
25	P	311	DMU	C19-C22-C25-C28
27	P	306	CDL	C57-C58-C59-C60
27	T	103	CDL	CB5-C51-C52-C53
19	N	610	TGL	CB2-CB1-OG2-CG2
19	Q	201	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	C20-C21-C22-C23
19	L	101	TGL	CB2-CB3-CB4-CB5
19	Q	201	TGL	C17-C18-C19-C33
28	P	309	PEK	C26-C27-C28-C29
27	T	103	CDL	C40-C41-C42-C43
27	T	103	CDL	C72-C73-C74-C75
27	T	103	CDL	C82-C83-C84-C85
28	T	102	PEK	C22-C23-C24-C25
27	T	103	CDL	OB6-CB4-CB6-OB8
28	P	309	PEK	O03-C01-C02-O01
25	C	302	DMU	O16-C18-C19-C22
19	A	608	TGL	C11-C12-C13-C14
20	C	308	PGV	C12-C13-C14-C15
20	P	305	PGV	C1-C2-C3-C4
19	D	201	TGL	CA6-CA7-CA8-CA9
20	C	308	PGV	O04-C19-O03-C01
27	T	103	CDL	OB9-CB7-OB8-CB6
27	T	103	CDL	OB7-CB5-OB6-CB4
19	A	608	TGL	CA5-CA6-CA7-CA8
27	C	305	CDL	C53-C54-C55-C56
27	G	102	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
28	C	307	PEK	C14-C15-C16-C17
25	P	310	DMU	C18-C19-C22-C25
20	C	304	PGV	C20-C21-C22-C23
27	P	306	CDL	C19-C20-C21-C22
25	C	309	DMU	O6-C11-C9-O1
20	P	302	PGV	C02-C03-O11-P
19	N	610	TGL	C14-C29-C30-C31
27	P	306	CDL	C77-C78-C79-C80
19	A	608	TGL	CC5-CC6-CC7-CC8
20	P	302	PGV	C30-C31-C32-C33
20	P	302	PGV	C3-C4-C5-C6
28	T	102	PEK	C15-C16-C17-C18
19	L	101	TGL	CB1-CB2-CB3-CB4
27	G	102	CDL	C72-C73-C74-C75
28	P	309	PEK	C29-C30-C31-C32
20	P	302	PGV	O12-C04-C05-C06
27	P	306	CDL	CA2-C1-CB2-OB2
27	C	305	CDL	C42-C43-C44-C45
28	T	102	PEK	C30-C31-C32-C33
19	A	608	TGL	CB9-C10-C11-C12
19	D	201	TGL	C10-C11-C12-C13
19	D	201	TGL	C21-C20-CA9-CA8
24	C	306	CHD	C20-C22-C23-C24
19	D	201	TGL	OG1-CG1-CG2-CG3
20	A	609	PGV	C26-C27-C28-C29
27	C	305	CDL	CA3-CA4-CA6-OA8
27	C	305	CDL	CB3-CB4-CB6-OB8
28	G	104	PEK	O03-C01-C02-C03
20	C	304	PGV	C10-C11-C12-C13
28	G	101	PEK	C4-C5-C6-C7
28	P	304	PEK	C4-C5-C6-C7
27	C	305	CDL	C84-C85-C86-C87
28	T	102	PEK	C32-C33-C34-C35
20	P	302	PGV	C31-C32-C33-C34
28	C	307	PEK	C35-C36-C37-C38
28	G	101	PEK	C34-C35-C36-C37
24	P	307	CHD	C21-C20-C22-C23
27	G	102	CDL	CB7-C71-C72-C73
27	G	102	CDL	C56-C57-C58-C59
27	C	305	CDL	C74-C75-C76-C77
20	N	609	PGV	C11-C10-C9-C8
27	C	305	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
27	P	306	CDL	C24-C25-C26-C27
19	Y	101	TGL	C16-C17-C18-C19
19	Y	101	TGL	C29-C30-C31-C32
28	P	309	PEK	C35-C36-C37-C38
25	P	310	DMU	O16-C18-C19-C22
27	C	305	CDL	C80-C81-C82-C83
19	Q	201	TGL	CB5-CB6-CB7-CB8
20	A	609	PGV	C31-C32-C33-C34
25	M	102	DMU	C34-C37-C40-C43
28	P	304	PEK	C26-C27-C28-C29
28	C	307	PEK	C01-C02-O01-C1
19	A	608	TGL	C29-C30-C31-C32
23	O	302	PSC	C31-C32-C33-C34
25	C	302	DMU	C31-C34-C37-C40
27	C	305	CDL	C11-C12-C13-C14
19	N	610	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	CB5-CB6-CB7-CB8
20	M	101	PGV	C31-C32-C33-C34
27	P	306	CDL	C17-C18-C19-C20
19	L	101	TGL	CC2-CC1-OG3-CG3
28	G	104	PEK	O01-C02-C03-O11
20	N	609	PGV	C10-C11-C12-C13
28	C	307	PEK	C13-C14-C15-C16
19	Y	101	TGL	CC4-CC5-CC6-CC7
28	C	307	PEK	C34-C35-C36-C37
21	A	612	EDO	O1-C1-C2-O2
21	C	312	EDO	O1-C1-C2-O2
20	N	609	PGV	C23-C24-C25-C26
25	Z	101	DMU	O16-C18-C19-C22
27	C	305	CDL	C21-C22-C23-C24
27	T	103	CDL	C34-C35-C36-C37
19	D	201	TGL	OG1-CG1-CG2-OG2
19	L	101	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	CC9-C15-C16-C17
25	M	102	DMU	C25-C28-C31-C34
27	C	305	CDL	C76-C77-C78-C79
20	P	305	PGV	C11-C12-C13-C14
19	A	608	TGL	CC4-CC5-CC6-CC7
19	D	201	TGL	C16-C17-C18-C19
27	C	305	CDL	C82-C83-C84-C85
27	P	306	CDL	C51-C52-C53-C54
28	P	309	PEK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	T	103	CDL	C51-CB5-OB6-CB4
27	C	305	CDL	C20-C21-C22-C23
27	P	306	CDL	C71-C72-C73-C74
19	Q	201	TGL	C29-C30-C31-C32
19	Y	101	TGL	C15-C16-C17-C18
27	G	102	CDL	C41-C42-C43-C44
20	N	608	PGV	C10-C11-C12-C13
28	P	304	PEK	C10-C11-C12-C13
20	C	308	PGV	C29-C30-C31-C32
25	P	308	DMU	O16-C18-C19-C22
27	C	305	CDL	C64-C65-C66-C67
28	P	309	PEK	C32-C33-C34-C35
20	P	302	PGV	C01-C02-C03-O11
27	G	102	CDL	OB5-CB3-CB4-CB6
27	P	306	CDL	OA5-CA3-CA4-CA6
27	T	103	CDL	OB5-CB3-CB4-CB6
28	C	307	PEK	C01-C02-C03-O11
28	P	309	PEK	C30-C31-C32-C33
23	O	302	PSC	C20-C21-C22-C23
19	N	610	TGL	CC2-CC3-CC4-CC5
28	C	307	PEK	C25-C26-C27-C28
19	D	201	TGL	C24-C25-C26-C27
27	C	305	CDL	C71-CB7-OB8-CB6
19	L	101	TGL	OG2-CB1-CB2-CB3
25	C	310	DMU	C31-C34-C37-C40
19	Q	201	TGL	CB9-C10-C11-C12
20	N	608	PGV	C24-C25-C26-C27
20	P	302	PGV	C28-C29-C30-C31
28	G	101	PEK	C25-C26-C27-C28
28	G	101	PEK	C28-C29-C30-C31
19	A	608	TGL	OG1-CG1-CG2-CG3
19	Q	201	TGL	OG1-CG1-CG2-CG3
23	B	302	PSC	O03-C01-C02-C03
27	G	102	CDL	CB3-CB4-CB6-OB8
27	P	306	CDL	CB3-CB4-CB6-OB8
28	P	309	PEK	O03-C01-C02-C03
19	L	101	TGL	C14-C29-C30-C31
28	G	101	PEK	C13-C14-C15-C16
19	L	101	TGL	CA2-CA3-CA4-CA5
27	G	102	CDL	C79-C80-C81-C82
28	P	304	PEK	C33-C34-C35-C36
23	B	302	PSC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	G	102	CDL	CB2-OB2-PB2-OB5
28	C	307	PEK	C11-C10-C9-C8
28	G	101	PEK	C9-C10-C11-C12
28	G	104	PEK	C5-C6-C7-C8
28	G	104	PEK	C6-C7-C8-C9
28	P	304	PEK	C12-C13-C14-C15
28	P	309	PEK	C11-C12-C13-C14
28	T	102	PEK	C11-C10-C9-C8
28	T	102	PEK	C9-C10-C11-C12
28	T	102	PEK	C12-C13-C14-C15
19	L	101	TGL	OC1-CC1-OG3-CG3
28	G	101	PEK	C35-C36-C37-C38
25	M	102	DMU	C22-C25-C28-C31
20	P	302	PGV	O01-C02-C03-O11
28	C	307	PEK	O01-C02-C03-O11
27	G	102	CDL	OB7-CB5-OB6-CB4
20	A	609	PGV	C11-C10-C9-C8
20	P	302	PGV	C11-C10-C9-C8
28	C	307	PEK	C28-C29-C30-C31
23	B	302	PSC	O03-C01-C02-O01
23	O	302	PSC	O03-C01-C02-O01
27	C	305	CDL	OA6-CA4-CA6-OA8
19	N	610	TGL	C21-C20-CA9-CA8
14	A	601	HEA	C15-C16-C17-C18
19	N	610	TGL	C16-C15-CC9-CC8
25	C	309	DMU	C19-C22-C25-C28
19	N	610	TGL	CA9-C20-C21-C22
27	P	306	CDL	C14-C15-C16-C17
27	P	306	CDL	C60-C61-C62-C63
20	C	304	PGV	C27-C28-C29-C30
28	P	304	PEK	C30-C31-C32-C33
20	P	305	PGV	C02-C03-O11-P
23	O	302	PSC	C02-C03-O11-P
27	C	305	CDL	CA4-CA3-OA5-PA1
27	P	306	CDL	C1-CA2-OA2-PA1
24	C	306	CHD	C16-C17-C20-C22
19	A	608	TGL	C21-C20-CA9-CA8
20	P	302	PGV	C19-C20-C21-C22
20	P	302	PGV	C29-C30-C31-C32
21	C	316	EDO	O1-C1-C2-O2
19	N	610	TGL	CC7-CC8-CC9-C15
27	G	102	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
27	P	306	CDL	C61-C62-C63-C64
28	G	104	PEK	C23-C24-C25-C26
20	N	608	PGV	C15-C16-C17-C18
20	N	608	PGV	C01-C02-C03-O11
27	C	305	CDL	OA5-CA3-CA4-CA6
19	Q	201	TGL	C16-C17-C18-C19
27	C	305	CDL	C60-C61-C62-C63
28	G	101	PEK	C32-C33-C34-C35
27	T	103	CDL	C54-C55-C56-C57
27	T	103	CDL	C57-C58-C59-C60
20	P	305	PGV	C24-C25-C26-C27
27	T	103	CDL	C53-C54-C55-C56
28	T	102	PEK	C27-C28-C29-C30
27	G	102	CDL	C51-CB5-OB6-CB4
20	N	609	PGV	C13-C14-C15-C16
27	C	305	CDL	C13-C14-C15-C16
19	D	201	TGL	C11-C12-C13-C14
25	P	311	DMU	C34-C37-C40-C43
20	P	302	PGV	C9-C10-C11-C12
23	O	302	PSC	C14-C15-C16-C17
19	D	201	TGL	C15-C16-C17-C18
19	L	101	TGL	C24-C25-C26-C27
19	Q	201	TGL	C15-C16-C17-C18
25	C	309	DMU	C34-C37-C40-C43
28	C	307	PEK	C22-C21-O03-C01
20	N	609	PGV	C31-C32-C33-C34
20	N	608	PGV	O03-C01-C02-C03
23	O	302	PSC	O03-C01-C02-C03
27	C	305	CDL	C1-CA2-OA2-PA1
20	N	608	PGV	O01-C02-C03-O11
27	G	102	CDL	OB5-CB3-CB4-OB6
27	G	102	CDL	C12-C11-CA5-OA6
20	C	308	PGV	C2-C3-C4-C5
19	Q	201	TGL	CA7-CA8-CA9-C20
27	G	102	CDL	C76-C77-C78-C79
27	C	305	CDL	OB9-CB7-OB8-CB6
28	C	307	PEK	O04-C21-O03-C01
20	P	302	PGV	C13-C14-C15-C16
19	A	608	TGL	OG1-CG1-CG2-OG2
19	N	610	TGL	OG2-CG2-CG3-OG3
20	N	608	PGV	O03-C01-C02-O01
27	C	305	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
27	P	306	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	C18-C19-C33-C34
19	D	201	TGL	CB2-CB1-OG2-CG2
20	P	305	PGV	C11-C10-C9-C8
27	P	306	CDL	CA5-C11-C12-C13
19	D	201	TGL	OB1-CB1-OG2-CG2
28	G	104	PEK	O02-C1-O01-C02
27	C	305	CDL	C81-C82-C83-C84
27	G	102	CDL	C18-C19-C20-C21
20	A	609	PGV	C23-C24-C25-C26
28	G	104	PEK	C29-C30-C31-C32
20	P	302	PGV	C23-C24-C25-C26
28	G	104	PEK	C7-C8-C9-C10
27	P	306	CDL	C20-C21-C22-C23
27	C	305	CDL	C41-C42-C43-C44
27	P	306	CDL	C37-C38-C39-C40
19	A	608	TGL	CB5-CB6-CB7-CB8
19	D	201	TGL	CA4-CA5-CA6-CA7
20	C	304	PGV	C31-C32-C33-C34
20	P	302	PGV	C03-O11-P-O12
23	B	302	PSC	C04-O12-P-O11
27	G	102	CDL	CB3-OB5-PB2-OB2
28	T	102	PEK	C04-O12-P-O11
20	M	101	PGV	O12-C04-C05-O05
20	C	304	PGV	C02-C03-O11-P
20	C	308	PGV	C03-O11-P-O13
20	M	101	PGV	C03-O11-P-O14
23	O	302	PSC	C03-O11-P-O13
27	C	305	CDL	CA3-OA5-PA1-OA3
27	C	305	CDL	CB2-OB2-PB2-OB3
27	P	306	CDL	CB3-OB5-PB2-OB3
27	T	103	CDL	CA2-OA2-PA1-OA4
27	T	103	CDL	CB3-OB5-PB2-OB3
28	C	307	PEK	C03-O11-P-O13
28	P	309	PEK	C03-O11-P-O14
28	P	309	PEK	C04-O12-P-O14
20	C	304	PGV	C1-C2-C3-C4
28	G	104	PEK	C01-C02-C03-O11
19	D	201	TGL	OG2-CB1-CB2-CB3
27	C	305	CDL	C17-C18-C19-C20
27	T	103	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	C	304	PGV	C15-C16-C17-C18
28	G	104	PEK	C30-C31-C32-C33
28	P	309	PEK	C2-C3-C4-C5
27	G	102	CDL	C24-C25-C26-C27
23	B	302	PSC	C22-C23-C24-C25
27	C	305	CDL	OA5-CA3-CA4-OA6
27	P	306	CDL	OA5-CA3-CA4-OA6
27	T	103	CDL	OB5-CB3-CB4-OB6
27	T	103	CDL	C56-C57-C58-C59
28	G	101	PEK	C31-C32-C33-C34
27	G	102	CDL	C53-C54-C55-C56
23	B	302	PSC	C04-C05-N-C08
19	D	201	TGL	CG1-CG2-CG3-OG3
19	N	610	TGL	CG1-CG2-CG3-OG3
19	Y	101	TGL	CA7-CA8-CA9-C20
19	Y	101	TGL	CG1-CG2-CG3-OG3
19	D	201	TGL	OG2-CG2-CG3-OG3
27	P	306	CDL	OA6-CA4-CA6-OA8
28	G	104	PEK	O03-C01-C02-O01
27	G	102	CDL	C74-C75-C76-C77
27	P	306	CDL	C39-C40-C41-C42
20	P	305	PGV	C05-C04-O12-P
19	L	101	TGL	C16-C15-CC9-CC8
28	P	309	PEK	C22-C21-O03-C01
27	P	306	CDL	C15-C16-C17-C18
19	A	608	TGL	C17-C18-C19-C33
20	C	308	PGV	O05-C05-C06-O06
27	P	306	CDL	C84-C85-C86-C87
20	M	101	PGV	C12-C13-C14-C15
23	B	302	PSC	C04-C05-N-C07
20	M	101	PGV	C15-C16-C17-C18
20	N	609	PGV	C29-C30-C31-C32
19	L	101	TGL	CC9-C15-C16-C17
27	C	305	CDL	C56-C57-C58-C59
25	C	302	DMU	C34-C37-C40-C43
19	D	201	TGL	CG3-CG2-OG2-CB1
25	C	302	DMU	C28-C31-C34-C37
19	Q	201	TGL	CC2-CC3-CC4-CC5
27	T	103	CDL	C17-C18-C19-C20
28	G	104	PEK	C25-C26-C27-C28
27	T	103	CDL	C35-C36-C37-C38
27	C	305	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	P	311	DMU	C18-C19-C22-C25
20	M	101	PGV	C21-C22-C23-C24
27	G	102	CDL	C20-C21-C22-C23
27	G	102	CDL	C64-C65-C66-C67
19	L	101	TGL	CA4-CA5-CA6-CA7
21	A	611	EDO	O1-C1-C2-O2
21	A	613	EDO	O1-C1-C2-O2
21	D	204	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
21	N	614	EDO	O1-C1-C2-O2
21	R	202	EDO	O1-C1-C2-O2
21	R	205	EDO	O1-C1-C2-O2
21	U	101	EDO	O1-C1-C2-O2
20	N	608	PGV	C31-C32-C33-C34
25	C	302	DMU	C22-C25-C28-C31
19	Q	201	TGL	CC1-CC2-CC3-CC4
28	G	104	PEK	C3-C4-C5-C6
19	Q	201	TGL	OG1-CG1-CG2-OG2
20	N	608	PGV	C03-O11-P-O12
20	P	302	PGV	C04-O12-P-O11
23	O	302	PSC	C04-O12-P-O11
27	G	102	CDL	CA2-OA2-PA1-OA5
27	G	102	CDL	CA3-OA5-PA1-OA2
27	P	306	CDL	CA3-OA5-PA1-OA2
27	T	103	CDL	CB2-OB2-PB2-OB5
28	G	104	PEK	C04-O12-P-O11
19	N	610	TGL	C20-C21-C22-C23
27	C	305	CDL	C51-C52-C53-C54
27	G	102	CDL	C36-C37-C38-C39
19	L	101	TGL	OG1-CG1-CG2-CG3
14	A	601	HEA	C26-C15-C16-C17
19	L	101	TGL	OG1-CA1-CA2-CA3
19	Q	201	TGL	OG2-CB1-CB2-CB3
28	G	104	PEK	C2-C1-O01-C02
23	B	302	PSC	C04-C05-N-C06
19	Y	101	TGL	C24-C25-C26-C27
27	T	103	CDL	C83-C84-C85-C86
25	Z	101	DMU	C25-C28-C31-C34
27	P	306	CDL	CA4-CA3-OA5-PA1
27	T	103	CDL	C1-CA2-OA2-PA1
27	P	306	CDL	OA7-CA5-OA6-CA4
19	A	608	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
28	G	101	PEK	C24-C25-C26-C27
19	L	101	TGL	C23-C24-C25-C26
19	Q	201	TGL	CB2-CB3-CB4-CB5
27	C	305	CDL	C24-C25-C26-C27
14	N	602[B]	HEA	CAA-CBA-CGA-O1A
19	L	101	TGL	C29-C30-C31-C32
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
24	G	103	CHD	C22-C23-C24-O26
24	P	307	CHD	C22-C23-C24-O26
19	A	608	TGL	CC9-C15-C16-C17
27	C	305	CDL	C72-C73-C74-C75
28	P	309	PEK	O04-C21-O03-C01
27	T	103	CDL	C42-C43-C44-C45
20	C	304	PGV	C21-C22-C23-C24
20	M	101	PGV	C05-C04-O12-P
19	Y	101	TGL	C17-C18-C19-C33
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
24	T	101	CHD	C22-C23-C24-O25
23	O	302	PSC	C7-C8-C9-C10
28	P	309	PEK	C3-C4-C5-C6
28	C	307	PEK	C17-C18-C19-C20
23	O	302	PSC	C4-C5-C6-C7
27	G	102	CDL	C44-C45-C46-C47
20	N	609	PGV	C12-C13-C14-C15
21	R	204	EDO	O1-C1-C2-O2
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
14	N	601	HEA	CAD-CBD-CGD-O1D
24	G	103	CHD	C22-C23-C24-O25
20	C	304	PGV	C28-C29-C30-C31
28	C	307	PEK	C33-C34-C35-C36
19	L	101	TGL	CA9-C20-C21-C22
19	Y	101	TGL	OG1-CA1-CA2-CA3
28	P	304	PEK	C15-C16-C17-C18
24	T	101	CHD	C22-C23-C24-O26
19	Y	101	TGL	C21-C22-C23-C24
23	O	302	PSC	C9-C10-C11-C12
28	C	307	PEK	C6-C7-C8-C9
28	C	307	PEK	C11-C12-C13-C14
28	G	101	PEK	C6-C7-C8-C9
28	G	104	PEK	C11-C10-C9-C8
28	G	104	PEK	C12-C13-C14-C15
28	P	304	PEK	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	CC7-CC8-CC9-C15
20	C	308	PGV	C15-C16-C17-C18
14	N	602[B]	HEA	CAA-CBA-CGA-O2A
27	T	103	CDL	C32-C33-C34-C35
27	C	305	CDL	C83-C84-C85-C86
23	B	302	PSC	O01-C1-C2-C3
14	N	601	HEA	CAD-CBD-CGD-O2D
24	P	307	CHD	C22-C23-C24-O25
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
27	G	102	CDL	OB9-CB7-OB8-CB6
19	L	101	TGL	OG2-CG2-CG3-OG3
23	B	302	PSC	C12-C13-C14-C15
25	C	309	DMU	C18-C19-C22-C25
19	D	201	TGL	CC7-CC8-CC9-C15
28	T	102	PEK	C13-C14-C15-C16
19	A	608	TGL	C15-C16-C17-C18
20	M	101	PGV	O12-C04-C05-C06
14	N	601	HEA	C26-C15-C16-C17
14	N	602[B]	HEA	C26-C15-C16-C17
27	T	103	CDL	C37-C38-C39-C40
28	P	304	PEK	C16-C17-C18-C19
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
19	L	101	TGL	CC6-CC7-CC8-CC9
20	N	608	PGV	C05-C04-O12-P
28	T	102	PEK	C33-C34-C35-C36
19	Q	201	TGL	OG1-CA1-CA2-CA3
28	P	304	PEK	O03-C21-C22-C23
20	C	304	PGV	C11-C12-C13-C14
19	L	101	TGL	CG1-CG2-CG3-OG3
14	A	601	HEA	CAD-CBD-CGD-O1D
19	D	201	TGL	C18-C19-C33-C34
19	Y	101	TGL	CB7-CB8-CB9-C10
20	A	609	PGV	C30-C31-C32-C33
27	P	306	CDL	C41-C42-C43-C44
27	P	306	CDL	OA9-CA7-OA8-CA6
23	O	302	PSC	C27-C28-C29-C30
20	C	308	PGV	C7-C8-C9-C10
20	M	101	PGV	O01-C02-C03-O11
27	T	103	CDL	C55-C56-C57-C58
20	A	609	PGV	O03-C19-C20-C21
27	P	306	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
25	P	311	DMU	C31-C34-C37-C40
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
19	N	610	TGL	C24-C25-C26-C27
25	Z	101	DMU	C22-C25-C28-C31
27	G	102	CDL	C42-C43-C44-C45
28	P	304	PEK	C32-C33-C34-C35
27	G	102	CDL	C71-CB7-OB8-CB6
23	B	302	PSC	C20-C21-C22-C23
19	N	610	TGL	C10-C11-C12-C13
25	M	102	DMU	O6-C11-C9-C8
28	G	104	PEK	C02-C03-O11-P
19	Y	101	TGL	OG2-CG2-CG3-OG3
23	B	302	PSC	O03-C19-C20-C21
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	A	601	HEA	C14-C15-C16-C17
23	B	302	PSC	C11-C12-C13-C14
20	P	302	PGV	C11-C12-C13-C14
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
24	P	301	CHD	C22-C23-C24-O26
19	D	201	TGL	CG1-CG2-OG2-CB1
23	O	302	PSC	C03-C02-O01-C1
19	L	101	TGL	C25-C26-C27-C28
23	B	302	PSC	C4-C5-C6-C7
19	D	201	TGL	OG3-CC1-CC2-CC3
19	D	201	TGL	CA7-CA8-CA9-C20
19	D	201	TGL	OG1-CA1-CA2-CA3
28	G	104	PEK	O03-C21-C22-C23
27	P	306	CDL	C62-C63-C64-C65
28	C	307	PEK	C2-C3-C4-C5
19	L	101	TGL	C17-C18-C19-C33
20	C	304	PGV	C05-C04-O12-P
27	P	306	CDL	CA3-CA4-CA6-OA8
19	L	101	TGL	CB3-CB4-CB5-CB6
25	P	311	DMU	C28-C31-C34-C37
27	C	305	CDL	C19-C20-C21-C22
19	L	101	TGL	C13-C14-C29-C30
27	C	305	CDL	C35-C36-C37-C38
21	A	617	EDO	O1-C1-C2-O2
21	C	314	EDO	O1-C1-C2-O2
21	E	205	EDO	O1-C1-C2-O2
21	N	612	EDO	O1-C1-C2-O2
21	O	305	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	CAD-CBD-CGD-O2D
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
24	C	306	CHD	C22-C23-C24-O26
20	A	609	PGV	C11-C12-C13-C14
20	C	304	PGV	C9-C10-C11-C12
24	C	301	CHD	C22-C23-C24-O25
24	C	306	CHD	C22-C23-C24-O25
27	G	102	CDL	C23-C24-C25-C26
24	C	301	CHD	C22-C23-C24-O26
24	P	301	CHD	C22-C23-C24-O25
28	G	101	PEK	C14-C15-C16-C17
28	T	102	PEK	C3-C4-C5-C6
20	P	302	PGV	O01-C1-C2-C3
19	Q	201	TGL	C14-C29-C30-C31
14	N	602[B]	HEA	C14-C15-C16-C17
20	N	609	PGV	C11-C12-C13-C14
14	N	601	HEA	CAA-CBA-CGA-O1A
19	Y	101	TGL	CC2-CC3-CC4-CC5
19	Q	201	TGL	OG3-CC1-CC2-CC3
19	Q	201	TGL	CC3-CC4-CC5-CC6
27	G	102	CDL	C12-C13-C14-C15
19	A	608	TGL	CC7-CC8-CC9-C15
28	G	104	PEK	O04-C21-C22-C23
14	N	601	HEA	C27-C19-C20-C21
14	N	601	HEA	C14-C15-C16-C17
27	G	102	CDL	C84-C85-C86-C87
19	D	201	TGL	CA5-CA6-CA7-CA8
28	P	309	PEK	C27-C28-C29-C30
23	B	302	PSC	O04-C19-C20-C21
27	G	102	CDL	C57-C58-C59-C60
19	Y	101	TGL	OG1-CG1-CG2-CG3
19	N	610	TGL	OG1-CA1-CA2-CA3
19	L	101	TGL	CC4-CC5-CC6-CC7
20	M	101	PGV	C02-C03-O11-P
19	L	101	TGL	C10-C11-C12-C13
27	P	306	CDL	C36-C37-C38-C39
28	P	304	PEK	C17-C18-C19-C20
20	N	608	PGV	C03-O11-P-O13
20	N	608	PGV	C04-O12-P-O13
23	O	302	PSC	C04-O12-P-O14
27	G	102	CDL	CA2-OA2-PA1-OA3
27	P	306	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	C	305	CDL	CA5-C11-C12-C13
19	L	101	TGL	OB1-CB1-CB2-CB3
19	Q	201	TGL	OC1-CC1-CC2-CC3
28	P	309	PEK	C01-C02-C03-O11
28	C	307	PEK	O12-C04-C05-N
19	D	201	TGL	OA1-CA1-CA2-CA3
19	D	201	TGL	OC1-CC1-CC2-CC3
21	E	204	EDO	O1-C1-C2-O2
21	N	619	EDO	O1-C1-C2-O2
21	S	103	EDO	O1-C1-C2-O2
19	D	201	TGL	C12-C13-C14-C29
19	Q	201	TGL	CG3-CG2-OG2-CB1
23	B	302	PSC	C05-C04-O12-P
23	O	302	PSC	C05-C04-O12-P
27	G	102	CDL	C33-C34-C35-C36
20	N	609	PGV	O03-C19-C20-C21
20	M	101	PGV	O05-C05-C06-O06
19	L	101	TGL	C16-C17-C18-C19
20	P	302	PGV	O02-C1-C2-C3
20	C	308	PGV	O01-C1-C2-C3
27	G	102	CDL	C32-C31-CA7-OA8
19	Q	201	TGL	C33-C34-C35-C36
25	P	308	DMU	C25-C28-C31-C34
23	O	302	PSC	C25-C26-C27-C28
23	O	302	PSC	O03-C19-C20-C21
19	A	608	TGL	OC1-CC1-CC2-CC3
14	A	602[B]	HEA	C26-C15-C16-C17
27	P	306	CDL	C74-C75-C76-C77
28	P	309	PEK	O01-C02-C03-O11
14	A	601	HEA	CAA-CBA-CGA-O1A
19	Y	101	TGL	C12-C13-C14-C29
27	C	305	CDL	C12-C11-CA5-OA6
20	M	101	PGV	C1-C2-C3-C4
28	P	309	PEK	O01-C1-C2-C3
28	C	307	PEK	C29-C30-C31-C32
23	O	302	PSC	O04-C19-C20-C21
19	A	608	TGL	OG3-CC1-CC2-CC3

There are no ring outliers.

70 monomers are involved in 436 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	314	EDO	1	0
19	D	201	TGL	13	0
14	N	602[A]	HEA	7	0
19	Q	201	TGL	12	0
25	P	308	DMU	12	0
21	G	105	EDO	1	0
18	N	607	AZI	6	0
19	L	101	TGL	17	0
25	C	310	DMU	7	0
24	C	306	CHD	5	0
27	G	102	CDL	24	0
21	D	203	EDO	4	0
21	F	104	EDO	1	0
14	N	601	HEA	7	0
23	B	302	PSC	13	0
20	C	304	PGV	2	0
20	N	609	PGV	2	0
21	Q	204	EDO	5	0
24	P	301	CHD	2	0
21	A	616	EDO	1	0
14	A	601	HEA	8	0
21	P	312	EDO	1	0
21	A	612	EDO	4	0
14	A	602[A]	HEA	6	0
20	P	302	PGV	10	0
19	N	610	TGL	4	0
21	C	313	EDO	1	0
21	D	206	EDO	2	0
21	S	103	EDO	3	0
21	D	202	EDO	6	0
21	A	614	EDO	7	0
21	N	621	EDO	8	0
28	G	104	PEK	14	0
24	G	103	CHD	1	0
14	N	602[B]	HEA	12	0
20	A	609	PGV	4	0
21	N	612	EDO	2	0
19	A	608	TGL	4	0
25	C	302	DMU	12	0
21	A	618	EDO	4	0
20	P	305	PGV	2	0
24	P	307	CHD	4	0
23	O	302	PSC	16	0

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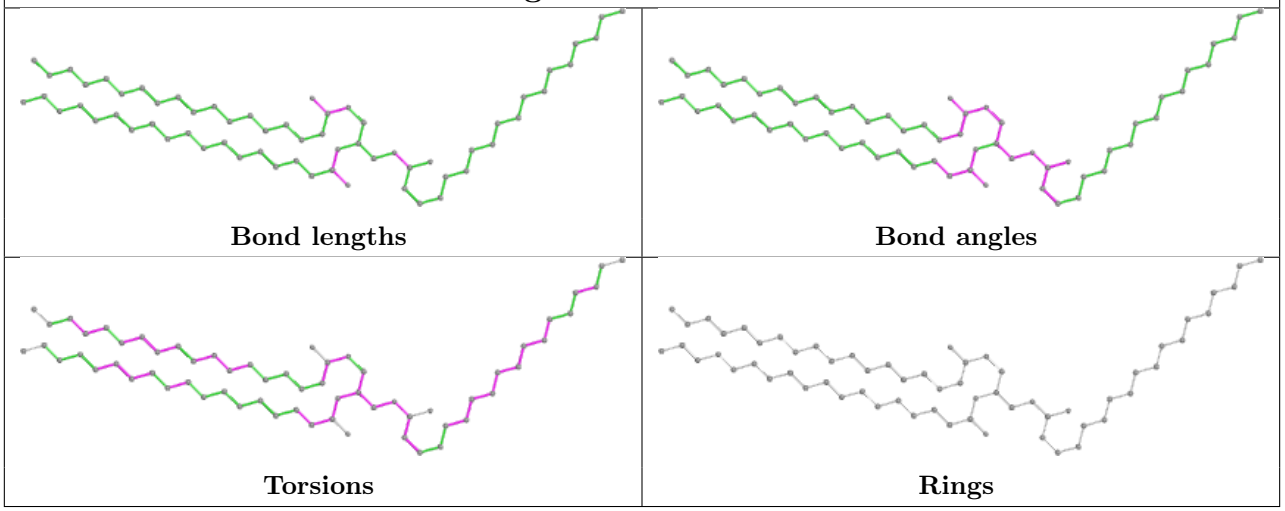
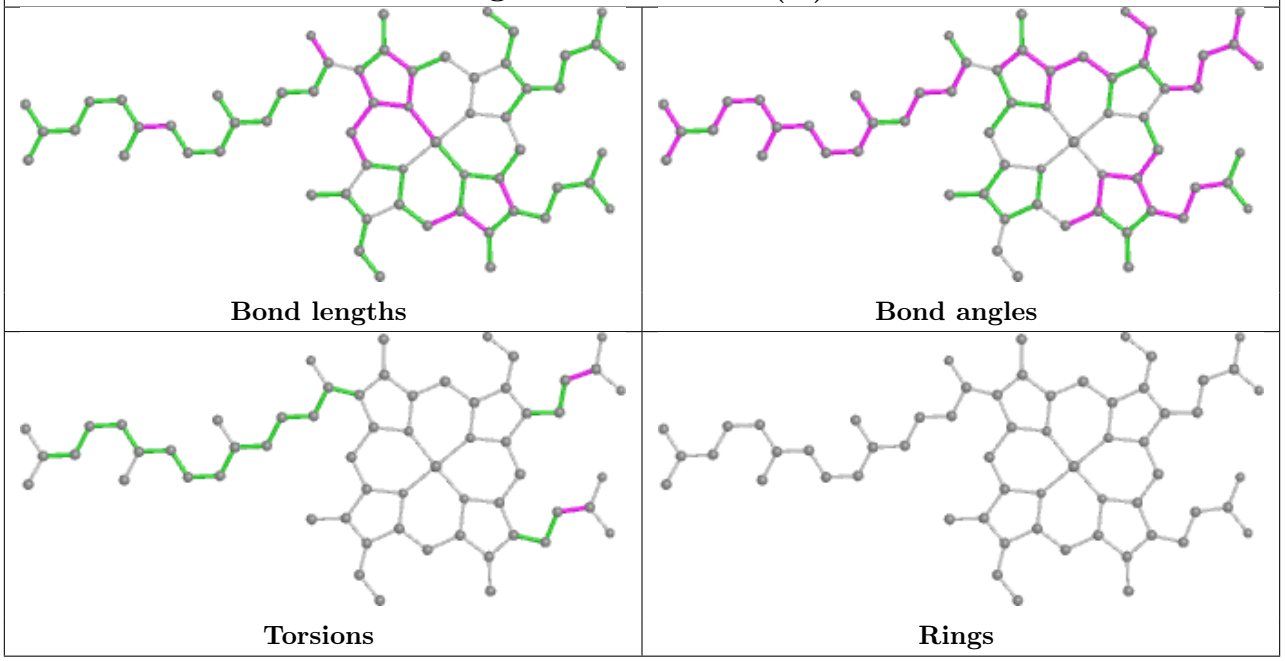
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	620	EDO	2	0
21	A	617	EDO	2	0
27	P	306	CDL	22	0
28	P	309	PEK	2	0
20	M	101	PGV	3	0
21	H	101	EDO	3	0
28	P	304	PEK	3	0
21	A	610	EDO	1	0
20	C	308	PGV	2	0
25	P	310	DMU	2	0
18	A	606	AZI	1	0
18	N	606	AZI	1	0
25	C	309	DMU	2	0
21	N	618	EDO	5	0
28	G	101	PEK	9	0
18	A	607	AZI	6	0
21	C	312	EDO	1	0
19	Y	101	TGL	16	0
21	Q	203	EDO	1	0
28	C	307	PEK	12	0
27	T	103	CDL	25	0
20	N	608	PGV	12	0
14	A	602[B]	HEA	11	0
28	T	102	PEK	10	0
21	R	204	EDO	3	0
21	C	317	EDO	1	0
27	C	305	CDL	26	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.

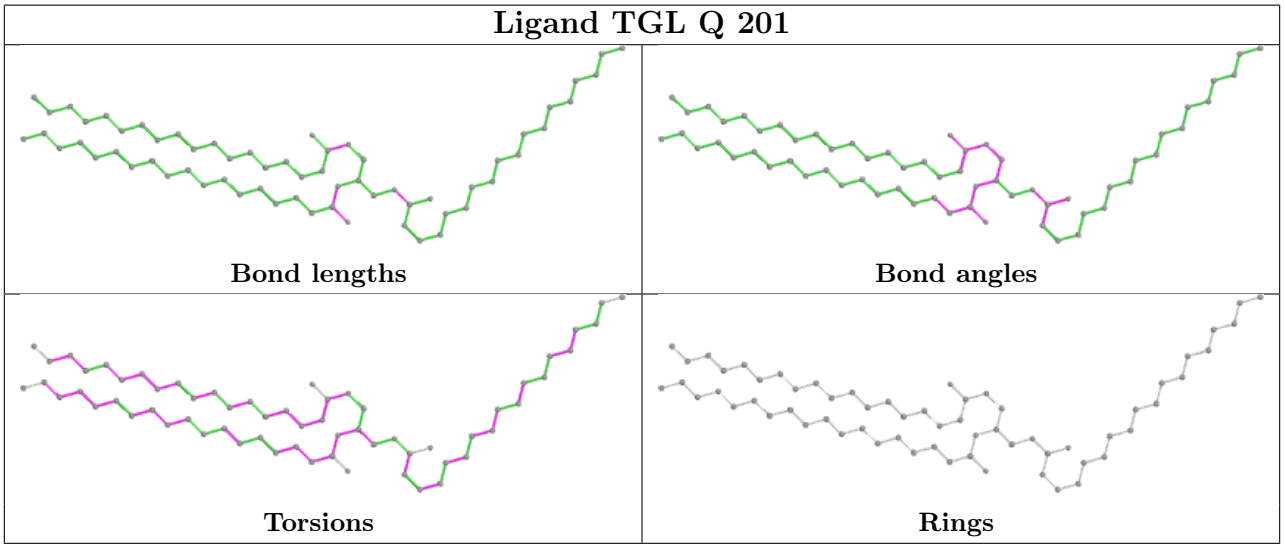
Ligand TGL D 201



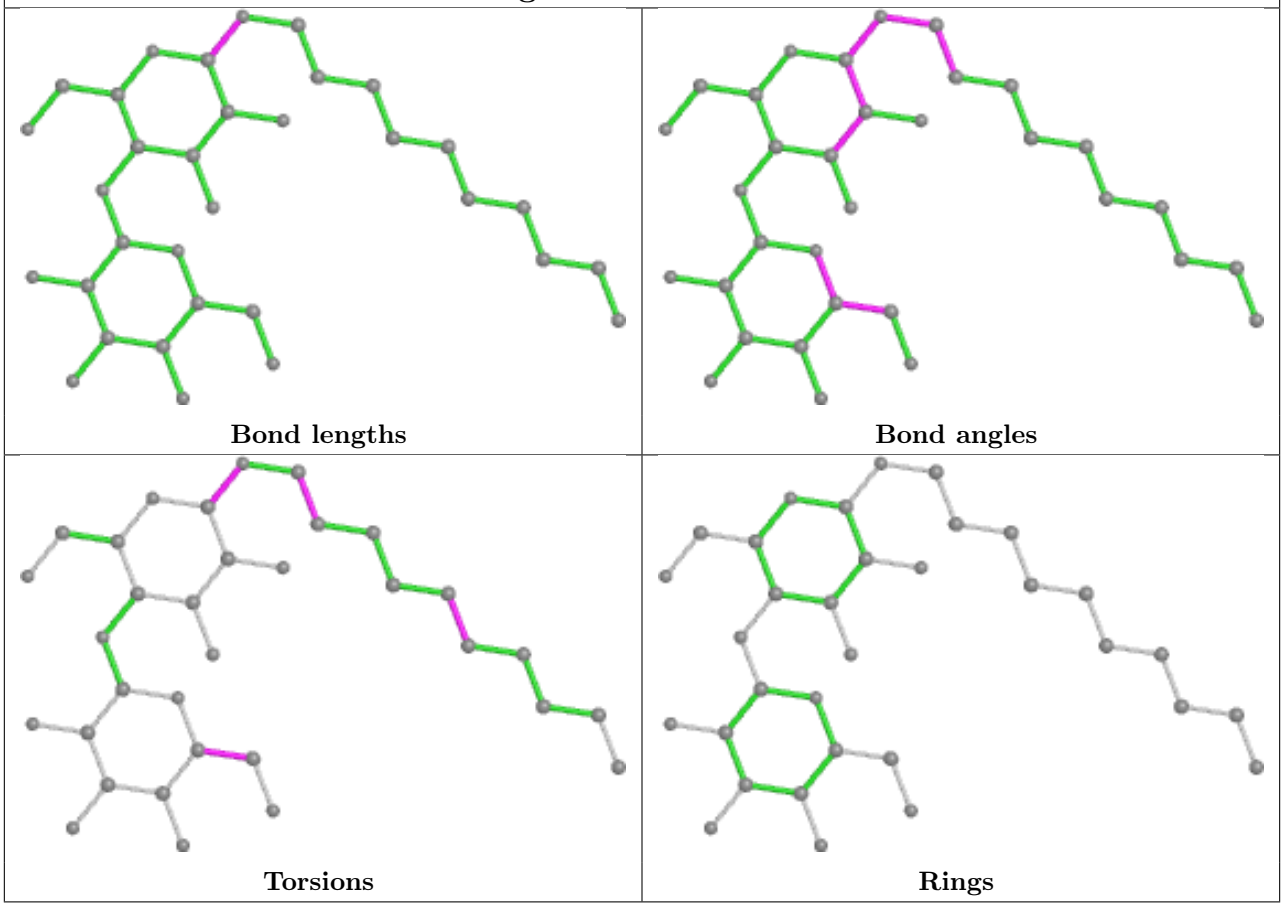
Ligand HEA N 602 (A)



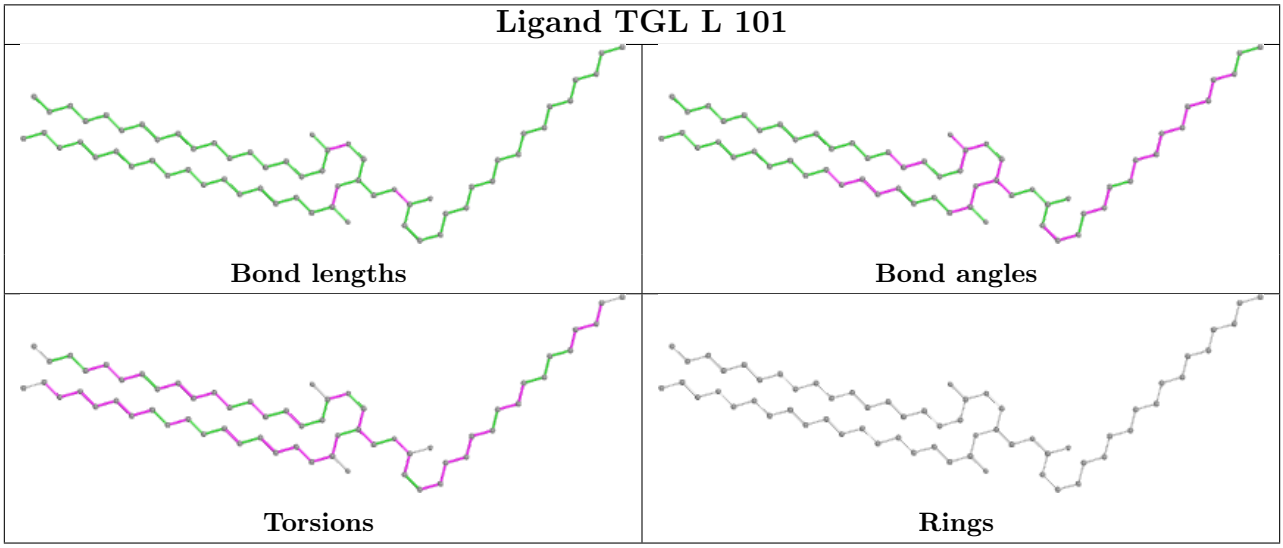
Ligand TGL Q 201



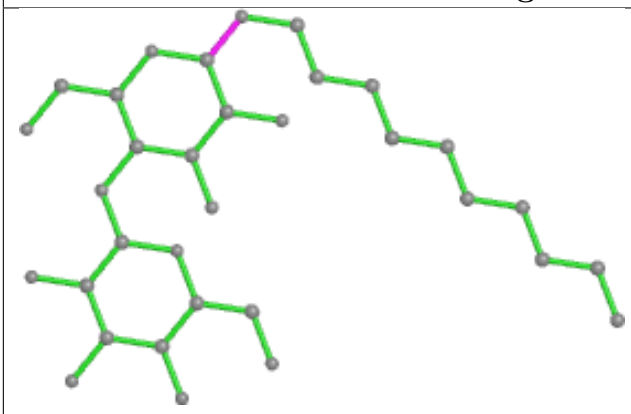
Ligand DMU P 308



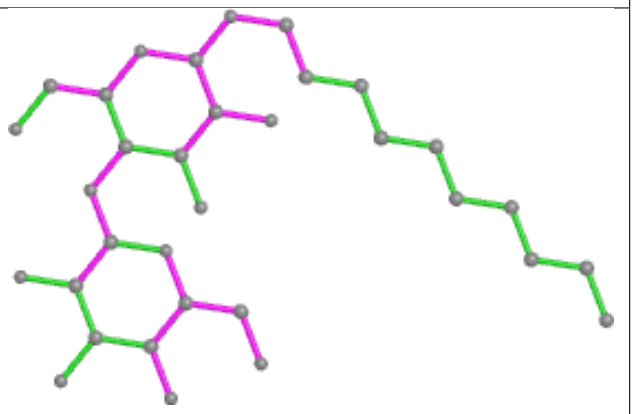
Ligand TGL L 101



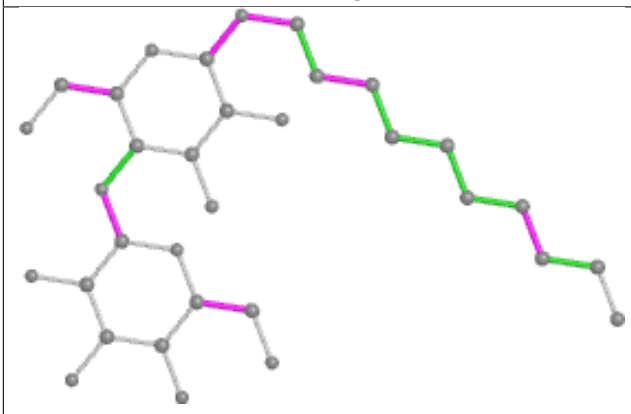
Ligand DMU C 310



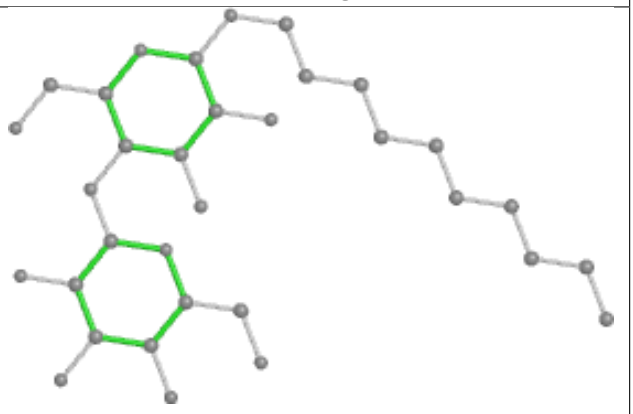
Bond lengths



Bond angles

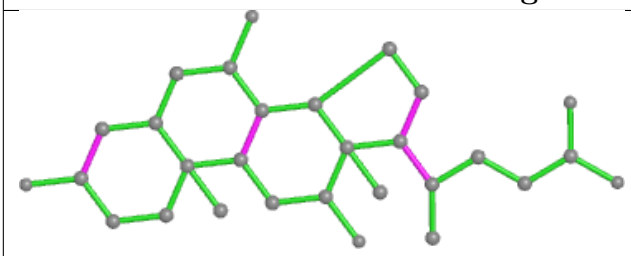


Torsions

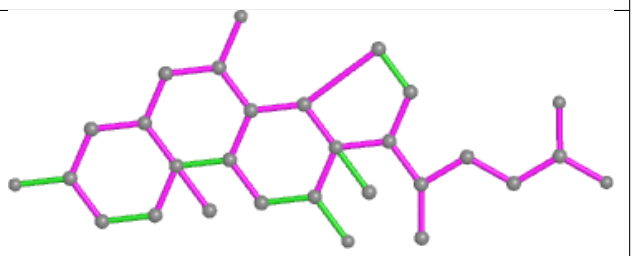


Rings

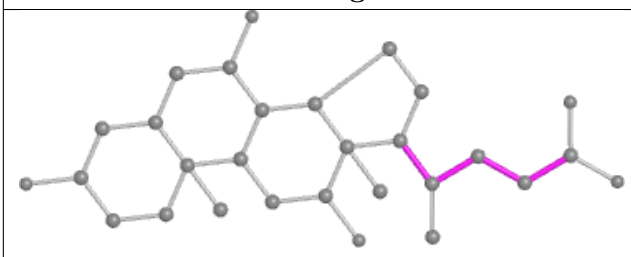
Ligand CHD C 306



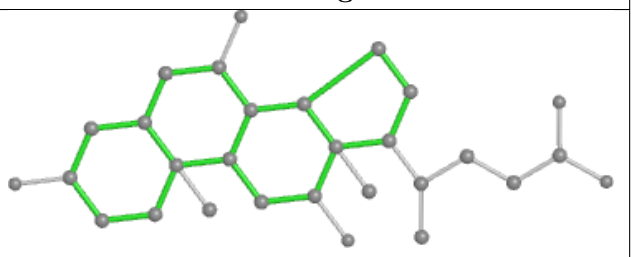
Bond lengths



Bond angles

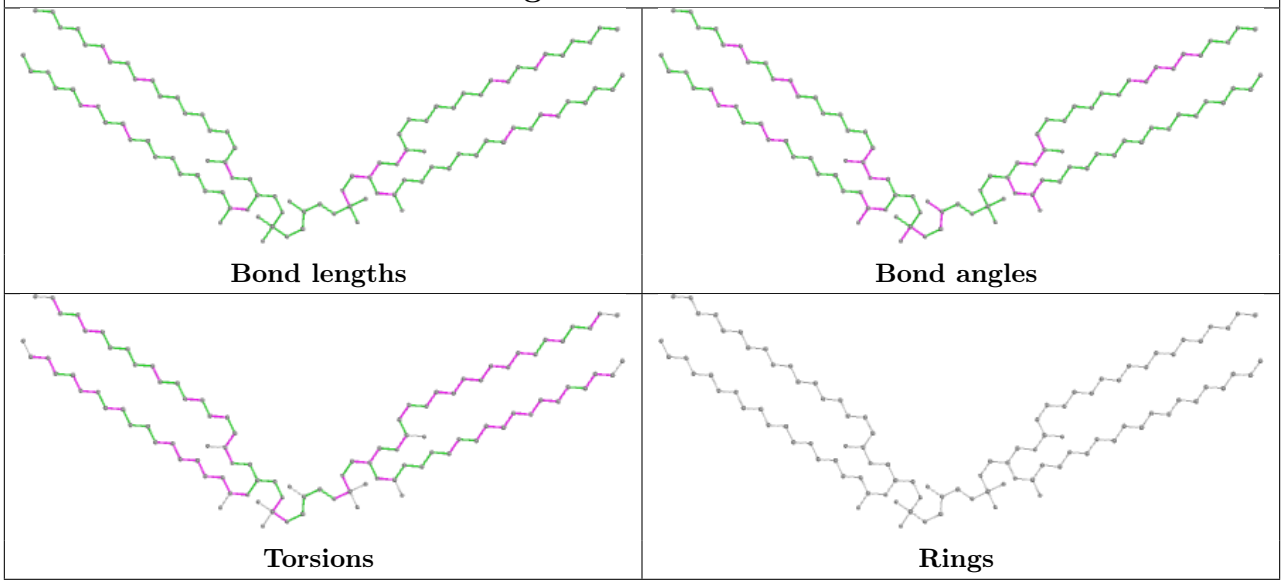


Torsions

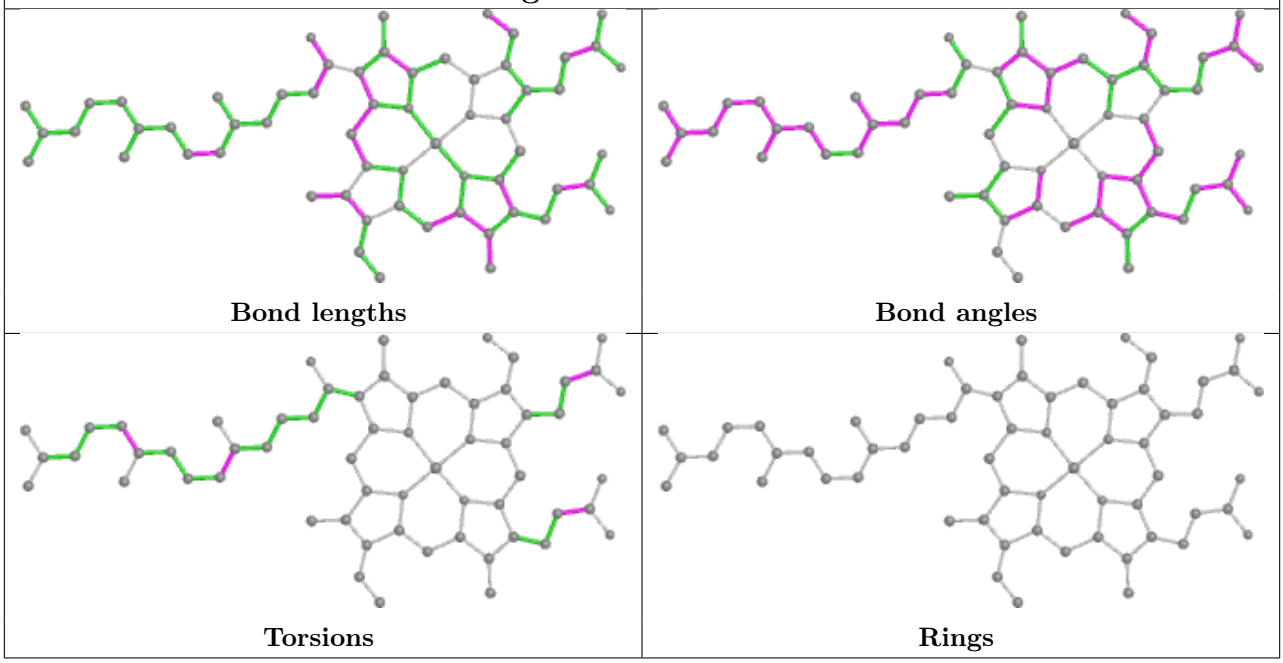


Rings

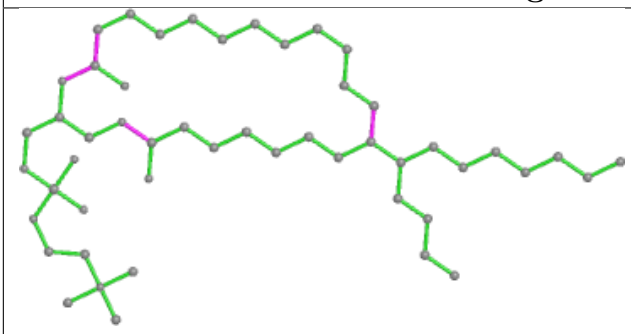
Ligand CDL G 102



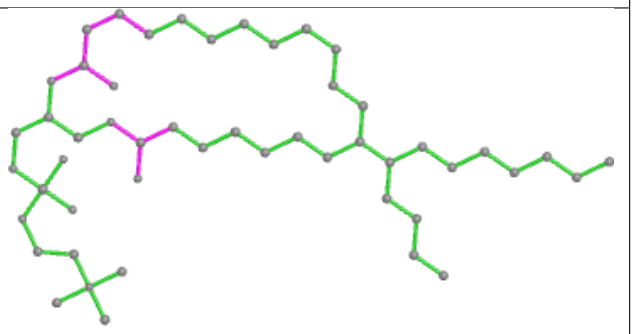
Ligand HEA N 601



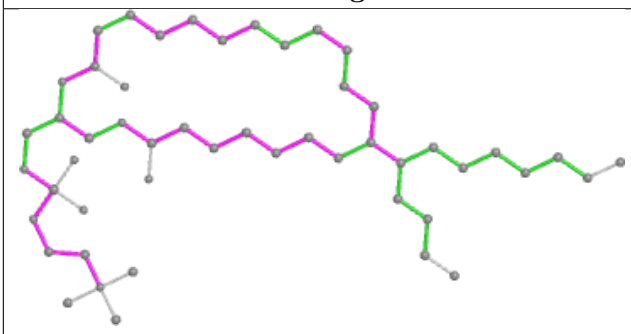
Ligand PSC B 302



Bond lengths



Bond angles



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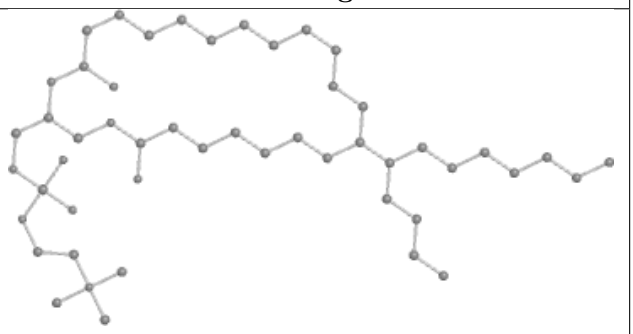
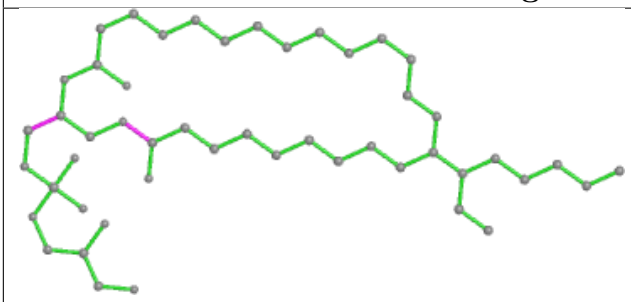
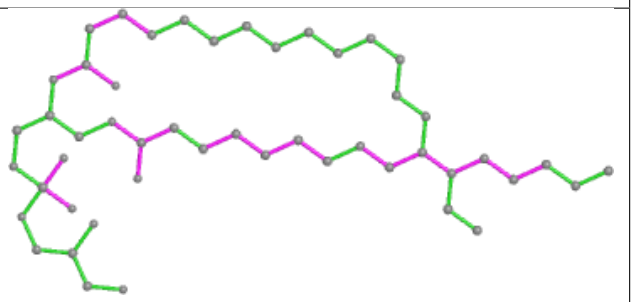


Rings

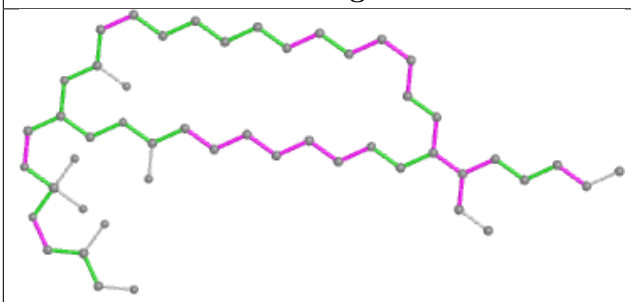
Ligand PGV C 304



Bond lengths



Bond angles



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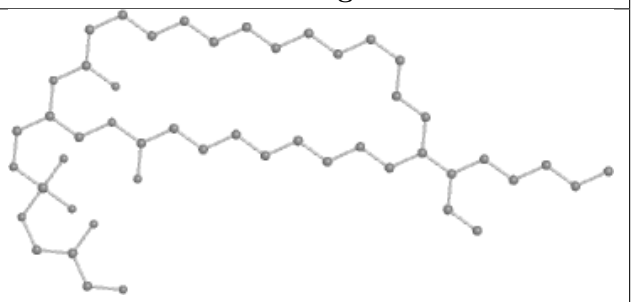
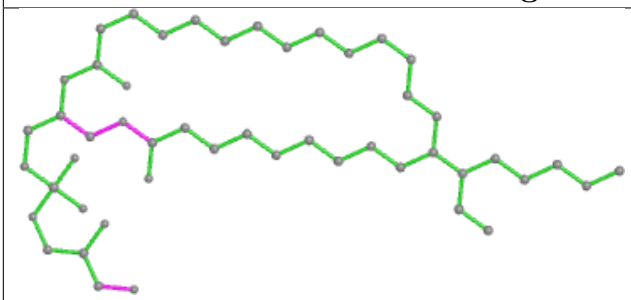
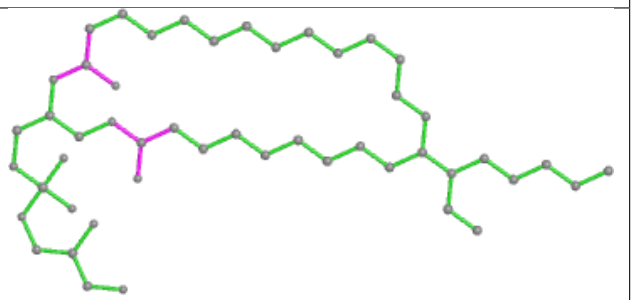


Rings

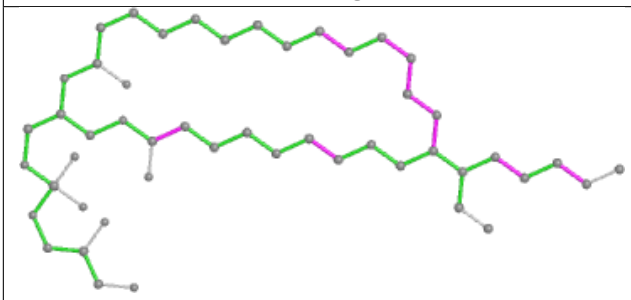
Ligand PGV N 609



Bond lengths



Bond angles



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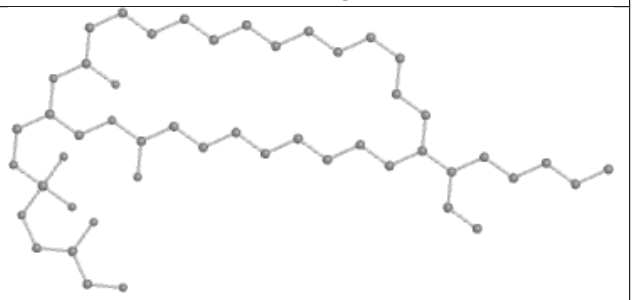
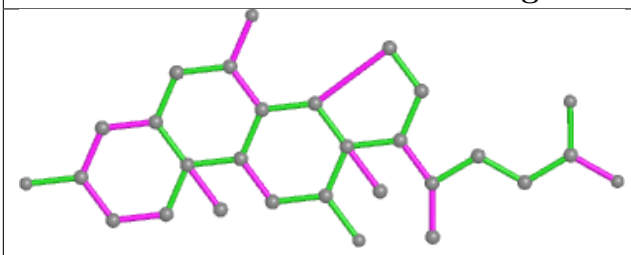
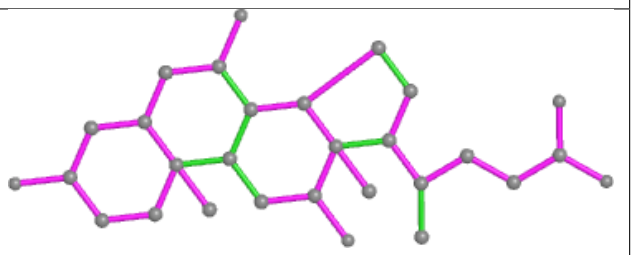


Rings

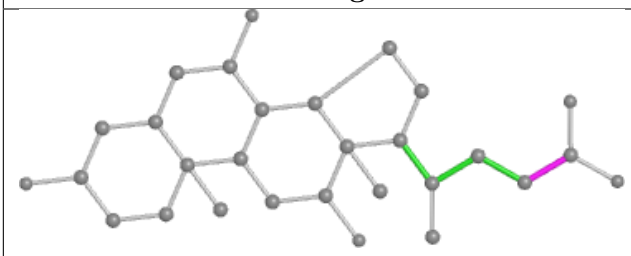
Ligand CHD T 101



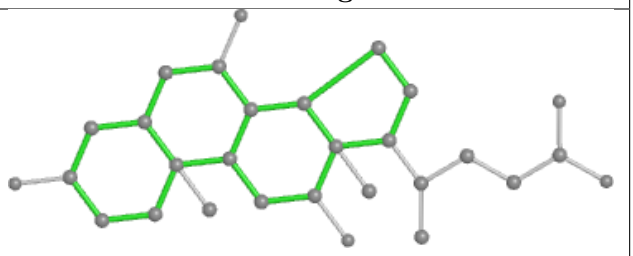
Bond lengths



Bond angles

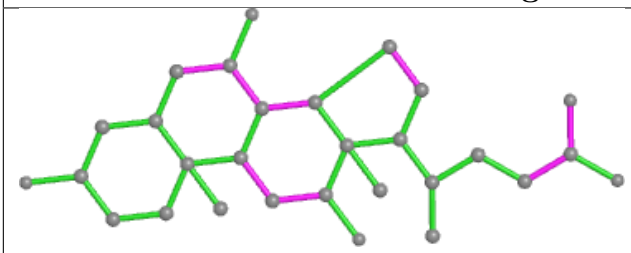


Torsions

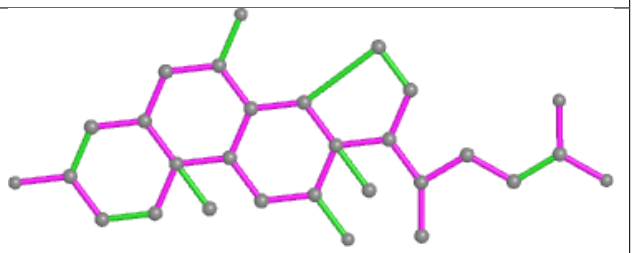


Rings

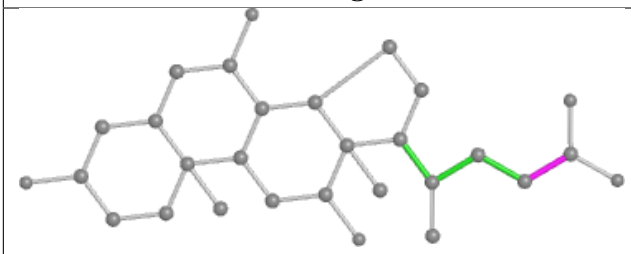
Ligand CHD P 301



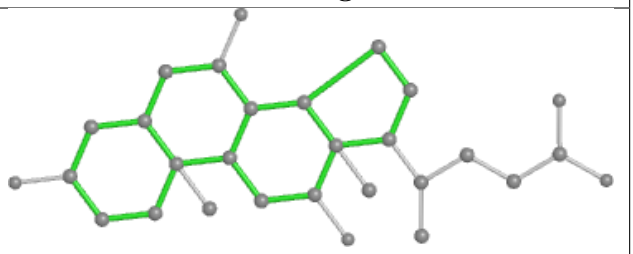
Bond lengths



Bond angles

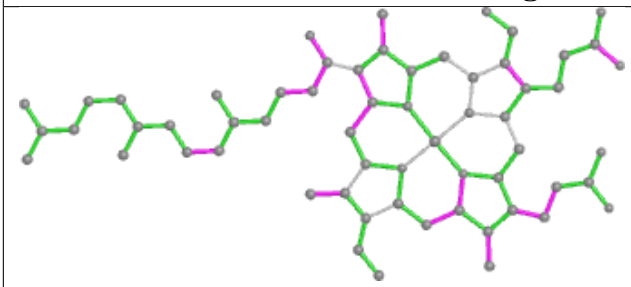


Torsions

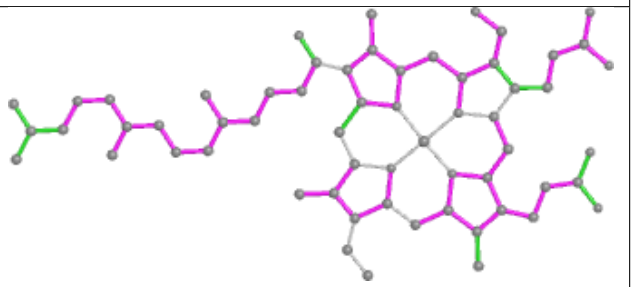


Rings

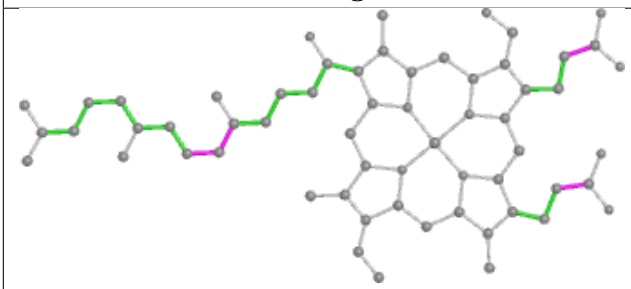
Ligand HEA A 601



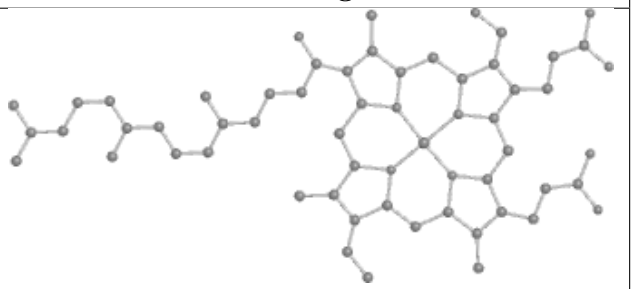
Bond lengths



Bond angles

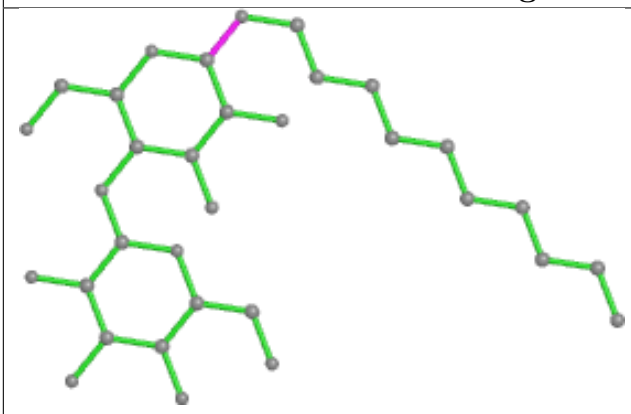


Torsions

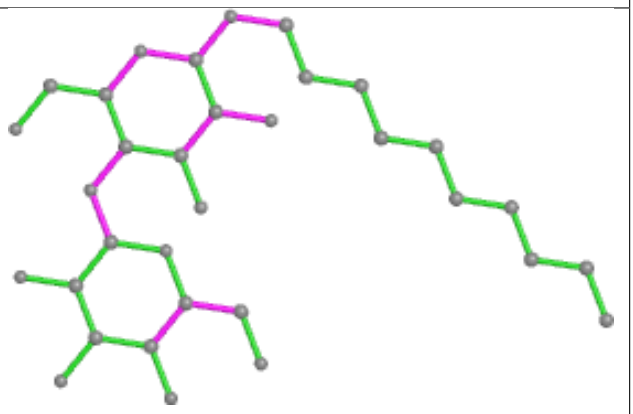


Rings

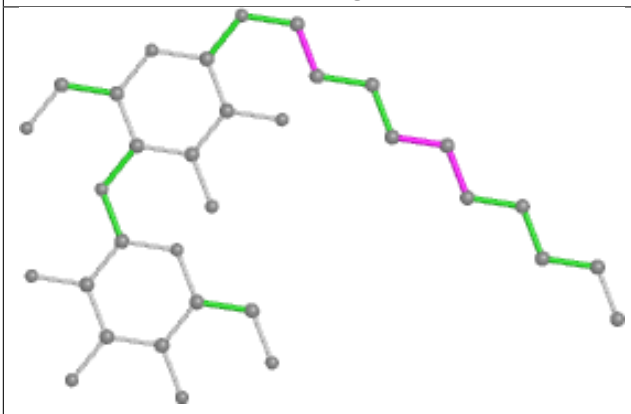
Ligand DMU Z 101



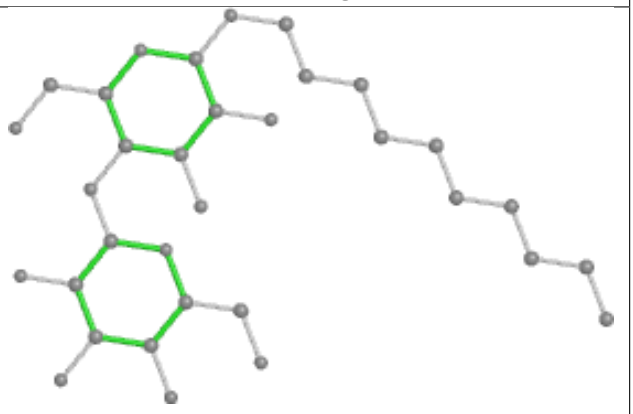
Bond lengths



Bond angles

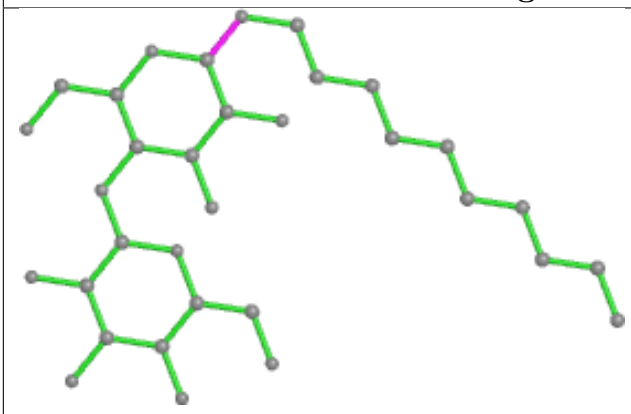


Torsions

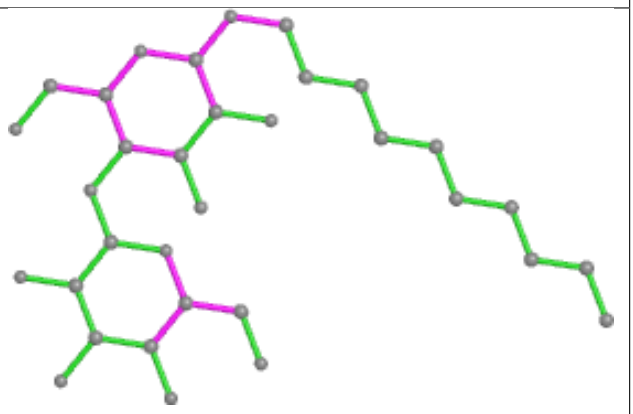


Rings

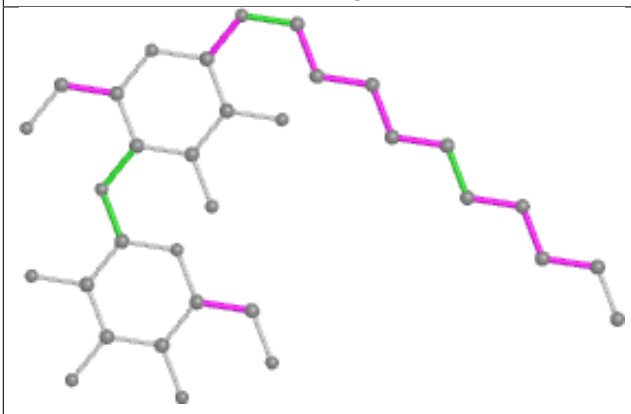
Ligand DMU P 311



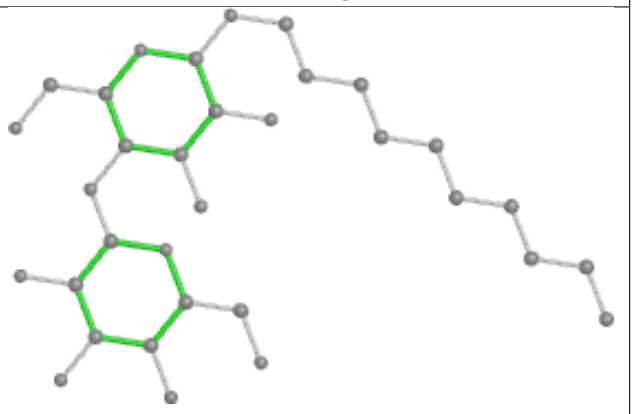
Bond lengths



Bond angles

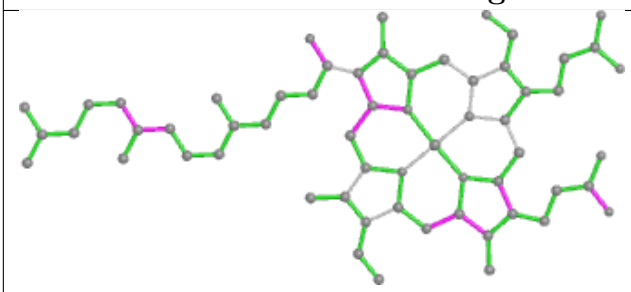


Torsions

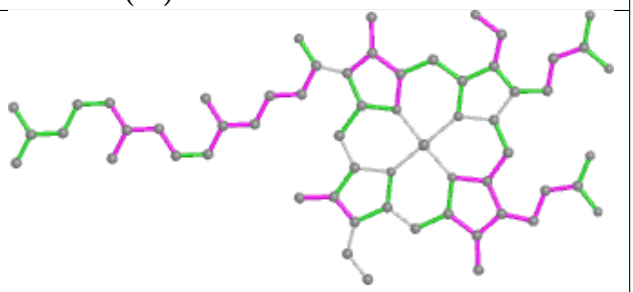


Rings

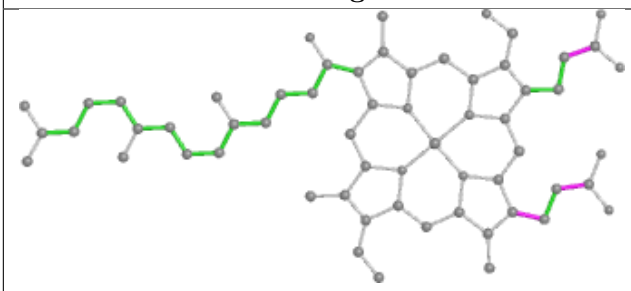
Ligand HEA A 602 (A)



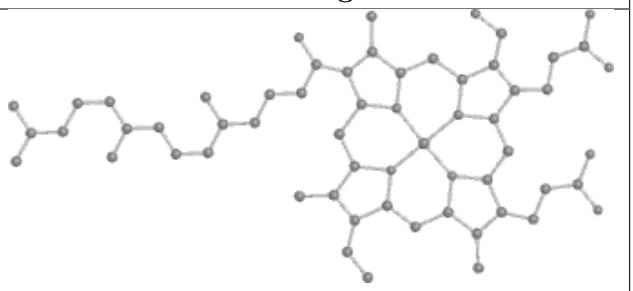
Bond lengths



Bond angles

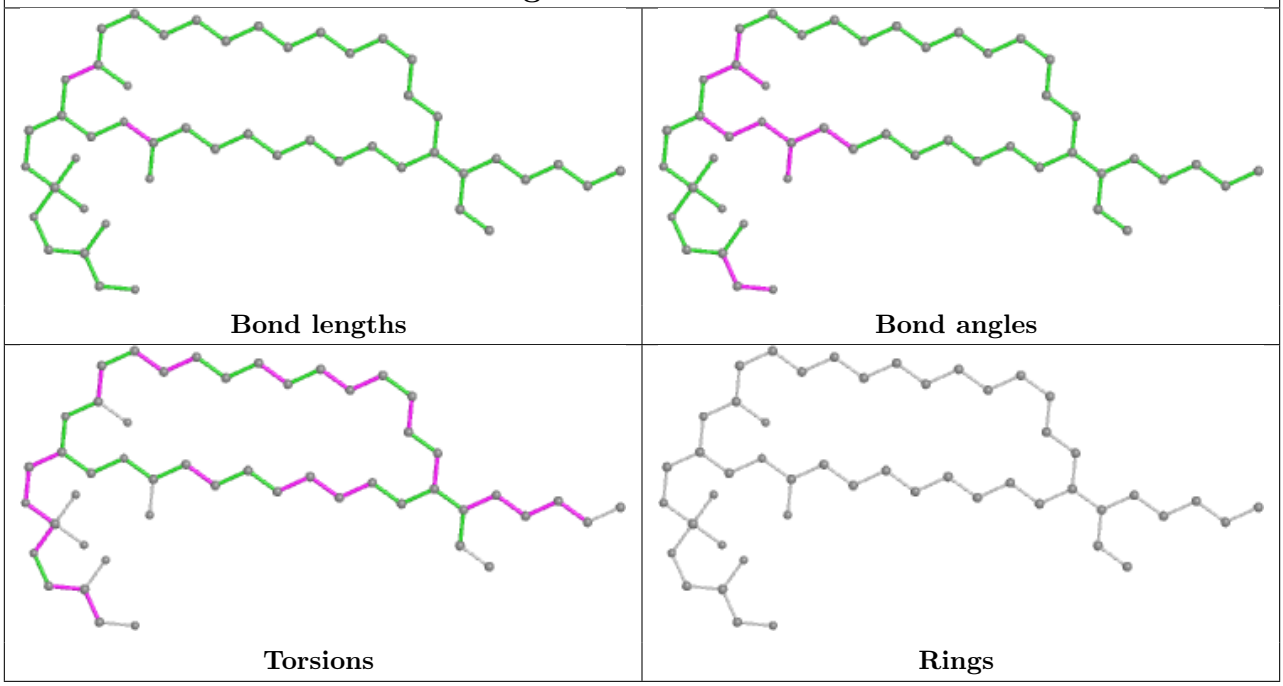


Torsions

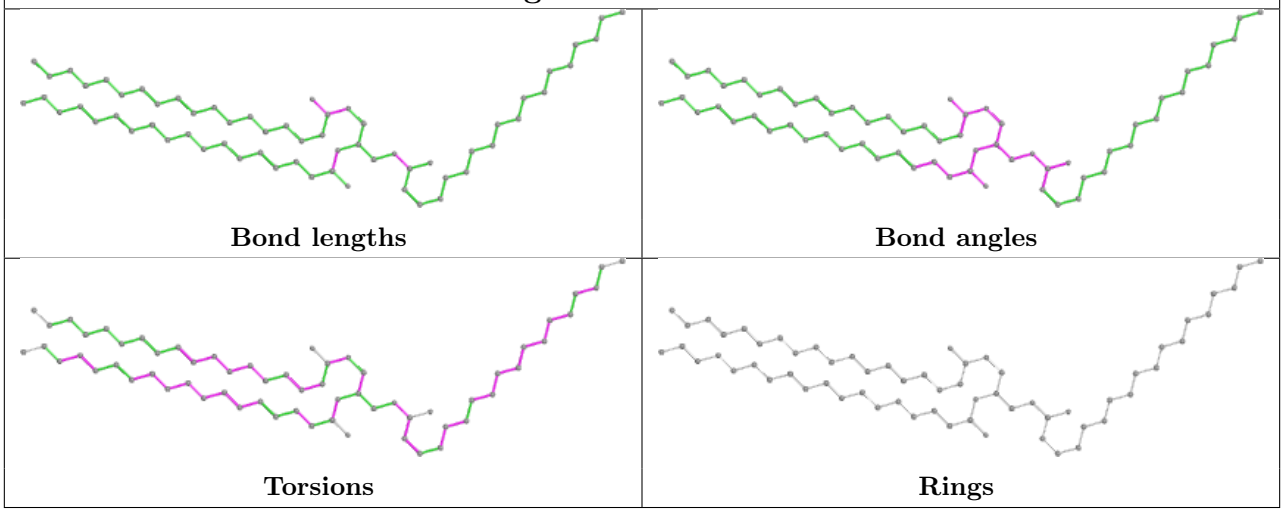


Rings

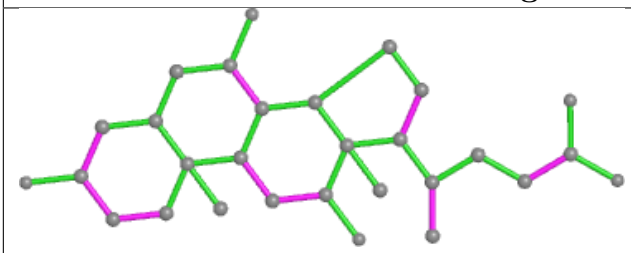
Ligand PGV P 302



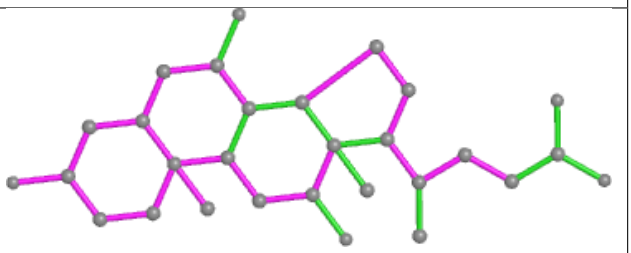
Ligand TGL N 610



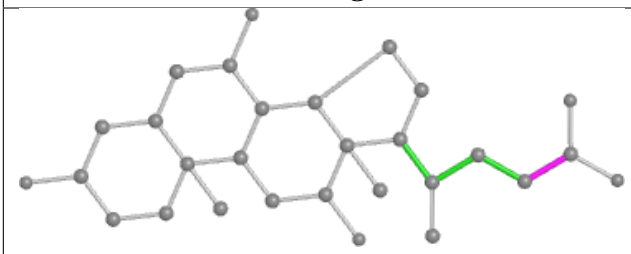
Ligand CHD C 301



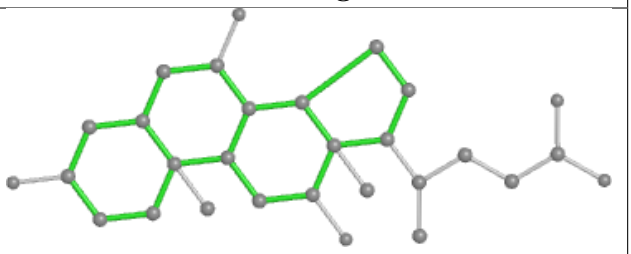
Bond lengths



Bond angles

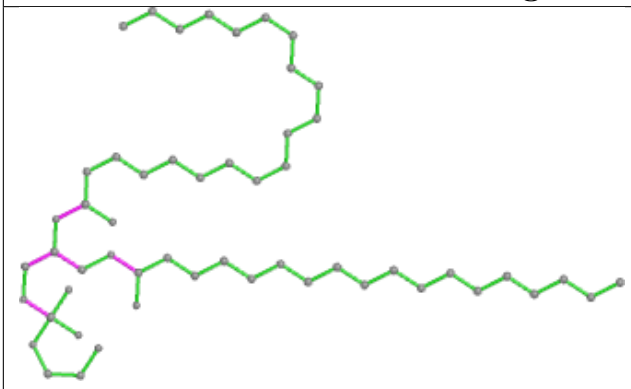


Torsions

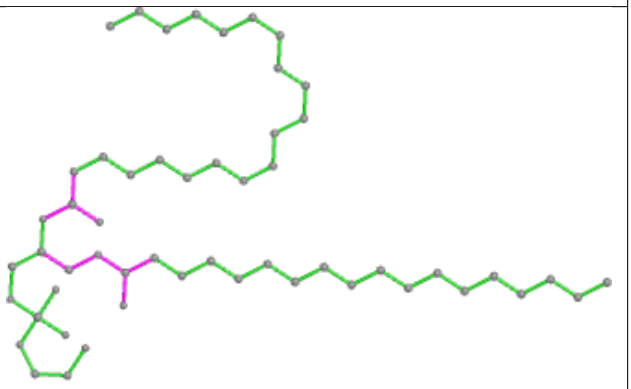


Rings

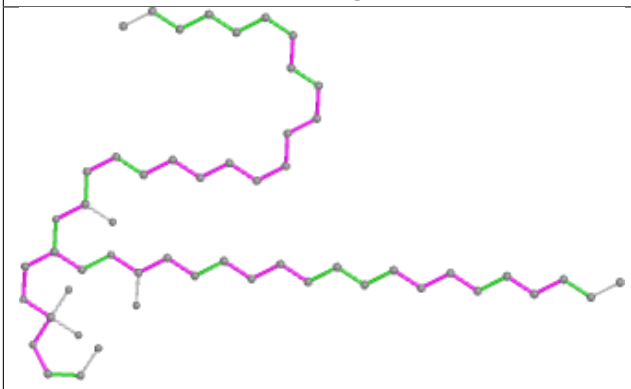
Ligand PEK G 104



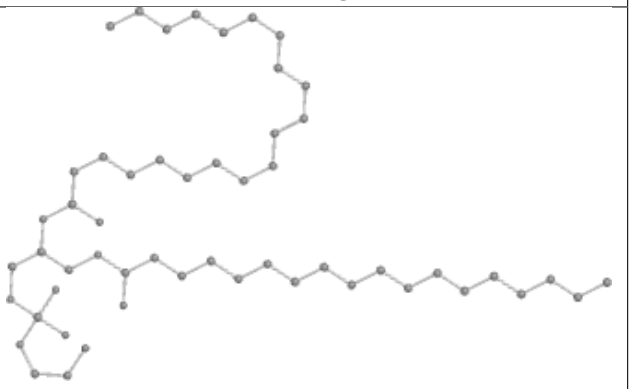
Bond lengths



Bond angles

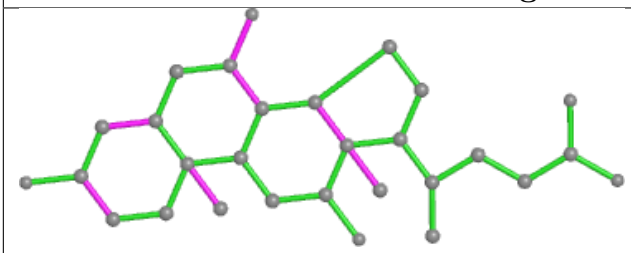


Torsions

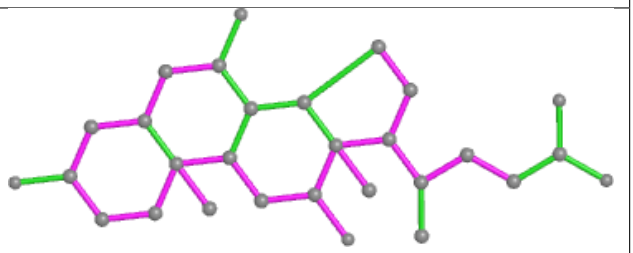


Rings

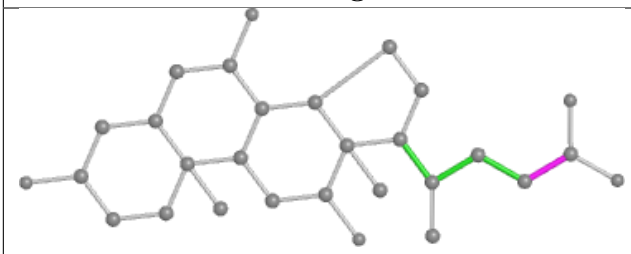
Ligand CHD G 103



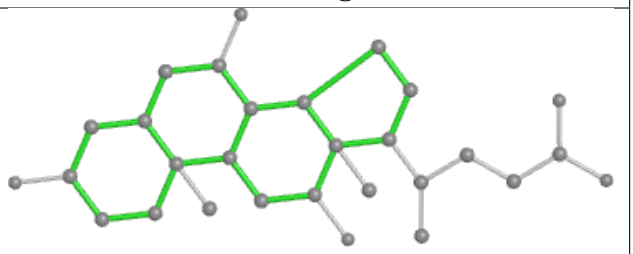
Bond lengths



Bond angles

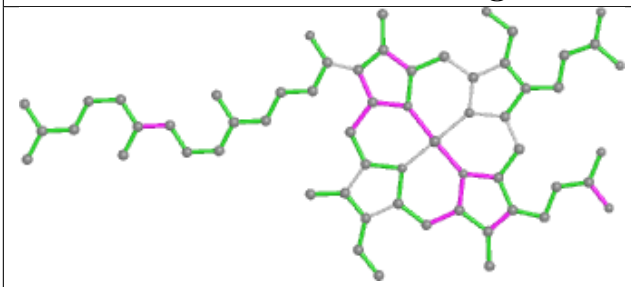


Torsions

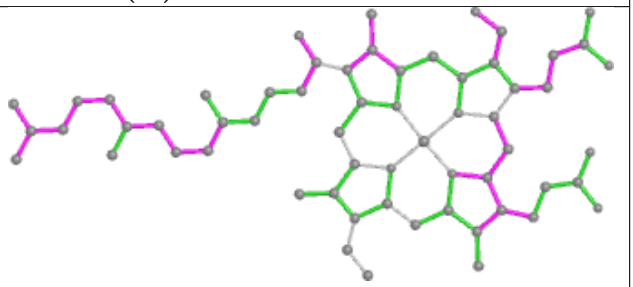


Rings

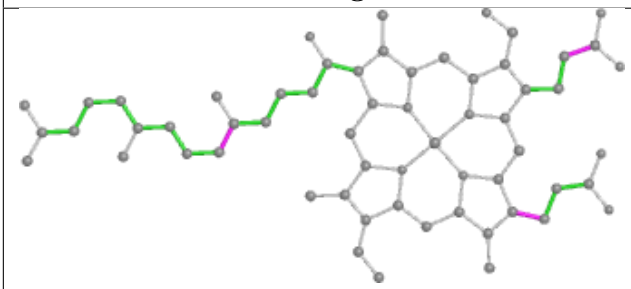
Ligand HEA N 602 (B)



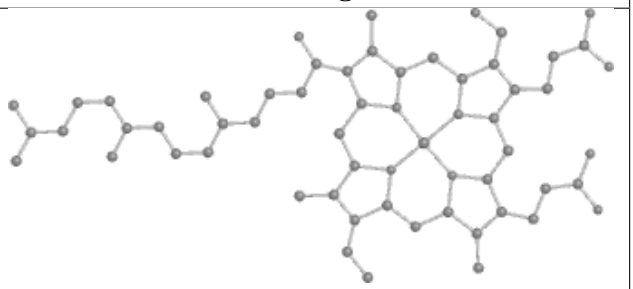
Bond lengths



Bond angles

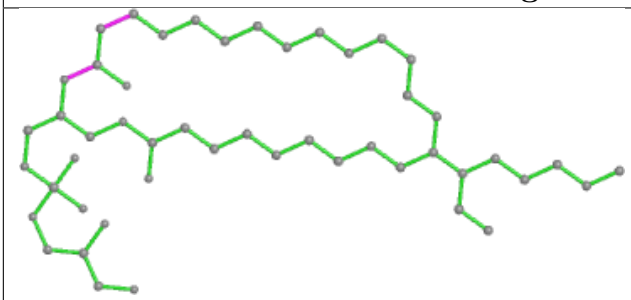


Torsions

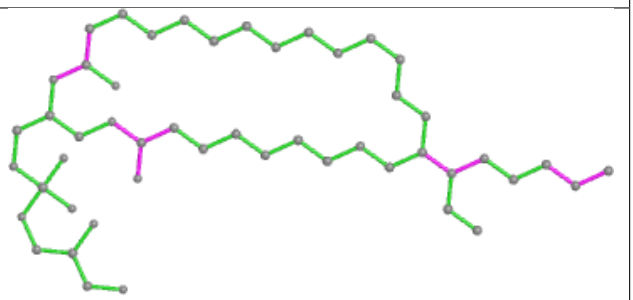


Rings

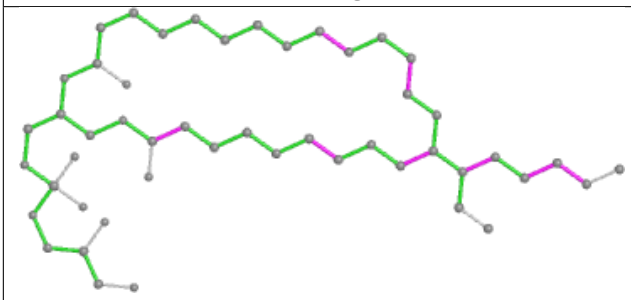
Ligand PGV A 609



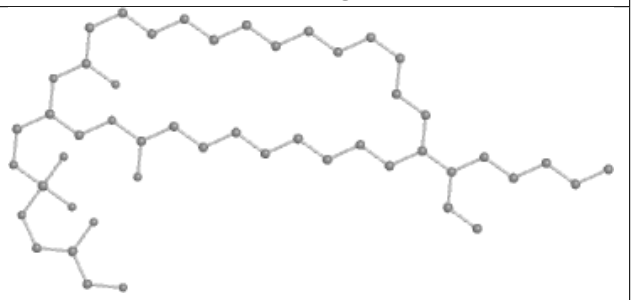
Bond lengths



Bond angles

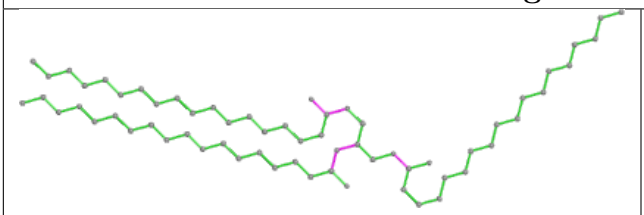


Torsions

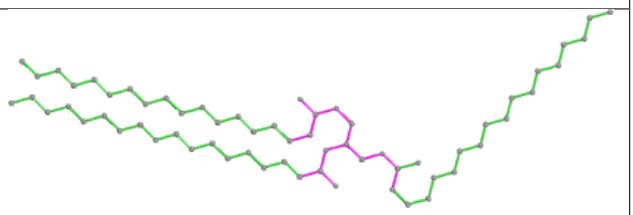


Rings

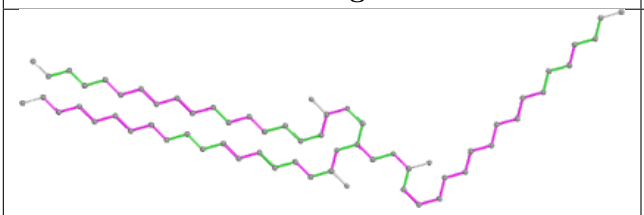
Ligand TGL A 608



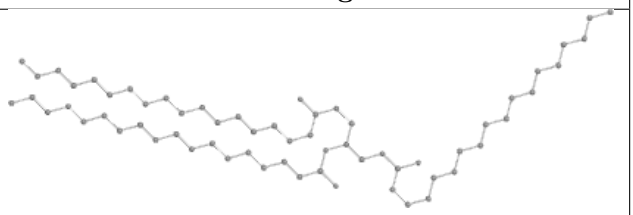
Bond lengths



Bond angles

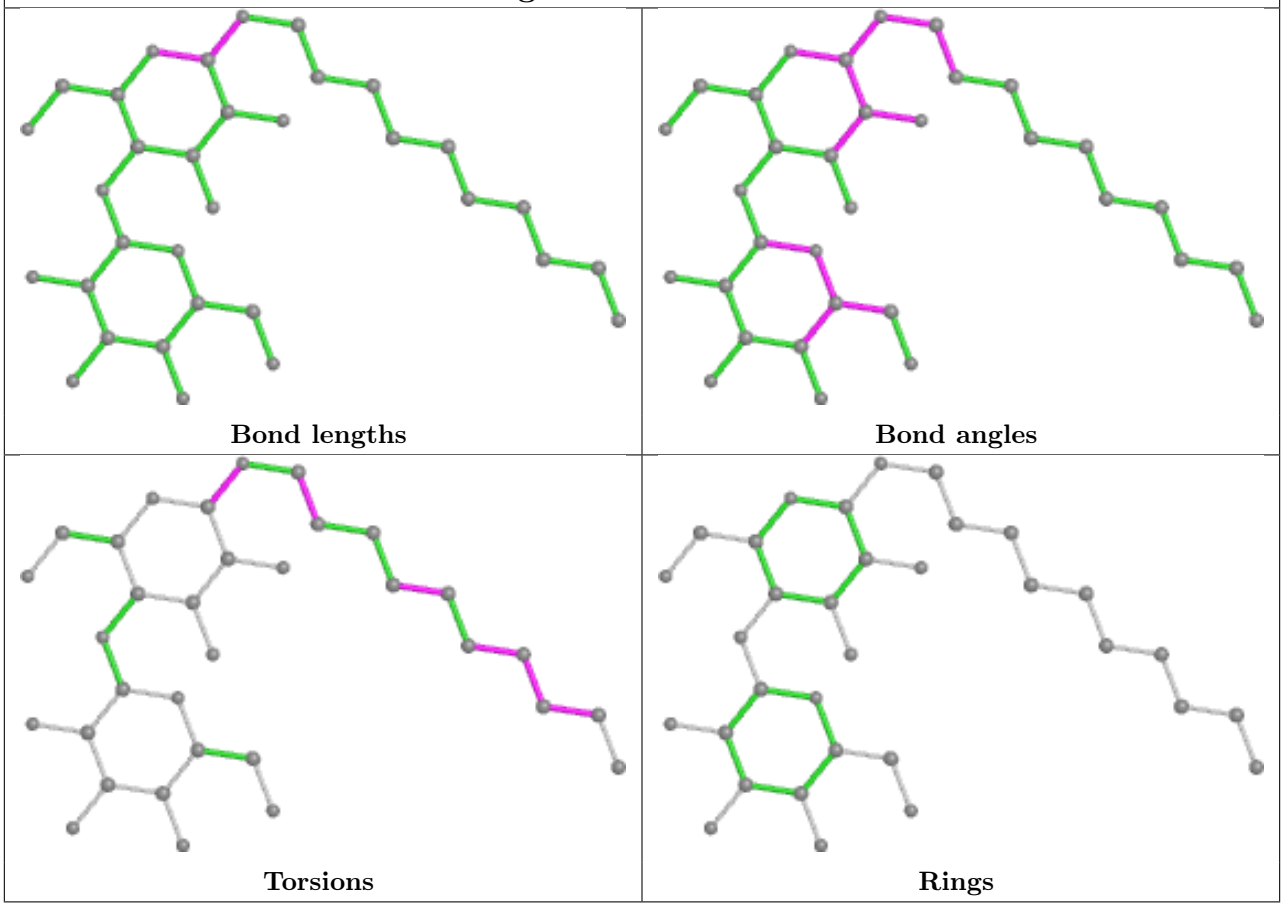


Torsions

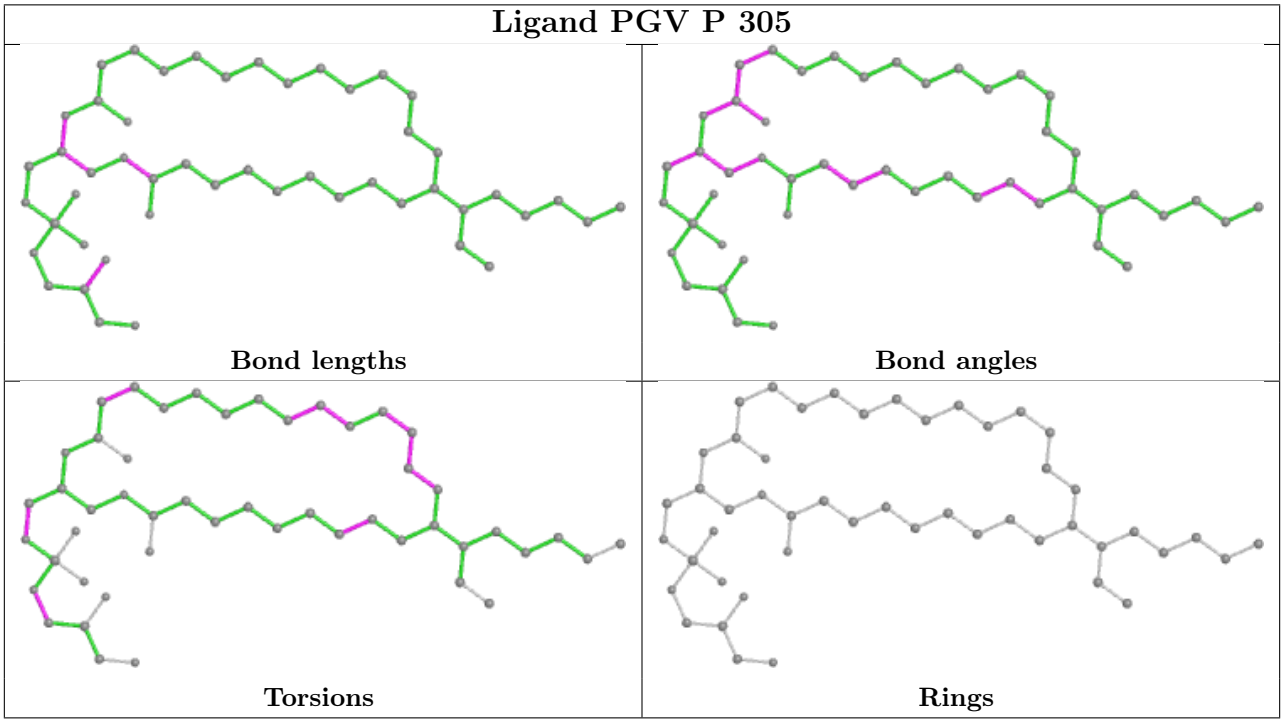


Rings

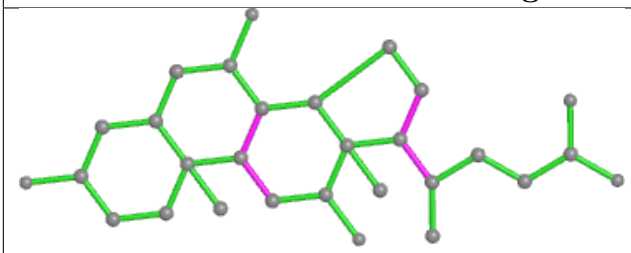
Ligand DMU C 302



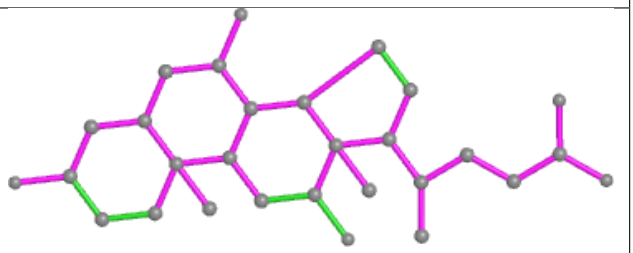
Ligand PGV P 305



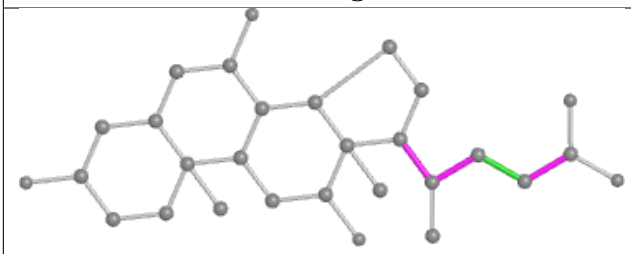
Ligand CHD P 307



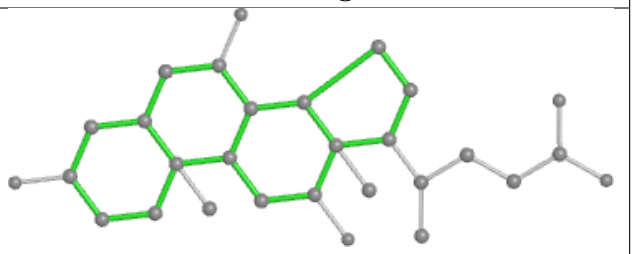
Bond lengths



Bond angles

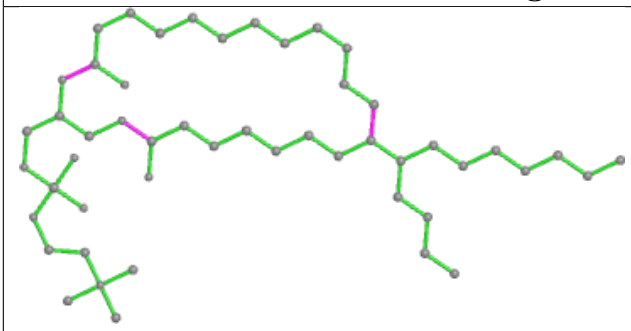


Torsions

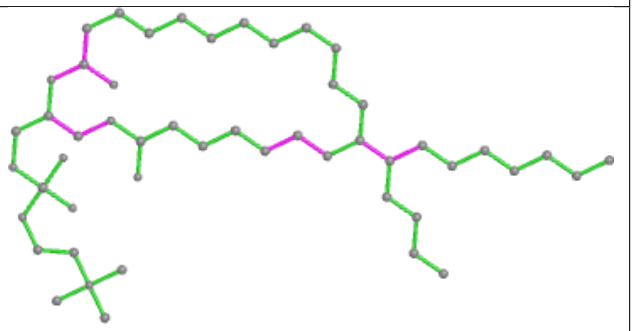


Rings

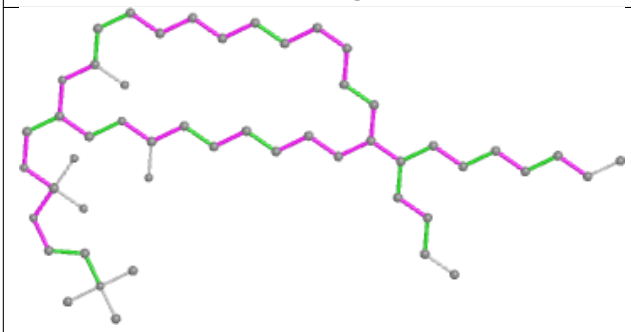
Ligand PSC O 302



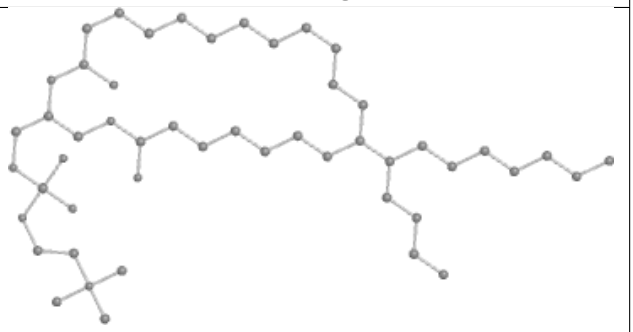
Bond lengths



Bond angles

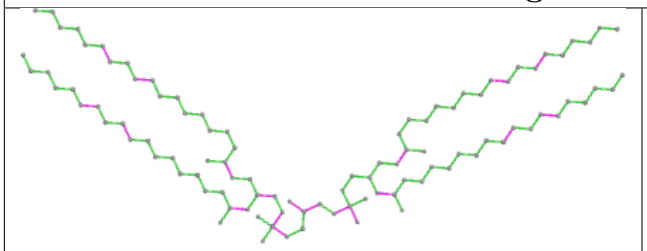


Torsions

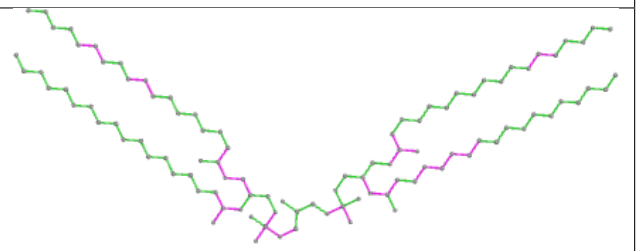


Rings

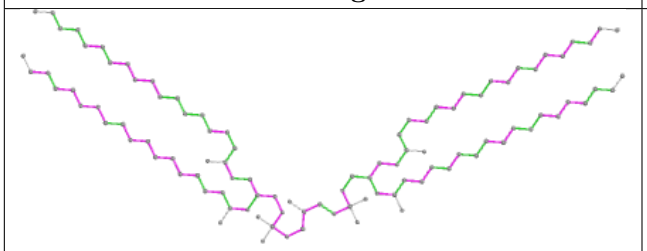
Ligand CDL P 306



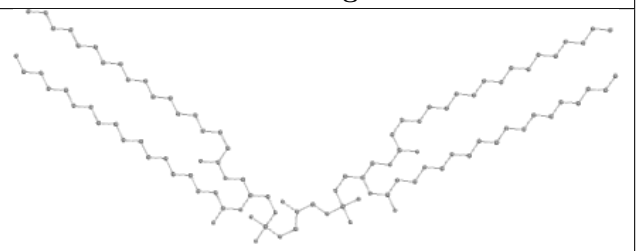
Bond lengths



Bond angles

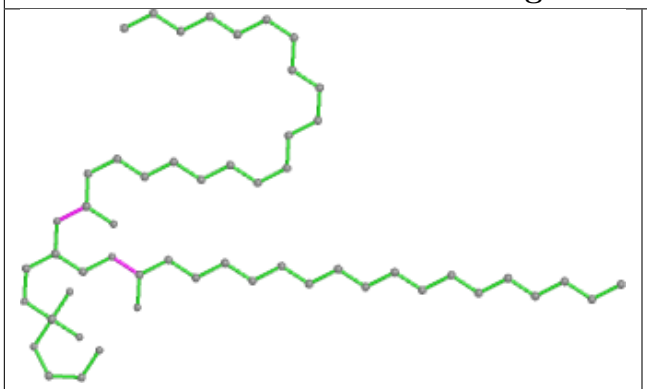


Torsions

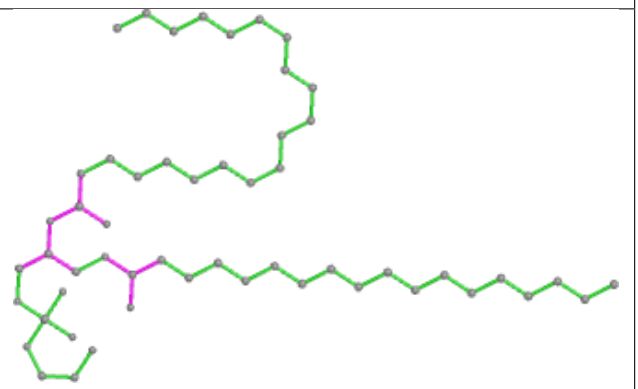


Rings

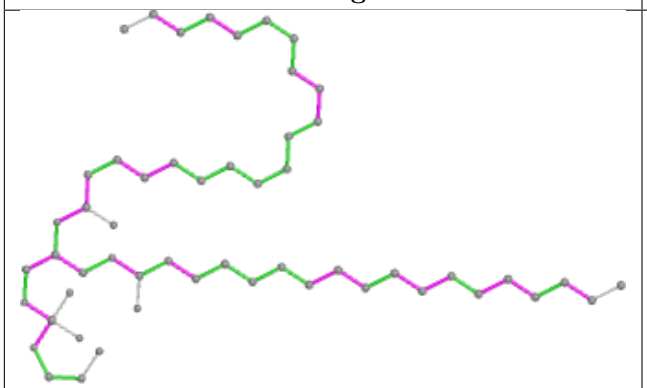
Ligand PEK P 309



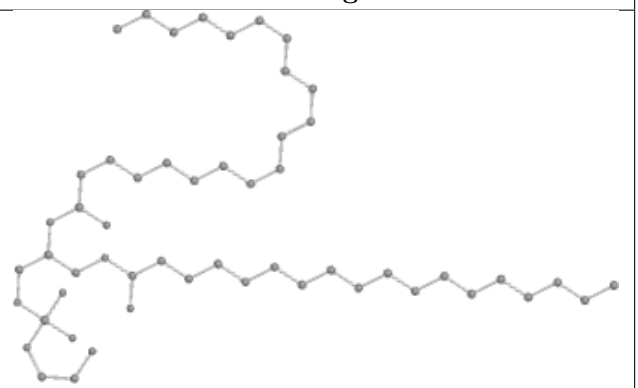
Bond lengths



Bond angles

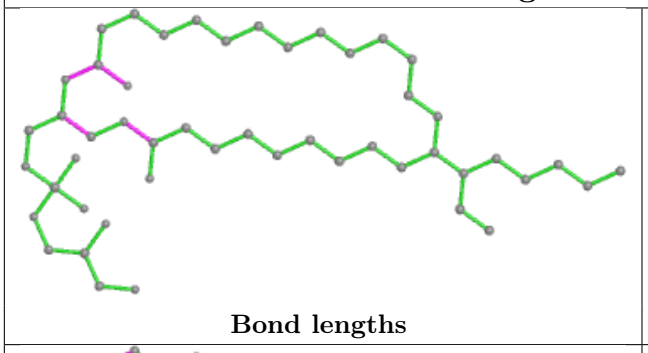


Torsions

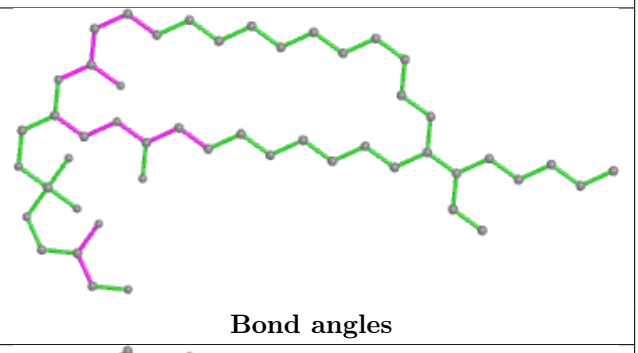


Rings

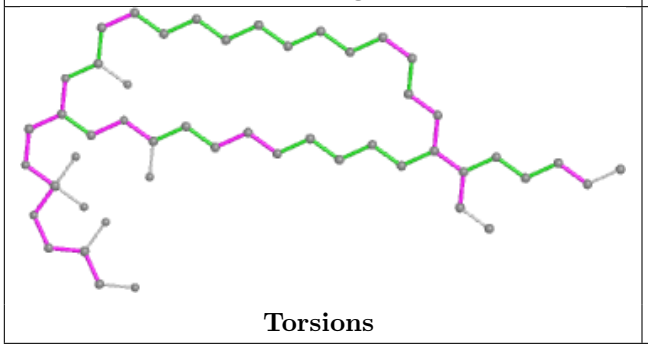
Ligand PGV M 101



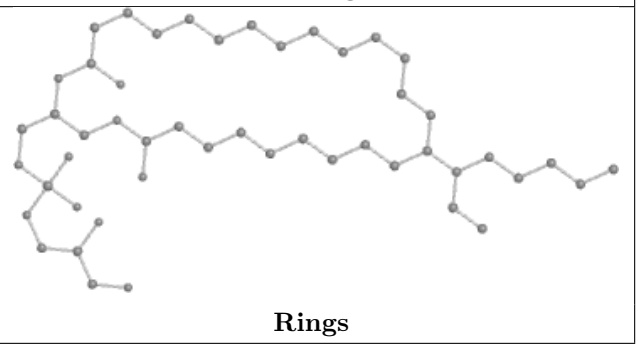
Bond lengths



Bond angles

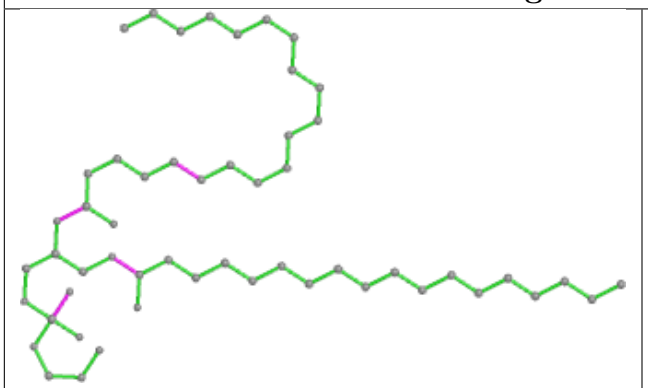


Torsions

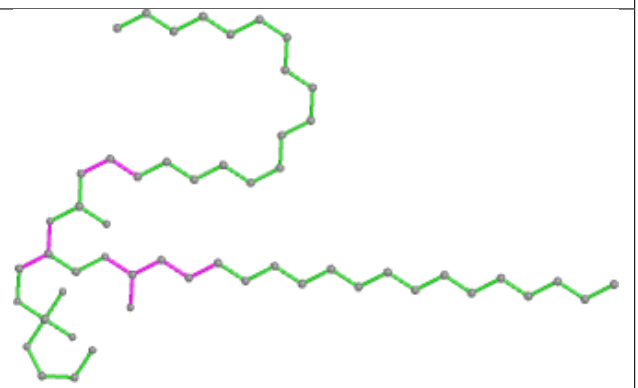


Rings

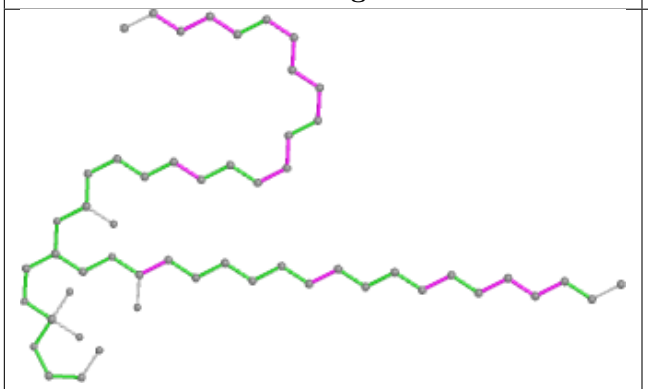
Ligand PEK P 304



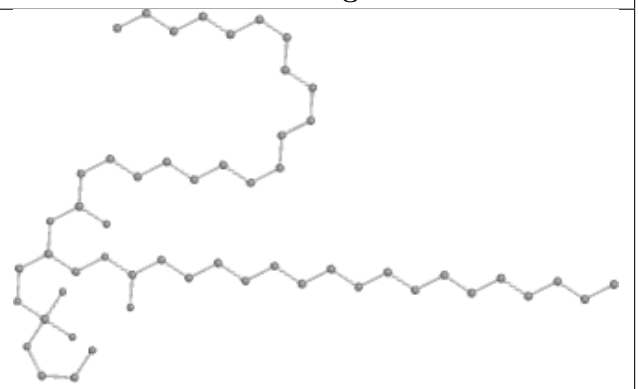
Bond lengths



Bond angles

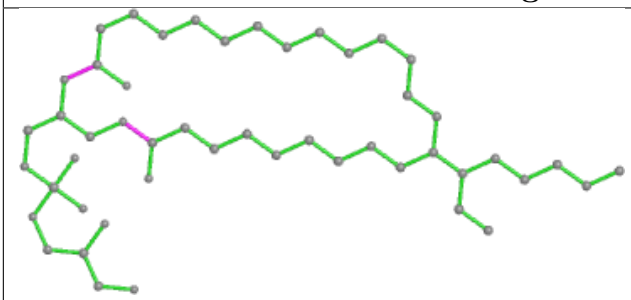


Torsions

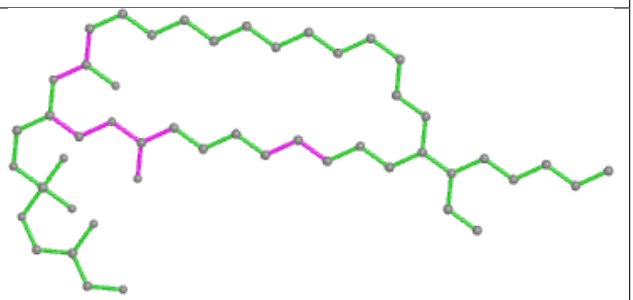


Rings

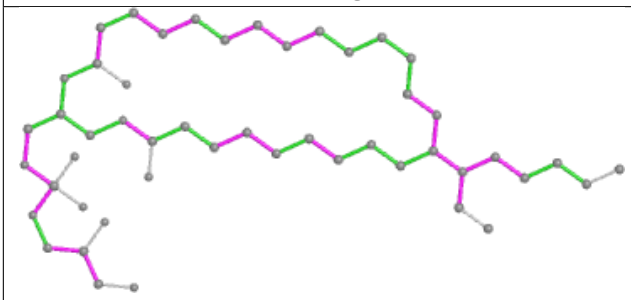
Ligand PGV C 308



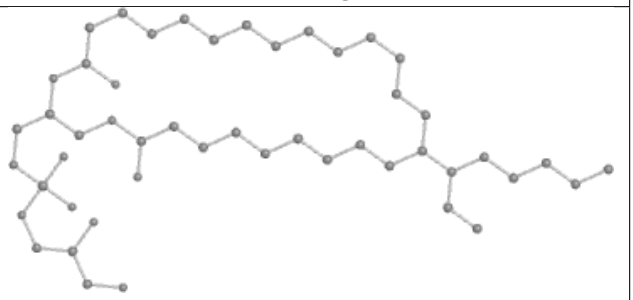
Bond lengths



Bond angles

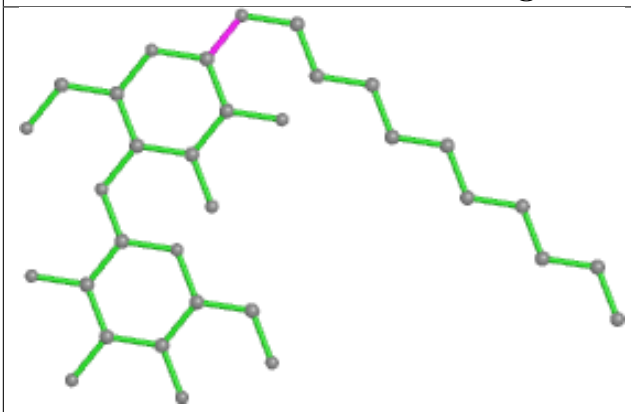


Torsions

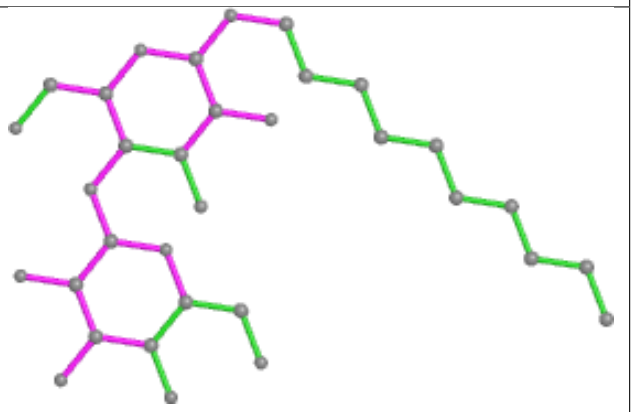


Rings

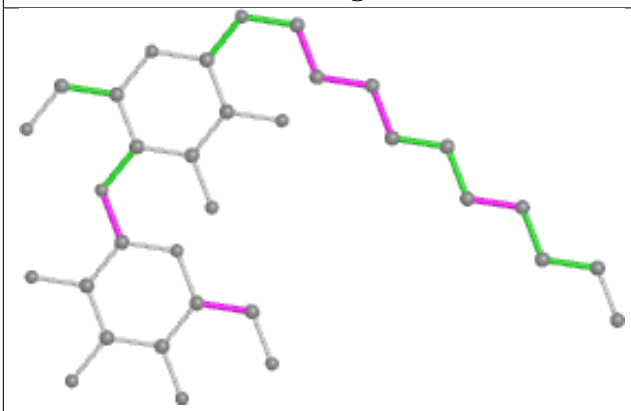
Ligand DMU P 310



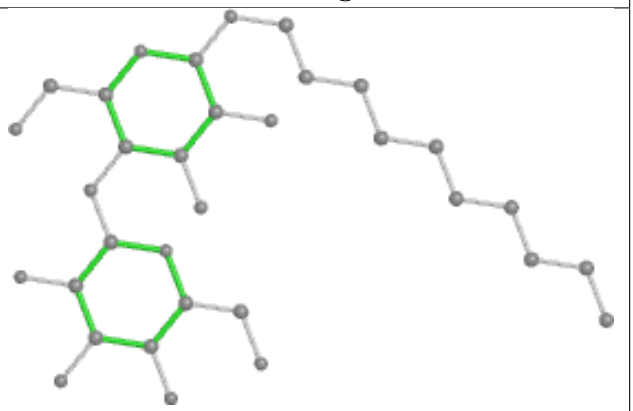
Bond lengths



Bond angles

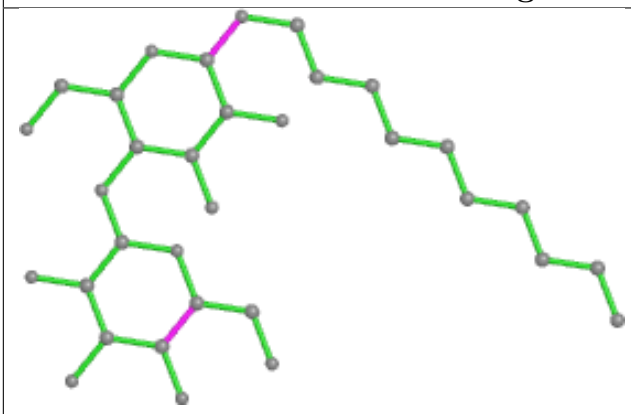


Torsions

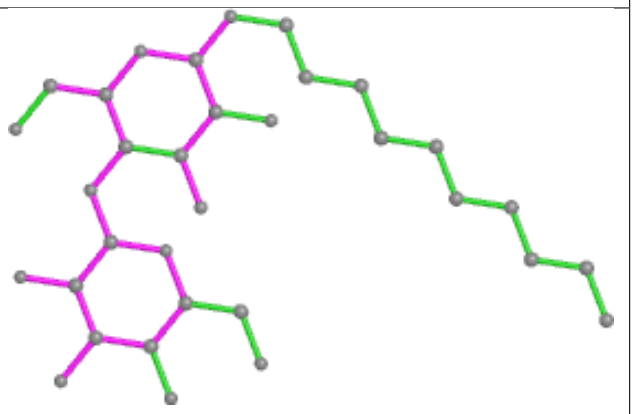


Rings

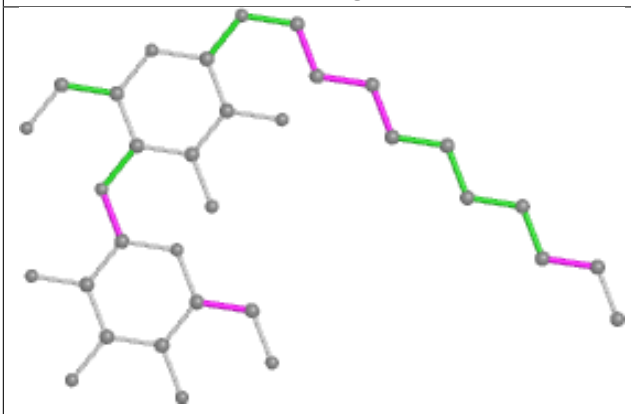
Ligand DMU C 309



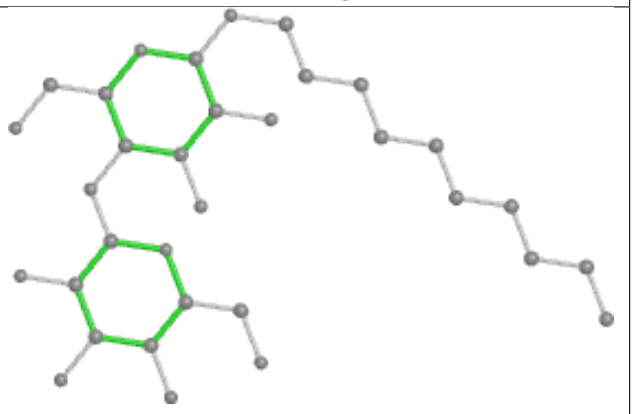
Bond lengths



Bond angles

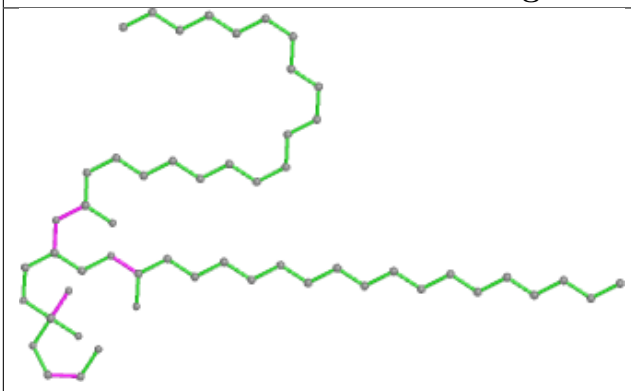


Torsions

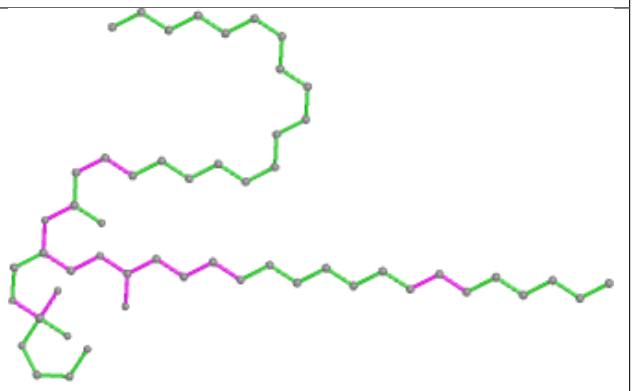


Rings

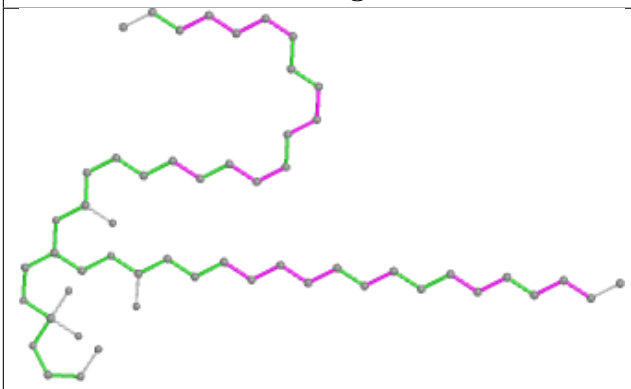
Ligand PEK G 101



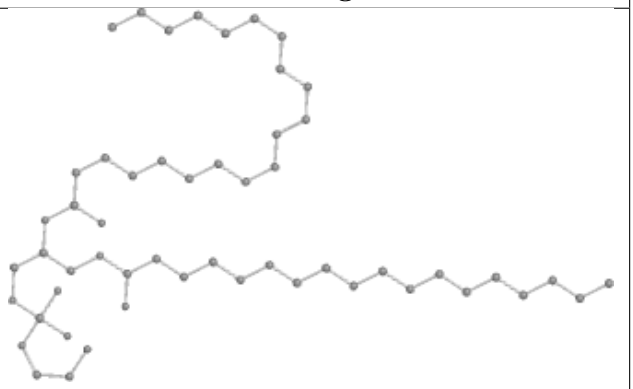
Bond lengths



Bond angles

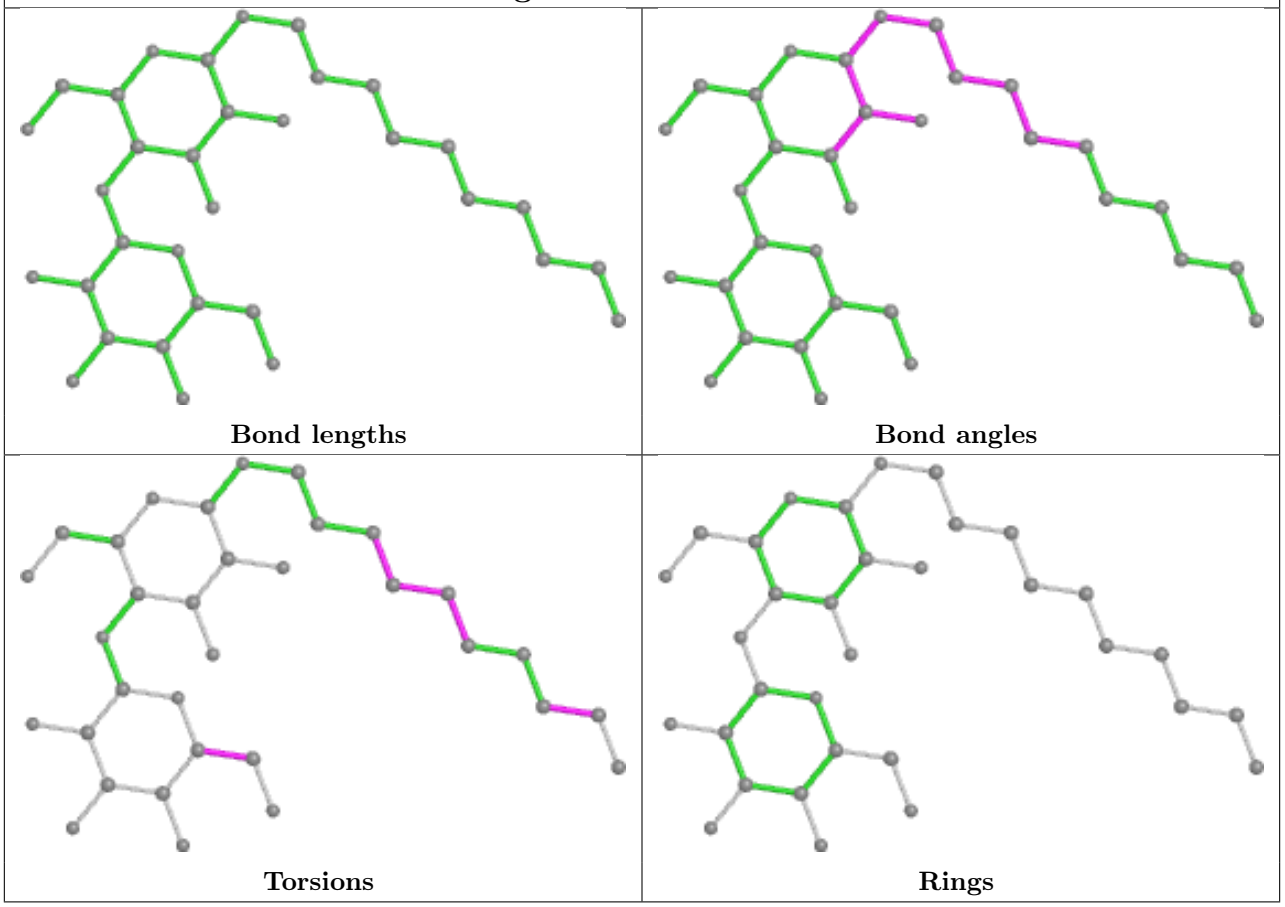


Torsions

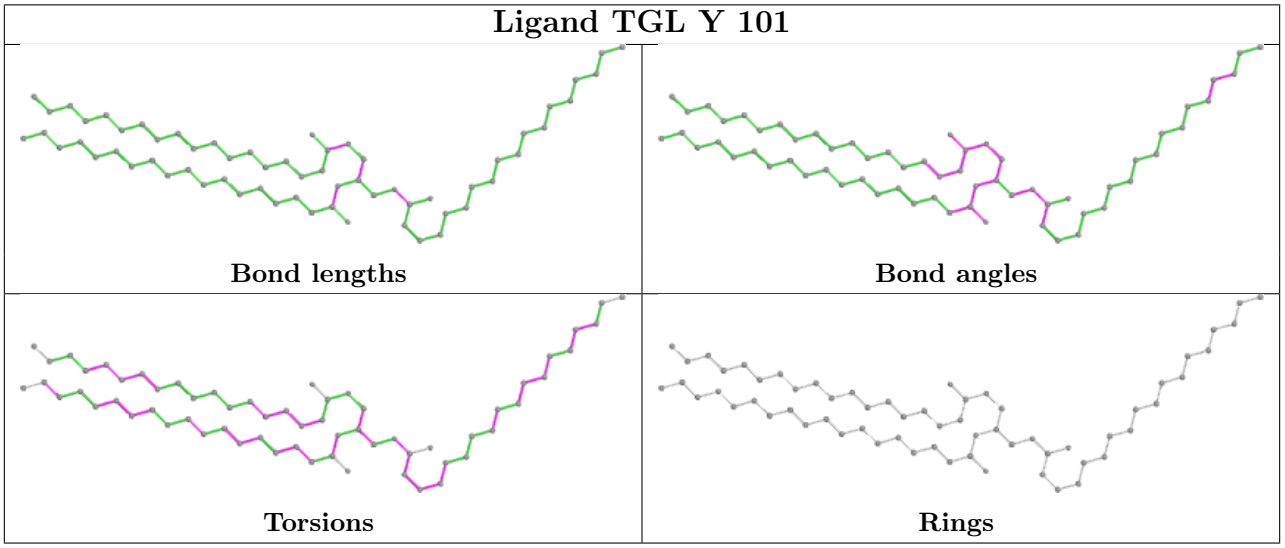


Rings

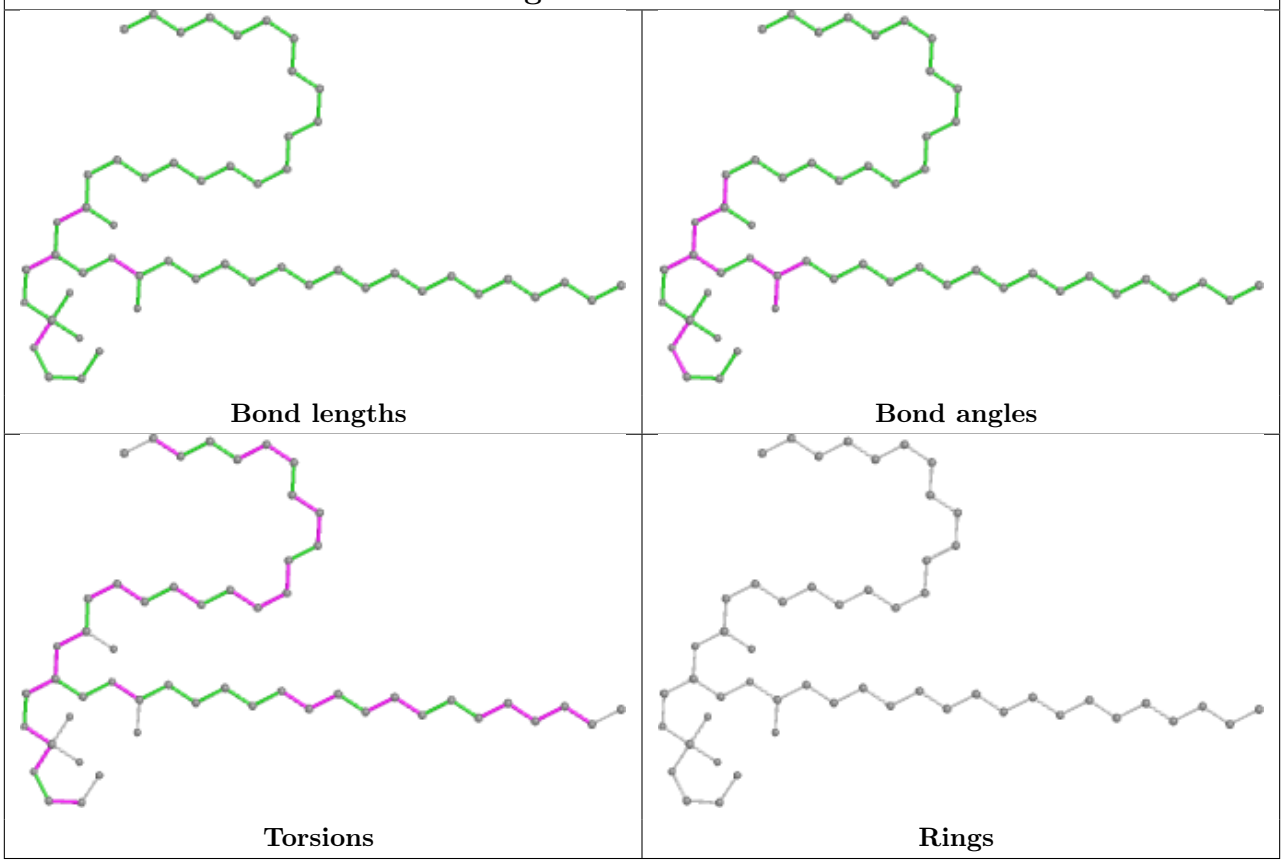
Ligand DMU M 102



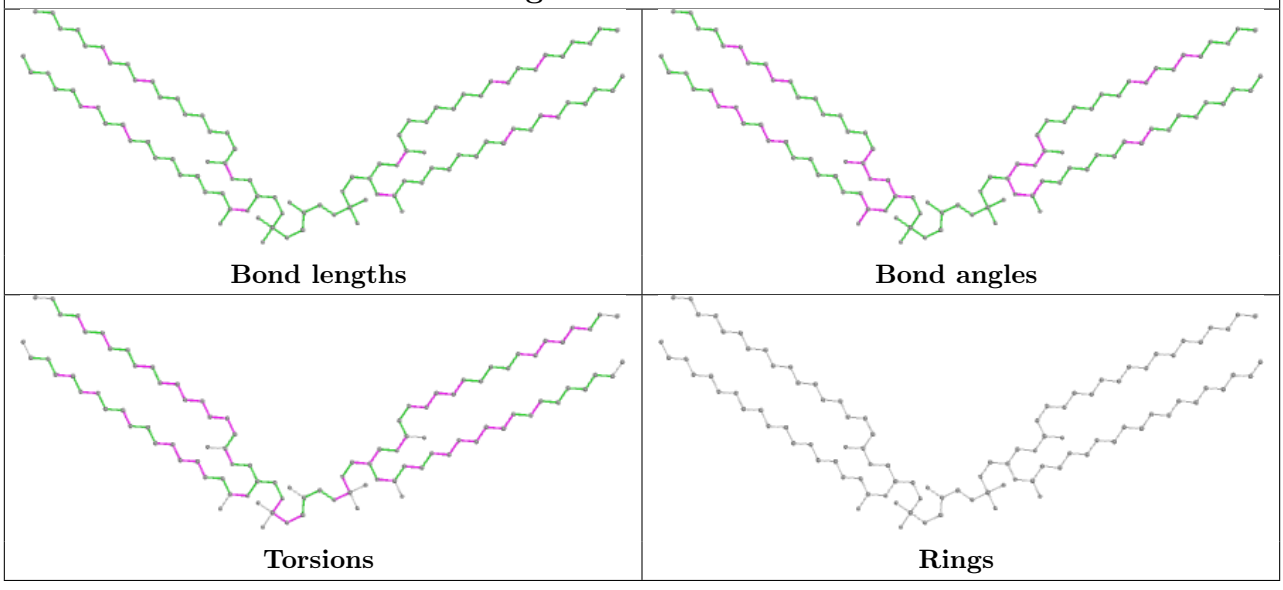
Ligand TGL Y 101



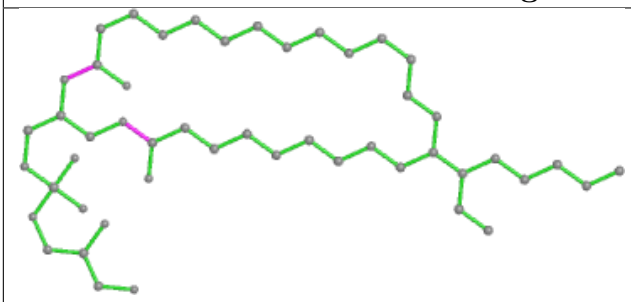
Ligand PEK C 307



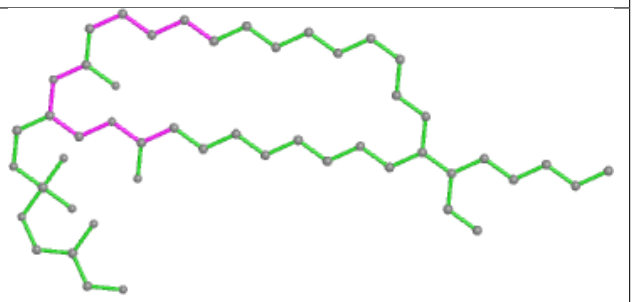
Ligand CDL T 103



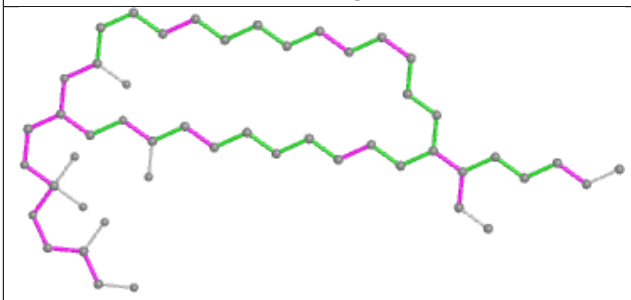
Ligand PGV N 608



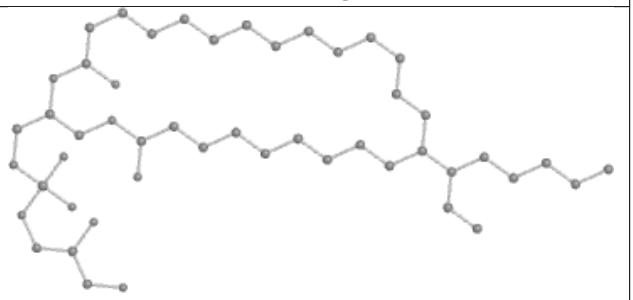
Bond lengths



Bond angles

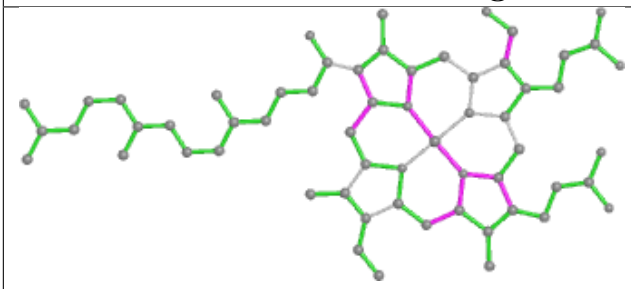


Torsions

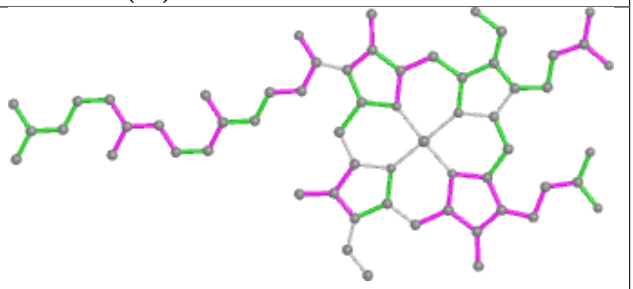


Rings

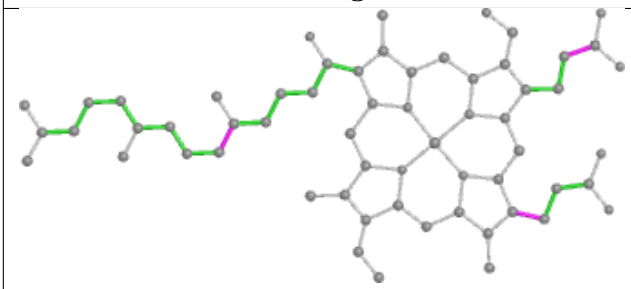
Ligand HEA A 602 (B)



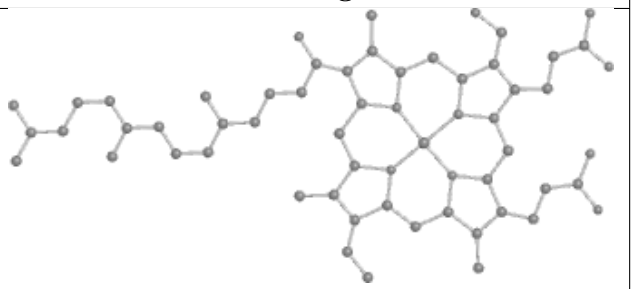
Bond lengths



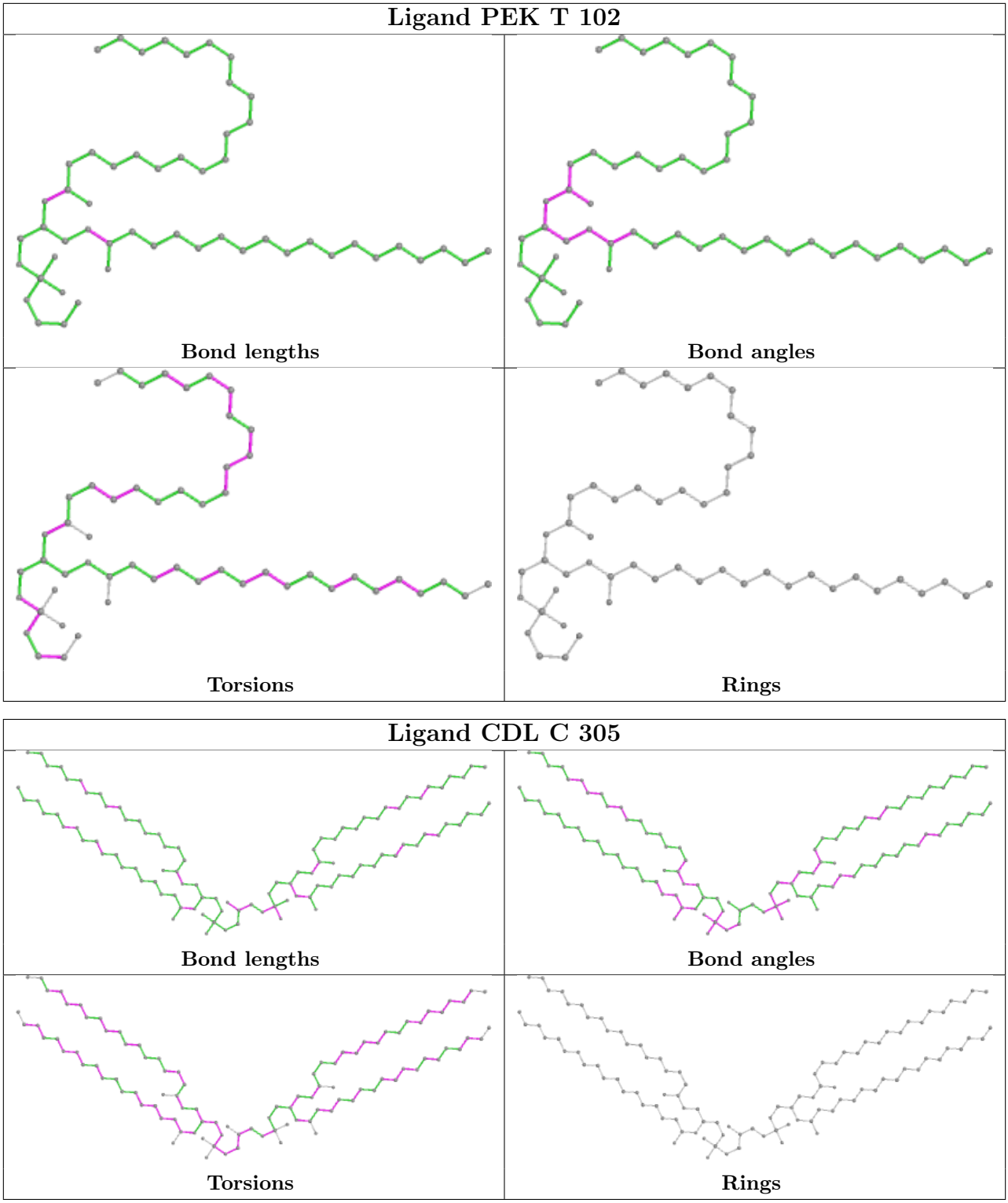
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.04	0 100 100	20, 25, 33, 69	0
1	N	513/514 (99%)	-0.09	1 (0%) 95 94	22, 30, 40, 72	0
2	B	226/227 (99%)	-0.04	3 (1%) 77 78	23, 33, 53, 77	0
2	O	226/227 (99%)	-0.02	3 (1%) 77 78	29, 40, 65, 85	0
3	C	259/261 (99%)	-0.03	0 100 100	22, 29, 41, 79	0
3	P	259/261 (99%)	-0.05	3 (1%) 79 79	24, 30, 42, 65	0
4	D	144/147 (97%)	-0.16	2 (1%) 75 76	25, 34, 55, 77	0
4	Q	144/147 (97%)	0.46	9 (6%) 20 19	35, 48, 74, 125	0
5	E	105/109 (96%)	-0.17	2 (1%) 66 66	26, 33, 57, 116	0
5	R	105/109 (96%)	-0.13	2 (1%) 66 66	32, 41, 60, 113	0
6	F	98/98 (100%)	0.36	7 (7%) 16 15	25, 37, 93, 130	0
6	S	98/98 (100%)	0.54	8 (8%) 11 11	25, 37, 91, 133	0
7	G	83/85 (97%)	0.87	14 (16%) 1 1	28, 38, 109, 137	0
7	T	83/85 (97%)	0.85	16 (19%) 1 1	27, 40, 97, 133	0
8	H	79/85 (92%)	0.23	7 (8%) 9 9	30, 41, 90, 95	0
8	U	79/85 (92%)	0.41	6 (7%) 13 13	35, 45, 96, 124	0
9	I	72/73 (98%)	0.36	5 (6%) 16 16	31, 44, 75, 89	0
9	V	72/73 (98%)	0.45	5 (6%) 16 16	31, 53, 77, 99	0
10	J	58/59 (98%)	0.29	4 (6%) 16 16	29, 39, 65, 120	0
10	W	58/59 (98%)	0.21	2 (3%) 45 42	33, 44, 70, 110	0
11	K	49/56 (87%)	-0.04	0 100 100	33, 40, 55, 60	0
11	X	49/56 (87%)	0.35	4 (8%) 11 11	42, 50, 70, 78	0
12	L	46/47 (97%)	-0.01	1 (2%) 62 61	26, 32, 50, 85	0
12	Y	46/47 (97%)	0.04	1 (2%) 62 61	33, 41, 58, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.10	1 (2%) 60 59	27, 31, 66, 101	0
13	Z	43/46 (93%)	0.42	4 (9%) 8 8	39, 44, 76, 115	0
All	All	3550/3614 (98%)	0.10	110 (3%) 49 47	20, 34, 66, 137	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.0
7	G	10	GLY	15.2
4	Q	6	VAL	13.4
6	S	1	ALA	12.6
4	Q	5	VAL	10.5
6	F	1	ALA	10.4
10	J	58	LYS	10.2
7	G	3	ALA	9.9
6	F	98	HIS	9.7
4	Q	8	SER	9.6
6	F	97	ALA	8.9
7	T	3	ALA	8.8
5	R	109	VAL	8.6
13	Z	43	SER	8.3
4	Q	4	SER	8.0
8	U	45	ALA	7.5
6	S	96	LEU	7.4
4	Q	7	LYS	7.2
10	W	58	LYS	7.0
7	G	40	GLY	6.9
6	F	96	LEU	6.8
6	S	94	HIS	6.7
6	S	98	HIS	6.5
8	U	7	LYS	6.4
6	S	2	SER	6.3
13	Z	42	LYS	6.0
7	T	10	GLY	5.6
5	R	5	HIS	5.5
8	U	8	ILE	5.4
9	V	2	THR	5.4
6	F	95	GLN	5.1
7	T	1	ALA	5.0
6	F	94	HIS	5.0
7	G	6	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
7	T	40	GLY	4.9
9	V	37	PHE	4.8
6	F	2	SER	4.8
9	I	25	PHE	4.8
7	G	2	SER	4.8
8	H	46	LYS	4.7
7	G	9	GLY	4.6
9	I	30	GLY	4.6
2	O	227	LEU	4.6
7	T	39	SER	4.6
7	T	2	SER	4.6
7	T	8	HIS	4.5
10	J	1	PHE	4.4
5	E	5	HIS	4.1
7	T	36	TRP	4.1
9	V	25	PHE	4.1
7	G	42	ARG	4.0
7	G	36	TRP	4.0
6	S	93	PRO	4.0
9	I	37	PHE	4.0
7	G	1	ALA	3.9
7	T	5	LYS	3.9
7	T	4	ALA	3.8
9	V	29	LEU	3.8
2	O	91	ASN	3.8
7	T	9	GLY	3.8
6	S	95	GLN	3.8
8	U	10	ASN	3.7
12	Y	47	LYS	3.7
7	G	5	LYS	3.7
7	G	7	ASP	3.7
2	O	113	TYR	3.6
11	X	13	TYR	3.6
7	T	6	GLY	3.6
7	T	42	ARG	3.5
9	I	29	LEU	3.5
10	W	57	HIS	3.5
9	I	33	THR	3.4
9	V	34	PHE	3.3
8	H	44	THR	3.3
7	T	84	LYS	3.2
8	H	45	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	109	VAL	3.2
4	D	4	SER	3.1
13	M	42	LYS	3.0
8	U	49	ASP	3.0
4	Q	147	LYS	2.9
11	X	7	PRO	2.9
8	H	48	GLY	2.9
3	P	3	HIS	2.9
11	X	6	ALA	2.8
8	H	47	GLY	2.8
4	Q	87[A]	PHE	2.7
10	J	52	TRP	2.6
7	T	41	HIS	2.5
3	P	33[A]	MET	2.5
8	H	7	LYS	2.5
4	Q	10	ASP	2.3
7	G	84	LYS	2.3
2	B	59	GLN	2.2
8	H	43	MET	2.2
10	J	57	HIS	2.2
12	L	2	HIS	2.2
3	P	38	ASN	2.2
8	U	48	GLY	2.2
13	Z	40	TYR	2.2
4	D	5	VAL	2.1
7	G	4	ALA	2.1
2	B	60	GLU	2.1
11	X	52	GLU	2.1
7	T	7	ASP	2.1
2	B	40	TYR	2.1
1	N	311[A]	ILE	2.1
7	G	41	HIS	2.0
13	Z	41	LYS	2.0
4	Q	33	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	0.27	0.44	113,119,130,131	0
7	TPO	G	11	11/12	0.36	0.39	91,100,118,123	0
7	TPO	T	11	11/12	0.37	0.43	104,118,157,157	0
9	SAC	I	1	9/10	0.84	0.25	64,73,78,78	0
1	FME	A	1	10/11	0.96	0.12	36,45,72,87	0
1	FME	N	1	10/11	0.97	0.13	41,50,72,76	0
2	FME	O	1	10/11	0.98	0.11	37,39,48,60	0
2	FME	B	1	10/11	0.99	0.13	29,30,41,66	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	C	318	4/4	0.45	0.83	74,101,105,116	0
21	EDO	Q	204	4/4	0.61	0.21	64,68,71,77	0
21	EDO	D	204	4/4	0.66	0.42	59,71,80,85	0
28	PEK	T	102	53/53	0.66	0.34	52,89,154,154	0
27	CDL	T	103	100/100	0.68	0.24	52,89,137,160	0
28	PEK	C	307	53/53	0.70	0.27	47,77,139,164	0
27	CDL	G	102	100/100	0.70	0.25	53,89,128,159	0
27	CDL	P	306	100/100	0.71	0.28	39,84,113,122	0
23	PSC	B	302	52/52	0.71	0.27	40,78,152,157	0
28	PEK	P	309	53/53	0.74	0.28	42,74,121,135	0
19	TGL	Q	201	63/63	0.75	0.21	48,73,95,107	0
28	PEK	G	104	53/53	0.75	0.26	48,77,135,152	0
21	EDO	S	103	4/4	0.76	0.29	61,68,69,70	0
21	EDO	Q	203	4/4	0.76	0.27	52,54,57,67	0
20	PGV	C	308	51/51	0.76	0.23	44,78,123,132	0
25	DMU	C	302	33/33	0.77	0.28	32,72,98,105	0
23	PSC	O	302	52/52	0.77	0.27	42,78,156,162	0
21	EDO	C	317	4/4	0.78	0.39	59,74,76,85	0
21	EDO	N	611	4/4	0.78	0.18	65,65,66,69	0
25	DMU	C	309	33/33	0.78	0.24	55,75,100,104	0
25	DMU	C	310	33/33	0.78	0.22	53,80,105,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	DMU	P	308	33/33	0.78	0.30	45,74,113,121	0
21	EDO	C	312	4/4	0.78	0.14	79,82,85,92	0
25	DMU	P	311	33/33	0.79	0.21	62,82,105,108	0
25	DMU	P	310	33/33	0.79	0.24	59,76,103,104	0
27	CDL	C	305	100/100	0.80	0.23	37,77,110,115	0
19	TGL	Y	101	63/63	0.80	0.23	41,74,110,136	0
24	CHD	P	307	29/29	0.81	0.25	53,67,73,77	0
20	PGV	P	302	51/51	0.82	0.23	48,76,122,137	0
19	TGL	L	101	63/63	0.83	0.21	32,59,93,112	0
21	EDO	A	616	4/4	0.83	0.21	47,50,53,66	0
19	TGL	D	201	63/63	0.83	0.18	33,61,85,90	0
20	PGV	N	608	51/51	0.83	0.26	47,78,115,127	0
24	CHD	C	306	29/29	0.83	0.28	49,64,71,73	0
21	EDO	C	314	4/4	0.84	0.25	55,65,65,66	0
21	EDO	R	204	4/4	0.84	0.35	52,55,58,60	0
21	EDO	A	619	4/4	0.84	0.19	55,58,58,60	0
25	DMU	Z	101	33/33	0.84	0.17	47,56,73,77	0
21	EDO	O	305	4/4	0.84	0.14	72,74,75,82	0
20	PGV	M	101	51/51	0.84	0.23	31,63,99,110	0
21	EDO	N	618	4/4	0.85	0.23	42,43,51,55	0
21	EDO	C	315	4/4	0.86	0.17	35,45,47,50	0
19	TGL	N	610	63/63	0.86	0.19	48,74,101,115	0
21	EDO	A	615	4/4	0.86	0.17	41,42,45,45	0
21	EDO	G	105	4/4	0.87	0.34	51,62,74,87	0
21	EDO	C	313	4/4	0.87	0.16	56,60,64,81	0
21	EDO	A	611	4/4	0.87	0.17	46,60,61,62	0
21	EDO	C	316	4/4	0.88	0.17	61,63,71,83	0
25	DMU	M	102	33/33	0.88	0.12	39,47,56,66	0
21	EDO	E	203	4/4	0.89	0.25	48,52,54,60	0
21	EDO	P	315	4/4	0.89	0.26	46,54,57,72	0
19	TGL	A	608	63/63	0.89	0.17	40,74,96,112	0
21	EDO	U	101	4/4	0.89	0.14	62,65,66,72	0
26	UNX	C	303	1/1	0.90	0.14	30,30,30,30	0
21	EDO	H	101	4/4	0.90	0.12	51,57,59,66	0
21	EDO	A	617	4/4	0.90	0.29	44,66,70,75	0
21	EDO	D	203	4/4	0.91	0.28	54,54,66,72	0
21	EDO	V	101	4/4	0.91	0.22	63,67,68,70	0
21	EDO	O	304	4/4	0.91	0.22	61,62,65,76	0
26	UNX	P	303	1/1	0.91	0.18	29,29,29,29	0
21	EDO	N	614	4/4	0.92	0.17	58,61,62,72	0
21	EDO	D	202	4/4	0.92	0.48	39,45,50,65	0
21	EDO	D	206	4/4	0.92	0.17	49,59,60,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	R	201	4/4	0.92	0.18	56,62,64,83	0
21	EDO	R	202	4/4	0.92	0.17	49,58,63,63	0
21	EDO	A	613	4/4	0.92	0.17	59,63,69,80	0
21	EDO	R	205	4/4	0.92	0.19	42,49,53,53	0
21	EDO	P	312	4/4	0.92	0.13	32,33,45,52	0
21	EDO	N	612	4/4	0.93	0.24	30,37,45,57	0
21	EDO	E	201	4/4	0.93	0.11	41,41,47,56	0
21	EDO	P	314	4/4	0.93	0.26	48,56,63,65	0
21	EDO	A	614	4/4	0.93	0.17	19,25,27,39	0
21	EDO	F	104	4/4	0.93	0.25	47,48,53,55	0
21	EDO	E	205	4/4	0.94	0.13	52,55,58,67	0
21	EDO	N	621	4/4	0.94	0.17	40,45,52,57	0
21	EDO	S	104	4/4	0.94	0.23	39,54,65,66	0
21	EDO	Q	202	4/4	0.95	0.12	58,58,64,64	0
21	EDO	A	618	4/4	0.95	0.43	43,51,65,69	0
21	EDO	C	319	4/4	0.95	0.23	32,42,46,58	0
16	MG	N	604	1/1	0.95	0.08	31,31,31,31	0
21	EDO	N	615	4/4	0.95	0.11	33,33,39,43	0
21	EDO	R	203	4/4	0.95	0.09	44,44,46,46	0
24	CHD	C	301	29/29	0.95	0.09	27,31,34,38	0
28	PEK	P	304	53/53	0.95	0.14	29,47,85,94	0
21	EDO	N	617	4/4	0.95	0.13	41,42,44,52	0
21	EDO	A	620	4/4	0.95	0.34	45,45,48,65	0
21	EDO	N	619	4/4	0.96	0.15	45,46,55,56	0
21	EDO	T	104	4/4	0.96	0.14	34,36,39,42	0
21	EDO	A	612	4/4	0.96	0.17	31,32,37,74	0
24	CHD	P	301	29/29	0.96	0.08	27,32,36,40	0
21	EDO	G	106	4/4	0.96	0.10	29,34,38,40	0
21	EDO	E	204	4/4	0.96	0.10	37,39,42,46	0
20	PGV	A	609	51/51	0.97	0.12	23,32,62,65	0
20	PGV	C	304	51/51	0.97	0.13	26,32,80,91	0
21	EDO	F	103	4/4	0.97	0.10	36,37,37,39	0
28	PEK	G	101	53/53	0.97	0.14	27,44,79,97	0
20	PGV	N	609	51/51	0.97	0.12	27,35,62,66	0
21	EDO	N	620	4/4	0.97	0.17	42,55,55,65	0
21	EDO	N	613	4/4	0.97	0.15	36,44,45,49	0
18	AZI	N	607	3/3	0.97	0.18	32,32,34,38	0
21	EDO	D	205	4/4	0.98	0.14	35,36,53,55	0
18	AZI	A	607	3/3	0.98	0.17	30,30,31,34	0
21	EDO	P	313	4/4	0.98	0.15	41,42,43,46	0
14	HEA	A	602[B]	60/60	0.98	0.14	18,22,33,37	60
14	HEA	N	601	60/60	0.98	0.11	25,28,48,50	0

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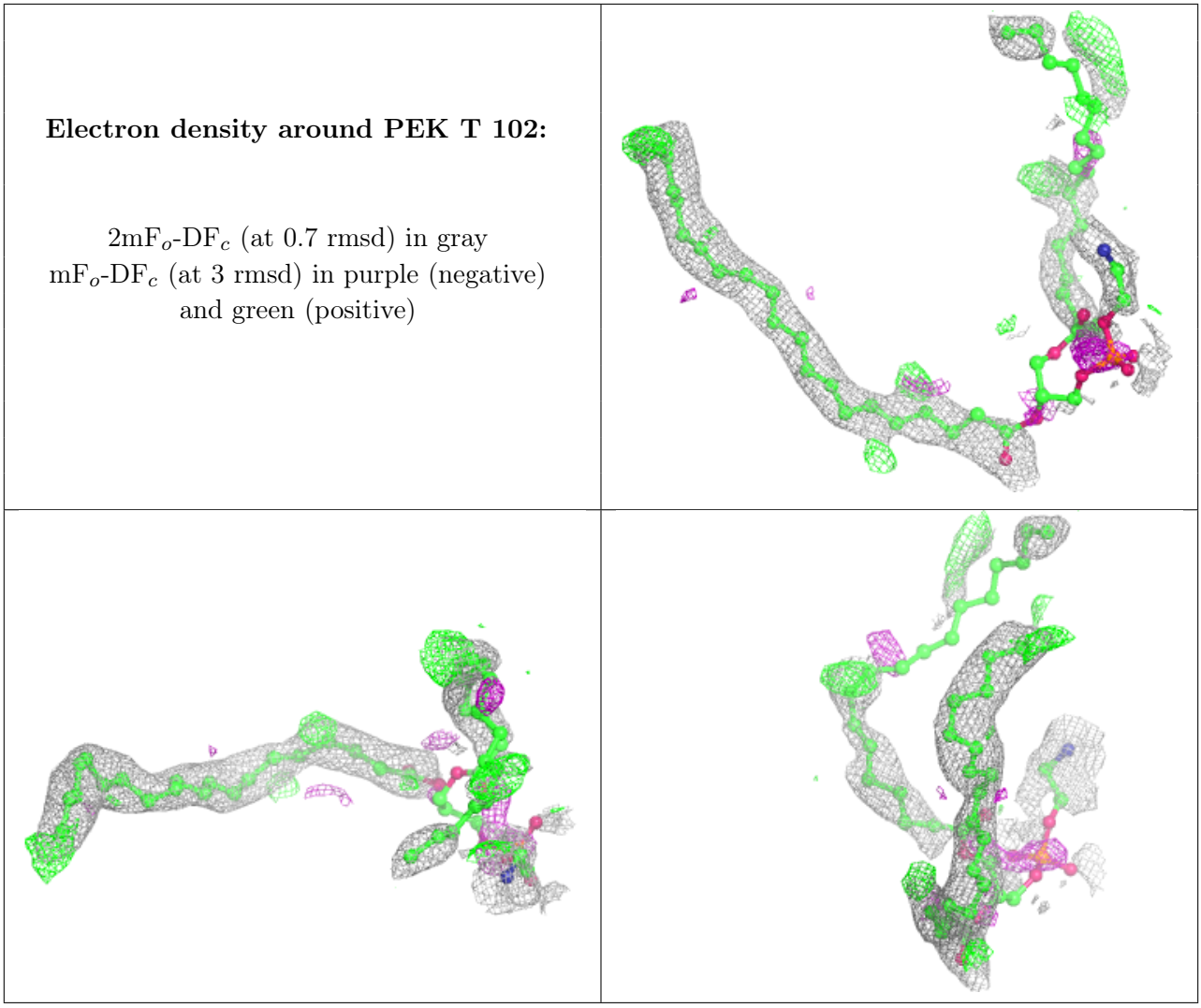
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	PGV	P	305	51/51	0.98	0.12	26,35,72,76	0
21	EDO	N	616	4/4	0.98	0.11	26,31,33,35	0
21	EDO	A	610	4/4	0.98	0.13	36,38,39,45	0
24	CHD	G	103	29/29	0.98	0.09	26,30,33,38	0
14	HEA	N	602[A]	60/60	0.98	0.15	21,25,29,31	60
14	HEA	N	602[B]	60/60	0.98	0.15	21,26,39,42	60
24	CHD	T	101	29/29	0.98	0.10	26,28,31,39	0
21	EDO	B	303	4/4	0.98	0.11	28,28,34,34	0
21	EDO	C	311	4/4	0.98	0.09	38,39,39,41	0
21	EDO	O	303	4/4	0.98	0.14	37,37,37,38	0
14	HEA	A	602[A]	60/60	0.98	0.14	18,22,25,27	60
21	EDO	E	202	4/4	0.99	0.15	37,39,43,45	0
21	EDO	S	102	4/4	0.99	0.13	28,29,30,31	0
17	NA	N	605	1/1	0.99	0.07	35,35,35,35	0
18	AZI	A	606	3/3	0.99	0.15	28,28,28,28	0
16	MG	A	604	1/1	0.99	0.09	24,24,24,24	0
21	EDO	F	102	4/4	0.99	0.10	24,25,26,28	0
14	HEA	A	601	60/60	0.99	0.12	19,23,45,45	0
22	CUA	O	301	2/2	0.99	0.14	31,31,31,32	0
17	NA	A	605	1/1	0.99	0.10	28,28,28,28	0
15	CU	N	603	1/1	1.00	0.16	28,28,28,28	0
18	AZI	N	606	3/3	1.00	0.13	33,33,34,35	0
22	CUA	B	301	2/2	1.00	0.17	25,25,25,26	0
15	CU	A	603	1/1	1.00	0.15	25,25,25,25	0
29	ZN	F	101	1/1	1.00	0.14	30,30,30,30	0
29	ZN	S	101	1/1	1.00	0.13	32,32,32,32	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.

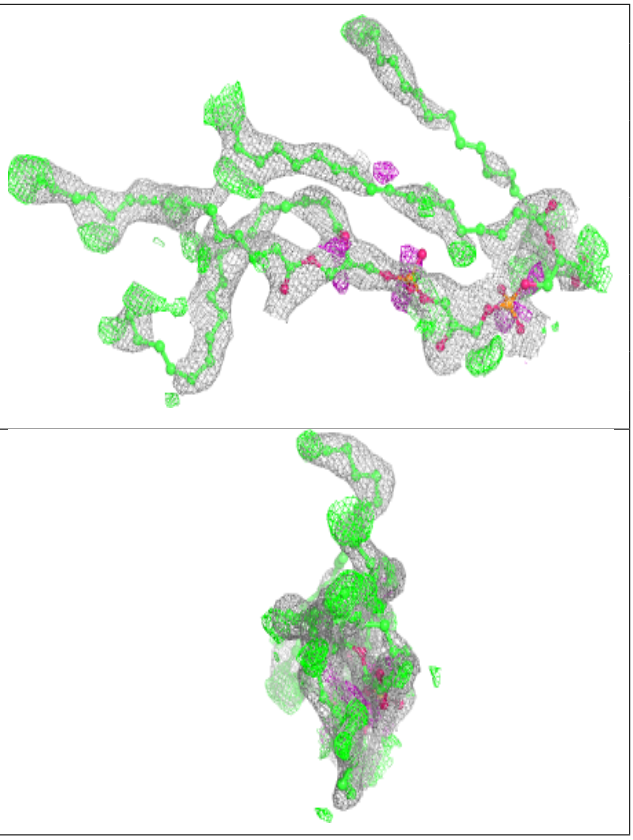
Electron density around PEK T 102:

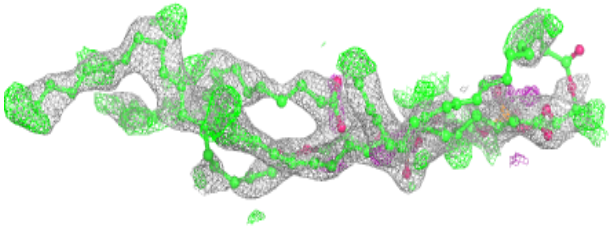
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CDL T 103:

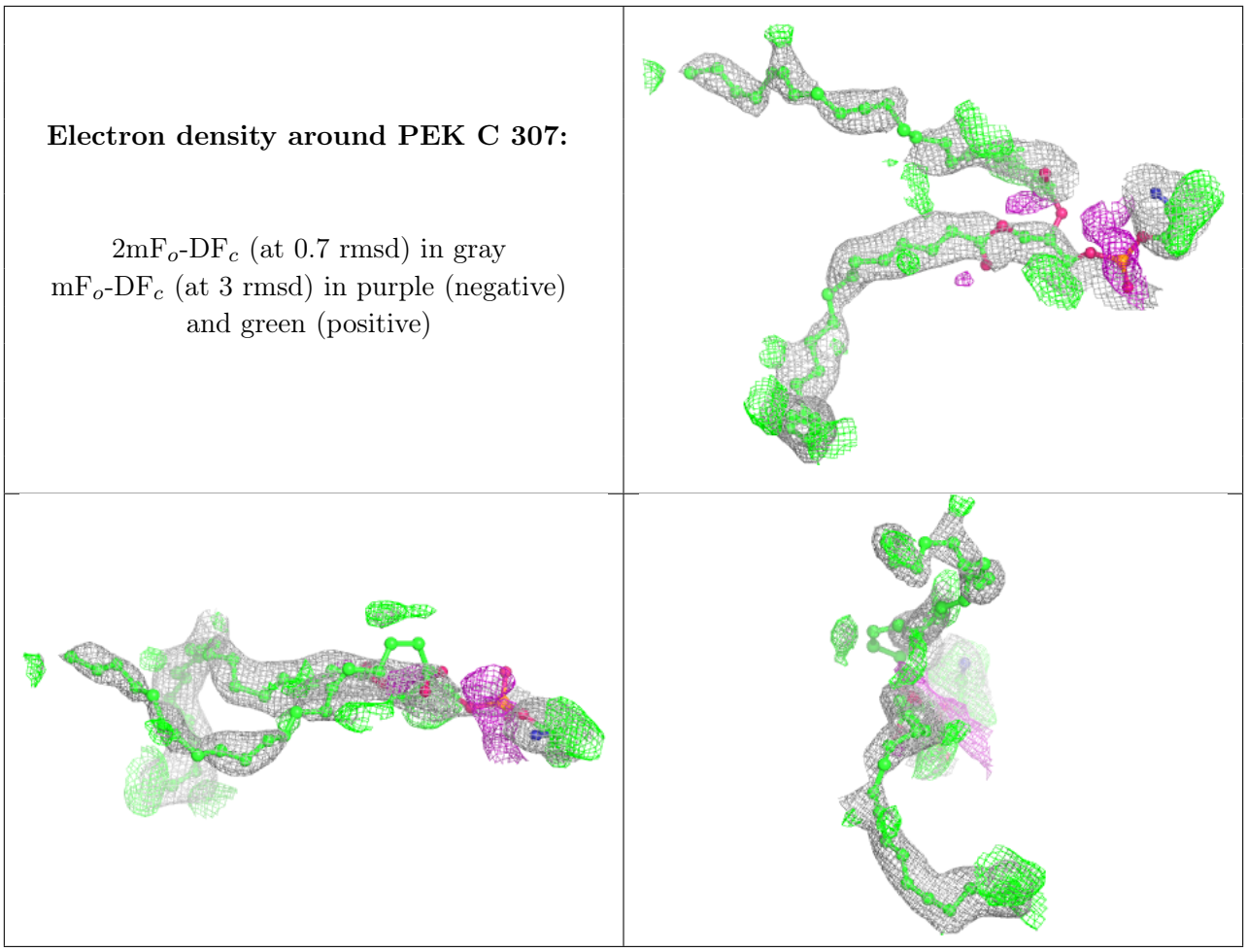
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





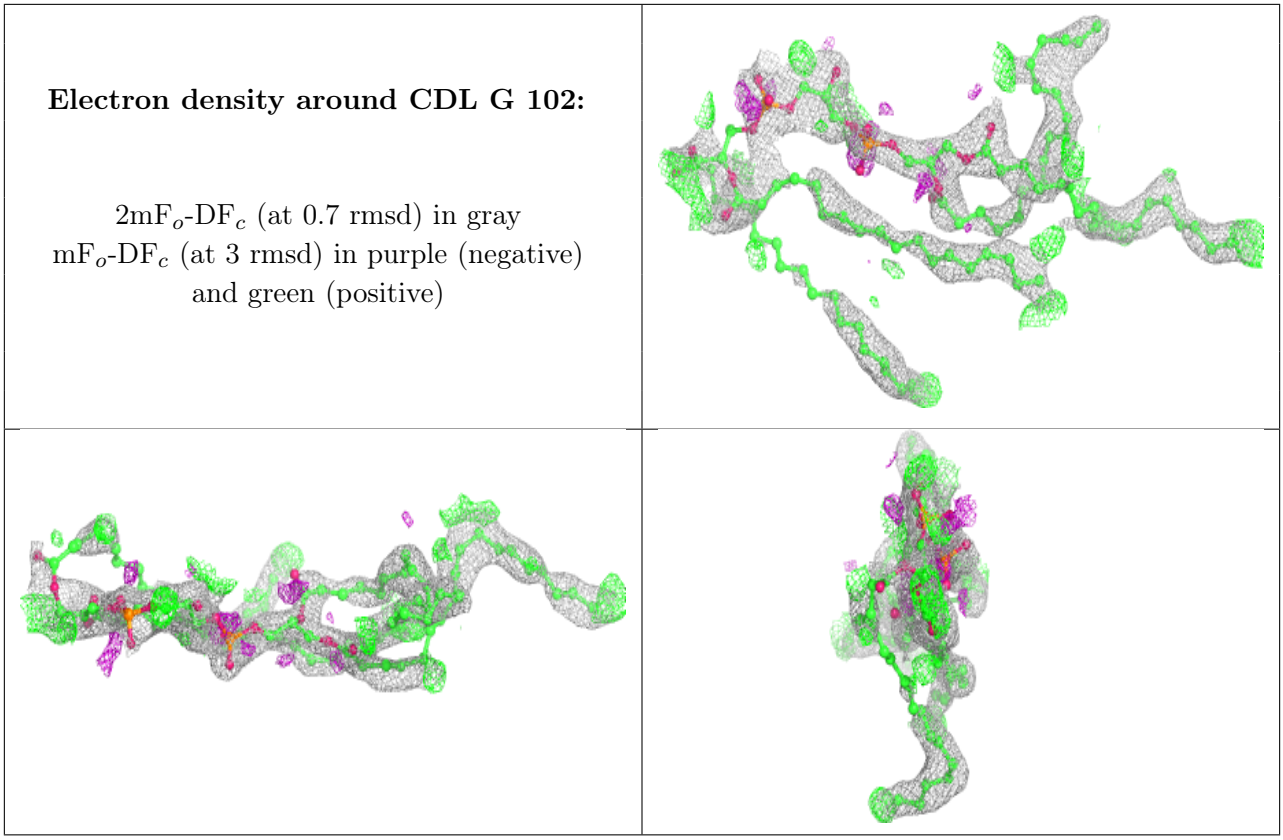
Electron density around PEK C 307:

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



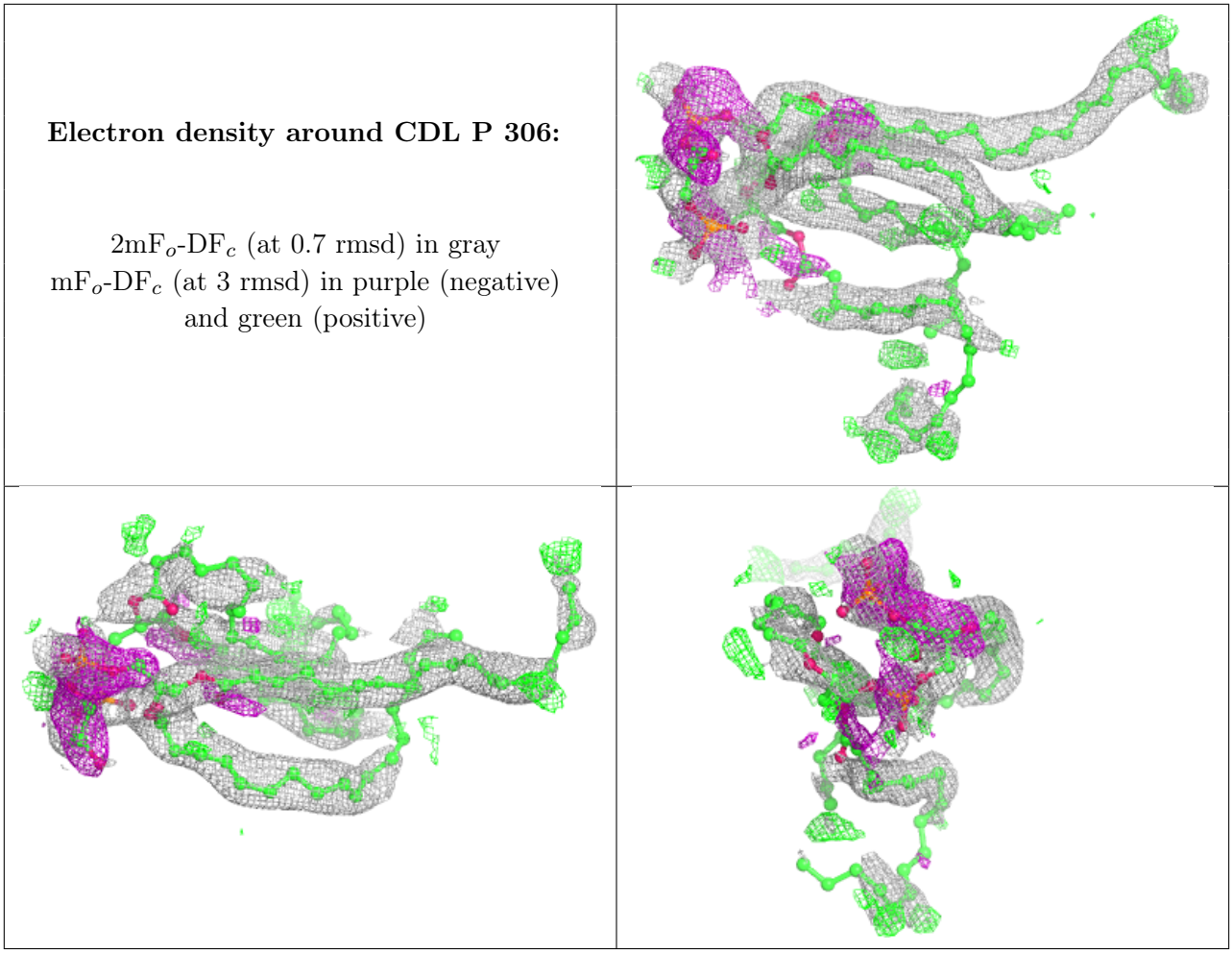
Electron density around CDL G 102:

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



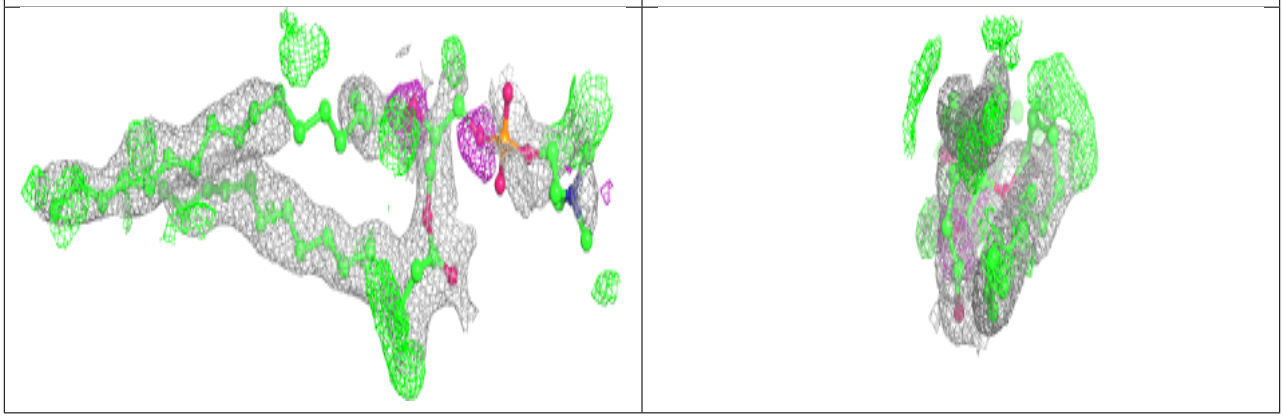
Electron density around CDL P 306:

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



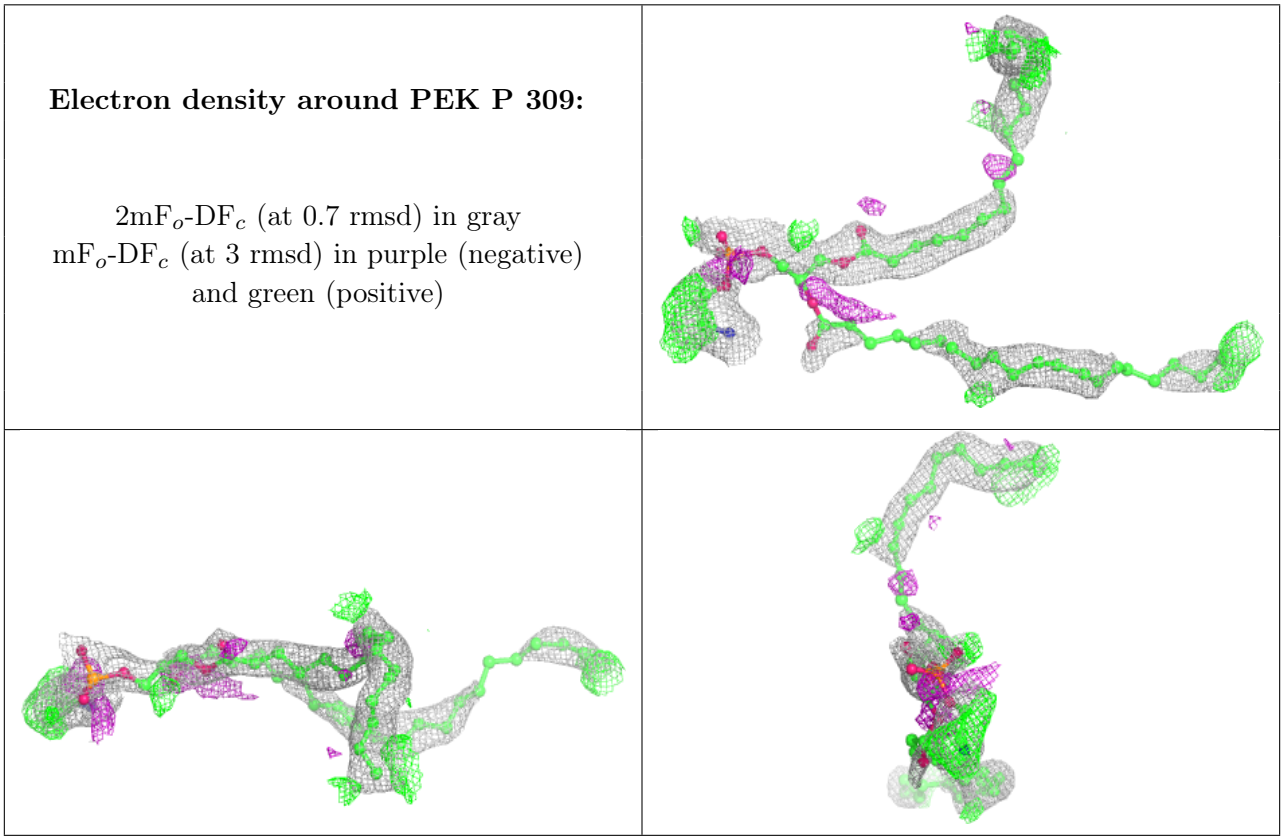
Electron density around PSC B 302:

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



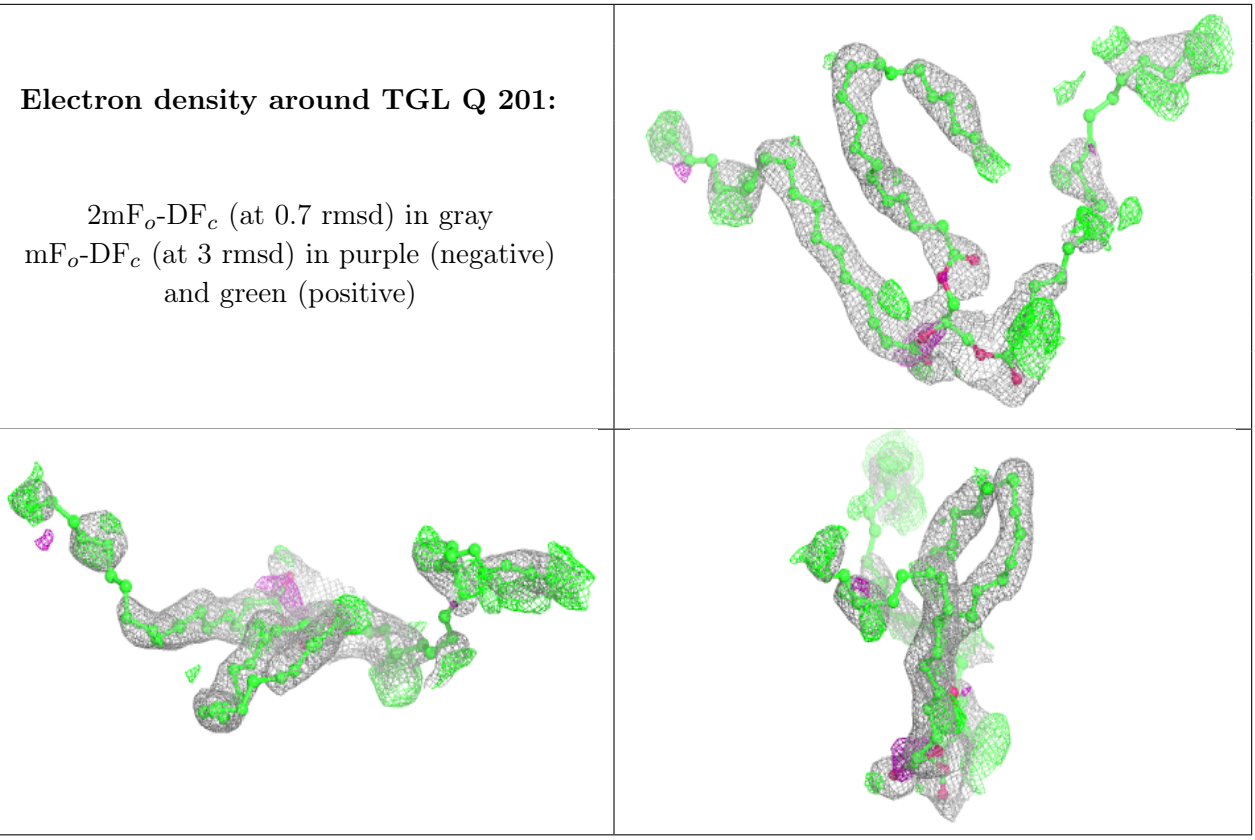
Electron density around PEK P 309:

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



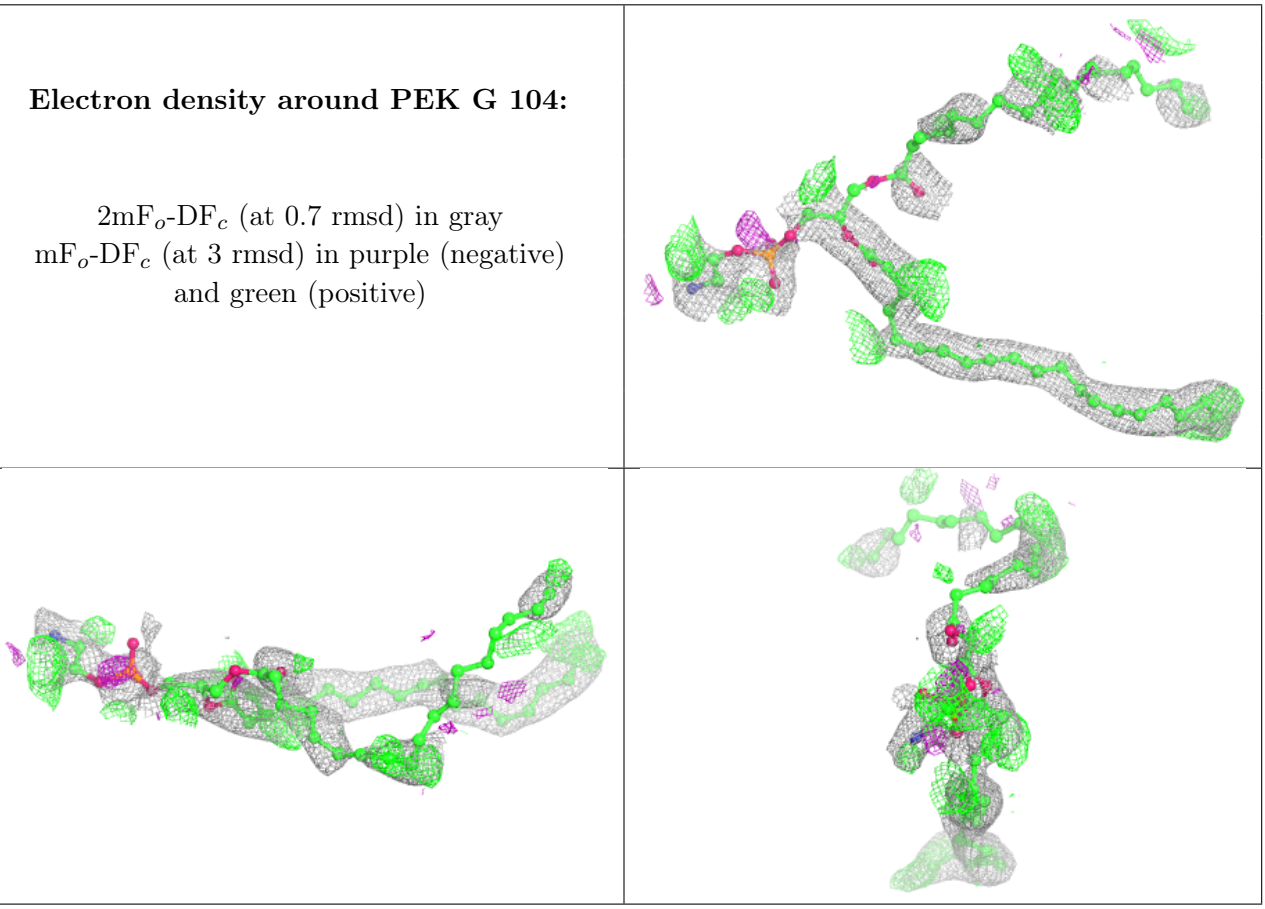
Electron density around TGL Q 201:

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



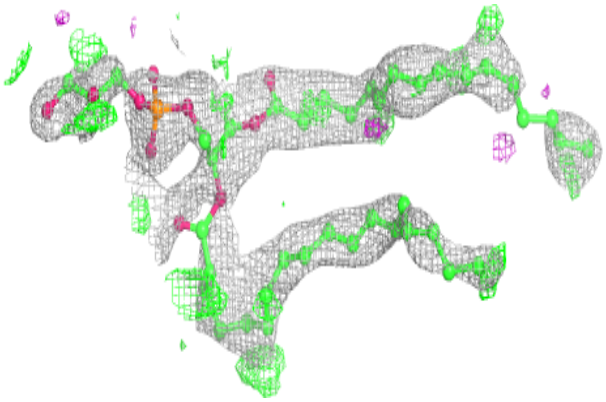
Electron density around PEK G 104:

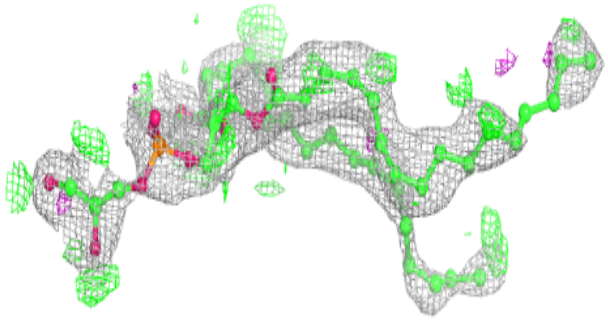
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

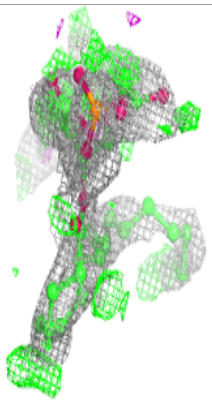


Electron density around PGV C 308:

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

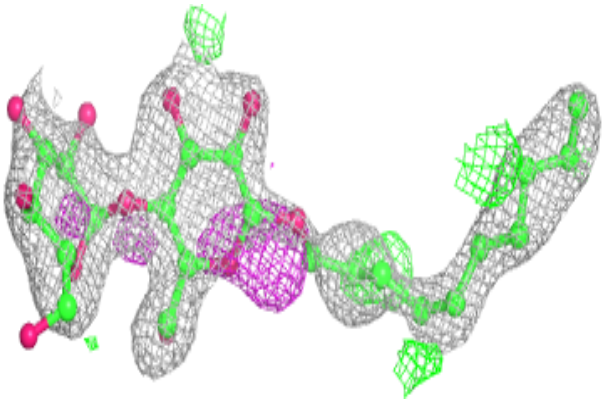


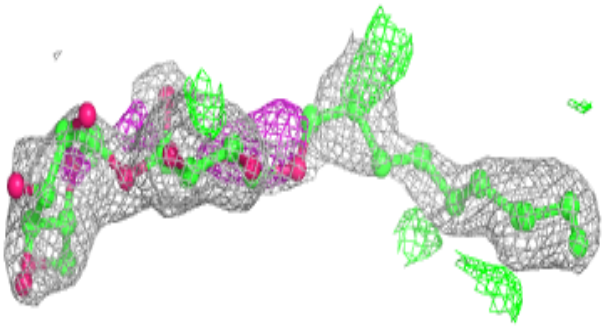


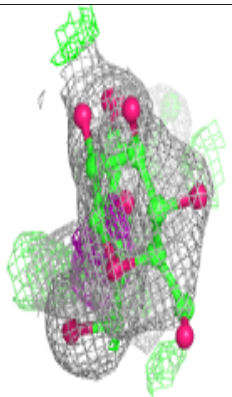


Electron density around DMU C 302:

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

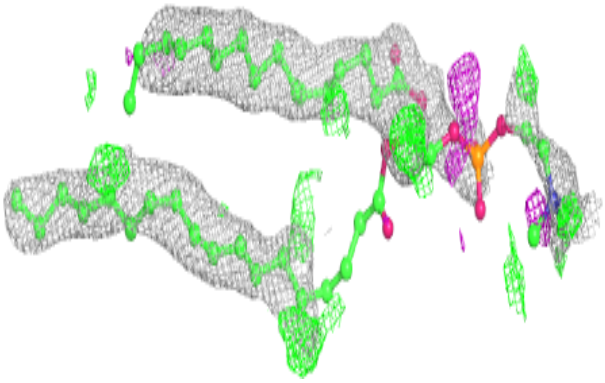


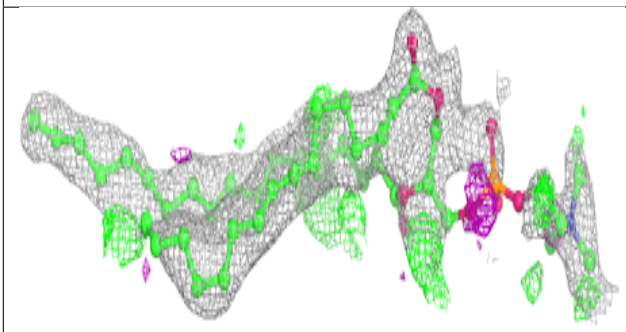


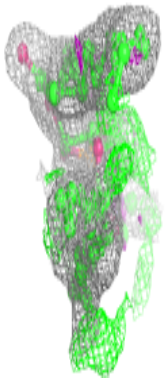


Electron density around PSC O 302:

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

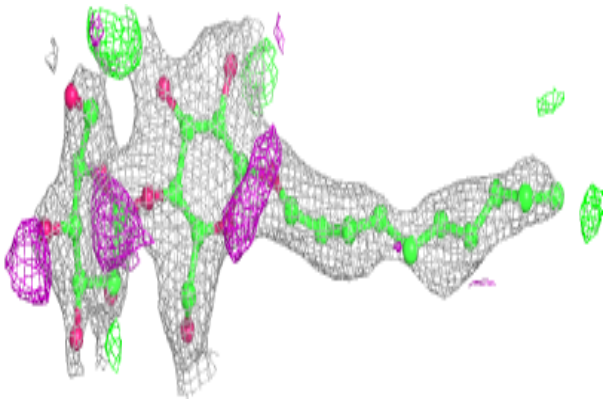


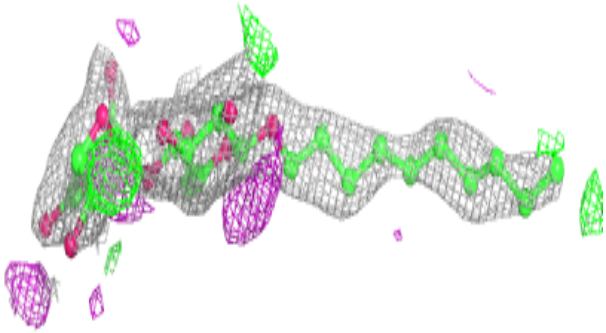


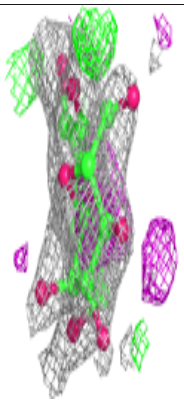


Electron density around DMU C 309:

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

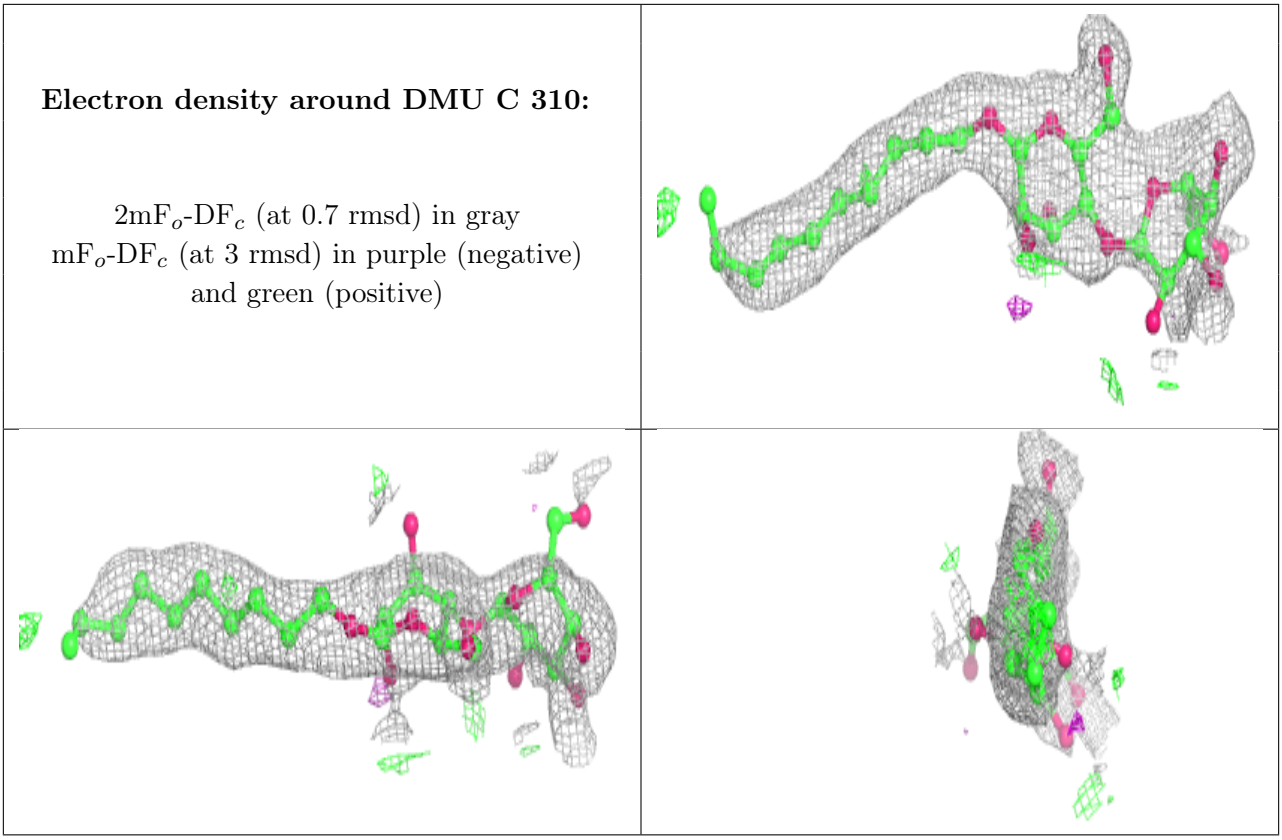






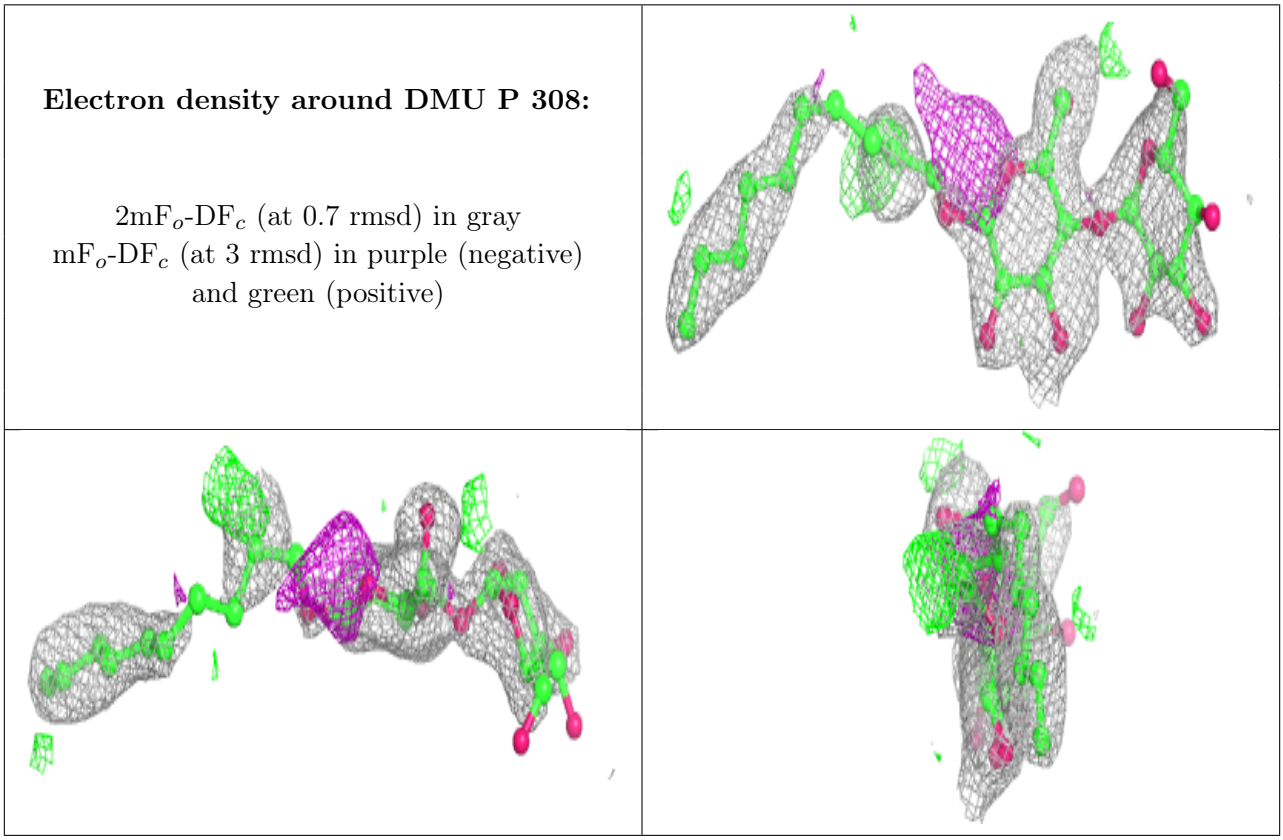
Electron density around DMU C 310:

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



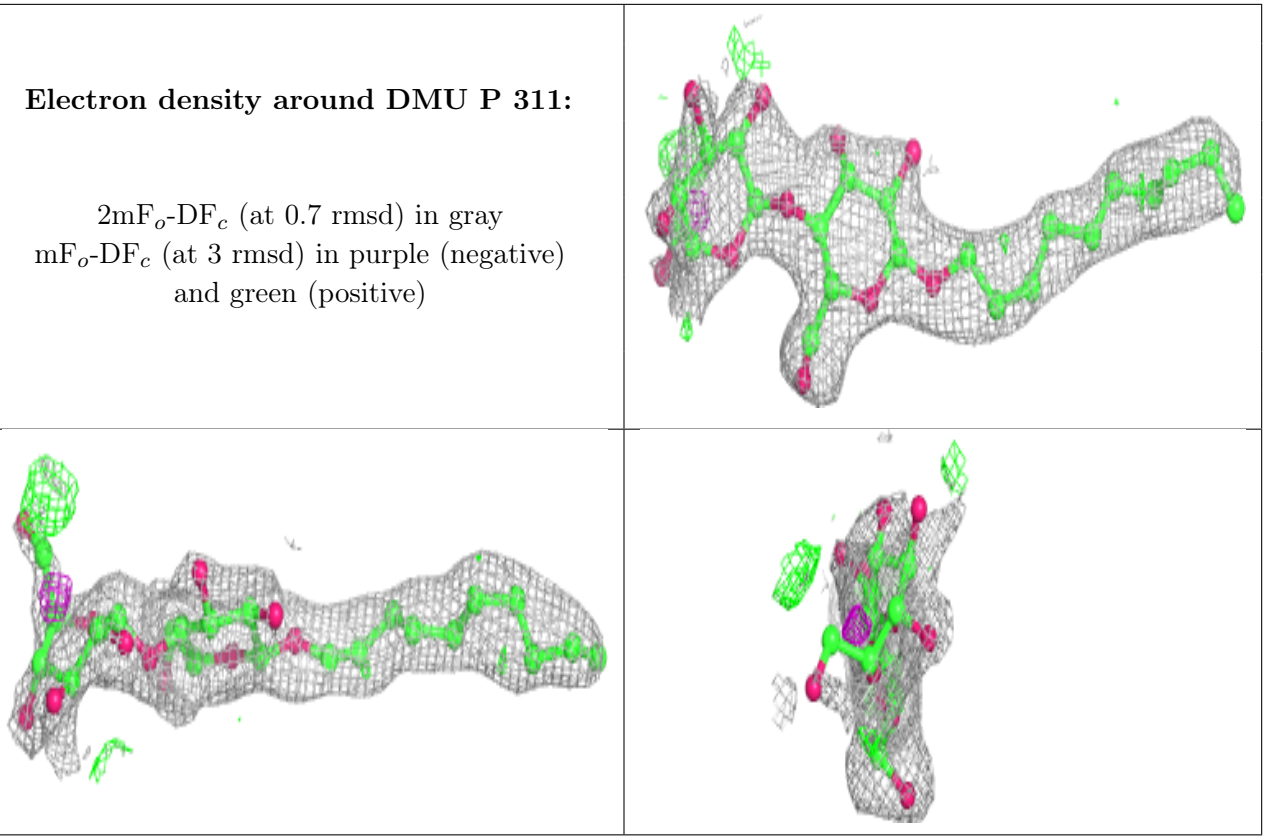
Electron density around DMU P 308:

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



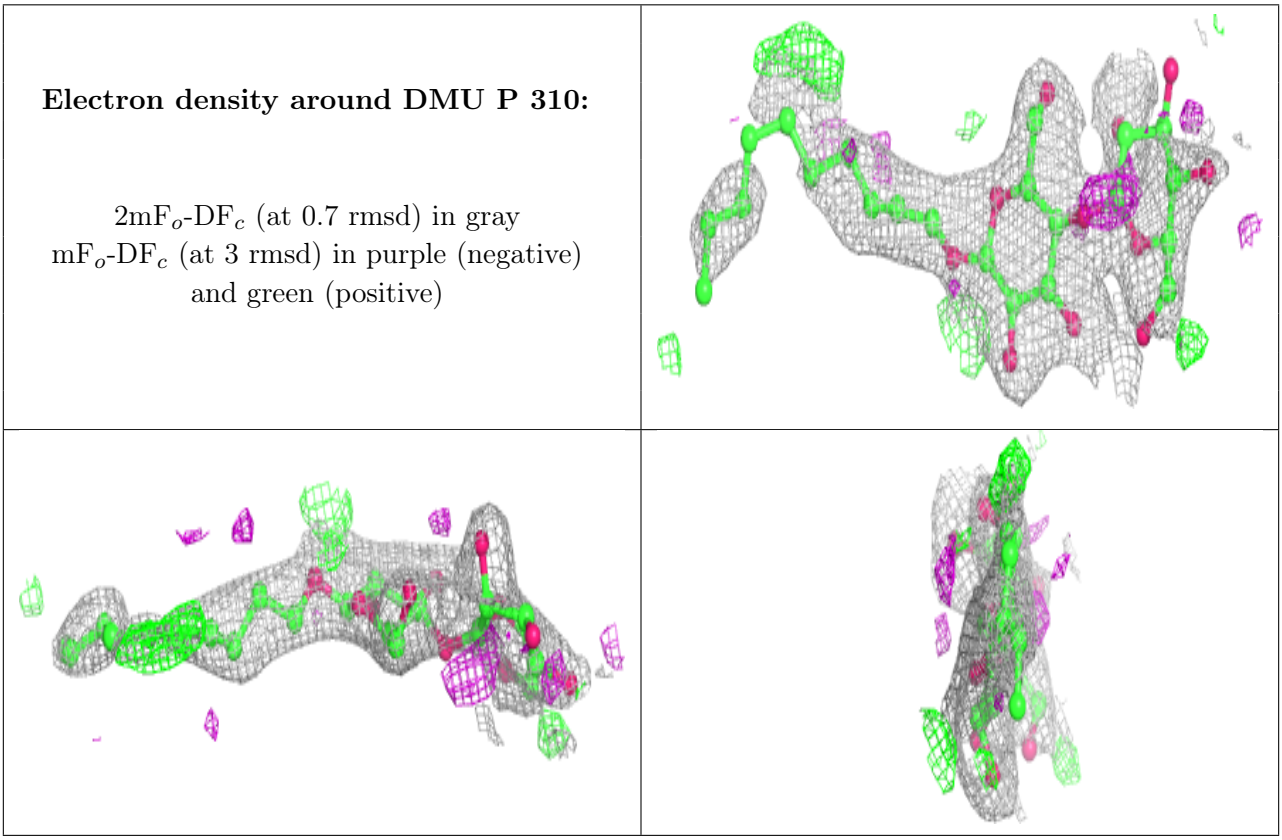
Electron density around DMU P 311:

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



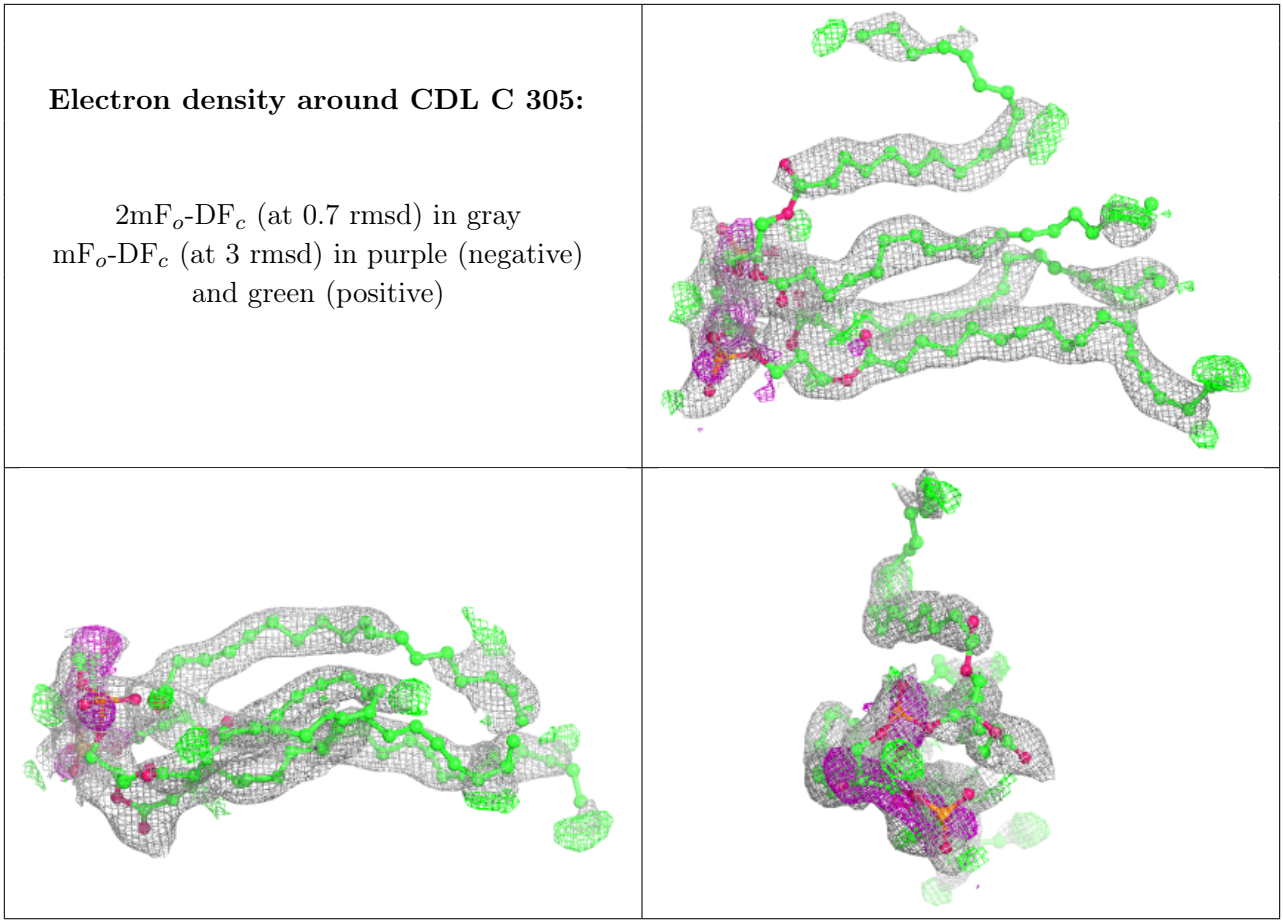
Electron density around DMU P 310:

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



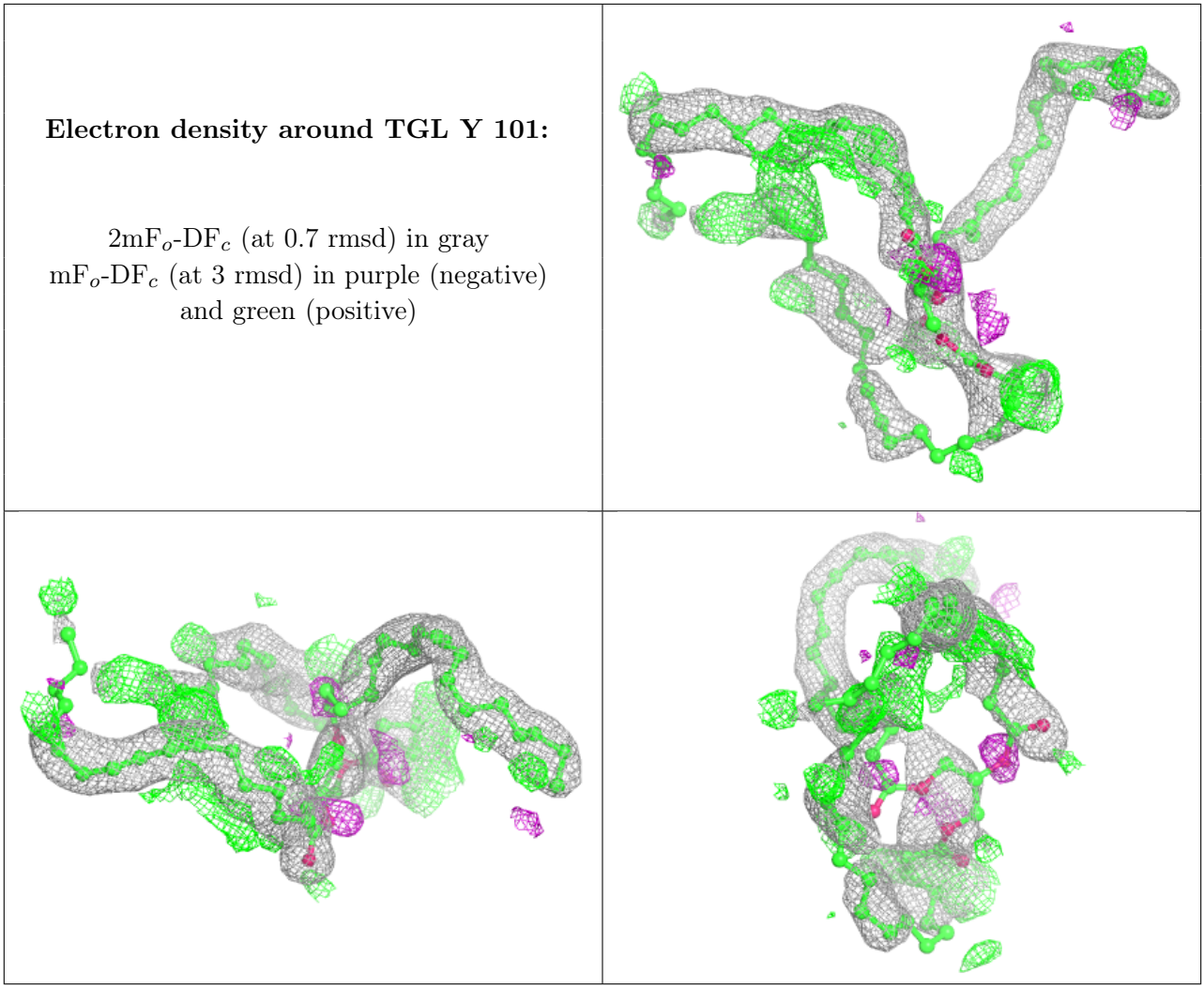
Electron density around CDL C 305:

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



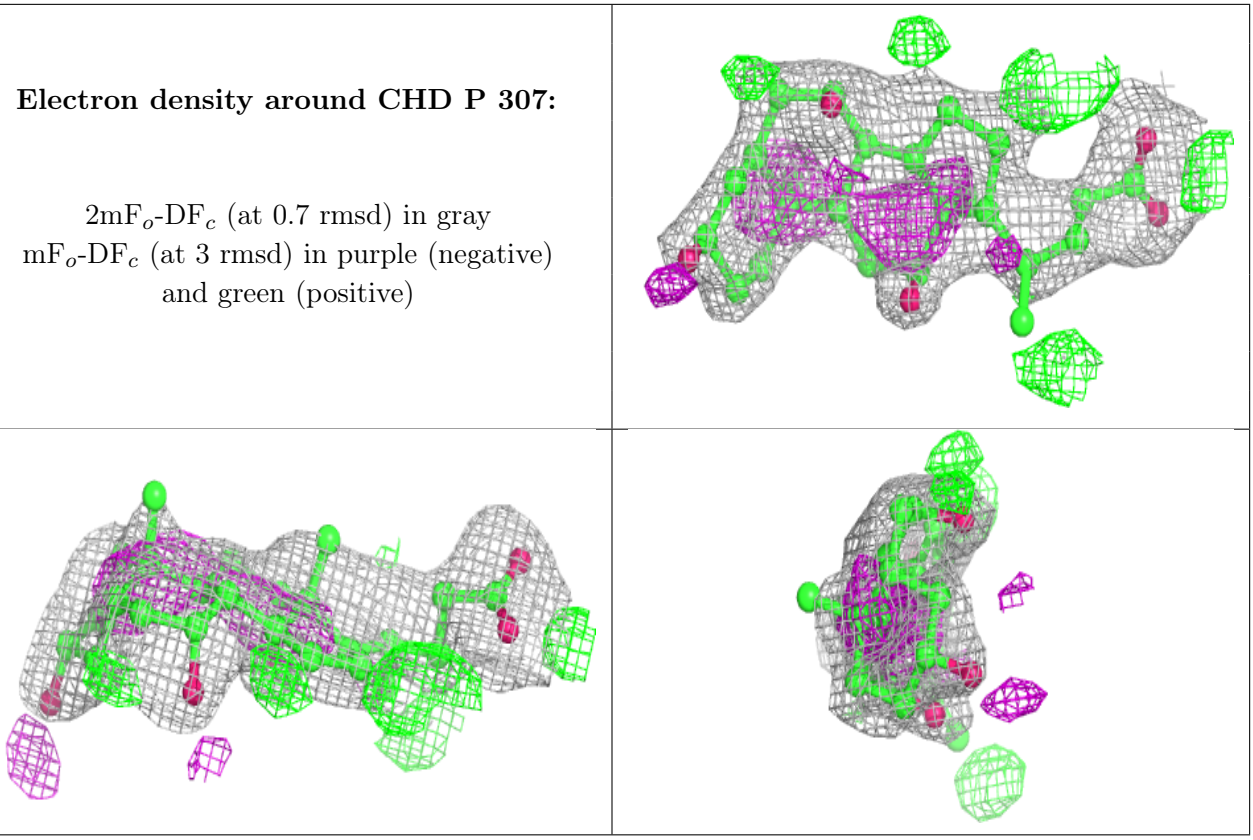
Electron density around TGL Y 101:

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



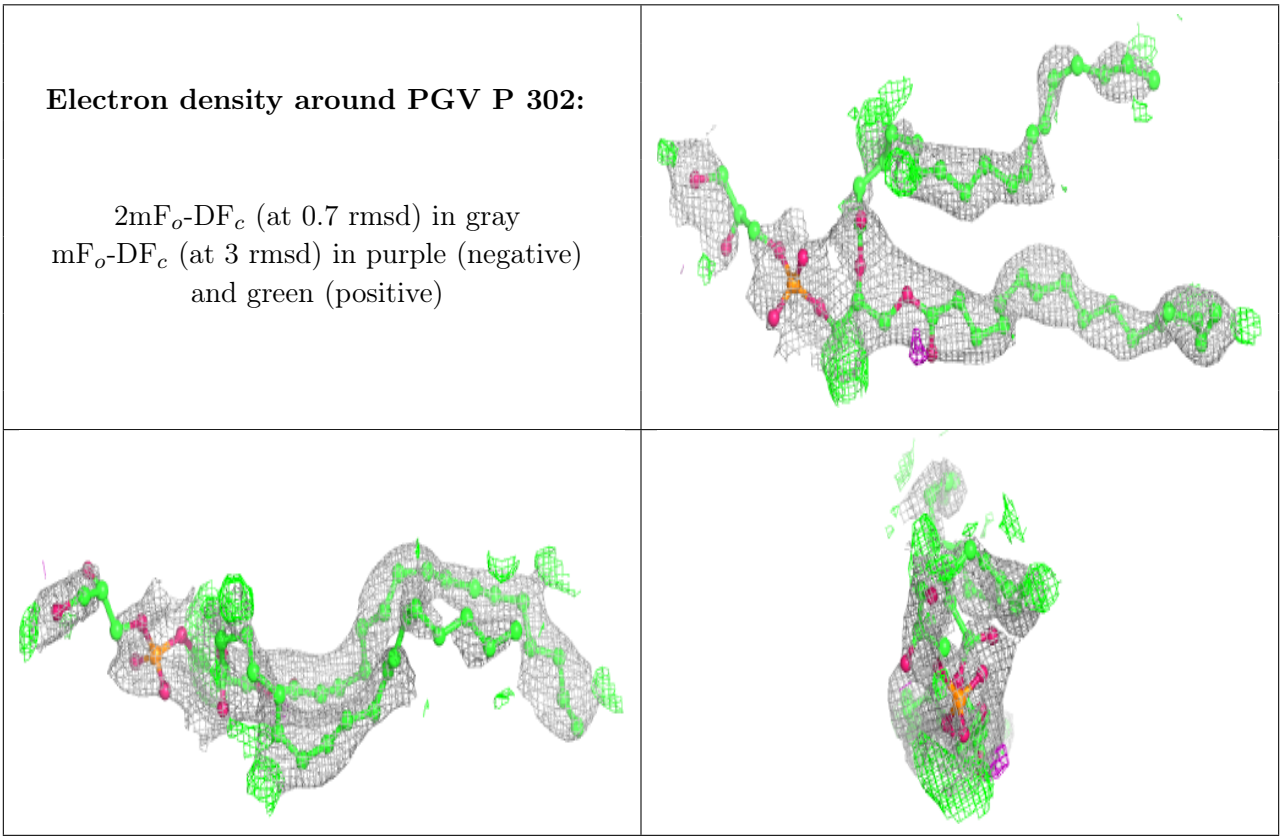
Electron density around CHD P 307:

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



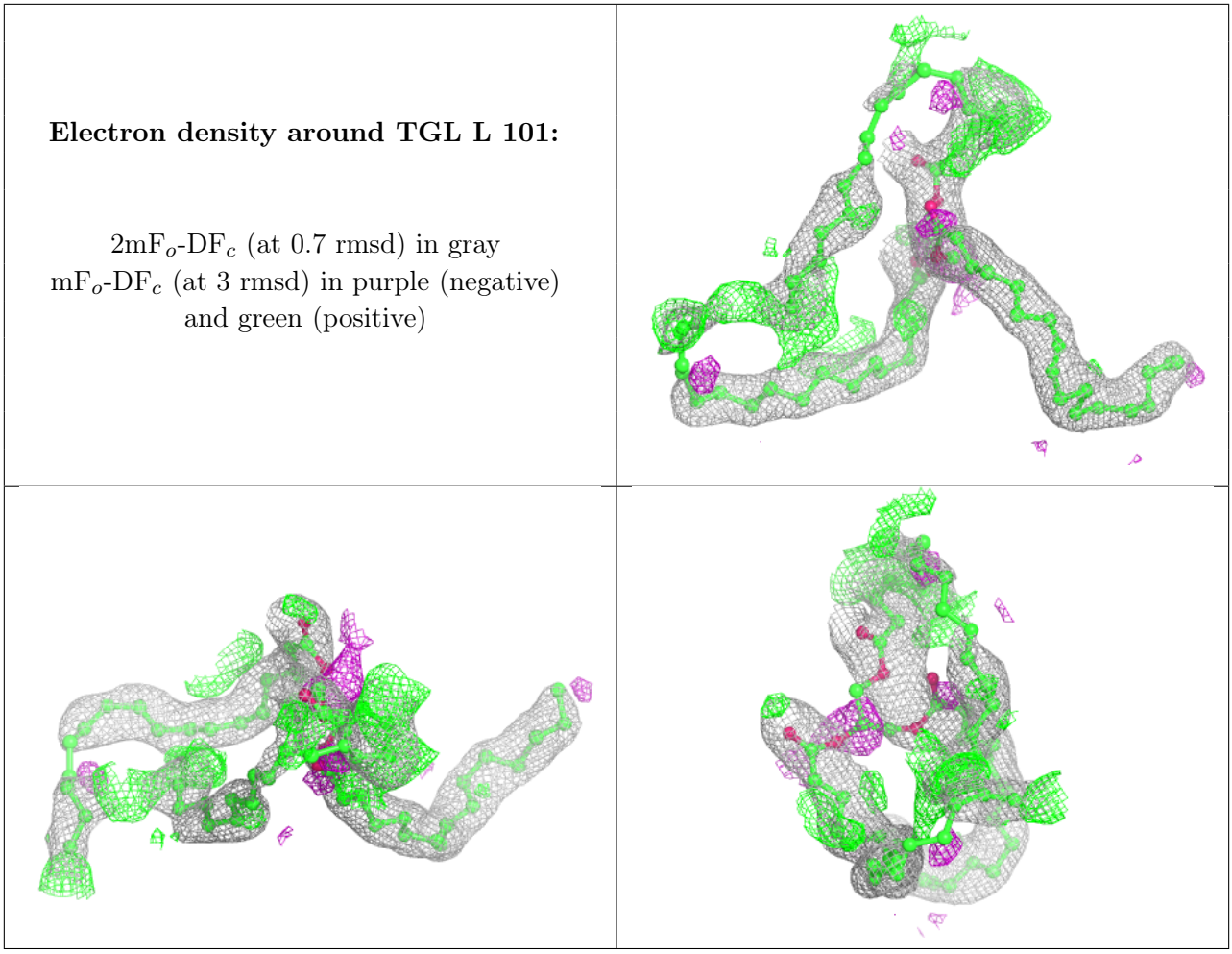
Electron density around PGV P 302:

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



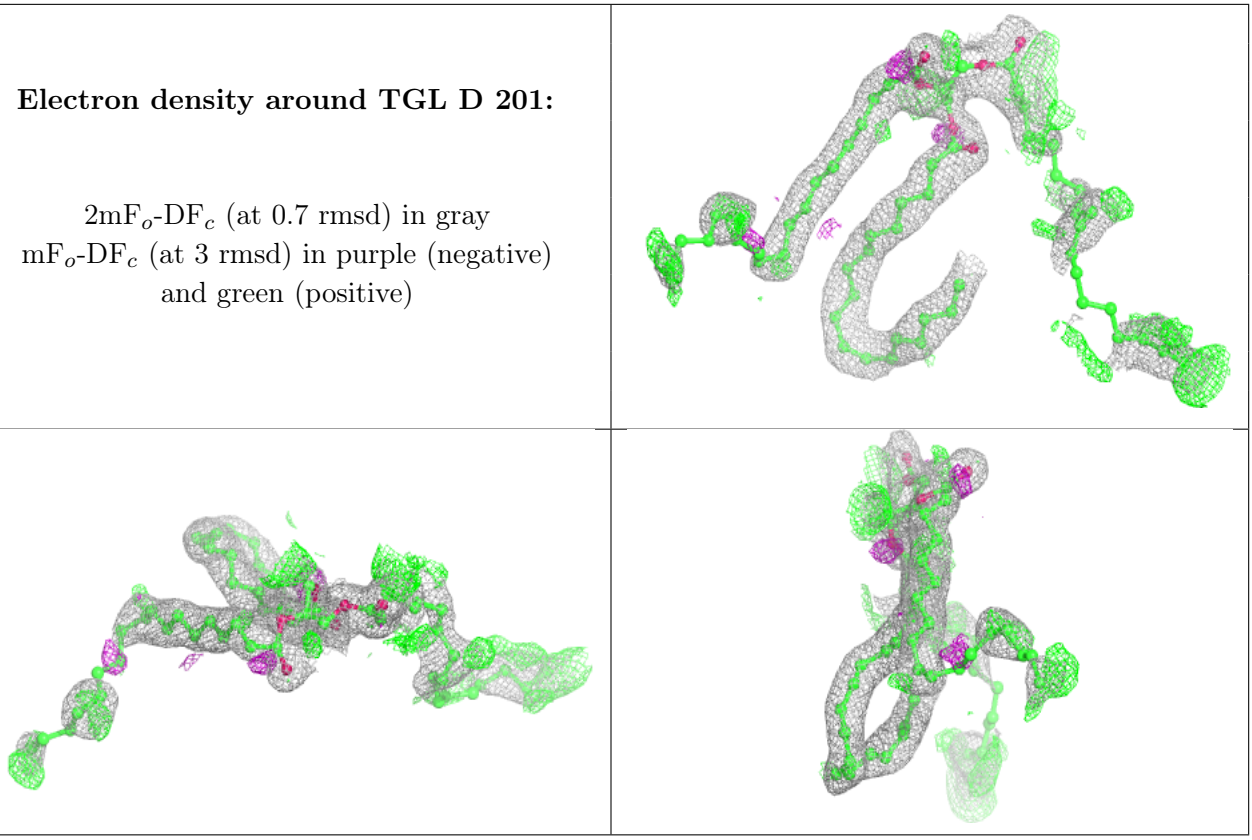
Electron density around TGL L 101:

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



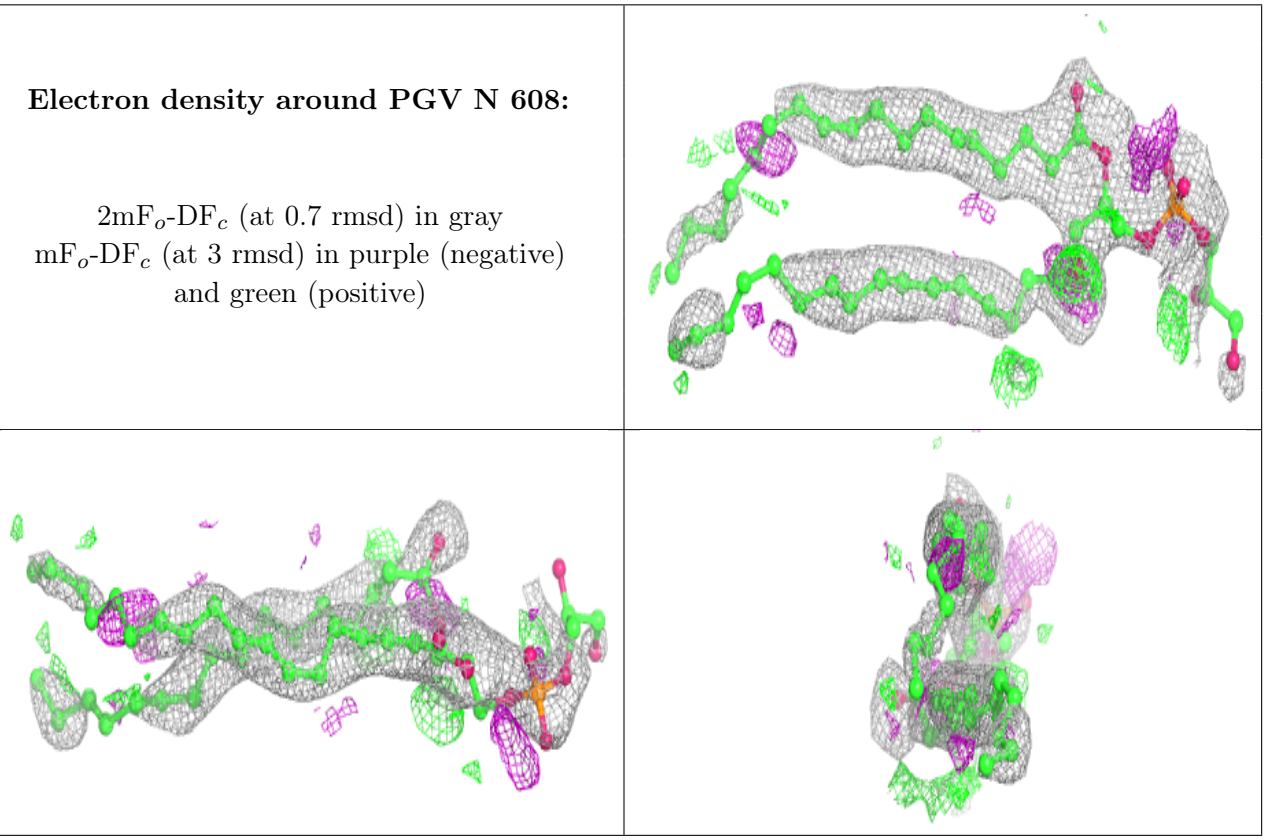
Electron density around TGL D 201:

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



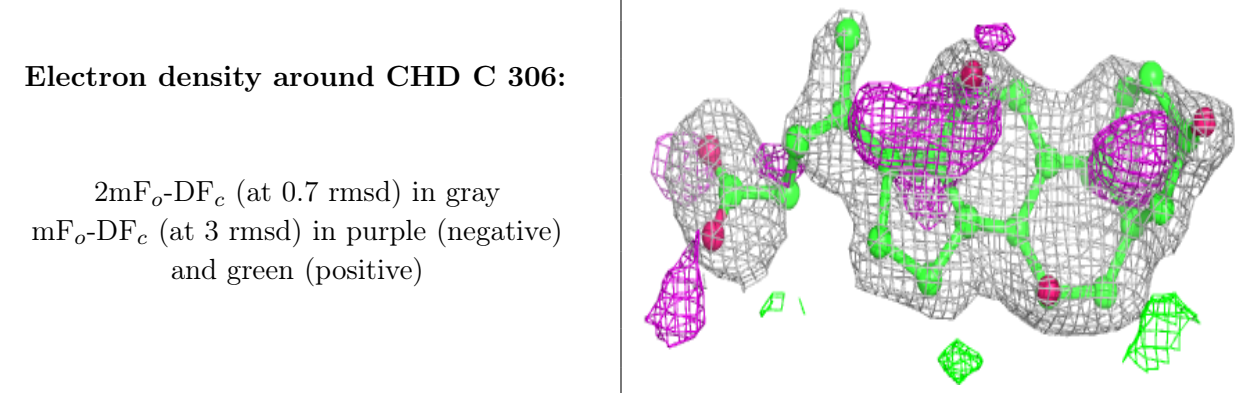
Electron density around PGV N 608:

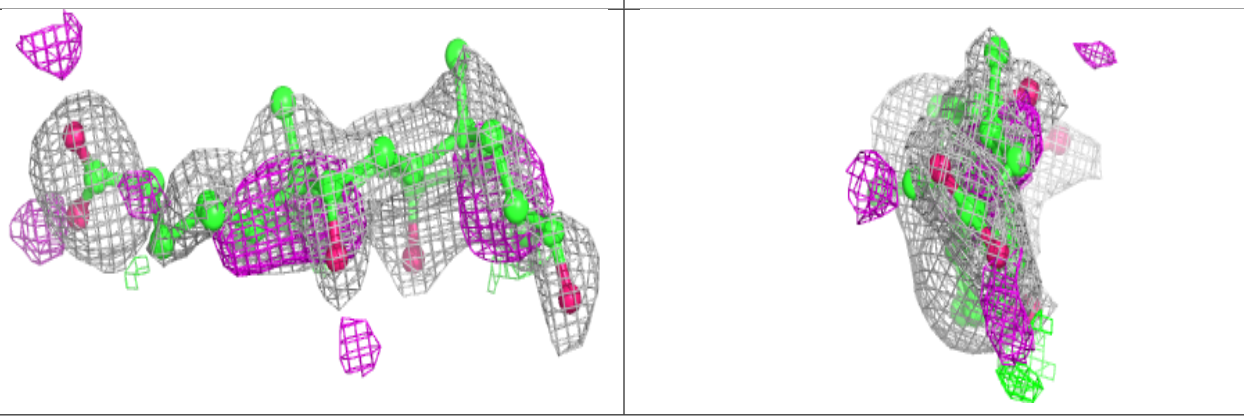
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CHD C 306:

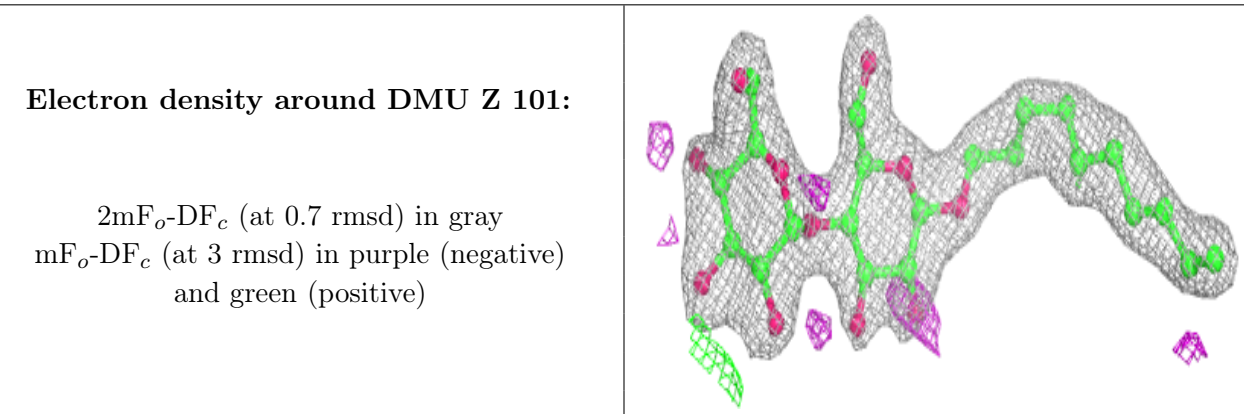
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

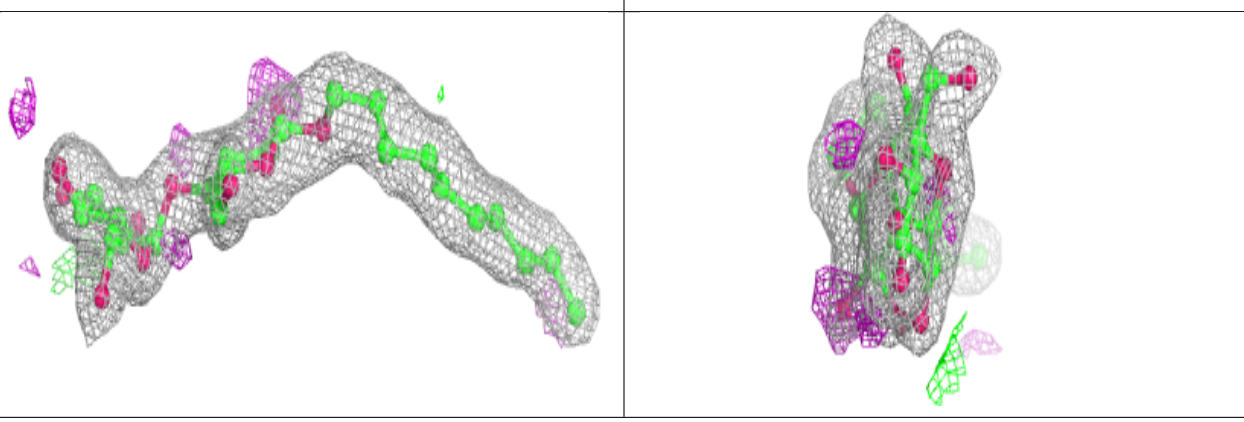




Electron density around DMU Z 101:

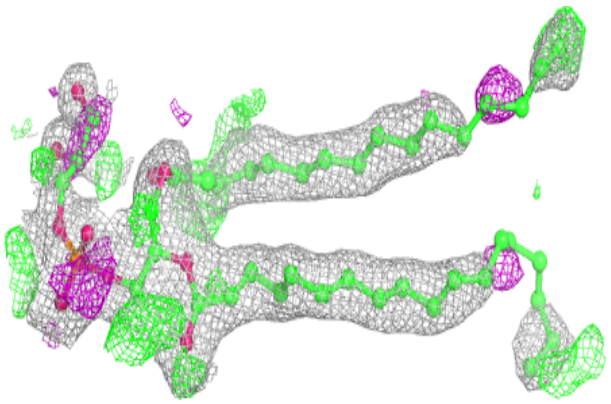
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

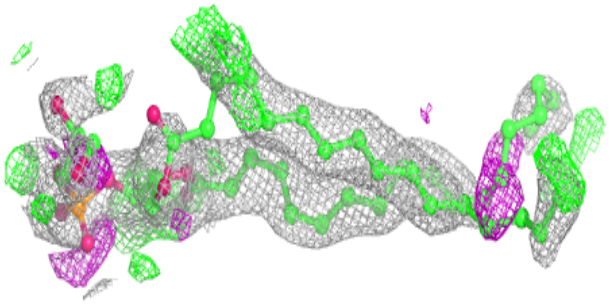


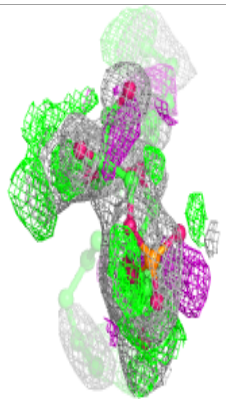


Electron density around PGV M 101:

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

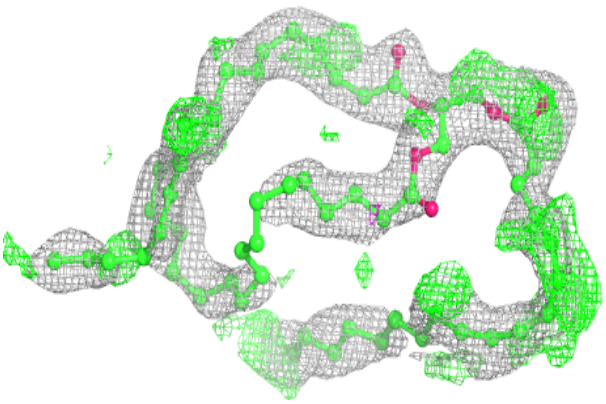


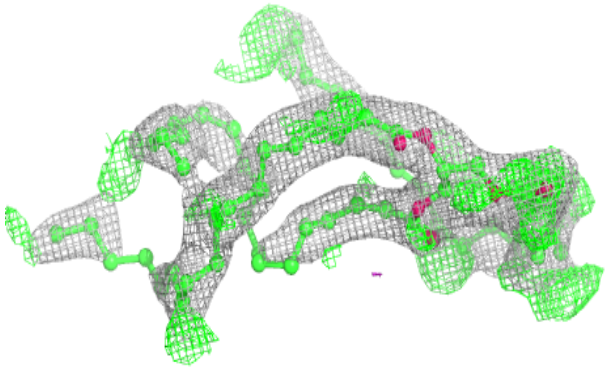


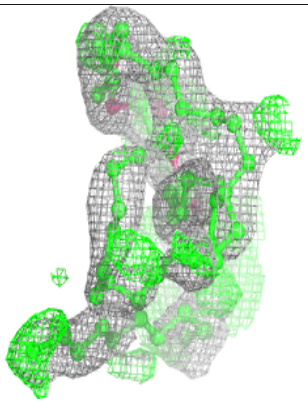


Electron density around TGL N 610:

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

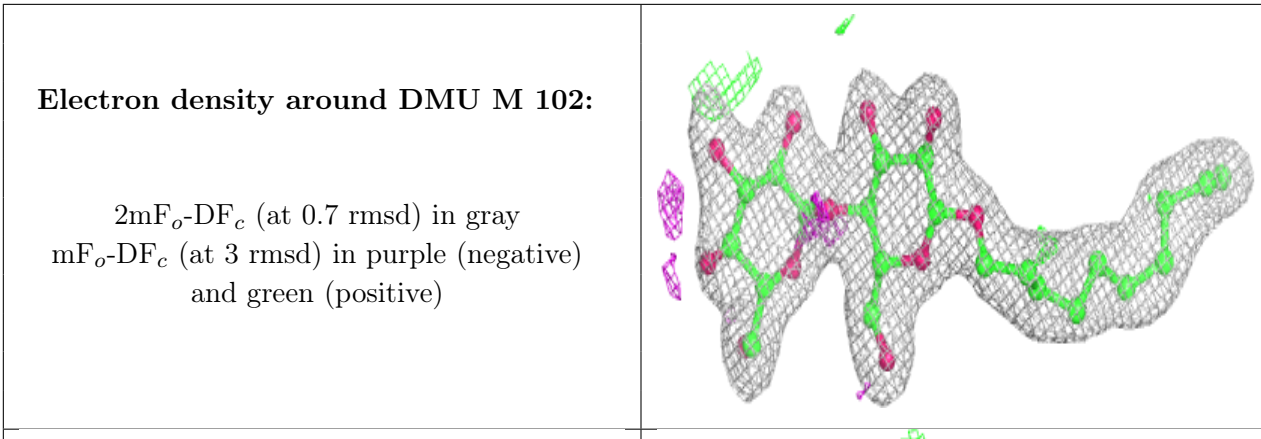






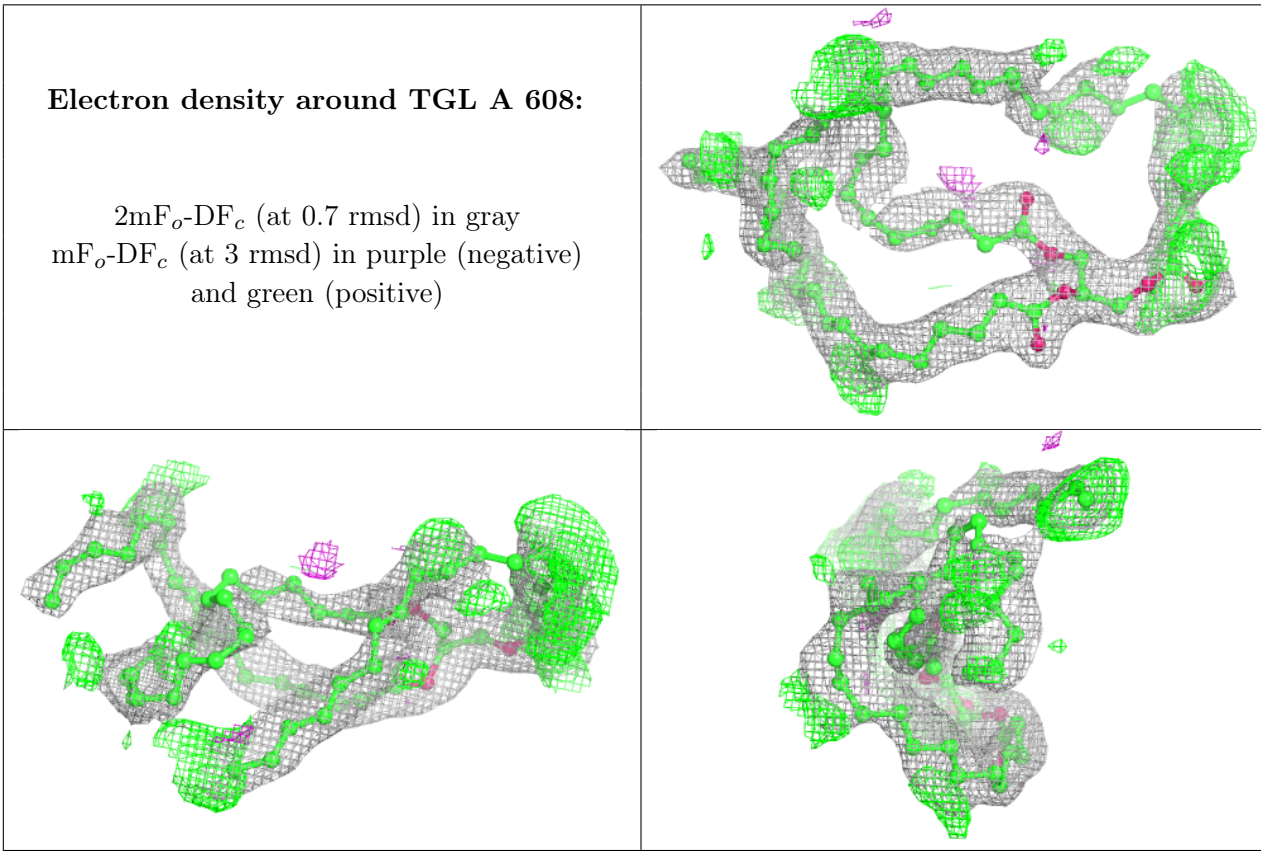
Electron density around DMU M 102:

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



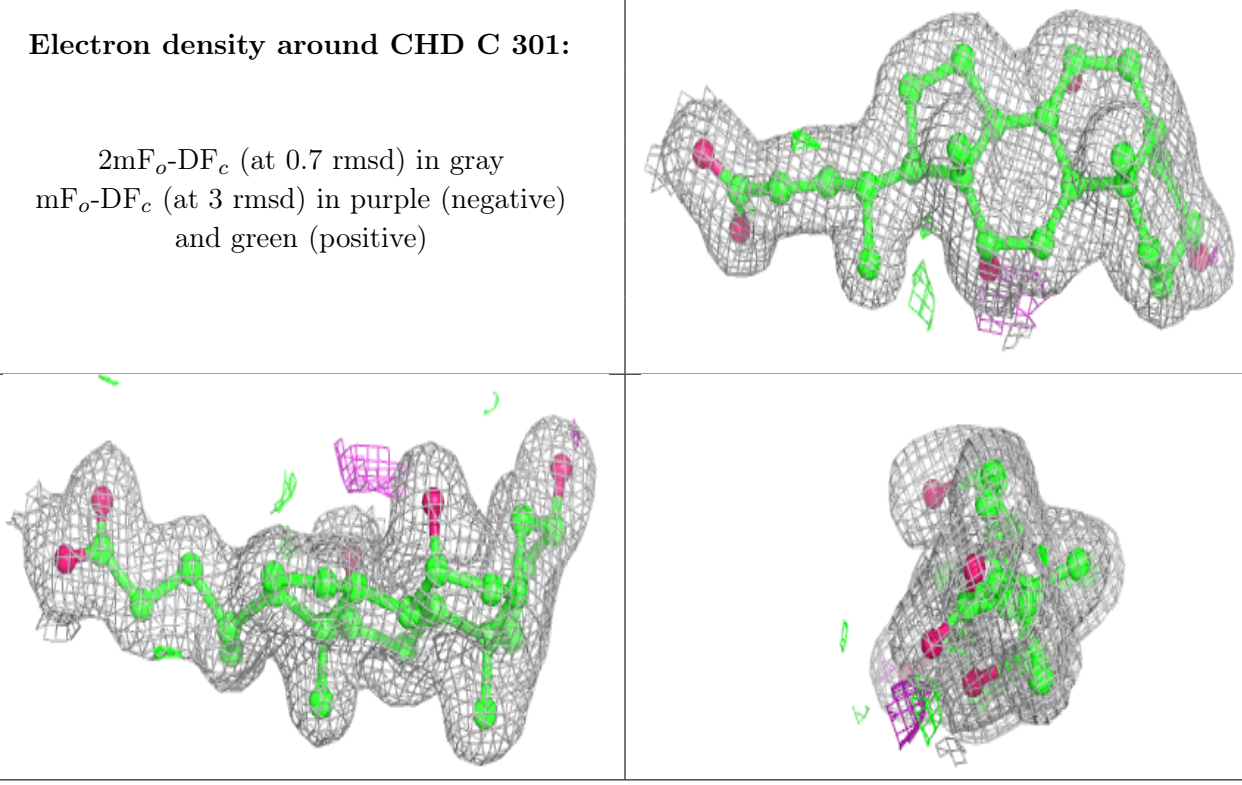
Electron density around TGL A 608:

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



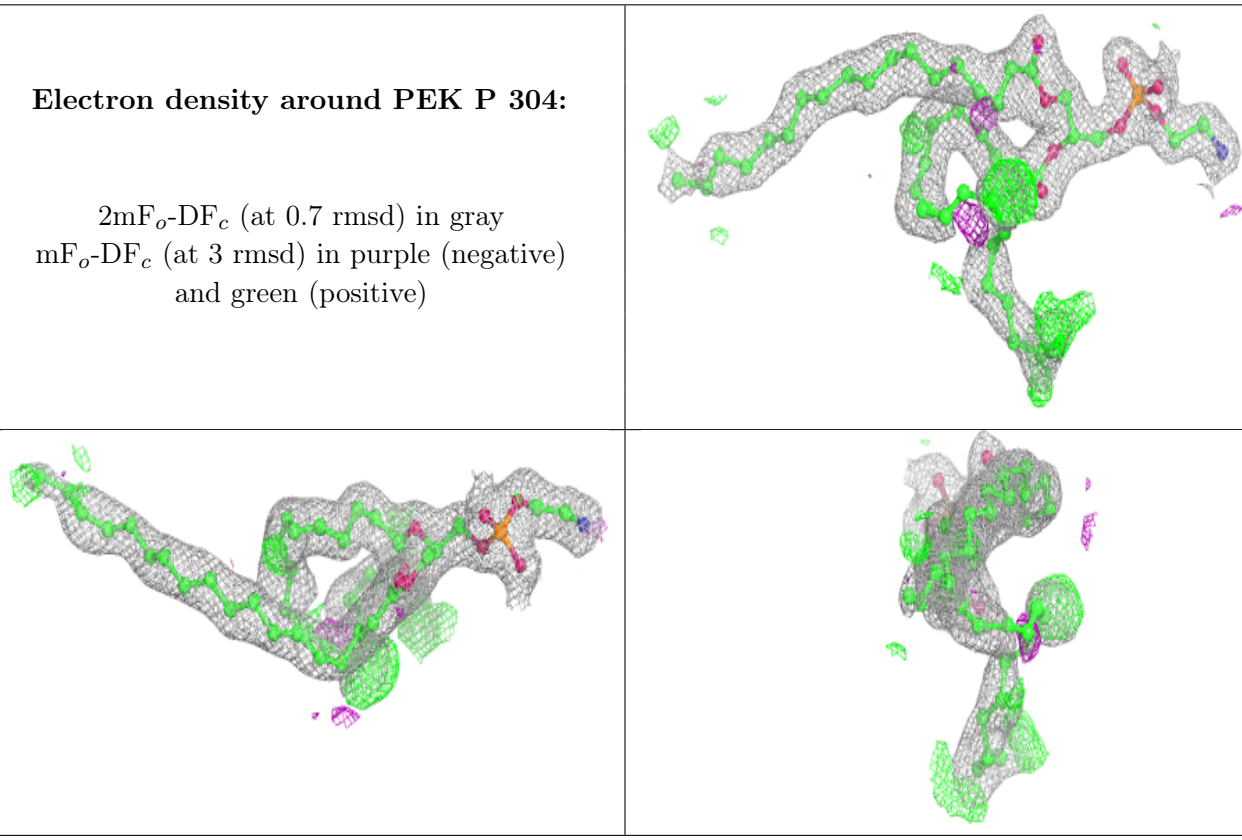
Electron density around CHD C 301:

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



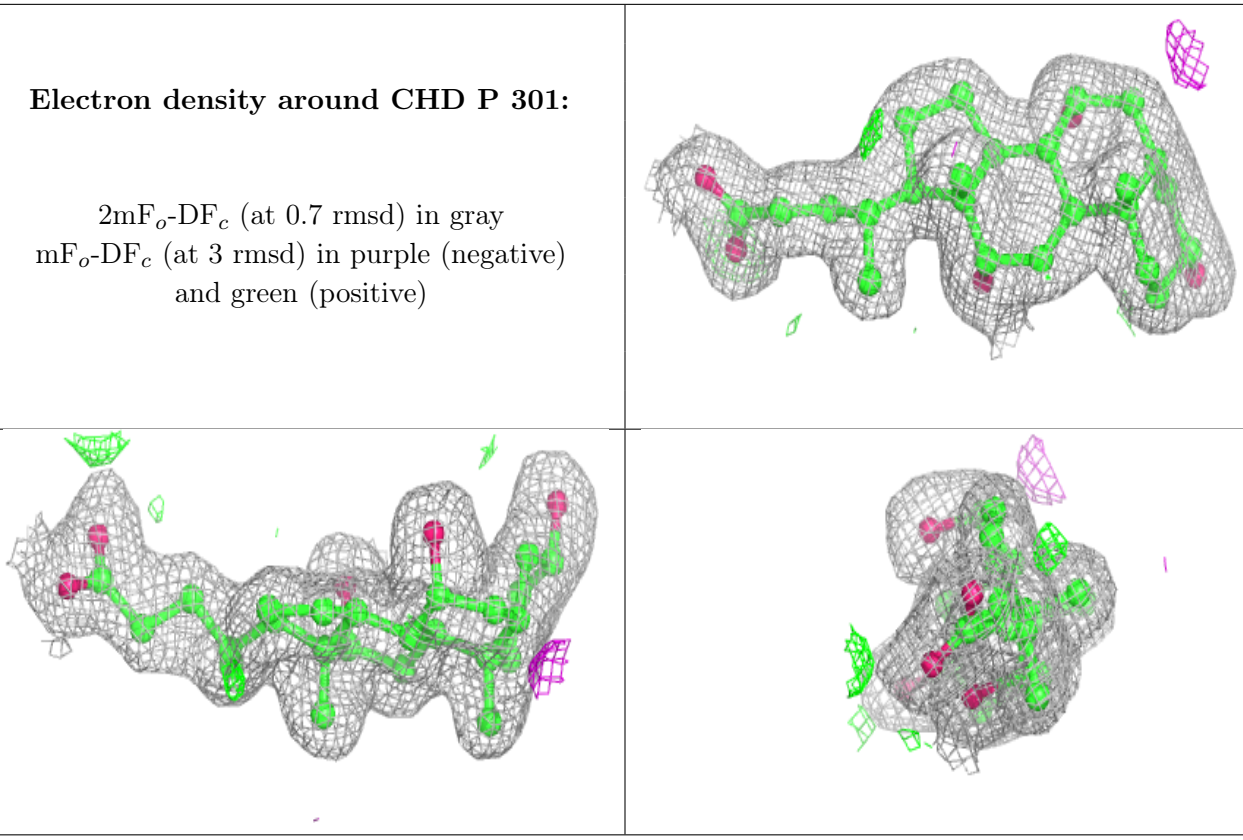
Electron density around PEK P 304:

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



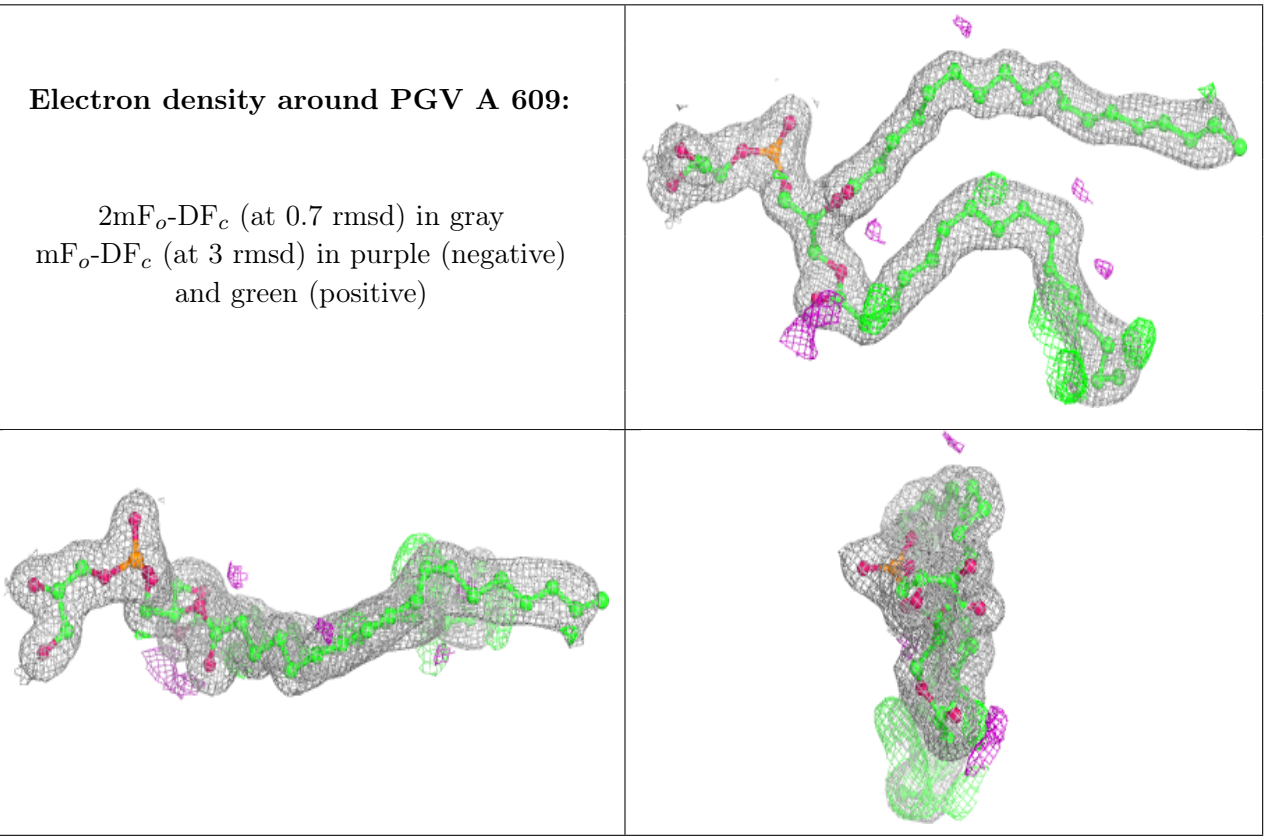
Electron density around CHD P 301:

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



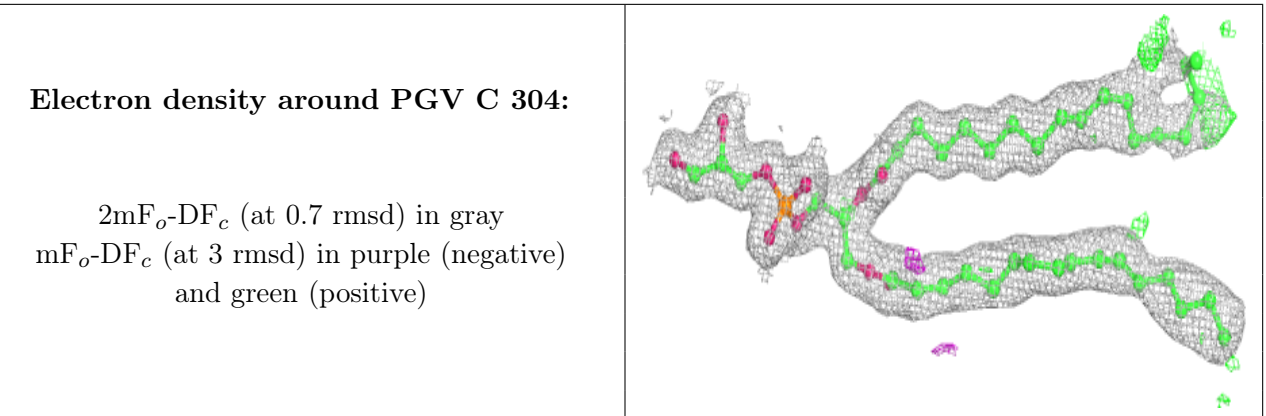
Electron density around PGV A 609:

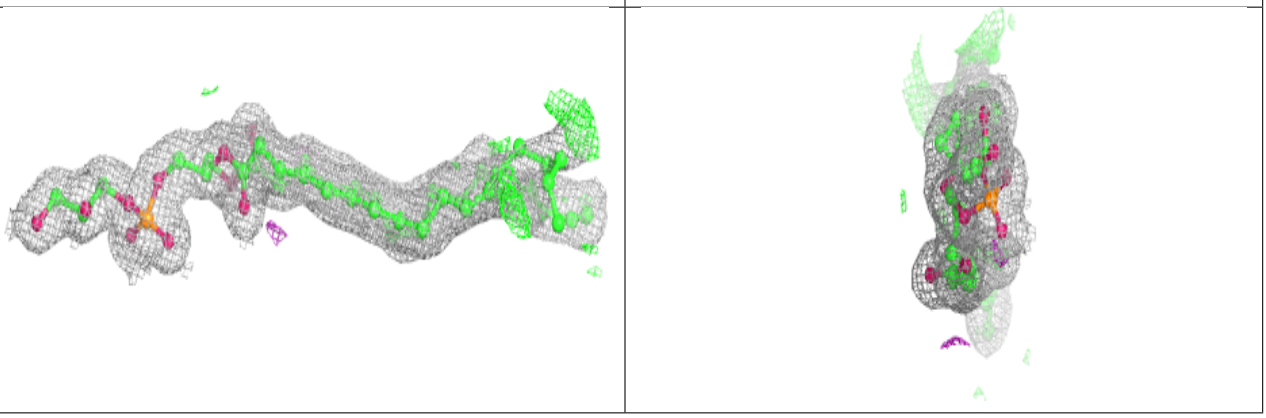
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGV C 304:

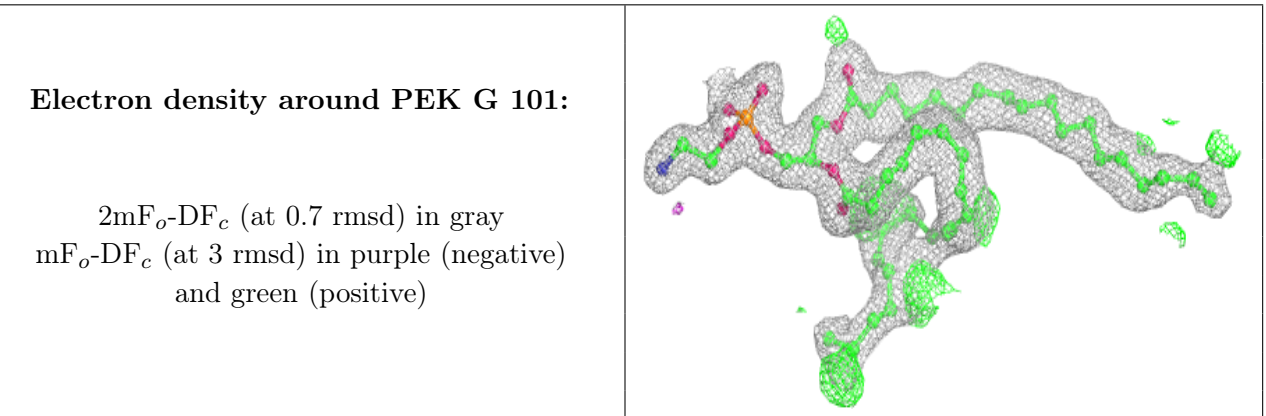
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

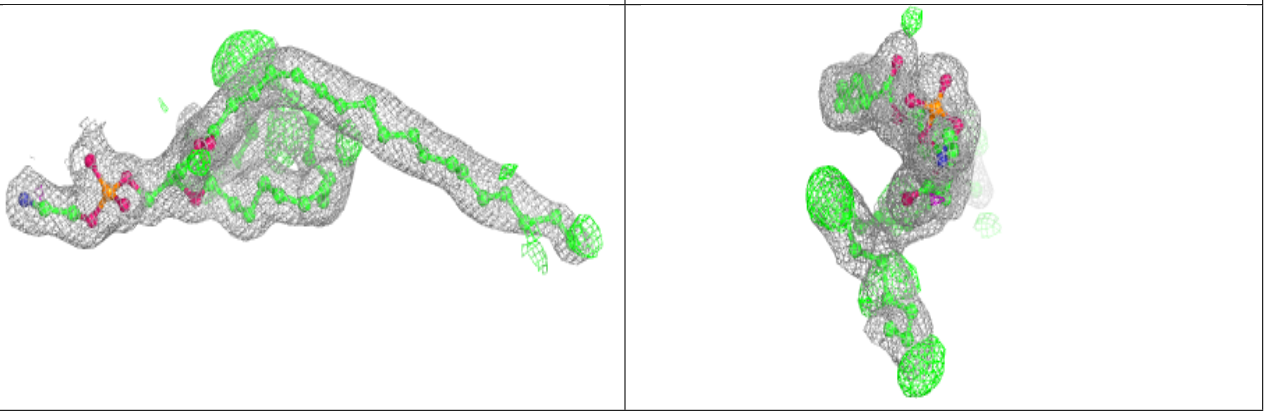




Electron density around PEK G 101:

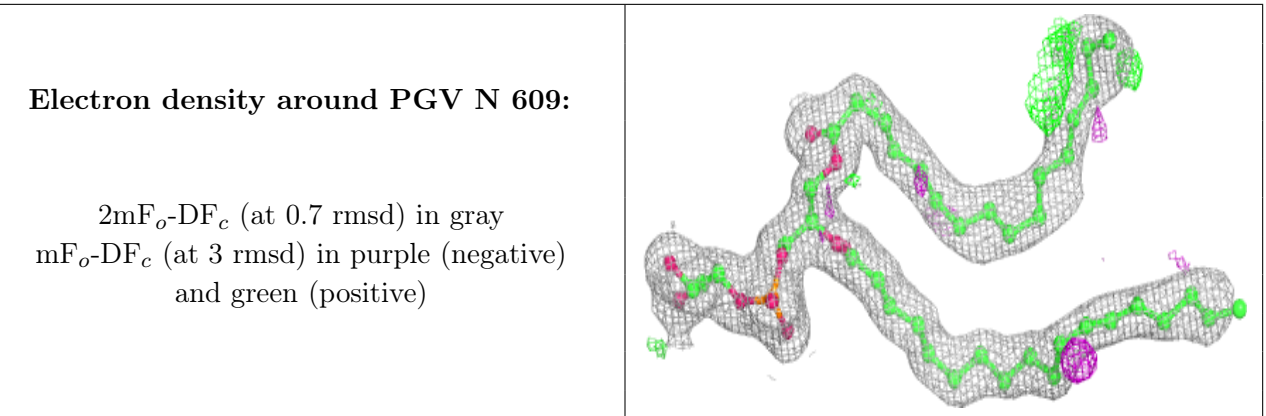
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

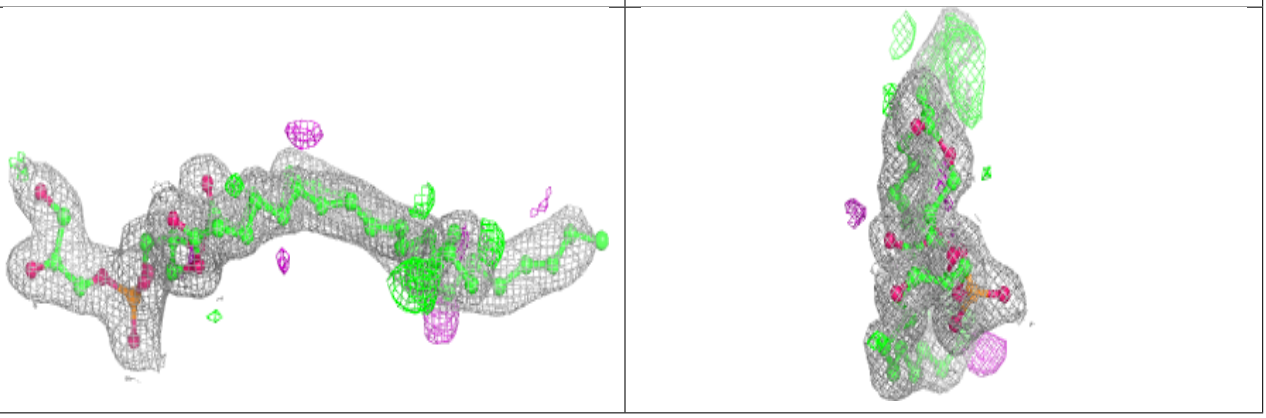




Electron density around PGV N 609:

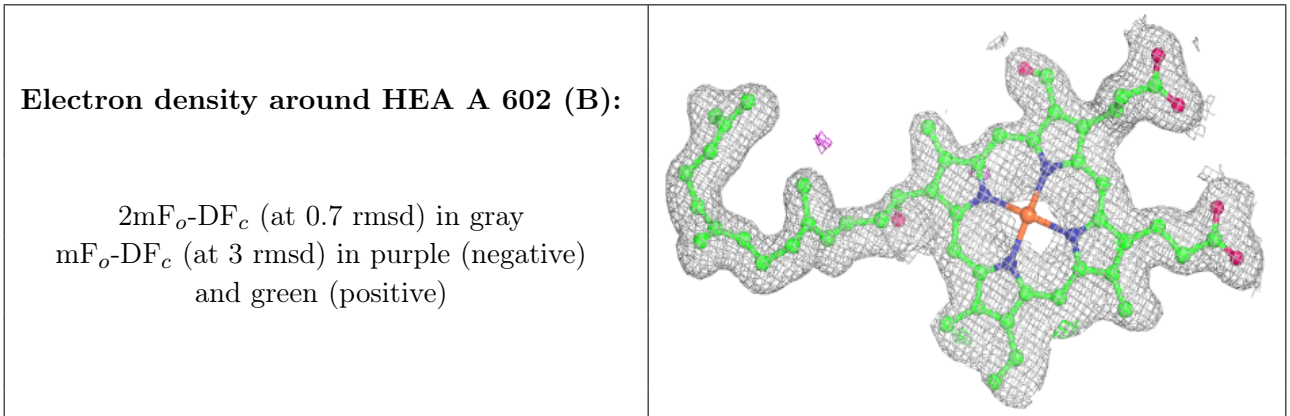
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

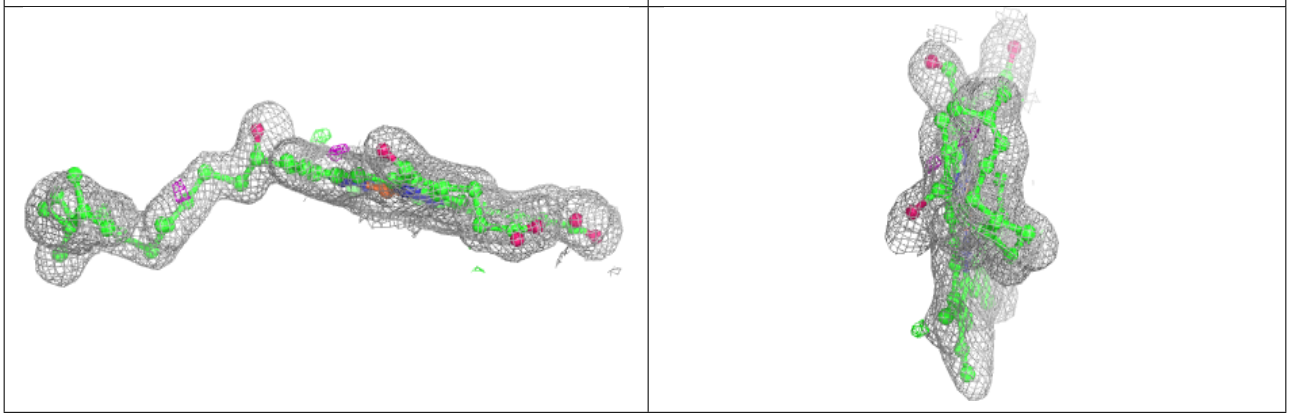




Electron density around HEA A 602 (B):

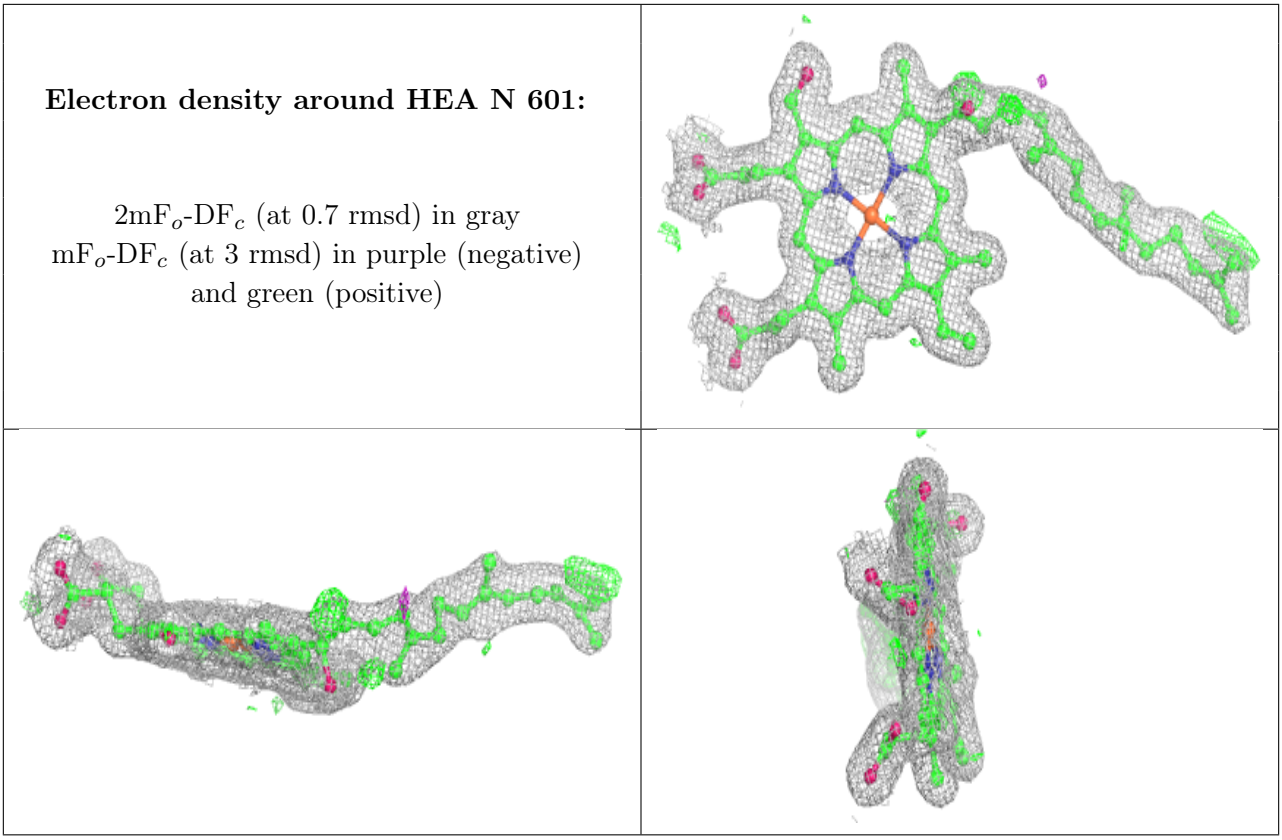
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





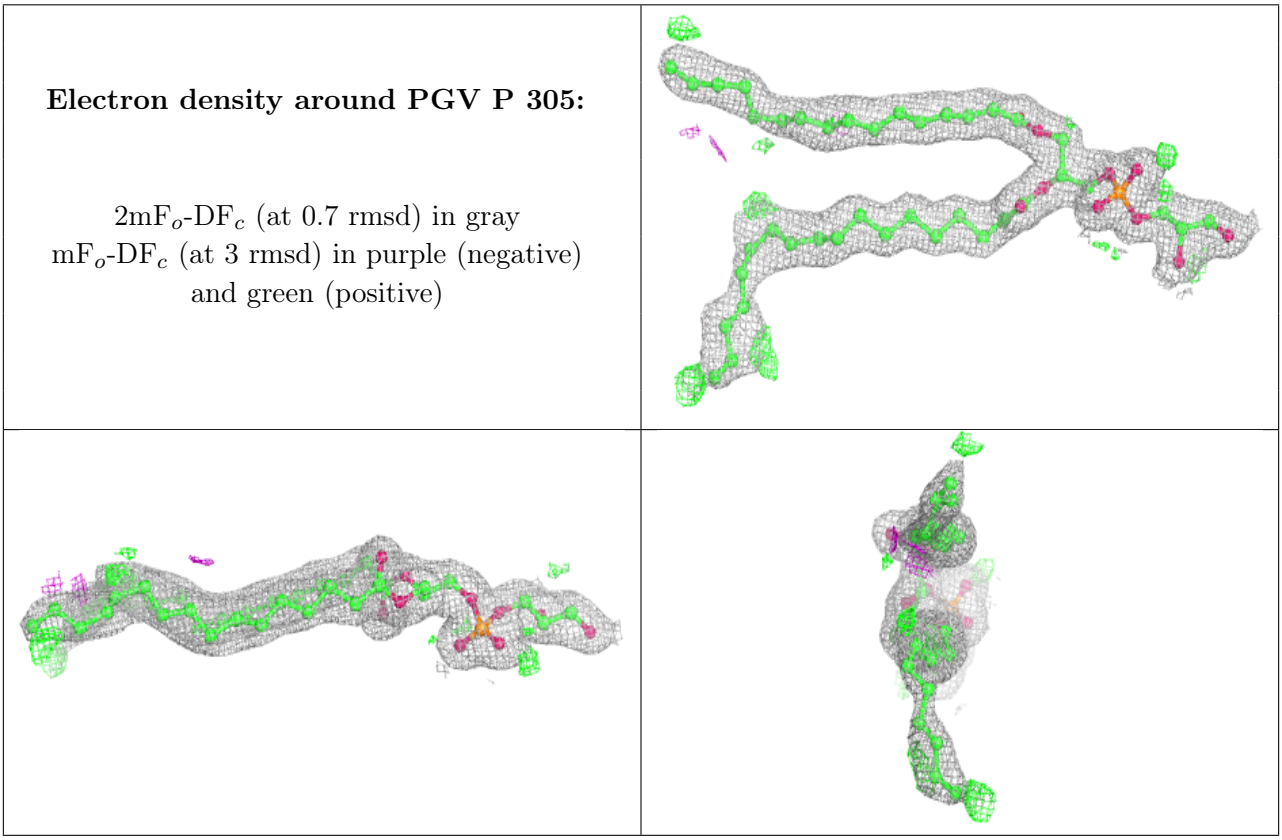
Electron density around HEA N 601:

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



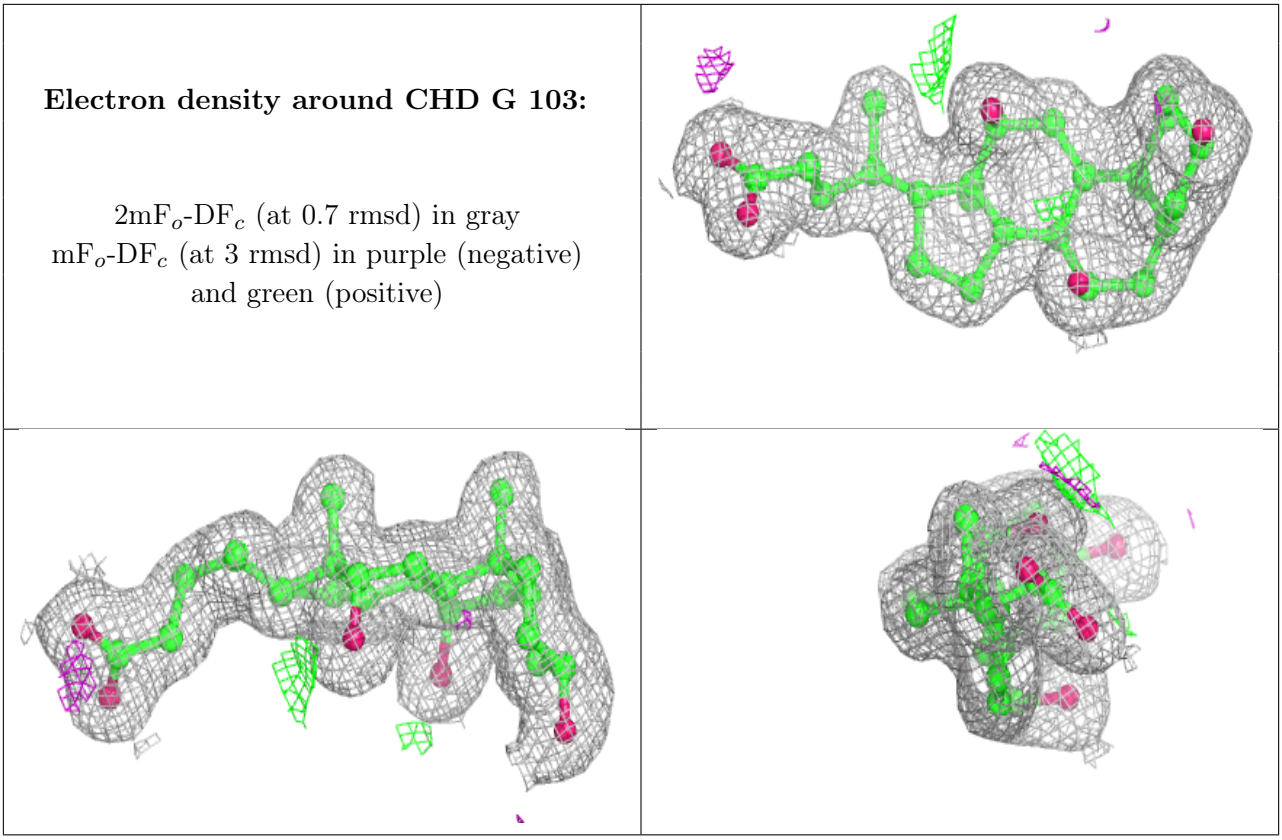
Electron density around PGV P 305:

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



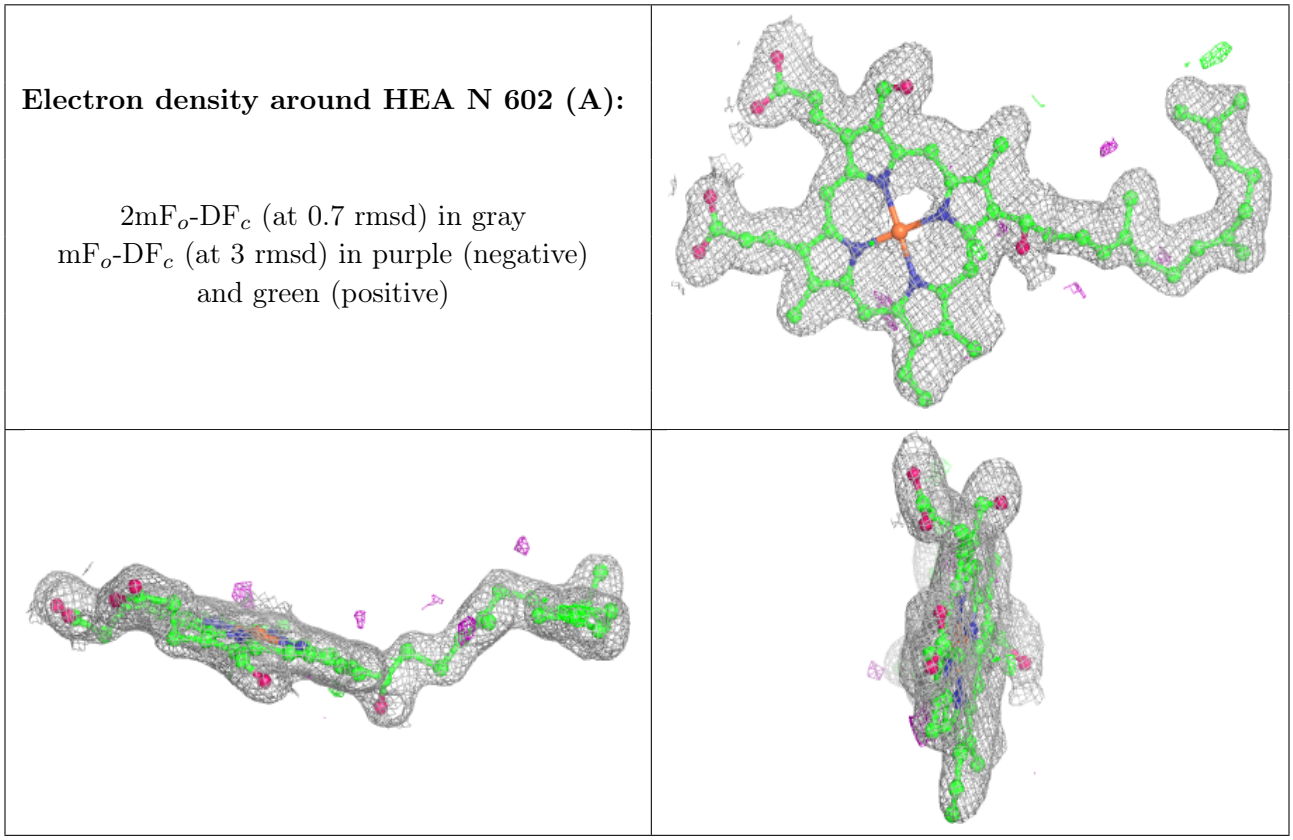
Electron density around CHD G 103:

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



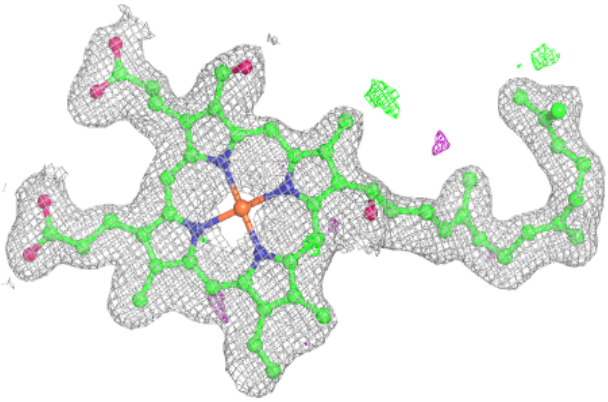
Electron density around HEA N 602 (A):

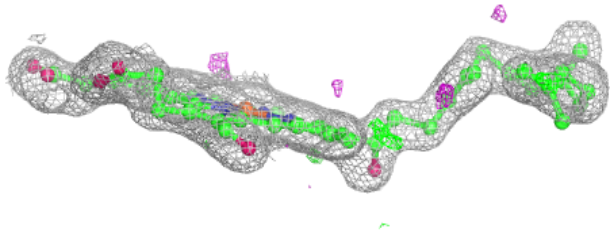
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

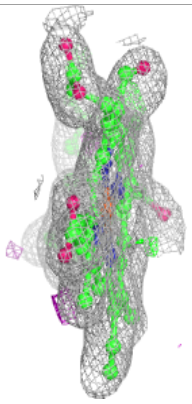


Electron density around HEA N 602 (B):

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

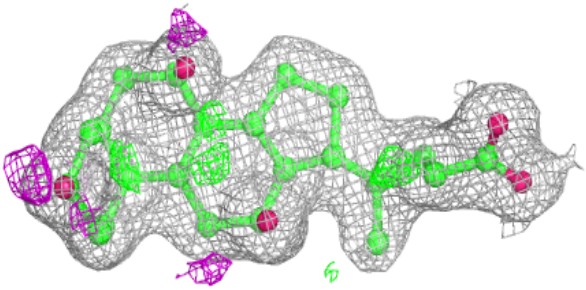


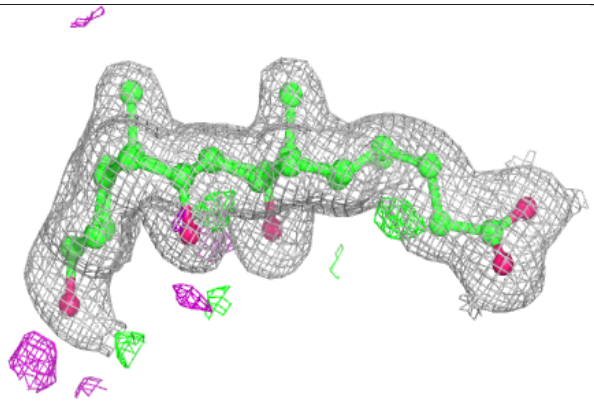


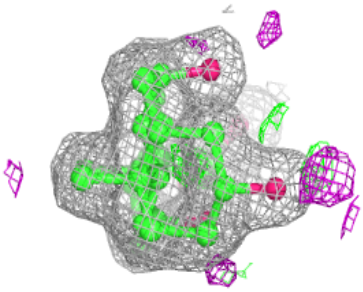


Electron density around CHD T 101:

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

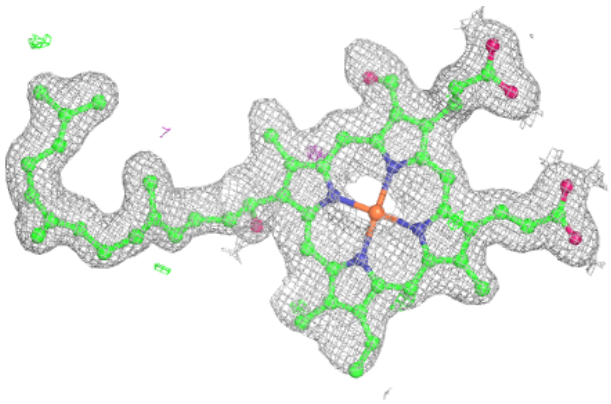


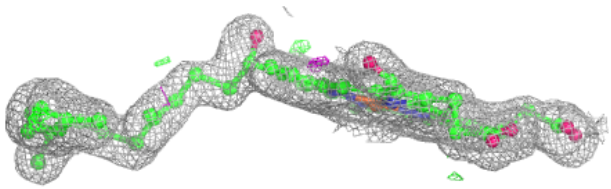


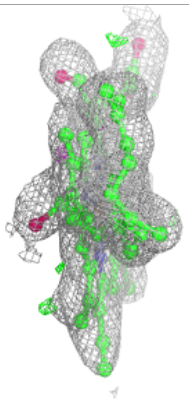


Electron density around HEA A 602 (A):

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

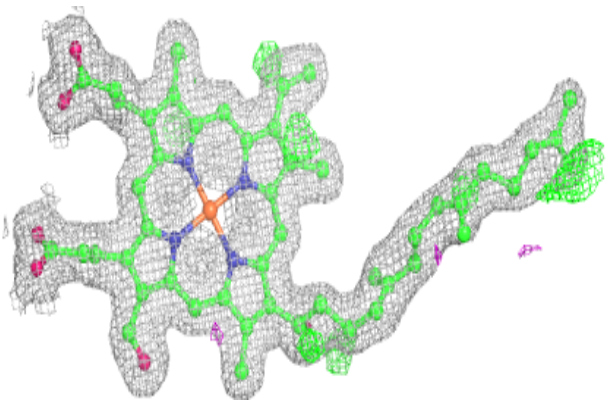


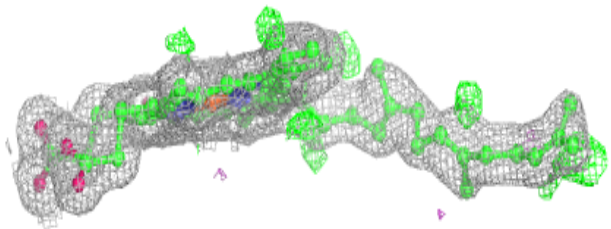


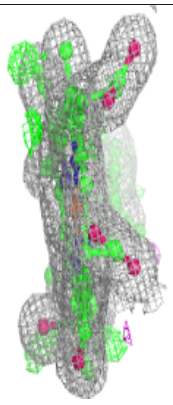


Electron density around HEA A 601:

$2mF_o$-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.