Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 02:08 PM JST

PDB ID	:	5ZCO
Title	:	azide-bound cytochrome c oxidase structure determined using the crystals exposed to 2 mM azide solution for 2 days
Authors	:	Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on	:	2018-02-19
Resolution	:	1.90 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:

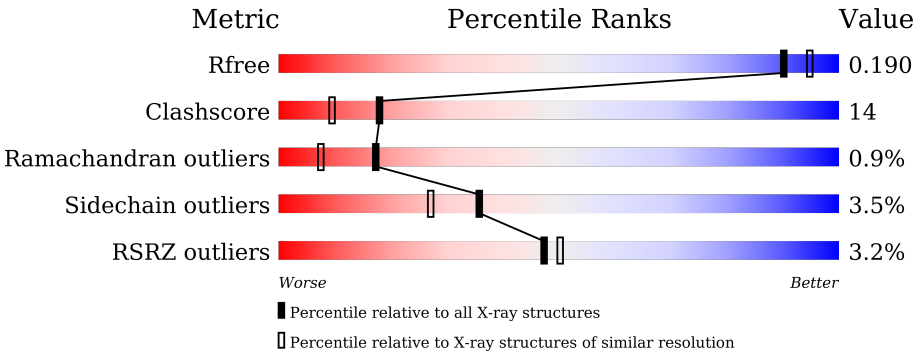
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	79% 18% ·
1	N	514	% 79% 18% ·
2	B	227	% 71% 26% ·
2	O	227	% 74% 24% ·
3	C	261	80% 18% ··
3	P	261	% 79% 18% ··

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Mol	Chain	Length	Quality of chain
4	D	147	80% 16%
4	Q	147	8% 73% 21%
5	E	109	3% 83% 12%
5	R	109	2% 78% 16%
6	F	98	8% 73% 22%
6	S	98	8% 71% 18% 8%
7	G	85	18% 60% 26% 9%
7	T	85	16% 69% 20% 8%
8	H	85	7% 67% 19% 6% 7%
8	U	85	6% 69% 21% 7%
9	I	73	7% 79% 21%
9	V	73	5% 81% 15%
10	J	59	5% 83% 15%
10	W	59	3% 88% 8%
11	K	56	75% 9% 12%
11	X	56	7% 77% 11% 12%
12	L	47	2% 81% 11% 6%
12	Y	47	4% 74% 23%
13	M	46	4% 72% 20% 7%
13	Z	46	9% 72% 22% 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
14	HEA	A	602[B]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	608[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	615	-	X	X	-
20	EDO	B	304	-	-	X	-
20	EDO	D	202	-	-	X	-
20	EDO	G	105	-	-	X	-
20	EDO	N	620	-	-	X	-
21	TGL	Y	101	-	-	X	-
26	CDL	C	305	-	-	X	-
26	CDL	N	601	-	-	X	-
26	CDL	P	304	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33609 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	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	9	0
			1899	1234	292	353	20			
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	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1233	803	204	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

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

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

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

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

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

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

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

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

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

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

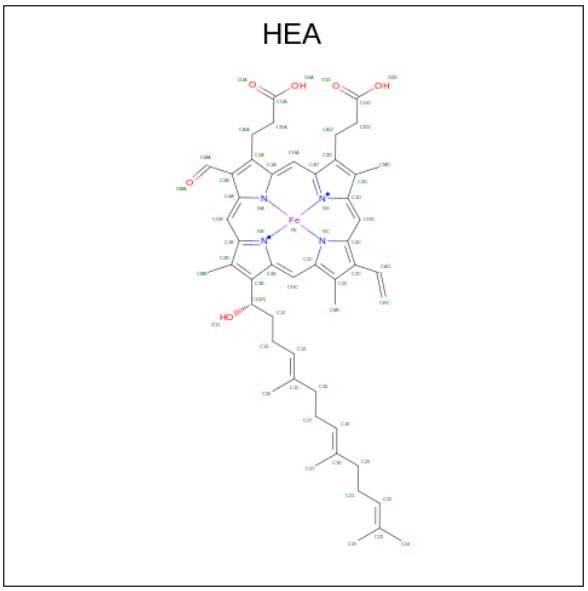
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

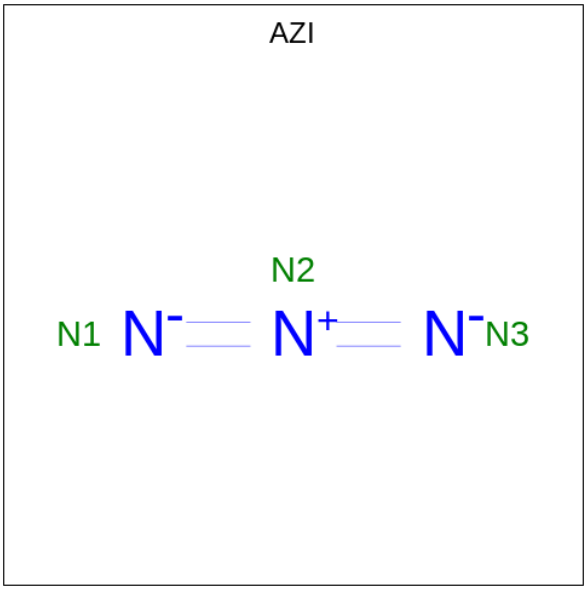
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

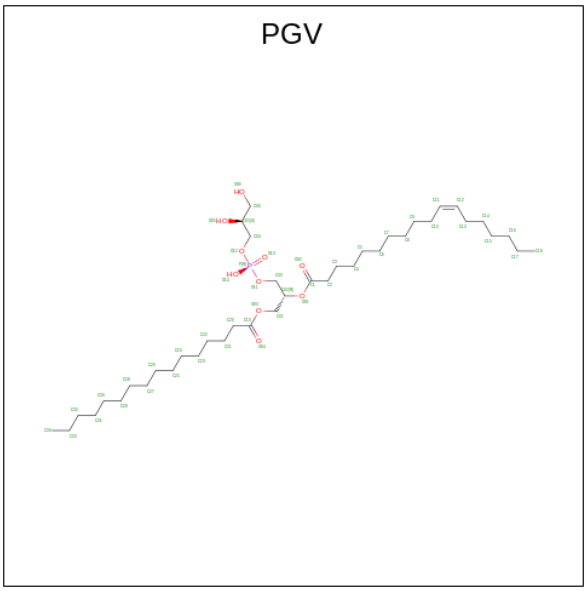
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



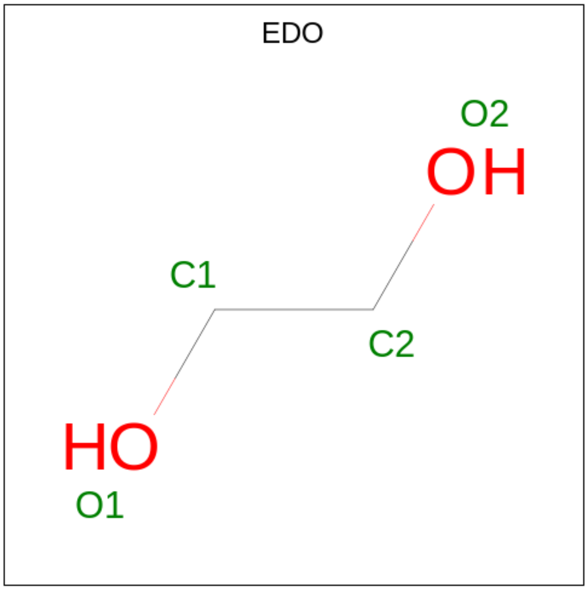
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

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



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

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



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

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

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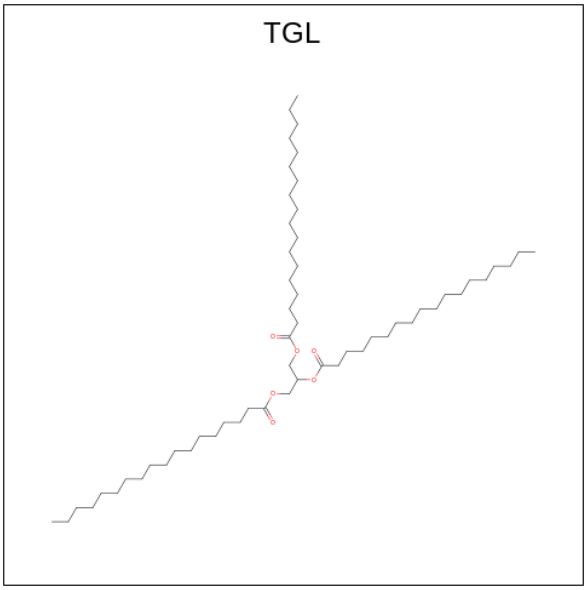
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C O 4 2 2	0	0
20	O	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	R	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	T	1	Total C O 4 2 2	0	0
20	Y	1	Total C O 4 2 2	0	0

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



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

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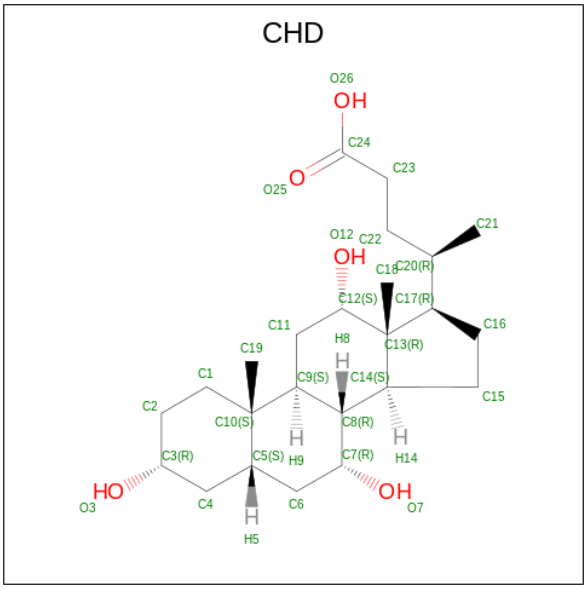
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	D	1	Total C O 63 57 6	0	0
21	L	1	Total C O 63 57 6	0	0
21	N	1	Total C O 63 57 6	0	0
21	Q	1	Total C O 63 57 6	0	0
21	Y	1	Total C O 63 57 6	0	0

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



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

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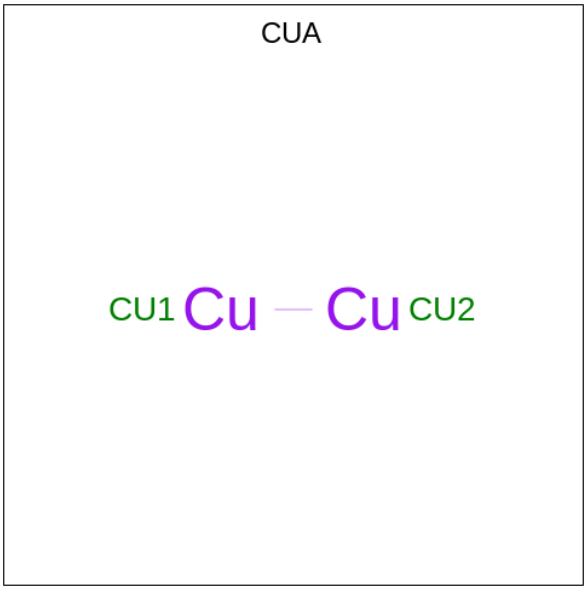
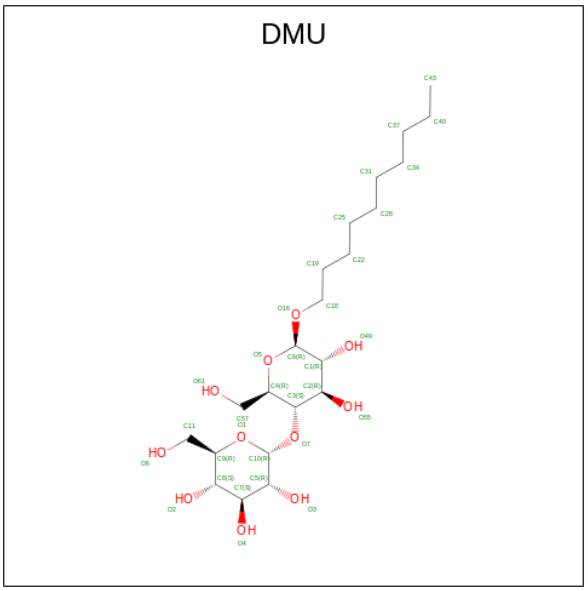
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

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



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

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

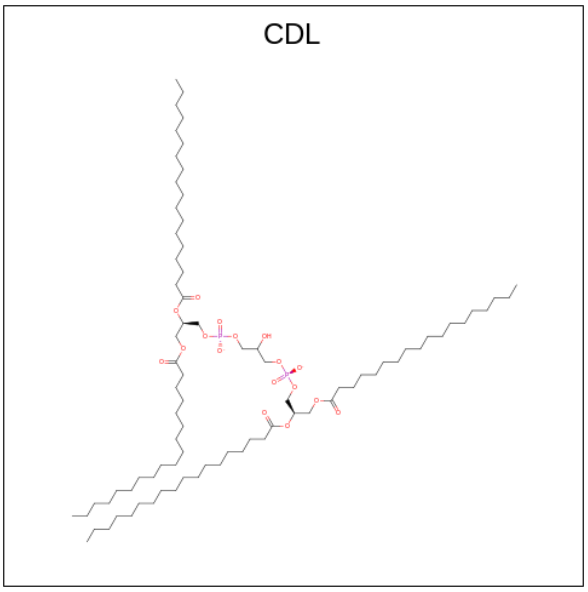


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	C	1	Total C O 33 22 11	0	0
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

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

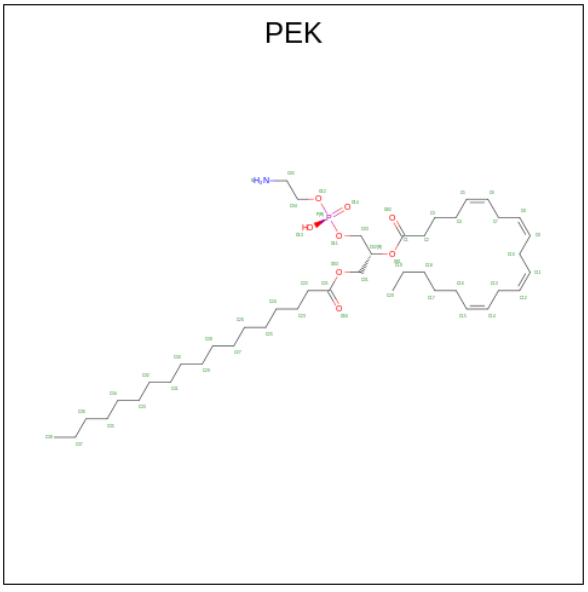
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

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



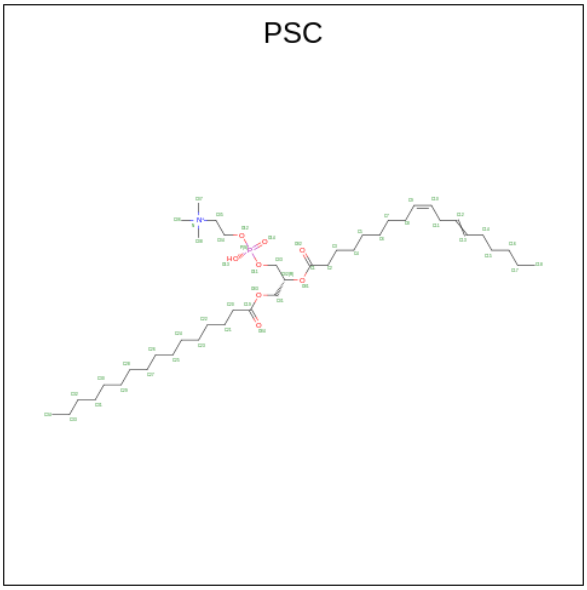
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	N	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

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



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

- Molecule 28 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(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
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	238	Total O 238 238	0	0
30	B	156	Total O 157 157	0	1
30	C	102	Total O 102 102	0	0
30	D	124	Total O 124 124	0	0
30	E	91	Total O 91 91	0	0
30	F	97	Total O 97 97	0	0
30	G	43	Total O 43 43	0	0
30	H	45	Total O 45 45	0	0
30	I	28	Total O 28 28	0	0
30	J	23	Total O 23 23	0	0
30	K	25	Total O 25 25	0	0
30	L	38	Total O 38 38	0	0
30	M	26	Total O 26 26	0	0
30	N	206	Total O 206 206	0	0
30	O	100	Total O 101 101	0	1
30	P	90	Total O 90 90	0	0
30	Q	29	Total O 29 29	0	0
30	R	40	Total O 40 40	0	0

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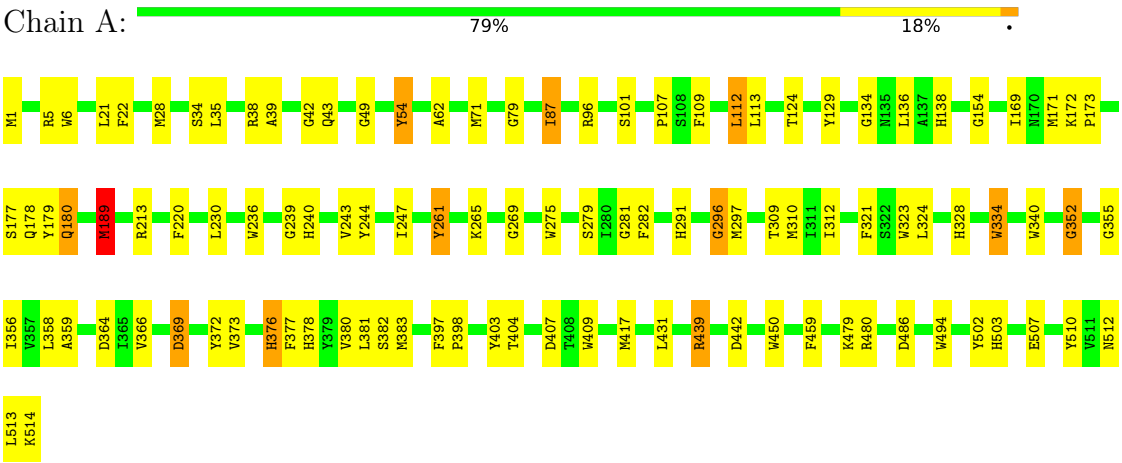
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	S	45	Total O 45 45	0	0
30	T	36	Total O 36 36	0	0
30	U	31	Total O 31 31	0	0
30	V	13	Total O 13 13	0	0
30	W	6	Total O 6 6	0	0
30	X	12	Total O 12 12	0	0
30	Y	12	Total O 12 12	0	0
30	Z	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

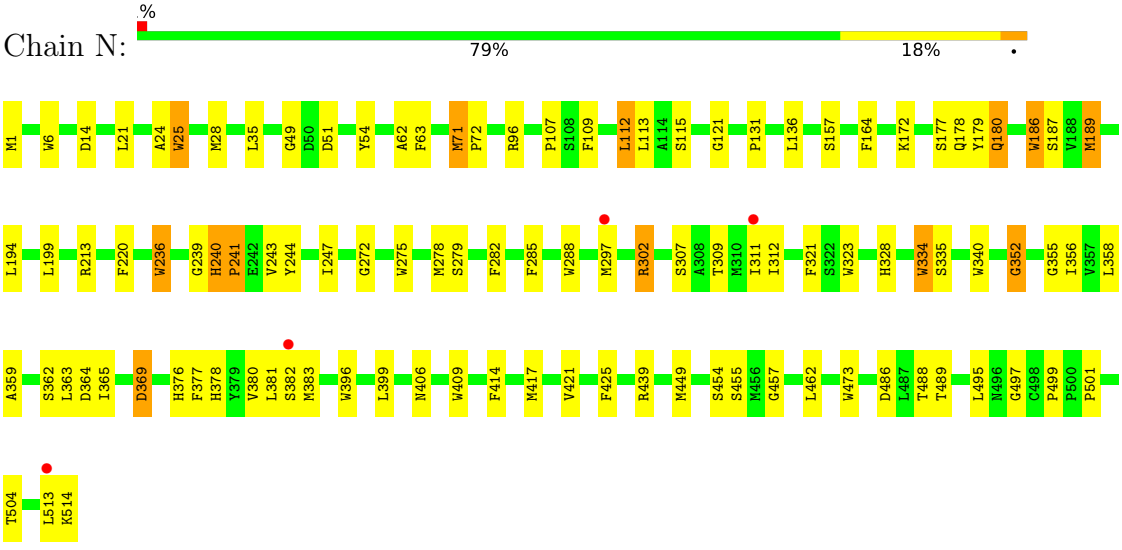
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



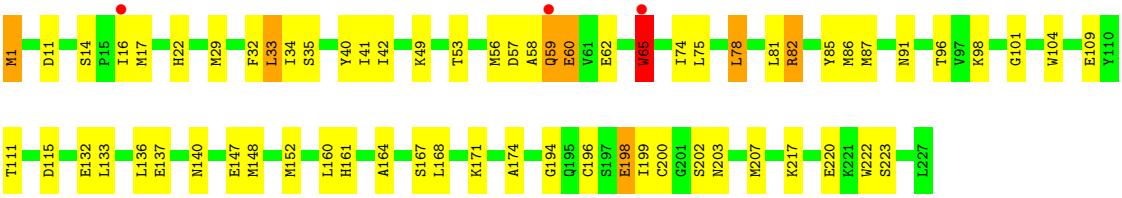
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

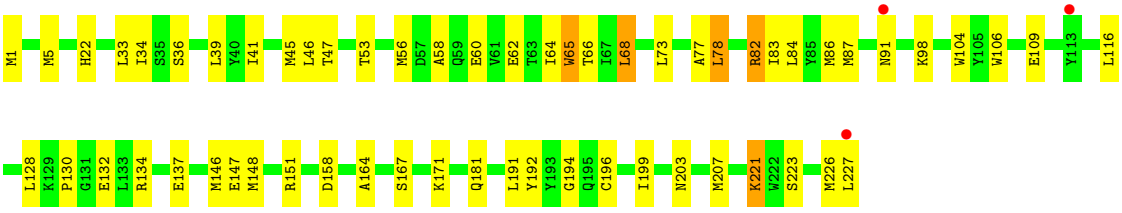


• Molecule 2: Cytochrome c oxidase subunit 2

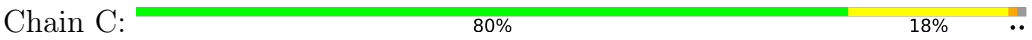
Chain B:

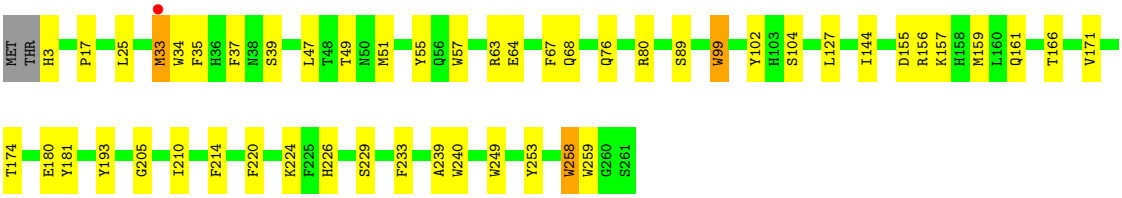


• Molecule 2: Cytochrome c oxidase subunit 2

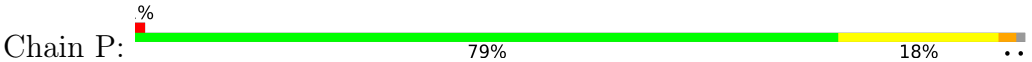


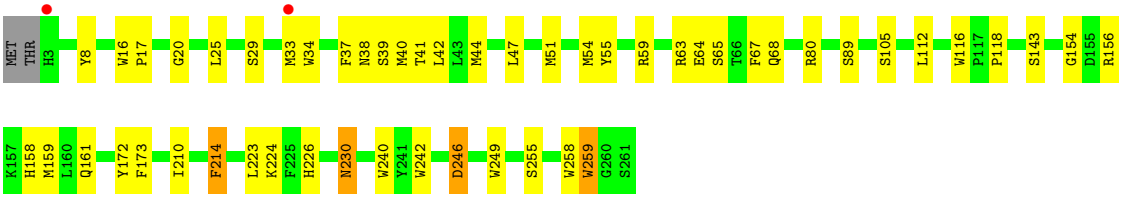
• Molecule 3: Cytochrome c oxidase subunit 3



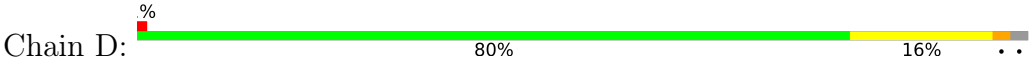


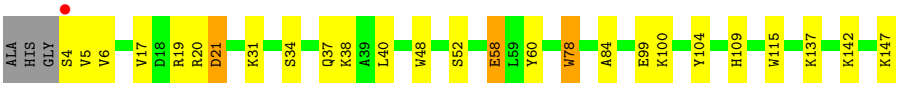
• Molecule 3: Cytochrome c oxidase subunit 3



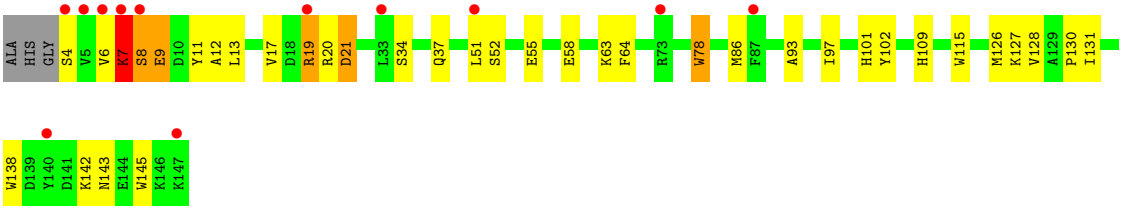


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

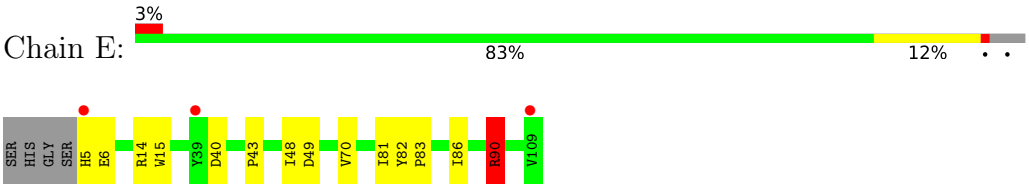




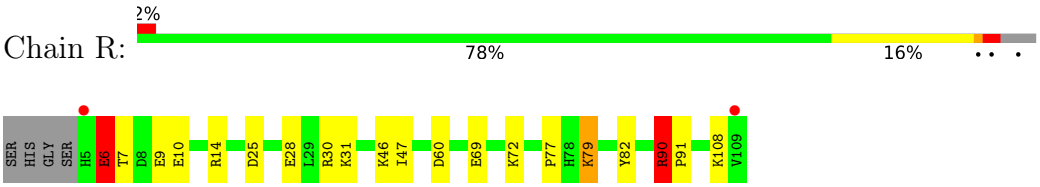
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



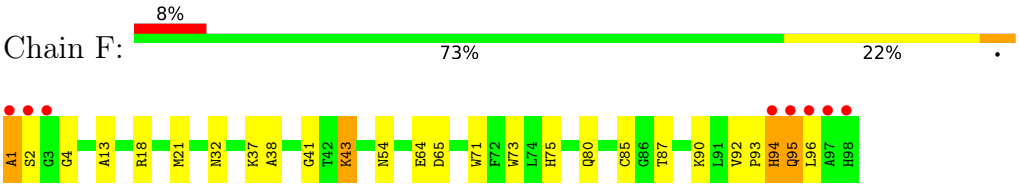
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



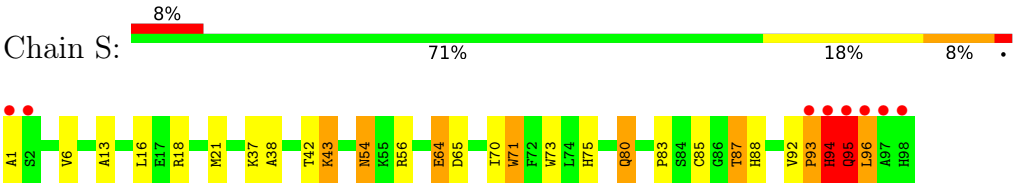
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



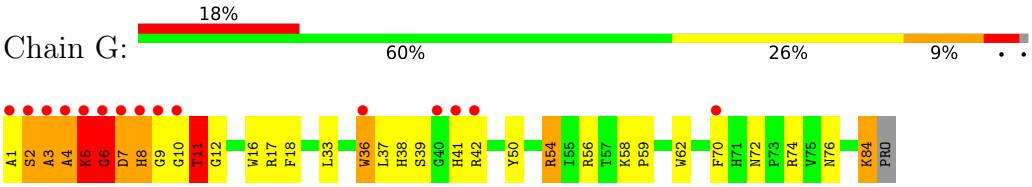
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



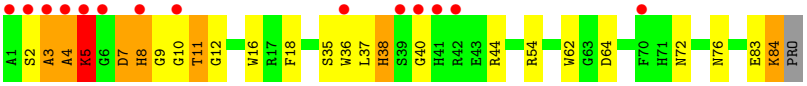
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



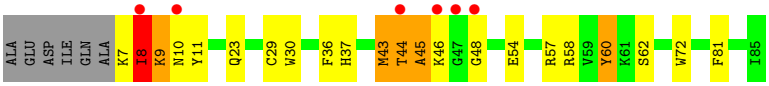
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



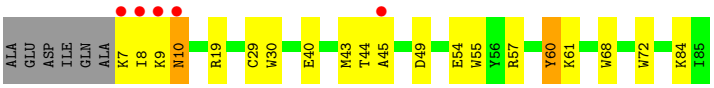
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



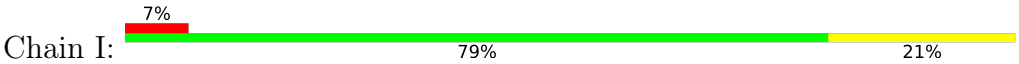
• Molecule 8: Cytochrome c oxidase subunit 6B1

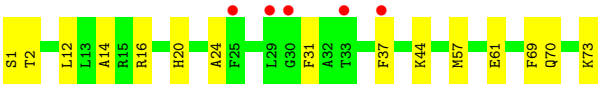


• Molecule 8: Cytochrome c oxidase subunit 6B1

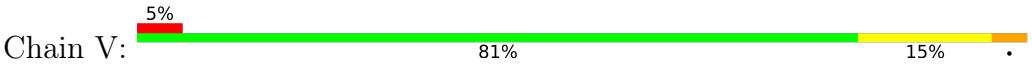


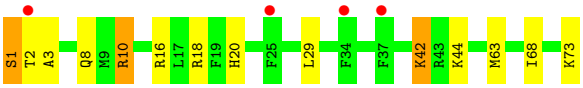
• Molecule 9: Cytochrome c oxidase subunit 6C



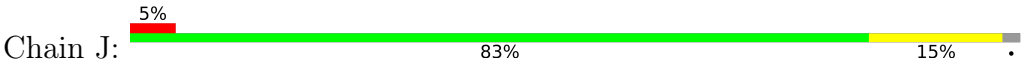


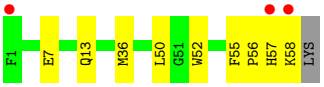
• Molecule 9: Cytochrome c oxidase subunit 6C



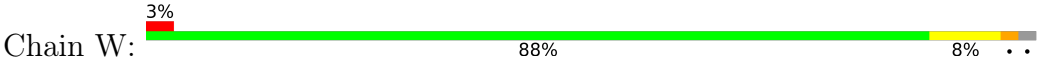


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



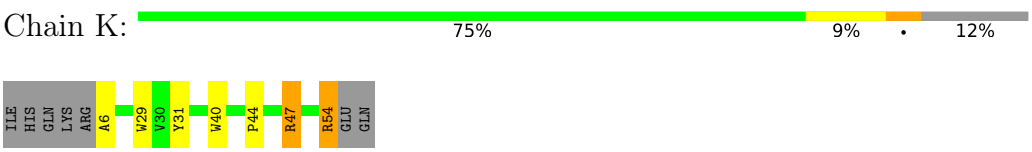


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



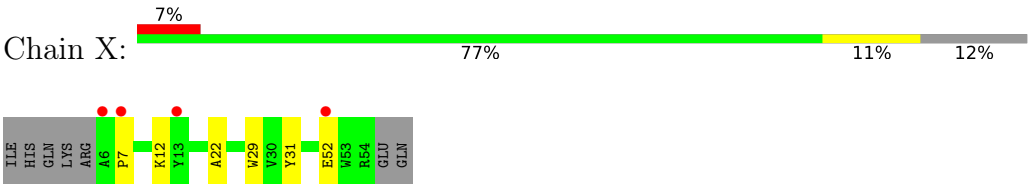
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



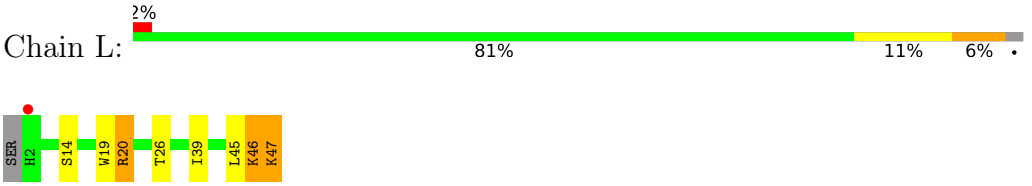
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



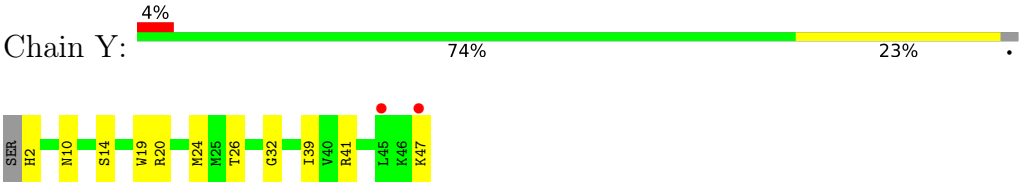
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



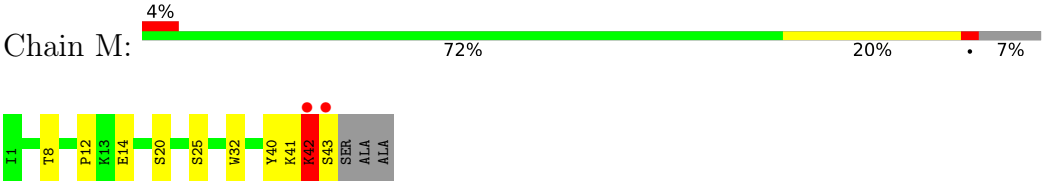
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



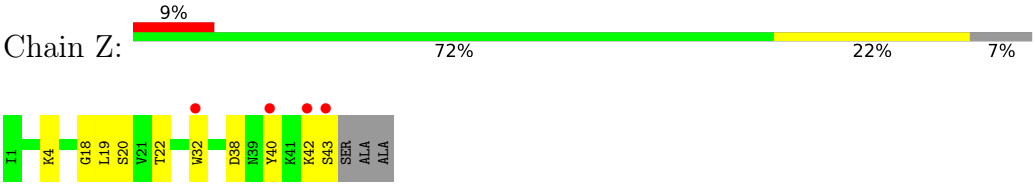
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.38Å 206.66Å 177.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 137.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.90) 99.7 (137.16-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.24 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.164 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	26414 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.62	35/4322 (0.8%)	1.28	25/5897 (0.4%)
1	N	1.57	33/4308 (0.8%)	1.22	15/5878 (0.3%)
2	B	1.44	12/1937 (0.6%)	1.22	6/2637 (0.2%)
2	O	1.23	5/1908 (0.3%)	1.11	7/2597 (0.3%)
3	C	1.53	16/2272 (0.7%)	1.10	1/3102 (0.0%)
3	P	1.51	18/2272 (0.8%)	1.12	6/3102 (0.2%)
4	D	1.48	7/1268 (0.6%)	1.17	3/1709 (0.2%)
4	Q	1.15	4/1259 (0.3%)	1.09	5/1698 (0.3%)
5	E	1.42	1/871 (0.1%)	1.36	6/1182 (0.5%)
5	R	1.16	1/882 (0.1%)	1.09	5/1196 (0.4%)
6	F	1.42	4/795 (0.5%)	1.21	3/1079 (0.3%)
6	S	1.24	1/780 (0.1%)	1.15	3/1058 (0.3%)
7	G	1.46	5/702 (0.7%)	1.14	4/953 (0.4%)
7	T	1.42	5/702 (0.7%)	1.12	3/953 (0.3%)
8	H	1.34	4/682 (0.6%)	1.00	0/921
8	U	1.24	5/682 (0.7%)	1.00	1/921 (0.1%)
9	I	1.14	1/605 (0.2%)	1.11	0/802
9	V	1.02	0/605	1.09	1/802 (0.1%)
10	J	1.20	0/471	1.00	1/636 (0.2%)
10	W	1.23	0/480	1.08	2/648 (0.3%)
11	K	1.36	3/398 (0.8%)	1.25	4/546 (0.7%)
11	X	1.18	2/405 (0.5%)	0.92	0/556
12	L	1.44	1/393 (0.3%)	1.18	2/526 (0.4%)
12	Y	1.36	2/401 (0.5%)	1.01	0/536
13	M	1.44	3/345 (0.9%)	1.14	0/470
13	Z	1.27	4/345 (1.2%)	1.04	1/470 (0.2%)
All	All	1.43	172/30090 (0.6%)	1.16	104/40875 (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
6	F	0	1
6	S	0	2
7	G	0	1
7	T	0	1
All	All	0	9

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	9.44	1.36	1.25
3	C	181	TYR	CE1-CZ	9.34	1.50	1.38
3	C	89	SER	CB-OG	9.28	1.54	1.42
1	N	179	TYR	CE1-CZ	8.87	1.50	1.38
2	B	65	TRP	CD2-CE2	8.14	1.51	1.41
1	N	409	TRP	CD2-CE2	7.83	1.50	1.41
2	B	198	GLU	CD-OE2	-7.83	1.17	1.25
7	T	62	TRP	CD2-CE2	7.63	1.50	1.41
6	F	4	GLY	N-CA	7.25	1.56	1.46
4	Q	78	TRP	CD2-CE2	7.16	1.50	1.41
1	A	101	SER	CB-OG	7.04	1.51	1.42
11	K	29	TRP	CD2-CE2	7.04	1.49	1.41
1	N	25	TRP	CG-CD1	7.03	1.46	1.36
3	C	249	TRP	CD2-CE2	7.03	1.49	1.41
3	C	240	TRP	CG-CD1	6.94	1.46	1.36
1	N	49	GLY	C-O	6.93	1.34	1.23
8	H	72	TRP	CD2-CE2	6.90	1.49	1.41
2	O	65	TRP	CD2-CE2	6.77	1.49	1.41
1	A	96	ARG	CZ-NH1	6.77	1.41	1.33
11	X	29	TRP	CD2-CE2	6.74	1.49	1.41
4	Q	138	TRP	CD2-CE2	6.71	1.49	1.41
3	C	259	TRP	CD2-CE2	6.68	1.49	1.41
2	B	167	SER	CB-OG	-6.63	1.33	1.42
1	A	323	TRP	CZ3-CH2	6.54	1.50	1.40
3	C	34	TRP	CD2-CE2	6.54	1.49	1.41
1	A	34	SER	CB-OG	-6.51	1.33	1.42
2	B	222	TRP	CG-CD1	6.50	1.45	1.36
3	P	258	TRP	CD2-CE2	6.50	1.49	1.41
1	N	340	TRP	CD2-CE2	6.48	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	TYR	CE2-CZ	6.42	1.47	1.38
8	U	68	TRP	CD2-CE2	6.42	1.49	1.41
3	C	104	SER	CB-OG	6.42	1.50	1.42
8	U	68	TRP	CG-CD1	6.39	1.45	1.36
4	D	115	TRP	CD2-CE2	6.39	1.49	1.41
3	P	20	GLY	N-CA	6.38	1.55	1.46
1	A	340	TRP	CD2-CE2	6.37	1.49	1.41
1	N	335	SER	CB-OG	6.35	1.50	1.42
2	B	109	GLU	CD-OE2	6.34	1.32	1.25
1	N	63	PHE	CG-CD1	6.34	1.48	1.38
7	G	16	TRP	CD2-CE2	6.32	1.49	1.41
7	G	36	TRP	CD2-CE2	6.31	1.49	1.41
1	N	279	SER	CA-CB	6.31	1.62	1.52
5	R	69	GLU	CD-OE2	-6.29	1.18	1.25
1	A	279	SER	CA-CB	6.26	1.62	1.52
1	A	409	TRP	CD2-CE2	6.24	1.48	1.41
3	P	249	TRP	CD2-CE2	6.24	1.48	1.41
2	O	167	SER	CB-OG	-6.24	1.34	1.42
3	C	229	SER	CA-CB	6.20	1.62	1.52
1	N	157	SER	CB-OG	6.19	1.50	1.42
1	A	129	TYR	CD1-CE1	6.17	1.48	1.39
1	N	275	TRP	CG-CD1	6.13	1.45	1.36
2	B	220	GLU	CD-OE1	-6.12	1.19	1.25
1	A	372	TYR	CG-CD1	6.09	1.47	1.39
6	F	1	ALA	C-O	6.09	1.34	1.23
2	O	147	GLU	CD-OE1	-6.08	1.19	1.25
2	B	223	SER	CA-CB	6.08	1.62	1.52
1	A	403	TYR	CG-CD1	6.03	1.47	1.39
3	P	259	TRP	CD2-CE2	6.03	1.48	1.41
1	A	323	TRP	CD2-CE2	6.03	1.48	1.41
1	A	275	TRP	CG-CD1	6.01	1.45	1.36
4	D	48	TRP	CD2-CE2	6.01	1.48	1.41
13	M	32	TRP	CD2-CE2	6.00	1.48	1.41
1	N	288	TRP	CE3-CZ3	5.98	1.48	1.38
1	A	352	GLY	N-CA	5.96	1.54	1.46
3	C	258	TRP	CD2-CE2	5.96	1.48	1.41
8	U	72	TRP	CD2-CE2	5.95	1.48	1.41
12	L	19	TRP	CD2-CE2	5.94	1.48	1.41
8	H	30	TRP	CD2-CE2	5.94	1.48	1.41
1	N	454	SER	CB-OG	5.92	1.50	1.42
5	E	15	TRP	CD2-CE2	5.91	1.48	1.41
1	A	79	GLY	N-CA	5.91	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	143	SER	CA-CB	5.87	1.61	1.52
1	N	186	TRP	CD2-CE2	5.85	1.48	1.41
12	Y	32	GLY	N-CA	5.84	1.54	1.46
3	P	246	ASP	CB-CG	5.83	1.64	1.51
1	A	179	TYR	CE1-CZ	5.83	1.46	1.38
1	N	25	TRP	CD2-CE2	5.83	1.48	1.41
2	B	147	GLU	CD-OE1	-5.80	1.19	1.25
1	N	6	TRP	CD2-CE2	5.76	1.48	1.41
3	C	35	PHE	CG-CD2	5.75	1.47	1.38
4	D	60	TYR	CG-CD1	5.75	1.46	1.39
1	N	457	GLY	N-CA	5.75	1.54	1.46
3	P	16	TRP	CG-CD2	5.72	1.53	1.43
13	Z	32	TRP	CD2-CE2	5.71	1.48	1.41
4	D	78	TRP	CD2-CE2	5.68	1.48	1.41
13	Z	18	GLY	N-CA	5.68	1.54	1.46
8	H	81	PHE	CE2-CZ	5.67	1.48	1.37
1	A	6	TRP	CD2-CE2	5.65	1.48	1.41
3	P	89	SER	CB-OG	5.65	1.49	1.42
1	N	473	TRP	CE3-CZ3	5.64	1.48	1.38
1	N	334	TRP	CD2-CE2	5.63	1.48	1.41
11	K	31	TYR	CG-CD1	5.63	1.46	1.39
13	M	20	SER	CA-CB	5.62	1.61	1.52
8	U	30	TRP	CD2-CE2	5.62	1.48	1.41
6	S	71	TRP	CE3-CZ3	5.60	1.48	1.38
1	A	334	TRP	CD2-CE2	5.59	1.48	1.41
1	N	473	TRP	CD2-CE2	5.59	1.48	1.41
3	P	8	TYR	CG-CD1	5.56	1.46	1.39
13	Z	20	SER	CA-CB	5.55	1.61	1.52
6	F	73	TRP	CD2-CE2	5.54	1.48	1.41
7	T	62	TRP	CG-CD1	5.54	1.44	1.36
1	A	376	HIS	CG-CD2	5.52	1.45	1.35
9	I	69	PHE	CG-CD1	5.51	1.47	1.38
3	P	34	TRP	CD2-CE2	5.50	1.48	1.41
4	D	60	TYR	CE1-CZ	5.49	1.45	1.38
1	N	236	TRP	CD1-NE1	5.46	1.47	1.38
7	G	36	TRP	CG-CD2	5.46	1.52	1.43
3	P	242	TRP	CD2-CE2	5.45	1.47	1.41
3	C	99	TRP	CD2-CE2	5.42	1.47	1.41
1	A	154	GLY	N-CA	5.42	1.54	1.46
7	G	62	TRP	CD2-CE2	5.41	1.47	1.41
2	O	106	TRP	CG-CD1	5.41	1.44	1.36
2	B	222	TRP	CD2-CE2	5.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	14	GLU	CD-OE1	-5.38	1.19	1.25
1	N	396	TRP	CD2-CE2	5.38	1.47	1.41
8	H	58	ARG	CZ-NH1	5.38	1.40	1.33
8	U	55	TRP	CD2-CE2	5.38	1.47	1.41
1	N	187	SER	CA-CB	5.37	1.61	1.52
1	A	502	TYR	CE1-CZ	-5.36	1.31	1.38
1	A	275	TRP	CZ2-CH2	5.35	1.47	1.37
6	F	71	TRP	CD2-CE2	5.35	1.47	1.41
1	A	134	GLY	C-O	5.35	1.32	1.23
7	T	36	TRP	CD2-CE2	5.33	1.47	1.41
1	A	261	TYR	CE2-CZ	5.32	1.45	1.38
1	N	455	SER	CB-OG	5.30	1.49	1.42
13	Z	22	THR	N-CA	5.29	1.56	1.46
12	Y	19	TRP	CD2-CE2	5.29	1.47	1.41
3	P	173	PHE	CG-CD1	5.29	1.46	1.38
11	K	40	TRP	CD2-CE2	5.26	1.47	1.41
1	A	275	TRP	CD2-CE2	5.25	1.47	1.41
1	A	49	GLY	C-O	5.25	1.32	1.23
1	N	239	GLY	N-CA	5.24	1.53	1.46
3	C	240	TRP	CD2-CE2	5.24	1.47	1.41
3	C	193	TYR	CD2-CE2	5.24	1.47	1.39
1	N	220	PHE	CE2-CZ	5.23	1.47	1.37
11	X	31	TYR	CG-CD1	5.23	1.46	1.39
1	A	507	GLU	CD-OE1	-5.22	1.20	1.25
7	T	16	TRP	CD2-CE2	5.21	1.47	1.41
4	Q	145	TRP	CD2-CE2	5.20	1.47	1.41
1	A	38	ARG	CZ-NH1	5.20	1.39	1.33
1	N	352	GLY	N-CA	5.18	1.53	1.46
2	B	59	GLN	CG-CD	5.17	1.62	1.51
1	N	288	TRP	CD2-CE2	5.17	1.47	1.41
1	N	497	GLY	N-CA	5.16	1.53	1.46
1	A	494	TRP	N-CA	5.15	1.56	1.46
1	N	323	TRP	CD2-CE2	5.15	1.47	1.41
3	P	116	TRP	CD2-CE2	5.14	1.47	1.41
2	B	220	GLU	CD-OE2	-5.14	1.20	1.25
4	Q	78	TRP	CG-CD1	5.14	1.44	1.36
1	A	87	ILE	N-CA	5.14	1.56	1.46
3	P	240	TRP	CG-CD1	5.14	1.44	1.36
1	N	244	TYR	CE2-CZ	5.13	1.45	1.38
3	P	172	TYR	CG-CD1	5.13	1.45	1.39
2	O	36	SER	CB-OG	5.13	1.49	1.42
4	D	52	SER	CB-OG	5.13	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	65	SER	CB-OG	5.12	1.49	1.42
1	A	43	GLN	CG-CD	5.11	1.62	1.51
3	C	102	TYR	CG-CD2	-5.11	1.32	1.39
1	N	25	TRP	CD2-CE3	5.11	1.48	1.40
1	N	414	PHE	CG-CD1	5.11	1.46	1.38
3	C	57	TRP	CD2-CE2	5.10	1.47	1.41
3	P	105	SER	CB-OG	5.10	1.48	1.42
3	C	226	HIS	CG-CD2	5.07	1.44	1.35
7	T	83	GLU	CD-OE1	5.07	1.31	1.25
1	A	510	TYR	CG-CD2	5.05	1.45	1.39
1	A	236	TRP	CE3-CZ3	5.05	1.47	1.38
1	A	269	GLY	N-CA	5.05	1.53	1.46
3	P	255	SER	CA-CB	5.04	1.60	1.52
7	G	50	TYR	CG-CD2	5.02	1.45	1.39
2	B	202	SER	N-CA	5.01	1.56	1.46
1	A	239	GLY	N-CA	5.01	1.53	1.46
1	N	272	GLY	N-CA	5.01	1.53	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	90	ARG	NE-CZ-NH1	18.45	129.53	120.30
5	E	90	ARG	NE-CZ-NH2	-15.05	112.78	120.30
4	Q	20	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	N	71	MET	CG-SD-CE	-14.65	76.76	100.20
1	A	71	MET	CG-SD-CE	-14.45	77.09	100.20
11	K	47	ARG	NE-CZ-NH1	13.34	126.97	120.30
5	R	90	ARG	NE-CZ-NH2	-9.98	115.31	120.30
4	Q	20	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	213	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	96	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	B	82	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	O	82	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	N	213	ARG	NE-CZ-NH2	-8.13	116.24	120.30
5	E	14	ARG	NE-CZ-NH1	8.11	124.35	120.30
4	D	21	ASP	CB-CG-OD2	8.10	125.59	118.30
6	F	18	ARG	NE-CZ-NH1	7.80	124.20	120.30
5	E	49	ASP	CB-CG-OD1	7.75	125.27	118.30
7	T	7	ASP	N-CA-C	7.71	131.83	111.00
1	A	38	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	B	65	TRP	CB-CA-C	7.35	125.11	110.40
1	N	51	ASP	CB-CG-OD1	7.35	124.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	164	PHE	CB-CG-CD1	-7.26	115.72	120.80
3	P	223	LEU	CB-CG-CD1	-7.08	98.96	111.00
4	Q	21	ASP	CB-CG-OD2	7.08	124.67	118.30
6	F	18	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	112	LEU	CD1-CG-CD2	-6.90	89.79	110.50
9	V	10	ARG	NE-CZ-NH2	-6.90	116.85	120.30
4	Q	20	ARG	CG-CD-NE	-6.84	97.44	111.80
7	G	54	ARG	NE-CZ-NH2	-6.78	116.91	120.30
6	S	94	HIS	N-CA-C	6.69	129.06	111.00
1	N	369	ASP	CB-CG-OD1	6.57	124.21	118.30
1	N	302[A]	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	N	302[B]	ARG	NE-CZ-NH1	6.55	123.58	120.30
7	G	6	GLY	N-CA-C	6.47	129.28	113.10
1	A	442	ASP	CB-CG-OD2	-6.47	112.48	118.30
7	G	5	LYS	CB-CA-C	6.20	122.80	110.40
1	A	373	VAL	CA-CB-CG2	-6.18	101.63	110.90
1	A	5	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	213	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	302[A]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	N	302[B]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
11	K	47	ARG	CD-NE-CZ	6.05	132.07	123.60
13	Z	4	LYS	CD-CE-NZ	-6.04	97.81	111.70
1	A	38	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	35	LEU	CB-CG-CD2	6.01	121.22	111.00
1	A	179	TYR	CD1-CE1-CZ	-6.01	114.39	119.80
1	A	369	ASP	CB-CG-OD1	5.95	123.66	118.30
2	B	136	LEU	CB-CG-CD1	-5.95	100.89	111.00
2	B	82	ARG	NE-CZ-NH1	5.93	123.27	120.30
3	C	49	THR	CA-CB-CG2	-5.90	104.14	112.40
3	P	214	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	A	54	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
1	N	194	LEU	CB-CG-CD1	5.79	120.84	111.00
3	P	214	PHE	CB-CG-CD1	5.77	124.84	120.80
12	L	20	ARG	NE-CZ-NH2	-5.74	117.43	120.30
5	E	90	ARG	CB-CG-CD	5.74	126.51	111.60
4	Q	127	LYS	CD-CE-NZ	5.72	124.86	111.70
1	A	310	MET	CA-CB-CG	-5.71	103.60	113.30
11	K	54	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	N	112	LEU	CD1-CG-CD2	-5.67	93.48	110.50
5	E	40	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	21	LEU	CB-CG-CD2	-5.67	101.36	111.00
10	W	27	THR	CB-CA-C	-5.64	96.36	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	129	TYR	CB-CG-CD2	-5.59	117.64	121.00
7	T	64	ASP	CB-CG-OD1	5.57	123.32	118.30
2	B	152	MET	CG-SD-CE	5.55	109.08	100.20
6	S	16	LEU	CB-CG-CD1	-5.54	101.59	111.00
2	O	82	ARG	NE-CZ-NH1	5.53	123.06	120.30
10	W	40	LEU	CB-CG-CD2	5.50	120.35	111.00
5	R	90	ARG	CG-CD-NE	-5.46	100.32	111.80
2	O	158	ASP	CB-CG-OD1	5.43	123.19	118.30
5	R	90	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	96	ARG	NE-CZ-NH1	5.36	122.98	120.30
8	U	19	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	480	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	189	MET	CB-CG-SD	-5.30	96.51	112.40
1	A	171	MET	CA-CB-CG	-5.28	104.33	113.30
4	D	20	ARG	NE-CZ-NH1	-5.27	117.67	120.30
12	L	20	ARG	CG-CD-NE	-5.27	100.74	111.80
2	O	65	TRP	CB-CA-C	5.25	120.91	110.40
1	A	124	THR	CA-CB-CG2	-5.22	105.09	112.40
1	N	96	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	O	227	LEU	CA-CB-CG	5.20	127.25	115.30
1	N	199	LEU	CB-CG-CD1	-5.19	102.18	111.00
5	R	60	ASP	CB-CG-OD1	5.19	122.97	118.30
5	R	30	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	O	73	LEU	CB-CG-CD1	-5.12	102.30	111.00
11	K	47	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	N	179	TYR	CD1-CE1-CZ	-5.08	115.22	119.80
4	D	137	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	N	189	MET	CB-CG-SD	-5.07	97.18	112.40
6	S	56	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	49	GLY	N-CA-C	-5.06	100.46	113.10
6	F	1	ALA	C-N-CA	5.06	134.34	121.70
1	A	439	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	O	192	TYR	CA-CB-CG	-5.04	103.82	113.40
1	A	366	VAL	CA-CB-CG2	-5.04	103.35	110.90
3	P	80[A]	ARG	NE-CZ-NH1	-5.03	117.79	120.30
3	P	80[B]	ARG	NE-CZ-NH1	-5.03	117.79	120.30
2	B	11	ASP	CB-CG-OD1	5.02	122.82	118.30
10	J	36	MET	CG-SD-CE	-5.01	92.18	100.20
3	P	223	LEU	CB-CG-CD2	5.01	119.52	111.00
7	T	5	LYS	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (9) 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
1	N	240	HIS	Sidechain
4	Q	7	LYS	Peptide
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide
7	T	40	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	110	0
1	N	4179	0	4154	101	0
2	B	1899	0	1898	70	0
2	O	1870	0	1868	51	0
3	C	2185	0	2097	61	0
3	P	2185	0	2097	51	0
4	D	1233	0	1223	37	0
4	Q	1224	0	1211	33	0
5	E	852	0	845	7	0
5	R	863	0	857	9	0
6	F	778	0	754	23	0
6	S	763	0	742	34	0
7	G	686	0	652	32	0
7	T	686	0	651	26	0
8	H	662	0	623	16	0
8	U	662	0	623	11	0
9	I	601	0	613	17	0
9	V	601	0	613	16	0
10	J	460	0	459	7	0
10	W	469	0	464	3	0
11	K	384	0	366	2	0
11	X	391	0	374	4	0
12	L	380	0	380	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	388	0	388	17	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	180	0	162	36	0
14	N	180	0	162	32	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	9	0	0	4	0
18	N	9	0	0	2	0
19	A	102	0	152	12	0
19	C	102	0	152	8	0
19	N	51	0	76	0	0
19	P	51	0	76	2	0
19	U	51	0	76	1	0
19	Z	51	0	76	11	0
20	A	40	0	60	12	0
20	B	16	0	24	5	0
20	D	8	0	12	12	0
20	E	12	0	18	0	0
20	F	12	0	18	0	0
20	G	8	0	12	6	0
20	L	4	0	6	0	0
20	M	4	0	6	0	0
20	N	40	0	60	7	0
20	O	4	0	6	0	0
20	P	12	0	18	0	0
20	R	4	0	6	0	0
20	S	8	0	12	0	0
20	T	4	0	6	0	0
20	Y	4	0	6	0	0
21	B	63	0	110	4	0
21	D	63	0	110	16	0
21	L	63	0	110	10	0
21	N	63	0	110	6	0
21	Q	63	0	110	13	0
21	Y	63	0	110	23	0
22	B	29	0	39	0	0
22	C	58	0	78	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	G	29	0	39	1	0
22	J	29	0	38	1	0
22	P	58	0	78	4	0
22	W	29	0	38	2	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	99	0	126	20	0
24	M	33	0	42	0	0
24	P	99	0	126	19	0
24	Z	33	0	42	1	0
25	C	1	0	0	0	0
25	P	1	0	0	1	0
26	C	100	0	156	25	0
26	N	100	0	156	26	0
26	P	100	0	156	25	0
26	T	100	0	156	19	0
27	C	106	0	154	27	0
27	G	106	0	154	12	0
27	P	53	0	77	5	0
27	T	53	0	77	1	0
28	E	52	0	80	12	0
28	O	52	0	80	15	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	238	0	0	32	0
30	B	157	0	0	30	2
30	C	102	0	0	6	0
30	D	124	0	0	18	2
30	E	91	0	0	1	0
30	F	97	0	0	4	0
30	G	43	0	0	7	0
30	H	45	0	0	1	0
30	I	28	0	0	4	1
30	J	23	0	0	3	0
30	K	25	0	0	1	0
30	L	38	0	0	3	0
30	M	26	0	0	7	1
30	N	206	0	0	15	0
30	O	101	0	0	3	0
30	P	90	0	0	4	0
30	Q	29	0	0	4	0
30	R	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	S	45	0	0	2	0
30	T	36	0	0	5	0
30	U	31	0	0	0	0
30	V	13	0	0	2	0
30	W	6	0	0	0	0
30	X	12	0	0	0	0
30	Y	12	0	0	1	0
30	Z	11	0	0	0	0
All	All	33609	0	32572	876	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (876) 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)
20:A:615:EDO:C2	20:A:615:EDO:C1	1.76	1.55
6:S:43:LYS:H	6:S:43:LYS:CD	1.19	1.45
19:Z:101:PGV:C2	19:Z:101:PGV:H011	1.50	1.38
20:A:615:EDO:C2	20:A:615:EDO:O1	1.70	1.33
9:I:73:LYS:HE2	30:I:118:HOH:O	1.16	1.32
20:B:305:EDO:H12	30:B:412:HOH:O	1.23	1.32
28:E:201:PSC:O02	9:I:14:ALA:HB2	1.25	1.30
30:B:410:HOH:O	8:H:62:SER:HA	1.29	1.29
1:A:512:ASN:HB3	30:A:701:HOH:O	1.31	1.28
1:A:503:HIS:HD2	30:A:813:HOH:O	0.94	1.27
21:D:201:TGL:HG31	30:D:353:HOH:O	1.34	1.25
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.38	1.24
1:A:39:ALA:HA	20:D:202:EDO:O1	1.35	1.22
1:A:136[B]:LEU:CD2	30:G:233:HOH:O	1.68	1.19
12:L:20:ARG:NH2	21:L:101:TGL:HC32	1.58	1.18
27:G:103:PEK:H312	27:G:103:PEK:H272	1.24	1.17
26:T:102:CDL:H321	26:T:102:CDL:OA7	1.43	1.17
6:S:43:LYS:HD3	6:S:43:LYS:N	1.49	1.16
6:S:43:LYS:CD	6:S:43:LYS:N	1.98	1.15
2:B:160:LEU:HB2	30:B:462:HOH:O	1.45	1.15
1:A:136[B]:LEU:HD21	30:G:233:HOH:O	1.20	1.15
30:A:706:HOH:O	21:D:201:TGL:HG11	1.46	1.12
1:A:512:ASN:CB	30:A:701:HOH:O	1.86	1.12
20:B:304:EDO:H21	30:B:404:HOH:O	0.95	1.11
6:S:43:LYS:H	6:S:43:LYS:HD2	1.10	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HG3	8:H:10:ASN:H	1.07	1.10
1:A:297[B]:MET:HB2	30:A:815:HOH:O	1.50	1.10
1:A:297[B]:MET:CB	30:A:815:HOH:O	1.96	1.10
20:A:618:EDO:H12	30:A:861:HOH:O	1.52	1.09
4:D:4:SER:HA	30:D:384:HOH:O	1.51	1.09
8:U:9:LYS:HG3	8:U:10:ASN:H	1.08	1.09
20:A:615:EDO:O1	20:A:615:EDO:H21	1.50	1.09
21:Y:101:TGL:CG1	21:Y:101:TGL:HA31	1.83	1.09
26:P:304:CDL:H272	26:P:304:CDL:H381	1.36	1.07
3:P:67:PHE:HE2	26:P:304:CDL:H1	1.16	1.06
26:P:304:CDL:H452	26:P:304:CDL:H411	1.06	1.06
24:P:306:DMU:H35	24:P:306:DMU:H29	1.32	1.06
1:A:512:ASN:ND2	30:A:701:HOH:O	1.88	1.04
1:A:112:LEU:HG	30:A:914:HOH:O	1.53	1.04
10:J:56:PRO:HD2	30:J:217:HOH:O	1.58	1.04
2:B:200:CYS:HB3	30:B:401:HOH:O	0.87	1.04
7:G:84:LYS:HD2	7:G:84:LYS:N	1.70	1.03
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.16	1.03
2:B:96:THR:HG22	30:B:531:HOH:O	1.57	1.03
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.99	1.02
19:Z:101:PGV:H011	19:Z:101:PGV:H21	1.06	1.02
26:P:304:CDL:H411	26:P:304:CDL:C45	1.87	1.02
19:Z:101:PGV:C2	19:Z:101:PGV:C01	2.36	1.02
28:O:302:PSC:C13	28:O:302:PSC:H343	1.90	1.02
11:K:6:ALA:N	30:K:101:HOH:O	1.92	1.01
3:C:67:PHE:HE2	26:C:305:CDL:H1	1.26	1.01
7:G:84:LYS:HD2	7:G:84:LYS:H	0.84	1.01
26:N:601:CDL:H611	26:N:601:CDL:C66	1.91	1.00
2:B:101:GLY:HA3	30:B:463:HOH:O	1.60	1.00
6:S:43:LYS:H	6:S:43:LYS:HD3	0.87	1.00
21:Y:101:TGL:HA31	21:Y:101:TGL:HG11	1.43	1.00
7:G:84:LYS:H	7:G:84:LYS:CD	1.73	0.99
20:B:304:EDO:H11	30:B:405:HOH:O	0.82	0.99
19:Z:101:PGV:H011	19:Z:101:PGV:H22	1.45	0.99
1:A:479:LYS:HB2	30:M:201:HOH:O	1.62	0.98
26:T:102:CDL:H571	26:T:102:CDL:H782	1.42	0.98
1:A:312:ILE:HD12	30:A:719:HOH:O	1.61	0.98
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:OD1	1.62	0.98
3:C:51[B]:MET:HE2	26:C:305:CDL:H392	1.45	0.98
10:J:55:PHE:HB2	30:J:205:HOH:O	1.62	0.98
1:N:356:ILE:HD13	14:N:603[B]:HEA:HMB1	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.12	0.98
1:N:417[A]:MET:CE	30:N:854:HOH:O	2.10	0.97
14:N:603[B]:HEA:HBC1	14:N:603[B]:HEA:HMC1	1.42	0.97
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	1.79	0.97
2:B:49:LYS:HE2	30:D:404:HOH:O	1.64	0.97
26:N:601:CDL:H321	26:N:601:CDL:OA7	1.64	0.97
27:C:309:PEK:H361	26:T:102:CDL:H872	1.43	0.96
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.13	0.96
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.30	0.96
1:A:514:LYS:CE	30:A:702:HOH:O	2.11	0.96
28:E:201:PSC:O02	9:I:14:ALA:CB	2.14	0.96
19:Z:101:PGV:H21	19:Z:101:PGV:C01	1.96	0.95
1:A:39:ALA:CA	20:D:202:EDO:O1	2.14	0.95
7:G:10:GLY:O	7:G:11:TPO:HB	1.65	0.95
30:A:926:HOH:O	21:D:201:TGL:HC31	1.66	0.95
1:A:513:LEU:O	1:A:514:LYS:HB2	1.64	0.95
3:C:33[A]:MET:HB2	24:C:302:DMU:C25	1.97	0.95
1:N:136[B]:LEU:HG	30:N:882:HOH:O	1.66	0.94
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	1.98	0.94
1:N:513:LEU:O	1:N:514:LYS:HB2	1.68	0.93
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.69	0.93
18:A:606[B]:AZI:N3	18:A:607[B]:AZI:N1	2.17	0.92
12:L:20:ARG:HH22	21:L:101:TGL:HC32	1.12	0.92
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.52	0.92
1:A:503:HIS:CD2	30:A:813:HOH:O	1.78	0.91
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:HBD2	1.49	0.91
1:A:39:ALA:HA	20:D:202:EDO:HO1	1.30	0.91
21:B:301:TGL:HA42	21:B:301:TGL:HA91	1.50	0.91
3:P:67:PHE:CE2	26:P:304:CDL:H1	2.04	0.91
26:P:304:CDL:H452	26:P:304:CDL:C41	1.97	0.90
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.52	0.90
1:A:230:LEU:HB3	30:A:704:HOH:O	1.71	0.89
6:S:95:GLN:HA	6:S:95:GLN:HE21	1.36	0.89
28:O:302:PSC:H343	28:O:302:PSC:H1	1.51	0.89
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.71	0.89
26:N:601:CDL:H371	2:O:78:LEU:HD12	1.53	0.89
8:H:9:LYS:HG3	8:H:10:ASN:N	1.85	0.89
21:N:610:TGL:CC4	30:N:906:HOH:O	2.20	0.89
3:C:33[A]:MET:HB2	24:C:302:DMU:C22	2.03	0.89
8:H:43:MET:O	8:H:45:ALA:N	2.05	0.89
1:A:514:LYS:NZ	30:A:702:HOH:O	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:PRO:O	20:G:105:EDO:H12	1.72	0.88
25:P:302:UNX:UNK	30:P:484:HOH:O	1.52	0.88
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.56	0.87
8:U:9:LYS:CG	8:U:10:ASN:H	1.85	0.87
12:L:20:ARG:HH22	21:L:101:TGL:CC3	1.86	0.87
4:D:100[B]:LYS:HE3	30:D:338:HOH:O	1.74	0.87
8:U:9:LYS:HG3	8:U:10:ASN:N	1.89	0.87
1:A:282:PHE:HA	7:T:4:ALA:CB	2.05	0.87
21:N:610:TGL:HC41	30:N:906:HOH:O	1.73	0.86
1:A:459:PHE:CE1	20:D:202:EDO:H11	2.12	0.85
2:B:98:LYS:HG3	30:B:531:HOH:O	1.77	0.85
1:N:356:ILE:HD13	14:N:603[B]:HEA:CMB	2.04	0.85
1:A:328:HIS:NE2	28:E:201:PSC:H31	1.90	0.85
19:A:608:PGV:H183	27:G:101:PEK:H322	1.57	0.85
27:G:103:PEK:H312	27:G:103:PEK:C27	2.04	0.85
3:C:63:ARG:HE	26:C:305:CDL:CA2	1.89	0.85
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.12	0.84
3:C:67:PHE:CE2	26:C:305:CDL:H1	2.13	0.84
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.79	0.83
26:N:601:CDL:H611	26:N:601:CDL:H661	1.58	0.83
3:C:180[B]:GLU:HG2	30:C:410:HOH:O	1.78	0.83
1:N:356:ILE:HA	14:N:603[B]:HEA:HMB3	1.60	0.82
8:U:9:LYS:O	8:U:10:ASN:HB2	1.79	0.82
24:P:306:DMU:H29	24:P:306:DMU:C9	2.09	0.82
2:B:16[B]:ILE:HG23	30:B:516:HOH:O	1.78	0.82
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.61	0.82
6:F:75:HIS:H	6:F:80:GLN:HE22	1.26	0.82
2:B:1:FME:HE3	2:B:133:LEU:HD22	1.62	0.82
5:E:90:ARG:HD2	30:E:372:HOH:O	1.79	0.82
30:A:838:HOH:O	4:D:17[A]:VAL:CG1	2.28	0.81
26:N:601:CDL:H591	26:N:601:CDL:H761	1.62	0.81
3:C:33[A]:MET:HB2	24:C:302:DMU:H13	1.61	0.81
12:Y:20:ARG:HH12	21:Y:101:TGL:HC32	1.44	0.81
4:D:19[A]:ARG:HD2	4:D:21:ASP:OD1	1.78	0.81
30:B:548:HOH:O	21:D:201:TGL:H281	1.79	0.81
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.26	0.81
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.79	0.81
6:S:75:HIS:H	6:S:80:GLN:HE22	1.26	0.80
28:O:302:PSC:C07	9:V:10:ARG:HH21	1.95	0.80
21:Y:101:TGL:HC41	21:Y:101:TGL:OC1	1.80	0.80
4:D:38:LYS:HD2	30:D:415:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:LYS:HB3	30:L:227:HOH:O	1.82	0.79
21:Y:101:TGL:OG1	21:Y:101:TGL:OG3	1.99	0.79
4:D:100[B]:LYS:CE	30:D:338:HOH:O	2.30	0.79
12:L:14:SER:H	21:L:101:TGL:HC31	1.47	0.79
30:B:548:HOH:O	21:D:201:TGL:C28	2.30	0.79
7:T:38:HIS:CE1	26:T:102:CDL:H141	2.18	0.79
2:B:160:LEU:O	30:B:401:HOH:O	2.00	0.78
19:C:304:PGV:H172	26:C:305:CDL:H632	1.64	0.78
3:C:51[B]:MET:CE	26:C:305:CDL:H392	2.13	0.78
1:N:28:MET:CE	14:N:602:HEA:H271	2.13	0.78
1:N:297[B]:MET:HB3	30:N:743:HOH:O	1.82	0.78
3:C:161[A]:GLN:HE22	27:C:307:PEK:H41	1.49	0.78
3:P:33[B]:MET:SD	24:P:306:DMU:H8	2.24	0.78
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.64	0.78
6:F:1:ALA:HB3	6:S:65:ASP:OD2	1.84	0.78
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.64	0.77
2:B:82:ARG:HA	26:T:102:CDL:H322	1.66	0.77
6:S:43:LYS:N	6:S:43:LYS:HD2	1.78	0.77
20:B:304:EDO:C2	30:B:404:HOH:O	1.71	0.77
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.24	0.77
20:A:615:EDO:H11	30:M:214:HOH:O	1.83	0.77
7:T:7:ASP:O	7:T:9:GLY:N	2.16	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.32	0.77
7:T:84:LYS:HA	7:T:84:LYS:HE3	1.65	0.77
1:N:28:MET:CE	14:N:602:HEA:C27	2.63	0.77
1:N:302[B]:ARG:HH12	1:N:365:ILE:CD1	1.96	0.76
22:C:306:CHD:H162	22:C:306:CHD:H231	1.67	0.76
1:A:398:PRO:HG3	30:A:710:HOH:O	1.84	0.76
2:B:29[B]:MET:SD	2:B:33:LEU:HD22	2.26	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.34	0.76
3:C:63:ARG:HE	26:C:305:CDL:HA22	1.51	0.76
30:A:838:HOH:O	4:D:17[A]:VAL:HG11	1.83	0.76
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.68	0.75
24:C:302:DMU:H22	10:J:50:LEU:HB2	1.67	0.75
1:A:297[B]:MET:HB3	30:A:815:HOH:O	1.68	0.75
3:P:63:ARG:HE	26:P:304:CDL:CA2	1.99	0.75
1:A:514:LYS:HE3	30:A:702:HOH:O	1.78	0.75
21:Y:101:TGL:HG11	21:Y:101:TGL:CA3	2.16	0.75
28:O:302:PSC:H02	28:O:302:PSC:H212	1.68	0.75
4:Q:78:TRP:CA	21:Q:201:TGL:HB22	2.18	0.74
7:G:7:ASP:HB2	1:N:178[A]:GLN:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92:VAL:HG21	30:F:293:HOH:O	1.86	0.74
7:G:72:ASN:H	7:G:76:ASN:HD22	1.35	0.73
1:N:356:ILE:CD1	14:N:603[B]:HEA:HMB1	2.18	0.73
6:S:43:LYS:HE3	30:S:238:HOH:O	1.88	0.73
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.54	0.73
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.71	0.73
1:A:28:MET:HE2	14:A:601:HEA:H273	1.71	0.73
8:H:9:LYS:HZ1	8:H:9:LYS:HA	1.54	0.73
3:P:224:LYS:CD	26:P:304:CDL:HB31	2.19	0.73
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	1.89	0.72
1:A:112:LEU:C	1:A:112:LEU:HD23	2.10	0.72
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.03	0.72
1:A:136[B]:LEU:HD11	30:A:933:HOH:O	1.88	0.72
2:B:53:THR:HG21	30:D:323:HOH:O	1.88	0.72
21:B:301:TGL:HA42	21:B:301:TGL:CA9	2.18	0.72
1:N:312:ILE:HD12	30:N:707:HOH:O	1.90	0.72
26:N:601:CDL:H322	2:O:82:ARG:HA	1.70	0.72
3:C:3:HIS:N	30:C:401:HOH:O	2.23	0.71
4:D:19[A]:ARG:HH21	4:D:21:ASP:CG	1.93	0.71
28:E:201:PSC:C1	9:I:14:ALA:HB2	2.19	0.71
20:N:620:EDO:H11	12:Y:10:ASN:HD22	1.55	0.71
27:C:309:PEK:H351	7:T:5:LYS:HB2	1.73	0.71
26:N:601:CDL:H611	26:N:601:CDL:C65	2.17	0.71
7:T:2:SER:OG	30:T:201:HOH:O	2.07	0.71
1:A:324:LEU:HD13	2:B:41[B]:ILE:HG21	1.73	0.71
26:P:304:CDL:HB21	26:P:304:CDL:OB6	1.92	0.70
4:D:99:GLU:OE2	20:D:202:EDO:H22	1.92	0.70
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:CBD	2.22	0.70
2:O:116:LEU:HD13	2:O:226:MET:CG	2.22	0.70
3:P:224:LYS:HD3	26:P:304:CDL:HB31	1.71	0.70
6:F:64:GLU:O	6:F:65:ASP:HB2	1.92	0.70
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.73	0.70
2:B:1:FME:HE3	2:B:133:LEU:CD2	2.21	0.70
3:C:63:ARG:HE	26:C:305:CDL:HA21	1.55	0.70
2:O:41:ILE:HD13	28:O:302:PSC:H342	1.73	0.70
26:C:305:CDL:HB32	26:C:305:CDL:HB21	1.73	0.69
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.05	0.69
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.57	0.69
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.27	0.69
3:C:47:LEU:O	3:C:51[A]:MET:HG2	1.92	0.69
9:V:18:ARG:HD3	30:V:112:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:609:PGV:H152	19:A:609:PGV:H322	1.75	0.69
12:Y:26:THR:OG1	30:Y:201:HOH:O	2.10	0.69
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.73	0.69
6:F:54[A]:ASN:ND2	6:F:54[A]:ASN:H	1.91	0.68
3:P:38:ASN:O	24:P:309:DMU:H32	1.93	0.68
7:T:76:ASN:HD21	27:T:101:PEK:HN2	1.38	0.68
1:N:417[A]:MET:HE2	30:N:854:HOH:O	1.80	0.68
3:C:33[B]:MET:HG2	3:C:39:SER:O	1.92	0.68
2:O:41:ILE:CD1	28:O:302:PSC:H342	2.24	0.68
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.29	0.68
21:Y:101:TGL:OC1	21:Y:101:TGL:CC4	2.42	0.68
24:C:302:DMU:H36	24:C:311:DMU:H41	1.74	0.68
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.92	0.68
6:F:87[A]:THR:HG21	30:F:273:HOH:O	1.93	0.68
2:B:87[B]:MET:HB3	30:B:472:HOH:O	1.93	0.67
21:Q:201:TGL:HG31	30:Q:315:HOH:O	1.94	0.67
4:D:4:SER:HB3	30:D:302:HOH:O	1.93	0.67
1:A:28:MET:CE	14:A:601:HEA:C27	2.73	0.67
2:B:56:MET:HB3	28:E:201:PSC:H251	1.77	0.67
21:Y:101:TGL:HA31	21:Y:101:TGL:HG12	1.76	0.67
19:A:608:PGV:H343	27:G:101:PEK:H382	1.75	0.67
28:O:302:PSC:H1	28:O:302:PSC:C34	2.25	0.67
13:M:8:THR:OG1	30:M:201:HOH:O	2.11	0.67
26:C:305:CDL:HB21	26:C:305:CDL:CB3	2.25	0.67
6:F:87[B]:THR:HG21	30:F:275:HOH:O	1.93	0.67
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.24	0.67
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	1.77	0.66
2:B:81:LEU:HD12	26:T:102:CDL:H382	1.76	0.66
28:O:302:PSC:H111	28:O:302:PSC:H321	1.77	0.66
4:D:4:SER:CB	30:D:302:HOH:O	2.43	0.66
27:C:307:PEK:H292	30:O:497:HOH:O	1.94	0.66
19:Z:101:PGV:C01	19:Z:101:PGV:H22	2.16	0.66
3:P:33[A]:MET:HE1	3:P:42:LEU:N	2.08	0.66
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.43	0.66
26:T:102:CDL:H361	26:T:102:CDL:H121	1.76	0.66
27:P:307:PEK:H042	6:S:1:ALA:N	2.11	0.66
4:Q:6:VAL:O	4:Q:7:LYS:HB2	1.94	0.66
7:T:44:ARG:HH22	7:T:84:LYS:HZ1	1.43	0.66
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	1.93	0.66
1:N:136[B]:LEU:HD11	30:N:905:HOH:O	1.96	0.66
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:310:DMU:H32	24:C:310:DMU:H29	1.78	0.65
2:B:1:FME:CE	2:B:133:LEU:HD13	2.26	0.65
2:B:174:ALA:HB1	30:B:463:HOH:O	1.95	0.65
27:G:103:PEK:H012	27:G:103:PEK:H22	1.78	0.65
7:T:11:TPO:CG2	30:T:233:HOH:O	2.43	0.65
3:C:157:LYS:NZ	27:C:307:PEK:H051	2.11	0.65
21:N:610:TGL:HC42	30:N:906:HOH:O	1.92	0.65
3:P:63:ARG:HE	26:P:304:CDL:HA22	1.59	0.65
4:D:34:SER:H	4:D:37:GLN:NE2	1.94	0.64
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	1.78	0.64
1:N:28:MET:HE1	14:N:602:HEA:C27	2.27	0.64
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.15	0.64
26:N:601:CDL:H371	2:O:78:LEU:CD1	2.26	0.64
27:C:307:PEK:H382	26:N:601:CDL:C27	2.28	0.64
4:D:19[A]:ARG:HG3	4:D:21:ASP:OD1	1.98	0.64
1:N:177:SER:H	1:N:180:GLN:HE21	1.45	0.64
3:C:80[B]:ARG:HH22	27:C:309:PEK:H032	1.62	0.64
1:N:28:MET:HE1	14:N:602:HEA:H271	1.79	0.64
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.37	0.64
9:V:18:ARG:HG3	30:V:108:HOH:O	1.98	0.64
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:CBC	2.28	0.63
1:N:302[B]:ARG:HH21	2:O:84:LEU:HD12	1.63	0.63
7:G:4:ALA:CB	1:N:282:PHE:HA	2.28	0.63
2:O:39:LEU:HD11	21:Q:201:TGL:H221	1.80	0.63
4:D:19[A]:ARG:CD	4:D:21:ASP:OD1	2.47	0.63
21:D:201:TGL:H242	21:D:201:TGL:HA91	1.79	0.63
27:P:307:PEK:C04	6:S:1:ALA:N	2.62	0.63
1:A:356:ILE:HA	14:A:602[B]:HEA:HMB3	1.81	0.63
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.13	0.63
21:B:301:TGL:HC22	30:I:127:HOH:O	1.99	0.62
2:B:29[B]:MET:SD	2:B:29[B]:MET:C	2.77	0.62
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:OD1	1.97	0.62
2:B:22[B]:HIS:ND1	9:I:44:LYS:HE2	2.15	0.62
9:I:70:GLN:NE2	30:I:103:HOH:O	2.32	0.62
1:N:383[B]:MET:SD	1:N:421:VAL:HG11	2.40	0.62
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.81	0.62
6:F:54[A]:ASN:H	6:F:54[A]:ASN:HD22	1.46	0.62
1:N:28:MET:HE2	14:N:602:HEA:H273	1.81	0.62
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.80	0.62
26:P:304:CDL:H272	26:P:304:CDL:C38	2.24	0.62
3:P:63:ARG:HE	26:P:304:CDL:HA21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.35	0.61
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	1.98	0.61
22:P:305:CHD:H231	22:P:305:CHD:H162	1.80	0.61
1:A:177:SER:H	1:A:180:GLN:HE21	1.48	0.61
26:P:304:CDL:H222	26:P:304:CDL:H651	1.81	0.61
1:A:28:MET:CE	14:A:601:HEA:H271	2.30	0.61
19:Z:101:PGV:H202	19:Z:101:PGV:H42	1.82	0.61
1:A:459:PHE:CE1	20:D:202:EDO:C1	2.84	0.61
4:Q:78:TRP:HB3	21:Q:201:TGL:HB22	1.82	0.61
12:L:47:LYS:CB	30:L:227:HOH:O	2.43	0.61
1:A:136[B]:LEU:HD23	30:G:233:HOH:O	1.63	0.61
1:A:220:PHE:HD1	30:A:704:HOH:O	1.84	0.61
1:A:417[A]:MET:CE	14:A:601:HEA:H263	2.31	0.61
3:C:224:LYS:HD2	26:C:305:CDL:HB31	1.83	0.60
6:S:94:HIS:HD2	6:S:95:GLN:HA	1.65	0.60
27:C:307:PEK:O14	27:C:307:PEK:N	2.34	0.60
1:N:311[B]:ILE:HD11	26:N:601:CDL:H232	1.82	0.60
28:O:302:PSC:H111	28:O:302:PSC:C32	2.32	0.60
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.84	0.60
1:A:324:LEU:HD13	2:B:41[B]:ILE:CG2	2.31	0.60
30:A:838:HOH:O	4:D:17[A]:VAL:HG12	1.97	0.60
1:N:356:ILE:CA	14:N:603[B]:HEA:HMB3	2.31	0.60
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.32	0.60
27:P:307:PEK:H042	6:S:1:ALA:H1	1.66	0.60
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.85	0.60
4:Q:4:SER:O	4:Q:9:GLU:HB3	2.01	0.60
21:Q:201:TGL:HA91	21:Q:201:TGL:H231	1.84	0.60
27:C:307:PEK:H382	26:N:601:CDL:H271	1.84	0.60
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.32	0.60
21:Q:201:TGL:H362	9:V:20:HIS:CE1	2.36	0.60
1:N:28:MET:HE2	14:N:602:HEA:C27	2.32	0.59
6:S:64:GLU:O	6:S:65:ASP:HB2	2.00	0.59
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:CE	2.76	0.59
2:B:140:ASN:HB3	30:B:510:HOH:O	2.01	0.59
26:N:601:CDL:H241	26:N:601:CDL:H531	1.82	0.59
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.96	0.59
20:A:618:EDO:H22	30:M:214:HOH:O	2.02	0.59
2:O:22[B]:HIS:CE1	9:V:44:LYS:NZ	2.70	0.59
4:Q:78:TRP:CB	21:Q:201:TGL:HB22	2.33	0.59
26:C:305:CDL:H641	26:C:305:CDL:H232	1.85	0.59
2:B:161:HIS:HB3	30:B:403:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:302[B]:ARG:HH21	2:O:84:LEU:CD1	2.15	0.58
22:P:305:CHD:H212	22:P:305:CHD:H12	1.84	0.58
7:G:38:HIS:CE1	26:N:601:CDL:H141	2.38	0.58
13:M:8:THR:N	30:M:201:HOH:O	2.36	0.58
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.84	0.58
21:N:610:TGL:HB92	21:N:610:TGL:C28	2.33	0.58
27:C:309:PEK:H361	26:T:102:CDL:C87	2.26	0.58
3:C:155:ASP:OD2	6:F:2:SER:HA	2.04	0.58
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:HG23	2.04	0.58
3:C:55:TYR:CE1	26:C:305:CDL:H521	2.38	0.57
3:C:80[B]:ARG:HH22	27:C:309:PEK:C03	2.16	0.57
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.39	0.57
3:C:174:THR:HG21	26:C:305:CDL:H861	1.86	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.57
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.69	0.57
8:H:9:LYS:HE3	8:H:11:TYR:H	1.70	0.57
1:A:291:HIS:CE1	18:A:607[B]:AZI:N2	2.72	0.57
1:A:356:ILE:HD13	14:A:602[B]:HEA:CMB	2.32	0.57
19:A:608:PGV:H312	19:C:304:PGV:H321	1.86	0.57
3:C:33[A]:MET:CB	24:C:302:DMU:C22	2.81	0.57
7:T:38:HIS:HE1	26:T:102:CDL:H141	1.67	0.57
1:N:307:SER:O	1:N:311[A]:ILE:HG13	2.04	0.57
4:Q:9:GLU:HG3	4:Q:11:TYR:CE2	2.39	0.57
7:G:12:GLY:N	30:G:203:HOH:O	2.36	0.57
21:B:301:TGL:HA72	21:B:301:TGL:H101	1.87	0.57
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.85	0.57
1:A:261:TYR:OH	20:A:615:EDO:H12	2.05	0.57
2:B:200:CYS:CB	30:B:401:HOH:O	1.75	0.57
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
1:N:382[B]:SER:O	1:N:383[B]:MET:CE	2.53	0.56
13:Z:19:LEU:HD23	19:Z:101:PGV:H311	1.85	0.56
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.56
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	1.86	0.56
1:A:382[B]:SER:O	1:A:383[B]:MET:HE2	2.05	0.56
14:A:602[B]:HEA:HBC1	14:A:602[B]:HEA:CMC	2.34	0.56
26:C:305:CDL:HB21	26:C:305:CDL:OB6	2.06	0.56
27:C:307:PEK:C38	26:N:601:CDL:C27	2.84	0.56
3:P:54[A]:MET:HE1	19:P:303:PGV:H131	1.88	0.56
2:B:111:THR:C	30:B:410:HOH:O	2.43	0.56
2:B:198:GLU:CG	30:B:462:HOH:O	2.53	0.56
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33[A]:MET:HB2	24:P:306:DMU:C19	2.35	0.56
27:P:307:PEK:C04	6:S:1:ALA:H2	2.18	0.56
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.88	0.56
4:Q:78:TRP:HA	21:Q:201:TGL:HB22	1.88	0.56
20:A:615:EDO:C2	20:A:615:EDO:HO1	2.08	0.55
3:C:33[A]:MET:CB	24:C:302:DMU:H13	2.35	0.55
27:C:309:PEK:C36	26:T:102:CDL:H872	2.29	0.55
5:R:31:LYS:HE2	6:S:83:PRO:O	2.07	0.55
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.87	0.55
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.88	0.55
7:G:1:ALA:O	7:G:3:ALA:N	2.39	0.55
1:N:417[A]:MET:HE1	30:N:854:HOH:O	1.88	0.55
1:A:358:LEU:O	14:A:602[B]:HEA:HMA	2.06	0.55
7:G:11:TPO:C	30:G:203:HOH:O	2.54	0.55
7:G:70[B]:PHE:HB2	27:G:101:PEK:H041	1.88	0.55
1:A:243:VAL:HG11	18:A:607[B]:AZI:N3	2.21	0.55
12:L:47:LYS:HG3	30:L:227:HOH:O	2.07	0.55
14:N:602:HEA:HHC	14:N:602:HEA:H122	1.89	0.55
26:P:304:CDL:H391	26:P:304:CDL:H351	1.87	0.55
7:T:11:TPO:HG22	30:T:233:HOH:O	2.06	0.55
24:C:302:DMU:C10	24:C:311:DMU:H41	2.37	0.55
1:A:281:GLY:C	7:T:4:ALA:HB1	2.27	0.55
14:N:603[A]:HEA:HMC1	14:N:603[A]:HEA:HBC1	1.88	0.55
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.55
4:Q:19[B]:ARG:NH1	30:Q:301:HOH:O	2.04	0.55
1:A:28:MET:HE2	14:A:601:HEA:C27	2.35	0.55
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.89	0.55
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.89	0.55
21:Q:201:TGL:H362	9:V:20:HIS:HE1	1.72	0.55
27:C:309:PEK:H351	7:T:5:LYS:HG3	1.88	0.55
7:G:8:HIS:CD2	7:G:9:GLY:H	2.25	0.55
2:B:29[B]:MET:SD	2:B:29[B]:MET:O	2.65	0.54
21:Y:101:TGL:CG1	21:Y:101:TGL:CA3	2.68	0.54
1:A:28:MET:HE1	14:A:601:HEA:H271	1.89	0.54
27:C:309:PEK:C35	7:T:5:LYS:HG3	2.37	0.54
7:G:36:TRP:HE3	7:G:39:SER:HB3	1.71	0.54
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.53	0.54
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.89	0.54
3:P:51[A]:MET:SD	3:P:54[A]:MET:CE	2.95	0.54
1:A:397:PHE:HD2	30:A:710:HOH:O	1.91	0.54
12:L:20:ARG:HH21	21:L:101:TGL:HC32	1.62	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:382[B]:SER:O	1:N:383[B]:MET:HE2	2.07	0.54
1:A:380[B]:VAL:CG1	1:A:381[B]:LEU:N	2.70	0.54
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.90	0.54
28:E:201:PSC:H011	28:E:201:PSC:H41	1.90	0.54
27:G:103:PEK:H012	27:G:103:PEK:C2	2.37	0.54
19:A:609:PGV:C22	30:M:222:HOH:O	2.55	0.53
2:B:96:THR:CG2	30:B:531:HOH:O	2.33	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53
10:W:32:TYR:OH	22:W:101:CHD:H213	2.08	0.53
27:C:309:PEK:H351	7:T:5:LYS:CB	2.38	0.53
1:N:178[B]:GLN:HG3	1:N:186:TRP:CE2	2.43	0.53
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.91	0.53
3:C:3:HIS:CA	30:C:401:HOH:O	2.57	0.53
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.09	0.53
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.44	0.52
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.09	0.52
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.90	0.52
6:F:75:HIS:H	6:F:80:GLN:NE2	2.02	0.52
3:C:220:PHE:HB2	26:C:305:CDL:H711	1.91	0.52
12:Y:24[B]:MET:SD	21:Y:101:TGL:HC21	2.49	0.52
1:N:14:ASP:OD1	20:N:620:EDO:H22	2.09	0.52
22:C:306:CHD:H162	22:C:306:CHD:C23	2.38	0.52
7:T:8:HIS:CD2	7:T:8:HIS:O	2.62	0.52
1:A:355:GLY:C	14:A:602[B]:HEA:HMB3	2.30	0.52
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.35	0.52
1:N:514:LYS:HE2	30:S:213:HOH:O	2.10	0.52
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.90	0.52
1:A:459:PHE:HE1	20:D:202:EDO:C1	2.22	0.52
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.92	0.52
3:C:156:ARG:HH21	22:C:306:CHD:C24	2.22	0.52
1:N:131:PRO:HB3	20:N:617:EDO:H12	1.90	0.52
1:N:247:ILE:HB	14:N:603[B]:HEA:HBC2	1.91	0.52
1:A:22:PHE:HA	21:L:101:TGL:HB71	1.91	0.52
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.92	0.52
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.40	0.51
12:L:45:LEU:O	12:L:46:LYS:C	2.48	0.51
3:C:258:TRP:CZ3	26:N:601:CDL:H642	2.45	0.51
13:M:40:TYR:O	13:M:43:SER:HB2	2.10	0.51
2:O:66:THR:CG2	30:O:497:HOH:O	2.58	0.51
1:A:39:ALA:CA	20:D:202:EDO:HO1	2.09	0.51
14:A:601:HEA:HHC	14:A:601:HEA:H122	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.93	0.51
2:B:174:ALA:CB	30:B:463:HOH:O	2.56	0.51
12:Y:20:ARG:HH22	21:Y:101:TGL:HC62	1.74	0.51
1:A:378:HIS:O	1:A:383[B]:MET:HG2	2.11	0.51
3:C:210:ILE:HG12	19:C:304:PGV:H132	1.91	0.51
12:L:47:LYS:HE2	12:L:47:LYS:HA	1.93	0.51
2:B:198:GLU:HG2	30:B:462:HOH:O	2.09	0.51
27:C:307:PEK:N	27:C:307:PEK:P	2.84	0.51
26:T:102:CDL:H161	26:T:102:CDL:OB3	2.10	0.51
4:D:17[A]:VAL:HG23	4:D:17[A]:VAL:O	2.11	0.51
21:D:201:TGL:CG3	30:D:353:HOH:O	2.13	0.51
3:P:33[A]:MET:HB2	24:P:306:DMU:H9	1.93	0.51
3:C:253:TYR:HE2	26:N:601:CDL:H641	1.76	0.51
27:G:101:PEK:H172	27:G:101:PEK:C12	2.41	0.51
3:P:59:ARG:HA	26:P:304:CDL:H512	1.93	0.51
5:R:14[B]:ARG:HG2	30:R:301:HOH:O	2.10	0.51
21:D:201:TGL:H363	9:I:20:HIS:HE1	1.76	0.50
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.59	0.50
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	1.93	0.50
1:A:378:HIS:HA	1:A:382[B]:SER:CB	2.42	0.50
6:S:95:GLN:HA	6:S:95:GLN:NE2	2.17	0.50
26:T:102:CDL:H601	26:T:102:CDL:H651	1.93	0.50
1:A:380[B]:VAL:HG13	1:A:381[B]:LEU:N	2.26	0.50
2:B:1:FME:HE1	2:B:133:LEU:HD13	1.92	0.50
3:C:33[B]:MET:HB2	24:C:302:DMU:C22	2.41	0.50
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.41	0.50
7:G:58:LYS:NZ	20:G:105:EDO:H11	2.27	0.50
3:P:224:LYS:HD3	26:P:304:CDL:CB3	2.39	0.50
7:T:44:ARG:HH22	7:T:84:LYS:NZ	2.08	0.50
1:A:358:LEU:C	14:A:602[B]:HEA:HMA	2.31	0.50
1:A:417[A]:MET:HE3	14:A:601:HEA:H263	1.93	0.50
13:M:41:LYS:O	13:M:43:SER:N	2.41	0.50
26:N:601:CDL:H531	26:N:601:CDL:H261	1.92	0.50
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE1	1.91	0.50
1:N:309:THR:HG22	14:N:603[A]:HEA:HMB2	1.92	0.50
3:P:156:ARG:HE	22:P:305:CHD:C24	2.24	0.50
8:U:57:ARG:O	8:U:61:LYS:HB2	2.12	0.50
1:N:136[B]:LEU:HD11	30:T:235:HOH:O	2.11	0.50
1:N:358:LEU:O	14:N:603[B]:HEA:HMA	2.11	0.50
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.76	0.50
10:J:7:GLU:HG3	30:J:215:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:201:PSC:H32	9:I:14:ALA:HA	1.94	0.50
2:O:39:LEU:CD1	21:Q:201:TGL:H221	2.41	0.50
1:A:514:LYS:HG3	6:F:38:ALA:HB2	1.93	0.49
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.11	0.49
3:P:246:ASP:HB2	30:P:482:HOH:O	2.12	0.49
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.12	0.49
12:Y:20:ARG:HH22	21:Y:101:TGL:HC82	1.76	0.49
3:P:33[A]:MET:HB2	24:P:306:DMU:H8	1.94	0.49
3:P:33[B]:MET:HE3	24:P:306:DMU:H6	1.94	0.49
3:C:37:PHE:CD2	24:C:302:DMU:H8	2.47	0.49
2:O:47:THR:HB	21:Q:201:TGL:H181	1.95	0.49
1:A:439:ARG:HD3	2:B:199:ILE:HB	1.94	0.49
24:P:306:DMU:O1	24:P:309:DMU:H40	2.12	0.49
12:Y:24[A]:MET:SD	21:Y:101:TGL:H172	2.53	0.49
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.11	0.49
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.95	0.49
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.48	0.49
8:H:7:LYS:O	8:H:8:ILE:HD12	2.13	0.49
3:P:33[B]:MET:SD	24:P:306:DMU:C19	3.00	0.49
3:P:158:HIS:CE1	6:S:1:ALA:HA	2.48	0.49
26:T:102:CDL:H111	26:T:102:CDL:OA5	2.13	0.49
1:A:136[B]:LEU:CD1	30:A:933:HOH:O	2.56	0.49
4:D:19[A]:ARG:CG	4:D:21:ASP:OD1	2.59	0.49
1:A:356:ILE:CD1	14:A:602[B]:HEA:HMB1	2.37	0.48
4:D:100[B]:LYS:HE3	30:D:301:HOH:O	2.12	0.48
1:N:321:PHE:CD1	28:O:302:PSC:H331	2.48	0.48
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.95	0.48
26:P:304:CDL:H392	26:P:304:CDL:H252	1.94	0.48
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:CG	2.30	0.48
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.12	0.48
7:T:8:HIS:O	7:T:8:HIS:HD2	1.96	0.48
8:U:9:LYS:CG	8:U:10:ASN:N	2.58	0.48
26:C:305:CDL:H212	26:C:305:CDL:H602	1.94	0.48
8:H:8:ILE:CG2	8:H:8:ILE:O	2.61	0.48
19:A:609:PGV:H132	19:A:609:PGV:H302	1.94	0.48
27:C:307:PEK:P	27:C:307:PEK:HN1	2.36	0.48
4:D:5:VAL:HA	30:D:303:HOH:O	2.12	0.48
3:P:33[B]:MET:HA	24:P:306:DMU:H9	1.94	0.48
26:T:102:CDL:H762	26:T:102:CDL:H551	1.95	0.48
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.91	0.48
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:601:CDL:HA21	26:N:601:CDL:H131	1.96	0.48
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.48
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.32	0.48
7:T:3:ALA:O	7:T:4:ALA:CB	2.62	0.48
28:O:302:PSC:H212	28:O:302:PSC:C02	2.40	0.48
26:P:304:CDL:PA1	26:P:304:CDL:HB22	2.52	0.48
1:A:404:THR:HA	30:A:710:HOH:O	2.13	0.48
2:B:217:LYS:HG2	30:B:490:HOH:O	2.13	0.48
20:B:304:EDO:C1	30:B:405:HOH:O	1.71	0.48
3:C:33[A]:MET:CB	24:C:302:DMU:H11	2.44	0.48
3:C:156:ARG:HE	22:C:306:CHD:C24	2.27	0.48
7:G:3:ALA:O	7:G:4:ALA:CB	2.62	0.48
5:R:77:PRO:O	5:R:79:LYS:HD2	2.14	0.48
4:D:6:VAL:N	30:D:303:HOH:O	2.22	0.48
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.96	0.48
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.49	0.47
11:X:7:PRO:HB2	11:X:12:LYS:HZ3	1.79	0.47
3:P:33[A]:MET:HA	24:P:306:DMU:H9	1.95	0.47
1:A:355:GLY:O	14:A:602[B]:HEA:HMB3	2.14	0.47
11:X:7:PRO:HB2	11:X:12:LYS:HZ2	1.80	0.47
19:A:609:PGV:H221	30:M:222:HOH:O	2.14	0.47
22:C:301:CHD:H212	22:C:301:CHD:H12	1.97	0.47
21:L:101:TGL:OA1	21:L:101:TGL:OG3	2.32	0.47
2:O:58:ALA:O	2:O:62:GLU:HG3	2.13	0.47
1:A:417[B]:MET:CE	30:A:836:HOH:O	2.62	0.47
30:Q:322:HOH:O	9:V:42:LYS:HD2	2.14	0.47
12:Y:20:ARG:NH1	21:Y:101:TGL:HC32	2.22	0.47
1:A:243:VAL:CG1	14:A:602[B]:HEA:HMD2	2.45	0.47
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.50	0.47
5:R:72:LYS:HB2	5:R:82:TYR:CD1	2.49	0.47
1:A:359:ALA:CA	14:A:602[B]:HEA:OMA	2.53	0.47
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.64	0.47
12:L:14:SER:N	21:L:101:TGL:HC31	2.24	0.47
1:N:136[B]:LEU:CD2	30:N:882:HOH:O	2.61	0.47
19:A:609:PGV:H231	19:A:609:PGV:H202	1.70	0.47
3:C:3:HIS:HA	30:C:401:HOH:O	2.15	0.47
7:G:8:HIS:HD2	7:G:9:GLY:H	1.62	0.47
1:N:399:LEU:O	1:N:499:PRO:HA	2.15	0.47
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.47
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.46
1:N:136[B]:LEU:CD1	30:N:905:HOH:O	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.15	0.46
3:C:33[B]:MET:HB2	24:C:302:DMU:C25	2.45	0.46
3:C:157:LYS:HZ1	27:C:307:PEK:H051	1.77	0.46
6:F:90:LYS:HD2	30:F:290:HOH:O	2.14	0.46
3:P:33[B]:MET:CE	24:P:306:DMU:H6	2.45	0.46
1:N:501:PRO:HD2	1:N:504:THR:CG2	2.45	0.46
26:N:601:CDL:OA7	26:N:601:CDL:C32	2.51	0.46
13:Z:19:LEU:HD23	19:Z:101:PGV:C31	2.46	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.46
1:N:328:HIS:HB2	2:O:45:MET:SD	2.56	0.46
2:O:22[B]:HIS:CE1	9:V:44:LYS:HZ1	2.32	0.46
12:Y:24[B]:MET:SD	21:Y:101:TGL:CC3	3.04	0.46
3:C:171:VAL:HG22	26:C:305:CDL:H851	1.98	0.46
1:N:243:VAL:HG11	18:N:608[B]:AZI:N2	2.30	0.46
1:N:359:ALA:CA	14:N:603[B]:HEA:OMA	2.58	0.46
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.71	0.46
19:A:609:PGV:H102	4:D:84:ALA:HB2	1.98	0.46
3:C:224:LYS:CD	26:C:305:CDL:HB31	2.46	0.46
12:L:47:LYS:HE2	12:L:47:LYS:OXT	2.16	0.46
8:U:54:GLU:HA	8:U:54:GLU:OE1	2.16	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.46
7:G:12:GLY:N	30:G:202:HOH:O	2.35	0.46
1:N:406:ASN:HD21	19:Z:101:PGV:H21	1.80	0.46
2:O:146:MET:O	2:O:148:MET:HG3	2.16	0.46
26:C:305:CDL:H761	26:C:305:CDL:H791	1.78	0.46
26:N:601:CDL:H161	26:N:601:CDL:OB3	2.15	0.46
30:A:926:HOH:O	21:D:201:TGL:CC3	2.43	0.46
28:E:201:PSC:H232	28:E:201:PSC:O03	2.16	0.46
1:N:513:LEU:O	1:N:514:LYS:CB	2.43	0.46
27:P:307:PEK:C38	26:T:102:CDL:H273	2.46	0.46
6:S:18:ARG:HA	6:S:21[B]:MET:HE3	1.98	0.46
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.51	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.45
5:E:86:ILE:O	5:E:90:ARG:HG2	2.16	0.45
3:C:33[B]:MET:HA	24:C:302:DMU:H11	1.98	0.45
4:D:38:LYS:CD	30:D:415:HOH:O	2.51	0.45
22:G:102:CHD:H12	22:G:102:CHD:H212	1.98	0.45
9:I:57:MET:O	9:I:61:GLU:HG2	2.17	0.45
30:A:703:HOH:O	6:F:96:LEU:HD13	2.15	0.45
2:B:32[A]:PHE:HD1	2:B:32[A]:PHE:HA	1.65	0.45
27:C:307:PEK:C38	26:N:601:CDL:H271	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	2.16	0.45
1:N:236:TRP:HZ3	18:N:608[B]:AZI:N3	2.14	0.45
1:N:311[A]:ILE:HD11	26:N:601:CDL:H212	1.98	0.45
20:N:619:EDO:H12	6:S:70:ILE:HD12	1.99	0.45
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.99	0.45
5:R:6:GLU:HA	5:R:10:GLU:OE1	2.16	0.45
12:Y:14:SER:H	21:Y:101:TGL:HC31	1.81	0.45
1:A:178[B]:GLN:OE1	7:T:10:GLY:N	2.49	0.45
2:B:82:ARG:HD2	2:B:86:MET:HE3	1.98	0.45
3:C:33[B]:MET:CA	24:C:302:DMU:H13	2.47	0.45
28:O:302:PSC:H071	9:V:10:ARG:HH21	1.76	0.45
6:S:42:THR:HB	6:S:43:LYS:HD3	1.99	0.45
1:A:334:TRP:CZ3	21:D:201:TGL:HA52	2.52	0.45
1:A:376:HIS:CE1	1:A:380[B]:VAL:HG11	2.52	0.45
20:A:617:EDO:C1	30:A:708:HOH:O	2.64	0.45
2:O:221:LYS:HD2	2:O:221:LYS:O	2.17	0.45
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.31	0.45
2:B:58:ALA:O	2:B:62:GLU:HG3	2.17	0.45
8:H:7:LYS:HG2	8:U:45:ALA:O	2.16	0.45
1:N:112:LEU:HD23	1:N:112:LEU:C	2.37	0.45
21:Y:101:TGL:HC32	21:Y:101:TGL:HC62	1.55	0.45
1:A:54:TYR:HB2	30:A:768:HOH:O	2.17	0.45
1:N:352:GLY:O	14:N:603[B]:HEA:H121	2.17	0.45
3:P:55:TYR:CE1	26:P:304:CDL:C52	3.00	0.45
4:Q:4:SER:O	4:Q:9:GLU:CB	2.65	0.45
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	2.35	0.45
3:C:157:LYS:HZ2	27:C:307:PEK:C05	2.29	0.45
1:N:112:LEU:HG	30:N:888:HOH:O	2.17	0.45
1:N:358:LEU:C	14:N:603[B]:HEA:CMA	2.85	0.45
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.14	0.45
3:P:158:HIS:HE1	6:S:1:ALA:HA	1.83	0.45
3:P:210:ILE:HD13	19:P:303:PGV:H301	1.97	0.45
3:C:99:TRP:CD1	19:C:308:PGV:H232	2.52	0.44
3:C:157:LYS:HZ2	27:C:307:PEK:H051	1.81	0.44
1:N:21:LEU:HD23	21:Y:101:TGL:H211	1.99	0.44
4:Q:109:HIS:HD2	30:Q:319:HOH:O	1.99	0.44
27:C:309:PEK:H351	7:T:5:LYS:CG	2.47	0.44
4:D:99:GLU:OE2	20:D:202:EDO:C2	2.64	0.44
13:M:42:LYS:HE3	13:M:42:LYS:HA	2.00	0.44
20:N:620:EDO:H11	12:Y:10:ASN:ND2	2.28	0.44
4:Q:7:LYS:HD3	4:Q:7:LYS:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:7:THR:HB	5:R:9:GLU:OE2	2.18	0.44
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.17	0.44
3:C:205:GLY:HA3	27:G:101:PEK:H202	1.98	0.44
19:C:304:PGV:H181	26:C:305:CDL:H652	1.99	0.44
4:D:78:TRP:N	21:D:201:TGL:HB21	2.31	0.44
7:G:59:PRO:HB2	20:G:105:EDO:H22	1.99	0.44
1:N:383[B]:MET:SD	1:N:421:VAL:CG1	3.05	0.44
3:P:41:THR:HA	3:P:44[B]:MET:CE	2.47	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.44
1:N:439:ARG:HD3	2:O:199:ILE:HB	1.98	0.44
3:P:29:SER:HB2	24:P:306:DMU:H21	1.99	0.44
1:A:28:MET:HE1	14:A:601:HEA:C27	2.44	0.44
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.53	0.44
2:B:1:FME:HE3	2:B:133:LEU:HD13	2.00	0.44
2:B:56:MET:HA	28:E:201:PSC:H231	2.00	0.44
2:B:82:ARG:CA	26:T:102:CDL:H322	2.43	0.44
3:C:157:LYS:NZ	27:C:307:PEK:C05	2.80	0.44
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.53	0.44
1:N:35:LEU:HB3	24:Z:102:DMU:H24	2.00	0.44
2:O:56:MET:HG2	28:O:302:PSC:H211	2.00	0.44
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.44
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.99	0.44
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.18	0.44
3:P:33[A]:MET:CB	24:P:306:DMU:H9	2.48	0.44
3:P:158:HIS:HD2	3:P:161[B]:GLN:OE1	2.00	0.44
10:W:33:ARG:HG2	22:W:101:CHD:H151	1.99	0.44
1:A:265:LYS:NZ	20:A:617:EDO:H22	2.33	0.44
21:L:101:TGL:HA92	21:L:101:TGL:H222	1.18	0.44
1:A:42:GLY:HA3	20:D:202:EDO:H21	2.00	0.43
2:B:57:ASP:H	28:E:201:PSC:H221	1.83	0.43
1:N:355:GLY:O	14:N:603[B]:HEA:CHB	2.65	0.43
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.31	0.43
2:B:85:TYR:CE2	26:T:102:CDL:H112	2.53	0.43
4:D:109:HIS:HD2	30:D:357:HOH:O	2.00	0.43
5:E:43:PRO:HB2	5:E:48:ILE:HD11	2.00	0.43
1:N:311[B]:ILE:CD1	26:N:601:CDL:H232	2.48	0.43
2:O:66:THR:HG22	30:O:497:HOH:O	2.18	0.43
24:C:310:DMU:H36	24:C:310:DMU:H34	1.06	0.43
6:F:92:VAL:HG23	6:F:92:VAL:O	2.18	0.43
3:P:55:TYR:CE1	26:P:304:CDL:H521	2.53	0.43
2:B:74:ILE:HG22	2:B:78:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:TRP:CZ3	24:C:310:DMU:H12	2.54	0.43
5:E:5:HIS:N	28:E:201:PSC:H061	2.33	0.43
8:H:37:HIS:HD2	30:H:102:HOH:O	2.01	0.43
8:U:9:LYS:O	8:U:10:ASN:CB	2.59	0.43
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.83	0.43
1:A:113[B]:LEU:CD1	12:L:39:ILE:HD11	2.49	0.43
3:C:99:TRP:NE1	19:C:308:PGV:H232	2.32	0.43
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.18	0.43
1:A:352:GLY:O	14:A:602[B]:HEA:H121	2.18	0.43
3:C:76:GLN:O	3:C:80[A]:ARG:HG3	2.18	0.43
27:G:101:PEK:O04	30:G:201:HOH:O	2.21	0.43
14:N:603[B]:HEA:HMB1	14:N:603[B]:HEA:H11	1.83	0.43
12:Y:24[B]:MET:SD	21:Y:101:TGL:CC2	3.07	0.43
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.53	0.43
19:C:304:PGV:C18	26:C:305:CDL:H652	2.49	0.43
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.48	0.43
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.68	0.43
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	3.06	0.43
21:N:610:TGL:H201	21:N:610:TGL:H231	1.58	0.43
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.54	0.43
1:A:247:ILE:HB	14:A:602[B]:HEA:HBC2	2.01	0.43
19:A:609:PGV:H062	19:A:609:PGV:O14	2.19	0.43
12:L:47:LYS:HA	12:L:47:LYS:CE	2.49	0.43
20:N:620:EDO:H11	12:Y:10:ASN:HB2	2.00	0.43
3:P:259:TRP:CD1	24:P:308:DMU:H30	2.54	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.91	0.43
21:Y:101:TGL:HA51	21:Y:101:TGL:HA22	1.29	0.43
1:A:364:ASP:OD1	14:A:602[B]:HEA:O1A	2.37	0.42
19:A:609:PGV:H32	19:A:609:PGV:H011	2.01	0.42
5:E:6:GLU:HG2	28:E:201:PSC:H072	2.01	0.42
7:G:59:PRO:HD2	20:G:105:EDO:H21	2.00	0.42
21:L:101:TGL:H262	21:L:101:TGL:H231	1.83	0.42
3:C:161[A]:GLN:NE2	27:C:307:PEK:H41	2.27	0.42
10:J:52:TRP:O	10:J:57:HIS:HE1	2.02	0.42
14:N:603[B]:HEA:C22	2:O:34:ILE:HD13	2.49	0.42
26:P:304:CDL:H812	26:P:304:CDL:H842	1.71	0.42
24:P:306:DMU:H11	10:W:49:CYS:HB3	2.00	0.42
21:N:610:TGL:C28	21:N:610:TGL:CB9	2.98	0.42
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.01	0.42
2:B:42:ILE:HG21	21:D:201:TGL:H231	2.00	0.42
2:B:82:ARG:HH11	2:B:86:MET:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144[B]:ILE:HB	3:C:166:THR:HG21	2.02	0.42
4:D:104:TYR:OH	20:D:202:EDO:H21	2.19	0.42
21:D:201:TGL:H342	9:I:16:ARG:HE	1.84	0.42
1:N:113[B]:LEU:HD13	12:Y:39:ILE:HD11	2.01	0.42
2:O:82:ARG:NH1	2:O:86:MET:HE3	2.34	0.42
2:O:82:ARG:HH11	2:O:86:MET:CE	2.32	0.42
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.17	0.42
2:B:60:GLU:H	2:B:60:GLU:CD	2.23	0.42
21:D:201:TGL:H363	9:I:20:HIS:CE1	2.53	0.42
27:G:101:PEK:H101	27:G:101:PEK:H42	2.00	0.42
1:N:321:PHE:CD1	28:O:302:PSC:C33	3.03	0.42
11:K:44:PRO:HA	11:K:47:ARG:HH21	1.85	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.42
24:C:302:DMU:H6	10:J:52:TRP:CE3	2.54	0.42
7:G:6:GLY:H	1:N:278[B]:MET:HE1	1.84	0.42
14:N:603[B]:HEA:OMA	14:N:603[B]:HEA:HHB	2.20	0.42
30:N:801:HOH:O	2:O:53:THR:HG21	2.19	0.42
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.01	0.42
12:L:26:THR:HG23	13:M:25:SER:CB	2.50	0.42
20:N:620:EDO:C1	12:Y:10:ASN:HD22	2.29	0.42
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.42
2:B:198:GLU:HG3	30:B:462:HOH:O	2.17	0.41
26:N:601:CDL:H411	2:O:77:ALA:CB	2.50	0.41
3:P:246:ASP:HB2	30:P:475:HOH:O	2.20	0.41
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.02	0.41
21:Y:101:TGL:OC1	21:Y:101:TGL:CC5	2.68	0.41
13:Z:19:LEU:HD23	19:Z:101:PGV:H302	2.02	0.41
2:B:148:MET:HB3	30:B:541:HOH:O	2.20	0.41
3:C:253:TYR:CE2	26:N:601:CDL:H641	2.54	0.41
30:C:458:HOH:O	10:J:13:GLN:HG2	2.20	0.41
8:H:9:LYS:CG	8:H:10:ASN:N	2.66	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.20	0.41
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.55	0.41
22:P:305:CHD:H183	22:P:305:CHD:H20	1.91	0.41
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.20	0.41
26:T:102:CDL:H792	26:T:102:CDL:H821	1.81	0.41
3:C:144[A]:ILE:CD1	3:C:239:ALA:HA	2.50	0.41
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.36	0.41
7:G:3:ALA:O	7:G:4:ALA:HB2	2.20	0.41
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	2.02	0.41
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:22[B]:HIS:CE1	9:V:44:LYS:HZ2	2.38	0.41
28:O:302:PSC:H012	28:O:302:PSC:O13	2.20	0.41
1:A:358:LEU:C	14:A:602[B]:HEA:CMA	2.89	0.41
1:A:407:ASP:OD2	20:A:618:EDO:H11	2.21	0.41
14:A:602[A]:HEA:HHA	14:A:602[A]:HEA:HAD2	1.84	0.41
3:C:51[A]:MET:CE	19:C:304:PGV:H161	2.50	0.41
24:C:310:DMU:H32	24:C:310:DMU:C57	2.48	0.41
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.02	0.41
2:O:223:SER:O	2:O:226:MET:HB2	2.20	0.41
3:P:44[B]:MET:HB2	3:P:44[B]:MET:HE3	1.96	0.41
3:P:226:HIS:CE1	26:P:304:CDL:HB32	2.55	0.41
4:Q:8:SER:HB3	4:Q:13:LEU:HD11	2.02	0.41
1:A:172:LYS:NZ	1:A:178[A]:GLN:NE2	2.63	0.41
3:C:51[B]:MET:HB3	26:C:305:CDL:H381	2.02	0.41
6:S:92:VAL:O	6:S:92:VAL:HG23	2.21	0.41
1:A:169:ILE:HD11	1:A:189:MET:HE3	2.02	0.41
1:A:417[B]:MET:HE2	30:A:836:HOH:O	2.21	0.41
2:B:41[B]:ILE:N	2:B:41[B]:ILE:HD13	2.33	0.41
26:P:304:CDL:H651	26:P:304:CDL:C22	2.49	0.41
8:U:43:MET:HE3	8:U:49:ASP:N	2.35	0.41
19:A:609:PGV:H241	13:M:12:PRO:HG3	2.02	0.41
7:G:58:LYS:HZ3	20:G:105:EDO:H11	1.83	0.41
1:N:54:TYR:HB2	30:N:804:HOH:O	2.20	0.41
2:O:64:ILE:HG23	2:O:68:LEU:HD13	2.02	0.41
19:U:101:PGV:H242	19:U:101:PGV:H11	2.03	0.41
2:B:148:MET:HE1	30:B:541:HOH:O	2.20	0.41
27:C:309:PEK:H221	30:C:488:HOH:O	2.21	0.41
9:I:73:LYS:O	30:I:102:HOH:O	2.21	0.41
1:N:24:ALA:HA	14:N:602:HEA:H22	2.03	0.41
1:N:25:TRP:CE3	21:Y:101:TGL:HB91	2.56	0.41
1:N:378:HIS:CG	1:N:425:PHE:CE1	3.09	0.41
24:P:308:DMU:H36	24:P:308:DMU:H34	1.41	0.41
1:A:291:HIS:HE1	18:A:607[B]:AZI:N2	2.15	0.41
1:A:459:PHE:HE1	20:D:202:EDO:H11	1.70	0.41
2:B:78:LEU:HD12	26:T:102:CDL:H371	2.02	0.41
3:C:33[A]:MET:CA	24:C:302:DMU:H13	2.51	0.41
3:C:51[B]:MET:HG2	26:C:305:CDL:H601	2.03	0.41
5:E:81:ILE:HD11	9:I:12:LEU:HD11	2.01	0.41
7:G:36:TRP:CE3	7:G:39:SER:HB3	2.55	0.41
7:G:59:PRO:O	20:G:105:EDO:C1	2.57	0.41
1:N:488:THR:HB	1:N:495:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.86	0.41
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:CG2	2.69	0.41
12:Y:24[B]:MET:SD	21:Y:101:TGL:HC31	2.61	0.41
26:P:304:CDL:H471	26:P:304:CDL:H331	2.03	0.41
4:Q:86:MET:CE	11:X:22:ALA:HA	2.51	0.41
14:A:602[B]:HEA:C22	2:B:34:ILE:HD13	2.51	0.40
6:F:43:LYS:HB2	6:F:43:LYS:HE2	1.74	0.40
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.03	0.40
3:P:37:PHE:CB	24:P:306:DMU:H7	2.50	0.40
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.01	0.40
26:C:305:CDL:PA1	26:C:305:CDL:HB22	2.62	0.40
4:D:100[B]:LYS:HE2	30:D:338:HOH:O	2.08	0.40
26:N:601:CDL:H112	26:N:601:CDL:OA5	2.21	0.40
9:V:1:SAC:OAC	9:V:3:ALA:HB3	2.21	0.40
20:A:619:EDO:H22	6:F:32:ASN:HD21	1.86	0.40
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.56	0.40
2:B:148:MET:CB	30:B:541:HOH:O	2.70	0.40
3:C:161[A]:GLN:HE22	27:C:307:PEK:C4	2.27	0.40
4:D:4:SER:OG	30:D:302:HOH:O	2.21	0.40
1:N:240:HIS:O	1:N:241:PRO:C	2.57	0.40
3:P:230:ASN:HB2	30:P:470:HOH:O	2.22	0.40
5:R:46:LYS:HG3	5:R:47:ILE:N	2.36	0.40
7:T:12:GLY:CA	30:T:230:HOH:O	2.70	0.40
1:A:356:ILE:CA	14:A:602[B]:HEA:HMB3	2.49	0.40
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.04	0.40
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.03	0.40
6:S:13:ALA:CB	6:S:21[B]:MET:HE1	2.51	0.40
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.70	0.40
22:J:101:CHD:H193	22:J:101:CHD:H111	1.85	0.40
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	2.62	0.40

All (3) 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:I:126:HOH:O	30:M:211:HOH:O[2_584]	1.94	0.26
30:B:540:HOH:O	30:D:394:HOH:O[2_584]	1.95	0.25
30:B:459:HOH:O	30:D:385:HOH:O[2_584]	2.07	0.13

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/514 (104%)	520 (97%)	14 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	234/227 (103%)	223 (95%)	11 (5%)	0	100	100
2	O	230/227 (101%)	222 (96%)	8 (4%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	142 (97%)	4 (3%)	0	100	100
4	Q	145/147 (99%)	137 (94%)	6 (4%)	2 (1%)	11	3
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	104/109 (95%)	103 (99%)	0	1 (1%)	15	6
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1
6	S	98/98 (100%)	91 (93%)	3 (3%)	4 (4%)	3	0
7	G	82/85 (96%)	69 (84%)	6 (7%)	7 (8%)	1	0
7	T	82/85 (96%)	73 (89%)	5 (6%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	1 (1%)	6 (8%)	1	0
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	5	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	55 (96%)	2 (4%)	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%)	41 (93%)	2 (4%)	1 (2%)	6	1
12	Y	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
All	All	3597/3614 (100%)	3456 (96%)	111 (3%)	30 (1%)	17 9

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	2	SER
7	G	4	ALA
8	H	44	THR
4	Q	7	LYS
6	S	94	HIS
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
8	U	10	ASN
7	G	3	ALA
7	G	5	LYS
7	G	6	GLY
7	G	37	LEU
8	H	43	MET
8	H	45	ALA
13	M	42	LYS
6	S	95	GLN
6	S	96	LEU
7	T	4	ALA
6	F	95	GLN
7	G	8	HIS
12	L	46	LYS
5	R	6	GLU
8	H	46	LYS
8	H	48	GLY
4	Q	8	SER
8	H	8	ILE
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	447/426 (105%)	442 (99%)	5 (1%)	73 73
1	N	445/426 (104%)	439 (99%)	6 (1%)	69 68
2	B	219/210 (104%)	210 (96%)	9 (4%)	30 21
2	O	215/210 (102%)	207 (96%)	8 (4%)	34 25
3	C	233/226 (103%)	227 (97%)	6 (3%)	46 39
3	P	233/226 (103%)	229 (98%)	4 (2%)	60 57
4	D	132/129 (102%)	129 (98%)	3 (2%)	50 45
4	Q	131/129 (102%)	123 (94%)	8 (6%)	18 9
5	E	92/95 (97%)	90 (98%)	2 (2%)	52 47
5	R	93/95 (98%)	89 (96%)	4 (4%)	29 19
6	F	85/81 (105%)	83 (98%)	2 (2%)	49 43
6	S	83/81 (102%)	73 (88%)	10 (12%)	5 1
7	G	68/68 (100%)	61 (90%)	7 (10%)	7 2
7	T	68/68 (100%)	62 (91%)	6 (9%)	10 4
8	H	71/75 (95%)	66 (93%)	5 (7%)	15 7
8	U	71/75 (95%)	65 (92%)	6 (8%)	10 4
9	I	57/57 (100%)	55 (96%)	2 (4%)	36 27
9	V	57/57 (100%)	53 (93%)	4 (7%)	15 7
10	J	49/50 (98%)	48 (98%)	1 (2%)	55 51
10	W	50/50 (100%)	48 (96%)	2 (4%)	31 22
11	K	39/46 (85%)	38 (97%)	1 (3%)	46 39
11	X	40/46 (87%)	39 (98%)	1 (2%)	47 41
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 39
12	Y	40/40 (100%)	38 (95%)	2 (5%)	24 15
13	M	37/38 (97%)	36 (97%)	1 (3%)	44 38
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11 4
All	All	3131/3082 (102%)	3022 (96%)	109 (4%)	36 27

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	189	MET
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	17	PRO
3	C	33[A]	MET
3	C	33[B]	MET
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	31	LYS
4	D	142	LYS
4	D	147	LYS
5	E	70	VAL
5	E	90	ARG
6	F	37	LYS
6	F	43	LYS
7	G	2	SER
7	G	7	ASP
7	G	18	PHE
7	G	33	LEU
7	G	42	ARG
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	44	THR
8	H	60	TYR
9	I	2	THR
9	I	37	PHE
10	J	58	LYS
11	K	54	ARG

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Mol	Chain	Res	Type
12	L	47	LYS
13	M	42	LYS
1	N	109	PHE
1	N	180	GLN
1	N	189	MET
1	N	241	PRO
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	171	LYS
2	O	221	LYS
3	P	17	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	7	LYS
4	Q	9	GLU
4	Q	19[A]	ARG
4	Q	19[B]	ARG
4	Q	51	LEU
4	Q	58	GLU
4	Q	142	LYS
4	Q	143	ASN
5	R	6	GLU
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
6	S	37	LYS
6	S	43	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	94	HIS
6	S	95	GLN
6	S	96	LEU

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Mol	Chain	Res	Type
7	T	18	PHE
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	7	LYS
8	U	29	CYS
8	U	40	GLU
8	U	44	THR
8	U	60	TYR
8	U	84	LYS
9	V	2	THR
9	V	8	GLN
9	V	29	LEU
9	V	42	LYS
10	W	27	THR
10	W	50	LEU
11	X	52	GLU
12	Y	2	HIS
12	Y	47	LYS
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN

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Mol	Chain	Res	Type
6	F	80	GLN
6	F	95	GLN
7	G	8	HIS
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
9	I	20	HIS
10	J	29	ASN
10	J	57	HIS
1	N	180	GLN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	8	HIS
7	T	76	ASN
8	U	37	HIS
9	V	8	GLN
10	W	29	ASN
11	X	35	GLN
13	Z	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	1.59	1 (14%)	8,9,11	1.58	2 (25%)
2	FME	O	1	2	8,9,10	1.12	0	7,9,11	1.95	3 (42%)
7	TPO	G	11	7	8,10,11	2.13	2 (25%)	10,14,16	1.22	1 (10%)
9	SAC	I	1	9	7,8,9	1.26	1 (14%)	8,9,11	2.07	2 (25%)
1	FME	N	1	1	8,9,10	1.42	1 (12%)	7,9,11	1.63	2 (28%)
1	FME	A	1	1	8,9,10	0.96	0	7,9,11	2.29	4 (57%)
2	FME	B	1	2	8,9,10	1.67	2 (25%)	7,9,11	2.32	3 (42%)
7	TPO	T	11	7	8,10,11	1.69	1 (12%)	10,14,16	1.49	2 (20%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.05	1.52	1.46
7	G	11	TPO	P-O1P	3.54	1.62	1.50
1	N	1	FME	CA-N	3.45	1.51	1.46
7	T	11	TPO	P-O1P	3.21	1.60	1.50
9	I	1	SAC	CA-N	3.03	1.50	1.46
7	G	11	TPO	P-OG1	2.97	1.64	1.59
2	B	1	FME	CA-N	2.70	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CB-CA	2.32	1.57	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-4.55	100.30	112.95
9	I	1	SAC	OG-CB-CA	-4.39	99.77	110.97
1	A	1	FME	CE-SD-CG	3.96	114.02	100.40
2	O	1	FME	CG-CB-CA	-3.05	104.47	112.95
2	B	1	FME	C-CA-N	-2.99	104.34	109.73
9	I	1	SAC	C-CA-N	2.97	115.09	109.73
7	T	11	TPO	CG2-CB-CA	2.88	118.84	113.16
1	A	1	FME	CA-N-CN	2.66	126.91	122.82
9	V	1	SAC	CA-N-C1A	2.52	127.80	123.15
1	N	1	FME	C-CA-N	2.39	114.04	109.73
7	T	11	TPO	O3P-P-O2P	2.38	116.73	107.64
1	A	1	FME	O-C-CA	-2.37	118.57	124.78
2	B	1	FME	CE-SD-CG	2.34	108.44	100.40
1	A	1	FME	C-CA-N	2.33	113.94	109.73
7	G	11	TPO	O2P-P-OG1	2.29	116.26	105.99
2	O	1	FME	CA-N-CN	2.27	126.31	122.82
9	V	1	SAC	O-C-CA	-2.24	118.92	124.78
2	O	1	FME	CE-SD-CG	2.16	107.82	100.40
1	N	1	FME	O1-CN-N	-2.03	119.93	125.27

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0
7	G	11	TPO	2	0
2	B	1	FME	5	0
7	T	11	TPO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 111 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	EDO	A	611	-	3,3,3	0.61	0	2,2,2	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	AZI	N	608[B]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	E	203	-	3,3,3	0.70	0	2,2,2	0.11	0
20	EDO	L	102	-	3,3,3	0.70	0	2,2,2	0.77	0
18	AZI	A	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
23	CUA	O	301	2	0,1,1	-	-	-		
27	PEK	T	101	-	52,52,52	1.37	7 (13%)	55,57,57	2.19	9 (16%)
20	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.70	0
24	DMU	P	309	-	34,34,34	1.09	2 (5%)	45,45,45	1.89	11 (24%)
26	CDL	T	102	-	99,99,99	1.43	13 (13%)	105,111,111	1.41	14 (13%)
24	DMU	P	306	-	34,34,34	1.12	1 (2%)	45,45,45	1.67	8 (17%)
20	EDO	N	611	-	3,3,3	1.56	1 (33%)	2,2,2	1.01	0
22	CHD	P	305	-	32,32,32	1.22	4 (12%)	51,51,51	3.48	22 (43%)
14	HEA	A	602[A]	18,1	57,67,67	1.61	12 (21%)	61,103,103	2.19	21 (34%)
20	EDO	M	102	-	3,3,3	0.33	0	2,2,2	0.78	0
22	CHD	B	302	-	32,32,32	2.07	14 (43%)	51,51,51	2.11	20 (39%)
20	EDO	B	304	-	3,3,3	0.54	0	2,2,2	1.05	0
20	EDO	O	303	-	3,3,3	0.82	0	2,2,2	1.03	0
20	EDO	F	104	-	3,3,3	0.67	0	2,2,2	0.59	0
20	EDO	G	105	-	3,3,3	0.52	0	2,2,2	0.53	0
20	EDO	D	203	-	3,3,3	0.71	0	2,2,2	0.39	0
24	DMU	C	302	-	34,34,34	0.72	0	45,45,45	1.42	7 (15%)
19	PGV	P	303	-	50,50,50	0.90	2 (4%)	53,56,56	1.26	5 (9%)
19	PGV	Z	101	-	50,50,50	1.14	2 (4%)	53,56,56	1.33	7 (13%)
20	EDO	N	619	-	3,3,3	0.37	0	2,2,2	0.52	0
18	AZI	N	608[A]	15,14	0,2,2	-	-	0,1,1	-	-
14	HEA	N	603[A]	18,1	57,67,67	1.66	14 (24%)	61,103,103	2.47	28 (45%)
18	AZI	N	607[B]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	620	-	3,3,3	0.87	0	2,2,2	1.25	0
20	EDO	A	618	-	3,3,3	0.29	0	2,2,2	1.56	0
21	TGL	D	201	-	62,62,62	1.77	4 (6%)	65,65,65	2.27	10 (15%)
24	DMU	Z	102	-	34,34,34	0.70	1 (2%)	45,45,45	1.28	6 (13%)
27	PEK	G	103	-	52,52,52	1.14	2 (3%)	55,57,57	1.26	3 (5%)
24	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.21	14 (31%)
28	PSC	O	302	-	51,51,51	1.27	3 (5%)	57,59,59	1.26	4 (7%)
20	EDO	P	312	-	3,3,3	0.44	0	2,2,2	0.66	0
20	EDO	N	613	-	3,3,3	0.64	0	2,2,2	0.83	0
20	EDO	Y	102	-	3,3,3	0.50	0	2,2,2	0.67	0
26	CDL	C	305	-	99,99,99	1.50	16 (16%)	105,111,111	1.44	17 (16%)
20	EDO	A	616	-	3,3,3	1.13	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PSC	E	201	-	51,51,51	1.38	4 (7%)	57,59,59	1.47	6 (10%)
19	PGV	A	609	-	50,50,50	1.22	4 (8%)	53,56,56	1.46	8 (15%)
22	CHD	W	101	-	32,32,32	1.34	5 (15%)	51,51,51	2.84	24 (47%)
26	CDL	N	601	-	99,99,99	1.49	13 (13%)	105,111,111	1.50	15 (14%)
24	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.36	13 (28%)
20	EDO	A	613	-	3,3,3	1.59	1 (33%)	2,2,2	1.17	0
20	EDO	A	617	-	3,3,3	0.34	0	2,2,2	1.30	0
22	CHD	C	306	-	32,32,32	1.19	3 (9%)	51,51,51	3.23	19 (37%)
20	EDO	N	616	-	3,3,3	0.61	0	2,2,2	0.56	0
20	EDO	S	103	-	3,3,3	0.64	0	2,2,2	1.67	1 (50%)
19	PGV	A	608	-	50,50,50	1.13	4 (8%)	53,56,56	1.42	8 (15%)
24	DMU	M	101	-	34,34,34	0.82	1 (2%)	45,45,45	1.43	8 (17%)
22	CHD	G	102	-	32,32,32	1.72	8 (25%)	51,51,51	1.98	18 (35%)
20	EDO	A	610	-	3,3,3	0.38	0	2,2,2	1.09	0
22	CHD	J	101	-	32,32,32	0.89	0	51,51,51	2.84	22 (43%)
20	EDO	N	618	-	3,3,3	1.19	0	2,2,2	0.25	0
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
14	HEA	N	602	1	57,67,67	1.77	15 (26%)	61,103,103	2.41	28 (45%)
20	EDO	T	103	-	3,3,3	1.05	0	2,2,2	0.70	0
20	EDO	A	615	-	3,3,3	2.46	1 (33%)	2,2,2	4.78	1 (50%)
22	CHD	P	301	-	32,32,32	1.47	6 (18%)	51,51,51	2.33	14 (27%)
19	PGV	N	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.45	7 (13%)
20	EDO	E	204	-	3,3,3	0.77	0	2,2,2	0.42	0
21	TGL	B	301	-	62,62,62	1.23	4 (6%)	65,65,65	1.81	10 (15%)
26	CDL	P	304	-	99,99,99	1.56	17 (17%)	105,111,111	1.56	20 (19%)
23	CUA	B	303	2	0,1,1	-	-	-		
21	TGL	Y	101	-	62,62,62	1.44	5 (8%)	65,65,65	1.60	13 (20%)
20	EDO	B	305	-	3,3,3	0.43	0	2,2,2	0.52	0
21	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.39	6 (9%)
20	EDO	F	103	-	3,3,3	1.21	0	2,2,2	0.35	0
27	PEK	C	307	-	52,52,52	1.55	6 (11%)	55,57,57	1.59	9 (16%)
24	DMU	C	311	-	34,34,34	1.04	1 (2%)	45,45,45	2.42	11 (24%)
21	TGL	L	101	-	62,62,62	1.32	3 (4%)	65,65,65	1.91	17 (26%)
20	EDO	A	612	-	3,3,3	0.57	0	2,2,2	0.40	0
27	PEK	G	101	-	52,52,52	0.96	5 (9%)	55,57,57	1.17	4 (7%)
14	HEA	N	603[B]	18,1	57,67,67	1.60	10 (17%)	61,103,103	2.15	19 (31%)
19	PGV	C	308	-	50,50,50	1.40	2 (4%)	53,56,56	1.68	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	EDO	A	614	-	3,3,3	0.58	0	2,2,2	1.92	1 (50%)
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	615	-	3,3,3	0.91	0	2,2,2	0.14	0
20	EDO	G	104	-	3,3,3	0.88	0	2,2,2	0.63	0
20	EDO	N	617	-	3,3,3	0.80	0	2,2,2	0.53	0
20	EDO	F	102	-	3,3,3	1.11	0	2,2,2	0.60	0
22	CHD	C	301	-	32,32,32	1.96	13 (40%)	51,51,51	2.10	16 (31%)
20	EDO	B	306	-	3,3,3	1.79	1 (33%)	2,2,2	0.35	0
20	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.92	0
14	HEA	A	601	1	57,67,67	1.70	14 (24%)	61,103,103	2.26	21 (34%)
19	PGV	C	304	-	50,50,50	0.93	2 (4%)	53,56,56	1.13	5 (9%)
21	TGL	N	610	-	62,62,62	1.16	3 (4%)	65,65,65	1.68	9 (13%)
27	PEK	P	307	-	52,52,52	1.26	2 (3%)	55,57,57	1.37	7 (12%)
20	EDO	N	614	-	3,3,3	1.29	0	2,2,2	0.28	0
19	PGV	U	101	-	50,50,50	1.19	2 (4%)	53,56,56	1.53	8 (15%)
20	EDO	D	202	-	3,3,3	0.66	0	2,2,2	0.77	0
27	PEK	C	309	-	52,52,52	1.26	2 (3%)	55,57,57	1.40	6 (10%)
14	HEA	A	602[B]	18,1	57,67,67	1.64	12 (21%)	61,103,103	2.00	15 (24%)
20	EDO	R	201	-	3,3,3	0.82	0	2,2,2	0.35	0
20	EDO	P	310	-	3,3,3	1.03	0	2,2,2	0.32	0
20	EDO	B	307	-	3,3,3	0.80	0	2,2,2	0.71	0
20	EDO	S	102	-	3,3,3	1.27	0	2,2,2	0.76	0
20	EDO	P	311	-	3,3,3	0.70	0	2,2,2	1.87	1 (50%)
20	EDO	N	612	-	3,3,3	0.56	0	2,2,2	1.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	E	203	-	-	1/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
27	PEK	T	101	-	-	25/56/56/56	-
20	EDO	A	619	-	-	0/1/1/1	-
24	DMU	P	309	-	-	12/19/59/59	0/2/2/2
26	CDL	T	102	-	-	59/110/110/110	-
24	DMU	P	306	-	-	3/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	611	-	-	0/1/1/1	-
22	CHD	P	305	-	-	5/9/74/74	0/4/4/4
14	HEA	A	602[A]	18,1	-	5/32/76/76	-
20	EDO	M	102	-	-	0/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	B	304	-	-	0/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
24	DMU	C	302	-	-	9/19/59/59	0/2/2/2
19	PGV	P	303	-	-	14/55/55/55	-
19	PGV	Z	101	-	-	29/55/55/55	-
20	EDO	N	619	-	-	0/1/1/1	-
14	HEA	N	603[A]	18,1	-	4/32/76/76	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	A	618	-	-	1/1/1/1	-
21	TGL	D	201	-	-	41/65/65/65	-
24	DMU	Z	102	-	-	4/19/59/59	0/2/2/2
27	PEK	G	103	-	-	31/56/56/56	-
24	DMU	P	308	-	-	6/19/59/59	0/2/2/2
28	PSC	O	302	-	-	24/55/55/55	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
26	CDL	C	305	-	-	62/110/110/110	-
20	EDO	A	616	-	-	0/1/1/1	-
28	PSC	E	201	-	-	38/55/55/55	-
19	PGV	A	609	-	-	22/55/55/55	-
22	CHD	W	101	-	-	6/9/74/74	0/4/4/4
26	CDL	N	601	-	-	57/110/110/110	-
24	DMU	C	310	-	-	6/19/59/59	0/2/2/2
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
22	CHD	C	306	-	-	7/9/74/74	0/4/4/4
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	S	103	-	-	1/1/1/1	-
19	PGV	A	608	-	-	8/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	M	101	-	-	5/19/59/59	0/2/2/2
22	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	A	610	-	-	1/1/1/1	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
20	EDO	N	618	-	-	0/1/1/1	-
14	HEA	N	602	1	-	6/32/76/76	-
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
19	PGV	N	609	-	-	6/55/55/55	-
20	EDO	E	204	-	-	0/1/1/1	-
21	TGL	B	301	-	-	33/65/65/65	-
26	CDL	P	304	-	-	57/110/110/110	-
21	TGL	Y	101	-	-	41/65/65/65	-
20	EDO	B	305	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	29/65/65/65	-
20	EDO	F	103	-	-	0/1/1/1	-
27	PEK	C	307	-	-	32/56/56/56	-
24	DMU	C	311	-	-	9/19/59/59	0/2/2/2
21	TGL	L	101	-	-	41/65/65/65	-
20	EDO	A	612	-	-	0/1/1/1	-
27	PEK	G	101	-	-	17/56/56/56	-
14	HEA	N	603[B]	18,1	-	5/32/76/76	-
19	PGV	C	308	-	-	27/55/55/55	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
14	HEA	A	601	1	-	7/32/76/76	-
19	PGV	C	304	-	-	17/55/55/55	-
21	TGL	N	610	-	-	35/65/65/65	-
27	PEK	P	307	-	-	24/56/56/56	-
20	EDO	N	614	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	U	101	-	-	25/55/55/55	-
20	EDO	D	202	-	-	1/1/1/1	-
27	PEK	C	309	-	-	25/56/56/56	-
14	HEA	A	602[B]	18,1	-	4/32/76/76	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OB1-CB1	8.22	1.46	1.22
21	Y	101	TGL	OG2-CB1	6.50	1.52	1.34
19	C	308	PGV	O01-C1	6.36	1.52	1.34
27	C	307	PEK	O01-C1	6.35	1.52	1.34
21	L	101	TGL	OG2-CB1	6.30	1.52	1.34
21	D	201	TGL	OG1-CA1	6.20	1.51	1.33
27	C	307	PEK	O03-C21	6.13	1.51	1.33
21	Q	201	TGL	OG2-CB1	6.08	1.51	1.34
27	T	101	PEK	C2-C1	6.05	1.68	1.50
21	D	201	TGL	OG2-CB1	5.98	1.51	1.34
21	Y	101	TGL	OG3-CC1	5.98	1.50	1.33
19	Z	101	PGV	O03-C19	5.78	1.50	1.33
27	P	307	PEK	O01-C1	5.75	1.50	1.34
26	N	601	CDL	OB6-CB5	5.72	1.50	1.34
26	T	102	CDL	OB8-CB7	5.55	1.49	1.33
26	P	304	CDL	OA8-CA7	5.55	1.49	1.33
28	O	302	PSC	O01-C1	5.54	1.49	1.34
26	N	601	CDL	OB8-CB7	5.52	1.49	1.33
21	Q	201	TGL	OB1-CB1	5.50	1.38	1.22
26	P	304	CDL	OB8-CB7	5.41	1.49	1.33
21	B	301	TGL	OG1-CA1	5.33	1.48	1.33
26	C	305	CDL	OA8-CA7	5.31	1.48	1.33
27	C	309	PEK	O03-C21	5.28	1.48	1.33
19	C	308	PGV	O03-C19	5.24	1.48	1.33
26	T	102	CDL	OB6-CB5	5.20	1.49	1.34
27	G	103	PEK	O01-C1	5.18	1.48	1.34
27	C	309	PEK	O01-C1	5.12	1.48	1.34
21	L	101	TGL	OG3-CC1	5.11	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	610	TGL	OG1-CA1	5.01	1.48	1.33
28	E	201	PSC	O01-C1	5.00	1.48	1.34
24	P	306	DMU	O16-C6	4.99	1.48	1.40
14	N	603[A]	HEA	O11-C11	4.95	1.53	1.42
26	T	102	CDL	OA6-CA5	4.89	1.48	1.34
21	Q	201	TGL	OG1-CA1	4.87	1.47	1.33
19	U	101	PGV	O01-C1	4.86	1.48	1.34
26	N	601	CDL	OA8-CA7	4.82	1.47	1.33
19	A	609	PGV	O03-C19	4.79	1.47	1.33
26	C	305	CDL	OA6-CA5	4.76	1.47	1.34
27	P	307	PEK	O03-C21	4.74	1.47	1.33
27	G	103	PEK	O03-C21	4.73	1.47	1.33
26	N	601	CDL	OA6-CA5	4.73	1.47	1.34
26	P	304	CDL	OA6-CA5	4.69	1.47	1.34
26	T	102	CDL	OA8-CA7	4.69	1.47	1.33
28	E	201	PSC	O03-C19	4.67	1.47	1.33
21	L	101	TGL	OG1-CA1	4.61	1.46	1.33
26	C	305	CDL	OB8-CB7	4.60	1.46	1.33
21	Y	101	TGL	OG1-CA1	4.53	1.46	1.33
19	U	101	PGV	O03-C19	4.51	1.46	1.33
28	O	302	PSC	O03-C19	4.50	1.46	1.33
22	B	302	CHD	C8-C7	4.45	1.61	1.53
14	N	602	HEA	CMD-C2D	4.45	1.60	1.50
21	Q	201	TGL	OG3-CC1	4.43	1.46	1.33
21	N	610	TGL	OG2-CB1	4.39	1.46	1.34
19	A	609	PGV	O01-C1	4.39	1.46	1.34
26	C	305	CDL	PB2-OB3	4.37	1.66	1.50
14	A	602[B]	HEA	C4B-C3B	-4.31	1.37	1.44
21	B	301	TGL	OG2-CB1	4.30	1.46	1.34
21	N	610	TGL	OG3-CC1	4.13	1.45	1.33
14	A	601	HEA	CHD-C1D	4.06	1.45	1.35
28	E	201	PSC	C13-C12	4.06	1.55	1.31
26	C	305	CDL	OB6-CB5	4.04	1.45	1.34
22	C	301	CHD	C8-C7	4.03	1.60	1.53
20	A	615	EDO	C2-C1	4.02	1.76	1.48
14	A	602[B]	HEA	CHD-C1D	3.96	1.45	1.35
14	A	602[B]	HEA	CHC-C4B	3.95	1.45	1.35
22	G	102	CHD	C8-C7	3.94	1.60	1.53
28	O	302	PSC	C13-C12	3.93	1.54	1.31
19	Z	101	PGV	O01-C1	3.91	1.45	1.34
24	C	311	DMU	O16-C6	3.89	1.46	1.40
14	N	603[B]	HEA	FE-NB	3.85	2.15	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	609	PGV	O03-C19	3.79	1.44	1.33
14	A	601	HEA	C12-C13	3.76	1.65	1.53
26	P	304	CDL	PB2-OB3	3.72	1.64	1.50
22	B	302	CHD	C11-C9	3.71	1.59	1.53
22	C	301	CHD	C2-C3	3.70	1.60	1.51
27	T	101	PEK	C3-C2	3.62	1.65	1.52
26	P	304	CDL	OB6-CB5	3.61	1.44	1.34
21	D	201	TGL	OG3-CC1	3.59	1.43	1.33
22	P	301	CHD	C11-C9	3.54	1.59	1.53
24	P	309	DMU	O16-C6	3.49	1.46	1.40
22	C	301	CHD	C11-C9	3.48	1.59	1.53
26	C	305	CDL	C79-C78	-3.47	1.32	1.51
14	N	603[B]	HEA	FE-ND	3.47	2.14	1.96
14	N	603[B]	HEA	CHD-C1D	3.47	1.43	1.35
14	A	602[A]	HEA	C1D-C2D	-3.46	1.37	1.44
21	B	301	TGL	OG3-CC1	3.46	1.43	1.33
19	A	608	PGV	O03-C19	3.43	1.43	1.33
14	N	603[B]	HEA	C4B-C3B	-3.41	1.38	1.44
14	A	602[A]	HEA	CHD-C1D	3.39	1.43	1.35
14	N	603[B]	HEA	C1D-ND	-3.38	1.34	1.40
22	P	301	CHD	C8-C7	3.38	1.59	1.53
14	A	602[A]	HEA	CHC-C4B	3.36	1.43	1.35
26	N	601	CDL	C59-C58	-3.34	1.32	1.51
14	A	601	HEA	C1B-NB	-3.34	1.31	1.38
14	N	603[B]	HEA	CHC-C4B	3.33	1.43	1.35
14	N	602	HEA	CHC-C4B	3.31	1.43	1.35
14	A	601	HEA	C1D-ND	-3.26	1.34	1.40
14	N	602	HEA	C4B-NB	-3.21	1.34	1.40
22	C	306	CHD	C16-C17	3.18	1.61	1.54
14	A	602[B]	HEA	C1B-NB	-3.17	1.32	1.38
22	B	302	CHD	C4-C3	3.14	1.57	1.51
14	N	602	HEA	CMB-C2B	3.14	1.57	1.50
22	C	301	CHD	C13-C12	-3.14	1.49	1.54
22	C	301	CHD	C11-C12	3.13	1.58	1.53
14	N	602	HEA	O11-C11	3.11	1.49	1.42
14	N	603[A]	HEA	C12-C11	3.11	1.58	1.52
22	W	101	CHD	C20-C17	3.10	1.59	1.54
14	N	602	HEA	C1D-ND	-3.09	1.35	1.40
14	A	602[B]	HEA	C4D-ND	-3.08	1.32	1.38
22	G	102	CHD	C4-C5	3.07	1.58	1.53
14	A	602[A]	HEA	O11-C11	3.07	1.49	1.42
26	P	304	CDL	C79-C78	-3.04	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	601	CDL	C22-C21	-3.04	1.34	1.51
26	P	304	CDL	C82-C81	-3.04	1.34	1.51
14	N	602	HEA	C4D-ND	-3.03	1.32	1.38
27	G	101	PEK	O01-C1	3.02	1.42	1.34
26	C	305	CDL	C59-C58	-3.01	1.34	1.51
14	N	603[A]	HEA	CHC-C4B	3.01	1.42	1.35
26	T	102	CDL	C59-C58	-3.00	1.34	1.51
14	N	603[B]	HEA	C4B-NB	-2.99	1.35	1.40
22	G	102	CHD	C11-C9	2.99	1.58	1.53
26	N	601	CDL	C19-C18	-2.98	1.34	1.51
19	N	609	PGV	O03-C01	2.94	1.51	1.45
22	B	302	CHD	C19-C10	2.93	1.59	1.54
26	C	305	CDL	C19-C18	-2.93	1.35	1.51
14	A	602[A]	HEA	C20-C19	2.92	1.57	1.51
26	C	305	CDL	O1-C1	2.92	1.52	1.43
22	G	102	CHD	C2-C3	2.91	1.58	1.51
26	P	304	CDL	C62-C61	-2.90	1.35	1.51
26	P	304	CDL	C19-C18	-2.90	1.35	1.51
14	A	602[A]	HEA	CMB-C2B	2.90	1.56	1.50
26	C	305	CDL	C82-C81	-2.90	1.35	1.51
22	C	301	CHD	C23-C24	2.89	1.57	1.50
14	N	602	HEA	CBA-CGA	2.88	1.57	1.50
24	C	310	DMU	O16-C6	2.88	1.45	1.40
27	T	101	PEK	O02-C1	2.87	1.31	1.22
26	N	601	CDL	C42-C41	-2.87	1.35	1.51
26	N	601	CDL	C79-C78	-2.86	1.35	1.51
26	C	305	CDL	C22-C21	-2.85	1.35	1.51
22	P	301	CHD	C23-C24	2.85	1.57	1.50
26	P	304	CDL	C59-C58	-2.85	1.35	1.51
14	A	602[B]	HEA	C4D-C3D	-2.85	1.40	1.45
14	N	603[A]	HEA	CHD-C1D	2.85	1.42	1.35
22	G	102	CHD	C20-C17	2.85	1.59	1.54
26	C	305	CDL	C62-C61	-2.84	1.35	1.51
26	P	304	CDL	C42-C41	-2.84	1.35	1.51
14	A	602[A]	HEA	C4D-C3D	-2.82	1.40	1.45
26	T	102	CDL	C79-C78	-2.81	1.35	1.51
14	A	601	HEA	CMB-C2B	2.81	1.56	1.50
26	N	601	CDL	C82-C81	-2.80	1.35	1.51
14	A	601	HEA	CHC-C4B	2.80	1.42	1.35
26	N	601	CDL	C62-C61	-2.79	1.35	1.51
22	B	302	CHD	C10-C5	2.78	1.59	1.55
26	T	102	CDL	C22-C21	-2.77	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	101	PEK	O01-C1	2.77	1.42	1.34
14	N	603[A]	HEA	C1B-NB	-2.76	1.33	1.38
14	N	603[B]	HEA	C3A-C2A	-2.75	1.36	1.40
26	N	601	CDL	C39-C38	-2.75	1.36	1.51
14	N	603[A]	HEA	C1C-CHC	2.75	1.48	1.41
27	G	101	PEK	O03-C21	2.74	1.41	1.33
24	P	309	DMU	C10-C5	2.73	1.60	1.52
28	E	201	PSC	C3-C2	2.73	1.62	1.52
26	P	304	CDL	CB2-C1	2.73	1.60	1.51
22	B	302	CHD	C1-C2	2.72	1.59	1.53
27	C	307	PEK	O02-C1	2.72	1.30	1.22
26	P	304	CDL	C22-C21	-2.71	1.36	1.51
26	T	102	CDL	C39-C38	-2.69	1.36	1.51
22	C	306	CHD	O26-C24	-2.69	1.21	1.30
26	T	102	CDL	C42-C41	-2.68	1.36	1.51
22	P	305	CHD	C16-C17	2.68	1.59	1.54
14	N	602	HEA	C1B-NB	-2.67	1.33	1.38
22	B	302	CHD	C20-C17	2.67	1.59	1.54
14	N	603[B]	HEA	C4D-C3D	-2.66	1.40	1.45
26	T	102	CDL	C62-C61	-2.64	1.36	1.51
14	A	602[B]	HEA	C1D-ND	-2.64	1.35	1.40
26	P	304	CDL	C39-C38	-2.63	1.36	1.51
26	T	102	CDL	C82-C81	-2.63	1.36	1.51
26	C	305	CDL	C42-C41	-2.62	1.36	1.51
22	W	101	CHD	C13-C17	2.62	1.60	1.55
14	A	601	HEA	C18-C19	-2.62	1.26	1.33
14	A	601	HEA	CBD-CAD	2.62	1.60	1.52
14	N	603[A]	HEA	C20-C19	2.62	1.56	1.51
14	N	602	HEA	C1C-CHC	2.61	1.48	1.41
14	N	602	HEA	CBD-CAD	2.61	1.60	1.52
27	T	101	PEK	O03-C21	2.59	1.40	1.33
26	C	305	CDL	C39-C38	-2.59	1.37	1.51
22	P	305	CHD	C11-C9	2.59	1.58	1.53
14	N	602	HEA	CHD-C1D	2.59	1.41	1.35
22	P	301	CHD	C21-C20	2.58	1.59	1.53
14	A	602[A]	HEA	C18-C19	2.58	1.39	1.33
21	B	301	TGL	OC1-CC1	-2.57	1.14	1.22
14	N	603[B]	HEA	C1B-C2B	-2.55	1.39	1.44
14	N	603[A]	HEA	C4D-C3D	-2.54	1.40	1.45
22	C	301	CHD	C22-C20	2.53	1.60	1.54
22	C	301	CHD	C13-C14	2.52	1.59	1.55
26	T	102	CDL	C19-C18	-2.52	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	301	CHD	C16-C17	2.51	1.59	1.54
22	G	102	CHD	C21-C20	2.49	1.59	1.53
26	P	304	CDL	O1-C1	2.49	1.50	1.43
26	C	305	CDL	CB2-C1	2.49	1.60	1.51
22	B	302	CHD	C21-C20	2.48	1.59	1.53
14	N	603[A]	HEA	C4B-C3B	-2.48	1.40	1.44
14	A	602[B]	HEA	C1D-C2D	-2.47	1.39	1.44
22	W	101	CHD	C21-C20	2.47	1.59	1.53
22	C	301	CHD	C4-C3	2.46	1.56	1.51
22	B	302	CHD	C13-C17	-2.45	1.51	1.55
26	P	304	CDL	PB2-OB2	2.45	1.69	1.59
22	W	101	CHD	C8-C7	2.45	1.57	1.53
14	A	601	HEA	O11-C11	2.43	1.48	1.42
19	A	608	PGV	O01-C1	2.40	1.41	1.34
22	B	302	CHD	O25-C24	2.39	1.30	1.22
14	A	602[B]	HEA	C1B-C2B	-2.38	1.40	1.44
22	B	302	CHD	C18-C13	2.37	1.58	1.54
20	N	611	EDO	O2-C2	2.36	1.54	1.42
19	P	303	PGV	O03-C19	2.36	1.40	1.33
14	N	602	HEA	CBD-CGD	2.34	1.56	1.50
22	B	302	CHD	C13-C12	-2.33	1.50	1.54
14	N	603[A]	HEA	C4B-NB	-2.33	1.36	1.40
21	Y	101	TGL	CG3-CG2	2.33	1.57	1.50
14	A	602[A]	HEA	C4D-ND	-2.32	1.34	1.38
27	T	101	PEK	C3-C4	2.32	1.61	1.52
27	C	307	PEK	C2-C1	2.31	1.57	1.50
19	N	609	PGV	C01-C02	2.31	1.57	1.50
22	W	101	CHD	C8-C14	2.30	1.58	1.53
22	C	301	CHD	C21-C20	2.29	1.58	1.53
22	B	302	CHD	C2-C3	2.29	1.57	1.51
20	B	306	EDO	O1-C1	2.29	1.53	1.42
22	B	302	CHD	O12-C12	2.29	1.47	1.43
22	P	305	CHD	C20-C17	2.28	1.58	1.54
27	G	101	PEK	P-O13	-2.27	1.44	1.55
26	P	304	CDL	PA1-OA5	2.26	1.68	1.59
14	A	601	HEA	C16-C17	-2.26	1.46	1.53
19	A	609	PGV	C2-C1	-2.24	1.44	1.50
22	G	102	CHD	C13-C14	2.24	1.59	1.55
19	C	304	PGV	O01-C02	-2.23	1.41	1.46
14	N	603[A]	HEA	O1D-CGD	2.23	1.29	1.22
14	N	603[A]	HEA	C1D-C2D	-2.21	1.40	1.44
14	A	602[A]	HEA	O1A-CGA	2.20	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	O1A-CGA	2.20	1.29	1.22
14	N	602	HEA	C12-C11	-2.19	1.49	1.52
14	N	603[A]	HEA	C3A-C2A	2.19	1.43	1.40
19	A	608	PGV	C06-C05	2.18	1.60	1.51
14	A	602[B]	HEA	C3D-C2D	2.18	1.41	1.36
14	A	601	HEA	CMC-C2C	2.17	1.56	1.51
27	T	101	PEK	C05-C04	2.17	1.58	1.50
19	A	608	PGV	C01-C02	2.17	1.57	1.50
22	P	301	CHD	O26-C24	-2.17	1.23	1.30
14	A	601	HEA	C3C-CAC	2.16	1.52	1.47
24	M	101	DMU	O5-C6	2.16	1.47	1.41
14	A	602[B]	HEA	C4B-NB	-2.16	1.36	1.40
19	A	609	PGV	O02-C1	2.16	1.28	1.22
14	A	601	HEA	C1D-C2D	-2.15	1.40	1.44
27	G	101	PEK	P-O14	2.15	1.58	1.50
24	Z	102	DMU	O16-C6	2.14	1.43	1.40
14	N	603[A]	HEA	C3C-C2C	-2.14	1.37	1.40
14	N	602	HEA	OMA-CMA	2.14	1.28	1.21
19	P	303	PGV	O01-C02	-2.14	1.41	1.46
19	N	609	PGV	C20-C19	2.14	1.57	1.50
19	C	304	PGV	O03-C19	2.13	1.39	1.33
14	A	602[B]	HEA	FE-ND	2.13	2.07	1.96
27	G	101	PEK	C05-C04	2.13	1.58	1.50
26	T	102	CDL	CB6-CB4	2.13	1.57	1.50
27	C	307	PEK	C22-C21	2.13	1.56	1.50
14	A	602[A]	HEA	C4B-C3B	-2.13	1.41	1.44
22	C	301	CHD	C4-C5	2.12	1.57	1.53
14	A	602[A]	HEA	C13-C14	2.10	1.57	1.50
26	C	305	CDL	PB2-OB2	2.10	1.67	1.59
27	C	307	PEK	C03-C02	2.09	1.57	1.50
19	N	609	PGV	C06-C05	2.08	1.60	1.51
20	A	613	EDO	O2-C2	2.08	1.52	1.42
22	C	306	CHD	C20-C17	2.07	1.58	1.54
22	G	102	CHD	C13-C12	-2.07	1.51	1.54
21	Y	101	TGL	CB2-CB1	2.05	1.56	1.50
22	P	301	CHD	C16-C15	2.04	1.59	1.54
22	C	301	CHD	O26-C24	-2.04	1.23	1.30
26	N	601	CDL	CB3-CB4	2.03	1.56	1.50
22	P	305	CHD	C8-C9	2.02	1.57	1.53

All (607) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	305	CHD	C23-C22-C20	-16.38	84.59	114.52
22	C	306	CHD	C23-C22-C20	-14.41	88.20	114.52
24	C	311	DMU	O16-C6-C1	11.51	126.27	108.30
21	D	201	TGL	OG2-CB1-CB2	-10.50	88.87	111.50
27	T	101	PEK	C2-C3-C4	9.42	130.02	113.23
21	B	301	TGL	OG2-CB1-CB2	9.24	131.42	111.50
27	T	101	PEK	O01-C1-O02	-9.01	101.93	123.70
21	D	201	TGL	OG2-CB1-OB1	8.48	144.20	123.70
22	J	101	CHD	C17-C13-C14	-8.01	92.02	100.09
14	A	602[A]	HEA	C13-C12-C11	-7.99	102.35	114.35
22	W	101	CHD	C13-C17-C20	7.68	128.66	119.50
14	N	603[A]	HEA	C13-C12-C11	-7.60	102.94	114.35
24	C	310	DMU	C10-O1-C9	-7.30	99.37	113.69
22	J	101	CHD	C6-C5-C10	7.02	120.11	112.66
24	P	308	DMU	O16-C6-C1	6.98	119.21	108.30
22	C	306	CHD	C21-C20-C17	6.95	123.57	112.92
21	N	610	TGL	OG2-CB1-CB2	6.87	126.31	111.50
20	A	615	EDO	O1-C1-C2	-6.75	63.33	111.91
21	Y	101	TGL	OG2-CB1-CB2	6.74	126.02	111.50
22	P	301	CHD	C5-C6-C7	6.67	121.82	114.46
28	E	201	PSC	O01-C1-C2	6.64	125.80	111.50
27	C	309	PEK	O01-C1-C2	6.62	125.76	111.50
19	U	101	PGV	O03-C19-C20	6.59	132.60	111.91
21	D	201	TGL	CB3-CB2-CB1	6.32	136.60	113.62
21	L	101	TGL	OG2-CB1-CB2	6.31	125.11	111.50
26	N	601	CDL	OB6-CB5-C51	6.30	125.08	111.50
22	P	305	CHD	C13-C17-C20	-6.23	112.06	119.50
27	P	307	PEK	O01-C1-C2	6.17	124.80	111.50
22	J	101	CHD	C18-C13-C17	6.07	120.71	111.21
22	P	301	CHD	C4-C5-C10	-6.04	106.24	112.66
14	N	603[B]	HEA	OMA-CMA-C3A	-6.01	111.82	124.91
24	C	310	DMU	O16-C6-C1	5.98	117.64	108.30
22	W	101	CHD	C1-C10-C5	5.90	116.50	107.77
22	P	305	CHD	C5-C4-C3	-5.87	104.13	112.76
14	A	601	HEA	CHA-C4D-ND	5.83	130.76	124.43
24	C	310	DMU	C10-C5-C7	-5.81	97.90	110.00
22	P	301	CHD	C22-C20-C17	-5.80	98.30	110.28
22	C	306	CHD	C6-C7-C8	5.77	117.64	111.48
24	C	310	DMU	O7-C10-C5	5.76	123.02	108.10
21	N	610	TGL	OG1-CA1-CA2	5.74	129.92	111.91
22	J	101	CHD	C13-C17-C20	5.69	126.29	119.50
21	Q	201	TGL	OG2-CB1-CB2	-5.68	99.25	111.50
22	P	305	CHD	C16-C17-C20	5.67	120.93	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	306	DMU	O16-C6-C1	5.64	117.12	108.30
14	A	602[B]	HEA	CAA-CBA-CGA	-5.62	98.02	113.76
27	G	103	PEK	O01-C1-C2	5.53	123.41	111.50
21	L	101	TGL	OG3-CC1-CC2	5.42	128.93	111.91
24	P	308	DMU	C18-O16-C6	-5.39	104.91	113.84
22	C	301	CHD	C23-C22-C20	-5.35	104.75	114.52
19	A	609	PGV	C02-O01-C1	5.33	130.92	117.79
14	N	602	HEA	C13-C14-C15	-5.29	114.92	127.66
27	C	307	PEK	O01-C1-C2	5.29	122.90	111.50
22	P	305	CHD	C14-C13-C12	5.28	112.31	107.40
14	A	601	HEA	C26-C15-C16	-5.25	106.43	115.27
26	P	304	CDL	OA6-CA5-C11	5.24	122.80	111.50
21	L	101	TGL	CC4-CC3-CC2	-5.23	94.38	113.19
19	C	308	PGV	O01-C1-C2	5.18	122.66	111.50
22	C	306	CHD	C14-C13-C12	5.12	112.17	107.40
14	N	603[A]	HEA	OMA-CMA-C3A	-5.12	113.75	124.91
14	A	602[B]	HEA	CAD-C3D-C2D	5.12	137.41	127.88
26	T	102	CDL	OA6-CA5-C11	5.11	122.52	111.50
22	W	101	CHD	C6-C7-C8	5.09	116.92	111.48
19	C	308	PGV	C03-C02-C01	-5.06	99.82	111.79
14	N	603[B]	HEA	CMB-C2B-C3B	-5.06	120.69	130.34
22	P	301	CHD	C21-C20-C22	-5.03	102.47	110.36
28	O	302	PSC	O01-C1-C2	5.03	122.33	111.50
27	T	101	PEK	O02-C1-C2	5.03	143.34	123.73
22	P	305	CHD	C19-C10-C9	-4.93	104.39	111.18
22	W	101	CHD	C18-C13-C14	-4.89	103.55	111.21
27	C	307	PEK	O03-C21-C22	4.88	127.23	111.91
24	P	309	DMU	O7-C10-C5	4.87	120.73	108.10
24	P	309	DMU	O3-C5-C10	4.87	121.88	110.05
14	A	602[B]	HEA	C27-C19-C20	4.84	123.41	115.27
14	A	602[B]	HEA	C17-C18-C19	-4.78	116.15	127.66
22	J	101	CHD	C5-C6-C7	4.76	119.72	114.46
14	N	603[B]	HEA	CAA-CBA-CGA	-4.76	100.43	113.76
22	C	301	CHD	C22-C20-C17	-4.76	100.46	110.28
22	C	301	CHD	C5-C4-C3	-4.75	105.79	112.76
22	P	305	CHD	C21-C20-C17	4.72	120.15	112.92
26	C	305	CDL	OA6-CA5-C11	4.71	121.64	111.50
14	N	603[B]	HEA	C17-C18-C19	-4.69	116.37	127.66
22	P	301	CHD	C23-C22-C20	-4.69	105.96	114.52
22	J	101	CHD	C1-C10-C5	4.68	114.70	107.77
21	D	201	TGL	OG1-CA1-CA2	4.68	126.58	111.91
22	G	102	CHD	C11-C12-C13	4.66	116.03	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	603[A]	HEA	CBA-CAA-C2A	-4.65	104.76	112.60
22	C	306	CHD	C16-C17-C20	4.64	119.33	112.15
14	A	602[A]	HEA	CHA-C4D-ND	4.62	129.45	124.43
26	P	304	CDL	C52-C51-CB5	-4.61	96.85	113.62
22	W	101	CHD	C11-C12-C13	4.61	115.98	111.24
24	P	308	DMU	O7-C10-C5	4.61	120.03	108.10
14	A	602[A]	HEA	OMA-CMA-C3A	-4.60	114.88	124.91
22	C	306	CHD	C15-C14-C13	4.60	108.07	103.55
14	N	603[A]	HEA	C26-C15-C16	4.60	123.02	115.27
14	N	603[B]	HEA	CMC-C2C-C1C	-4.59	121.40	128.46
14	N	603[A]	HEA	CAD-CBD-CGD	-4.57	103.76	113.60
19	A	608	PGV	O03-C19-C20	4.54	126.14	111.91
22	W	101	CHD	C21-C20-C17	4.48	119.78	112.92
14	A	602[B]	HEA	CAD-C3D-C4D	-4.47	116.84	124.66
19	N	609	PGV	O03-C19-C20	4.46	125.91	111.91
22	P	305	CHD	C6-C7-C8	4.46	116.24	111.48
14	A	601	HEA	C13-C12-C11	-4.38	107.77	114.35
14	A	601	HEA	CHA-C4D-C3D	-4.38	118.40	124.84
22	C	306	CHD	C4-C5-C10	4.37	117.30	112.66
26	N	601	CDL	CB6-OB8-CB7	4.36	133.27	117.12
14	N	602	HEA	C1B-C2B-C3B	-4.35	101.60	106.80
22	J	101	CHD	C4-C3-C2	4.34	115.73	110.55
26	P	304	CDL	OB8-CB7-C71	4.33	125.49	111.91
22	B	302	CHD	C11-C9-C10	-4.33	109.26	113.73
22	B	302	CHD	C11-C12-C13	4.33	115.69	111.24
14	A	601	HEA	C3C-C4C-NC	4.32	114.80	109.21
22	W	101	CHD	C13-C14-C8	4.32	120.25	114.74
14	N	602	HEA	O2D-CGD-O1D	-4.31	112.55	123.30
14	A	602[A]	HEA	CAD-CBD-CGD	-4.29	104.38	113.60
22	W	101	CHD	C6-C5-C10	4.28	117.20	112.66
24	M	101	DMU	C18-O16-C6	-4.27	106.76	113.84
22	B	302	CHD	C17-C13-C12	4.27	121.56	117.67
21	B	301	TGL	OG2-CG2-CG3	4.26	123.82	108.40
21	Q	201	TGL	OG3-CC1-CC2	4.26	125.27	111.91
22	C	306	CHD	C13-C17-C20	-4.25	114.42	119.50
26	N	601	CDL	CB2-C1-CA2	-4.24	100.31	112.79
22	P	305	CHD	C16-C17-C13	4.20	107.67	103.55
26	T	102	CDL	OB6-CB5-C51	4.19	120.54	111.50
21	Q	201	TGL	OG3-CC1-OC1	-4.19	113.02	123.59
22	G	102	CHD	C1-C2-C3	-4.17	105.11	110.47
22	J	101	CHD	C16-C17-C13	4.17	107.64	103.55
21	Y	101	TGL	CG2-OG2-CB1	4.16	128.04	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	101	CHD	C14-C8-C7	4.15	117.31	111.81
14	A	601	HEA	C13-C14-C15	-4.14	117.69	127.66
28	E	201	PSC	O01-C1-O02	-4.14	113.69	123.70
14	N	602	HEA	C3C-C4C-NC	4.14	114.56	109.21
24	P	308	DMU	O49-C1-C2	-4.14	100.79	110.35
14	N	602	HEA	C1D-C2D-C3D	-4.13	102.61	106.96
22	P	301	CHD	C19-C10-C1	-4.12	101.62	108.26
14	N	603[B]	HEA	CMC-C2C-C3C	4.12	132.38	124.68
21	N	610	TGL	OG1-CA1-OA1	-4.12	113.20	123.59
24	P	309	DMU	C1-C2-C3	4.09	119.02	109.68
21	B	301	TGL	OG3-CC1-OC1	-4.07	113.31	123.59
19	N	609	PGV	O01-C1-O02	-4.07	113.87	123.70
24	P	309	DMU	O16-C6-C1	4.07	114.65	108.30
19	C	308	PGV	O03-C19-C20	4.06	124.66	111.91
14	N	602	HEA	CHC-C4B-NB	4.06	129.40	124.38
14	N	602	HEA	CHB-C1B-C2B	-4.04	118.67	124.98
14	N	602	HEA	C4D-CHA-C1A	-4.03	117.24	122.56
19	A	609	PGV	C4-C3-C2	-4.01	98.76	113.19
22	C	301	CHD	C1-C2-C3	-4.01	105.32	110.47
22	C	301	CHD	C21-C20-C22	-3.98	104.12	110.36
14	N	603[B]	HEA	C27-C19-C20	3.97	121.94	115.27
24	P	308	DMU	C10-O1-C9	-3.96	105.92	113.69
27	C	307	PEK	C02-O01-C1	3.95	127.52	117.79
27	G	101	PEK	C24-C23-C22	-3.95	98.99	113.19
14	N	603[A]	HEA	CHB-C1B-C2B	-3.95	118.81	124.98
21	B	301	TGL	OG3-CC1-CC2	3.93	124.23	111.91
26	C	305	CDL	OB8-CB7-C71	3.92	124.22	111.91
26	N	601	CDL	CB4-OB6-CB5	3.88	127.35	117.79
22	B	302	CHD	C13-C17-C20	-3.87	114.88	119.50
14	A	602[A]	HEA	C2B-C1B-NB	3.86	114.51	109.88
21	B	301	TGL	CG3-OG3-CC1	3.86	131.40	117.12
22	J	101	CHD	C1-C10-C9	-3.86	105.29	111.35
26	N	601	CDL	OA6-CA5-C11	3.85	119.81	111.50
22	P	305	CHD	O7-C7-C6	-3.84	100.43	109.94
14	N	603[A]	HEA	C2B-C1B-NB	3.83	114.47	109.88
19	U	101	PGV	C21-C20-C19	-3.82	99.72	113.62
14	A	601	HEA	C4A-CHB-C1B	3.79	127.56	122.56
22	B	302	CHD	C16-C17-C20	-3.79	106.28	112.15
14	N	602	HEA	C2D-C1D-ND	3.78	114.32	109.84
14	A	601	HEA	CMC-C2C-C3C	3.76	131.70	124.68
22	C	306	CHD	C22-C23-C24	-3.75	102.54	112.51
24	P	306	DMU	O16-C18-C19	3.73	122.64	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	101	CHD	C19-C10-C5	-3.69	104.11	110.36
19	A	608	PGV	O03-C19-O04	-3.68	114.30	123.59
14	N	602	HEA	C2B-C1B-NB	3.66	114.27	109.88
21	Y	101	TGL	OG3-CC1-CC2	3.65	123.35	111.91
26	P	304	CDL	OB8-CB7-OB9	-3.64	114.40	123.59
22	C	306	CHD	C17-C13-C12	-3.64	114.34	117.67
21	Y	101	TGL	OG3-CG3-CG2	3.64	119.02	108.43
19	P	303	PGV	O01-C1-O02	-3.64	114.91	123.70
14	N	603[A]	HEA	C4D-CHA-C1A	3.62	127.34	122.56
21	Q	201	TGL	OG2-CB1-OB1	3.62	132.46	123.70
24	P	309	DMU	C10-O1-C9	-3.62	106.58	113.69
19	Z	101	PGV	O03-C19-C20	3.61	123.23	111.91
24	C	311	DMU	O5-C4-C3	-3.61	102.15	109.75
22	P	305	CHD	C15-C14-C13	3.60	107.08	103.55
14	N	602	HEA	CHA-C4D-ND	3.60	128.34	124.43
19	U	101	PGV	O04-C19-C20	-3.57	109.81	123.73
21	D	201	TGL	CG1-OG1-CA1	3.56	130.32	117.12
14	A	601	HEA	CAD-CBD-CGD	-3.56	105.95	113.60
21	L	101	TGL	OG1-CA1-CA2	3.56	123.07	111.91
14	N	603[B]	HEA	CMB-C2B-C1B	3.56	130.45	125.04
22	B	302	CHD	C18-C13-C12	-3.54	105.46	109.07
24	P	308	DMU	O3-C5-C10	3.53	118.63	110.05
21	B	301	TGL	OB1-CB1-CB2	-3.53	109.96	123.73
21	N	610	TGL	OG3-CC1-OC1	-3.52	114.70	123.59
22	W	101	CHD	C15-C14-C13	-3.51	100.11	103.55
14	N	603[A]	HEA	C3D-C4D-ND	3.50	113.74	110.36
22	W	101	CHD	C10-C9-C8	3.50	115.57	111.82
22	P	305	CHD	C15-C14-C8	3.49	123.21	118.33
14	A	602[A]	HEA	CMB-C2B-C1B	3.49	130.35	125.04
19	C	304	PGV	O03-C19-O04	-3.48	114.80	123.59
24	M	101	DMU	C22-C19-C18	-3.48	98.05	113.49
22	C	306	CHD	C5-C6-C7	3.48	118.30	114.46
14	A	602[A]	HEA	C12-C13-C14	-3.47	103.07	112.23
27	P	307	PEK	O03-C21-O04	-3.47	114.85	123.59
22	J	101	CHD	C11-C9-C10	-3.45	110.17	113.73
22	J	101	CHD	C16-C17-C20	3.45	117.48	112.15
28	E	201	PSC	O03-C19-C20	3.44	122.71	111.91
21	Q	201	TGL	OG1-CA1-CA2	3.44	122.71	111.91
24	C	310	DMU	C7-C8-C9	3.44	116.37	110.24
21	N	610	TGL	OG3-CC1-CC2	3.43	122.67	111.91
14	N	603[A]	HEA	C17-C18-C19	3.43	135.91	127.66
14	N	602	HEA	CMD-C2D-C1D	3.42	130.25	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	608	PGV	O01-C1-C2	3.42	118.86	111.50
26	P	304	CDL	OA6-CA5-OA7	-3.40	115.49	123.70
21	Y	101	TGL	OG2-CB1-OB1	-3.39	115.51	123.70
19	A	609	PGV	C3-C2-C1	3.39	125.94	113.62
24	P	306	DMU	O49-C1-C2	-3.39	102.52	110.35
22	G	102	CHD	C11-C9-C10	-3.38	110.24	113.73
24	C	311	DMU	C10-O7-C3	-3.38	109.60	117.96
22	P	301	CHD	C11-C9-C10	-3.37	110.25	113.73
19	N	609	PGV	O03-C19-O04	-3.37	115.08	123.59
14	N	602	HEA	C27-C19-C20	3.36	120.93	115.27
21	D	201	TGL	OG3-CC1-OC1	-3.33	115.18	123.59
22	C	301	CHD	O3-C3-C2	-3.33	101.69	110.16
26	T	102	CDL	C83-C82-C81	3.33	131.32	114.42
24	C	310	DMU	C6-O5-C4	3.31	120.19	113.69
14	A	601	HEA	O2D-CGD-O1D	-3.31	115.05	123.30
27	T	101	PEK	O03-C21-C22	3.29	122.25	111.91
24	C	311	DMU	C18-O16-C6	3.29	119.30	113.84
27	T	101	PEK	C02-O01-C1	3.28	125.86	117.79
24	C	311	DMU	C10-O1-C9	3.28	120.12	113.69
22	G	102	CHD	C23-C22-C20	-3.28	108.53	114.52
22	J	101	CHD	C9-C10-C5	3.28	113.18	108.58
24	P	308	DMU	O5-C6-O16	-3.27	102.23	109.97
19	U	101	PGV	O01-C1-C2	3.26	118.53	111.50
27	C	307	PEK	O03-C21-O04	-3.26	115.38	123.59
19	P	303	PGV	O03-C19-O04	-3.25	115.38	123.59
22	C	306	CHD	C15-C14-C8	3.24	122.86	118.33
24	C	302	DMU	C25-C22-C19	-3.23	98.04	114.42
22	J	101	CHD	C19-C10-C5	-3.23	104.89	110.36
14	A	601	HEA	C4D-CHA-C1A	-3.23	118.30	122.56
14	N	603[A]	HEA	C4A-CHB-C1B	3.22	126.81	122.56
24	P	309	DMU	O1-C9-C11	3.22	114.45	106.44
19	Z	101	PGV	C01-O03-C19	3.22	129.04	117.12
27	C	307	PEK	O01-C1-O02	-3.21	115.94	123.70
22	G	102	CHD	C6-C5-C4	-3.21	107.50	111.19
22	B	302	CHD	C19-C10-C5	-3.20	104.93	110.36
19	A	609	PGV	O03-C19-C20	3.19	121.92	111.91
22	J	101	CHD	C11-C9-C8	3.19	115.54	110.88
21	Q	201	TGL	OG1-CA1-OA1	-3.17	115.58	123.59
14	A	601	HEA	CMC-C2C-C1C	-3.17	123.59	128.46
14	A	602[B]	HEA	C27-C19-C18	-3.17	115.55	123.68
22	P	305	CHD	C1-C2-C3	-3.16	106.41	110.47
24	C	311	DMU	O1-C9-C11	3.16	114.30	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	102	CDL	CB6-OB8-CB7	3.16	128.83	117.12
14	A	601	HEA	C1B-C2B-C3B	-3.16	103.02	106.80
24	C	302	DMU	O1-C9-C11	3.15	114.28	106.44
22	G	102	CHD	C21-C20-C17	-3.15	108.10	112.92
19	C	308	PGV	C02-O01-C1	3.14	125.53	117.79
27	G	101	PEK	O03-C21-O04	-3.14	115.67	123.59
22	P	305	CHD	C18-C13-C12	-3.14	105.87	109.07
19	C	308	PGV	O03-C19-O04	-3.13	115.69	123.59
26	P	304	CDL	OA8-CA7-C31	3.13	121.72	111.91
22	W	101	CHD	C18-C13-C17	3.13	116.11	111.21
14	N	602	HEA	CHA-C4D-C3D	-3.12	120.25	124.84
22	G	102	CHD	C4-C3-C2	-3.11	106.83	110.55
14	A	602[B]	HEA	CMD-C2D-C3D	3.11	134.57	126.12
14	N	603[A]	HEA	C27-C19-C20	3.11	120.50	115.27
14	N	602	HEA	O2D-CGD-CBD	3.09	123.96	114.03
21	L	101	TGL	C26-C25-C24	-3.09	98.74	114.42
21	D	201	TGL	CG3-OG3-CC1	3.09	128.56	117.12
22	P	305	CHD	O26-C24-O25	3.08	130.99	123.30
22	W	101	CHD	C17-C13-C12	3.08	120.48	117.67
22	C	306	CHD	C6-C5-C4	-3.08	107.65	111.19
21	D	201	TGL	OG1-CA1-OA1	-3.07	115.83	123.59
14	N	602	HEA	CMB-C2B-C1B	3.07	129.72	125.04
27	G	103	PEK	O03-C01-C02	3.07	117.36	108.43
24	C	302	DMU	O55-C2-C3	3.04	118.01	109.94
27	G	103	PEK	O03-C21-C22	3.04	121.46	111.91
24	Z	102	DMU	C6-O5-C4	3.04	119.65	113.69
24	P	309	DMU	O5-C6-C1	-3.04	103.92	110.35
26	N	601	CDL	OA8-CA7-C31	3.03	121.42	111.91
14	N	603[B]	HEA	C3B-C4B-NB	3.03	113.42	109.84
22	G	102	CHD	C6-C7-C8	-3.02	108.26	111.48
14	A	602[A]	HEA	C1B-C2B-C3B	-3.02	103.19	106.80
19	U	101	PGV	C03-C02-C01	-3.02	104.64	111.79
27	C	309	PEK	O03-C21-C22	3.01	121.36	111.91
21	L	101	TGL	CG2-OG2-CB1	3.01	125.21	117.79
26	T	102	CDL	OB8-CB6-CB4	3.01	117.19	108.43
19	Z	101	PGV	O01-C02-C01	3.01	119.28	108.40
24	Z	102	DMU	C10-O7-C3	-3.01	110.53	117.96
22	C	306	CHD	O26-C24-O25	3.00	130.77	123.30
14	N	603[A]	HEA	C3B-C4B-NB	2.99	113.38	109.84
22	W	101	CHD	C9-C10-C5	2.99	112.78	108.58
14	N	602	HEA	CAD-CBD-CGD	-2.99	107.18	113.60
24	C	302	DMU	C18-O16-C6	-2.98	108.89	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	302	DMU	C6-C1-C2	-2.96	103.83	110.00
22	G	102	CHD	O12-C12-C11	-2.96	103.10	109.12
28	O	302	PSC	C21-C20-C19	-2.96	102.86	113.62
19	A	608	PGV	O01-C02-C01	-2.95	97.72	108.40
22	G	102	CHD	C15-C14-C8	-2.94	114.22	118.33
22	B	302	CHD	C1-C10-C9	2.93	115.97	111.35
26	C	305	CDL	OB6-CB5-C51	2.93	117.82	111.50
22	W	101	CHD	C2-C1-C10	2.93	117.80	112.78
14	N	603[A]	HEA	C4B-NB-C1B	-2.92	102.06	105.07
21	L	101	TGL	OG3-CC1-OC1	-2.92	116.23	123.59
26	C	305	CDL	OB6-CB5-OB7	-2.90	116.69	123.70
22	J	101	CHD	C6-C7-C8	2.90	114.57	111.48
28	E	201	PSC	O01-C02-C03	2.89	118.85	108.40
28	O	302	PSC	O03-C19-C20	2.88	120.95	111.91
22	J	101	CHD	C5-C4-C3	2.88	116.99	112.76
21	N	610	TGL	CG3-CG2-CG1	-2.88	104.99	111.79
22	W	101	CHD	C1-C10-C9	-2.87	106.84	111.35
24	P	308	DMU	O4-C7-C8	2.86	116.97	110.35
22	B	302	CHD	C16-C17-C13	2.84	106.34	103.55
22	C	301	CHD	C16-C17-C13	-2.84	100.77	103.55
22	G	102	CHD	C5-C6-C7	2.84	117.59	114.46
19	Z	101	PGV	O01-C1-C2	2.84	117.61	111.50
24	C	311	DMU	O5-C4-C57	2.83	113.48	106.44
22	W	101	CHD	C4-C5-C10	2.83	115.66	112.66
19	C	308	PGV	O01-C02-C01	2.83	118.65	108.40
24	P	308	DMU	C8-C7-C5	-2.83	105.89	110.82
22	P	301	CHD	C19-C10-C5	-2.83	105.57	110.36
14	N	603[B]	HEA	O11-C11-C12	-2.82	101.52	109.42
14	N	603[B]	HEA	CBA-CAA-C2A	-2.82	107.85	112.60
22	C	301	CHD	C17-C13-C12	-2.81	115.10	117.67
24	P	306	DMU	O55-C2-C3	2.81	117.40	109.94
26	N	601	CDL	C44-C43-C42	-2.81	100.15	114.42
14	A	602[B]	HEA	CHD-C1D-ND	2.81	127.85	124.38
27	G	101	PEK	O03-C01-C02	-2.81	100.25	108.43
19	A	608	PGV	O01-C1-O02	-2.81	116.92	123.70
14	N	603[A]	HEA	CMC-C2C-C3C	2.79	129.89	124.68
22	C	301	CHD	C15-C14-C8	-2.78	114.44	118.33
14	N	602	HEA	CHD-C1D-C2D	-2.77	119.05	126.72
24	P	308	DMU	C7-C8-C9	2.77	115.19	110.24
14	N	602	HEA	C20-C21-C22	-2.77	102.79	111.88
26	C	305	CDL	OB2-PB2-OB3	2.77	119.88	109.07
14	A	601	HEA	C16-C15-C14	2.77	126.72	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	311	DMU	C6-C1-C2	2.76	115.75	110.00
22	J	101	CHD	C6-C5-C4	-2.76	108.01	111.19
14	A	602[A]	HEA	C4B-NB-C1B	-2.76	102.22	105.07
26	C	305	CDL	C39-C38-C37	2.75	128.40	114.42
22	B	302	CHD	C13-C14-C8	-2.75	111.23	114.74
22	C	301	CHD	C19-C10-C9	-2.75	107.40	111.18
21	B	301	TGL	OG1-CA1-CA2	2.74	120.51	111.91
22	C	306	CHD	O26-C24-C23	-2.74	105.23	114.03
22	C	306	CHD	C1-C10-C5	2.73	111.80	107.77
26	N	601	CDL	C23-C22-C21	2.73	128.28	114.42
24	C	311	DMU	O7-C3-C2	2.73	114.54	107.28
22	W	101	CHD	C6-C5-C4	-2.73	108.05	111.19
24	C	310	DMU	O7-C10-O1	2.72	118.28	110.67
26	C	305	CDL	PA1-OA2-CA2	2.72	137.65	121.68
24	P	306	DMU	C37-C34-C31	-2.72	100.60	114.42
24	Z	102	DMU	O3-C5-C7	2.72	116.64	110.35
27	C	309	PEK	C2-C3-C4	2.72	118.08	113.23
21	B	301	TGL	CB3-CB2-CB1	-2.71	103.75	113.62
14	A	602[B]	HEA	CMB-C2B-C3B	-2.71	125.18	130.34
14	N	602	HEA	C26-C15-C16	-2.71	110.72	115.27
26	T	102	CDL	OA8-CA7-C31	2.70	120.39	111.91
22	B	302	CHD	O26-C24-O25	-2.70	116.57	123.30
26	P	304	CDL	C83-C82-C81	2.70	128.13	114.42
27	C	307	PEK	C01-O03-C21	2.69	127.08	117.12
28	E	201	PSC	O03-C19-O04	-2.68	116.82	123.59
14	N	603[A]	HEA	O11-C11-C12	2.68	116.91	109.42
14	A	602[A]	HEA	O2A-CGA-CBA	2.67	122.62	114.03
14	N	603[A]	HEA	CMB-C2B-C1B	2.66	129.09	125.04
14	N	602	HEA	C25-C23-C24	-2.66	108.74	114.60
28	E	201	PSC	C27-C26-C25	-2.65	100.95	114.42
22	C	306	CHD	O7-C7-C6	-2.65	103.37	109.94
22	J	101	CHD	C11-C12-C13	2.65	113.96	111.24
14	N	602	HEA	OMA-CMA-C3A	-2.65	119.14	124.91
20	P	311	EDO	O1-C1-C2	-2.64	92.90	111.91
14	A	602[A]	HEA	C16-C15-C14	-2.64	115.77	121.12
22	B	302	CHD	O12-C12-C13	-2.64	106.57	111.03
19	C	304	PGV	C21-C20-C19	-2.63	104.05	113.62
21	L	101	TGL	CA4-CA3-CA2	-2.63	103.74	113.19
14	A	602[A]	HEA	C1D-ND-C4D	2.63	107.78	105.07
26	N	601	CDL	O1-C1-CA2	2.62	118.75	109.56
19	A	609	PGV	O01-C1-O02	2.61	130.01	123.70
22	P	305	CHD	C11-C9-C8	2.61	114.69	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	308	DMU	C10-C5-C7	-2.60	104.57	110.00
26	T	102	CDL	OA6-CA5-OA7	-2.60	117.41	123.70
26	T	102	CDL	OA2-PA1-OA3	-2.60	98.90	109.07
21	N	610	TGL	CG3-OG3-CC1	2.60	126.75	117.12
14	N	603[B]	HEA	C13-C12-C11	-2.59	110.45	114.35
14	A	602[B]	HEA	C1D-C2D-C3D	-2.59	104.24	106.96
21	N	610	TGL	OG2-CB1-OB1	-2.58	117.46	123.70
14	N	603[A]	HEA	O2A-CGA-CBA	2.58	122.32	114.03
19	A	608	PGV	C30-C29-C28	2.58	127.52	114.42
14	N	602	HEA	C27-C19-C18	-2.57	117.09	123.68
24	C	310	DMU	O5-C4-C57	2.56	112.80	106.44
26	P	304	CDL	PA1-OA2-CA2	2.56	136.70	121.68
22	C	306	CHD	C13-C14-C8	-2.56	111.47	114.74
14	N	602	HEA	C4A-CHB-C1B	2.55	125.93	122.56
27	C	309	PEK	O01-C1-O02	-2.55	117.55	123.70
22	J	101	CHD	C15-C14-C13	2.54	106.04	103.55
27	C	307	PEK	C24-C23-C22	2.54	122.31	113.19
14	N	603[A]	HEA	CMC-C2C-C1C	-2.53	124.58	128.46
14	A	602[B]	HEA	CMD-C2D-C1D	-2.53	121.19	125.04
19	N	609	PGV	C02-O01-C1	2.52	124.00	117.79
14	A	602[B]	HEA	C13-C12-C11	-2.52	110.56	114.35
26	P	304	CDL	C39-C38-C37	2.51	127.19	114.42
14	A	602[A]	HEA	CHA-C4D-C3D	-2.51	121.14	124.84
26	P	304	CDL	OB6-CB5-C51	2.51	116.91	111.50
22	P	305	CHD	O3-C3-C4	-2.50	104.87	109.85
24	C	311	DMU	O16-C18-C19	2.50	118.31	109.56
14	A	601	HEA	C2B-C1B-NB	2.49	112.87	109.88
26	C	305	CDL	OA8-CA7-C31	2.49	119.71	111.91
14	A	602[A]	HEA	CAD-C3D-C2D	2.48	132.51	127.88
26	C	305	CDL	CB6-CB4-CB3	-2.48	105.91	111.79
14	N	603[B]	HEA	C4B-C3B-C2B	-2.48	103.17	107.41
14	N	603[B]	HEA	C27-C19-C18	-2.48	117.32	123.68
22	B	302	CHD	C21-C20-C17	-2.46	109.15	112.92
14	A	602[B]	HEA	CHD-C1D-C2D	-2.46	119.92	126.72
19	U	101	PGV	C02-O01-C1	2.45	123.82	117.79
14	A	602[A]	HEA	C17-C18-C19	2.45	133.55	127.66
22	P	301	CHD	C13-C17-C20	-2.44	116.58	119.50
22	P	305	CHD	C1-C10-C9	2.43	115.18	111.35
14	N	603[A]	HEA	C1B-C2B-C3B	-2.43	103.89	106.80
14	A	602[A]	HEA	O1A-CGA-CBA	-2.43	115.27	123.08
26	T	102	CDL	C63-C62-C61	2.43	126.76	114.42
21	Y	101	TGL	CG3-OG3-CC1	2.43	126.12	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	O2D-CGD-CBD	2.43	121.83	114.03
26	N	601	CDL	OB7-CB5-C51	-2.42	114.28	123.73
26	N	601	CDL	C83-C82-C81	2.42	126.72	114.42
22	P	301	CHD	C1-C10-C5	2.42	111.34	107.77
22	G	102	CHD	O3-C3-C4	-2.41	105.05	109.85
26	C	305	CDL	CA6-OA8-CA7	2.41	126.03	117.12
26	C	305	CDL	C75-C74-C73	-2.41	102.21	114.42
14	A	602[B]	HEA	C12-C13-C14	-2.40	105.88	112.23
27	C	307	PEK	C3-C2-C1	2.40	122.36	113.62
19	C	304	PGV	C30-C29-C28	-2.39	102.28	114.42
22	C	301	CHD	C5-C6-C7	2.39	117.10	114.46
24	Z	102	DMU	O49-C1-C2	-2.39	104.82	110.35
14	N	602	HEA	CHB-C1B-NB	2.39	127.02	124.43
27	C	309	PEK	C01-O03-C21	2.39	125.96	117.12
22	W	101	CHD	O12-C12-C13	2.38	115.05	111.03
19	P	303	PGV	O02-C1-C2	2.38	133.00	123.73
19	U	101	PGV	O03-C19-O04	-2.38	117.59	123.59
24	P	309	DMU	O7-C10-O1	-2.37	104.04	110.67
14	N	603[A]	HEA	C2D-C1D-ND	2.37	112.64	109.84
22	P	301	CHD	O26-C24-O25	-2.37	117.40	123.30
24	C	310	DMU	O3-C5-C10	2.37	115.80	110.05
19	N	609	PGV	O12-P-O13	2.36	118.30	109.07
19	C	308	PGV	O06-C06-C05	2.36	121.53	110.20
21	L	101	TGL	C23-C22-C21	-2.36	102.43	114.42
26	T	102	CDL	C80-C79-C78	2.36	126.41	114.42
26	N	601	CDL	CA6-OA8-CA7	2.36	125.86	117.12
21	L	101	TGL	C22-C21-C20	-2.36	102.46	114.42
26	T	102	CDL	OB8-CB7-C71	2.34	119.26	111.91
19	N	609	PGV	O01-C02-C01	-2.34	99.92	108.40
21	Y	101	TGL	CB4-CB3-CB2	2.34	121.59	113.19
14	A	602[A]	HEA	C26-C15-C16	2.34	119.20	115.27
27	T	101	PEK	C3-C2-C1	-2.33	105.13	113.62
26	C	305	CDL	C42-C41-C40	2.33	126.24	114.42
19	C	304	PGV	O14-P-O13	2.32	123.73	112.24
24	P	309	DMU	C6-C1-C2	2.32	114.84	110.00
27	P	307	PEK	C23-C22-C21	2.32	122.07	113.62
22	C	301	CHD	C22-C23-C24	-2.32	106.35	112.51
19	C	304	PGV	C22-C21-C20	-2.32	104.86	113.19
14	N	603[A]	HEA	C1D-ND-C4D	-2.32	102.68	105.07
22	W	101	CHD	C5-C6-C7	2.31	117.02	114.46
19	P	303	PGV	C27-C26-C25	-2.31	102.68	114.42
19	C	308	PGV	O02-C1-C2	-2.31	114.72	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	310	DMU	O55-C2-C1	2.31	115.69	110.35
22	P	305	CHD	C19-C10-C5	2.30	114.27	110.36
19	A	608	PGV	C34-C33-C32	-2.30	96.00	113.42
19	Z	101	PGV	C6-C5-C4	-2.30	102.77	114.42
22	W	101	CHD	C9-C11-C12	2.30	117.33	114.30
19	U	101	PGV	O03-C01-C02	2.29	115.11	108.43
22	B	302	CHD	O3-C3-C4	-2.29	105.29	109.85
22	P	305	CHD	C6-C5-C4	-2.29	108.56	111.19
22	P	301	CHD	C9-C11-C12	-2.28	111.28	114.30
22	G	102	CHD	C19-C10-C1	-2.28	104.59	108.26
21	L	101	TGL	OC1-CC1-CC2	-2.28	114.84	123.73
14	A	602[A]	HEA	CMC-C2C-C3C	2.28	128.94	124.68
14	A	601	HEA	C3B-C4B-NB	-2.27	107.15	109.84
27	C	309	PEK	O03-C21-O04	-2.27	117.86	123.59
14	N	603[A]	HEA	C20-C19-C18	-2.27	116.53	121.12
27	G	101	PEK	O11-P-O14	-2.27	100.21	109.07
22	B	302	CHD	C9-C11-C12	-2.27	111.31	114.30
26	C	305	CDL	C43-C42-C41	2.27	125.92	114.42
22	P	305	CHD	O25-C24-C23	-2.26	115.81	123.08
26	P	304	CDL	OA8-CA6-CA4	2.26	115.02	108.43
22	C	301	CHD	C14-C13-C12	-2.26	105.30	107.40
26	P	304	CDL	C72-C71-CB7	2.26	121.84	113.62
21	L	101	TGL	CG3-OG3-CC1	2.25	125.46	117.12
21	L	101	TGL	C20-CA9-CA8	-2.25	103.00	114.42
21	B	301	TGL	OG2-CB1-OB1	-2.25	118.27	123.70
14	A	602[A]	HEA	C27-C19-C20	2.25	119.05	115.27
21	B	301	TGL	CG1-OG1-CA1	2.25	125.44	117.12
26	N	601	CDL	OA6-CA5-OA7	-2.25	118.28	123.70
22	J	101	CHD	C21-C20-C22	2.24	113.88	110.36
27	T	101	PEK	C24-C23-C22	-2.24	105.15	113.19
26	P	304	CDL	CB6-OB8-CB7	2.23	125.39	117.12
24	P	306	DMU	O1-C9-C11	2.23	111.99	106.44
14	N	603[B]	HEA	CHB-C1B-C2B	2.23	128.46	124.98
20	A	614	EDO	O1-C1-C2	-2.23	95.87	111.91
24	C	311	DMU	C1-C2-C3	2.23	114.77	109.68
24	M	101	DMU	O49-C1-C6	-2.22	104.66	110.05
26	C	305	CDL	OA8-CA6-CA4	2.22	114.89	108.43
14	N	603[B]	HEA	C3D-C4D-ND	2.21	112.50	110.36
24	C	310	DMU	O49-C1-C6	2.21	115.42	110.05
24	C	310	DMU	C8-C7-C5	-2.21	106.97	110.82
19	C	308	PGV	C21-C20-C19	2.20	121.64	113.62
21	L	101	TGL	OG2-CB1-OB1	-2.20	118.38	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	301	CHD	C11-C9-C10	-2.20	111.46	113.73
22	P	301	CHD	C1-C2-C3	-2.20	107.65	110.47
26	P	304	CDL	OB2-PB2-OB3	2.19	117.62	109.07
24	M	101	DMU	O61-C57-C4	-2.19	103.78	111.29
14	N	603[A]	HEA	C16-C15-C14	-2.18	116.70	121.12
22	C	301	CHD	C2-C1-C10	2.18	116.52	112.78
24	C	302	DMU	O16-C6-C1	2.18	111.71	108.30
26	C	305	CDL	CA6-CA4-CA3	-2.18	106.63	111.79
19	A	609	PGV	O02-C1-C2	-2.18	115.23	123.73
19	C	308	PGV	C01-O03-C19	2.18	125.19	117.12
27	P	307	PEK	O03-C21-C22	2.18	118.74	111.91
28	O	302	PSC	C02-O01-C1	2.17	123.13	117.79
27	C	307	PEK	O03-C01-C02	2.17	114.75	108.43
24	P	306	DMU	O5-C6-O16	2.16	115.10	109.97
22	W	101	CHD	C14-C8-C9	2.16	112.68	109.71
26	C	305	CDL	OA4-PA1-OA3	2.16	122.92	112.24
14	N	603[B]	HEA	C4A-CHB-C1B	2.16	125.41	122.56
14	A	602[A]	HEA	CAD-C3D-C4D	-2.16	120.89	124.66
22	G	102	CHD	C15-C14-C13	-2.15	101.45	103.55
24	M	101	DMU	O5-C6-C1	2.15	114.89	110.35
26	T	102	CDL	CA6-OA8-CA7	2.15	125.07	117.12
14	N	603[A]	HEA	CHC-C4B-C3B	-2.15	120.27	125.80
27	P	307	PEK	C35-C34-C33	2.15	125.31	114.42
14	N	603[A]	HEA	O1A-CGA-CBA	-2.14	116.19	123.08
26	C	305	CDL	C19-C18-C17	2.14	125.31	114.42
26	P	304	CDL	OB4-PB2-OB5	-2.14	97.80	107.75
19	Z	101	PGV	C3-C2-C1	-2.14	105.84	113.62
21	L	101	TGL	C21-C20-CA9	-2.14	103.56	114.42
21	Y	101	TGL	C24-C23-C22	-2.14	103.57	114.42
22	C	301	CHD	C18-C13-C17	2.13	114.55	111.21
27	P	307	PEK	O01-C1-O02	-2.13	118.55	123.70
24	M	101	DMU	O2-C8-C7	-2.13	105.42	110.35
19	C	308	PGV	O03-C01-C02	2.13	114.63	108.43
24	C	310	DMU	O5-C6-O16	-2.13	104.94	109.97
19	P	303	PGV	C02-O01-C1	2.13	123.03	117.79
26	T	102	CDL	C12-C11-CA5	2.13	121.35	113.62
22	J	101	CHD	C14-C13-C12	2.12	109.38	107.40
27	P	307	PEK	O01-C02-C03	2.12	116.07	108.40
26	P	304	CDL	OA8-CA7-OA9	-2.12	118.25	123.59
27	T	101	PEK	O03-C21-O04	-2.12	118.25	123.59
21	Y	101	TGL	OG1-CA1-CA2	2.12	118.55	111.91
22	B	302	CHD	C19-C10-C1	-2.12	104.85	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	102	CHD	O7-C7-C6	2.12	115.19	109.94
24	M	101	DMU	C10-O1-C9	2.11	117.83	113.69
21	Y	101	TGL	CG1-OG1-CA1	2.11	124.94	117.12
22	W	101	CHD	C16-C17-C20	2.11	115.41	112.15
26	N	601	CDL	C80-C79-C78	2.11	125.12	114.42
24	C	302	DMU	C10-O1-C9	-2.10	109.56	113.69
14	A	601	HEA	CBD-CAD-C3D	-2.10	106.80	112.63
26	P	304	CDL	C42-C41-C40	2.09	125.05	114.42
24	P	308	DMU	O1-C10-C5	2.09	114.78	110.35
21	L	101	TGL	CA8-CA7-CA6	-2.09	103.81	114.42
24	P	306	DMU	C8-C7-C5	2.09	114.47	110.82
14	A	602[A]	HEA	CMB-C2B-C3B	-2.08	126.37	130.34
21	D	201	TGL	CB5-CB4-CB3	2.08	125.00	114.42
21	Y	101	TGL	OG2-CG2-CG3	2.08	115.94	108.40
14	N	603[A]	HEA	CAA-CBA-CGA	-2.08	107.93	113.76
22	B	302	CHD	O26-C24-C23	2.08	120.70	114.03
14	N	602	HEA	C3A-C4A-NA	2.08	114.86	110.94
22	G	102	CHD	C1-C10-C9	2.07	114.61	111.35
26	P	304	CDL	C62-C61-C60	2.07	124.95	114.42
22	B	302	CHD	C22-C20-C17	2.07	114.56	110.28
21	D	201	TGL	CA3-CA2-CA1	2.07	121.15	113.62
14	N	602	HEA	C24-C23-C22	2.07	128.63	122.65
19	Z	101	PGV	C4-C3-C2	-2.06	105.78	113.19
22	C	306	CHD	C16-C17-C13	2.06	105.57	103.55
21	Y	101	TGL	OG3-CC1-OC1	-2.06	118.40	123.59
21	N	610	TGL	CB3-CB2-CB1	-2.06	106.14	113.62
22	J	101	CHD	O26-C24-C23	2.06	120.63	114.03
14	N	603[B]	HEA	CMD-C2D-C1D	2.06	128.17	125.04
26	T	102	CDL	C19-C18-C17	2.05	124.86	114.42
22	P	301	CHD	O3-C3-C2	-2.05	104.93	110.16
24	P	308	DMU	C6-O5-C4	-2.05	109.66	113.69
20	S	103	EDO	O1-C1-C2	-2.05	97.15	111.91
19	A	609	PGV	C01-O03-C19	2.05	124.71	117.12
14	A	601	HEA	C20-C21-C22	-2.04	105.17	111.88
24	P	308	DMU	O5-C4-C57	2.04	111.51	106.44
24	Z	102	DMU	C2-C3-C4	2.04	115.60	110.93
14	A	601	HEA	C20-C19-C18	2.04	125.24	121.12
14	N	602	HEA	C12-C13-C14	2.04	117.61	112.23
19	A	608	PGV	C25-C24-C23	2.03	124.75	114.42
26	N	601	CDL	C79-C78-C77	2.03	124.75	114.42
14	N	603[A]	HEA	C12-C13-C14	-2.03	106.86	112.23
22	G	102	CHD	O26-C24-C23	2.03	120.56	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	101	TGL	C25-C24-C23	-2.03	104.11	114.42
26	P	304	CDL	O1-C1-CB2	2.03	116.67	109.56
19	A	609	PGV	O03-C19-O04	-2.03	118.48	123.59
22	P	305	CHD	C14-C8-C9	-2.03	106.93	109.71
22	G	102	CHD	C9-C10-C5	-2.03	105.73	108.58
24	Z	102	DMU	C34-C31-C28	-2.02	104.14	114.42
14	N	603[B]	HEA	CHB-C1B-NB	-2.02	122.23	124.43
22	B	302	CHD	C5-C4-C3	-2.02	109.79	112.76
24	P	309	DMU	C10-C5-C7	2.02	114.20	110.00
24	P	309	DMU	C18-O16-C6	2.01	117.18	113.84
26	P	304	CDL	C22-C21-C20	2.01	124.64	114.42
24	M	101	DMU	C31-C28-C25	-2.01	104.22	114.42
19	N	609	PGV	O01-C1-C2	2.01	115.83	111.50
14	A	602[B]	HEA	C2D-C1D-ND	2.01	112.22	109.84
22	B	302	CHD	O7-C7-C8	-2.00	104.95	109.43
14	A	601	HEA	C16-C17-C18	-2.00	105.30	111.88
27	T	101	PEK	O13-P-O14	2.00	122.14	112.24
21	Y	101	TGL	CG3-CG2-CG1	-2.00	107.05	111.79

There are no chirality outliers.

All (949) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
19	A	609	PGV	C02-C03-O11-P
19	A	609	PGV	C04-C05-C06-O06
19	A	609	PGV	O02-C1-O01-C02
19	A	609	PGV	C2-C1-O01-C02
19	C	308	PGV	C03-O11-P-O12
19	C	308	PGV	C03-O11-P-O13
19	C	308	PGV	C03-O11-P-O14
19	C	308	PGV	C04-O12-P-O11
19	C	308	PGV	C04-O12-P-O13
19	C	308	PGV	C04-O12-P-O14
19	C	308	PGV	O03-C01-C02-O01
19	U	101	PGV	C02-C03-O11-P
19	Z	101	PGV	C01-C02-O01-C1
19	Z	101	PGV	C02-C03-O11-P
19	Z	101	PGV	C05-C04-O12-P
19	Z	101	PGV	C04-C05-C06-O06
19	Z	101	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	Z	101	PGV	C2-C1-O01-C02
21	D	201	TGL	CG2-CG1-OG1-CA1
21	D	201	TGL	OC1-CC1-OG3-CG3
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	CA2-CA1-OG1-CG1
21	Y	101	TGL	OA1-CA1-OG1-CG1
21	Y	101	TGL	OB1-CB1-OG2-CG2
22	W	101	CHD	C13-C17-C20-C22
24	C	311	DMU	C1-C6-O16-C18
24	C	311	DMU	O5-C6-O16-C18
24	C	311	DMU	C19-C18-O16-C6
24	P	306	DMU	C1-C6-O16-C18
24	P	306	DMU	O5-C6-O16-C18
24	P	309	DMU	O5-C6-O16-C18
26	C	305	CDL	CB2-C1-CA2-OA2
26	C	305	CDL	CA2-OA2-PA1-OA4
26	C	305	CDL	C11-CA5-OA6-CA4
26	C	305	CDL	CB2-OB2-PB2-OB3
26	C	305	CDL	CB2-OB2-PB2-OB4
26	C	305	CDL	CB2-OB2-PB2-OB5
26	C	305	CDL	C51-CB5-OB6-CB4
26	N	601	CDL	CA2-OA2-PA1-OA3
26	N	601	CDL	CA3-OA5-PA1-OA2
26	N	601	CDL	CA3-OA5-PA1-OA3
26	N	601	CDL	C11-CA5-OA6-CA4
26	N	601	CDL	CB2-OB2-PB2-OB3
26	N	601	CDL	CB2-OB2-PB2-OB4
26	N	601	CDL	CB2-OB2-PB2-OB5
26	N	601	CDL	CB3-OB5-PB2-OB2
26	N	601	CDL	CB3-OB5-PB2-OB3
26	N	601	CDL	CB3-OB5-PB2-OB4
26	N	601	CDL	OB6-CB4-CB6-OB8
26	P	304	CDL	CB2-C1-CA2-OA2
26	P	304	CDL	CA2-OA2-PA1-OA4
26	P	304	CDL	CA3-OA5-PA1-OA3
26	P	304	CDL	CB2-OB2-PB2-OB3
26	P	304	CDL	CB2-OB2-PB2-OB4
26	P	304	CDL	CB2-OB2-PB2-OB5
26	P	304	CDL	C51-CB5-OB6-CB4
26	T	102	CDL	OA6-CA4-CA6-OA8
26	T	102	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	CB2-OB2-PB2-OB3
26	T	102	CDL	CB2-OB2-PB2-OB5
26	T	102	CDL	CB3-OB5-PB2-OB3
27	C	307	PEK	C04-O12-P-O11
27	C	307	PEK	O12-C04-C05-N
27	C	307	PEK	O02-C1-O01-C02
27	C	307	PEK	C2-C1-O01-C02
27	C	307	PEK	C4-C5-C6-C7
27	C	307	PEK	C11-C12-C13-C14
27	C	309	PEK	C04-O12-P-O14
27	C	309	PEK	O03-C01-C02-O01
27	C	309	PEK	O12-C04-C05-N
27	G	101	PEK	C10-C11-C12-C13
27	G	103	PEK	C03-O11-P-O14
27	G	103	PEK	C2-C1-O01-C02
27	G	103	PEK	C12-C13-C14-C15
27	P	307	PEK	C03-O11-P-O14
27	P	307	PEK	O02-C1-O01-C02
27	P	307	PEK	C2-C1-O01-C02
27	T	101	PEK	C10-C11-C12-C13
27	T	101	PEK	C12-C13-C14-C15
28	E	201	PSC	C03-O11-P-O14
28	E	201	PSC	C04-O12-P-O14
28	E	201	PSC	O12-C04-C05-N
28	O	302	PSC	C03-O11-P-O12
28	O	302	PSC	C04-O12-P-O14
19	A	609	PGV	O04-C19-O03-C01
19	Z	101	PGV	O04-C19-O03-C01
28	O	302	PSC	O04-C19-O03-C01
24	C	310	DMU	C5-C10-O7-C3
24	P	308	DMU	C5-C10-O7-C3
19	A	609	PGV	C20-C19-O03-C01
19	Z	101	PGV	C20-C19-O03-C01
21	D	201	TGL	OA1-CA1-OG1-CG1
28	E	201	PSC	O04-C19-O03-C01
22	W	101	CHD	C16-C17-C20-C22
21	B	301	TGL	OB1-CB1-OG2-CG2
26	C	305	CDL	OA7-CA5-OA6-CA4
26	C	305	CDL	OB7-CB5-OB6-CB4
26	N	601	CDL	OA7-CA5-OA6-CA4
26	P	304	CDL	OA7-CA5-OA6-CA4
26	P	304	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CC2-CC1-OG3-CG3
28	E	201	PSC	C20-C19-O03-C01
28	O	302	PSC	C20-C19-O03-C01
21	Y	101	TGL	CB2-CB1-OG2-CG2
26	P	304	CDL	C11-CA5-OA6-CA4
26	T	102	CDL	C11-CA5-OA6-CA4
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
21	Y	101	TGL	CC3-CC4-CC5-CC6
21	B	301	TGL	CC2-CC1-OG3-CG3
21	D	201	TGL	CA2-CA1-OG1-CG1
21	Q	201	TGL	CC2-CC1-OG3-CG3
19	C	304	PGV	C10-C11-C12-C13
27	C	307	PEK	C7-C8-C9-C10
27	G	101	PEK	C7-C8-C9-C10
27	G	101	PEK	C13-C14-C15-C16
27	G	103	PEK	C7-C8-C9-C10
27	P	307	PEK	C13-C14-C15-C16
27	T	101	PEK	C4-C5-C6-C7
21	L	101	TGL	CA9-C20-C21-C22
26	T	102	CDL	C79-C80-C81-C82
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
27	G	103	PEK	O02-C1-O01-C02
21	B	301	TGL	OC1-CC1-OG3-CG3
24	C	302	DMU	O6-C11-C9-O1
24	C	311	DMU	O5-C4-C57-O61
24	P	308	DMU	O6-C11-C9-O1
21	Y	101	TGL	CA2-CA3-CA4-CA5
24	C	302	DMU	C19-C22-C25-C28
24	M	101	DMU	C28-C31-C34-C37
26	T	102	CDL	C42-C43-C44-C45
27	P	307	PEK	C33-C34-C35-C36
21	D	201	TGL	C21-C22-C23-C24
26	N	601	CDL	C81-C82-C83-C84
26	P	304	CDL	C41-C42-C43-C44
26	P	304	CDL	C53-C54-C55-C56
26	P	304	CDL	C81-C82-C83-C84
26	T	102	CDL	C61-C62-C63-C64
27	G	103	PEK	C28-C29-C30-C31
24	P	309	DMU	O6-C11-C9-C8
21	Q	201	TGL	CC1-CC2-CC3-CC4
28	E	201	PSC	C19-C20-C21-C22
19	A	609	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
19	C	308	PGV	C02-C03-O11-P
21	D	201	TGL	C16-C17-C18-C19
19	C	308	PGV	C2-C3-C4-C5
26	C	305	CDL	C76-C77-C78-C79
21	Y	101	TGL	CC1-CC2-CC3-CC4
24	C	302	DMU	O6-C11-C9-C8
22	C	306	CHD	C17-C20-C22-C23
22	P	305	CHD	C17-C20-C22-C23
21	Q	201	TGL	OC1-CC1-OG3-CG3
26	N	601	CDL	OA9-CA7-OA8-CA6
26	P	304	CDL	OB9-CB7-OB8-CB6
24	P	308	DMU	O6-C11-C9-C8
19	A	609	PGV	O12-C04-C05-C06
24	P	309	DMU	O6-C11-C9-O1
26	C	305	CDL	CA2-C1-CB2-OB2
21	N	610	TGL	OC1-CC1-OG3-CG3
28	E	201	PSC	C21-C22-C23-C24
28	E	201	PSC	C30-C31-C32-C33
21	N	610	TGL	CC2-CC1-OG3-CG3
26	N	601	CDL	C31-CA7-OA8-CA6
26	P	304	CDL	C71-CB7-OB8-CB6
24	C	311	DMU	C3-C4-C57-O61
21	B	301	TGL	CA2-CA3-CA4-CA5
21	N	610	TGL	C20-C21-C22-C23
26	N	601	CDL	C61-C62-C63-C64
26	P	304	CDL	C42-C43-C44-C45
19	A	608	PGV	C26-C27-C28-C29
24	P	309	DMU	C1-C6-O16-C18
19	U	101	PGV	O03-C01-C02-O01
22	W	101	CHD	C16-C17-C20-C21
22	J	101	CHD	C13-C17-C20-C21
21	B	301	TGL	CB2-CB1-OG2-CG2
26	T	102	CDL	C51-CB5-OB6-CB4
22	J	101	CHD	C13-C17-C20-C22
21	D	201	TGL	CA1-CA2-CA3-CA4
26	C	305	CDL	CA7-C31-C32-C33
26	N	601	CDL	CA5-C11-C12-C13
27	T	101	PEK	C1-C2-C3-C4
19	C	308	PGV	C10-C11-C12-C13
27	T	101	PEK	C13-C14-C15-C16
19	A	609	PGV	C20-C21-C22-C23
21	B	301	TGL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	O	302	PSC	C20-C21-C22-C23
21	D	201	TGL	CB1-CB2-CB3-CB4
26	C	305	CDL	CB7-C71-C72-C73
26	P	304	CDL	CB5-C51-C52-C53
27	G	103	PEK	C21-C22-C23-C24
27	P	307	PEK	C21-C22-C23-C24
26	T	102	CDL	OB7-CB5-OB6-CB4
22	P	305	CHD	C21-C20-C22-C23
24	P	309	DMU	O16-C18-C19-C22
19	C	308	PGV	C1-C2-C3-C4
21	B	301	TGL	CA1-CA2-CA3-CA4
21	B	301	TGL	CB1-CB2-CB3-CB4
21	L	101	TGL	CC1-CC2-CC3-CC4
20	L	102	EDO	O1-C1-C2-O2
22	W	101	CHD	C13-C17-C20-C21
22	C	306	CHD	C21-C20-C22-C23
21	N	610	TGL	CA1-CA2-CA3-CA4
24	Z	102	DMU	O16-C18-C19-C22
26	C	305	CDL	O1-C1-CA2-OA2
26	C	305	CDL	O1-C1-CB2-OB2
26	N	601	CDL	O1-C1-CB2-OB2
26	P	304	CDL	O1-C1-CA2-OA2
26	P	304	CDL	O1-C1-CB2-OB2
24	P	309	DMU	C4-C3-O7-C10
28	O	302	PSC	C2-C1-O01-C02
19	A	609	PGV	C03-O11-P-O12
19	U	101	PGV	C03-O11-P-O12
26	C	305	CDL	CA2-OA2-PA1-OA5
26	C	305	CDL	CA3-OA5-PA1-OA2
26	P	304	CDL	CA2-OA2-PA1-OA5
26	P	304	CDL	CA3-OA5-PA1-OA2
26	T	102	CDL	CA3-OA5-PA1-OA2
27	C	309	PEK	C03-O11-P-O12
27	C	309	PEK	C04-O12-P-O11
27	G	103	PEK	C03-O11-P-O12
27	G	103	PEK	C04-O12-P-O11
27	P	307	PEK	C04-O12-P-O11
26	N	601	CDL	C58-C59-C60-C61
21	L	101	TGL	CA2-CA1-OG1-CG1
21	N	610	TGL	CA2-CA1-OG1-CG1
26	T	102	CDL	C31-CA7-OA8-CA6
22	J	101	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
19	Z	101	PGV	C19-C20-C21-C22
26	N	601	CDL	CA2-C1-CB2-OB2
26	P	304	CDL	CA2-C1-CB2-OB2
21	N	610	TGL	OB1-CB1-OG2-CG2
28	O	302	PSC	O02-C1-O01-C02
19	U	101	PGV	C2-C3-C4-C5
26	N	601	CDL	C78-C79-C80-C81
19	U	101	PGV	C1-C2-C3-C4
21	N	610	TGL	C19-C33-C34-C35
26	N	601	CDL	C14-C15-C16-C17
26	P	304	CDL	C61-C62-C63-C64
21	N	610	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	C21-C22-C23-C24
21	N	610	TGL	CA5-CA6-CA7-CA8
21	N	610	TGL	C21-C20-CA9-CA8
21	N	610	TGL	C11-C10-CB9-CB8
21	N	610	TGL	CC4-CC5-CC6-CC7
21	Q	201	TGL	CB4-CB5-CB6-CB7
21	Y	101	TGL	CA9-C20-C21-C22
26	P	304	CDL	C14-C15-C16-C17
26	P	304	CDL	C17-C18-C19-C20
26	T	102	CDL	C71-CB7-OB8-CB6
21	D	201	TGL	C15-C16-C17-C18
21	Q	201	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CB3-CB4-CB5-CB6
21	Y	101	TGL	CB6-CB7-CB8-CB9
21	Y	101	TGL	CC4-CC5-CC6-CC7
24	C	302	DMU	O16-C18-C19-C22
26	N	601	CDL	C22-C23-C24-C25
26	P	304	CDL	C82-C83-C84-C85
27	G	103	PEK	C31-C32-C33-C34
28	E	201	PSC	C24-C25-C26-C27
28	O	302	PSC	C01-C02-O01-C1
19	Z	101	PGV	C3-C4-C5-C6
21	B	301	TGL	C10-C11-C12-C13
21	B	301	TGL	C16-C15-CC9-CC8
26	C	305	CDL	C18-C19-C20-C21
26	C	305	CDL	C56-C57-C58-C59
26	N	601	CDL	C32-C33-C34-C35
27	T	101	PEK	C26-C27-C28-C29
28	E	201	PSC	C23-C24-C25-C26
19	A	609	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	C	309	PEK	C13-C14-C15-C16
19	A	609	PGV	C14-C15-C16-C17
19	Z	101	PGV	C28-C29-C30-C31
21	Y	101	TGL	CB5-CB6-CB7-CB8
26	N	601	CDL	C13-C14-C15-C16
26	N	601	CDL	C35-C36-C37-C38
19	Z	101	PGV	C29-C30-C31-C32
26	C	305	CDL	C52-C53-C54-C55
28	O	302	PSC	C5-C6-C7-C8
24	C	302	DMU	C1-C6-O16-C18
26	P	304	CDL	C57-C58-C59-C60
21	B	301	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	C21-C22-C23-C24
21	L	101	TGL	CC6-CC7-CC8-CC9
24	P	309	DMU	C2-C3-O7-C10
27	G	103	PEK	C29-C30-C31-C32
21	B	301	TGL	C14-C29-C30-C31
21	L	101	TGL	CA3-CA4-CA5-CA6
21	N	610	TGL	CB9-C10-C11-C12
26	P	304	CDL	C31-C32-C33-C34
26	P	304	CDL	C39-C40-C41-C42
26	T	102	CDL	OA9-CA7-OA8-CA6
21	Q	201	TGL	C10-C11-C12-C13
24	P	309	DMU	C22-C25-C28-C31
26	N	601	CDL	C60-C61-C62-C63
26	T	102	CDL	C14-C15-C16-C17
27	G	101	PEK	C34-C35-C36-C37
27	G	103	PEK	C34-C35-C36-C37
28	E	201	PSC	C25-C26-C27-C28
19	C	308	PGV	C04-C05-C06-O06
19	U	101	PGV	C04-C05-C06-O06
28	E	201	PSC	O02-C1-O01-C02
28	E	201	PSC	C2-C1-O01-C02
19	C	304	PGV	C27-C28-C29-C30
21	Q	201	TGL	CA6-CA7-CA8-CA9
21	Q	201	TGL	C17-C18-C19-C33
21	Q	201	TGL	C19-C33-C34-C35
26	P	304	CDL	C77-C78-C79-C80
26	T	102	CDL	C13-C14-C15-C16
26	T	102	CDL	C41-C42-C43-C44
27	C	307	PEK	C15-C16-C17-C18
19	U	101	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	CC2-CC3-CC4-CC5
21	L	101	TGL	CC4-CC5-CC6-CC7
21	L	101	TGL	C16-C17-C18-C19
21	N	610	TGL	CC5-CC6-CC7-CC8
21	Q	201	TGL	CC9-C15-C16-C17
21	Y	101	TGL	CC6-CC7-CC8-CC9
26	P	304	CDL	C20-C21-C22-C23
26	P	304	CDL	C80-C81-C82-C83
26	T	102	CDL	C34-C35-C36-C37
26	T	102	CDL	C74-C75-C76-C77
26	T	102	CDL	C82-C83-C84-C85
28	O	302	PSC	C29-C30-C31-C32
21	B	301	TGL	C21-C20-CA9-CA8
21	N	610	TGL	C14-C29-C30-C31
26	C	305	CDL	C71-C72-C73-C74
27	G	101	PEK	C23-C24-C25-C26
27	P	307	PEK	C32-C33-C34-C35
19	A	608	PGV	C28-C29-C30-C31
19	C	304	PGV	C7-C8-C9-C10
19	C	308	PGV	C27-C28-C29-C30
19	P	303	PGV	C30-C31-C32-C33
19	U	101	PGV	C26-C27-C28-C29
19	Z	101	PGV	C30-C31-C32-C33
21	L	101	TGL	CC7-CC8-CC9-C15
21	N	610	TGL	C13-C14-C29-C30
26	T	102	CDL	C73-C74-C75-C76
27	G	103	PEK	C32-C33-C34-C35
21	N	610	TGL	OA1-CA1-OG1-CG1
26	N	601	CDL	C11-C12-C13-C14
26	N	601	CDL	C63-C64-C65-C66
26	P	304	CDL	C40-C41-C42-C43
26	T	102	CDL	C23-C24-C25-C26
27	C	307	PEK	C25-C26-C27-C28
28	O	302	PSC	C14-C15-C16-C17
21	B	301	TGL	C16-C17-C18-C19
26	N	601	CDL	C79-C80-C81-C82
21	N	610	TGL	CB7-CB8-CB9-C10
21	Y	101	TGL	C24-C25-C26-C27
27	G	101	PEK	C26-C27-C28-C29
27	T	101	PEK	C30-C31-C32-C33
21	L	101	TGL	OA1-CA1-OG1-CG1
19	P	303	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
19	P	303	PGV	C24-C25-C26-C27
21	B	301	TGL	CC4-CC5-CC6-CC7
21	L	101	TGL	CB2-CB3-CB4-CB5
21	Y	101	TGL	C18-C19-C33-C34
24	M	101	DMU	C19-C22-C25-C28
27	C	309	PEK	C27-C28-C29-C30
19	A	609	PGV	C19-C20-C21-C22
24	C	311	DMU	C18-C19-C22-C25
21	Q	201	TGL	CB5-CB6-CB7-CB8
26	T	102	CDL	OB9-CB7-OB8-CB6
26	C	305	CDL	C71-CB7-OB8-CB6
21	N	610	TGL	CA4-CA5-CA6-CA7
21	N	610	TGL	C21-C22-C23-C24
24	P	308	DMU	C19-C22-C25-C28
26	N	601	CDL	C72-C73-C74-C75
19	Z	101	PGV	C27-C28-C29-C30
21	B	301	TGL	CB4-CB5-CB6-CB7
21	Y	101	TGL	CA3-CA4-CA5-CA6
21	Y	101	TGL	C20-C21-C22-C23
24	C	310	DMU	C31-C34-C37-C40
28	O	302	PSC	C2-C3-C4-C5
27	P	307	PEK	C2-C3-C4-C5
27	T	101	PEK	C15-C16-C17-C18
26	N	601	CDL	C59-C60-C61-C62
21	N	610	TGL	CB6-CB7-CB8-CB9
26	N	601	CDL	C53-C54-C55-C56
19	U	101	PGV	C22-C23-C24-C25
21	D	201	TGL	C21-C20-CA9-CA8
21	L	101	TGL	C11-C12-C13-C14
24	P	308	DMU	C28-C31-C34-C37
26	C	305	CDL	C36-C37-C38-C39
28	O	302	PSC	C30-C31-C32-C33
20	A	615	EDO	O1-C1-C2-O2
20	A	617	EDO	O1-C1-C2-O2
20	N	617	EDO	O1-C1-C2-O2
26	P	304	CDL	C16-C17-C18-C19
28	E	201	PSC	C2-C3-C4-C5
21	Q	201	TGL	CB9-C10-C11-C12
21	Y	101	TGL	C10-C11-C12-C13
24	C	311	DMU	C31-C34-C37-C40
27	G	103	PEK	C24-C25-C26-C27
21	B	301	TGL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CC7-CC8-CC9-C15
21	Y	101	TGL	C11-C12-C13-C14
26	T	102	CDL	C58-C59-C60-C61
27	C	309	PEK	C10-C11-C12-C13
21	Q	201	TGL	C22-C23-C24-C25
27	T	101	PEK	C2-C3-C4-C5
21	L	101	TGL	CB1-CB2-CB3-CB4
26	N	601	CDL	C56-C57-C58-C59
26	C	305	CDL	C17-C18-C19-C20
26	N	601	CDL	C34-C35-C36-C37
27	G	101	PEK	C25-C26-C27-C28
19	U	101	PGV	C19-C20-C21-C22
24	Z	102	DMU	C28-C31-C34-C37
26	P	304	CDL	C15-C16-C17-C18
21	Y	101	TGL	CA1-CA2-CA3-CA4
27	P	307	PEK	O01-C02-C03-O11
19	U	101	PGV	C6-C7-C8-C9
26	N	601	CDL	C20-C21-C22-C23
19	C	304	PGV	C13-C14-C15-C16
21	L	101	TGL	CA6-CA7-CA8-CA9
27	C	309	PEK	C24-C25-C26-C27
26	N	601	CDL	OA6-CA4-CA6-OA8
26	N	601	CDL	C18-C19-C20-C21
21	N	610	TGL	C16-C15-CC9-CC8
26	P	304	CDL	C60-C61-C62-C63
27	C	309	PEK	C25-C26-C27-C28
27	C	309	PEK	C31-C32-C33-C34
19	P	303	PGV	C12-C13-C14-C15
19	Z	101	PGV	C11-C10-C9-C8
27	C	307	PEK	C2-C3-C4-C5
28	O	302	PSC	C13-C14-C15-C16
26	T	102	CDL	C20-C21-C22-C23
19	U	101	PGV	C30-C31-C32-C33
26	C	305	CDL	C77-C78-C79-C80
26	C	305	CDL	OB9-CB7-OB8-CB6
19	U	101	PGV	C13-C14-C15-C16
21	Y	101	TGL	C15-C16-C17-C18
24	Z	102	DMU	C25-C28-C31-C34
26	N	601	CDL	CA2-OA2-PA1-OA5
27	P	307	PEK	C03-O11-P-O12
21	Y	101	TGL	C16-C17-C18-C19
26	C	305	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	CB5-C51-C52-C53
26	C	305	CDL	CA4-CA3-OA5-PA1
26	C	305	CDL	OA5-CA3-CA4-CA6
27	C	309	PEK	C01-C02-C03-O11
21	N	610	TGL	CB1-CB2-CB3-CB4
28	E	201	PSC	C1-C2-C3-C4
21	Q	201	TGL	CB2-CB3-CB4-CB5
26	T	102	CDL	C36-C37-C38-C39
19	Z	101	PGV	C12-C13-C14-C15
27	C	307	PEK	C24-C25-C26-C27
21	Y	101	TGL	C13-C14-C29-C30
24	C	311	DMU	O16-C18-C19-C22
26	N	601	CDL	C19-C20-C21-C22
22	J	101	CHD	C21-C20-C22-C23
19	Z	101	PGV	C20-C21-C22-C23
21	Y	101	TGL	C12-C13-C14-C29
26	T	102	CDL	C75-C76-C77-C78
21	Q	201	TGL	CB2-CB1-OG2-CG2
27	T	101	PEK	C2-C1-O01-C02
21	Q	201	TGL	CC6-CC7-CC8-CC9
21	Y	101	TGL	C21-C20-CA9-CA8
27	C	307	PEK	C26-C27-C28-C29
28	E	201	PSC	C5-C6-C7-C8
19	U	101	PGV	O03-C01-C02-C03
19	Z	101	PGV	O03-C01-C02-C03
21	B	301	TGL	OG1-CG1-CG2-CG3
21	D	201	TGL	OG1-CG1-CG2-CG3
21	L	101	TGL	OG1-CG1-CG2-CG3
21	Q	201	TGL	C20-C21-C22-C23
26	C	305	CDL	CA3-CA4-CA6-OA8
26	C	305	CDL	CB3-CB4-CB6-OB8
26	N	601	CDL	CA3-CA4-CA6-OA8
26	T	102	CDL	CA3-CA4-CA6-OA8
26	T	102	CDL	CB3-CB4-CB6-OB8
28	E	201	PSC	O03-C01-C02-C03
28	O	302	PSC	O03-C01-C02-C03
26	C	305	CDL	C40-C41-C42-C43
27	C	307	PEK	C28-C29-C30-C31
27	C	307	PEK	C1-C2-C3-C4
19	A	609	PGV	C29-C30-C31-C32
21	D	201	TGL	C10-C11-C12-C13
28	O	302	PSC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	C12-C13-C14-C29
21	D	201	TGL	CC6-CC7-CC8-CC9
27	C	307	PEK	C35-C36-C37-C38
21	D	201	TGL	OG2-CB1-CB2-CB3
19	A	608	PGV	C31-C32-C33-C34
26	P	304	CDL	C19-C20-C21-C22
26	T	102	CDL	C24-C25-C26-C27
27	C	307	PEK	C17-C18-C19-C20
27	G	103	PEK	C25-C26-C27-C28
27	P	307	PEK	C35-C36-C37-C38
26	N	601	CDL	C44-C45-C46-C47
26	N	601	CDL	C77-C78-C79-C80
27	G	101	PEK	C33-C34-C35-C36
19	U	101	PGV	O05-C05-C06-O06
21	B	301	TGL	C25-C26-C27-C28
28	O	302	PSC	C6-C7-C8-C9
19	C	304	PGV	C15-C16-C17-C18
26	C	305	CDL	C84-C85-C86-C87
26	T	102	CDL	C32-C33-C34-C35
26	T	102	CDL	C64-C65-C66-C67
26	T	102	CDL	C52-C53-C54-C55
26	C	305	CDL	C24-C25-C26-C27
21	D	201	TGL	C19-C33-C34-C35
26	C	305	CDL	C64-C65-C66-C67
26	P	304	CDL	C18-C19-C20-C21
22	C	306	CHD	C20-C22-C23-C24
21	Y	101	TGL	C29-C30-C31-C32
21	B	301	TGL	C17-C18-C19-C33
26	T	102	CDL	C81-C82-C83-C84
19	P	303	PGV	C11-C12-C13-C14
21	B	301	TGL	CA9-C20-C21-C22
21	Y	101	TGL	CC9-C15-C16-C17
27	C	307	PEK	O01-C02-C03-O11
27	G	103	PEK	O01-C02-C03-O11
27	G	101	PEK	C24-C25-C26-C27
20	A	610	EDO	O1-C1-C2-O2
19	A	609	PGV	O12-C04-C05-O05
19	C	304	PGV	C20-C21-C22-C23
19	U	101	PGV	C12-C13-C14-C15
21	D	201	TGL	OG2-CG2-CG3-OG3
26	T	102	CDL	OB6-CB4-CB6-OB8
26	N	601	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	C33-C34-C35-C36
26	T	102	CDL	C62-C63-C64-C65
27	C	307	PEK	C34-C35-C36-C37
21	Y	101	TGL	C21-C22-C23-C24
19	A	608	PGV	C23-C24-C25-C26
19	P	303	PGV	C1-C2-C3-C4
26	N	601	CDL	C51-CB5-OB6-CB4
21	L	101	TGL	C24-C25-C26-C27
21	N	610	TGL	C24-C25-C26-C27
21	Y	101	TGL	C14-C29-C30-C31
19	C	304	PGV	C14-C15-C16-C17
21	Y	101	TGL	C22-C23-C24-C25
26	N	601	CDL	C41-C42-C43-C44
19	C	308	PGV	C01-C02-C03-O11
19	Z	101	PGV	C01-C02-C03-O11
26	P	304	CDL	OA5-CA3-CA4-CA6
27	P	307	PEK	C01-C02-C03-O11
28	E	201	PSC	C01-C02-C03-O11
19	N	609	PGV	C23-C24-C25-C26
21	N	610	TGL	C25-C26-C27-C28
19	C	304	PGV	C22-C23-C24-C25
26	C	305	CDL	C51-C52-C53-C54
19	C	308	PGV	C24-C25-C26-C27
21	B	301	TGL	C20-C21-C22-C23
21	L	101	TGL	C11-C10-CB9-CB8
19	C	304	PGV	C25-C26-C27-C28
24	C	311	DMU	C34-C37-C40-C43
21	L	101	TGL	C22-C23-C24-C25
21	Q	201	TGL	C13-C14-C29-C30
24	C	310	DMU	C19-C22-C25-C28
21	D	201	TGL	CC2-CC3-CC4-CC5
27	C	309	PEK	O03-C01-C02-C03
21	L	101	TGL	CB5-CB6-CB7-CB8
21	Y	101	TGL	C25-C26-C27-C28
28	E	201	PSC	C3-C4-C5-C6
27	C	309	PEK	C4-C5-C6-C7
21	L	101	TGL	C19-C33-C34-C35
21	Q	201	TGL	C21-C20-CA9-CA8
21	L	101	TGL	C13-C14-C29-C30
21	Q	201	TGL	C12-C13-C14-C29
27	T	101	PEK	C16-C17-C18-C19
19	U	101	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	P	304	CDL	C51-C52-C53-C54
26	P	304	CDL	CB3-OB5-PB2-OB2
27	C	307	PEK	C5-C6-C7-C8
27	C	307	PEK	C6-C7-C8-C9
27	C	307	PEK	C11-C10-C9-C8
27	C	309	PEK	C11-C10-C9-C8
27	C	309	PEK	C9-C10-C11-C12
27	C	309	PEK	C12-C13-C14-C15
27	G	101	PEK	C6-C7-C8-C9
27	G	101	PEK	C9-C10-C11-C12
27	G	103	PEK	C6-C7-C8-C9
27	P	307	PEK	C9-C10-C11-C12
27	P	307	PEK	C12-C13-C14-C15
27	T	101	PEK	C9-C10-C11-C12
28	E	201	PSC	C9-C10-C11-C12
28	E	201	PSC	C10-C11-C12-C13
19	C	308	PGV	C6-C7-C8-C9
26	P	304	CDL	OA5-CA3-CA4-OA6
22	C	306	CHD	C16-C17-C20-C22
21	B	301	TGL	C29-C30-C31-C32
24	P	309	DMU	C34-C37-C40-C43
26	N	601	CDL	C64-C65-C66-C67
21	Q	201	TGL	C29-C30-C31-C32
27	G	103	PEK	O03-C01-C02-O01
28	E	201	PSC	O03-C01-C02-O01
28	O	302	PSC	O03-C01-C02-O01
24	P	309	DMU	C19-C22-C25-C28
19	C	308	PGV	C14-C15-C16-C17
21	Q	201	TGL	OB1-CB1-OG2-CG2
28	O	302	PSC	C31-C32-C33-C34
28	E	201	PSC	C4-C5-C6-C7
19	P	303	PGV	C02-C03-O11-P
26	C	305	CDL	C1-CA2-OA2-PA1
28	O	302	PSC	C02-C03-O11-P
21	D	201	TGL	C16-C15-CC9-CC8
26	P	304	CDL	C83-C84-C85-C86
26	T	102	CDL	C33-C34-C35-C36
27	G	101	PEK	C28-C29-C30-C31
21	L	101	TGL	OG1-CA1-CA2-CA3
20	B	305	EDO	O1-C1-C2-O2
21	L	101	TGL	C15-C16-C17-C18
21	B	301	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
19	C	304	PGV	C1-C2-C3-C4
21	D	201	TGL	C20-C21-C22-C23
19	N	609	PGV	C31-C32-C33-C34
21	L	101	TGL	C29-C30-C31-C32
21	L	101	TGL	CA2-CA3-CA4-CA5
21	D	201	TGL	CC7-CC8-CC9-C15
26	C	305	CDL	C55-C56-C57-C58
26	T	102	CDL	C31-C32-C33-C34
26	T	102	CDL	OB5-CB3-CB4-CB6
21	N	610	TGL	CA9-C20-C21-C22
24	P	309	DMU	C31-C34-C37-C40
26	C	305	CDL	C35-C36-C37-C38
27	C	309	PEK	C15-C16-C17-C18
19	P	303	PGV	C22-C23-C24-C25
26	C	305	CDL	C62-C63-C64-C65
21	D	201	TGL	CC5-CC6-CC7-CC8
27	P	307	PEK	C26-C27-C28-C29
26	C	305	CDL	C22-C23-C24-C25
26	C	305	CDL	C59-C60-C61-C62
21	D	201	TGL	CG3-CG2-OG2-CB1
27	G	103	PEK	C01-C02-O01-C1
24	M	101	DMU	O6-C11-C9-C8
21	D	201	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	C11-C10-CB9-CB8
19	C	308	PGV	O03-C01-C02-C03
21	Y	101	TGL	OG1-CG1-CG2-CG3
21	Y	101	TGL	CG1-CG2-CG3-OG3
26	N	601	CDL	CB3-CB4-CB6-OB8
26	P	304	CDL	CA3-CA4-CA6-OA8
27	G	103	PEK	O03-C01-C02-C03
26	C	305	CDL	C82-C83-C84-C85
27	G	101	PEK	C4-C5-C6-C7
26	T	102	CDL	C53-C54-C55-C56
27	T	101	PEK	C17-C18-C19-C20
19	U	101	PGV	C31-C32-C33-C34
21	B	301	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	OA6-CA4-CA6-OA8
26	C	305	CDL	OB6-CB4-CB6-OB8
21	B	301	TGL	OA1-CA1-OG1-CG1
21	L	101	TGL	C25-C26-C27-C28
27	G	101	PEK	C35-C36-C37-C38
19	Z	101	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	CB4-CB5-CB6-CB7
24	C	310	DMU	C34-C37-C40-C43
24	Z	102	DMU	C22-C25-C28-C31
27	C	307	PEK	C29-C30-C31-C32
19	A	609	PGV	C22-C23-C24-C25
21	B	301	TGL	C11-C12-C13-C14
21	L	101	TGL	C10-C11-C12-C13
27	C	307	PEK	C22-C23-C24-C25
26	P	304	CDL	C56-C57-C58-C59
21	D	201	TGL	C11-C12-C13-C14
21	D	201	TGL	CB2-CB1-OG2-CG2
24	C	302	DMU	C25-C28-C31-C34
21	L	101	TGL	CC9-C15-C16-C17
26	C	305	CDL	C53-C54-C55-C56
26	C	305	CDL	C63-C64-C65-C66
26	T	102	CDL	CB3-OB5-PB2-OB2
28	E	201	PSC	C04-O12-P-O11
19	A	609	PGV	C15-C16-C17-C18
26	N	601	CDL	C42-C43-C44-C45
19	Z	101	PGV	C26-C27-C28-C29
19	C	304	PGV	C02-C03-O11-P
19	A	609	PGV	C03-O11-P-O13
19	U	101	PGV	C03-O11-P-O13
19	Z	101	PGV	C04-O12-P-O14
26	C	305	CDL	CA3-OA5-PA1-OA3
26	N	601	CDL	CA2-OA2-PA1-OA4
26	T	102	CDL	CA3-OA5-PA1-OA3
27	C	307	PEK	C04-O12-P-O13
27	C	309	PEK	C03-O11-P-O14
27	C	309	PEK	C04-O12-P-O13
27	G	103	PEK	C03-O11-P-O13
27	G	103	PEK	C04-O12-P-O13
27	G	103	PEK	C04-O12-P-O14
27	P	307	PEK	C03-O11-P-O13
27	P	307	PEK	C04-O12-P-O14
28	O	302	PSC	C03-O11-P-O13
21	N	610	TGL	CA7-CA8-CA9-C20
27	C	307	PEK	C01-C02-C03-O11
21	N	610	TGL	CA6-CA7-CA8-CA9
27	T	101	PEK	C7-C8-C9-C10
21	L	101	TGL	CB7-CB8-CB9-C10
26	T	102	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	C05-C04-O12-P
21	Y	101	TGL	CA5-CA6-CA7-CA8
19	U	101	PGV	C11-C10-C9-C8
26	N	601	CDL	C17-C18-C19-C20
19	C	308	PGV	O01-C02-C03-O11
19	Z	101	PGV	O01-C02-C03-O11
27	C	309	PEK	O01-C02-C03-O11
19	C	308	PGV	C15-C16-C17-C18
21	D	201	TGL	CG1-CG2-CG3-OG3
21	Q	201	TGL	CA5-CA6-CA7-CA8
26	C	305	CDL	C11-C12-C13-C14
28	O	302	PSC	O12-C04-C05-N
21	D	201	TGL	OG1-CG1-CG2-OG2
21	L	101	TGL	OG1-CG1-CG2-OG2
21	Y	101	TGL	OG2-CG2-CG3-OG3
19	A	608	PGV	C10-C11-C12-C13
19	U	101	PGV	C10-C11-C12-C13
26	T	102	CDL	C84-C85-C86-C87
19	A	608	PGV	C30-C31-C32-C33
26	T	102	CDL	C71-C72-C73-C74
24	C	302	DMU	O5-C6-O16-C18
19	A	609	PGV	C21-C22-C23-C24
21	N	610	TGL	C33-C34-C35-C36
26	C	305	CDL	C31-C32-C33-C34
19	N	609	PGV	C4-C5-C6-C7
26	P	304	CDL	C74-C75-C76-C77
27	T	101	PEK	C22-C23-C24-C25
19	C	304	PGV	C30-C31-C32-C33
21	L	101	TGL	CC5-CC6-CC7-CC8
21	D	201	TGL	C29-C30-C31-C32
19	C	304	PGV	C11-C12-C13-C14
28	E	201	PSC	C7-C8-C9-C10
27	G	103	PEK	C33-C34-C35-C36
21	B	301	TGL	CB9-C10-C11-C12
19	A	609	PGV	C31-C32-C33-C34
21	N	610	TGL	CA2-CA3-CA4-CA5
24	C	302	DMU	C18-C19-C22-C25
26	P	304	CDL	C73-C74-C75-C76
27	T	101	PEK	C34-C35-C36-C37
19	C	308	PGV	C30-C31-C32-C33
26	C	305	CDL	C31-CA7-OA8-CA6
26	C	305	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
28	E	201	PSC	O01-C02-C03-O11
27	T	101	PEK	O02-C1-O01-C02
20	S	103	EDO	O1-C1-C2-O2
21	D	201	TGL	CA4-CA5-CA6-CA7
19	Z	101	PGV	O03-C01-C02-O01
26	P	304	CDL	OA6-CA4-CA6-OA8
21	N	610	TGL	C10-C11-C12-C13
19	A	609	PGV	C04-O12-P-O11
19	U	101	PGV	C04-O12-P-O11
19	Z	101	PGV	C03-O11-P-O12
26	T	102	CDL	CA2-OA2-PA1-OA5
27	C	307	PEK	C03-O11-P-O12
28	E	201	PSC	C03-O11-P-O12
28	O	302	PSC	C04-O12-P-O11
26	T	102	CDL	C59-C60-C61-C62
27	T	101	PEK	C24-C25-C26-C27
19	C	308	PGV	C20-C21-C22-C23
26	T	102	CDL	C35-C36-C37-C38
24	P	308	DMU	C34-C37-C40-C43
26	P	304	CDL	C58-C59-C60-C61
27	C	307	PEK	C23-C24-C25-C26
27	P	307	PEK	C28-C29-C30-C31
21	L	101	TGL	C33-C34-C35-C36
26	T	102	CDL	C80-C81-C82-C83
27	G	101	PEK	C16-C17-C18-C19
21	Y	101	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	OA9-CA7-OA8-CA6
27	P	307	PEK	C10-C11-C12-C13
28	E	201	PSC	C11-C10-C9-C8
26	C	305	CDL	C78-C79-C80-C81
19	C	308	PGV	C3-C4-C5-C6
21	N	610	TGL	C16-C17-C18-C19
21	Q	201	TGL	C11-C12-C13-C14
19	U	101	PGV	C5-C6-C7-C8
26	C	305	CDL	C72-C73-C74-C75
22	C	306	CHD	C22-C23-C24-O26
27	C	309	PEK	C22-C23-C24-C25
28	E	201	PSC	C6-C7-C8-C9
27	T	101	PEK	C3-C4-C5-C6
21	N	610	TGL	CB2-CB3-CB4-CB5
21	Q	201	TGL	CA7-CA8-CA9-C20
27	P	307	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	P	305	CHD	C22-C23-C24-O26
24	M	101	DMU	C22-C25-C28-C31
28	E	201	PSC	C11-C12-C13-C14
22	B	302	CHD	C22-C23-C24-O25
22	W	101	CHD	C22-C23-C24-O25
26	P	304	CDL	C1-CA2-OA2-PA1
26	C	305	CDL	C19-C20-C21-C22
28	E	201	PSC	C12-C13-C14-C15
21	B	301	TGL	CC9-C15-C16-C17
21	D	201	TGL	C18-C19-C33-C34
27	T	101	PEK	C29-C30-C31-C32
20	D	202	EDO	O1-C1-C2-O2
19	C	304	PGV	C28-C29-C30-C31
21	Q	201	TGL	C15-C16-C17-C18
26	T	102	CDL	C19-C20-C21-C22
21	L	101	TGL	CA7-CA8-CA9-C20
26	P	304	CDL	CB3-CB4-CB6-OB8
14	N	602	HEA	CAD-CBD-CGD-O1D
14	N	603[A]	HEA	CAA-CBA-CGA-O2A
14	N	603[B]	HEA	CAA-CBA-CGA-O1A
22	G	102	CHD	C22-C23-C24-O25
22	G	102	CHD	C22-C23-C24-O26
27	G	103	PEK	C13-C14-C15-C16
19	N	609	PGV	C11-C10-C9-C8
21	D	201	TGL	C12-C13-C14-C29
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
14	N	603[A]	HEA	CAA-CBA-CGA-O1A
21	L	101	TGL	CG1-CG2-OG2-CB1
21	L	101	TGL	CG3-CG2-OG2-CB1
28	E	201	PSC	C01-C02-O01-C1
26	N	601	CDL	C71-C72-C73-C74
19	P	303	PGV	C21-C22-C23-C24
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O2D
22	J	101	CHD	C22-C23-C24-O26
22	P	305	CHD	C22-C23-C24-O25
27	C	309	PEK	C5-C6-C7-C8
27	G	101	PEK	C11-C12-C13-C14
27	G	101	PEK	C12-C13-C14-C15
27	G	103	PEK	C11-C12-C13-C14
27	T	101	PEK	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	302	CHD	C22-C23-C24-O26
22	J	101	CHD	C22-C23-C24-O25
21	D	201	TGL	OB1-CB1-CB2-CB3
19	A	608	PGV	O03-C19-C20-C21
26	C	305	CDL	C33-C34-C35-C36
14	N	603[B]	HEA	CAA-CBA-CGA-O2A
14	A	601	HEA	C26-C15-C16-C17
14	N	602	HEA	C27-C19-C20-C21
22	W	101	CHD	C22-C23-C24-O26
26	N	601	CDL	C16-C17-C18-C19
22	P	305	CHD	C16-C17-C20-C22
14	N	602	HEA	C15-C16-C17-C18
19	U	101	PGV	O12-C04-C05-C06
14	A	601	HEA	CAD-CBD-CGD-O1D
26	P	304	CDL	C78-C79-C80-C81
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
22	C	306	CHD	C22-C23-C24-O25
21	Q	201	TGL	OG2-CB1-CB2-CB3
26	P	304	CDL	C11-C12-C13-C14
21	D	201	TGL	CB9-C10-C11-C12
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
24	C	310	DMU	C18-C19-C22-C25
19	P	303	PGV	C05-C04-O12-P
22	C	306	CHD	C13-C17-C20-C22
21	L	101	TGL	C12-C13-C14-C29
26	T	102	CDL	C37-C38-C39-C40
24	P	306	DMU	C22-C25-C28-C31
26	P	304	CDL	C12-C13-C14-C15
26	T	102	CDL	C12-C13-C14-C15
20	E	203	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
19	P	303	PGV	C10-C11-C12-C13
26	N	601	CDL	C73-C74-C75-C76
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
26	N	601	CDL	C52-C53-C54-C55
19	U	101	PGV	C11-C12-C13-C14
27	T	101	PEK	O03-C21-C22-C23
28	E	201	PSC	C04-C05-N-C06
26	C	305	CDL	C20-C21-C22-C23
21	B	301	TGL	C23-C24-C25-C26
27	P	307	PEK	C3-C4-C5-C6
19	C	308	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	CC2-CC3-CC4-CC5
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
14	N	603[A]	HEA	CAD-CBD-CGD-O2D
26	C	305	CDL	C80-C81-C82-C83
26	N	601	CDL	C83-C84-C85-C86
22	P	301	CHD	C22-C23-C24-O26
21	Y	101	TGL	C19-C33-C34-C35
27	C	307	PEK	C30-C31-C32-C33
28	O	302	PSC	C4-C5-C6-C7
26	C	305	CDL	CA5-C11-C12-C13
21	N	610	TGL	C15-C16-C17-C18
21	D	201	TGL	OG1-CA1-CA2-CA3
21	Y	101	TGL	OG1-CA1-CA2-CA3
24	P	309	DMU	O1-C10-O7-C3
22	P	301	CHD	C22-C23-C24-O25
27	T	101	PEK	C28-C29-C30-C31
14	A	601	HEA	C14-C15-C16-C17
27	T	101	PEK	O01-C1-C2-C3
14	A	601	HEA	C12-C11-C3B-C2B
27	C	307	PEK	C02-C03-O11-P
14	A	601	HEA	CAA-CBA-CGA-O1A
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
28	E	201	PSC	C04-C05-N-C08
19	P	303	PGV	C28-C29-C30-C31
27	P	307	PEK	C29-C30-C31-C32
20	A	618	EDO	O1-C1-C2-O2
20	B	306	EDO	O1-C1-C2-O2
20	N	620	EDO	O1-C1-C2-O2
27	G	103	PEK	C3-C4-C5-C6
19	C	308	PGV	O01-C1-C2-C3
19	A	608	PGV	C11-C10-C9-C8
19	C	304	PGV	C26-C27-C28-C29
21	Y	101	TGL	OG1-CG1-CG2-OG2
24	M	101	DMU	O6-C11-C9-O1
19	A	609	PGV	C9-C10-C11-C12
27	C	307	PEK	C3-C4-C5-C6
27	G	103	PEK	C4-C5-C6-C7
19	C	308	PGV	C13-C14-C15-C16
26	T	102	CDL	C12-C11-CA5-OA6
27	G	103	PEK	O03-C21-C22-C23
14	A	601	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	P	304	CDL	C23-C24-C25-C26
26	T	102	CDL	C57-C58-C59-C60
19	C	304	PGV	C9-C10-C11-C12
19	Z	101	PGV	O03-C19-C20-C21
28	E	201	PSC	O03-C19-C20-C21
24	C	310	DMU	C25-C28-C31-C34
26	C	305	CDL	C54-C55-C56-C57
22	C	301	CHD	C16-C17-C20-C22
26	P	304	CDL	C13-C14-C15-C16
27	G	103	PEK	C1-C2-C3-C4
28	E	201	PSC	C04-C05-N-C07
19	C	308	PGV	O02-C1-C2-C3
21	B	301	TGL	C11-C10-CB9-CB8
19	P	303	PGV	C31-C32-C33-C34
21	N	610	TGL	CC7-CC8-CC9-C15
27	P	307	PEK	C27-C28-C29-C30
26	N	601	CDL	C36-C37-C38-C39
27	C	309	PEK	C26-C27-C28-C29
28	E	201	PSC	C02-C03-O11-P
21	D	201	TGL	OC1-CC1-CC2-CC3
19	N	609	PGV	C11-C12-C13-C14
19	Z	101	PGV	C03-O11-P-O13
19	Z	101	PGV	C04-O12-P-O13
26	T	102	CDL	CA2-OA2-PA1-OA3
27	C	307	PEK	C32-C33-C34-C35
26	P	304	CDL	C34-C35-C36-C37
21	D	201	TGL	CA7-CA8-CA9-C20
26	T	102	CDL	C12-C11-CA5-OA7
14	A	601	HEA	CAA-CBA-CGA-O2A
21	D	201	TGL	CG1-CG2-OG2-CB1
21	D	201	TGL	OA1-CA1-CA2-CA3
27	G	103	PEK	O04-C21-C22-C23
21	L	101	TGL	C18-C19-C33-C34
22	C	301	CHD	C22-C23-C24-O25
21	D	201	TGL	OG3-CC1-CC2-CC3
14	N	602	HEA	CAA-CBA-CGA-O2A
26	T	102	CDL	C83-C84-C85-C86
19	C	304	PGV	C05-C04-O12-P
14	N	603[B]	HEA	C26-C15-C16-C17
27	T	101	PEK	O02-C1-C2-C3
19	P	303	PGV	C20-C21-C22-C23
24	C	302	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
19	Z	101	PGV	O04-C19-C20-C21
28	E	201	PSC	O04-C19-C20-C21
27	C	309	PEK	O03-C21-C22-C23
19	N	609	PGV	O03-C19-C20-C21
21	Q	201	TGL	OG3-CC1-CC2-CC3
26	C	305	CDL	C12-C11-CA5-OA6

There are no ring outliers.

58 monomers are involved in 428 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	608[B]	AZI	2	0
27	T	101	PEK	1	0
20	A	619	EDO	1	0
24	P	309	DMU	2	0
26	T	102	CDL	19	0
24	P	306	DMU	16	0
22	P	305	CHD	4	0
14	A	602[A]	HEA	2	0
20	B	304	EDO	4	0
20	G	105	EDO	6	0
24	C	302	DMU	16	0
19	P	303	PGV	2	0
19	Z	101	PGV	11	0
20	N	619	EDO	1	0
14	N	603[A]	HEA	2	0
20	N	620	EDO	5	0
20	A	618	EDO	3	0
21	D	201	TGL	16	0
24	Z	102	DMU	1	0
27	G	103	PEK	4	0
24	P	308	DMU	2	0
28	O	302	PSC	15	0
26	C	305	CDL	25	0
28	E	201	PSC	12	0
19	A	609	PGV	9	0
22	W	101	CHD	2	0
26	N	601	CDL	26	0
24	C	310	DMU	4	0
20	A	617	EDO	2	0
22	C	306	CHD	4	0
19	A	608	PGV	3	0

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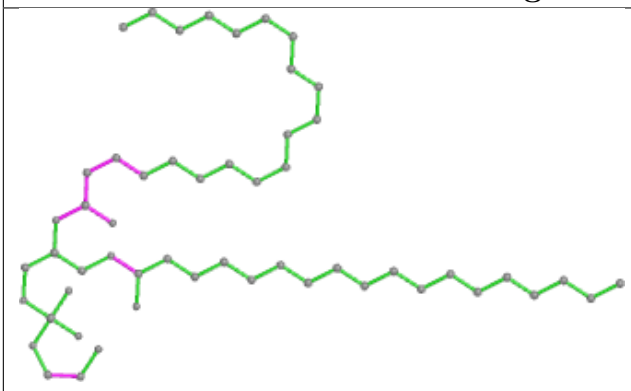
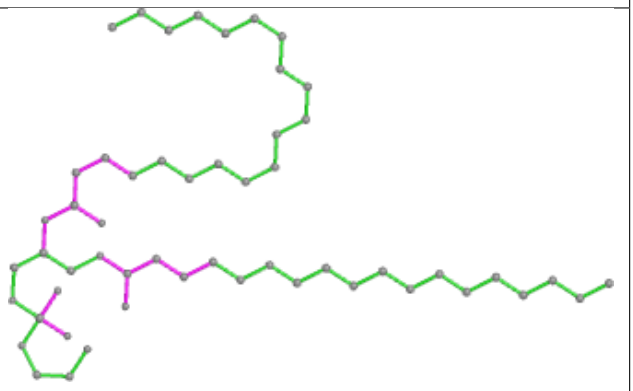
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	102	CHD	1	0
22	J	101	CHD	1	0
18	A	607[B]	AZI	4	0
14	N	602	HEA	10	0
20	A	615	EDO	6	0
21	B	301	TGL	4	0
26	P	304	CDL	25	0
21	Y	101	TGL	23	0
20	B	305	EDO	1	0
21	Q	201	TGL	13	0
27	C	307	PEK	16	0
24	C	311	DMU	2	0
21	L	101	TGL	10	0
27	G	101	PEK	8	0
14	N	603[B]	HEA	20	0
19	C	308	PGV	2	0
18	A	606[B]	AZI	1	0
20	N	617	EDO	1	0
22	C	301	CHD	1	0
14	A	601	HEA	11	0
19	C	304	PGV	6	0
21	N	610	TGL	6	0
27	P	307	PEK	5	0
19	U	101	PGV	1	0
20	D	202	EDO	12	0
27	C	309	PEK	11	0
14	A	602[B]	HEA	23	0

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

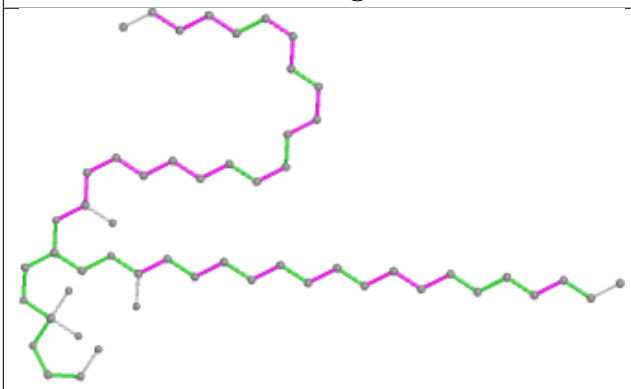
Ligand PEK T 101



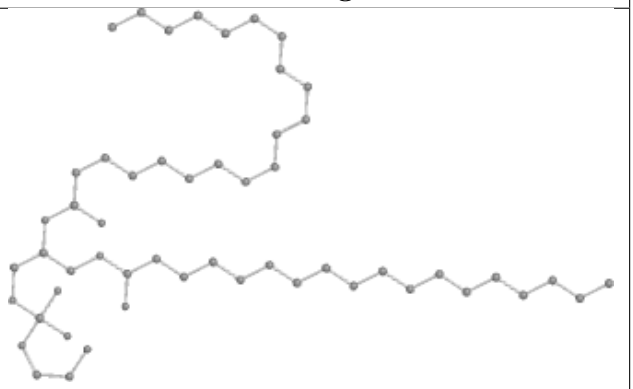
Bond lengths



Bond angles

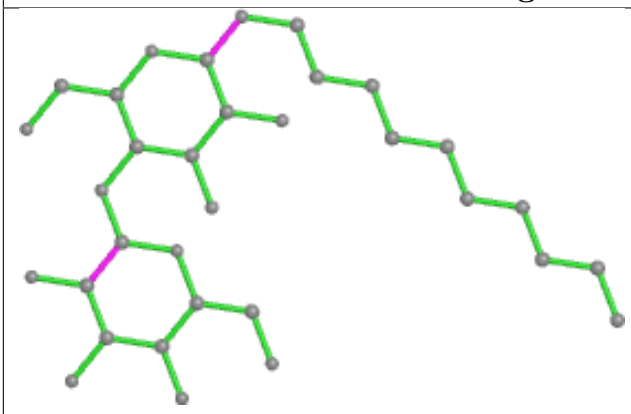


Torsions

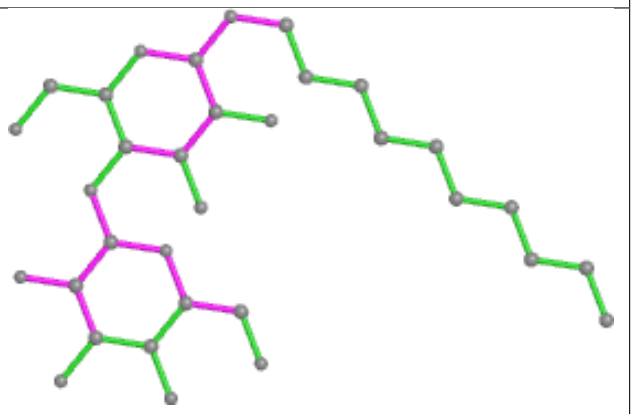


Rings

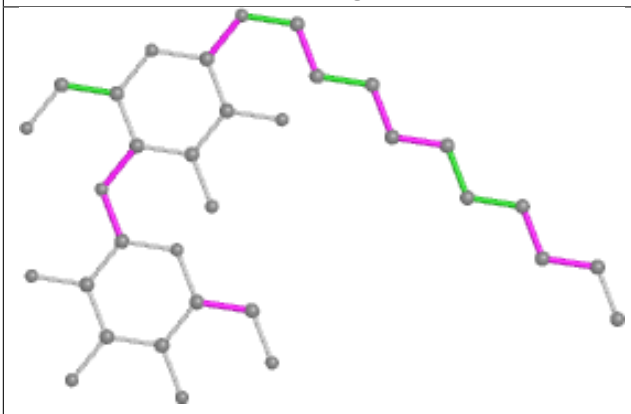
Ligand DMU P 309



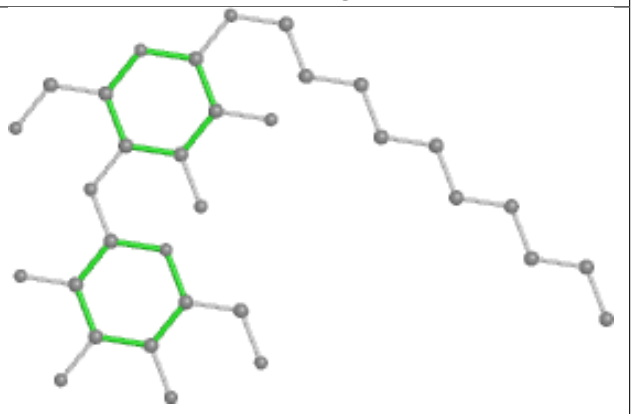
Bond lengths



Bond angles

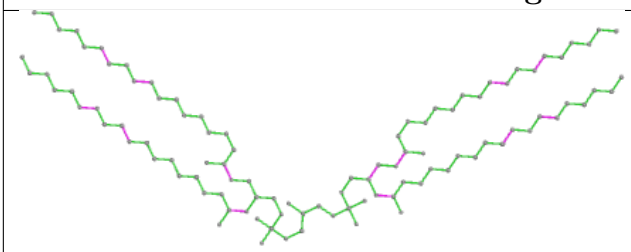


Torsions

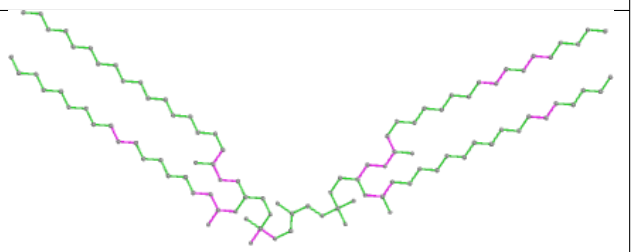


Rings

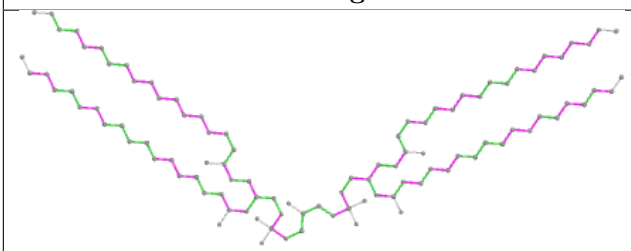
Ligand CDL T 102



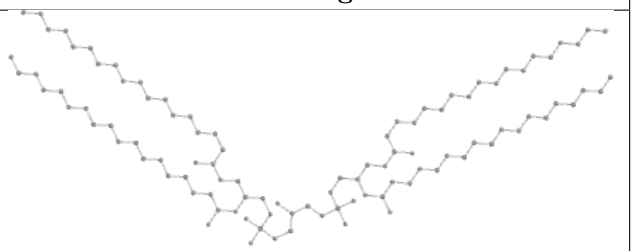
Bond lengths



Bond angles

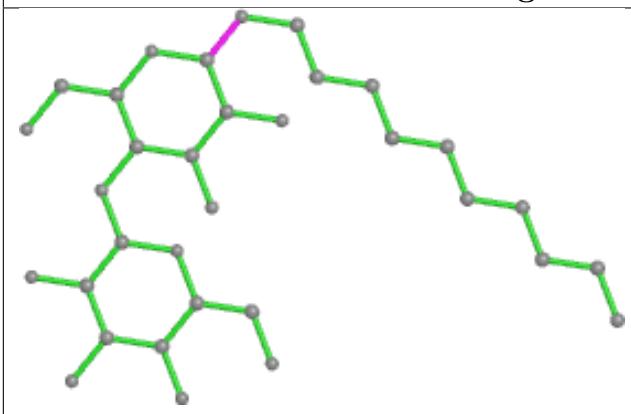


Torsions

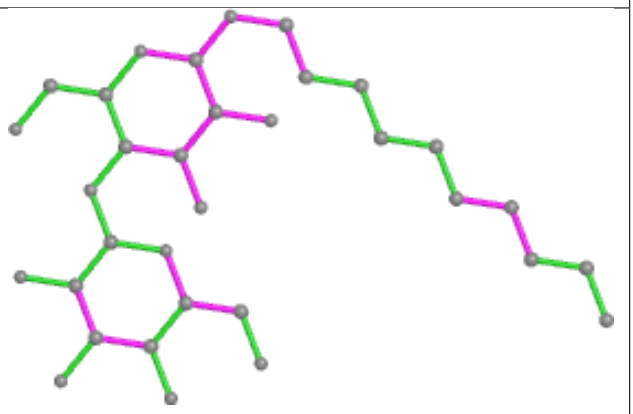


Rings

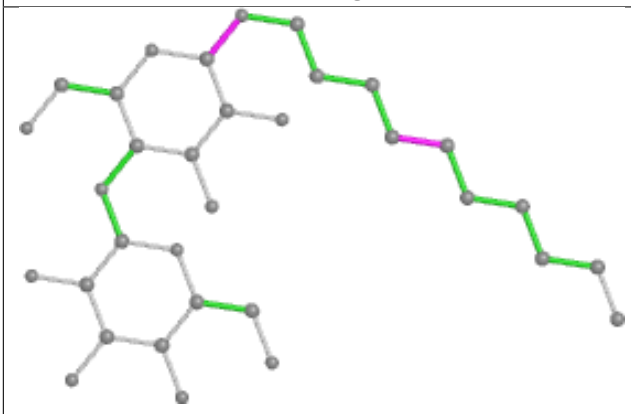
Ligand DMU P 306



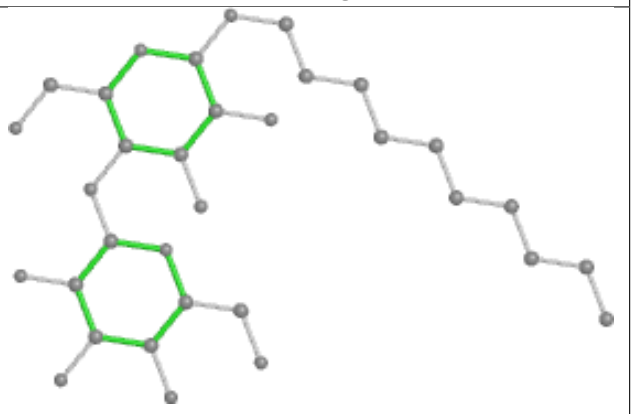
Bond lengths



Bond angles

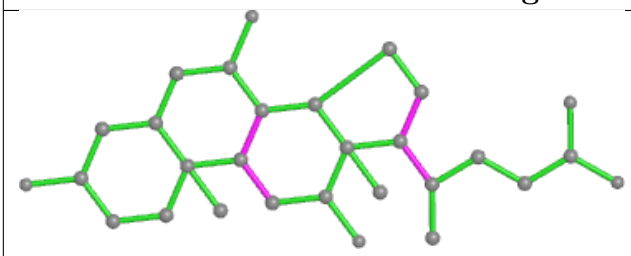


Torsions

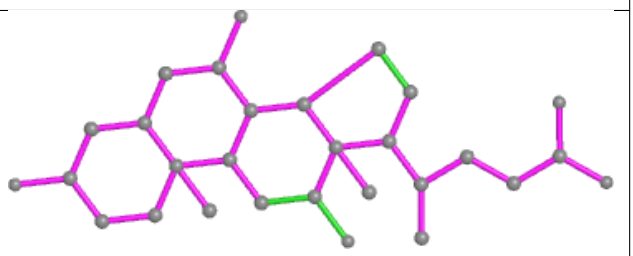


Rings

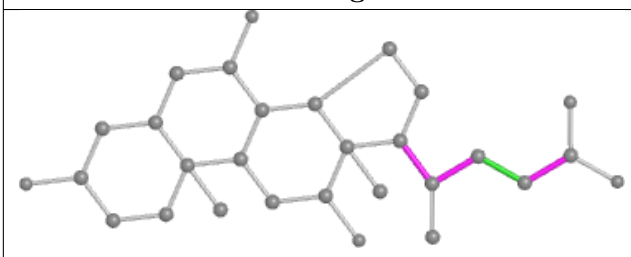
Ligand CHD P 305



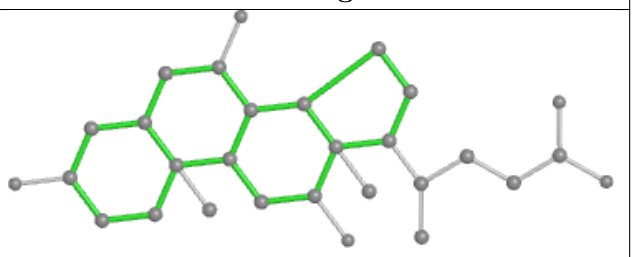
Bond lengths



Bond angles

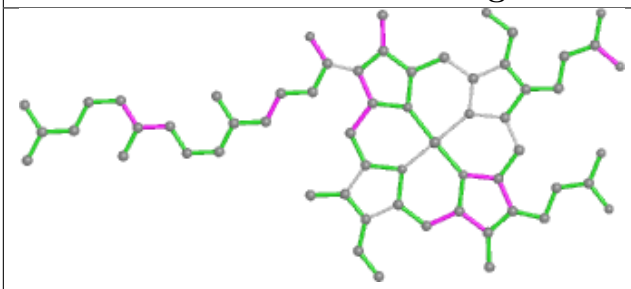


Torsions

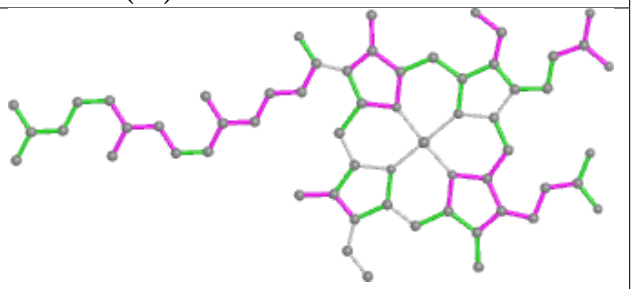


Rings

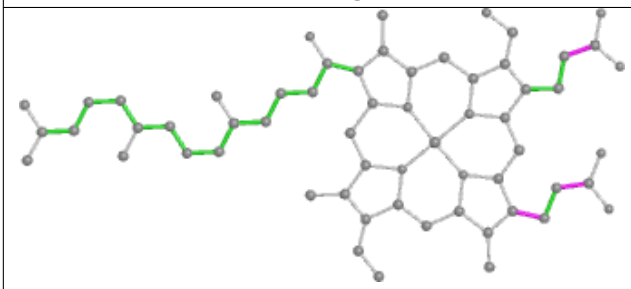
Ligand HEA A 602 (A)



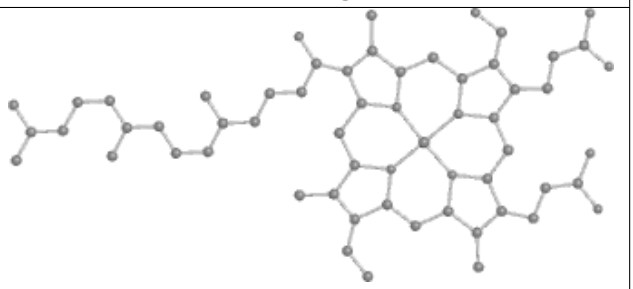
Bond lengths



Bond angles

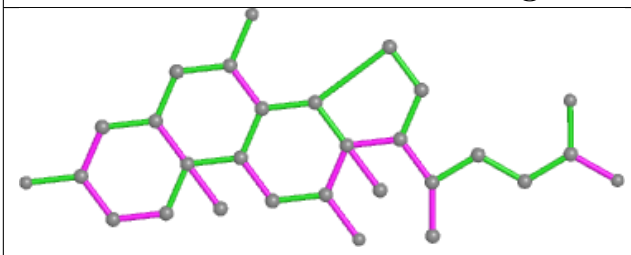


Torsions

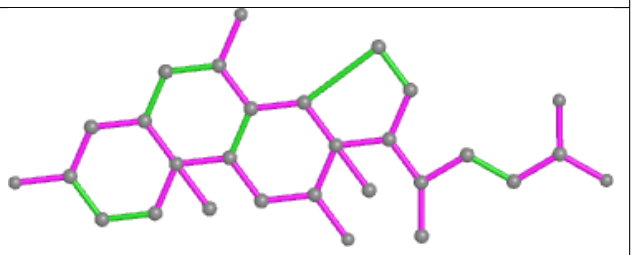


Rings

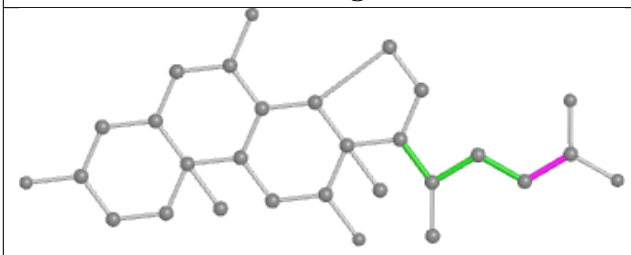
Ligand CHD B 302



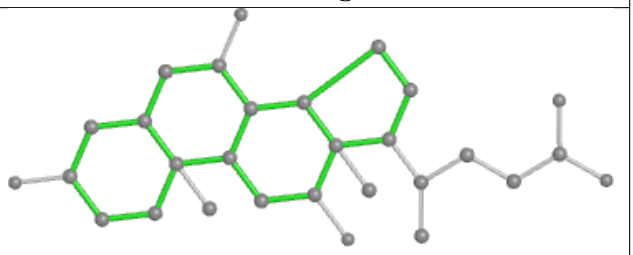
Bond lengths



Bond angles

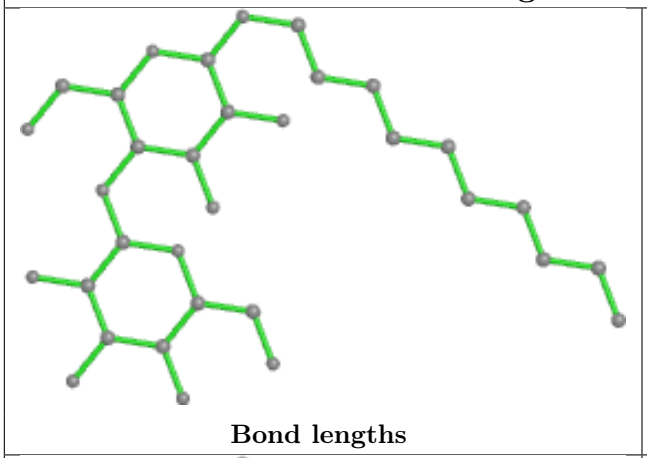


Torsions



Rings

Ligand DMU C 302



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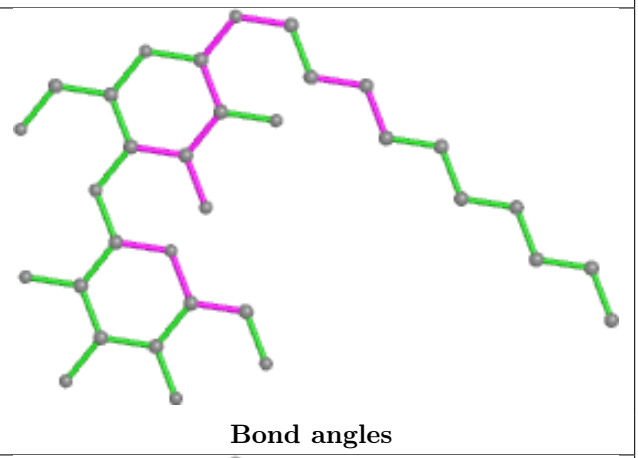
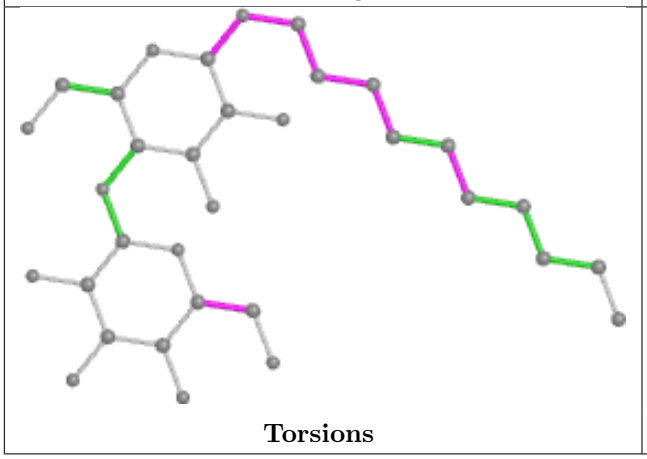
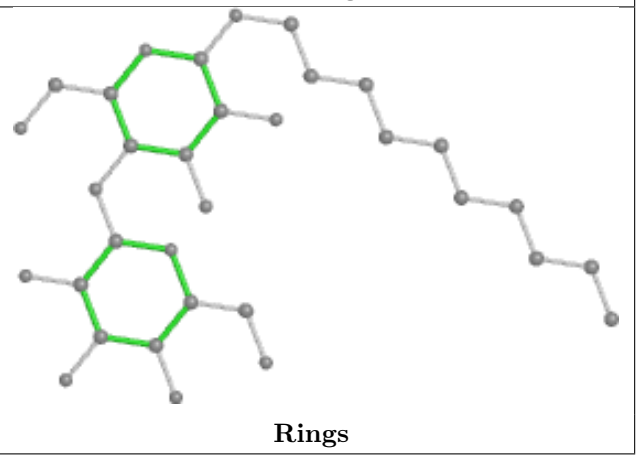


Bond angles

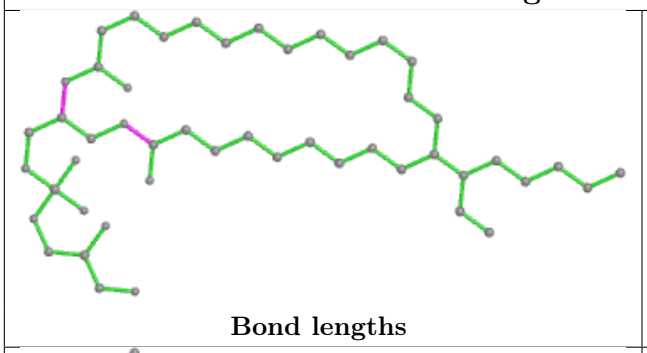


Torsions

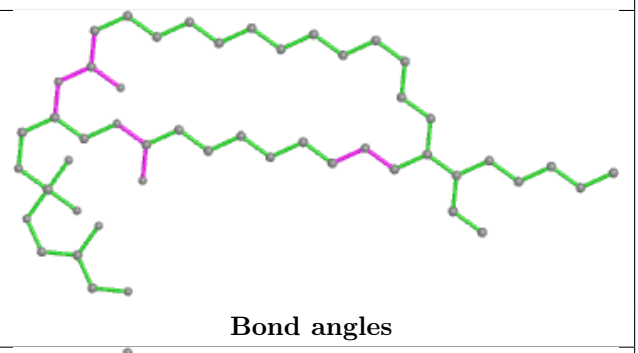


Rings

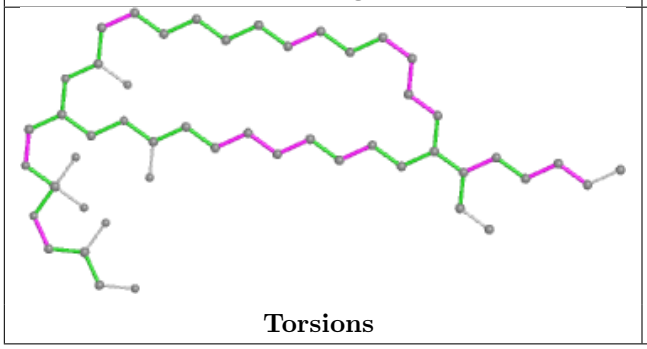
Ligand PGV P 303



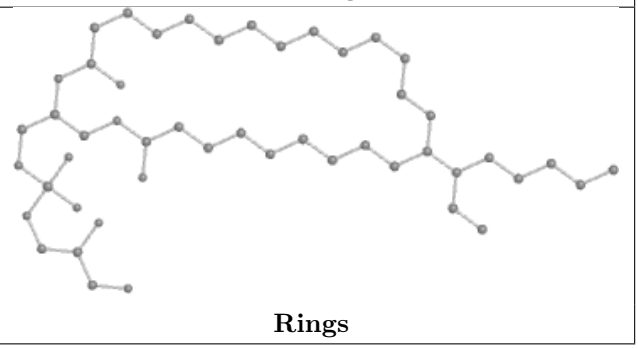
Bond lengths



Bond angles

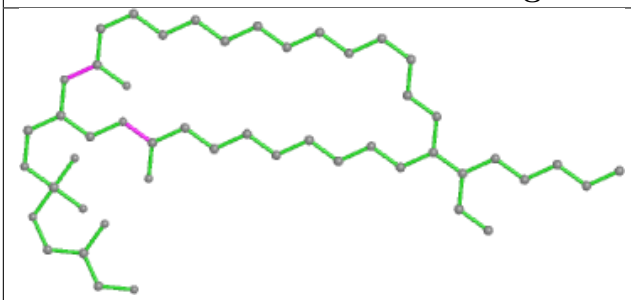


Torsions

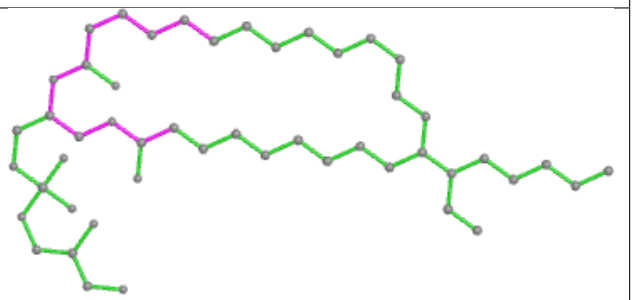


Rings

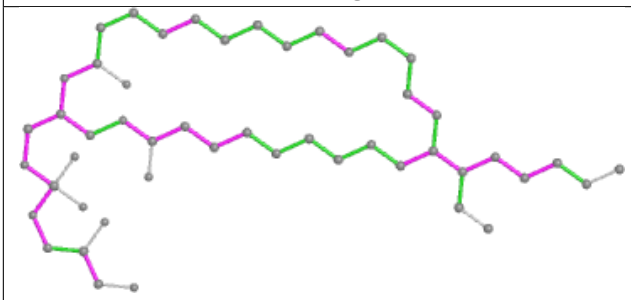
Ligand PGV Z 101



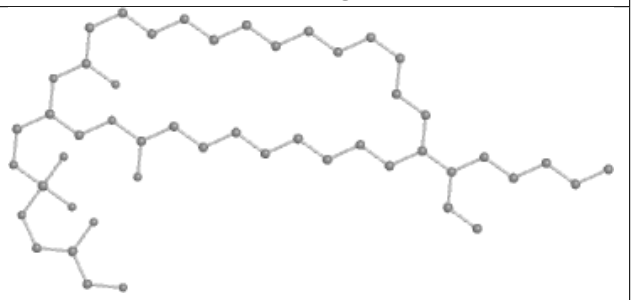
Bond lengths



Bond angles

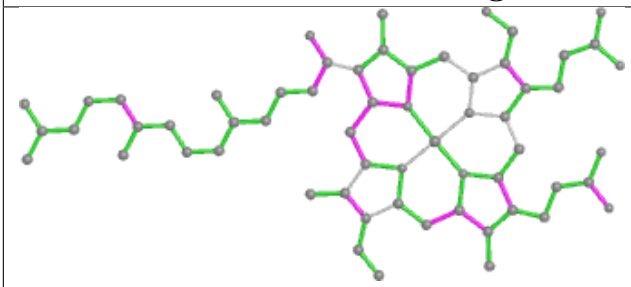


Torsions

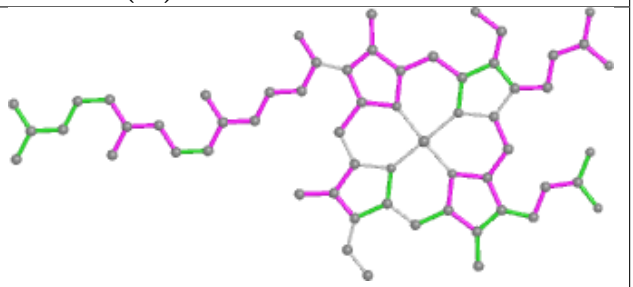


Rings

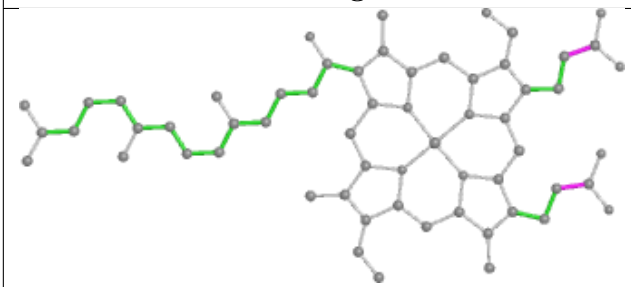
Ligand HEA N 603 (A)



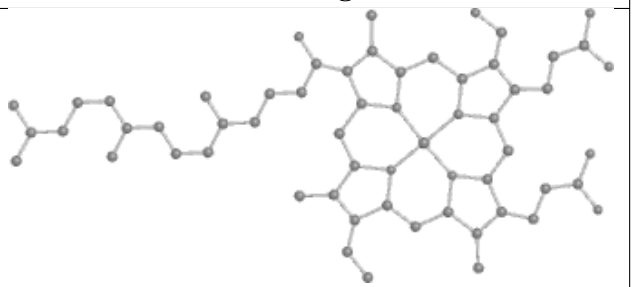
Bond lengths



Bond angles

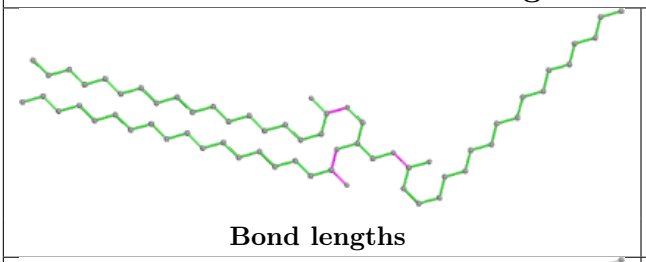


Torsions

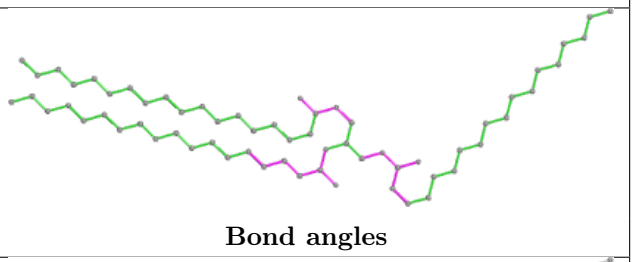


Rings

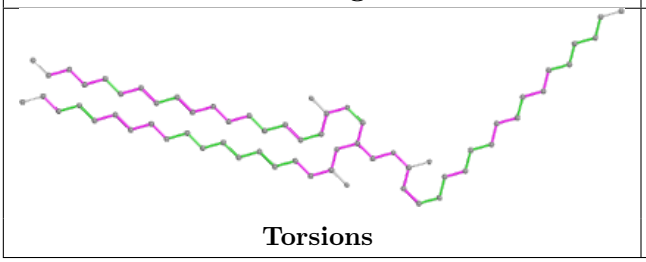
Ligand TGL D 201



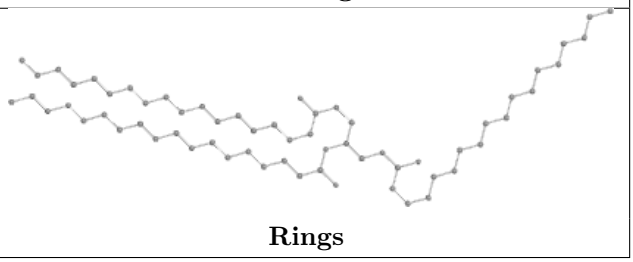
Bond lengths



Bond angles

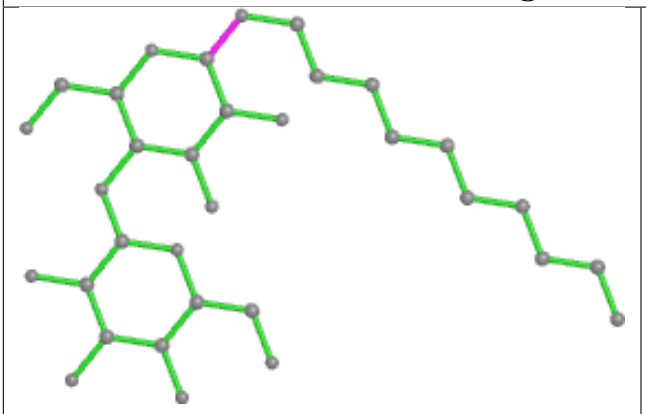


Torsions

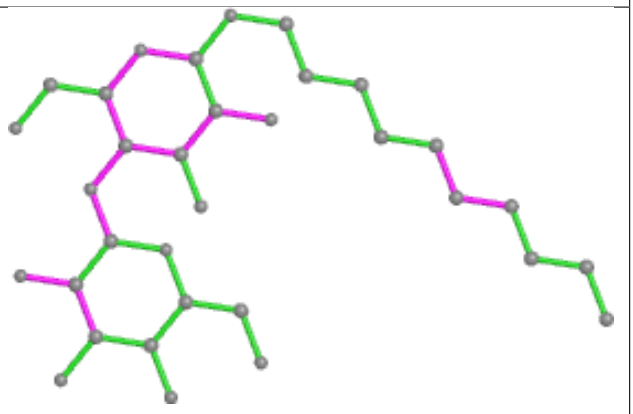


Rings

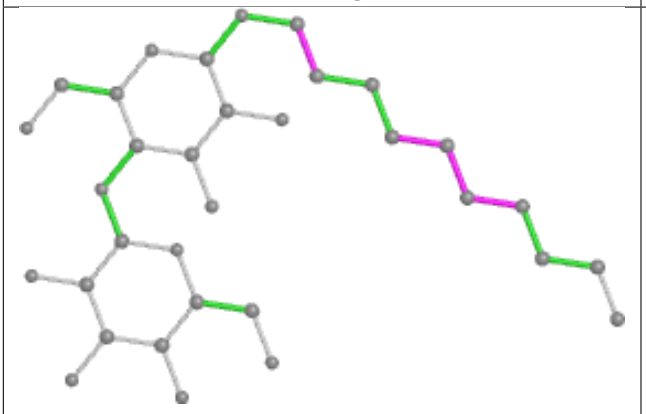
Ligand DMU Z 102



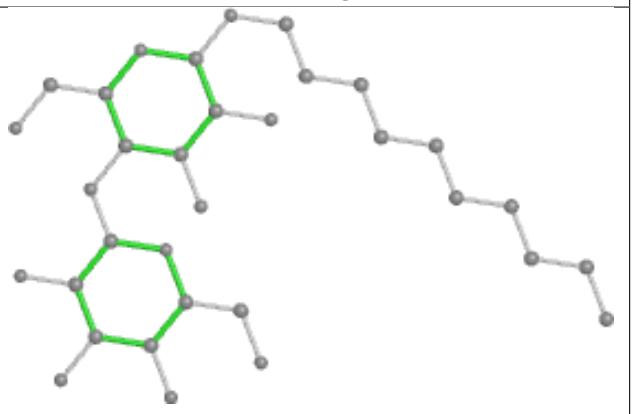
Bond lengths



Bond angles

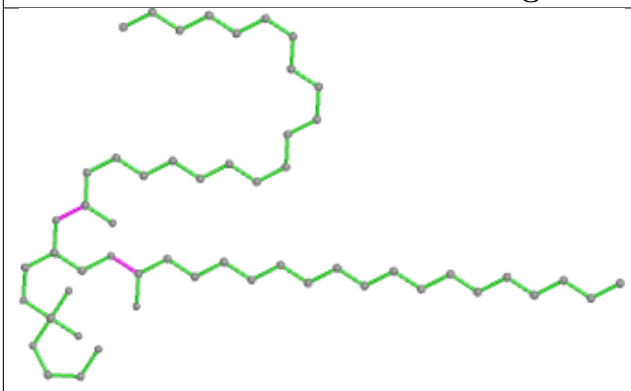


Torsions

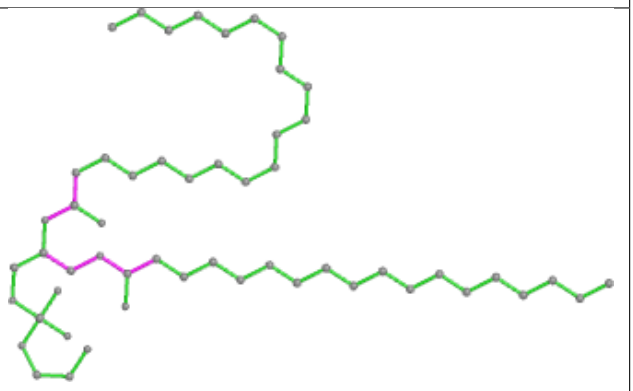


Rings

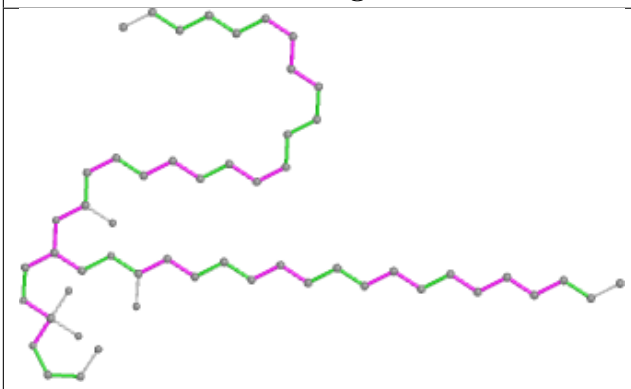
Ligand PEK G 103



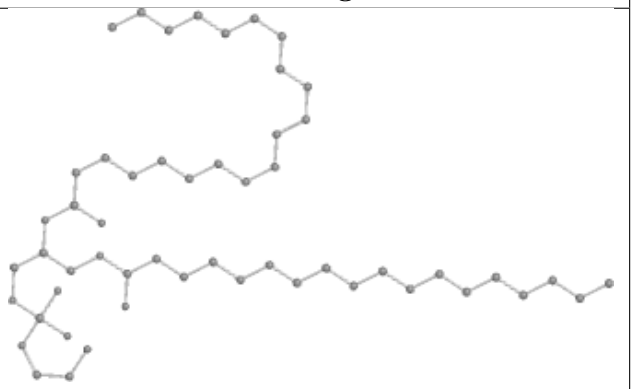
Bond lengths



Bond angles

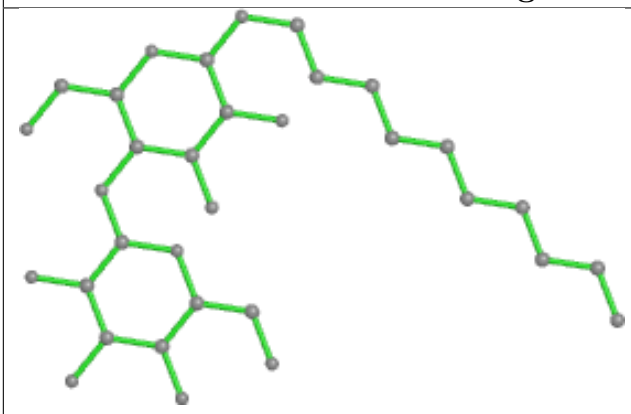


Torsions

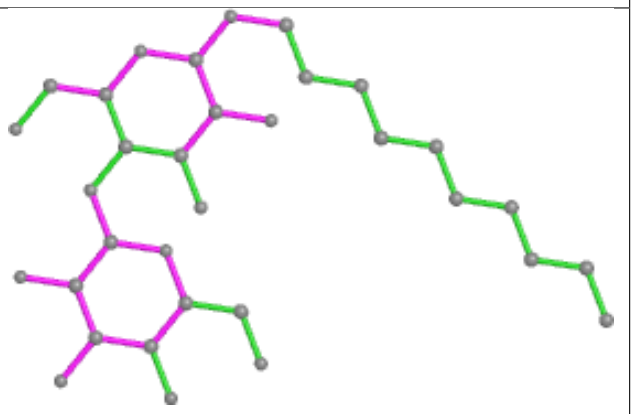


Rings

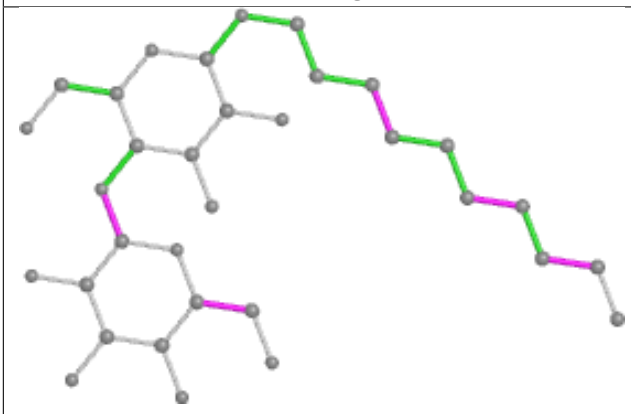
Ligand DMU P 308



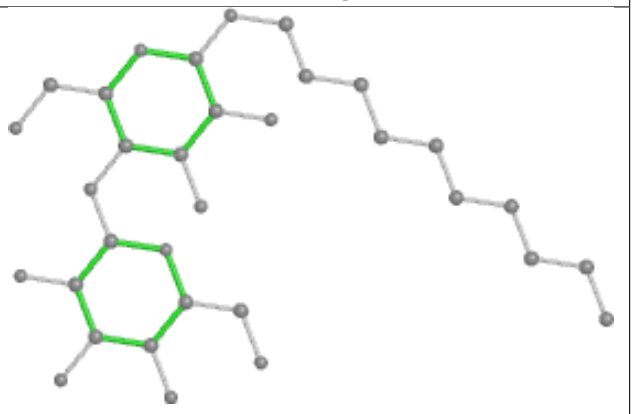
Bond lengths



Bond angles

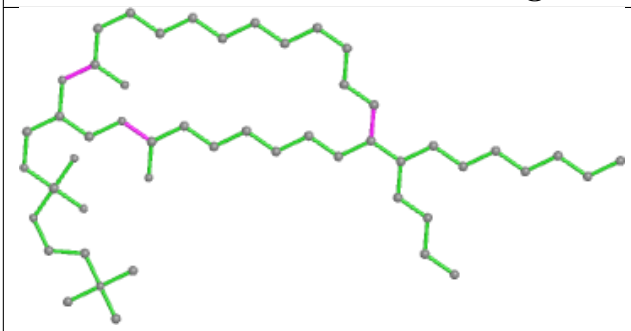


Torsions

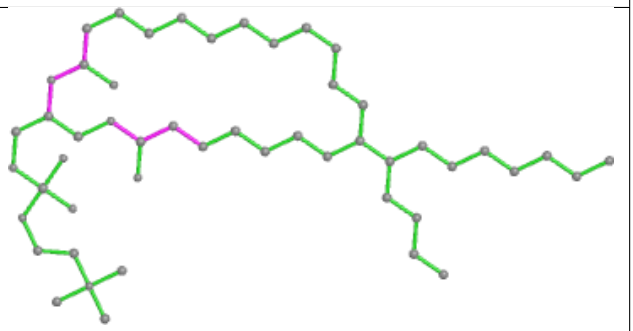


Rings

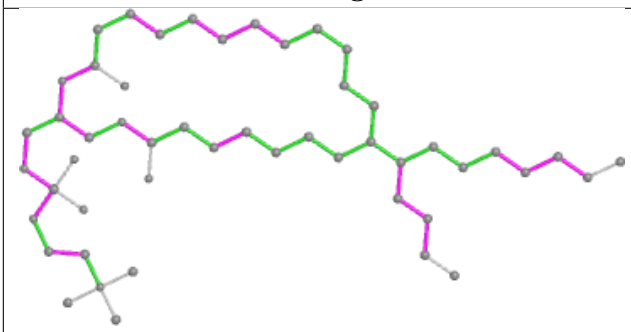
Ligand PSC O 302



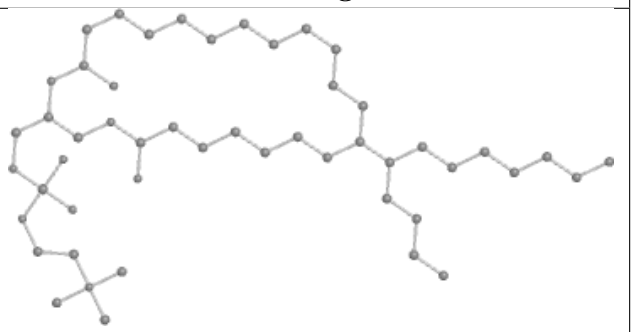
Bond lengths



Bond angles

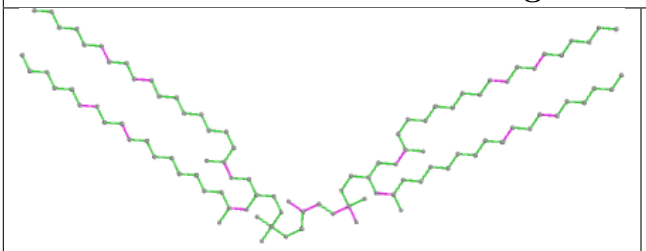


Torsions

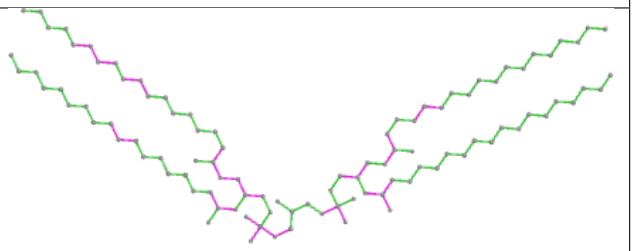


Rings

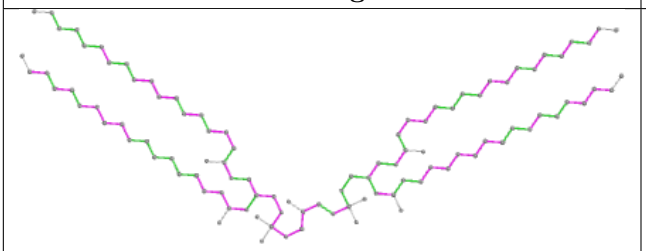
Ligand CDL C 305



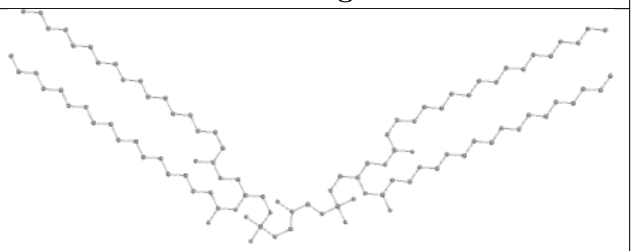
Bond lengths



Bond angles

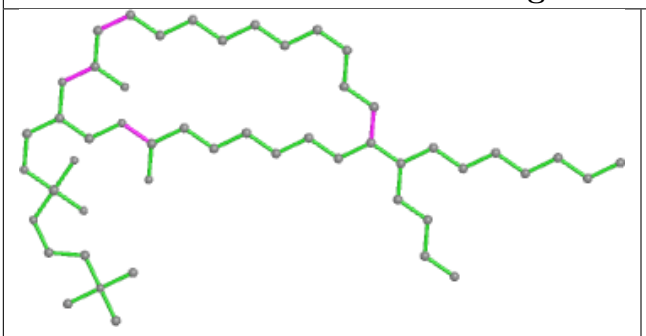


Torsions

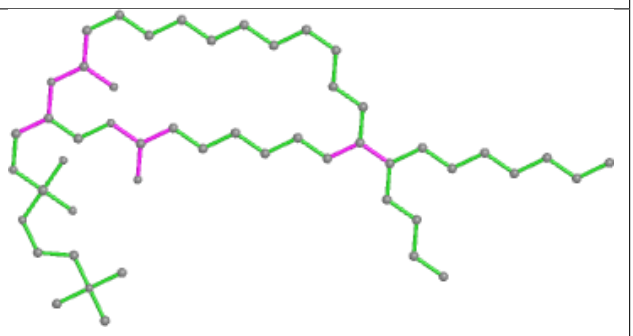


Rings

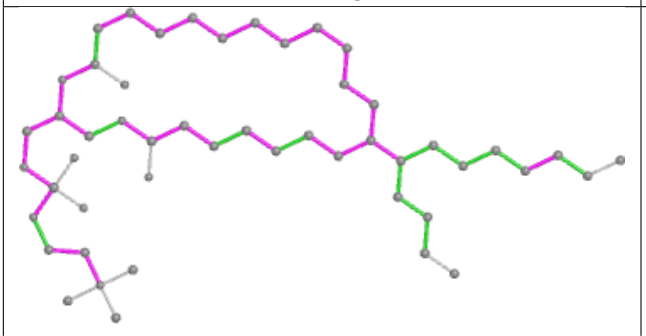
Ligand PSC E 201



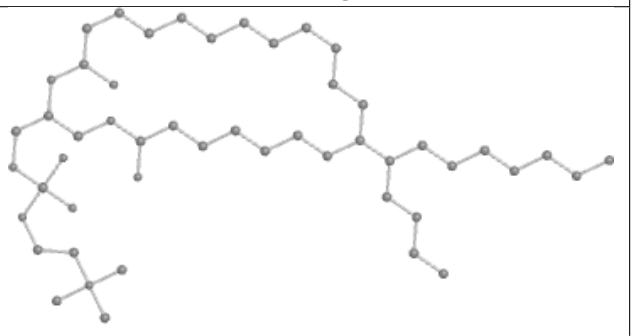
Bond lengths



Bond angles

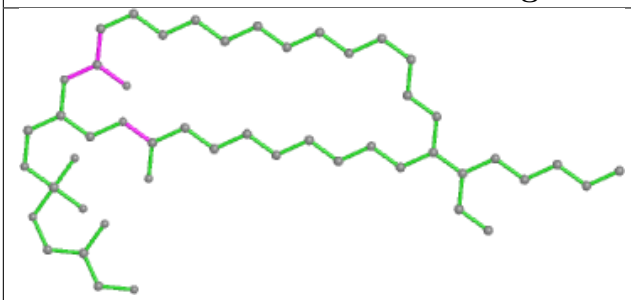


Torsions

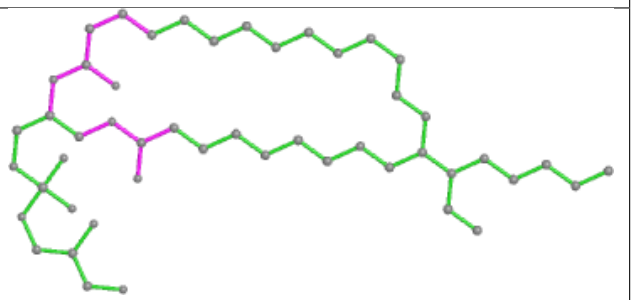


Rings

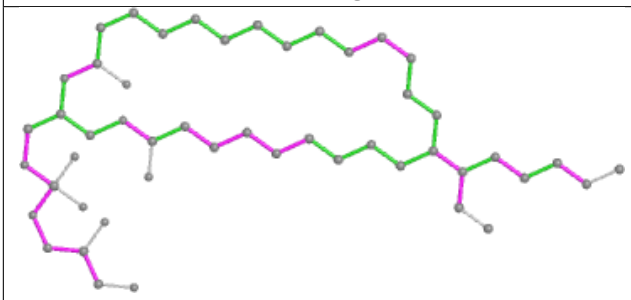
Ligand PGV A 609



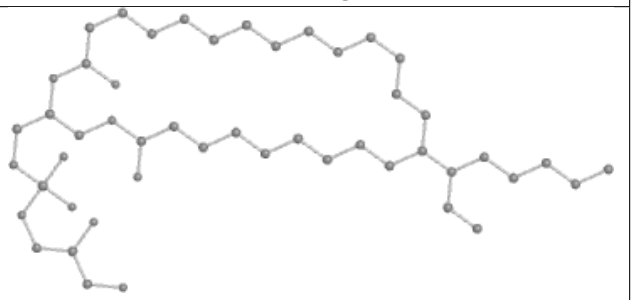
Bond lengths



Bond angles

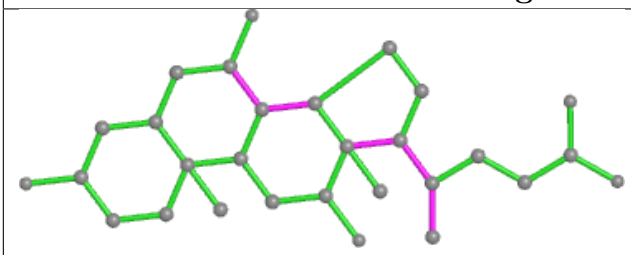


Torsions

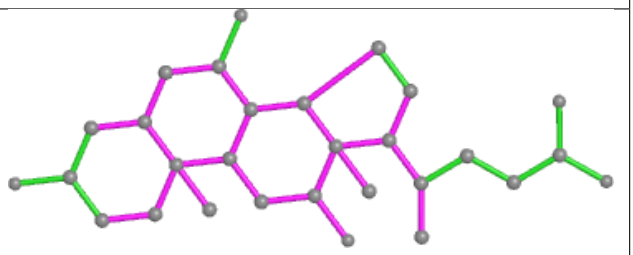


Rings

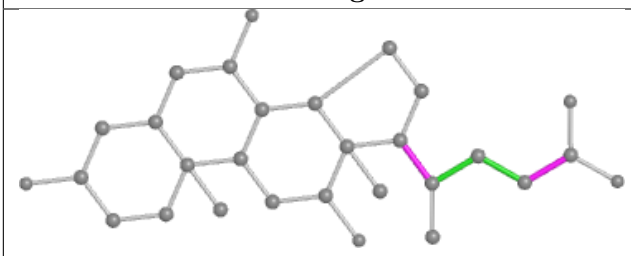
Ligand CHD W 101



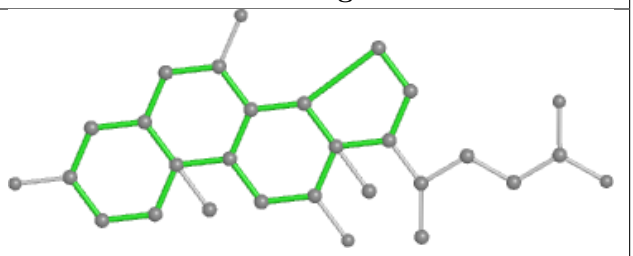
Bond lengths



Bond angles

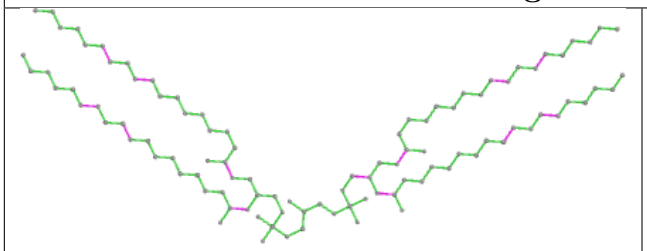


Torsions

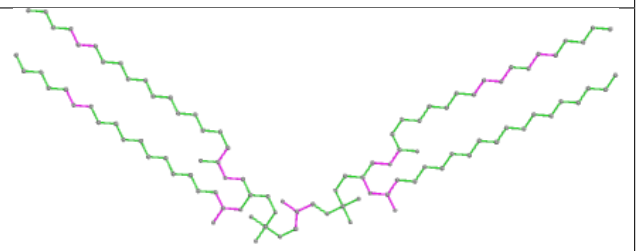


Rings

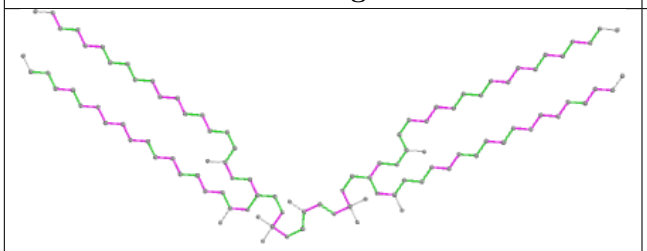
Ligand CDL N 601



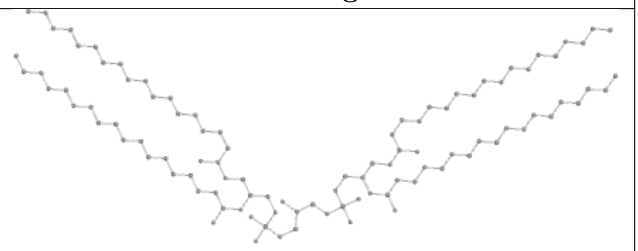
Bond lengths



Bond angles

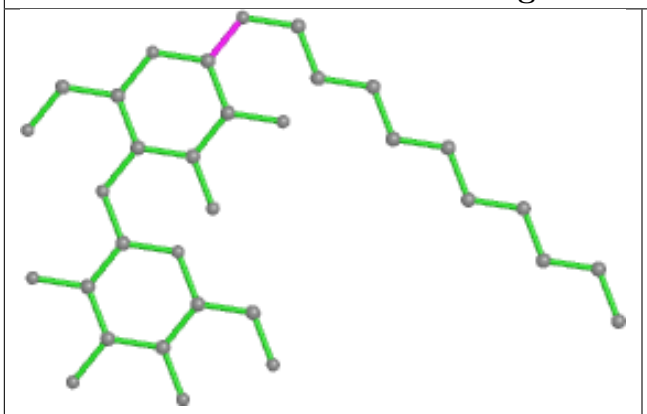


Torsions

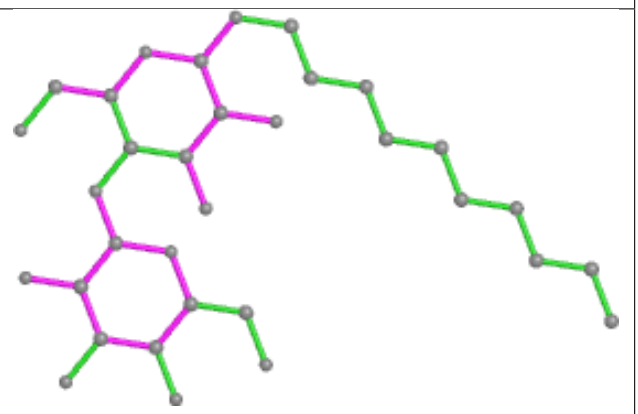


Rings

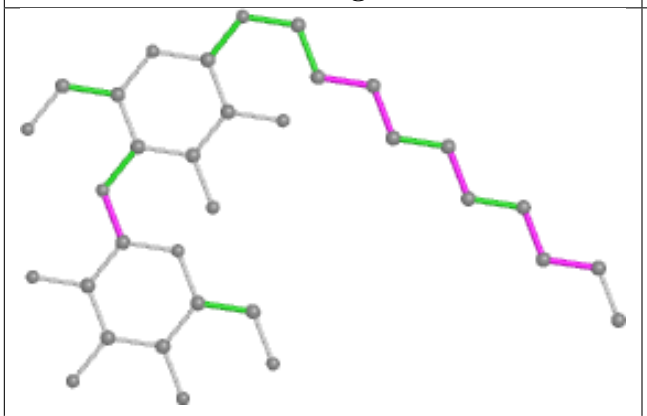
Ligand DMU C 310



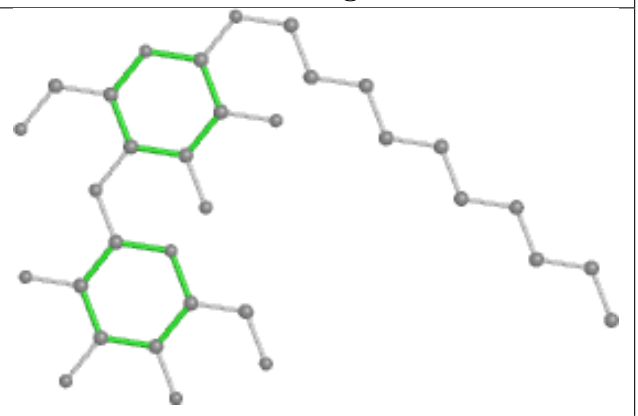
Bond lengths



Bond angles

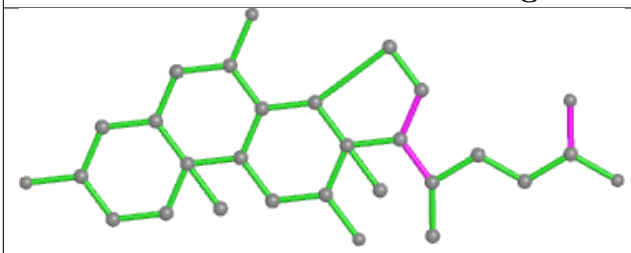


Torsions



Rings

Ligand CHD C 306



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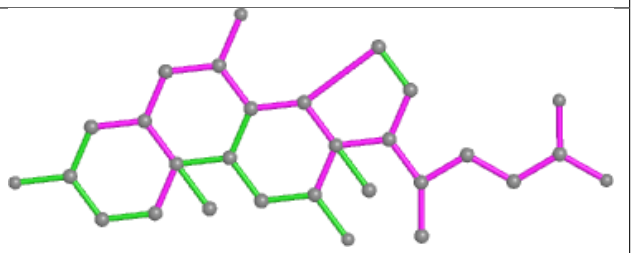
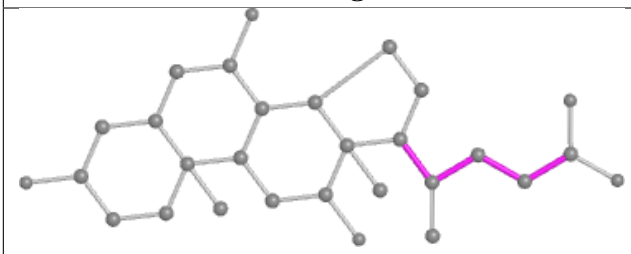
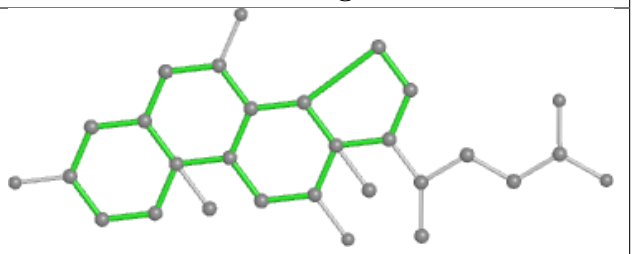


Bond angles

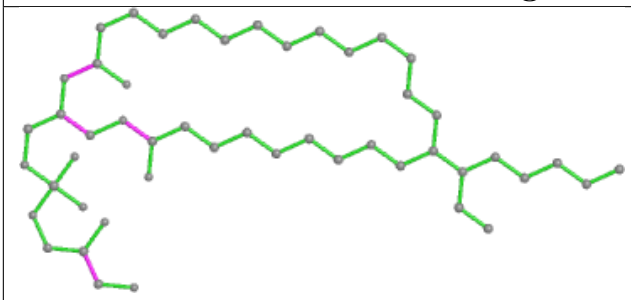


Torsions

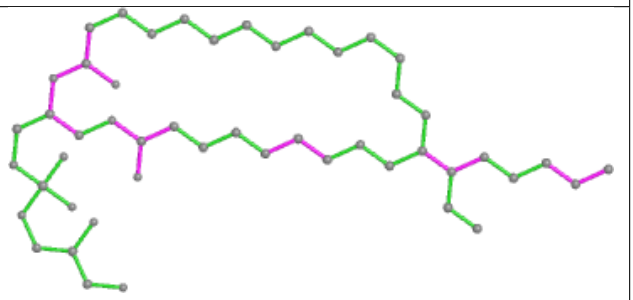


Rings

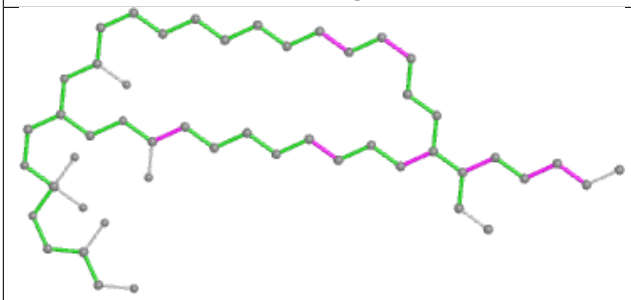
Ligand PGV A 608



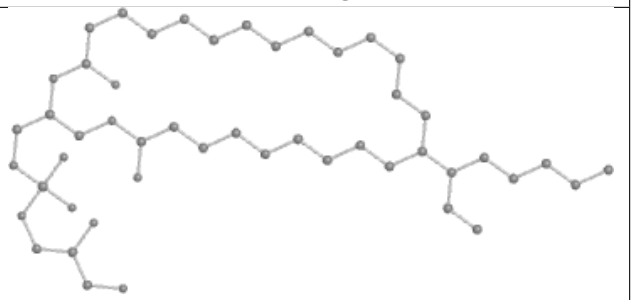
Bond lengths



Bond angles

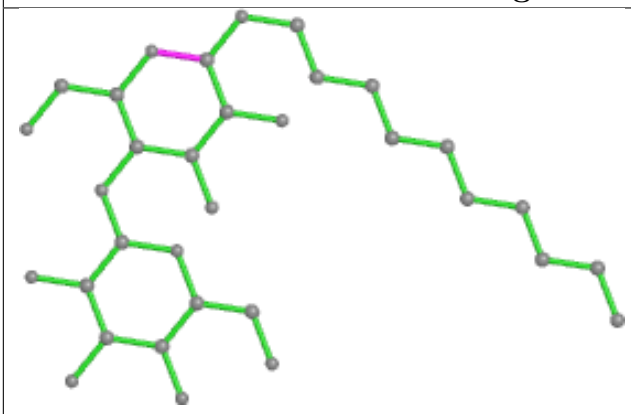


Torsions

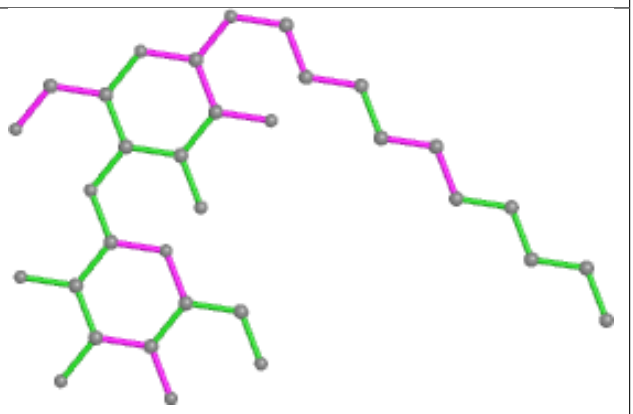


Rings

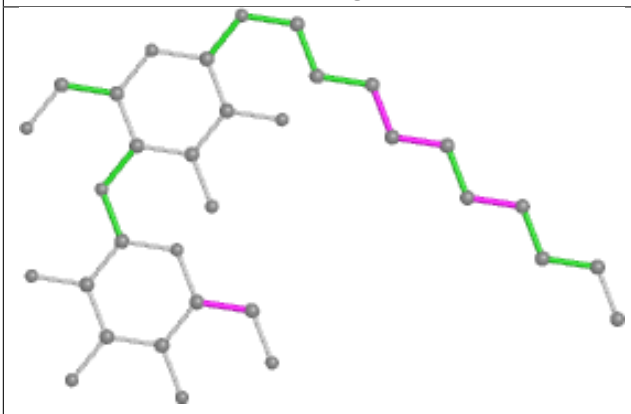
Ligand DMU M 101



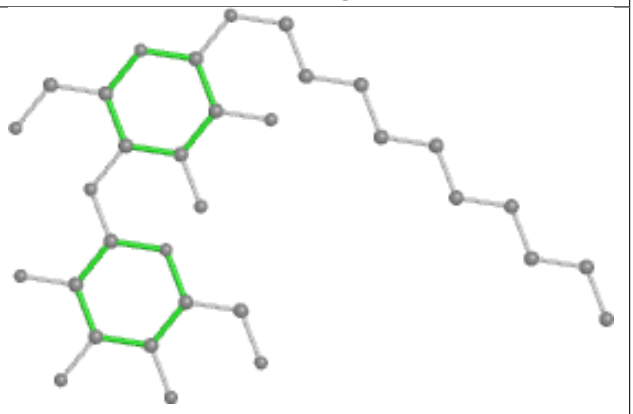
Bond lengths



Bond angles

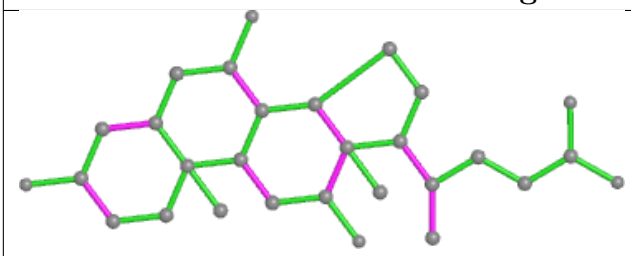


Torsions

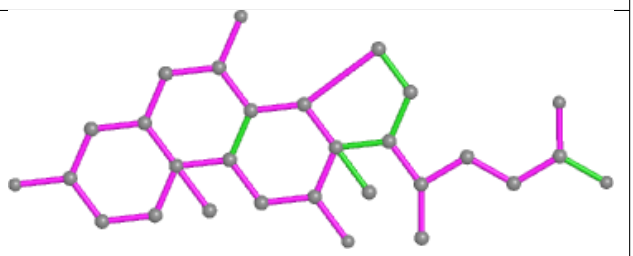


Rings

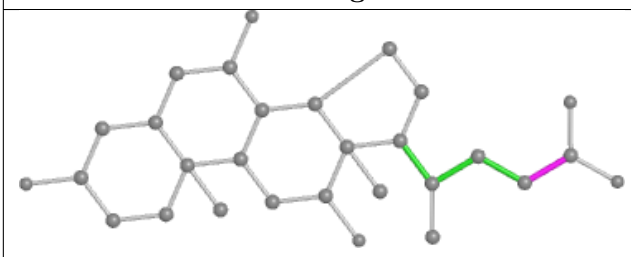
Ligand CHD G 102



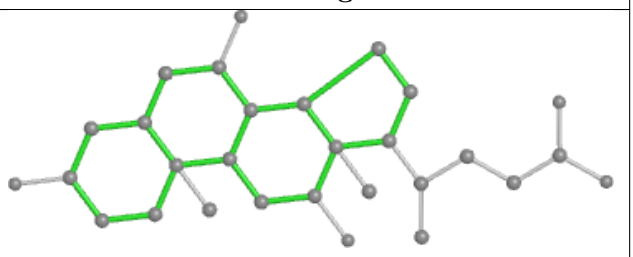
Bond lengths



Bond angles

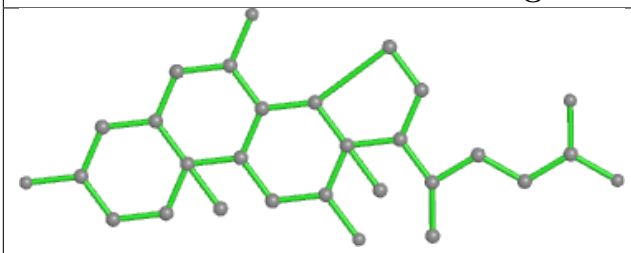


Torsions

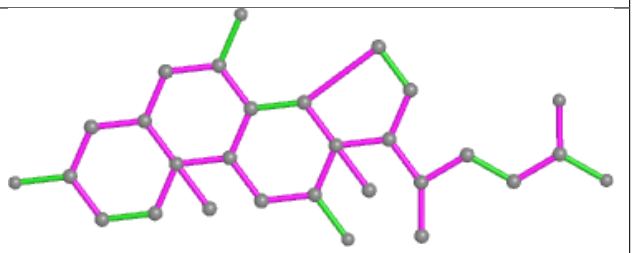


Rings

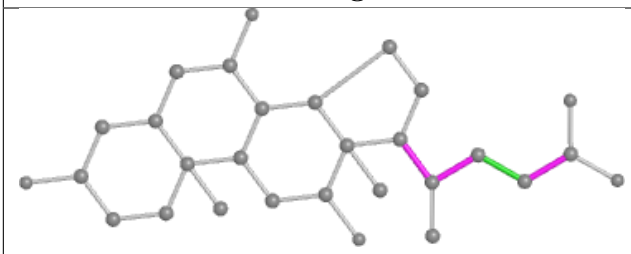
Ligand CHD J 101



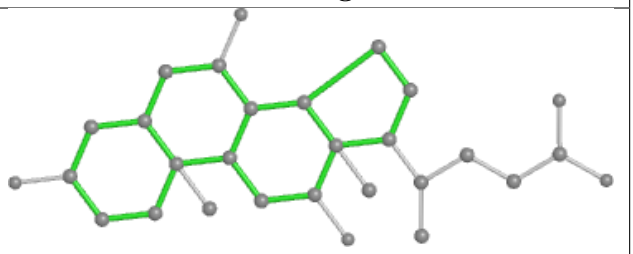
Bond lengths



Bond angles

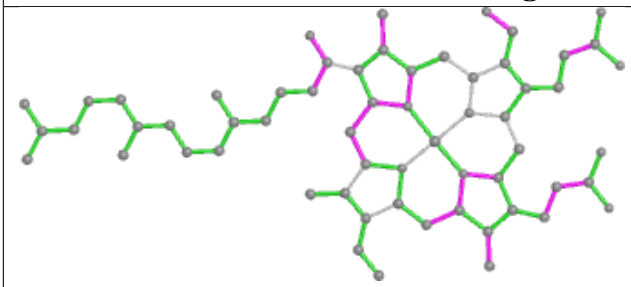


Torsions

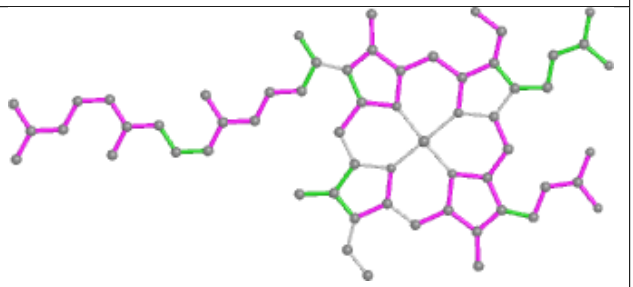


Rings

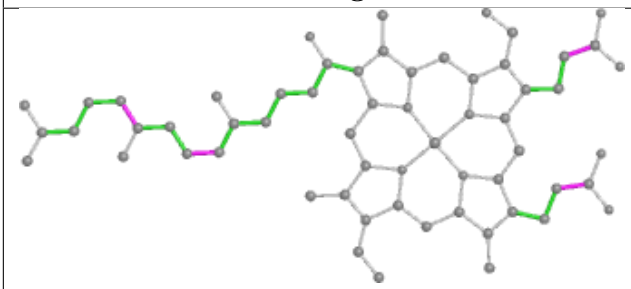
Ligand HEA N 602



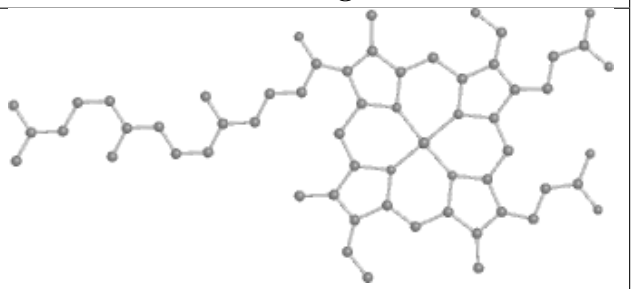
Bond lengths



Bond angles

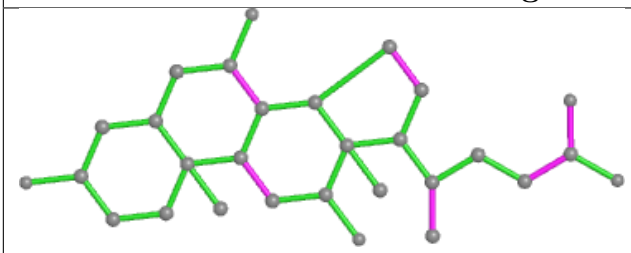


Torsions



Rings

Ligand CHD P 301



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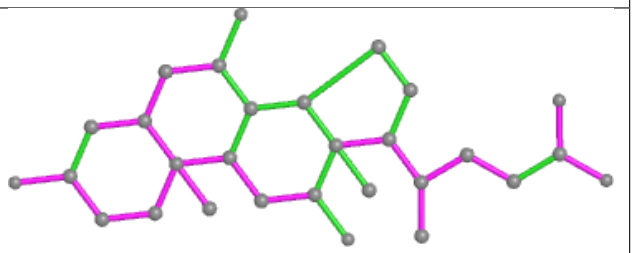
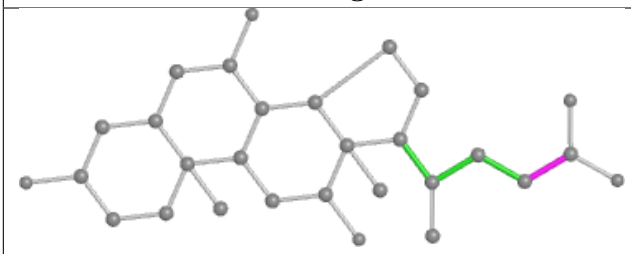
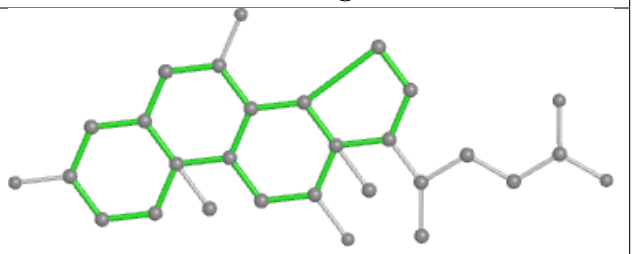


Bond angles

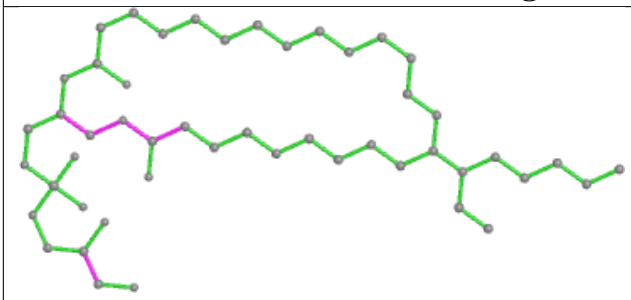


Torsions

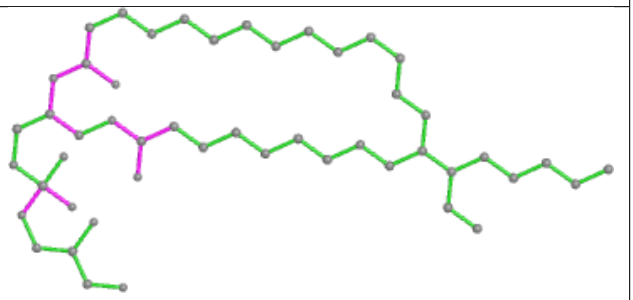


Rings

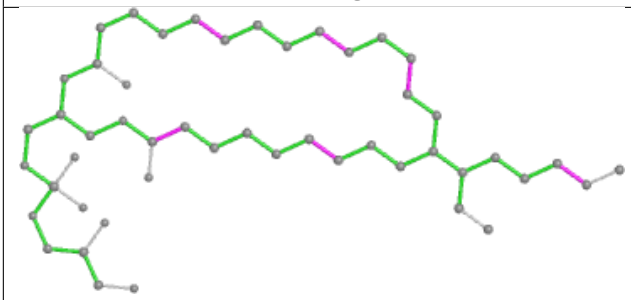
Ligand PGV N 609



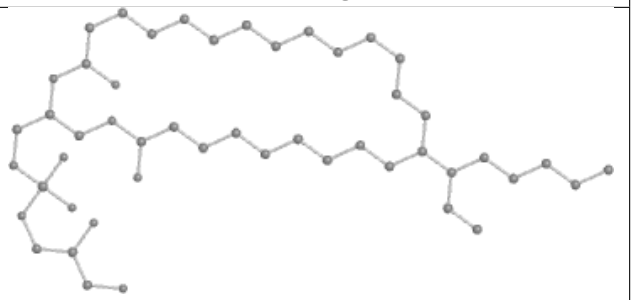
Bond lengths



Bond angles

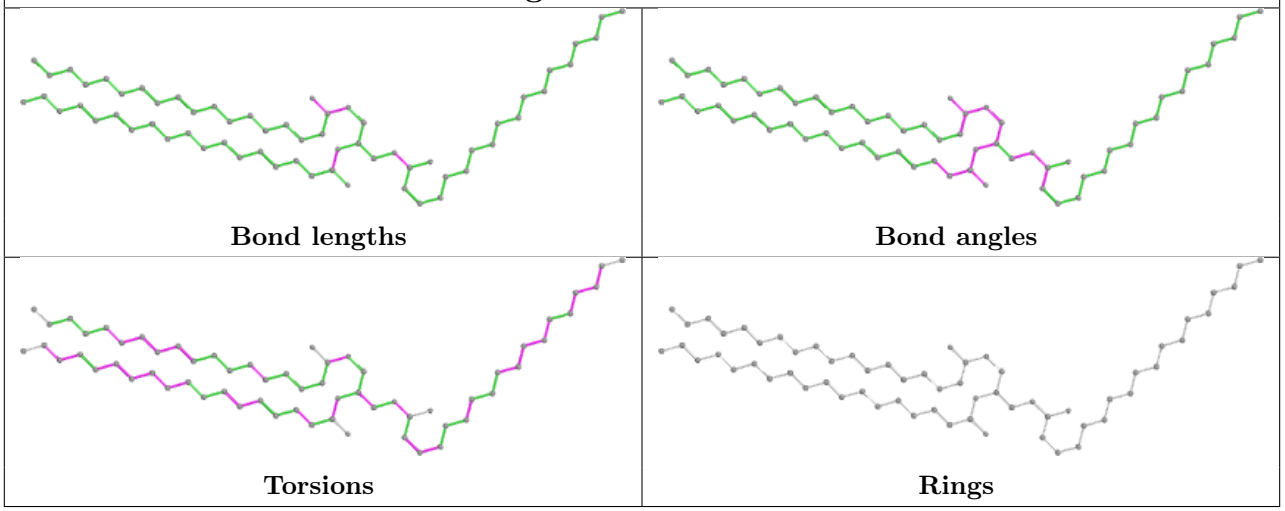


Torsions

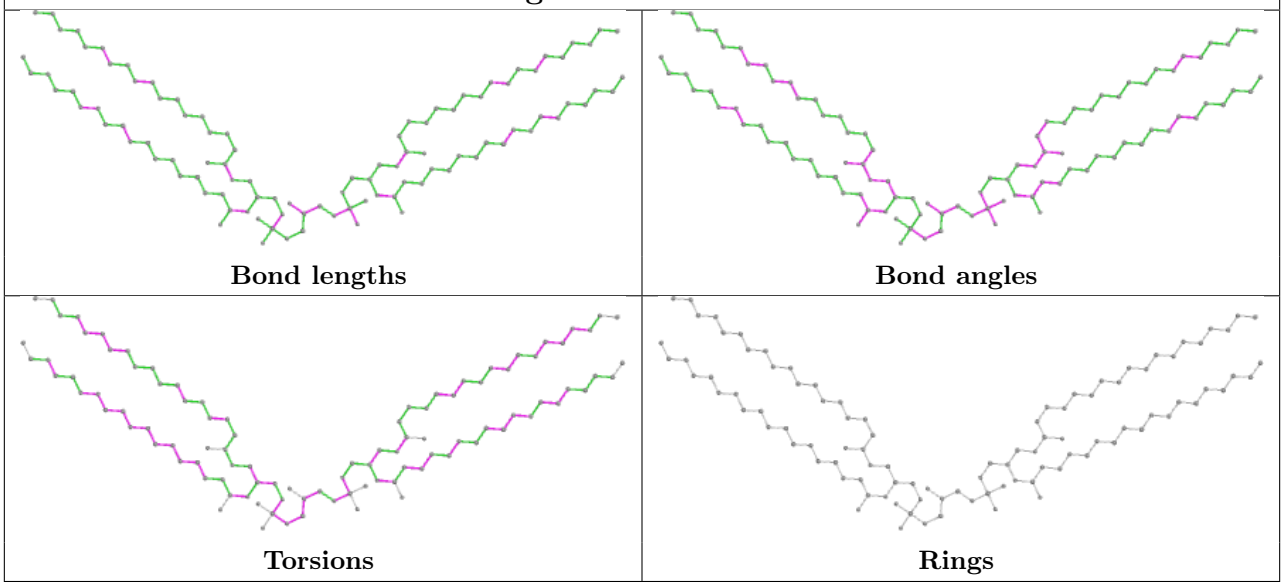


Rings

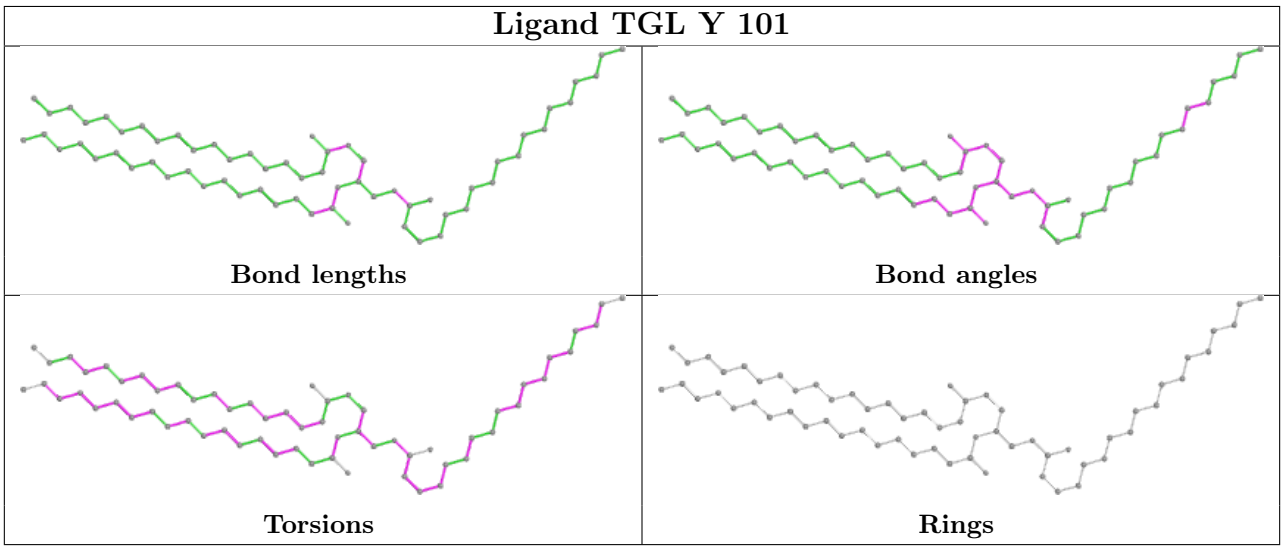
Ligand TGL B 301



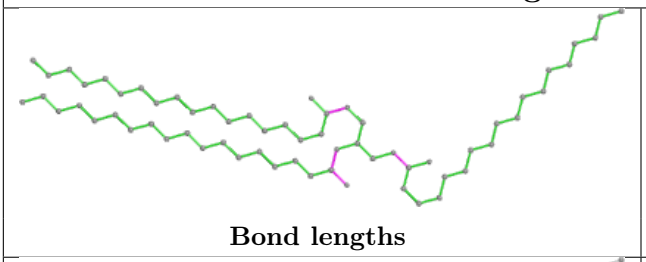
Ligand CDL P 304



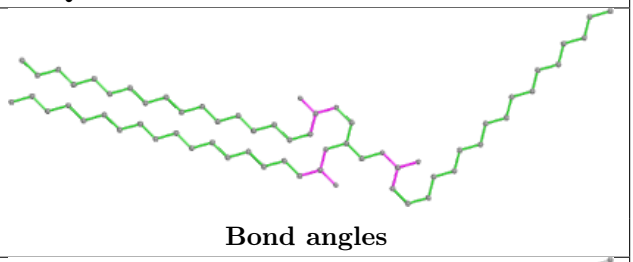
Ligand TGL Y 101



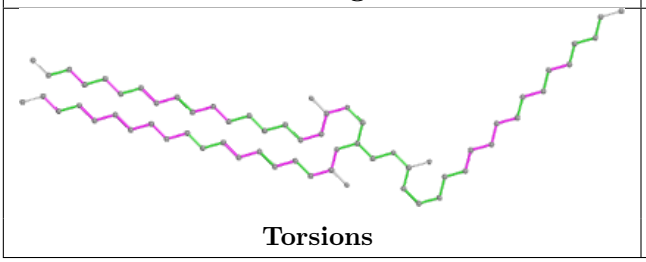
Ligand TGL Q 201



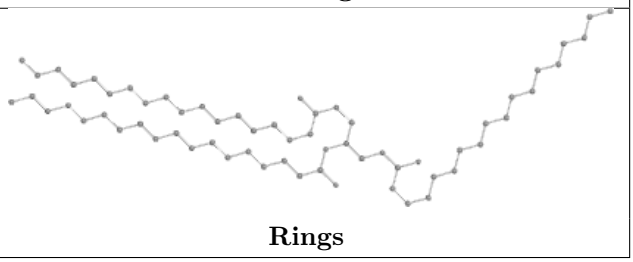
Bond lengths



Bond angles

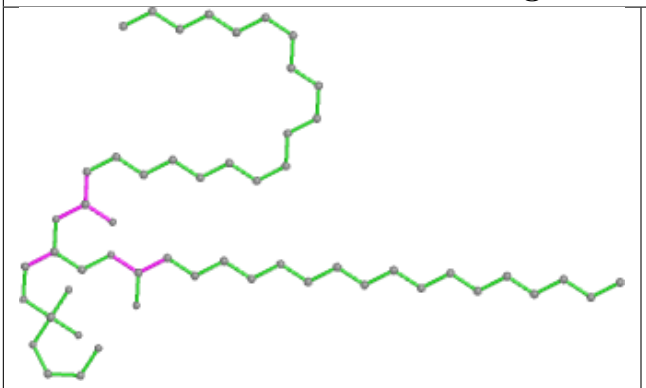


Torsions

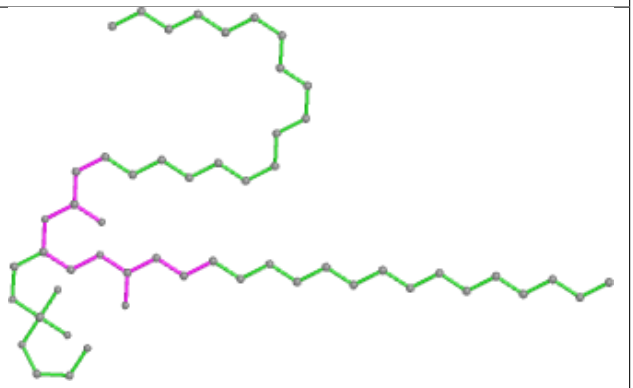


Rings

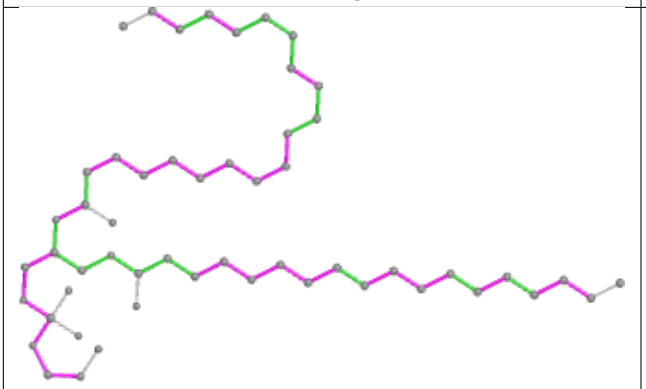
Ligand PEK C 307



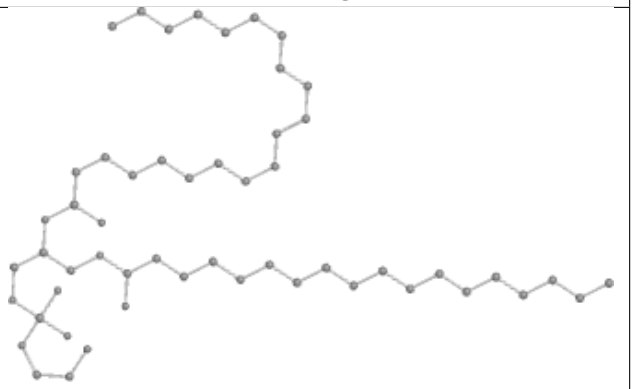
Bond lengths



Bond angles

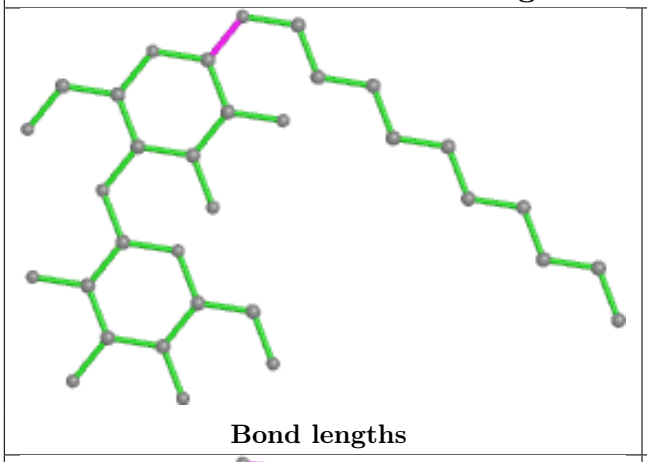


Torsions

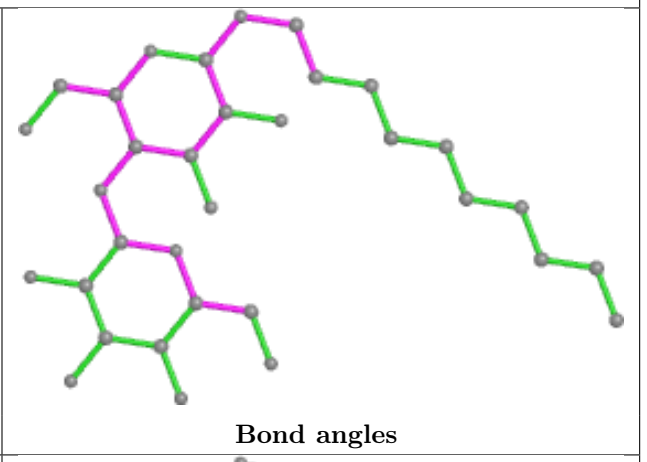


Rings

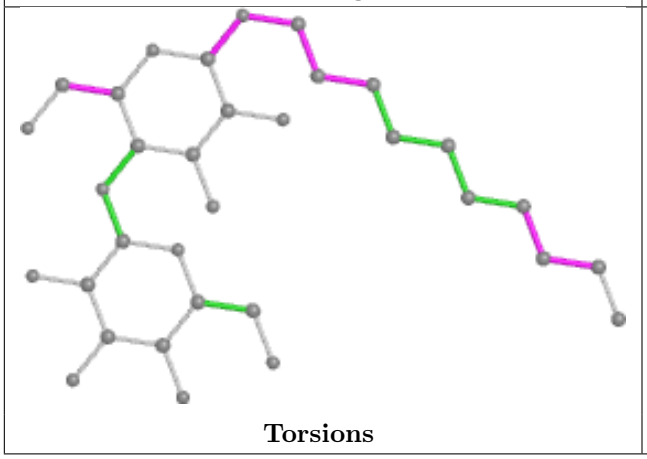
Ligand DMU C 311



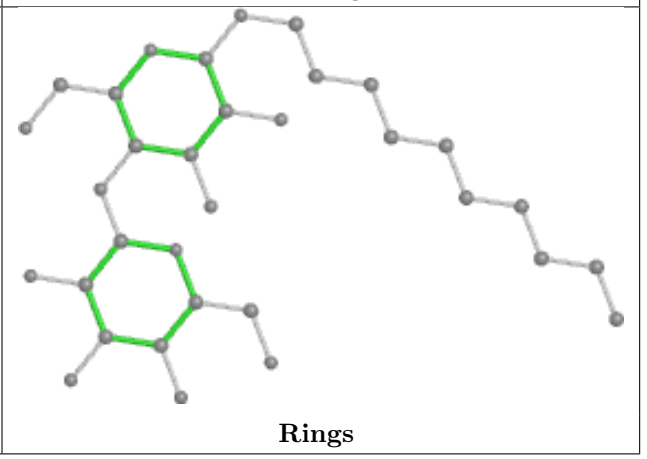
Bond lengths



Bond angles

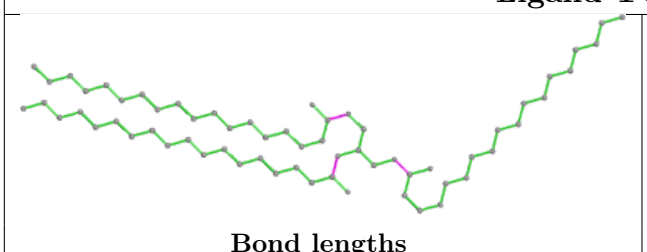


Torsions

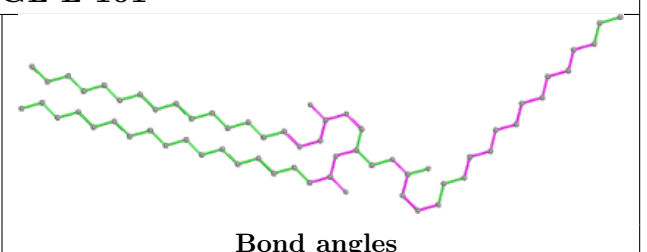


Rings

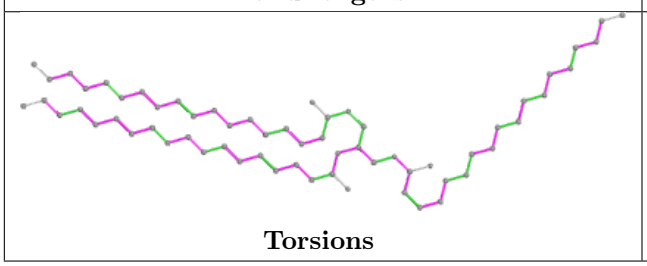
Ligand TGL L 101



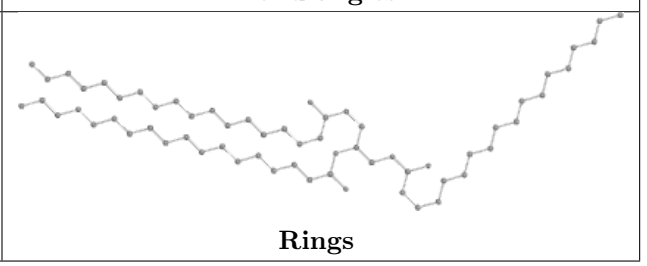
Bond lengths



Bond angles

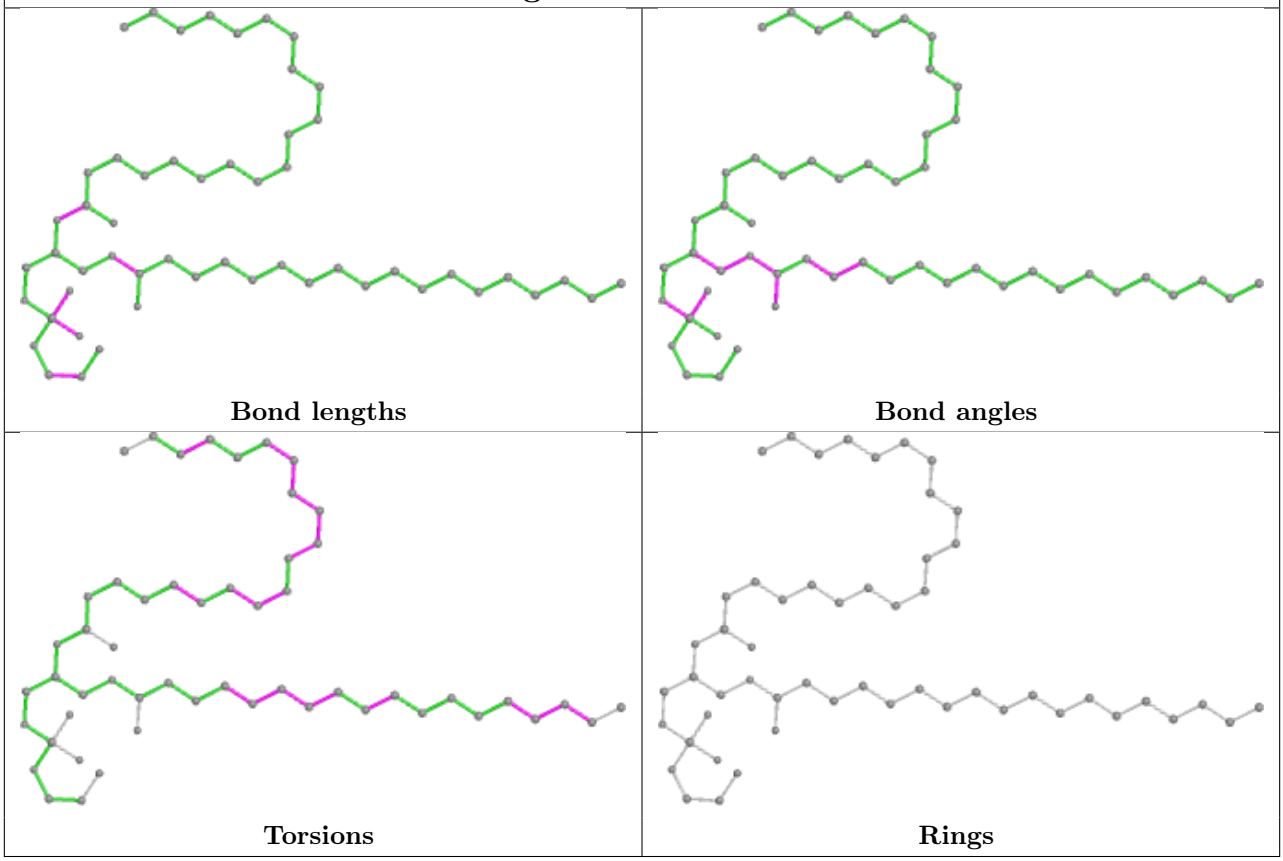


Torsions

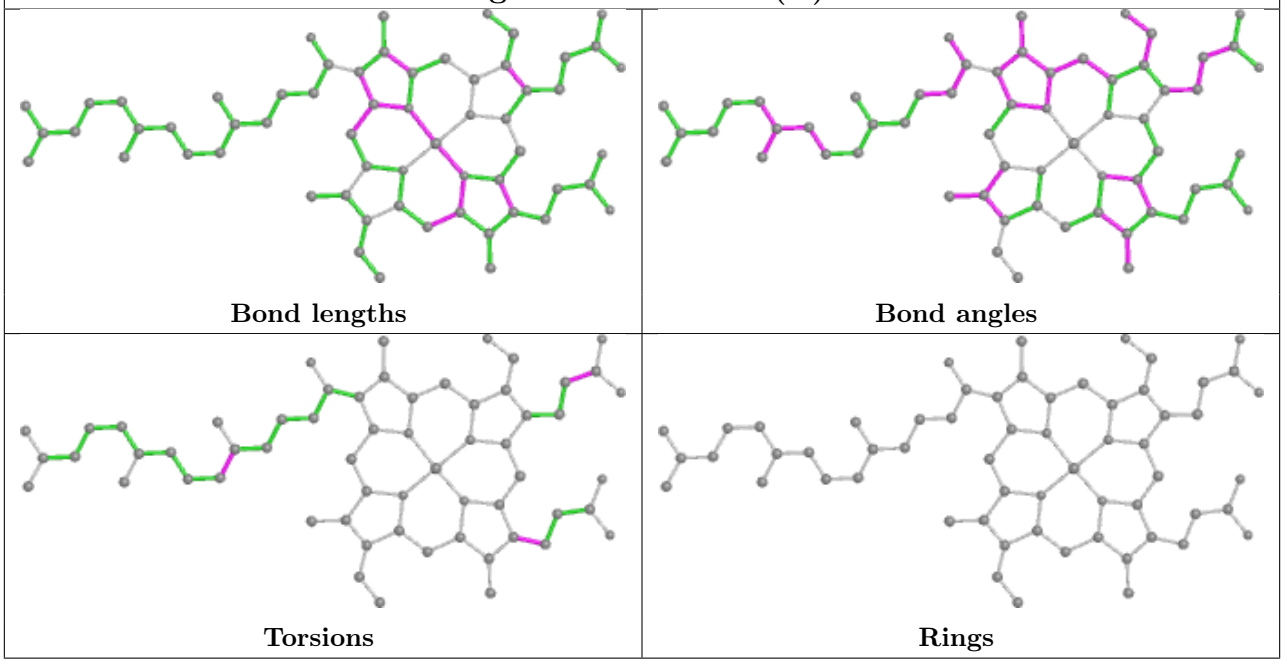


Rings

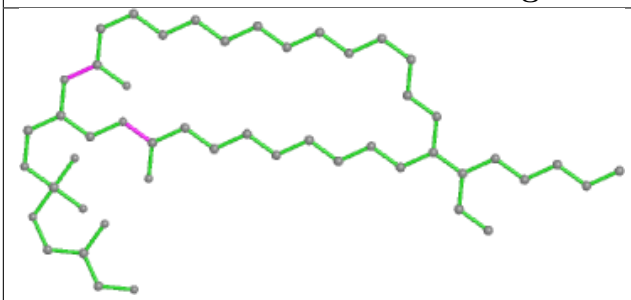
Ligand PEK G 101



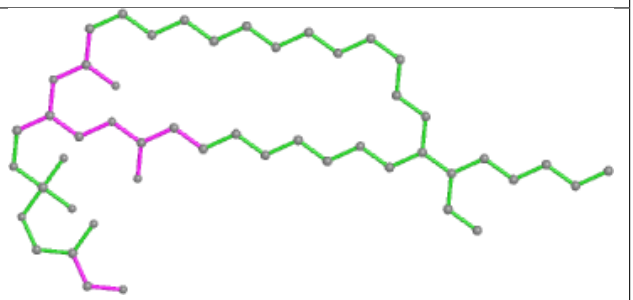
Ligand HEA N 603 (B)



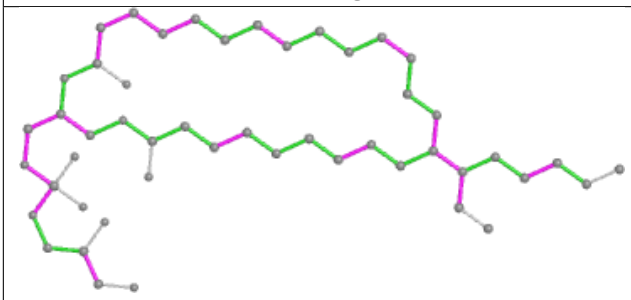
Ligand PGV C 308



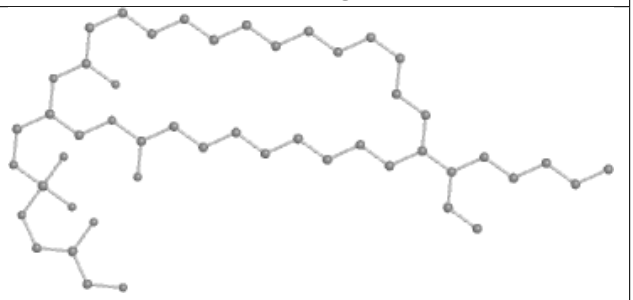
Bond lengths



Bond angles

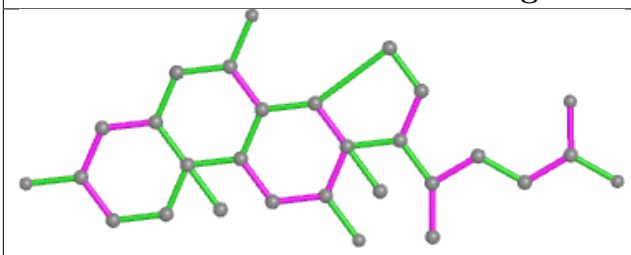


Torsions

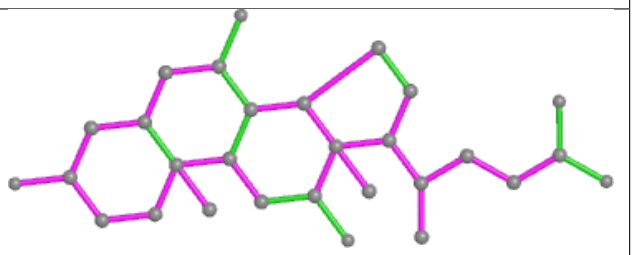


Rings

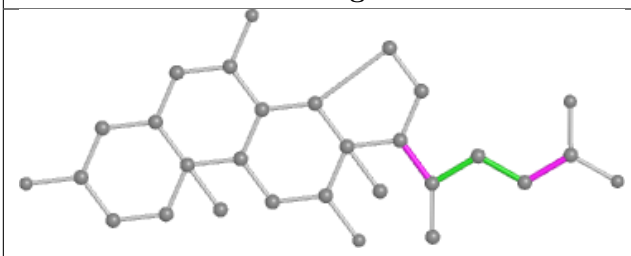
Ligand CHD C 301



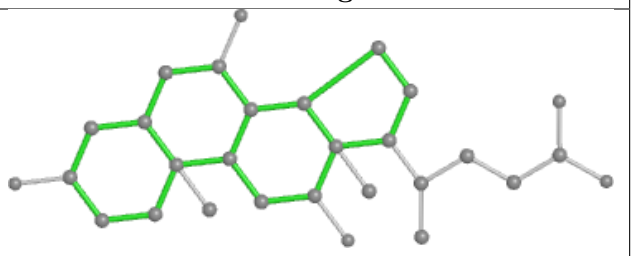
Bond lengths



Bond angles

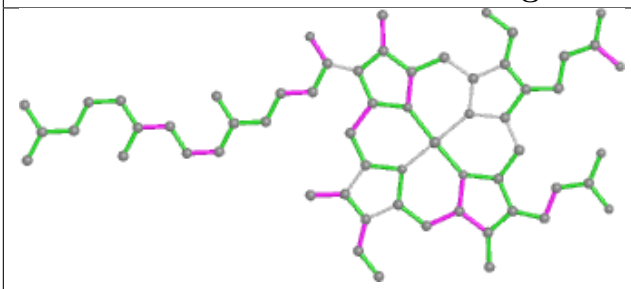


Torsions

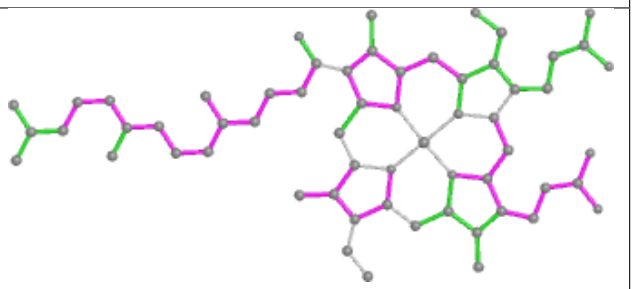


Rings

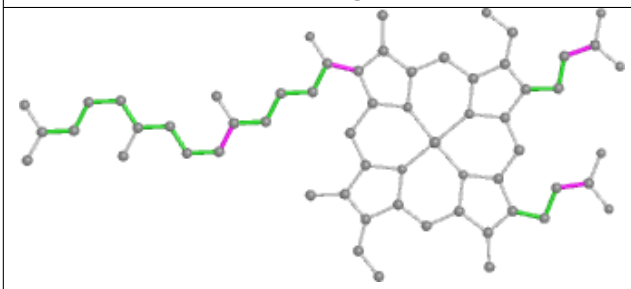
Ligand HEA A 601



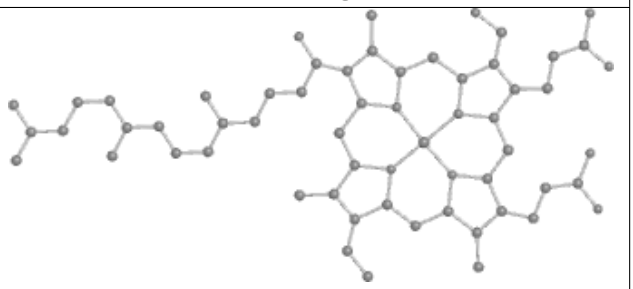
Bond lengths



Bond angles

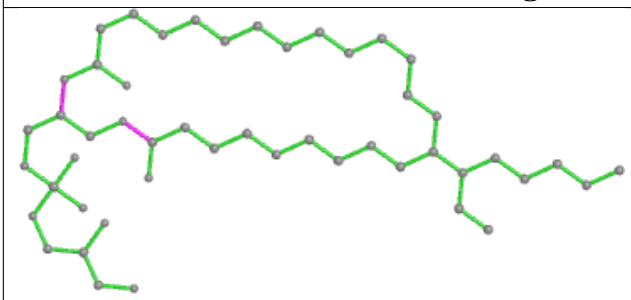


Torsions

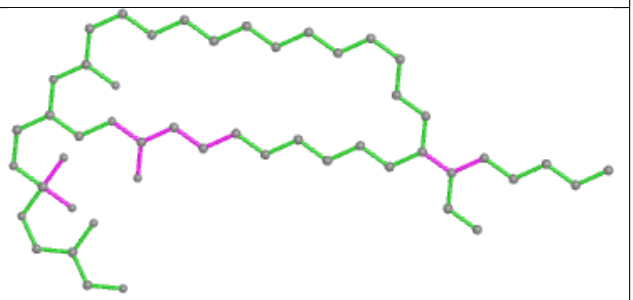


Rings

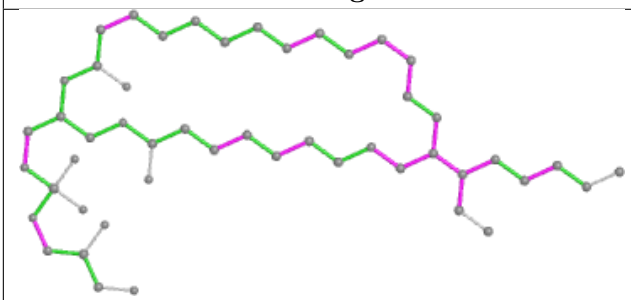
Ligand PGV C 304



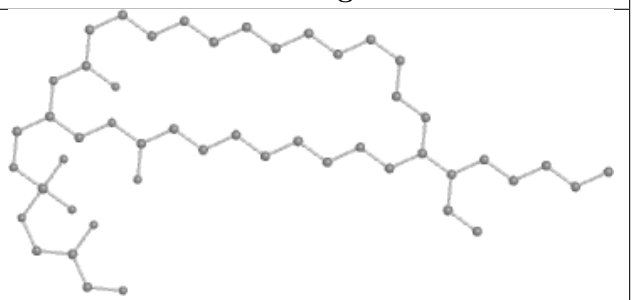
Bond lengths



Bond angles

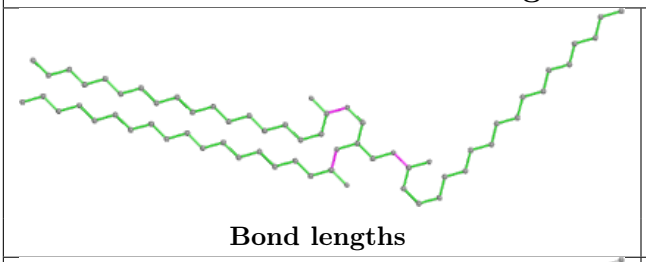


Torsions

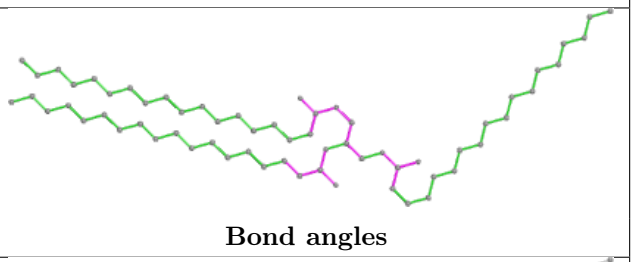


Rings

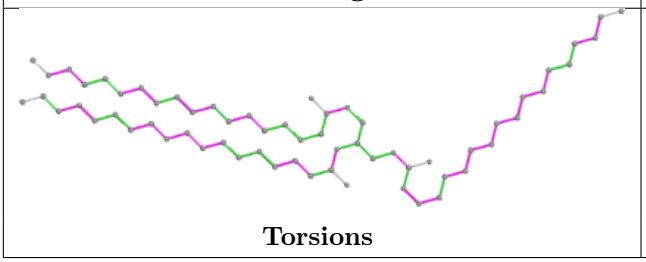
Ligand TGL N 610



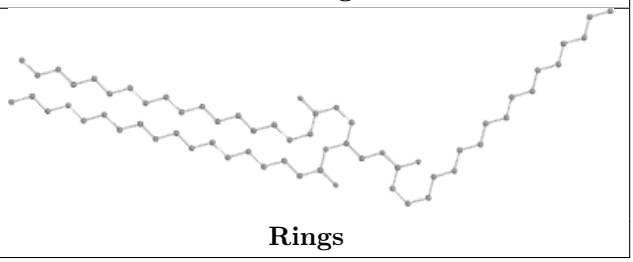
Bond lengths



Bond angles

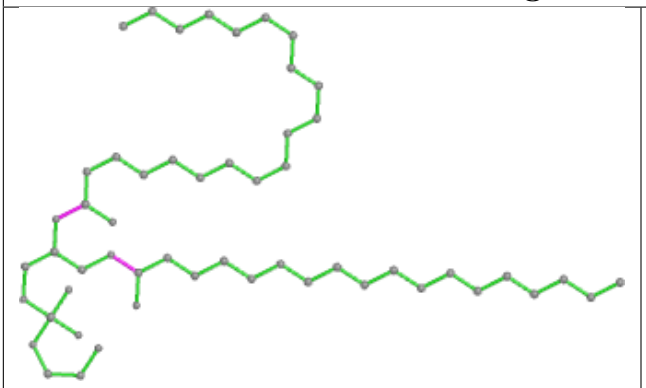


Torsions

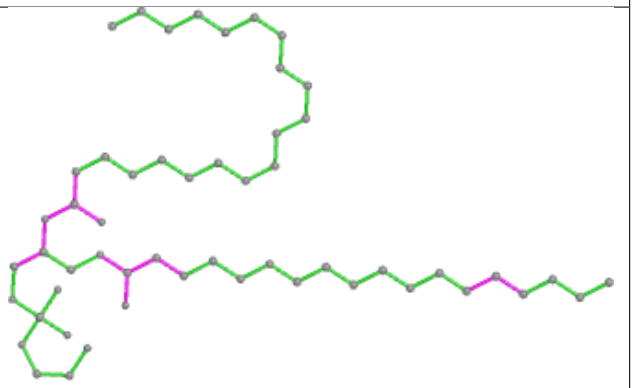


Rings

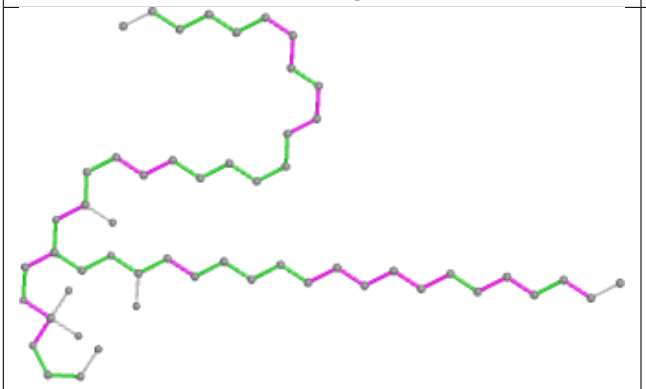
Ligand PEK P 307



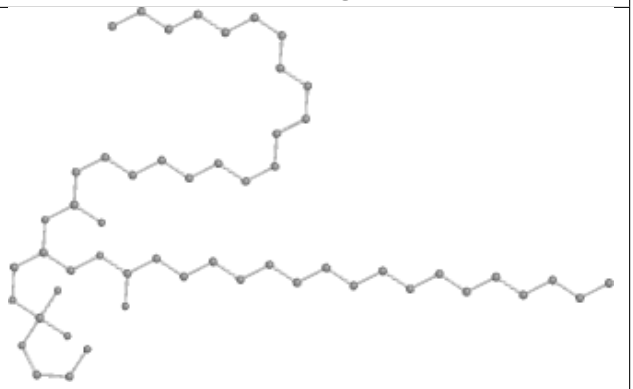
Bond lengths



Bond angles

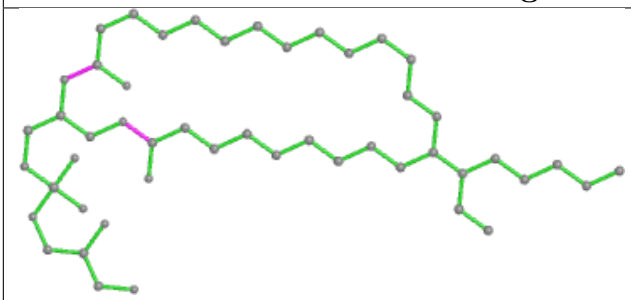


Torsions

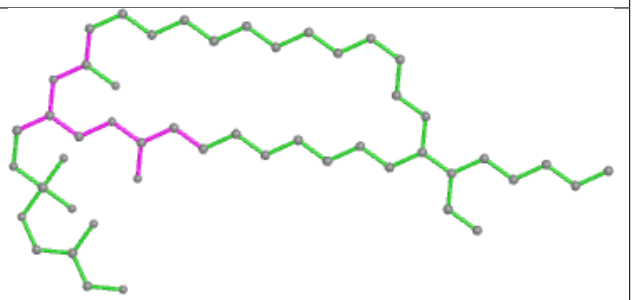


Rings

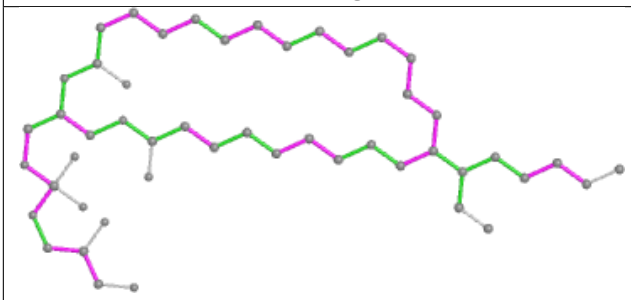
Ligand PGV U 101



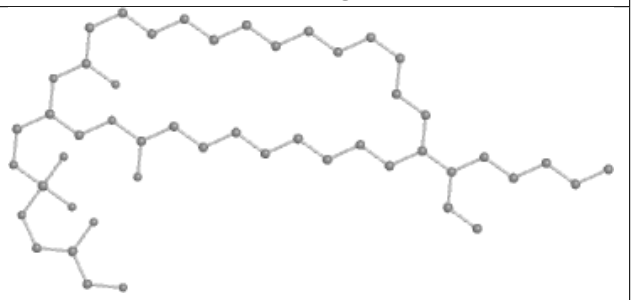
Bond lengths



Bond angles

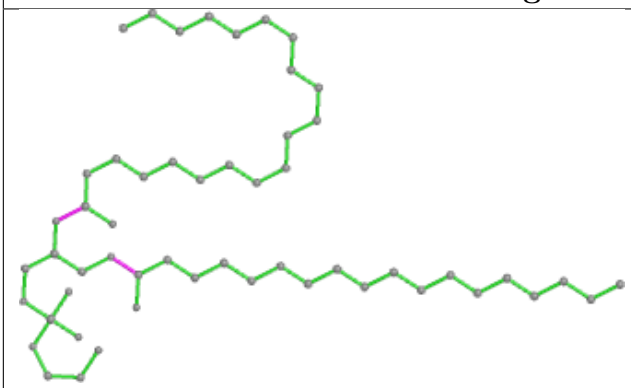


Torsions

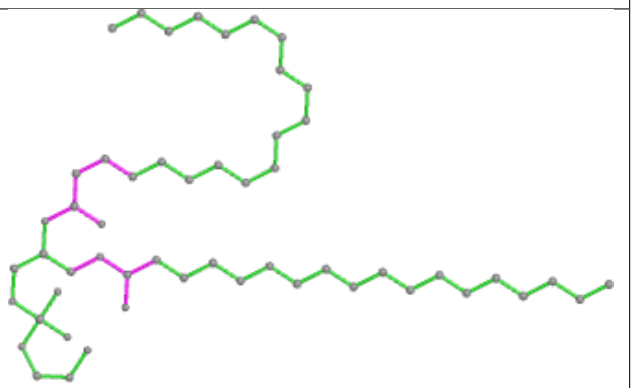


Rings

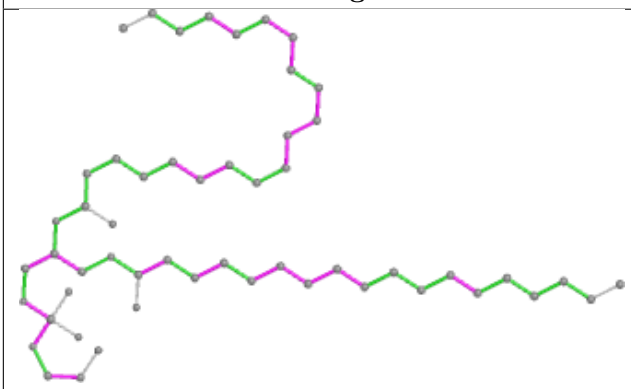
Ligand PEK C 309



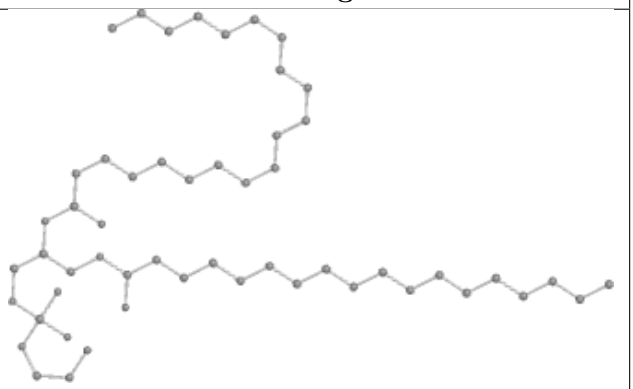
Bond lengths



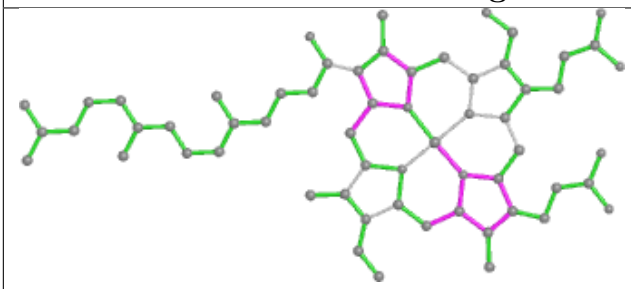
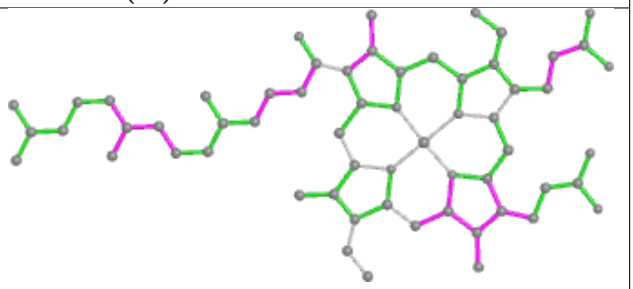
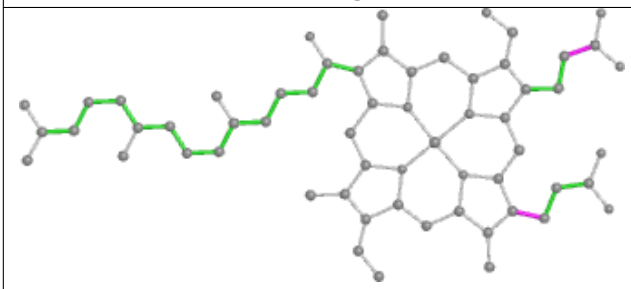
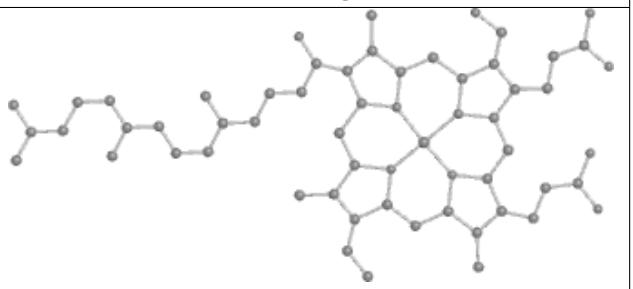
Bond angles



Torsions



Rings

Ligand HEA A 602 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

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%)	0.19	0 100 100	22, 28, 36, 73	0
1	N	513/514 (99%)	0.09	4 (0%) 86 87	25, 32, 41, 73	0
2	B	226/227 (99%)	0.13	3 (1%) 77 79	26, 35, 52, 74	0
2	O	226/227 (99%)	0.13	3 (1%) 77 79	32, 42, 66, 91	0
3	C	259/261 (99%)	0.16	1 (0%) 92 93	25, 32, 42, 79	0
3	P	259/261 (99%)	0.11	2 (0%) 86 87	26, 33, 45, 76	0
4	D	144/147 (97%)	0.00	1 (0%) 87 88	29, 37, 58, 79	0
4	Q	144/147 (97%)	0.78	12 (8%) 11 13	37, 51, 81, 145	0
5	E	105/109 (96%)	0.02	3 (2%) 51 54	29, 36, 59, 115	0
5	R	105/109 (96%)	0.05	2 (1%) 66 69	36, 44, 64, 121	0
6	F	98/98 (100%)	0.62	8 (8%) 11 13	29, 39, 92, 150	0
6	S	98/98 (100%)	0.69	8 (8%) 11 13	29, 40, 96, 144	0
7	G	83/85 (97%)	1.03	15 (18%) 1 1	30, 40, 110, 146	0
7	T	83/85 (97%)	0.92	14 (16%) 1 1	29, 41, 101, 137	0
8	H	79/85 (92%)	0.26	6 (7%) 13 15	32, 43, 92, 104	0
8	U	79/85 (92%)	0.31	5 (6%) 20 22	37, 47, 105, 121	0
9	I	72/73 (98%)	0.45	5 (6%) 16 19	34, 47, 78, 91	0
9	V	72/73 (98%)	0.38	4 (5%) 24 27	33, 56, 76, 104	0
10	J	58/59 (98%)	0.36	3 (5%) 27 30	32, 42, 65, 112	0
10	W	58/59 (98%)	0.33	2 (3%) 45 48	36, 47, 73, 117	0
11	K	49/56 (87%)	0.03	0 100 100	35, 42, 57, 66	0
11	X	49/56 (87%)	0.40	4 (8%) 11 13	45, 52, 77, 83	0
12	L	46/47 (97%)	0.22	1 (2%) 62 64	29, 35, 56, 94	0
12	Y	46/47 (97%)	0.29	2 (4%) 35 38	36, 42, 63, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.39	2 (4%) 31 34	30, 34, 70, 121	0
13	Z	43/46 (93%)	0.44	4 (9%) 8 10	40, 46, 84, 127	0
All	All	3550/3614 (98%)	0.26	114 (3%) 47 50	22, 36, 68, 150	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	27.1
4	Q	5	VAL	16.9
6	S	97	ALA	16.6
6	F	97	ALA	13.9
6	F	2	SER	11.9
7	G	10	GLY	10.8
10	J	58	LYS	10.7
4	Q	7	LYS	10.6
4	Q	4	SER	9.7
6	F	96	LEU	9.7
6	S	2	SER	9.7
6	F	1	ALA	9.0
7	T	3	ALA	8.7
7	G	3	ALA	8.6
6	S	1	ALA	8.0
6	S	98	HIS	7.9
6	F	98	HIS	7.4
6	S	94	HIS	7.0
7	G	9	GLY	6.9
6	S	96	LEU	6.8
13	M	42	LYS	6.3
10	W	58	LYS	6.3
13	Z	43	SER	6.3
12	Y	47	LYS	6.2
7	G	6	GLY	6.2
5	R	109	VAL	6.0
7	G	2	SER	5.8
9	I	37	PHE	5.4
7	T	10	GLY	5.3
4	Q	8	SER	5.3
8	U	7	LYS	5.2
13	Z	42	LYS	5.1
7	T	1	ALA	5.0
3	P	3	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	4.9
7	T	42	ARG	4.9
7	T	2	SER	4.8
6	F	95	GLN	4.7
7	T	8	HIS	4.6
8	U	8	ILE	4.3
7	T	36	TRP	4.2
5	E	109	VAL	4.2
13	M	43	SER	4.2
10	W	57	HIS	4.1
7	G	42	ARG	4.1
2	O	227	LEU	4.0
6	S	95	GLN	4.0
5	R	5	HIS	4.0
6	F	94	HIS	4.0
7	T	39	SER	3.9
7	G	8	HIS	3.9
7	T	40	GLY	3.9
2	O	113	TYR	3.8
2	O	91	ASN	3.8
8	U	10	ASN	3.7
7	G	1	ALA	3.7
6	S	93	PRO	3.6
8	H	44	THR	3.6
8	H	8	ILE	3.6
7	T	4	ALA	3.5
8	U	45	ALA	3.5
7	T	5	LYS	3.5
10	J	1	PHE	3.5
9	I	30	GLY	3.3
4	D	4	SER	3.2
7	G	5	LYS	3.2
7	G	36	TRP	3.1
7	G	7	ASP	3.1
7	T	6	GLY	3.1
9	V	34	PHE	3.1
11	X	13	TYR	3.1
9	I	29	LEU	3.1
3	C	33[A]	MET	3.0
11	X	7	PRO	3.0
8	H	46	LYS	2.9
9	I	25	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
12	L	2	HIS	2.9
4	Q	147	LYS	2.8
4	Q	87[A]	PHE	2.7
2	B	16[A]	ILE	2.7
9	V	37	PHE	2.7
9	V	2	THR	2.6
11	X	6	ALA	2.6
8	H	10	ASN	2.6
1	N	513	LEU	2.6
8	H	47	GLY	2.5
1	N	382[A]	SER	2.5
1	N	297[A]	MET	2.4
3	P	33[A]	MET	2.4
1	N	311[A]	ILE	2.4
9	I	33	THR	2.4
2	B	59	GLN	2.4
5	E	5	HIS	2.4
7	T	70[A]	PHE	2.3
13	Z	40	TYR	2.3
7	G	70[A]	PHE	2.3
8	U	9	LYS	2.3
5	E	39	TYR	2.2
10	J	57	HIS	2.2
4	Q	33	LEU	2.2
12	Y	45	LEU	2.2
11	X	52	GLU	2.2
4	Q	140	TYR	2.2
7	G	4	ALA	2.2
6	F	3	GLY	2.2
8	H	48	GLY	2.2
4	Q	19[A]	ARG	2.2
4	Q	51	LEU	2.1
2	B	65	TRP	2.1
13	Z	32	TRP	2.1
4	Q	73	ARG	2.1
9	V	25	PHE	2.1
7	T	41	HIS	2.1
7	G	41	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.44	0.36	82,111,131,134	0
7	TPO	T	11	11/12	0.60	0.29	97,108,122,128	0
9	SAC	V	1	9/10	0.84	0.33	103,119,127,139	0
9	SAC	I	1	9/10	0.87	0.18	67,77,80,86	0
2	FME	O	1	10/11	0.97	0.12	37,40,50,63	0
1	FME	A	1	10/11	0.97	0.14	42,48,75,93	0
1	FME	N	1	10/11	0.97	0.14	45,54,74,87	0
2	FME	B	1	10/11	0.98	0.13	31,33,43,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	D	203	4/4	0.68	0.21	61,64,65,67	0
22	CHD	W	101	29/29	0.68	0.34	59,93,115,119	0
28	PSC	E	201	52/52	0.69	0.30	38,84,156,157	0
27	PEK	C	307	53/53	0.71	0.23	42,81,145,153	0
27	PEK	C	309	53/53	0.72	0.34	52,97,147,150	0
24	DMU	C	302	33/33	0.73	0.38	32,83,118,129	0
27	PEK	G	103	53/53	0.74	0.27	50,84,152,154	0
26	CDL	T	102	100/100	0.74	0.24	53,88,128,152	0
26	CDL	N	601	100/100	0.76	0.27	58,91,133,158	0
19	PGV	C	308	51/51	0.76	0.22	46,76,120,137	0
21	TGL	Q	201	63/63	0.76	0.22	49,76,96,110	0
27	PEK	P	307	53/53	0.78	0.26	42,75,124,141	0
24	DMU	P	306	33/33	0.78	0.32	47,78,120,125	0
28	PSC	O	302	52/52	0.78	0.28	44,86,158,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CDL	P	304	100/100	0.79	0.26	38,82,120,130	0
20	EDO	G	105	4/4	0.79	0.31	55,63,64,79	0
24	DMU	C	311	33/33	0.80	0.21	56,79,102,119	0
21	TGL	Y	101	63/63	0.81	0.28	45,79,114,142	0
19	PGV	U	101	51/51	0.82	0.23	48,78,115,140	0
24	DMU	C	310	33/33	0.82	0.27	58,79,103,110	0
24	DMU	P	309	33/33	0.82	0.18	66,87,99,103	0
24	DMU	P	308	33/33	0.83	0.23	53,79,102,105	0
20	EDO	A	611	4/4	0.83	0.25	52,62,67,69	0
26	CDL	C	305	100/100	0.83	0.26	39,77,116,124	0
19	PGV	Z	101	51/51	0.83	0.25	50,75,113,131	0
20	EDO	L	102	4/4	0.84	0.32	59,72,89,95	0
20	EDO	A	616	4/4	0.85	0.27	46,48,49,51	0
20	EDO	N	620	4/4	0.85	0.32	43,52,54,68	0
22	CHD	J	101	29/29	0.85	0.23	54,79,113,116	0
21	TGL	D	201	63/63	0.85	0.21	35,64,87,100	0
21	TGL	L	101	63/63	0.85	0.20	34,59,94,111	0
21	TGL	N	610	63/63	0.86	0.20	53,78,101,119	0
24	DMU	Z	102	33/33	0.86	0.17	47,58,71,78	0
20	EDO	N	615	4/4	0.86	0.17	56,56,62,63	0
19	PGV	A	609	51/51	0.87	0.26	36,75,108,126	0
21	TGL	B	301	63/63	0.89	0.16	41,73,97,103	0
20	EDO	N	619	4/4	0.90	0.28	49,54,65,67	0
25	UNX	C	303	1/1	0.90	0.17	34,34,34,34	0
20	EDO	M	102	4/4	0.90	0.14	63,64,71,73	0
20	EDO	D	202	4/4	0.91	0.68	37,52,55,65	0
22	CHD	P	305	29/29	0.91	0.13	49,55,62,73	0
22	CHD	C	306	29/29	0.91	0.17	47,55,65,70	0
20	EDO	P	312	4/4	0.92	0.36	51,56,62,82	0
20	EDO	Y	102	4/4	0.92	0.26	64,67,70,77	0
20	EDO	B	306	4/4	0.92	0.21	33,46,51,53	0
20	EDO	N	616	4/4	0.92	0.21	53,59,64,68	0
20	EDO	A	612	4/4	0.92	0.24	53,55,58,59	0
20	EDO	B	305	4/4	0.92	0.48	54,58,72,89	0
16	MG	N	605	1/1	0.93	0.09	32,32,32,32	0
20	EDO	A	617	4/4	0.93	0.35	54,60,60,63	0
24	DMU	M	101	33/33	0.93	0.11	40,47,56,68	0
20	EDO	S	103	4/4	0.93	0.25	43,57,66,74	0
20	EDO	A	614	4/4	0.93	0.17	51,63,63,73	0
20	EDO	A	615	4/4	0.93	0.15	23,26,28,43	0
20	EDO	A	618	4/4	0.94	0.38	45,66,70,79	0
20	EDO	A	613	4/4	0.94	0.12	33,33,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	EDO	P	311	4/4	0.95	0.17	35,36,42,49	0
20	EDO	A	619	4/4	0.95	0.20	55,58,59,63	0
20	EDO	R	201	4/4	0.95	0.14	43,45,47,48	0
20	EDO	N	618	4/4	0.95	0.13	45,47,49,50	0
20	EDO	T	103	4/4	0.95	0.12	39,41,43,46	0
27	PEK	T	101	53/53	0.95	0.15	31,49,83,91	0
20	EDO	N	614	4/4	0.95	0.15	44,45,50,52	0
20	EDO	E	204	4/4	0.95	0.11	45,46,51,59	0
27	PEK	G	101	53/53	0.96	0.14	30,48,79,102	0
22	CHD	C	301	29/29	0.96	0.11	28,31,36,38	0
20	EDO	N	617	4/4	0.96	0.17	41,47,48,53	0
20	EDO	E	203	4/4	0.96	0.10	41,44,45,50	0
20	EDO	F	103	4/4	0.96	0.15	37,44,47,58	0
20	EDO	F	104	4/4	0.96	0.13	39,39,39,41	0
20	EDO	N	613	4/4	0.97	0.20	44,54,61,66	0
22	CHD	P	301	29/29	0.97	0.09	27,32,36,40	0
20	EDO	B	304	4/4	0.97	0.42	49,50,84,90	0
20	EDO	A	610	4/4	0.97	0.18	38,43,46,55	0
20	EDO	O	303	4/4	0.97	0.13	38,39,41,42	0
25	UNX	P	302	1/1	0.97	0.08	32,32,32,32	0
22	CHD	B	302	29/29	0.97	0.12	27,31,35,45	0
19	PGV	A	608	51/51	0.97	0.14	27,37,63,66	0
20	EDO	N	611	4/4	0.97	0.15	34,38,40,42	0
20	EDO	P	310	4/4	0.98	0.17	44,45,46,48	0
20	EDO	B	307	4/4	0.98	0.14	30,31,37,37	0
19	PGV	P	303	51/51	0.98	0.14	29,39,80,94	0
22	CHD	G	102	29/29	0.98	0.10	28,31,39,40	0
20	EDO	N	612	4/4	0.98	0.11	29,34,35,36	0
20	EDO	S	102	4/4	0.98	0.10	31,32,33,33	0
14	HEA	A	602[A]	60/60	0.98	0.16	20,24,29,35	60
20	EDO	E	202	4/4	0.98	0.12	40,45,45,46	0
18	AZI	N	607[B]	3/3	0.98	0.27	22,22,23,23	3
14	HEA	A	602[B]	60/60	0.98	0.16	17,25,28,30	60
14	HEA	N	603[A]	60/60	0.98	0.16	22,27,33,37	60
19	PGV	C	304	51/51	0.98	0.14	27,36,83,91	0
20	EDO	G	104	4/4	0.98	0.11	33,39,41,43	0
14	HEA	N	603[B]	60/60	0.98	0.16	24,30,41,44	60
19	PGV	N	609	51/51	0.98	0.12	30,41,66,76	0
14	HEA	N	602	60/60	0.99	0.12	25,31,56,65	0
18	AZI	N	608[A]	3/3	0.99	0.19	25,25,30,33	3
20	EDO	F	102	4/4	0.99	0.11	29,31,31,32	0
18	AZI	N	608[B]	3/3	0.99	0.19	22,22,22,23	3

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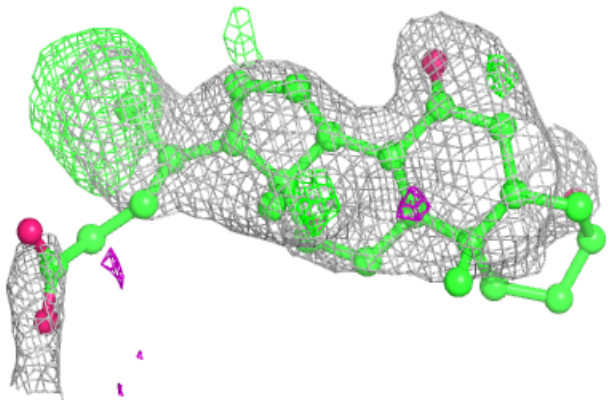
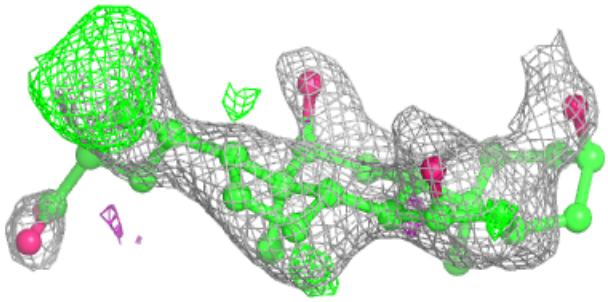
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	A	604	1/1	0.99	0.09	27,27,27,27	0
14	HEA	A	601	60/60	0.99	0.13	21,26,47,50	0
17	NA	N	606	1/1	0.99	0.06	35,35,35,35	0
18	AZI	A	606[B]	3/3	0.99	0.51	21,21,25,26	3
15	CU	A	603	1/1	1.00	0.18	28,28,28,28	0
15	CU	N	604	1/1	1.00	0.18	31,31,31,31	0
18	AZI	A	607[A]	3/3	1.00	0.19	25,25,27,29	3
18	AZI	A	607[B]	3/3	1.00	0.19	21,21,26,30	3
23	CUA	B	303	2/2	1.00	0.16	28,28,28,29	0
23	CUA	O	301	2/2	1.00	0.14	33,33,33,34	0
17	NA	A	605	1/1	1.00	0.09	29,29,29,29	0
29	ZN	F	101	1/1	1.00	0.15	34,34,34,34	0
29	ZN	S	101	1/1	1.00	0.15	36,36,36,36	0

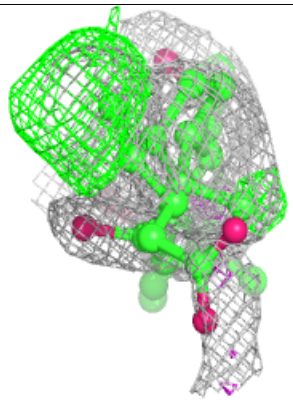
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD W 101:

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

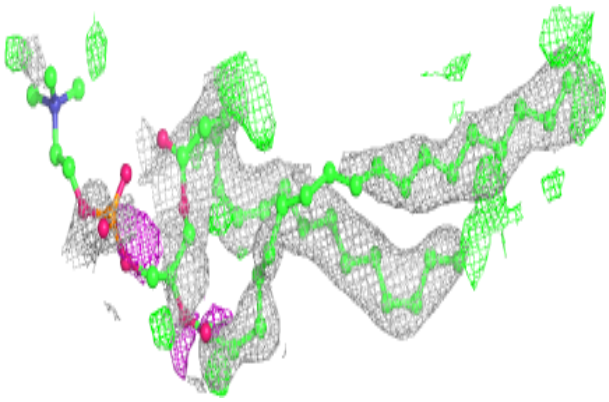


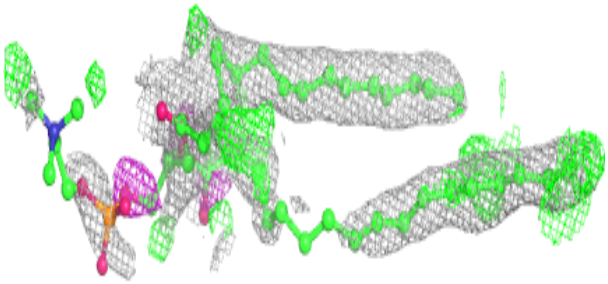


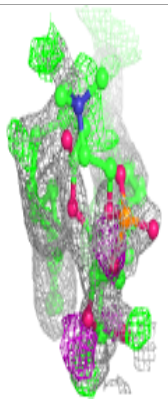


Electron density around PSC E 201:

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

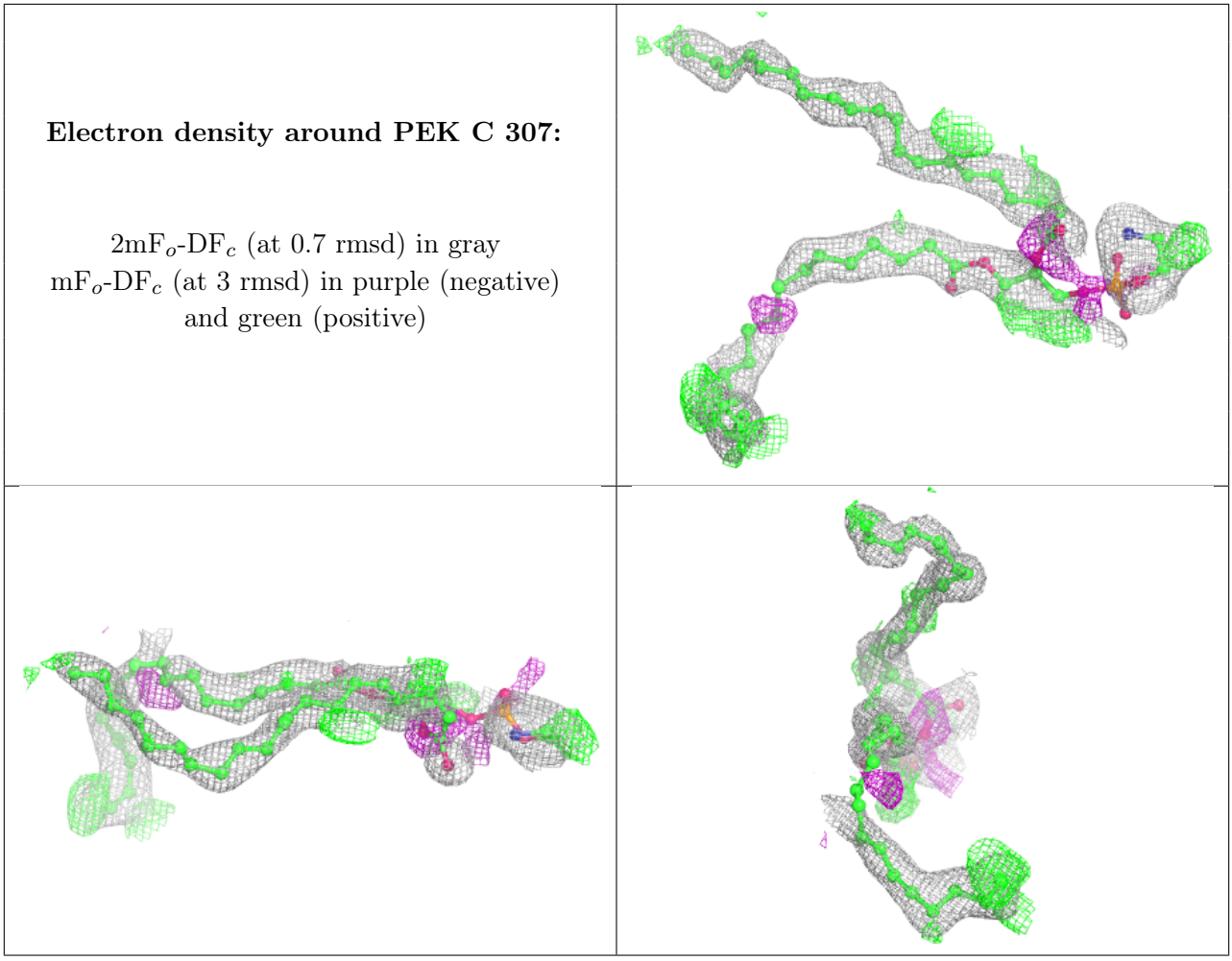






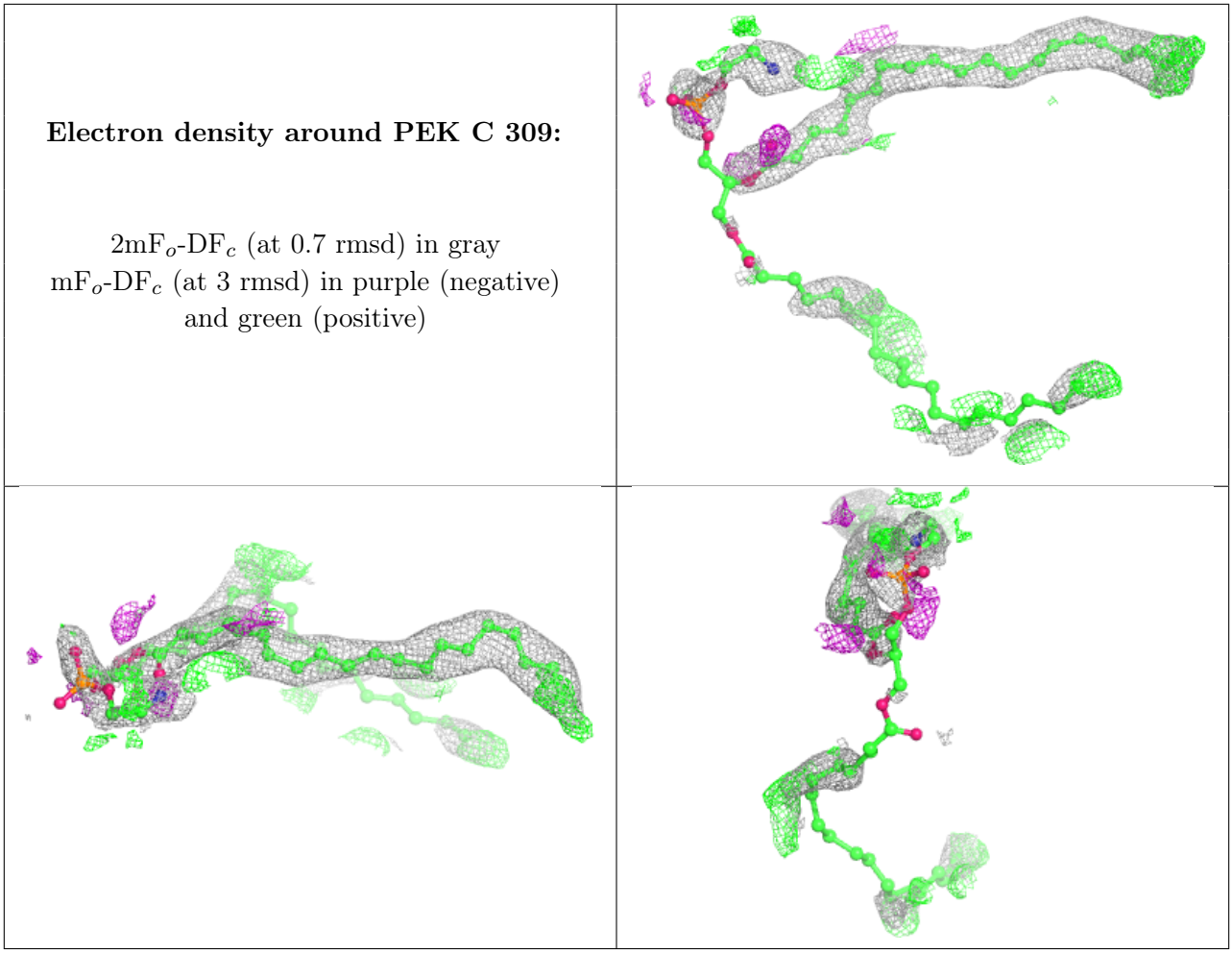
Electron density around PEK C 307:

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



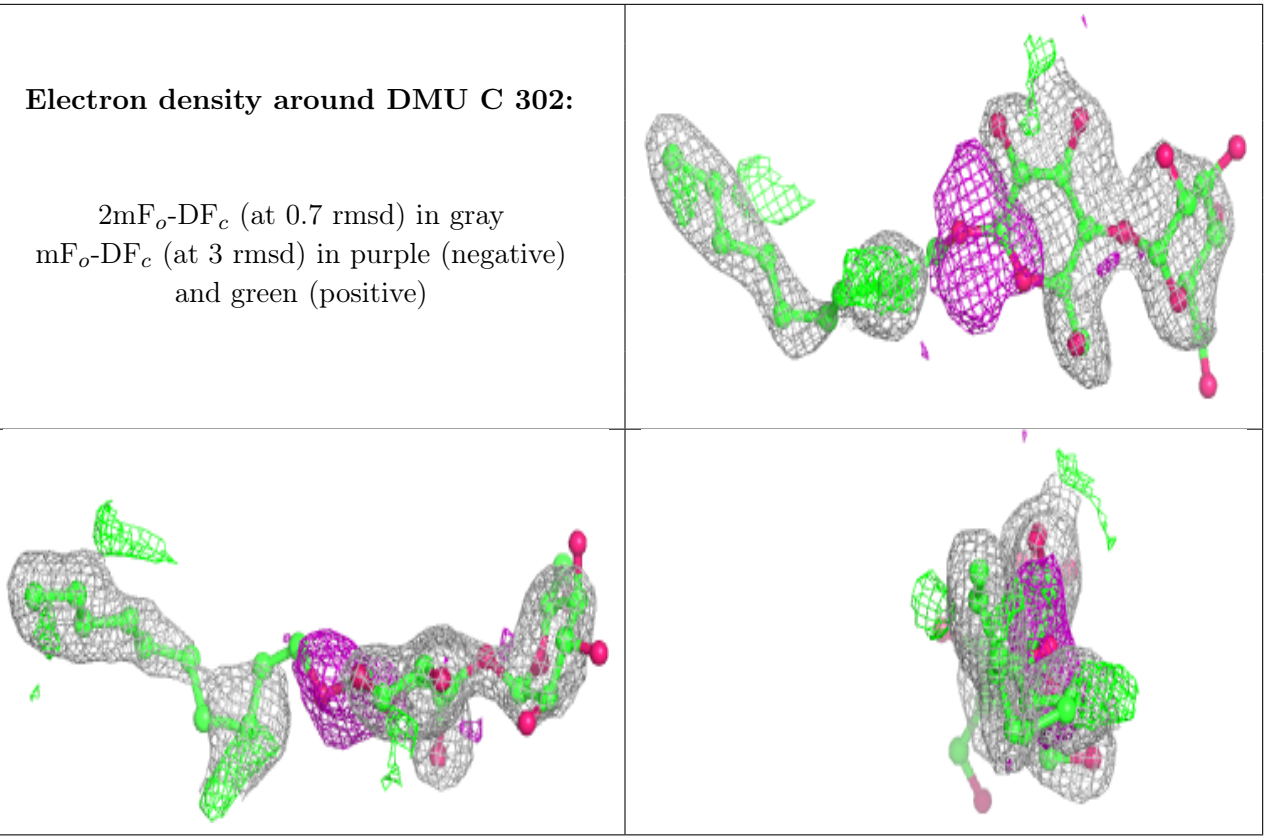
Electron density around PEK C 309:

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



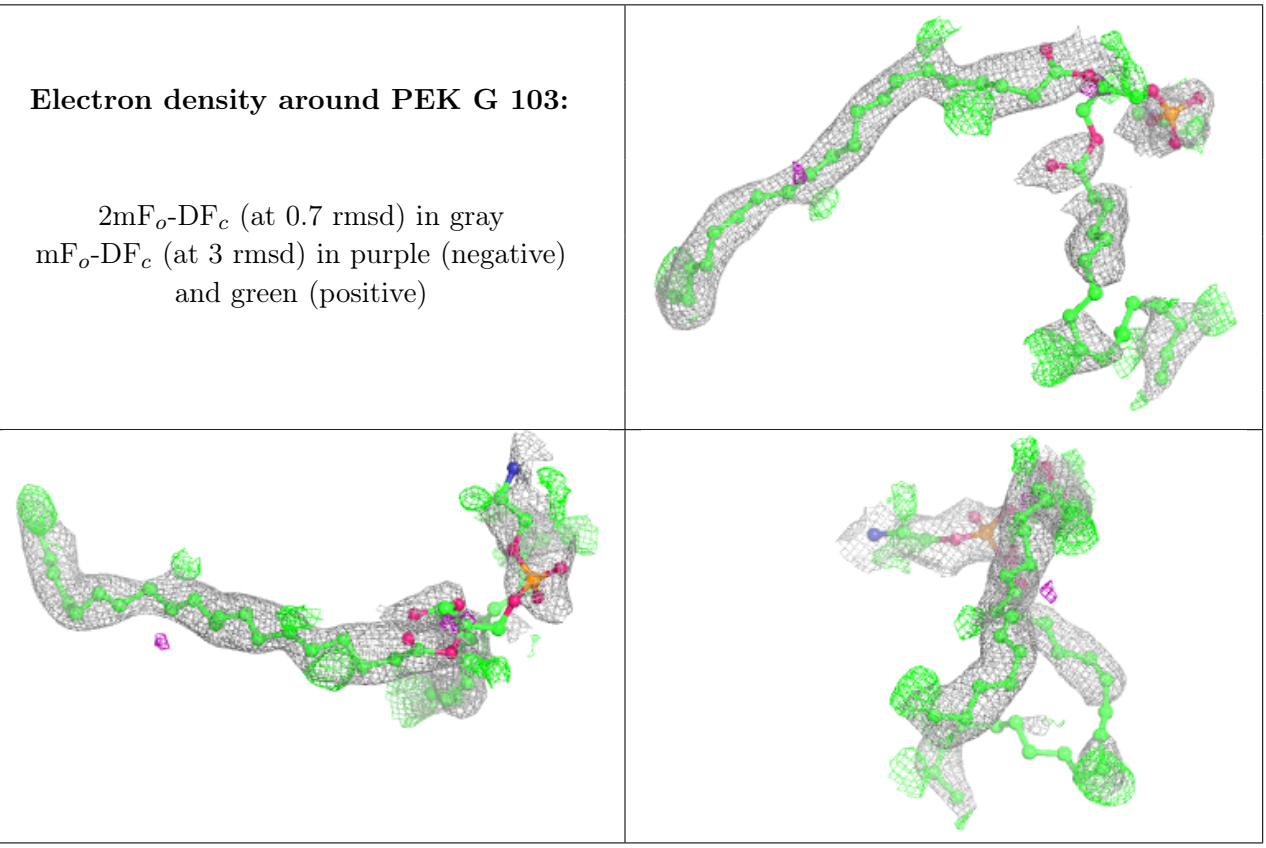
Electron density around DMU C 302:

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



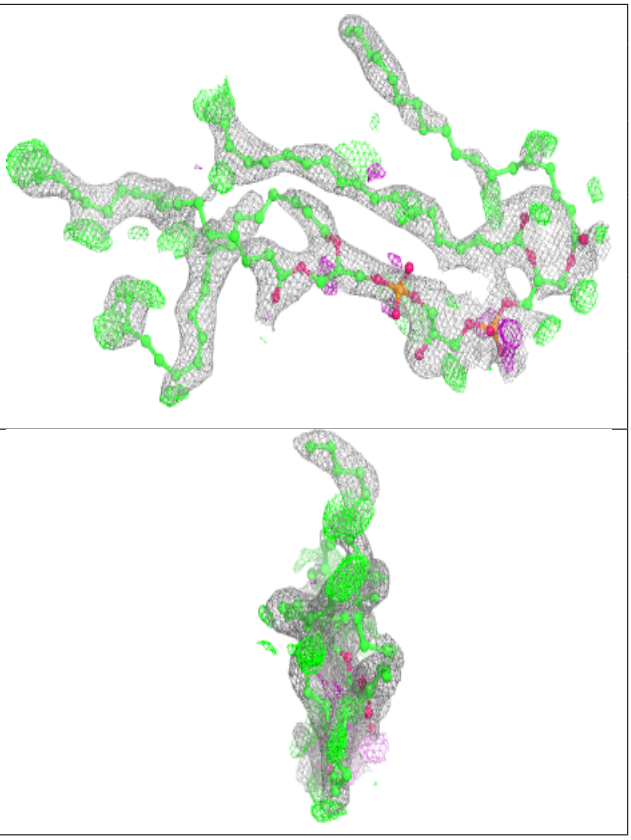
Electron density around PEK G 103:

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



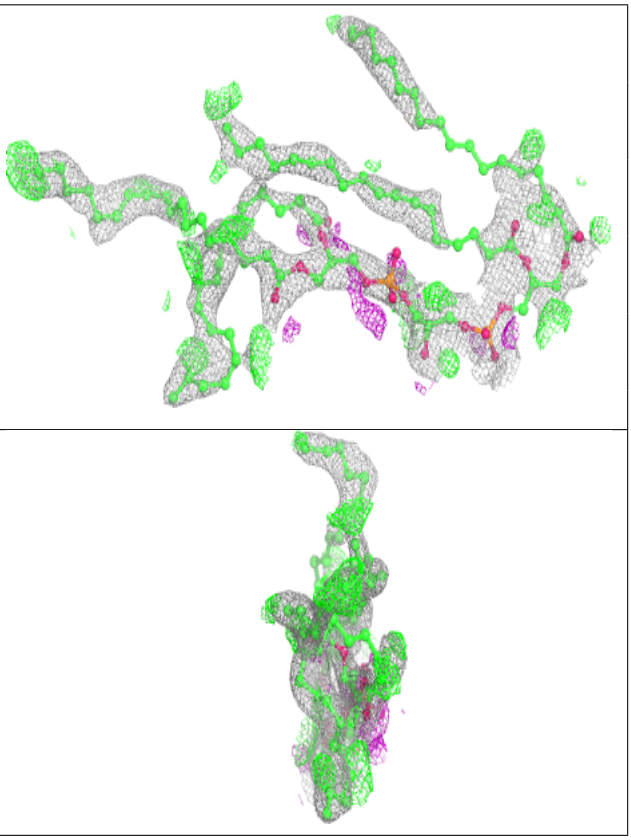
Electron density around CDL T 102:

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



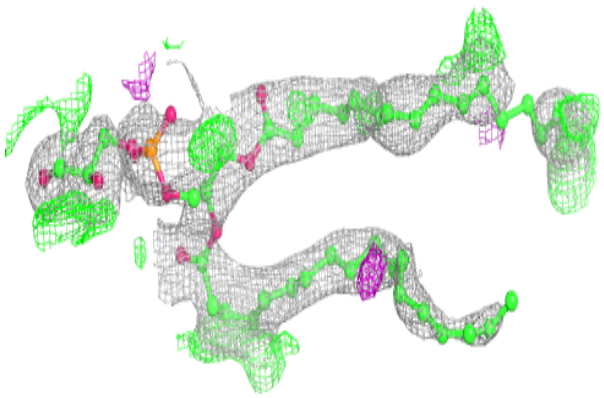
Electron density around CDL N 601:

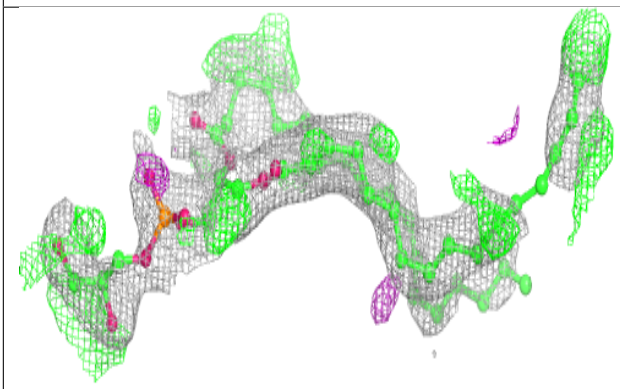
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

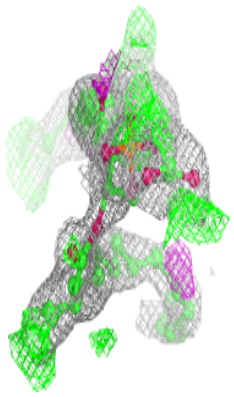


Electron density around PGV C 308:

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

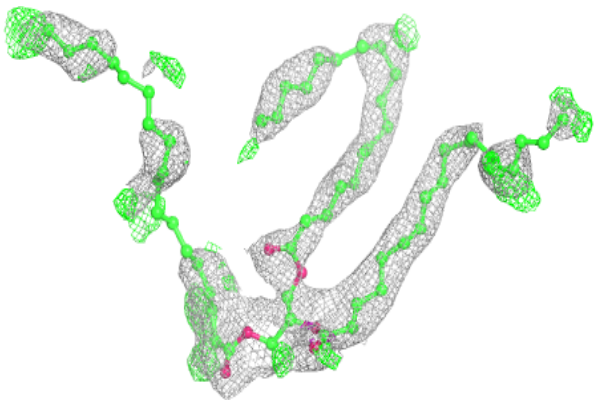


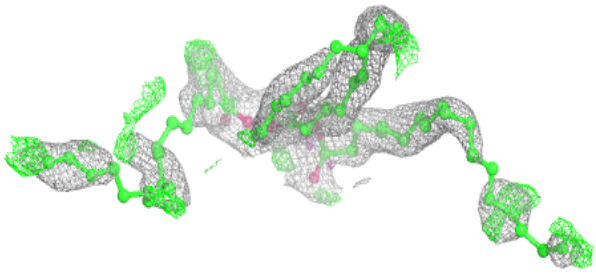


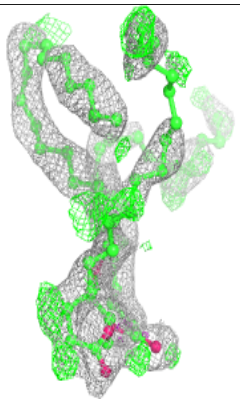


Electron density around TGL Q 201:

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

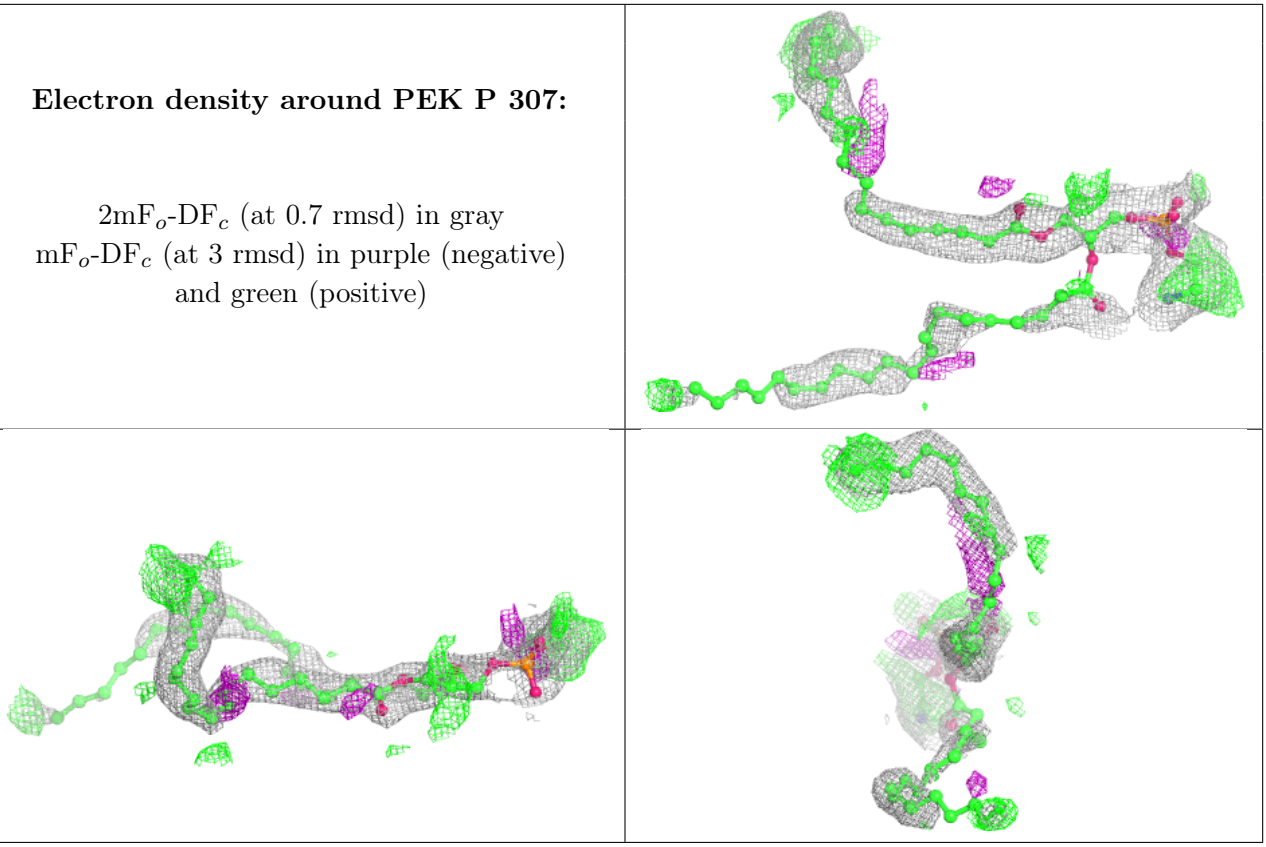






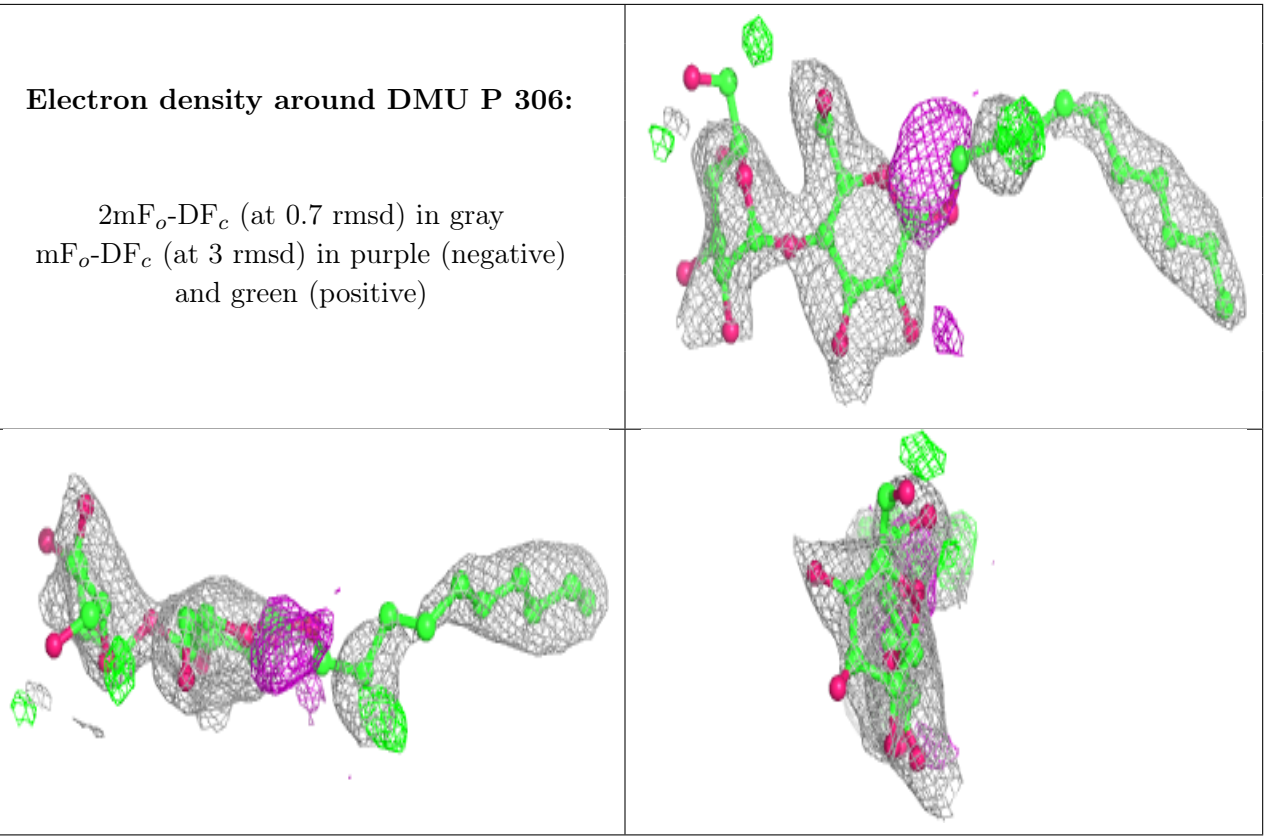
Electron density around PEK P 307:

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



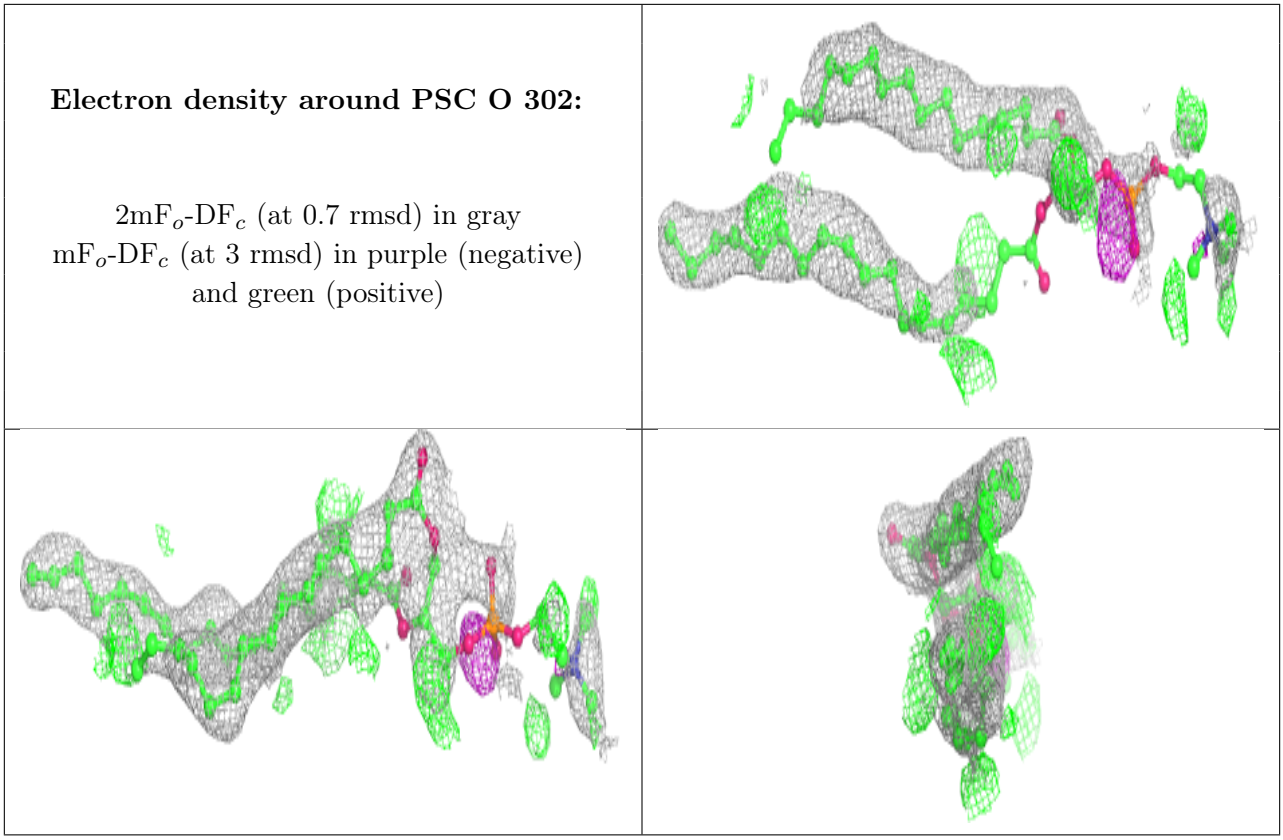
Electron density around DMU P 306:

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



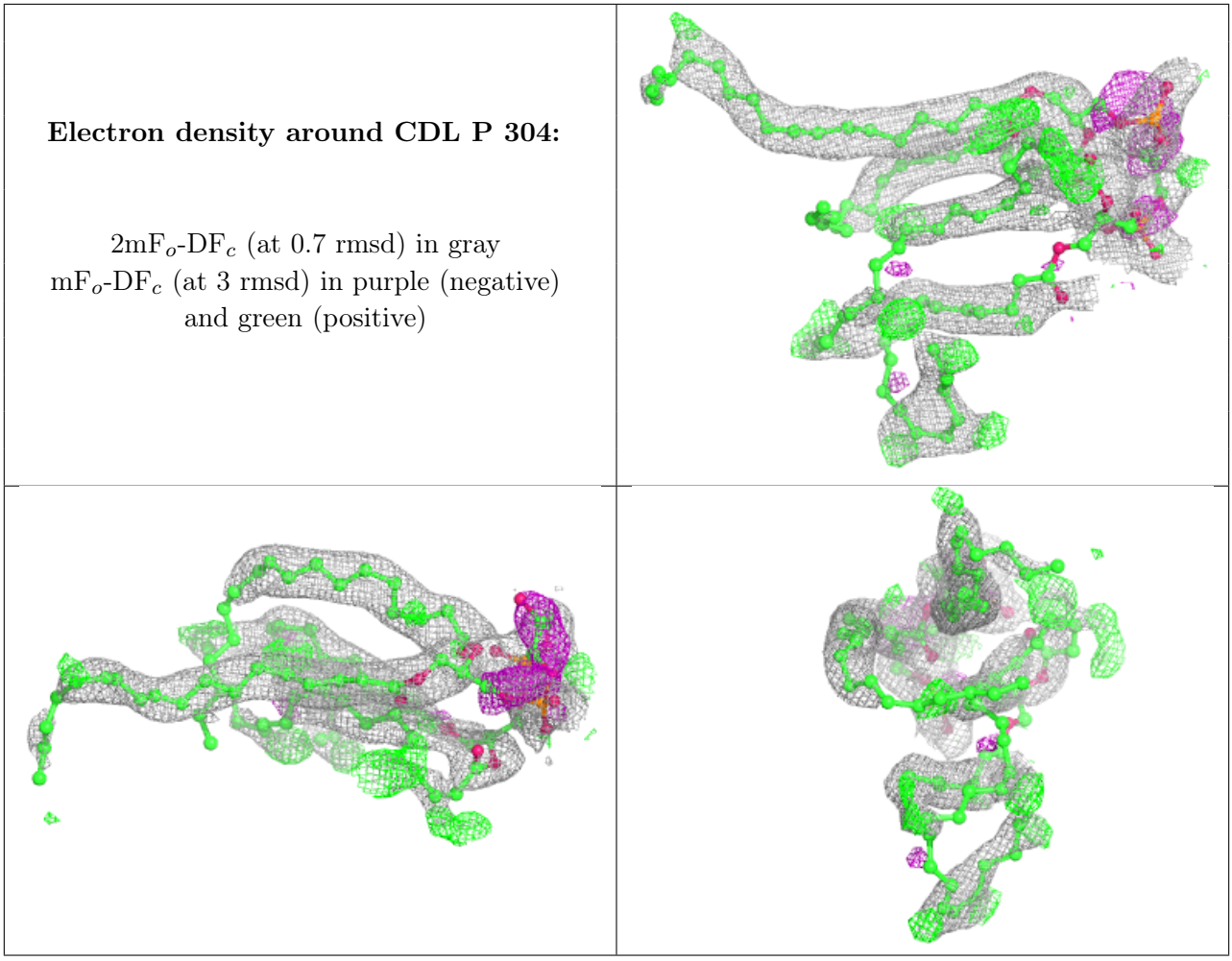
Electron density around PSC O 302:

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



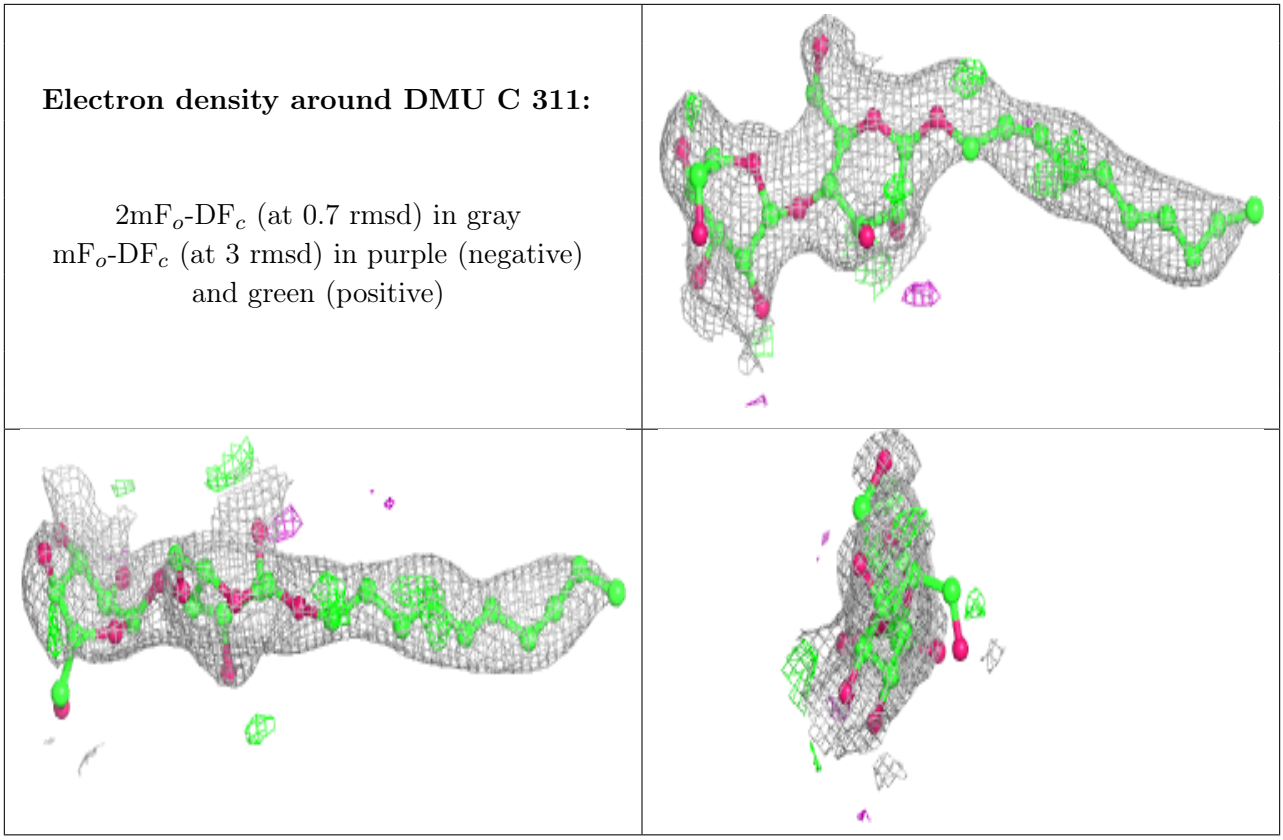
Electron density around CDL P 304:

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



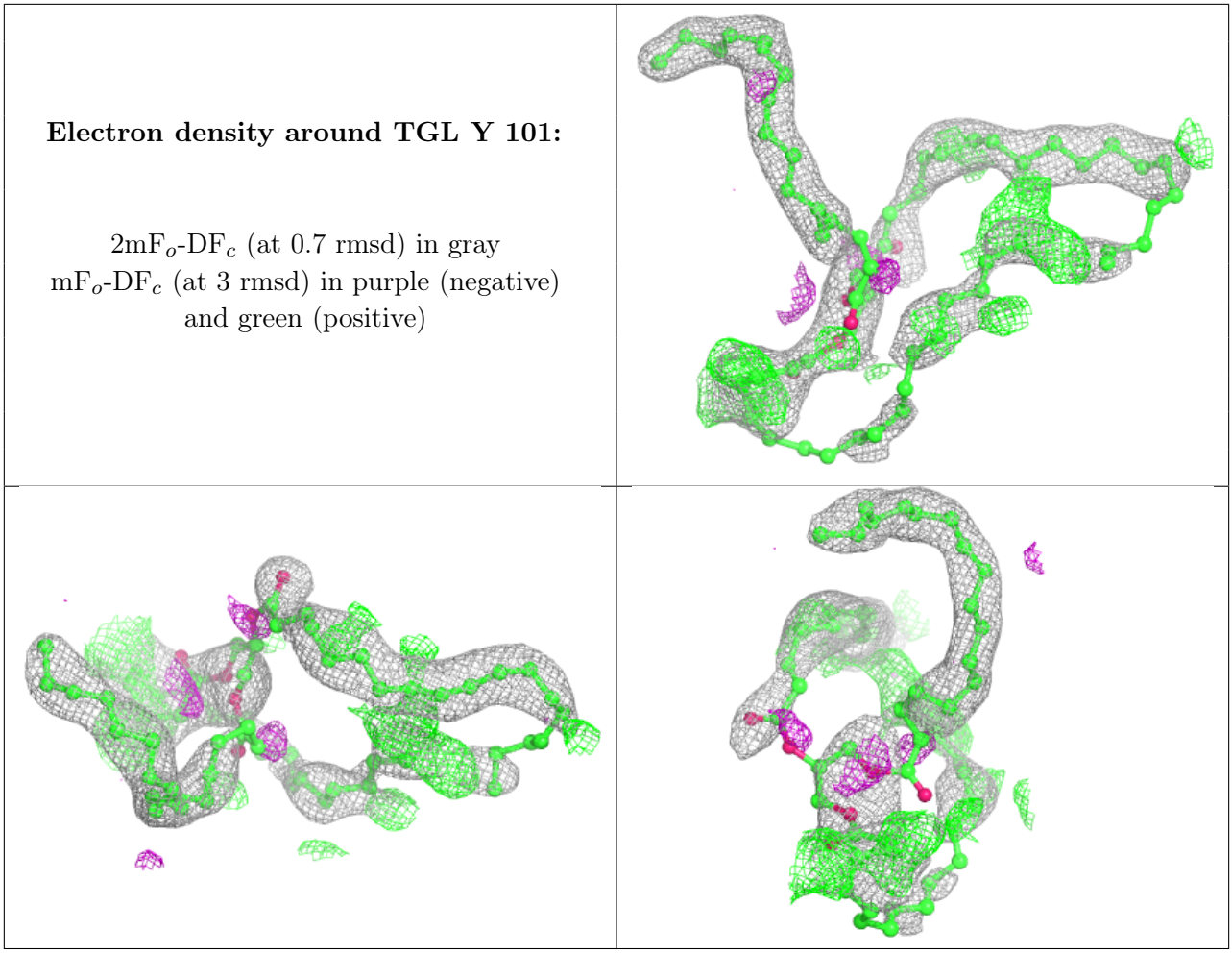
Electron density around DMU C 311:

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



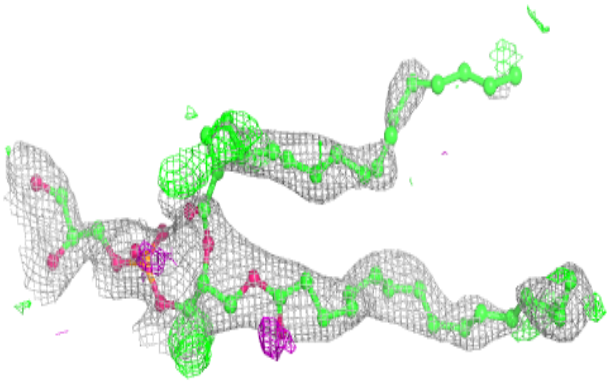
Electron density around TGL Y 101:

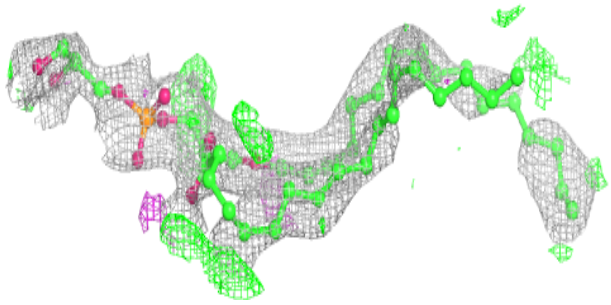
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

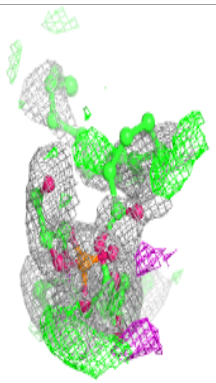


Electron density around PGV U 101:

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

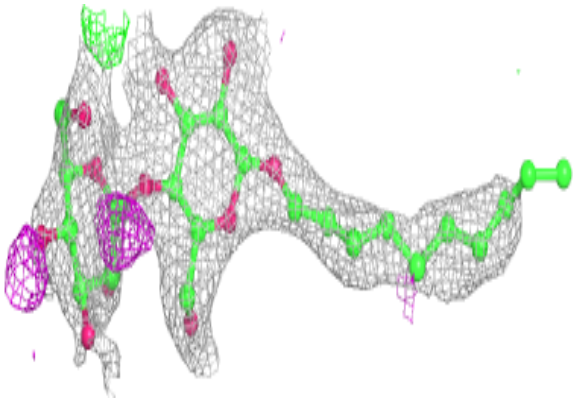


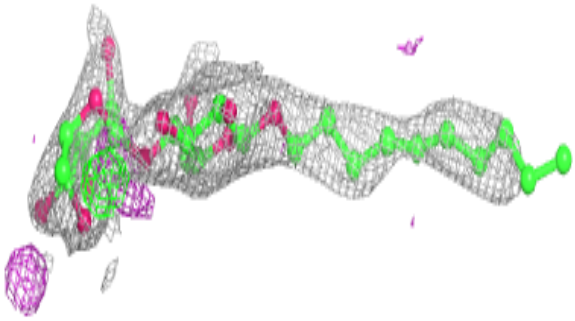


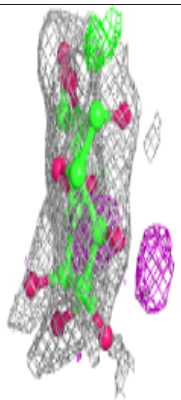


Electron density around DMU C 310:

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

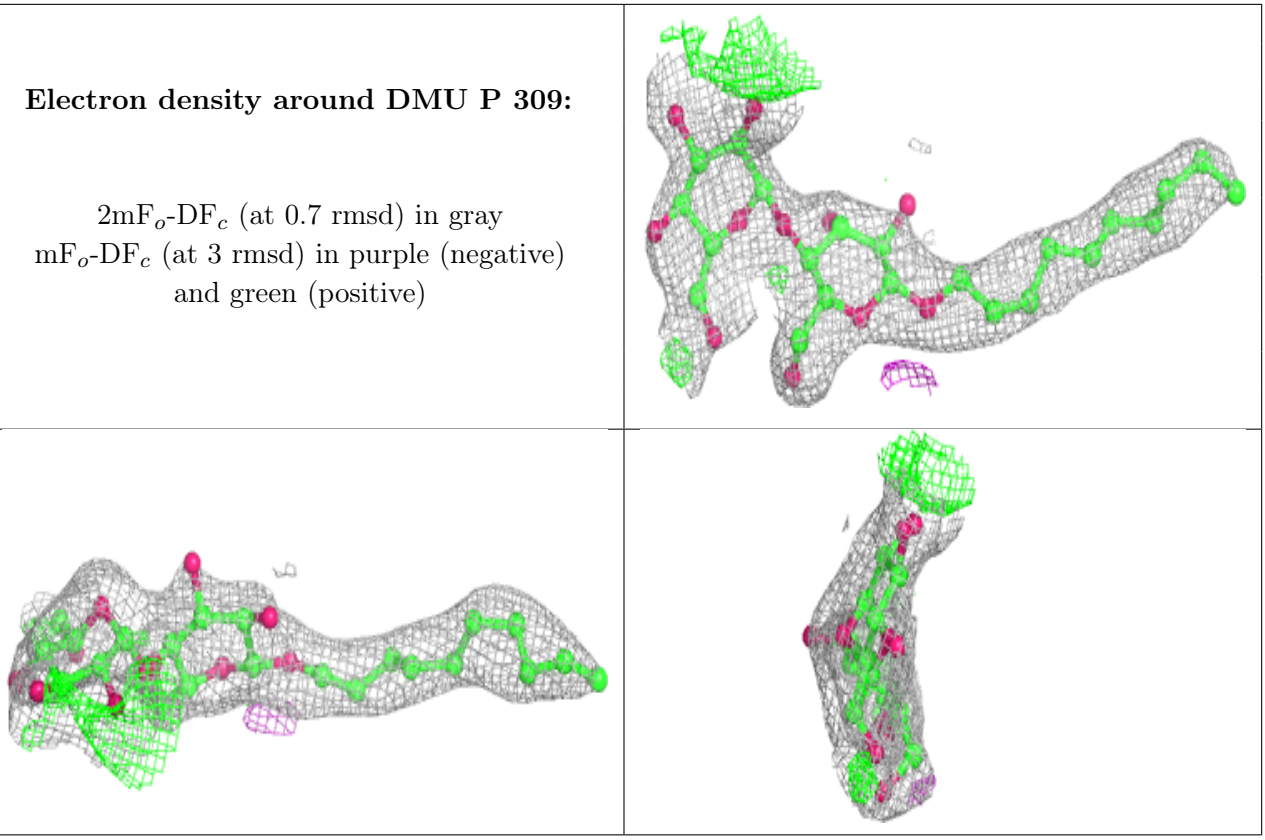






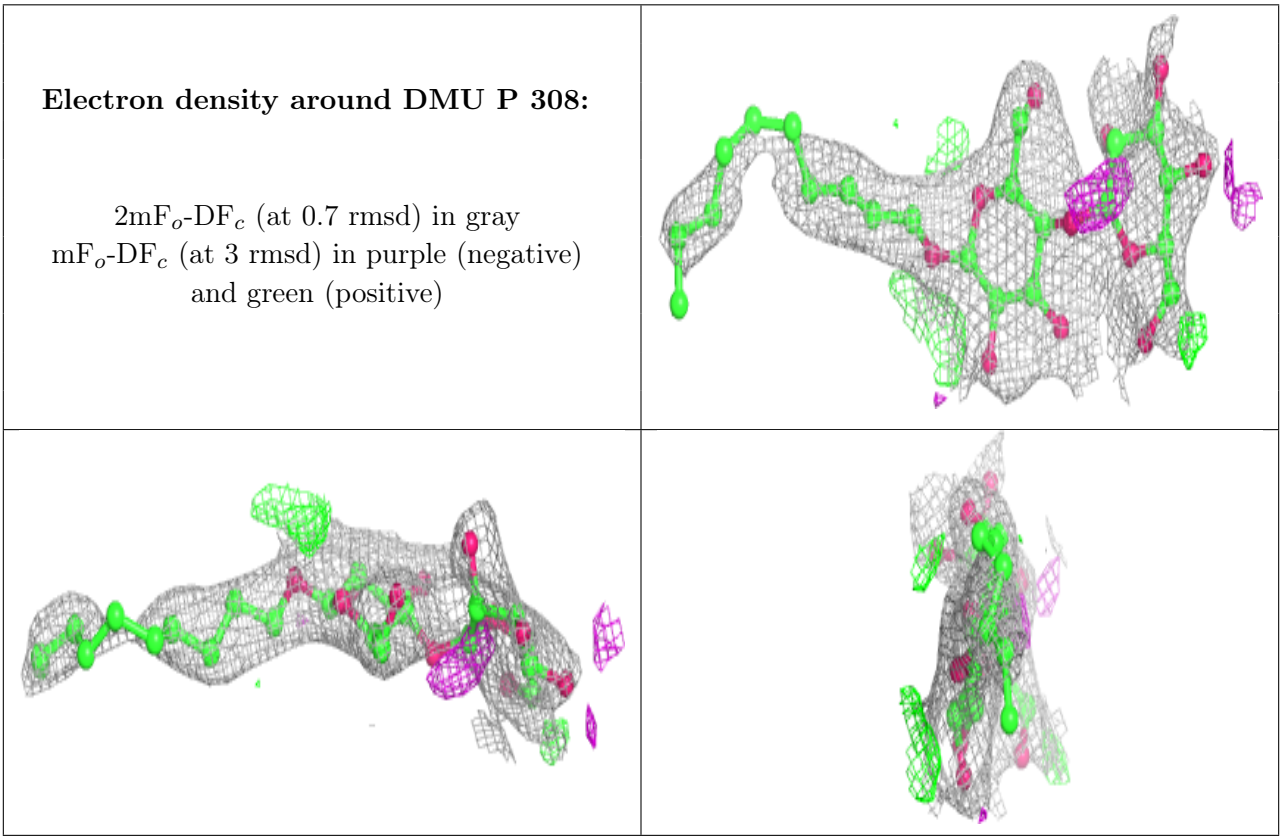
Electron density around DMU P 309:

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



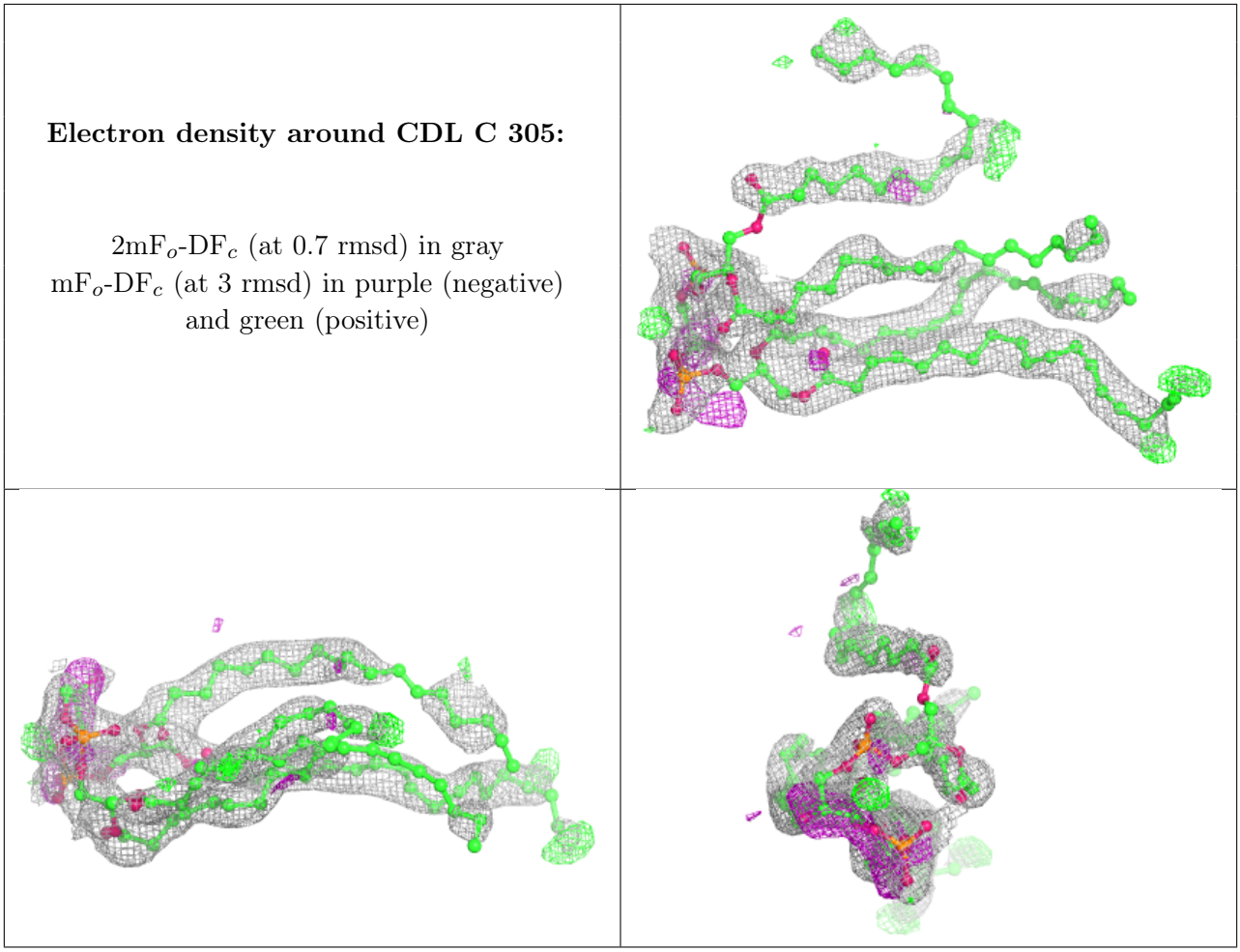
Electron density around DMU P 308:

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



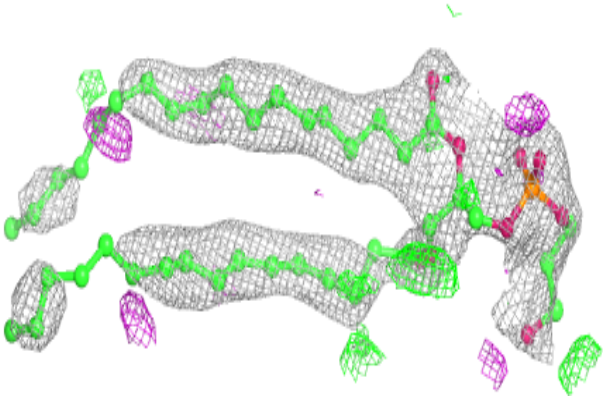
Electron density around CDL C 305:

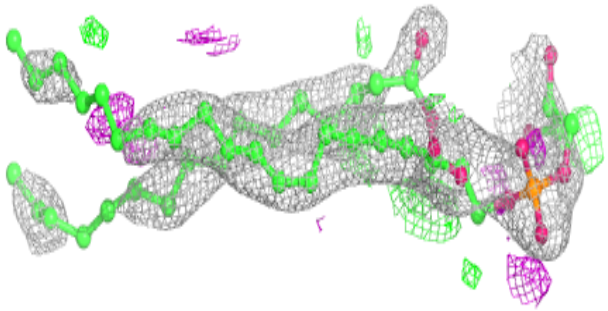
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

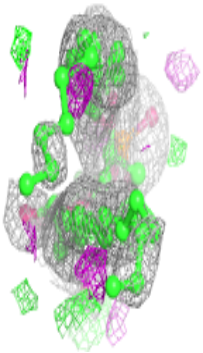


Electron density around PGV Z 101:

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

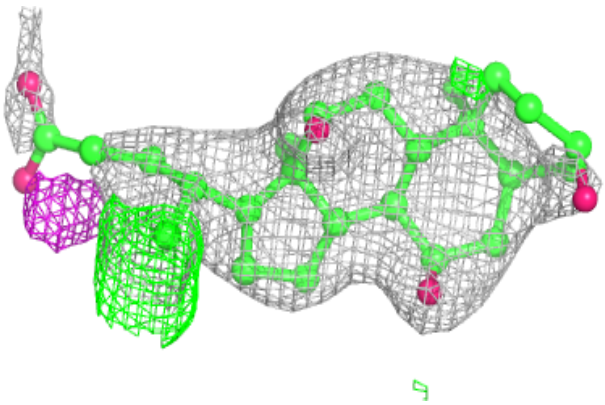


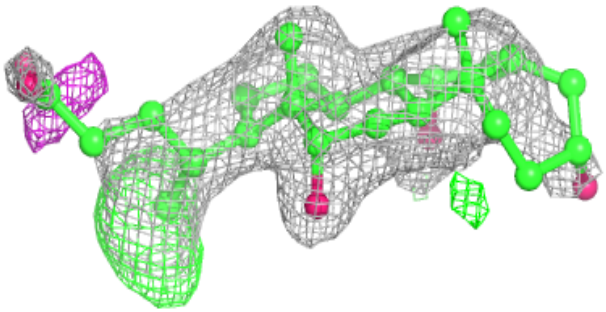


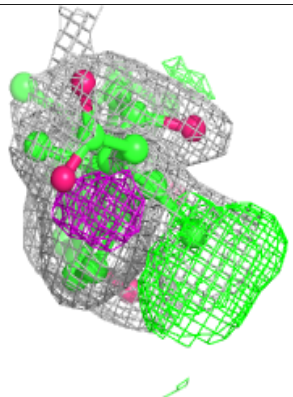


Electron density around CHD J 101:

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

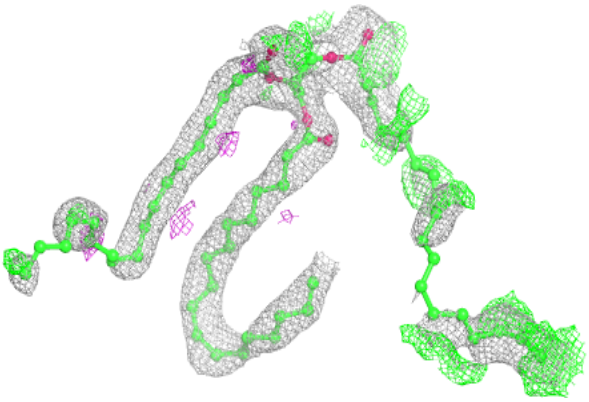


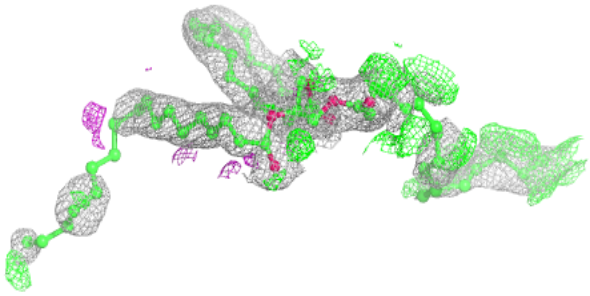


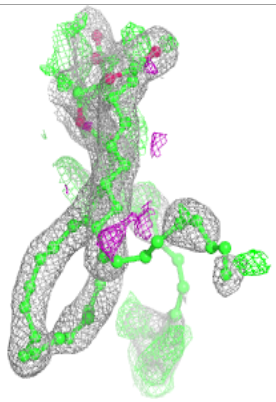


Electron density around TGL D 201:

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

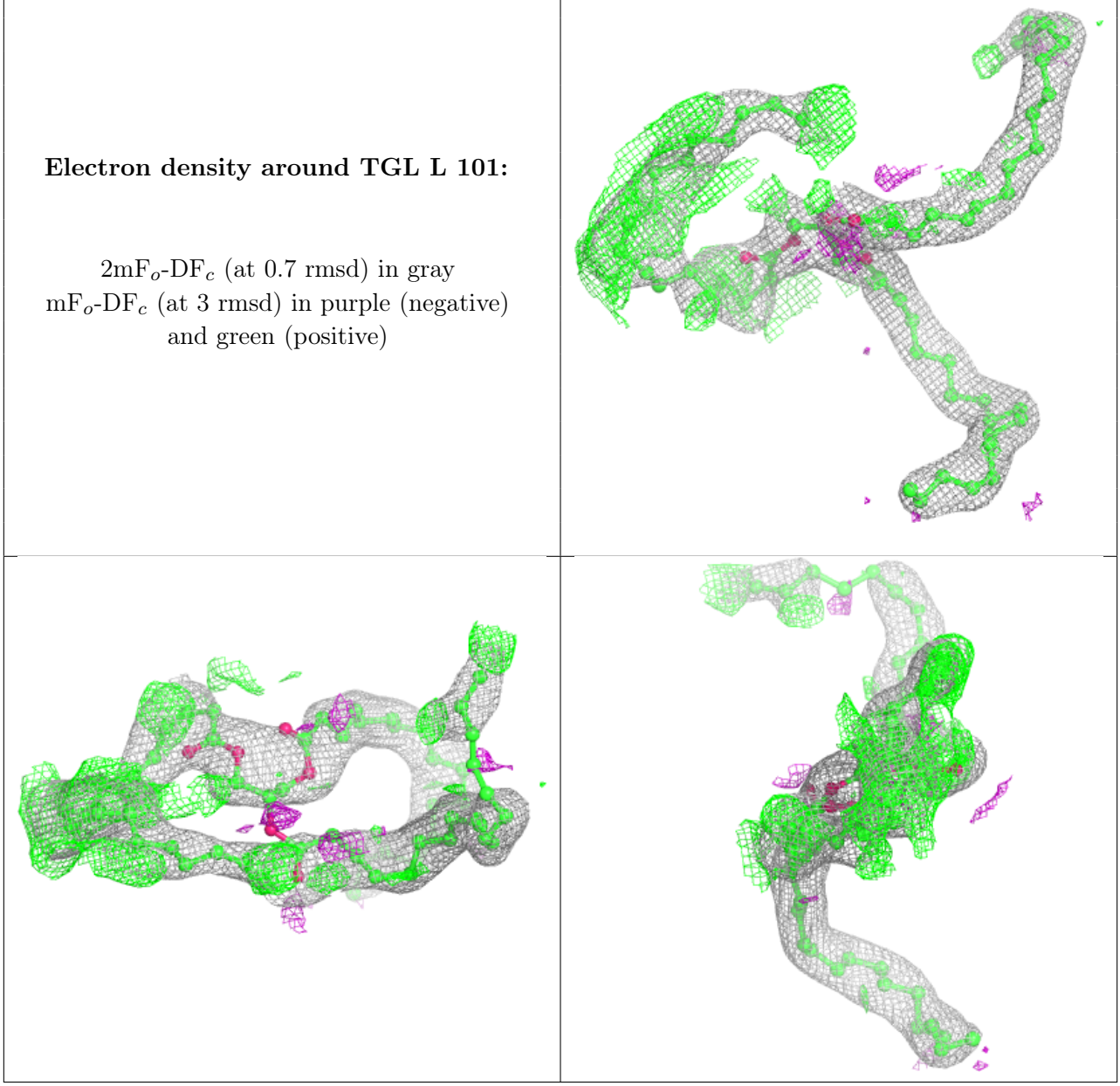






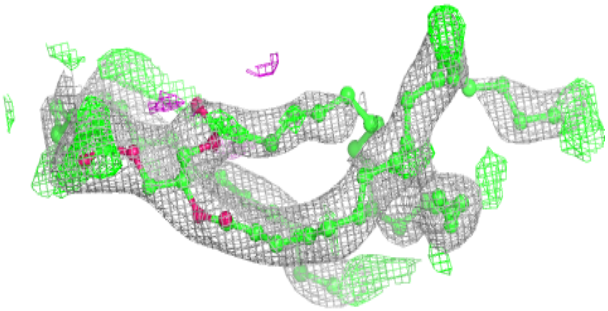
Electron density around TGL L 101:

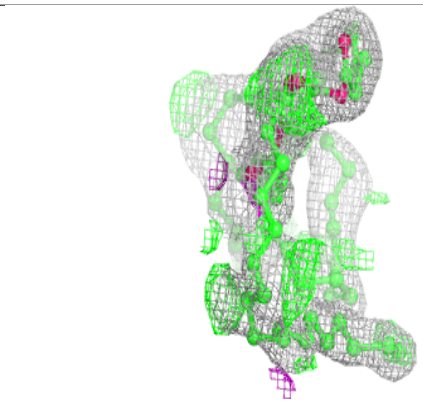
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around TGL N 610:

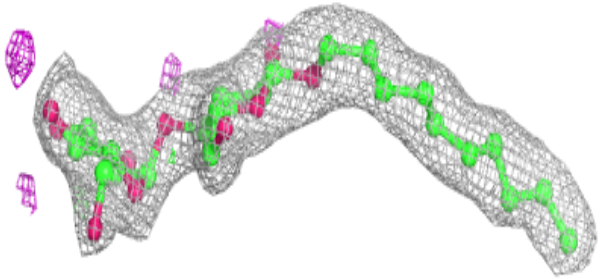
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

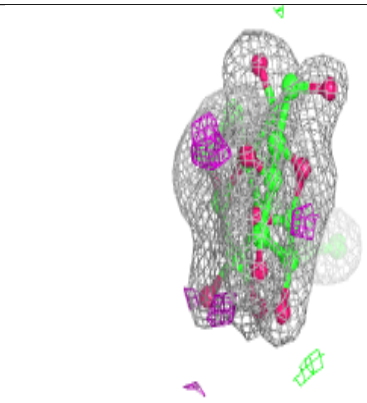




Electron density around DMU Z 102:

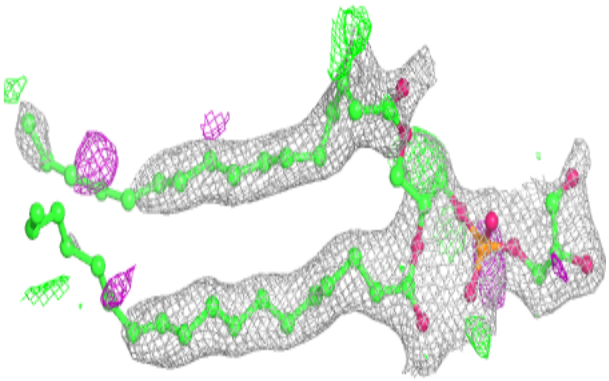
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

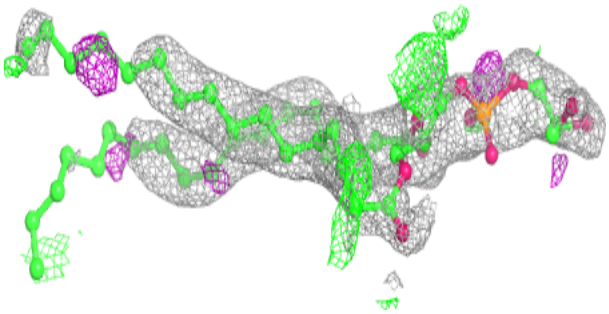


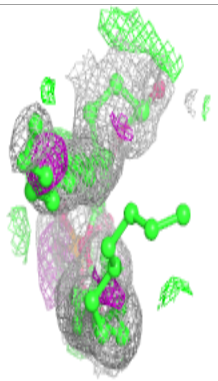


Electron density around PGV A 609:

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

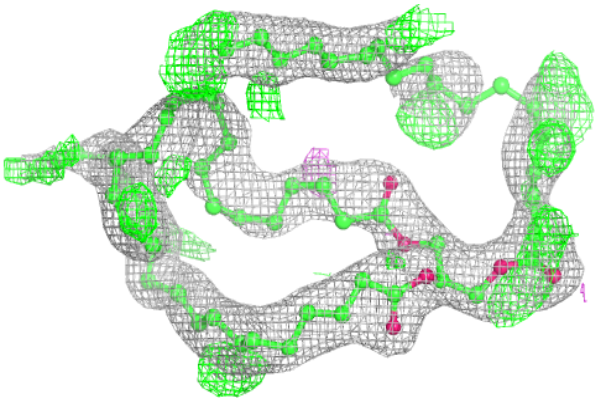


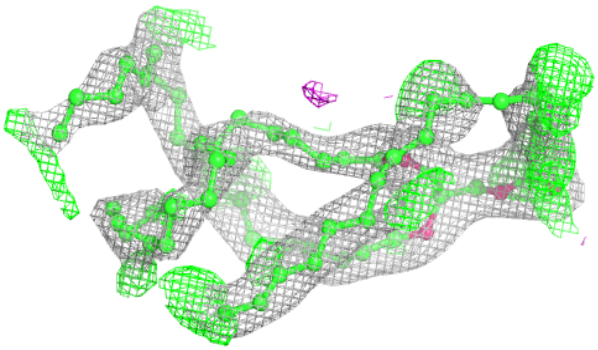


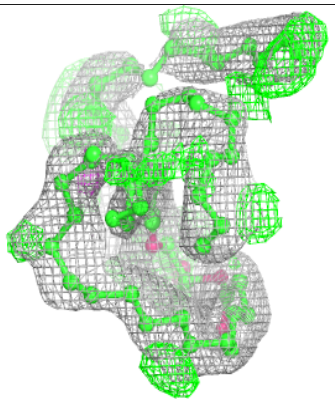


Electron density around TGL B 301:

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

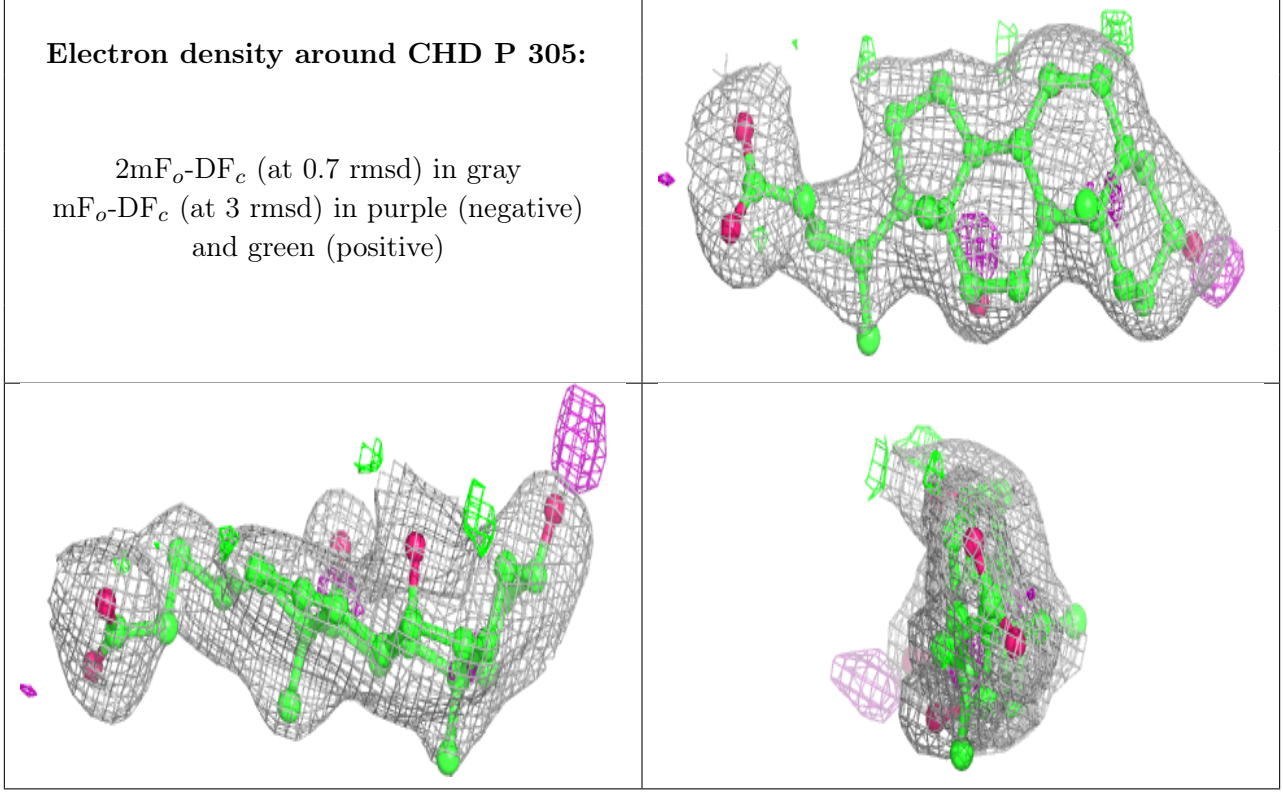






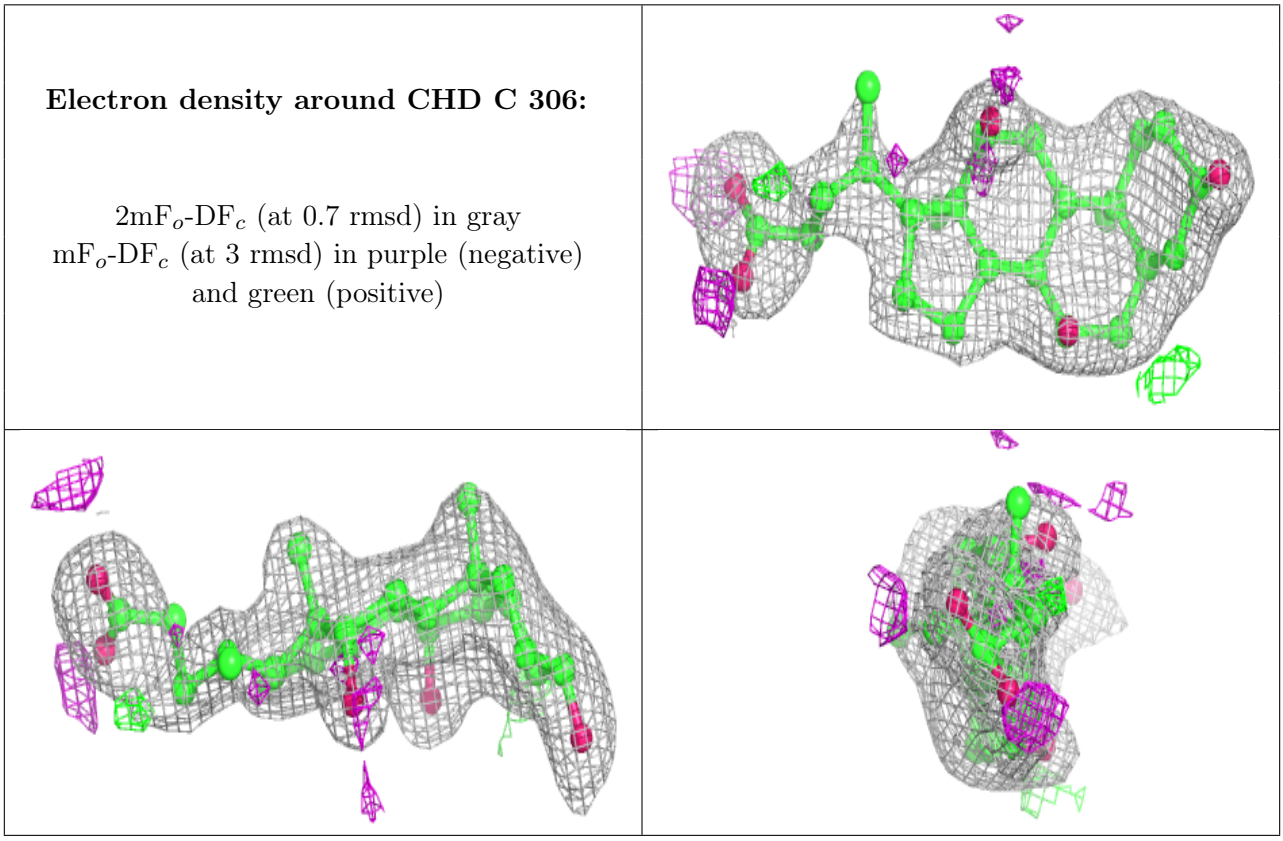
Electron density around CHD P 305:

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



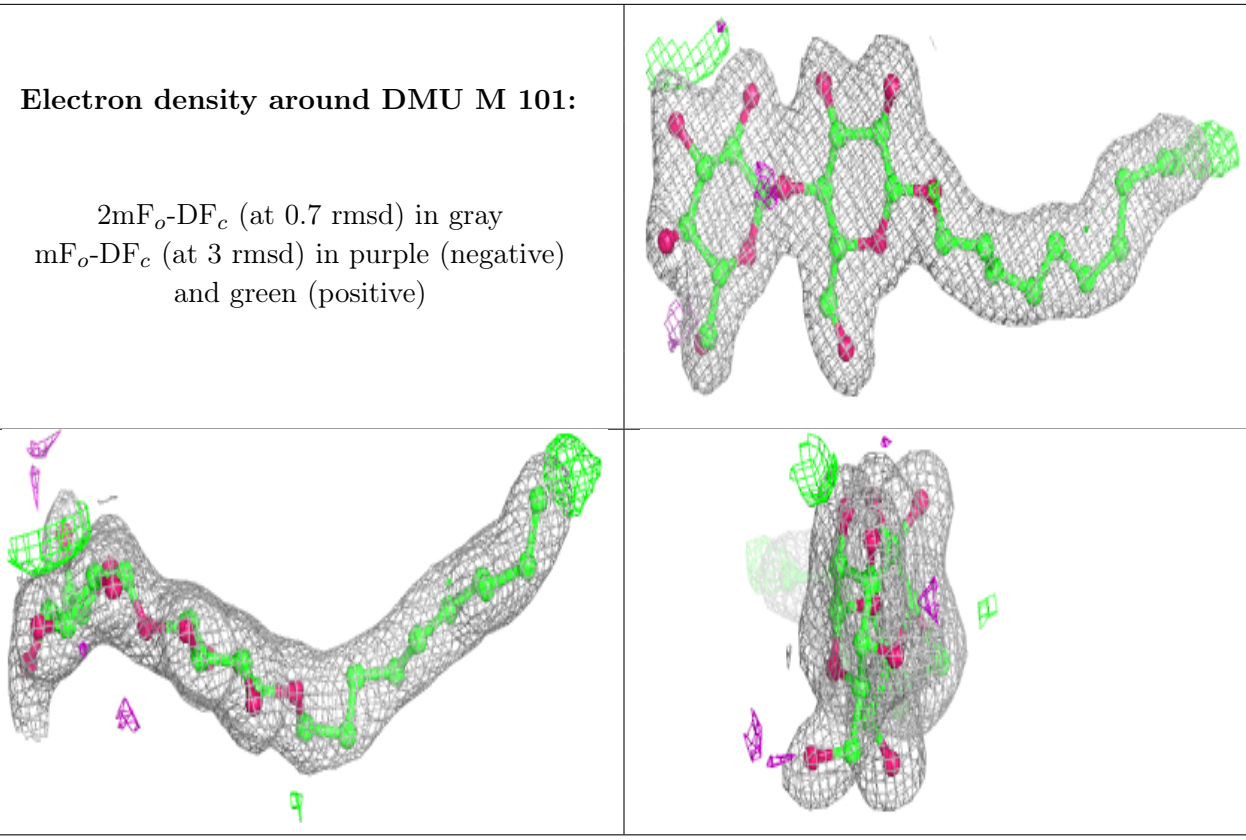
Electron density around CHD C 306:

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



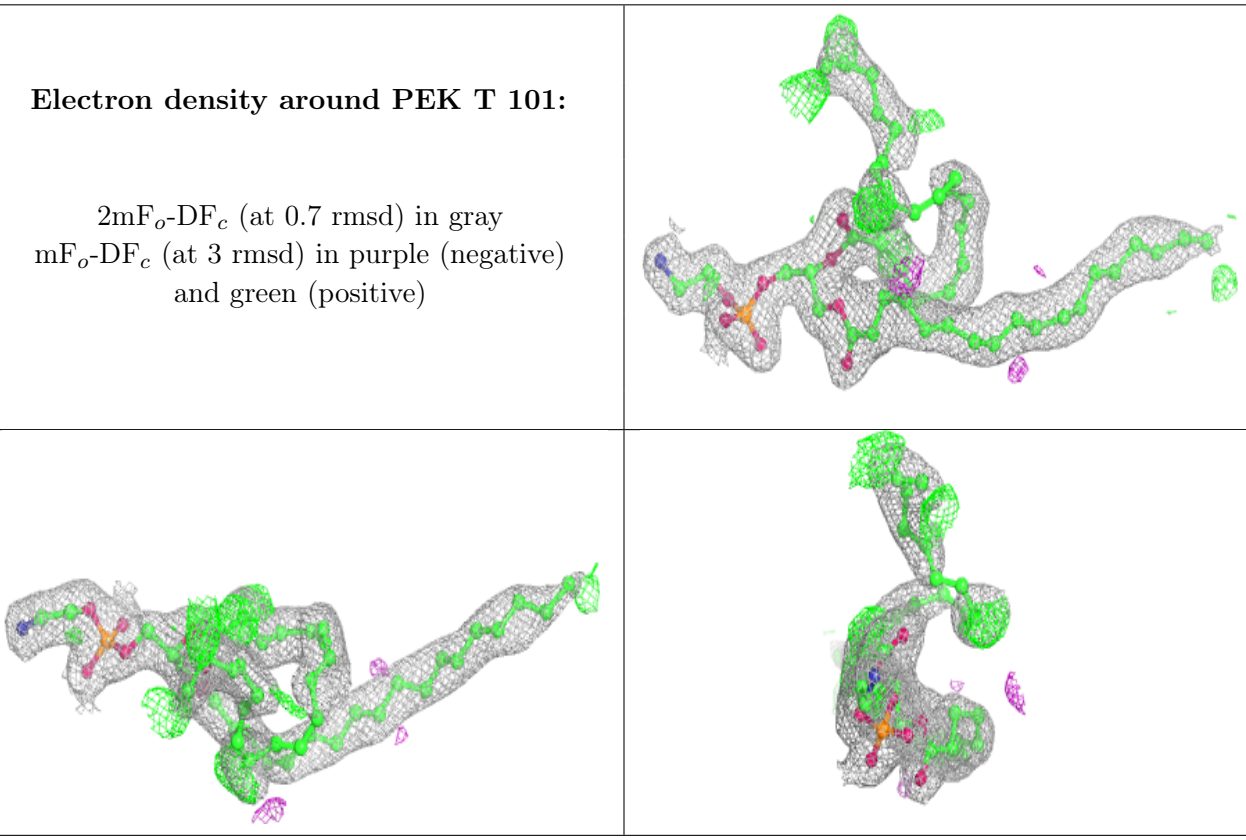
Electron density around DMU M 101:

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



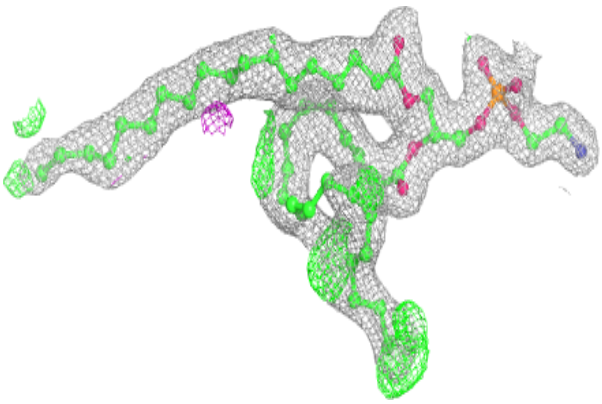
Electron density around PEK T 101:

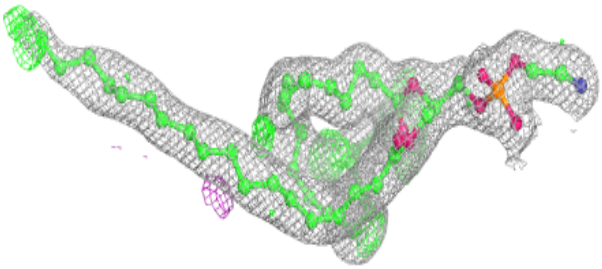
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

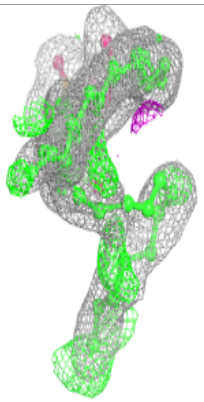


Electron density around PEK G 101:

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

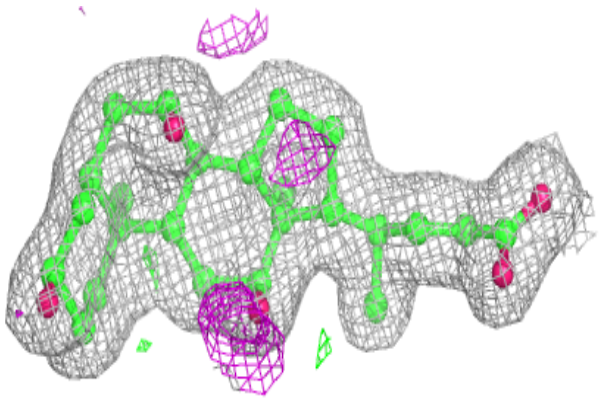


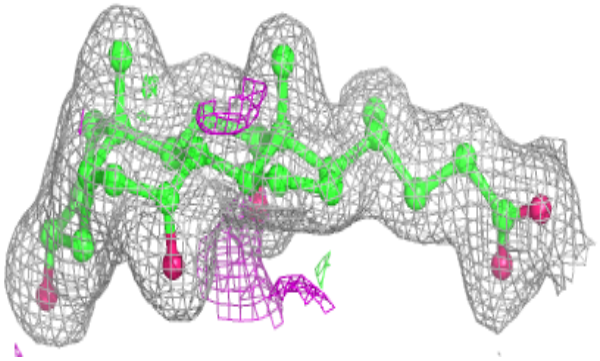


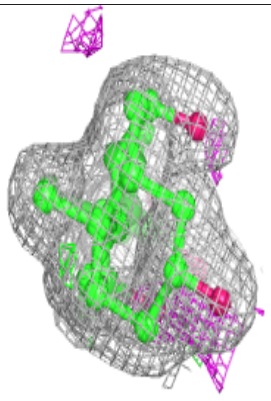


Electron density around CHD C 301:

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

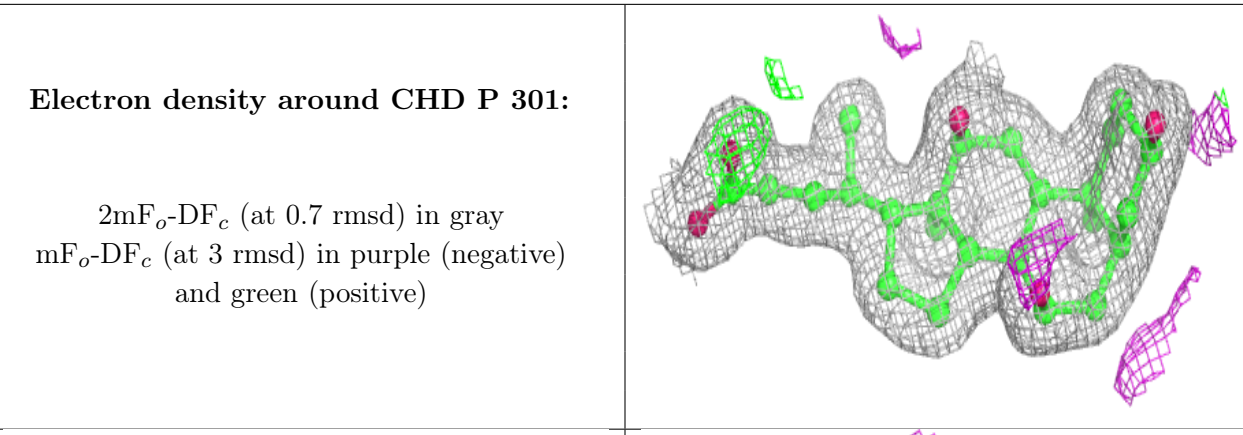


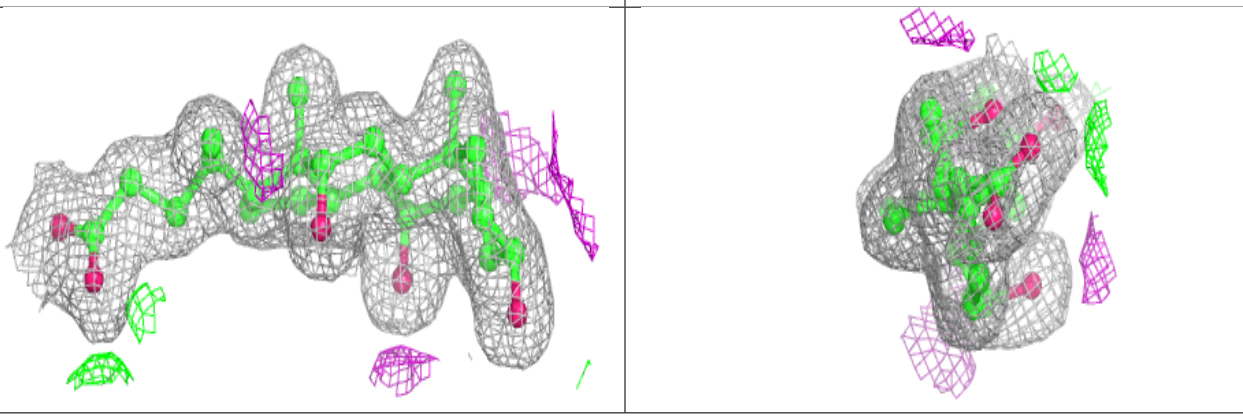




Electron density around CHD P 301:

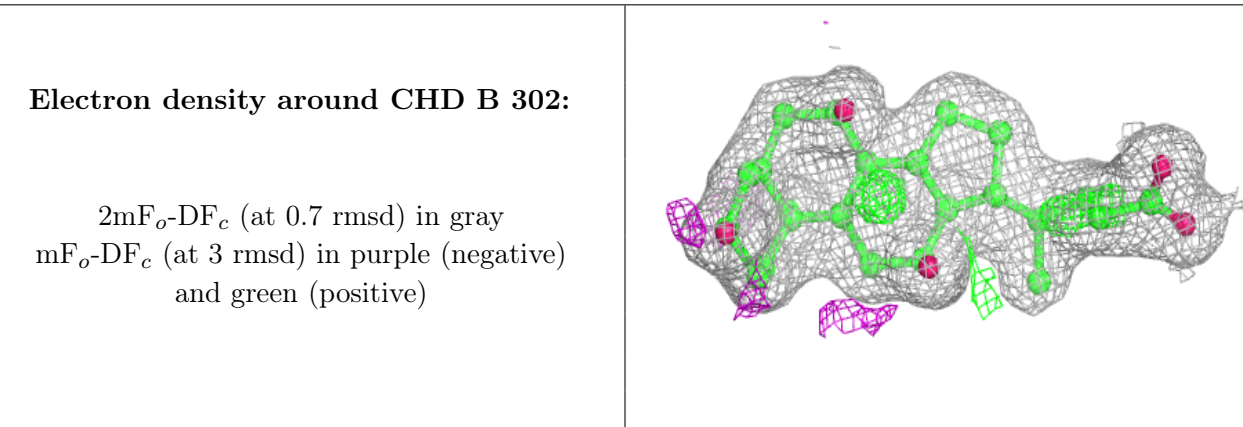
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

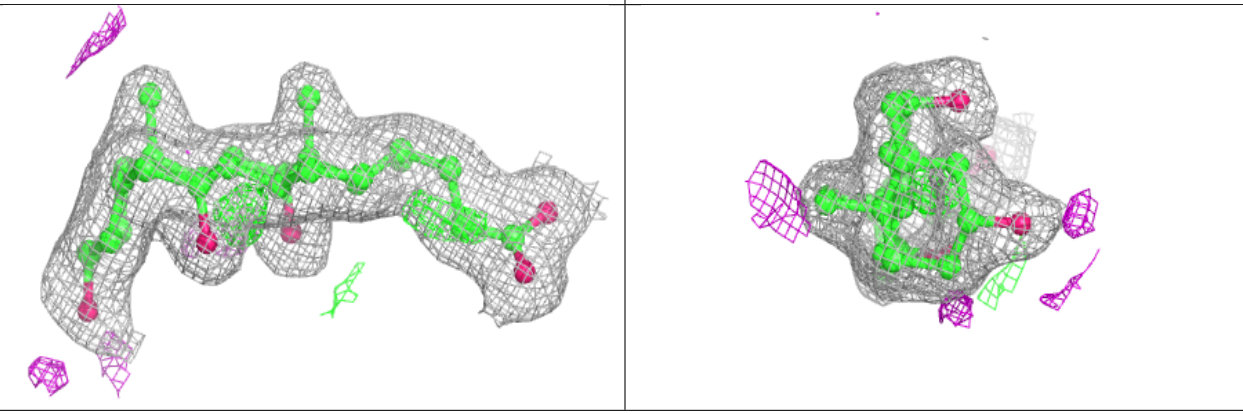




Electron density around CHD B 302:

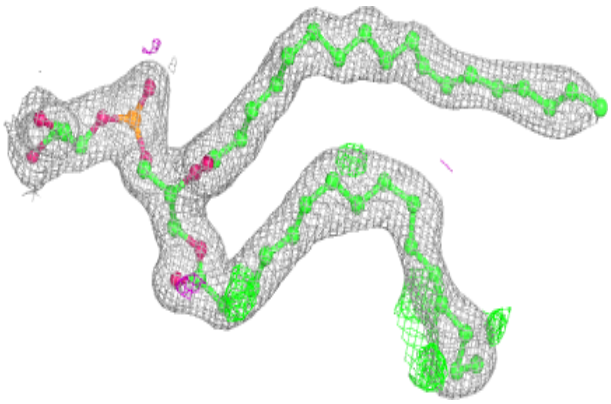
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

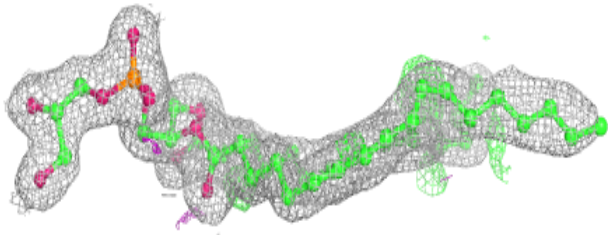


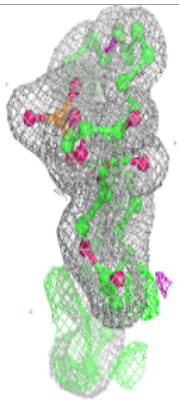


Electron density around PGV A 608:

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

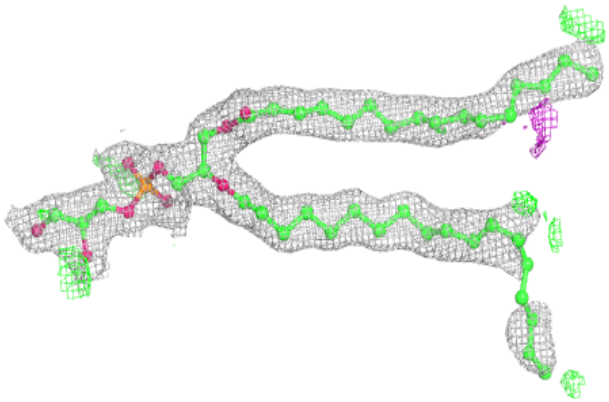


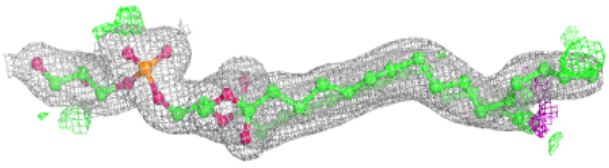


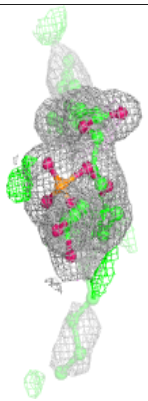


Electron density around PGV P 303:

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

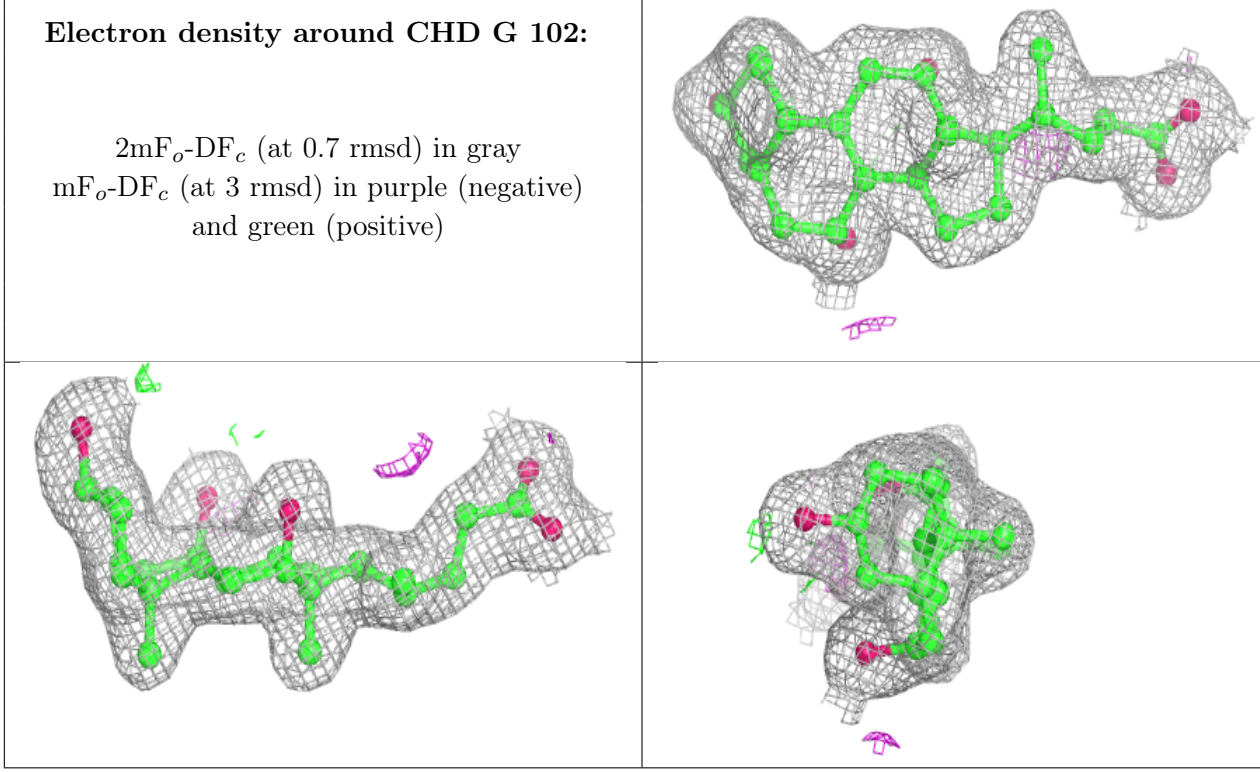






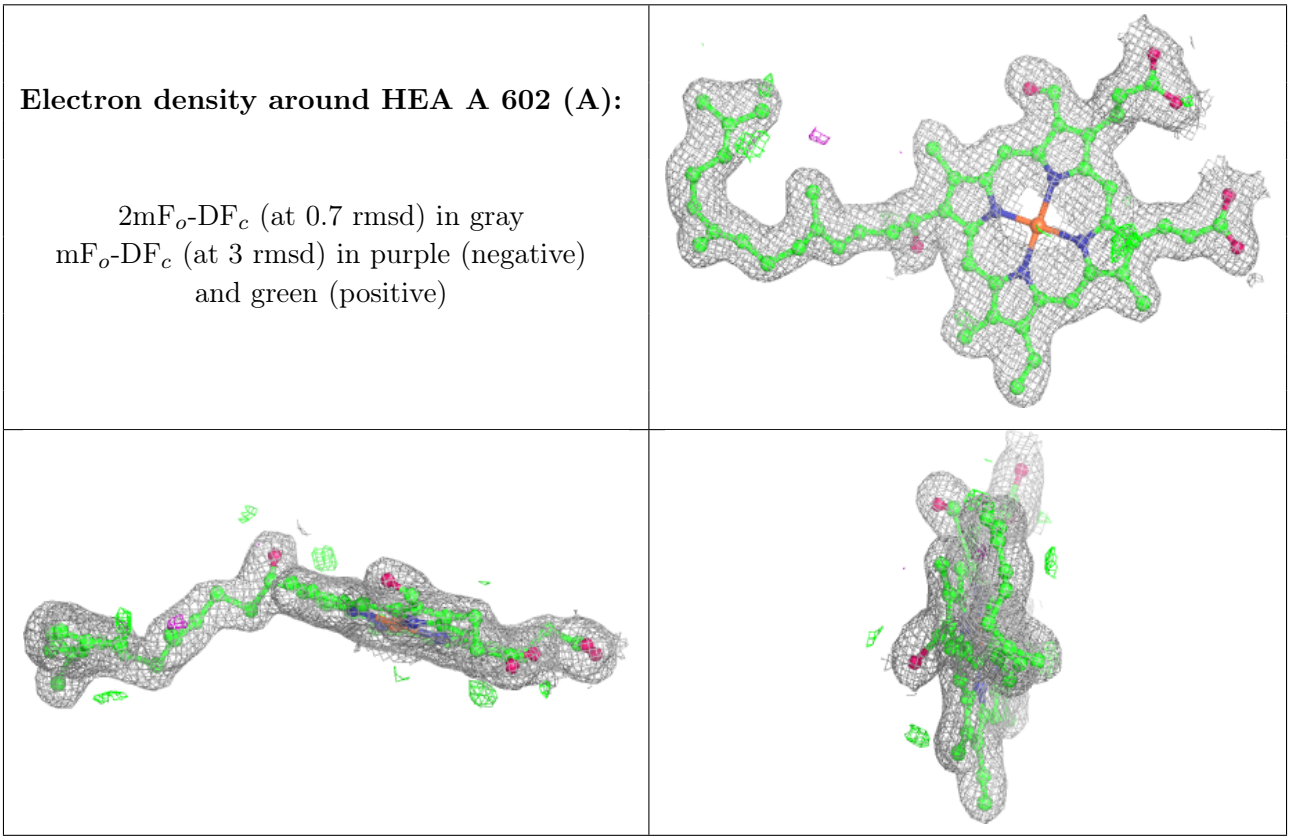
Electron density around CHD G 102:

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



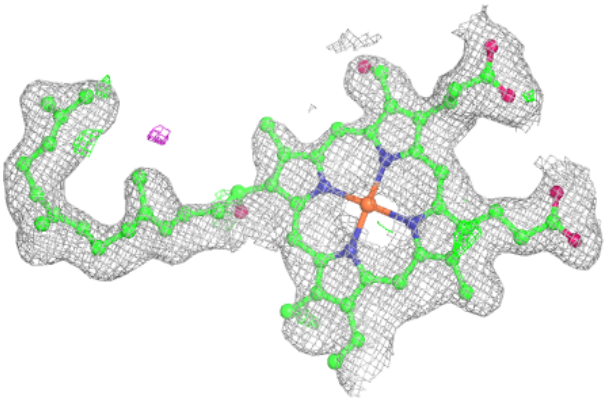
Electron density around HEA A 602 (A):

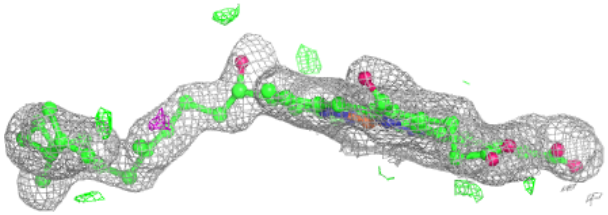
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

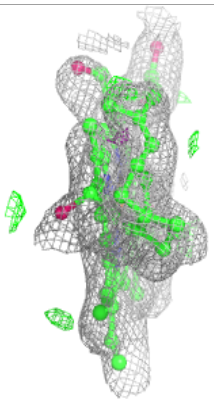


Electron density around HEA A 602 (B):

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

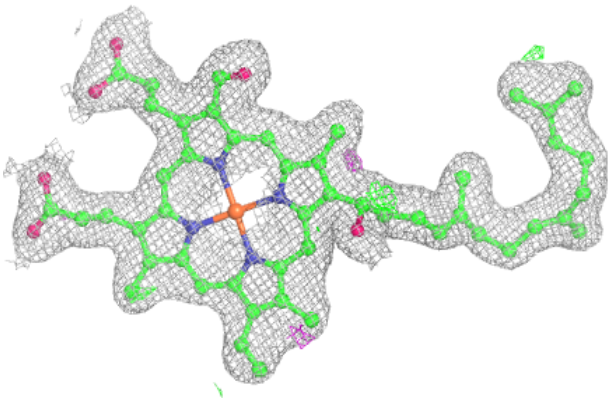


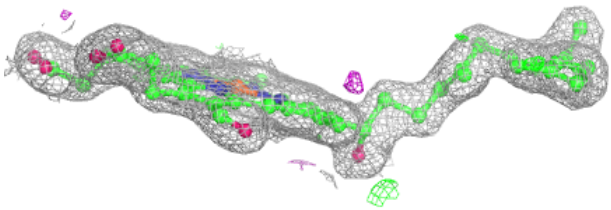


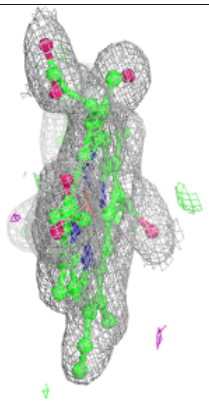


Electron density around HEA N 603 (A):

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

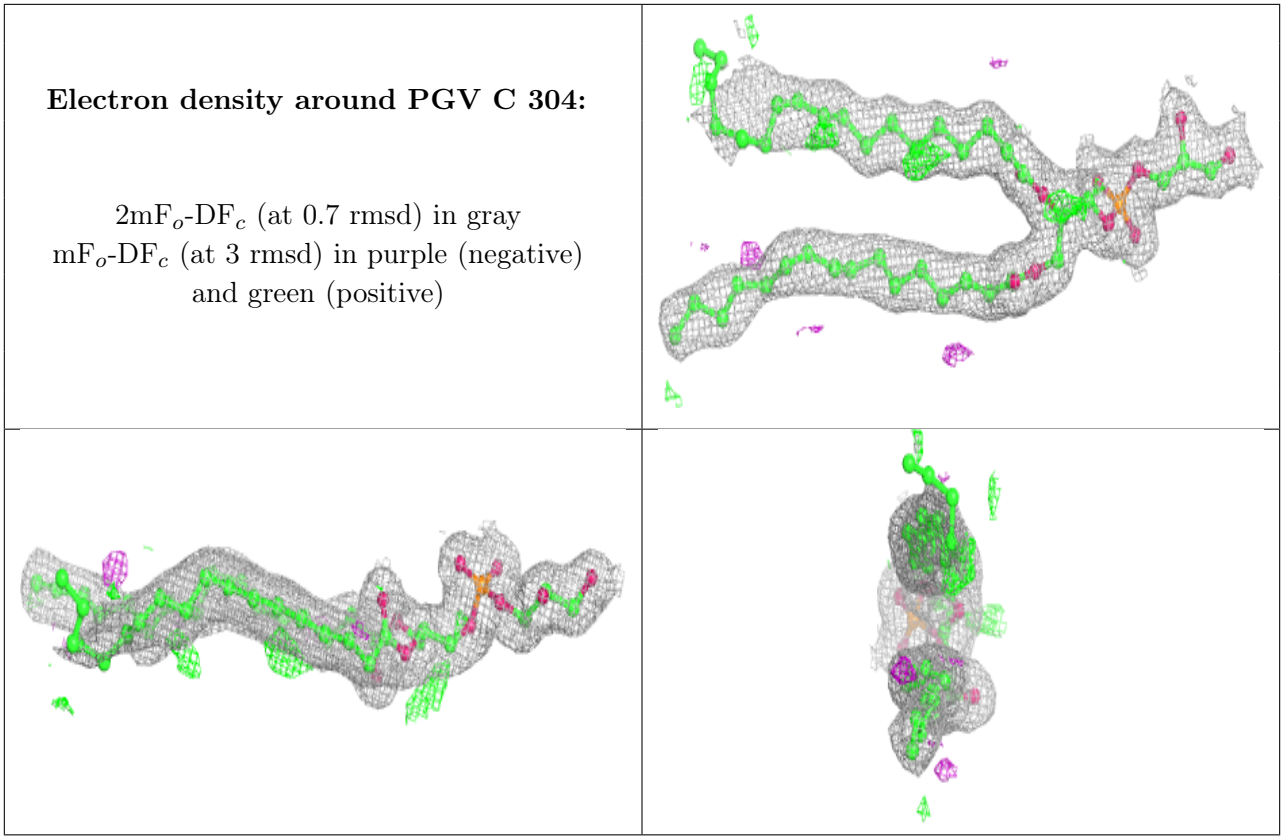






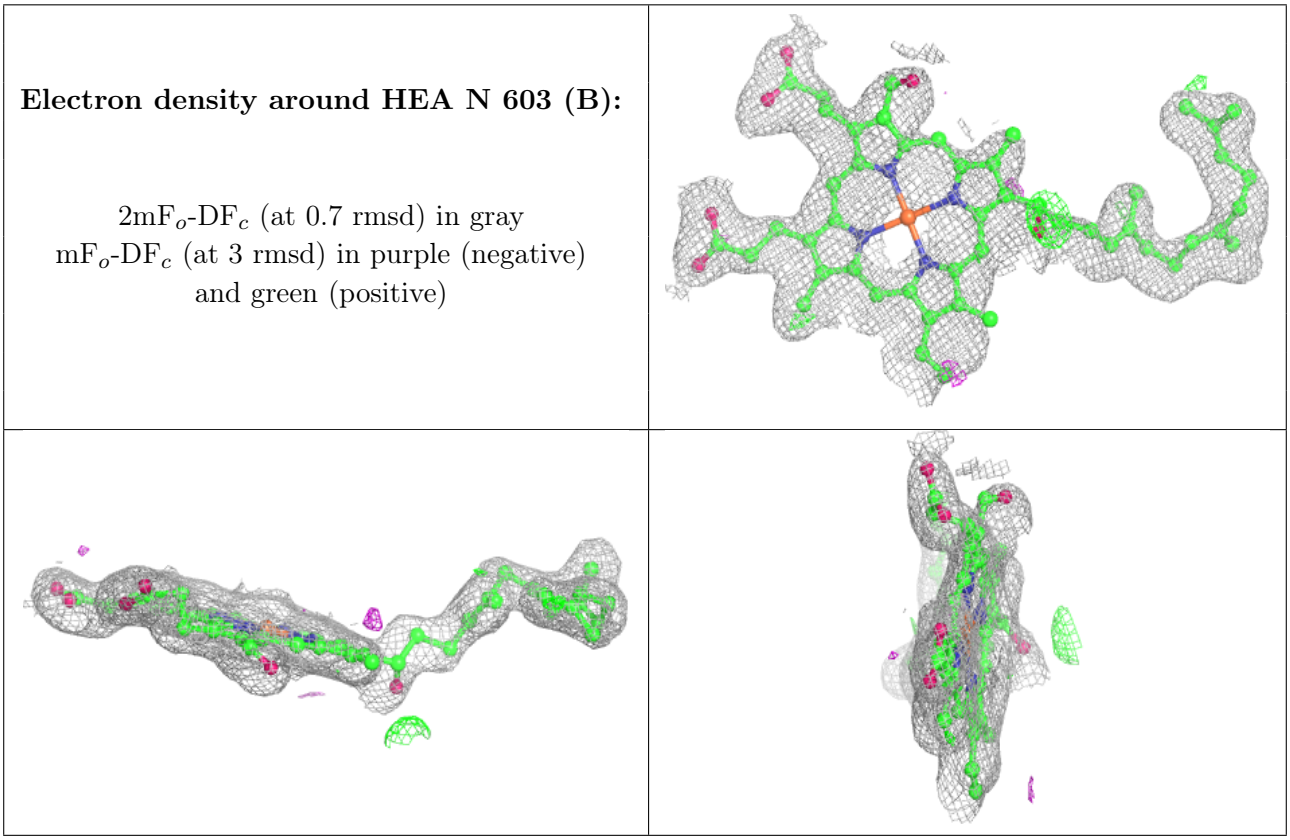
Electron density around PGV C 304:

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



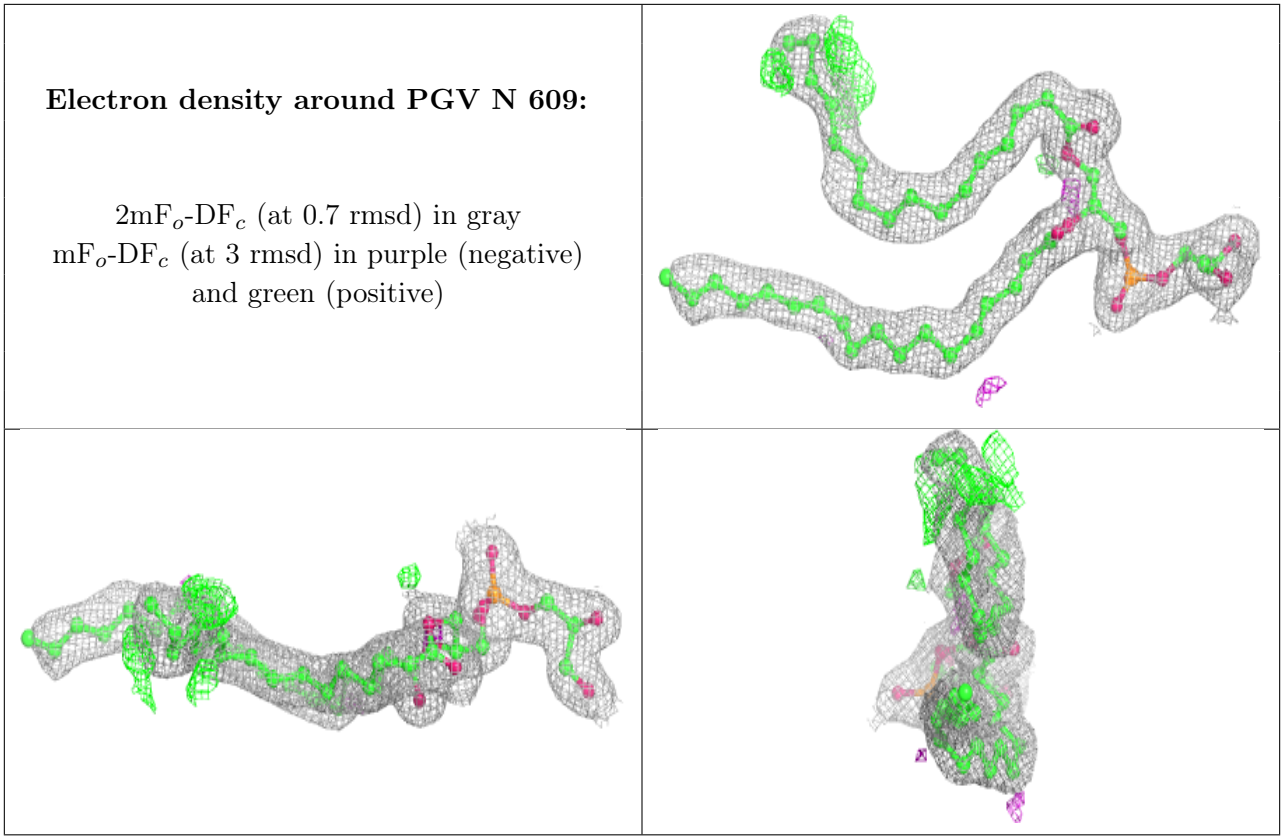
Electron density around HEA N 603 (B):

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



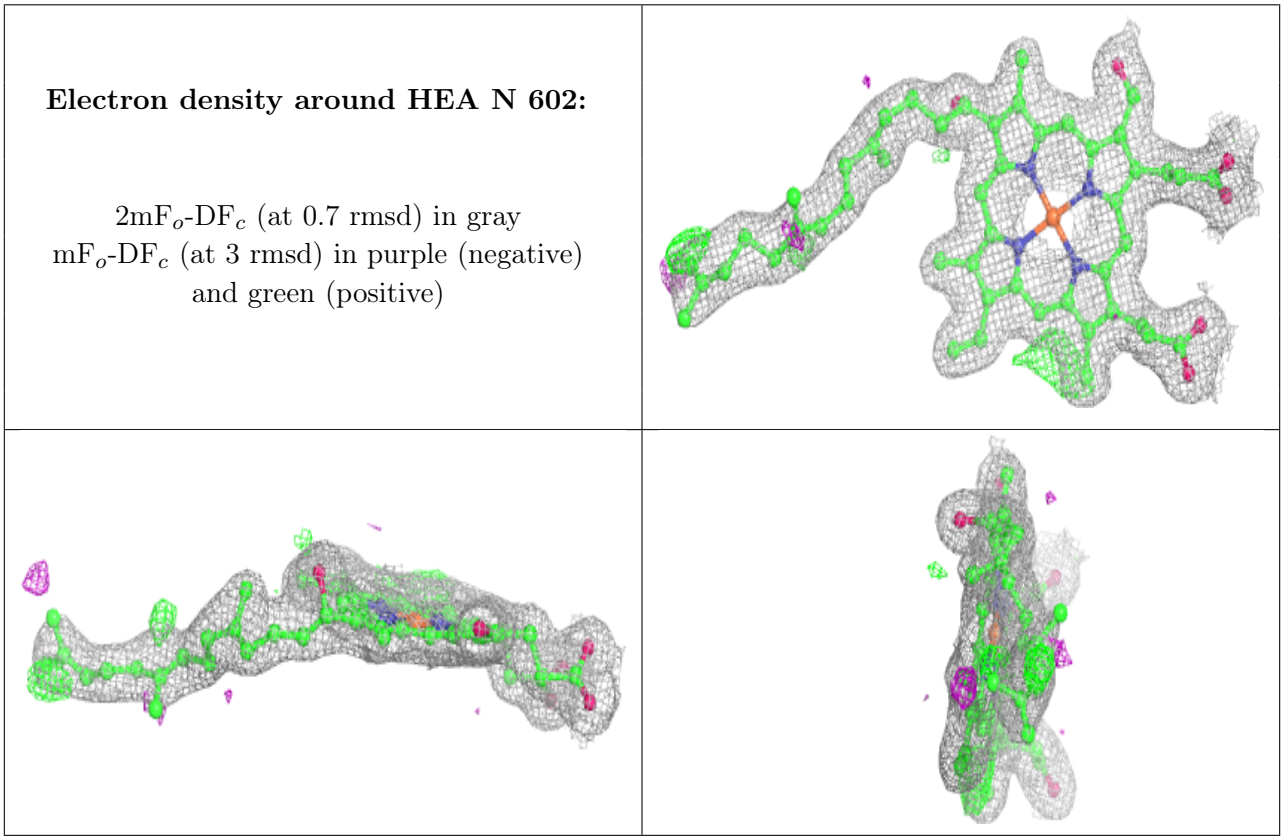
Electron density around PGV N 609:

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



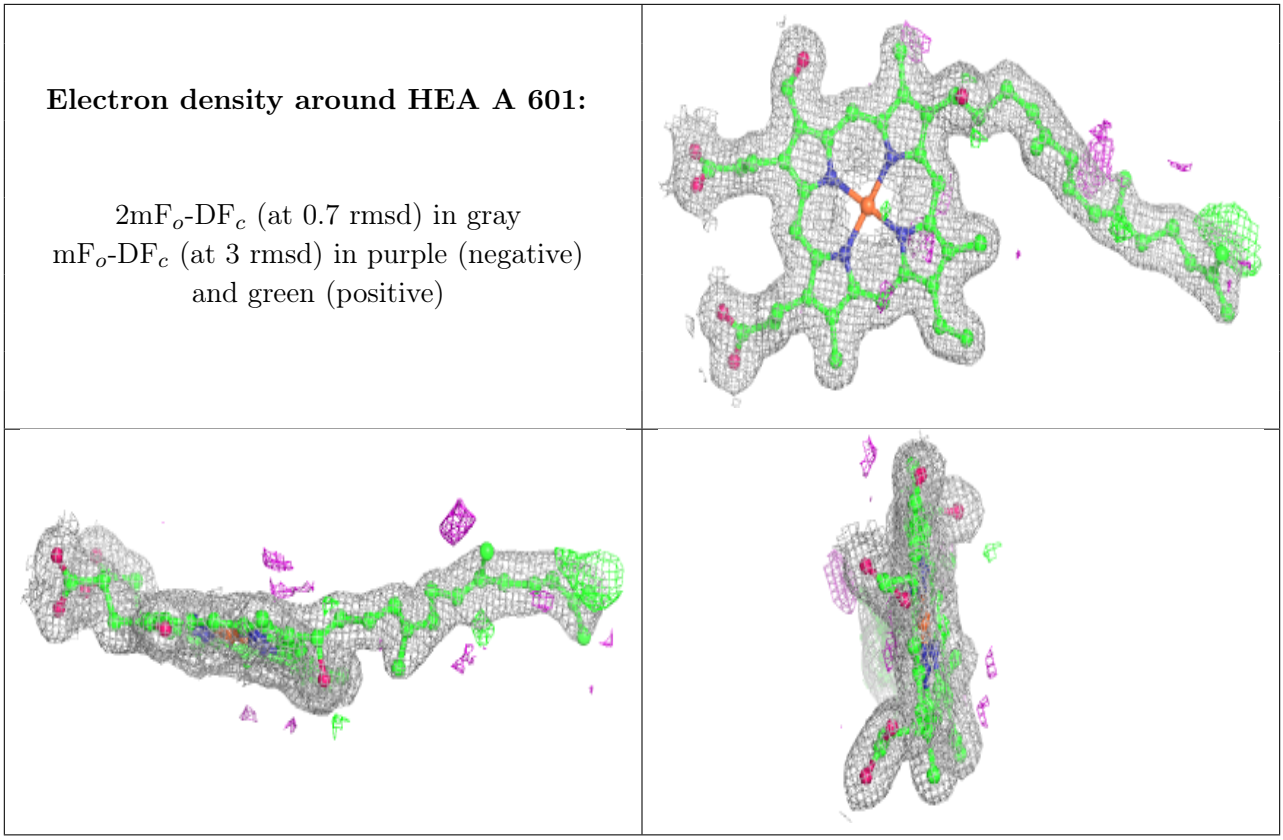
Electron density around HEA N 602:

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



Electron density around HEA A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.