Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 01:19 PM JST

PDB ID	:	5ZCQ
Title	:	Azide-bound cytochrome c oxidase structure determined using the crystals exposed to 10 mM azide solution for 2 days
Authors	:	Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on	:	2018-02-19
Resolution	:	1.65 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

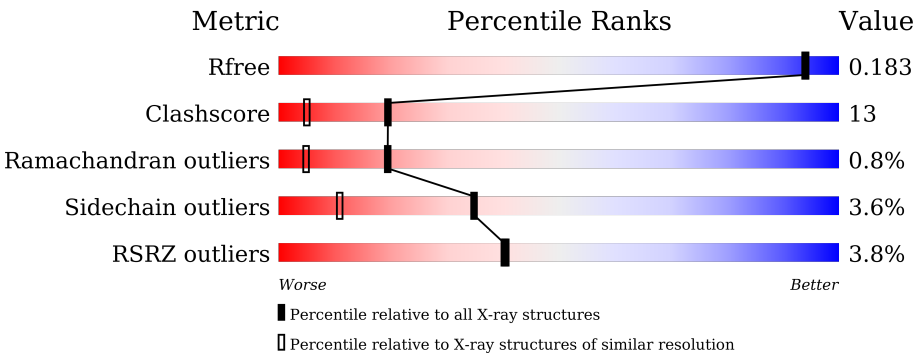
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	77% 20% •
1	N	514	79% 19% •
2	B	227	2% 72% 23% 5%
2	O	227	2% 72% 24% •
3	C	261	80% 18% ••
3	P	261	% 78% 19% • •

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Mol	Chain	Length	Quality of chain
4	D	147	%, 80%, 16%
4	Q	147	6%, 80%, 12%
5	E	109	2%, 81%, 13%
5	R	109	2%, 81%, 15%
6	F	98	8%, 78%, 16%, 5%
6	S	98	9%, 78%, 14%
7	G	85	20%, 65%, 19%, 13%
7	T	85	20%, 66%, 22%, 9%
8	H	85	9%, 64%, 20%, 8%, 7%
8	U	85	11%, 75%, 14%, 7%
9	I	73	11%, 77%, 21%
9	V	73	10%, 74%, 22%
10	J	59	7%, 78%, 17%
10	W	59	8%, 80%, 19%
11	K	56	75%, 12%, 12%
11	X	56	5%, 75%, 11%, 12%
12	L	47	2%, 68%, 23%, 6%
12	Y	47	2%, 79%, 17%
13	M	46	9%, 72%, 20%, 7%
13	Z	46	9%, 83%, 11%, 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	606[B]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	607[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FME	B	1	-	-	X	-
21	EDO	A	611	-	-	X	-
21	EDO	A	621	-	-	X	-
21	EDO	D	202	-	-	X	-
21	EDO	E	202	-	-	X	-
21	EDO	F	103	-	-	-	X
21	EDO	H	101	-	X	X	-
21	EDO	P	312	-	X	-	-
22	CHD	J	101	-	-	-	X
22	CHD	W	101	-	-	-	X
24	PSC	B	303	-	-	X	-
27	CDL	C	305	-	-	X	-
27	CDL	G	102	-	-	X	-
27	CDL	P	305	-	-	X	-
27	CDL	T	103	-	-	X	-
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 33657 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
			Total	C	N	O	S			
1	A	514	4193	2793	649	709	42	0	22	0
1	N	514	4179	2786	647	704	42	0	20	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1907	1238	293	356	20	0	10	0
2	O	227	1870	1215	288	347	20	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2168	1447	347	359	15	0	7	0
3	P	259	2185	1457	349	363	16	0	9	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1242	809	206	223	4	0	5	0
4	Q	144	1224	797	202	221	4	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	98	771	477	138	150	6	0	3	0
6	S	98	763	473	136	148	6	0	2	0

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

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

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

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

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

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

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

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

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

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

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

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

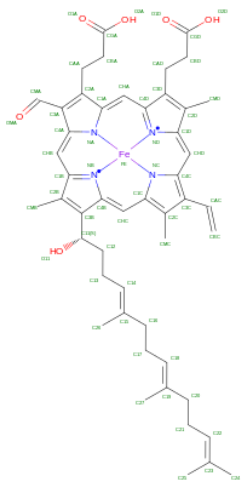
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	388	259	65	61	3	0	1	0

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

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

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

HEA



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

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

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

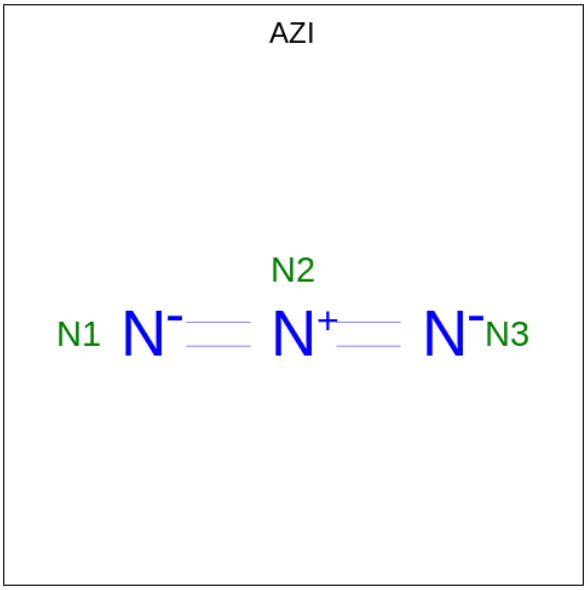
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

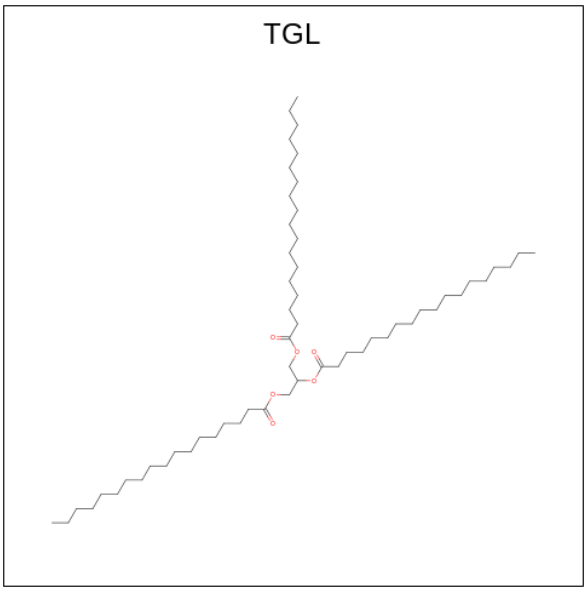
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

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



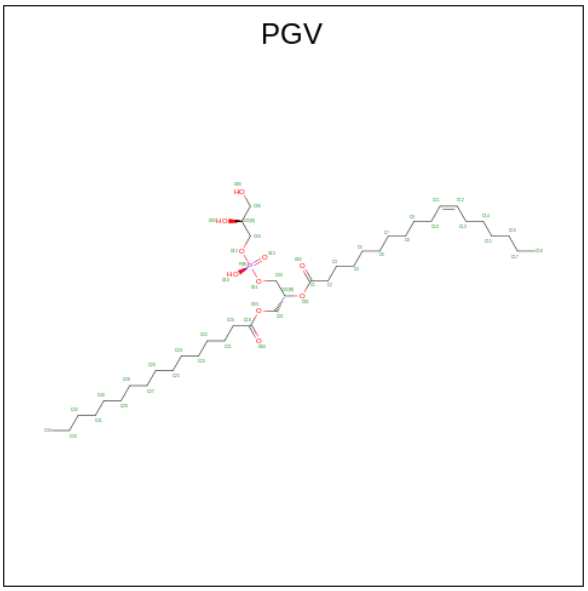
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
18	A	1	3	3	0	1
			Total	N		
18	A	1	6	6	0	1
			Total	N		
18	N	1	3	3	0	1
			Total	N		
18	N	1	6	6	0	1

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



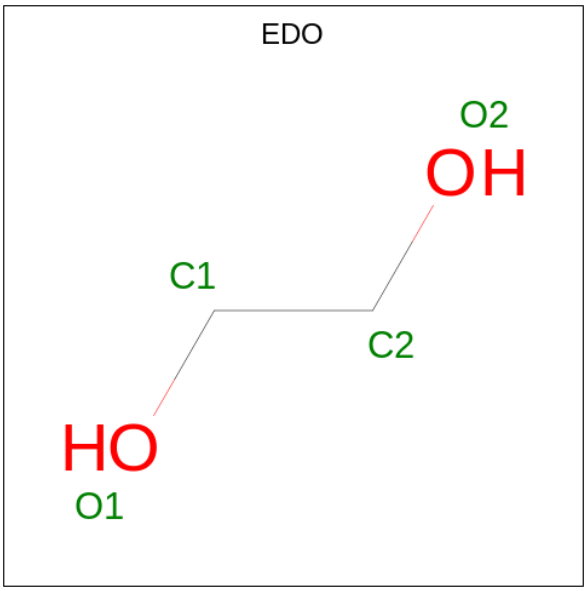
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

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



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

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



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

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

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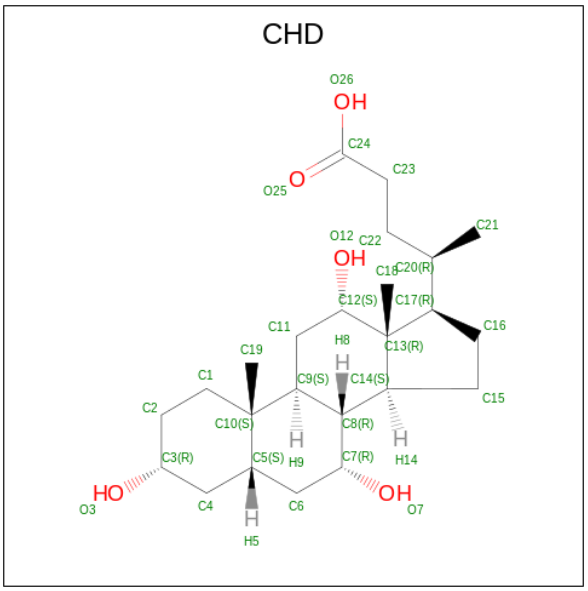
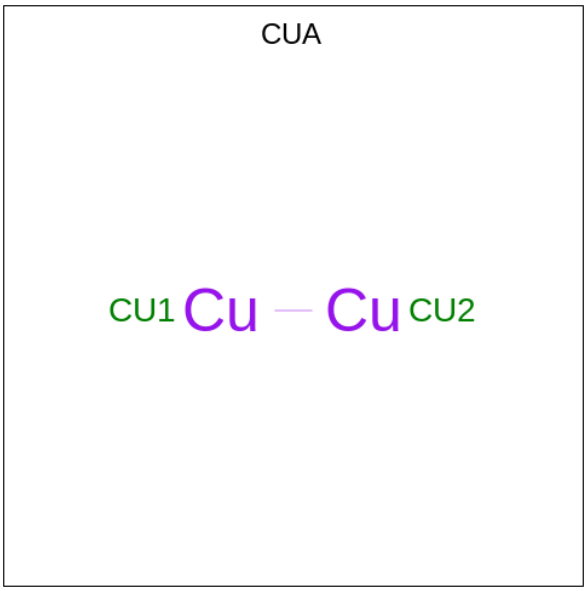
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	N	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	O	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	R	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	T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

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



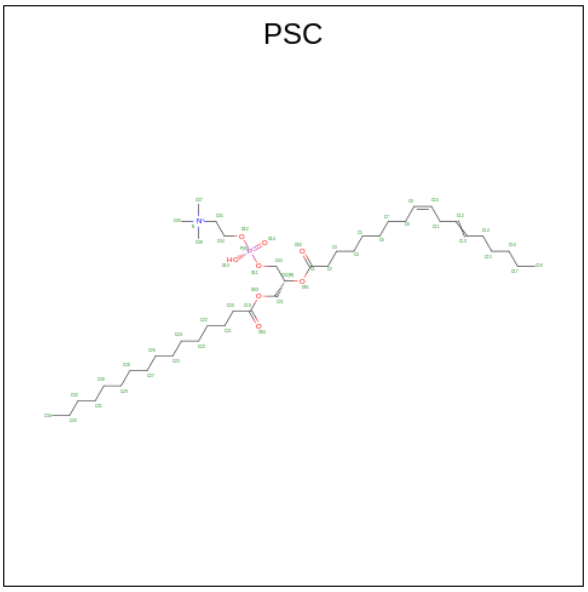
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	B	1	Total	C	O		0	0
			29	24	5			
22	C	1	Total	C	O		0	0
			29	24	5			
22	C	1	Total	C	O		0	0
			29	24	5			
22	G	1	Total	C	O		0	0
			29	24	5			
22	J	1	Total	C	O		0	0
			29	24	5			
22	P	1	Total	C	O		0	0
			29	24	5			
22	P	1	Total	C	O		0	0
			29	24	5			
22	W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

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



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

- Molecule 24 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
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0

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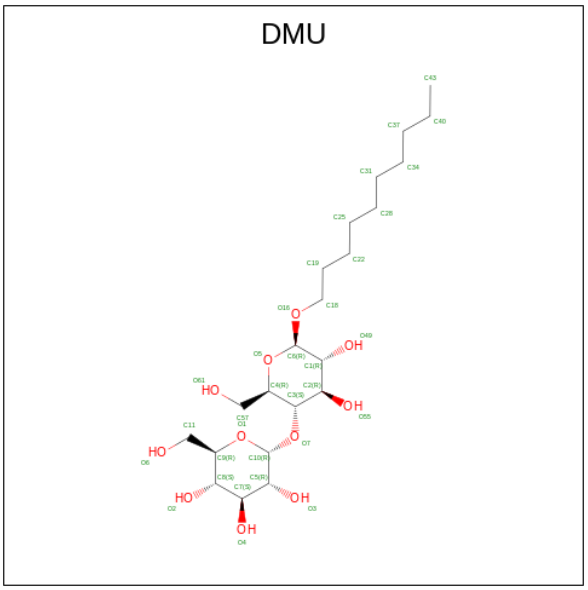
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	O	1	52	42	1	8	1	0	0

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

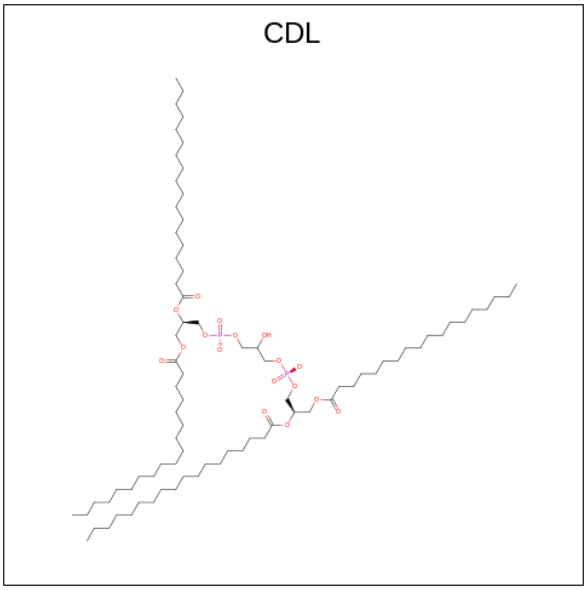


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	C	1	33	22	11	0	0
			Total	C	O		
25	L	1	33	22	11	0	0
			Total	C	O		
25	M	1	33	22	11	0	0
			Total	C	O		
25	P	1	33	22	11	0	0
			Total	C	O		
25	P	1	33	22	11	0	0
			Total	C	O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

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

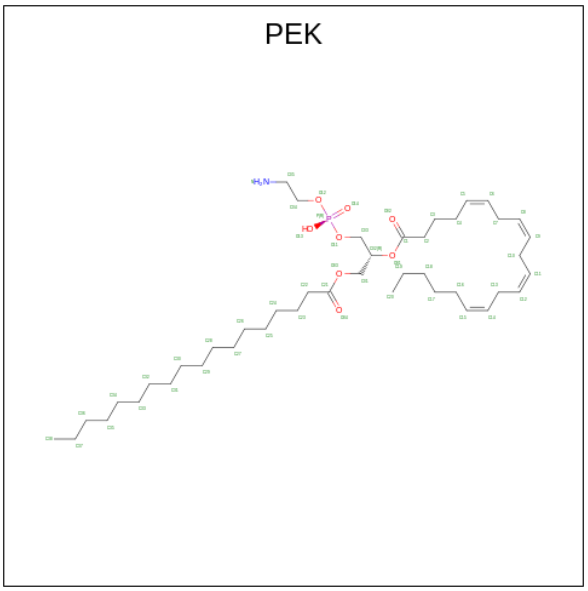
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
26	C	1	1	1	0	0
			Total	X		
26	P	1	1	1	0	0

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



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

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



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

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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	A	228	228	228	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	B	154	155	155	0	1
			Total	O		
30	C	101	101	101	0	0
			Total	O		
30	D	96	96	96	0	0
			Total	O		
30	E	80	80	80	0	0
			Total	O		
30	F	85	85	85	0	0
			Total	O		
30	G	46	46	46	0	0
			Total	O		
30	H	55	55	55	0	0
			Total	O		
30	I	26	26	26	0	0
			Total	O		
30	J	16	16	16	0	0
			Total	O		
30	K	15	15	15	0	0
			Total	O		
30	L	24	24	24	0	0
			Total	O		
30	M	19	19	19	0	0
			Total	O		
30	N	215	215	215	0	0
			Total	O		
30	O	109	110	110	0	1
			Total	O		
30	P	105	105	105	0	0
			Total	O		
30	Q	37	37	37	0	0
			Total	O		
30	R	49	49	49	0	0
			Total	O		
30	S	79	79	79	0	0
			Total	O		
30	T	36	36	36	0	0
			Total	O		
30	U	38	38	38	0	0
			Total	O		
30	V	14	14	14	0	0

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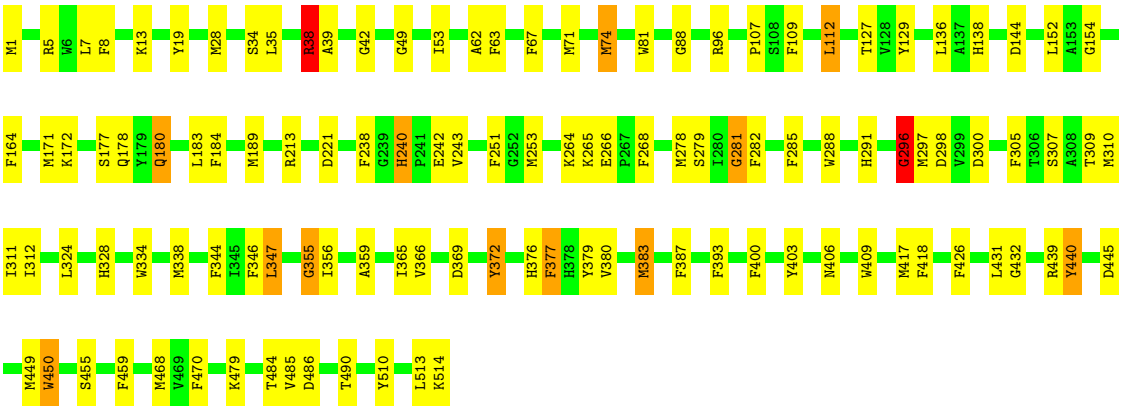
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	W	13	13	13	0	0
			Total	O		
30	X	11	11	11	0	0
			Total	O		
30	Y	13	13	13	0	0
			Total	O		
30	Z	12	12	12	0	0

3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

Chain A: 77% 20% •

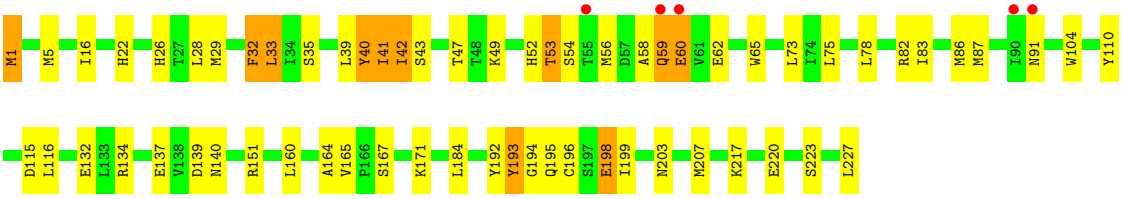


• Molecule 1: Cytochrome c oxidase subunit 1

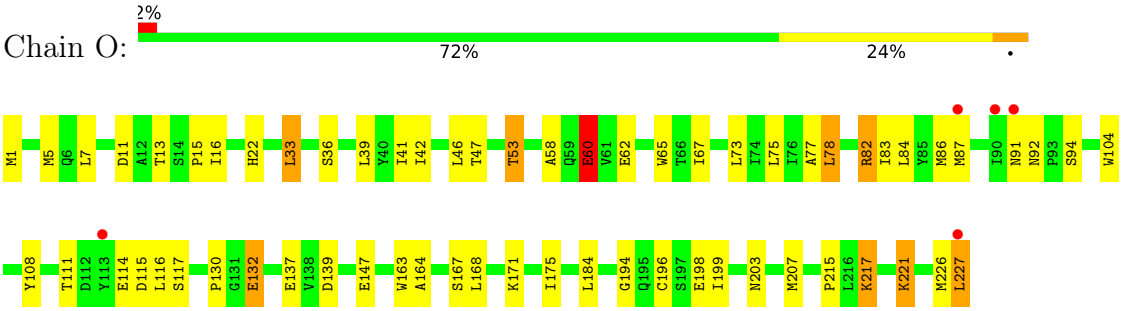
Chain N: 79% 19% •

• Molecule 2: Cytochrome c oxidase subunit 2

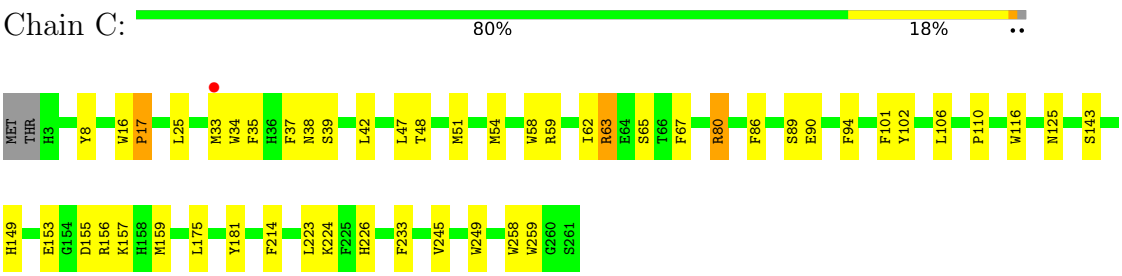
Chain B: 2% 72% 23% 5%



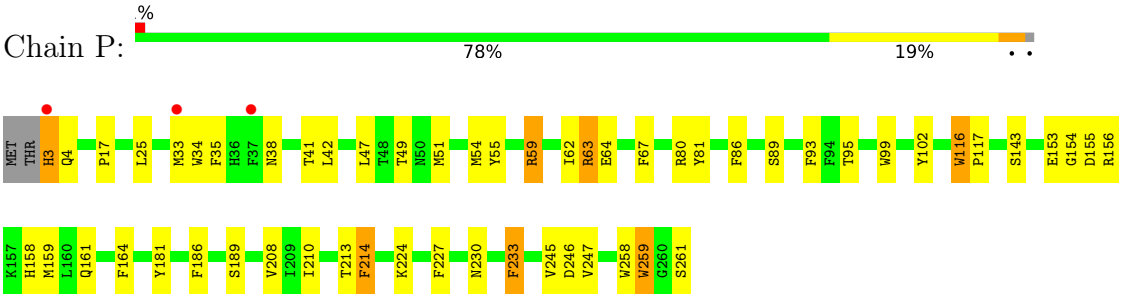
• Molecule 2: Cytochrome c oxidase subunit 2



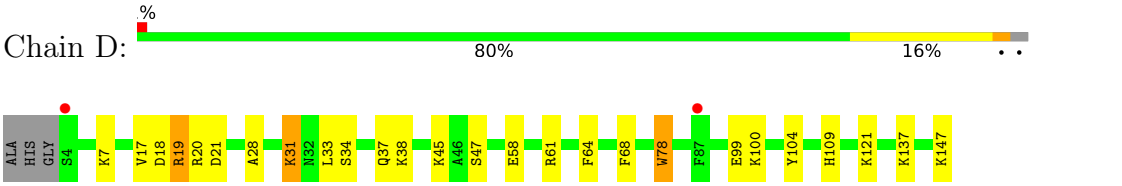
• Molecule 3: Cytochrome c oxidase subunit 3



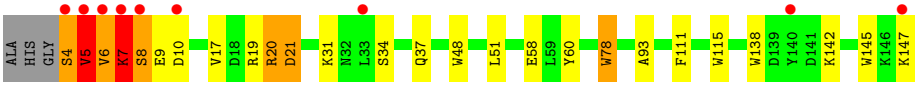
• Molecule 3: Cytochrome c oxidase subunit 3



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

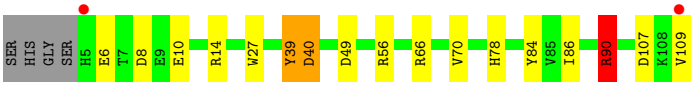


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



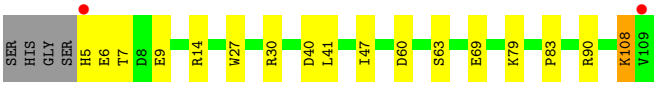
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



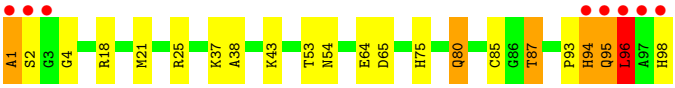
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



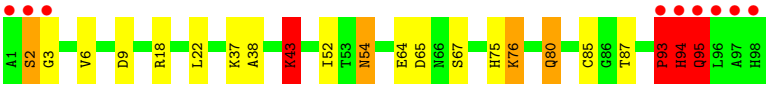
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



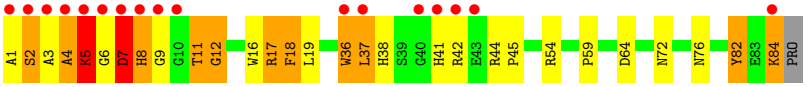
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



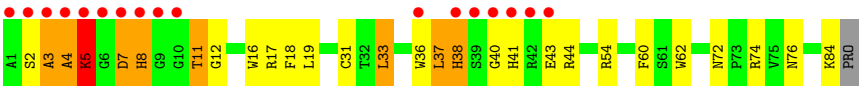
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



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

Chain T:

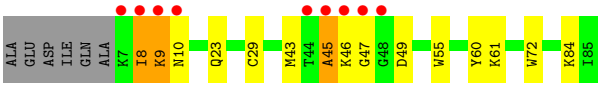


• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

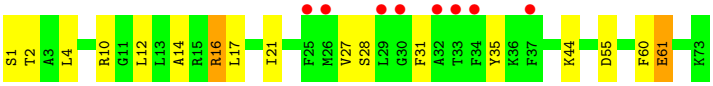
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



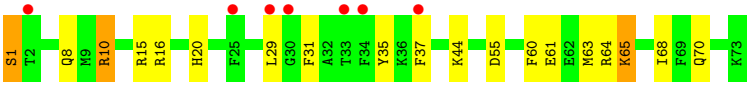
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:

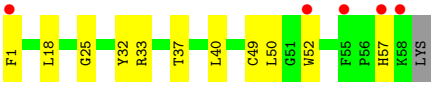


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:

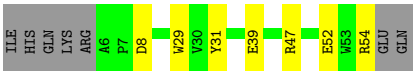
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



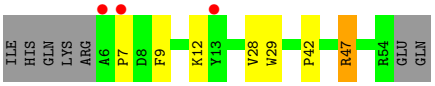
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



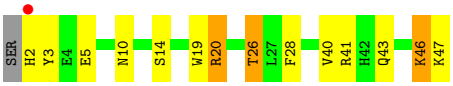
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



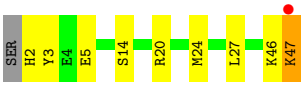
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



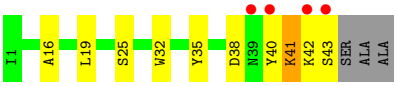
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



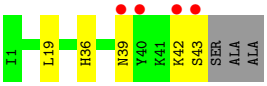
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.33Å 204.83Å 177.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 136.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.65) 99.9 (136.19-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.162 , 0.182 0.164 , 0.183	Depositor DCC
R_{free} test set	39619 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.6	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	0.97	EDS
Total number of atoms	33657	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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: DMU, CUA, CDL, PEK, PGV, SAC, PSC, UNX, EDO, FME, NA, CU, TGL, ZN, MG, CHD, AZI, HEA, TPO

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	1.66	30/4322 (0.7%)	1.51	49/5897 (0.8%)
1	N	1.62	33/4308 (0.8%)	1.39	35/5878 (0.6%)
2	B	1.64	17/1945 (0.9%)	1.45	15/2648 (0.6%)
2	O	1.37	12/1908 (0.6%)	1.21	9/2597 (0.3%)
3	C	1.64	17/2255 (0.8%)	1.33	13/3080 (0.4%)
3	P	1.58	17/2272 (0.7%)	1.33	16/3102 (0.5%)
4	D	1.60	9/1277 (0.7%)	1.37	6/1720 (0.3%)
4	Q	1.27	6/1259 (0.5%)	1.37	6/1698 (0.4%)
5	E	1.56	4/871 (0.5%)	1.75	12/1182 (1.0%)
5	R	1.39	6/871 (0.7%)	1.31	7/1182 (0.6%)
6	F	1.51	3/788 (0.4%)	1.37	6/1069 (0.6%)
6	S	1.40	2/780 (0.3%)	1.31	6/1058 (0.6%)
7	G	1.64	5/702 (0.7%)	1.36	8/953 (0.8%)
7	T	1.54	5/702 (0.7%)	1.27	6/953 (0.6%)
8	H	1.55	5/682 (0.7%)	1.23	3/921 (0.3%)
8	U	1.27	2/682 (0.3%)	1.05	0/921
9	I	1.44	4/605 (0.7%)	1.34	4/802 (0.5%)
9	V	1.15	0/605	1.15	2/802 (0.2%)
10	J	1.40	2/471 (0.4%)	1.18	1/636 (0.2%)
10	W	1.34	2/480 (0.4%)	1.22	2/648 (0.3%)
11	K	1.51	3/398 (0.8%)	1.34	5/546 (0.9%)
11	X	1.23	2/405 (0.5%)	0.92	0/556
12	L	1.60	5/393 (1.3%)	1.46	4/526 (0.8%)
12	Y	1.42	1/401 (0.2%)	1.15	0/536
13	M	1.51	2/345 (0.6%)	1.24	1/470 (0.2%)
13	Z	1.37	0/345	0.99	0/470
All	All	1.54	194/30072 (0.6%)	1.36	216/40851 (0.5%)

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	4
1	N	0	3
2	B	0	1
5	R	0	1
6	F	0	2
6	S	0	3
7	T	0	1
8	H	0	1
9	V	0	1
All	All	0	17

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	CD-OE2	-10.57	1.14	1.25
2	B	198	GLU	CD-OE1	-10.16	1.14	1.25
4	D	58	GLU	CD-OE1	10.12	1.36	1.25
12	Y	5	GLU	CD-OE2	-9.64	1.15	1.25
2	O	198	GLU	CD-OE2	-9.48	1.15	1.25
2	O	60	GLU	CD-OE1	9.39	1.35	1.25
2	B	65	TRP	CD2-CE2	9.08	1.52	1.41
1	A	34	SER	CB-OG	-9.03	1.30	1.42
3	C	102	TYR	CG-CD2	-8.95	1.27	1.39
1	A	74	MET	CB-CG	8.22	1.77	1.51
1	A	96	ARG	CZ-NH1	8.15	1.43	1.33
1	N	49	GLY	C-O	7.89	1.36	1.23
3	P	143	SER	CA-CB	7.89	1.64	1.52
6	F	1	ALA	C-O	7.79	1.38	1.23
3	C	143	SER	CA-CB	7.77	1.64	1.52
3	C	58	TRP	CD2-CE2	7.59	1.50	1.41
2	O	65	TRP	CD2-CE2	7.57	1.50	1.41
7	G	16	TRP	CD2-CE2	7.54	1.50	1.41
4	Q	78	TRP	CD2-CE2	7.49	1.50	1.41
1	N	126	TRP	CD2-CE2	7.38	1.50	1.41
2	O	60	GLU	CD-OE2	7.33	1.33	1.25
3	P	34	TRP	CD2-CE2	7.31	1.50	1.41
5	R	27	TRP	CD2-CE2	7.29	1.50	1.41
8	H	72	TRP	CD2-CE2	7.27	1.50	1.41
2	B	220	GLU	CD-OE1	-7.18	1.17	1.25
1	N	19	TYR	CE1-CZ	7.04	1.47	1.38
8	H	60	TYR	CG-CD2	6.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	334	TRP	CD2-CE2	6.95	1.49	1.41
1	N	279	SER	CA-CB	6.92	1.63	1.52
3	C	249	TRP	CD2-CE2	6.87	1.49	1.41
3	P	153	GLU	CG-CD	6.87	1.62	1.51
1	A	403	TYR	CG-CD1	6.66	1.47	1.39
4	D	78	TRP	CD2-CE2	6.62	1.49	1.41
11	X	29	TRP	CD2-CE2	6.61	1.49	1.41
7	T	60	PHE	CG-CD1	6.58	1.48	1.38
3	C	116	TRP	CD2-CE2	6.53	1.49	1.41
7	G	36	TRP	CD2-CE2	6.49	1.49	1.41
4	Q	138	TRP	CD2-CE2	6.48	1.49	1.41
2	O	167	SER	CB-OG	-6.47	1.33	1.42
8	U	72	TRP	CD2-CE2	6.32	1.49	1.41
1	A	450	TRP	CD2-CE2	6.32	1.49	1.41
9	I	28	SER	CB-OG	6.32	1.50	1.42
3	C	90	GLU	CD-OE1	6.29	1.32	1.25
4	D	18	ASP	N-CA	6.28	1.58	1.46
1	A	154	GLY	N-CA	6.28	1.55	1.46
1	A	88	GLY	N-CA	6.26	1.55	1.46
1	N	335	SER	CB-OG	6.24	1.50	1.42
1	A	213	ARG	CZ-NH1	6.22	1.41	1.33
1	N	5	ARG	CZ-NH1	6.19	1.41	1.33
3	C	258	TRP	CD2-CE2	6.13	1.48	1.41
1	N	74	MET	CB-CG	6.13	1.71	1.51
1	A	355	GLY	N-CA	6.12	1.55	1.46
3	C	259	TRP	CD2-CE2	6.11	1.48	1.41
1	N	323	TRP	CD2-CE2	6.11	1.48	1.41
3	P	258	TRP	CD2-CE2	6.11	1.48	1.41
1	A	5	ARG	CZ-NH1	6.09	1.41	1.33
8	H	30	TRP	CD2-CE2	6.05	1.48	1.41
1	N	25	TRP	CD2-CE2	6.04	1.48	1.41
3	P	64	GLU	CD-OE2	6.03	1.32	1.25
4	Q	145	TRP	CD2-CE2	6.03	1.48	1.41
3	P	99	TRP	CD2-CE2	6.02	1.48	1.41
3	P	102	TYR	CG-CD2	-6.00	1.31	1.39
2	B	167	SER	CB-OG	-6.00	1.34	1.42
3	C	259	TRP	CG-CD1	5.98	1.45	1.36
5	R	30	ARG	CZ-NH2	5.97	1.40	1.33
7	T	36	TRP	CD2-CE2	5.96	1.48	1.41
1	N	270	TYR	CG-CD1	5.94	1.46	1.39
3	P	181	TYR	CD1-CE1	5.93	1.48	1.39
3	C	35	PHE	CG-CD2	5.92	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	16	TRP	CD2-CE2	5.91	1.48	1.41
1	A	63	PHE	CG-CD1	5.90	1.47	1.38
1	A	279	SER	CA-CB	5.90	1.61	1.52
3	P	189	SER	CB-OG	5.89	1.50	1.42
5	R	27	TRP	CG-CD1	5.88	1.45	1.36
3	C	249	TRP	CE3-CZ3	5.87	1.48	1.38
2	B	193	TYR	CG-CD1	5.86	1.46	1.39
1	A	346	PHE	CD1-CE1	5.85	1.50	1.39
8	H	68	TRP	CD2-CE2	5.85	1.48	1.41
1	N	494	TRP	CD2-CE2	5.84	1.48	1.41
2	O	36	SER	CB-OG	5.83	1.49	1.42
1	A	288	TRP	CG-CD1	5.82	1.44	1.36
1	A	409	TRP	CD2-CE2	5.82	1.48	1.41
8	H	58	ARG	CZ-NH1	5.80	1.40	1.33
1	A	377	PHE	CE2-CZ	5.79	1.48	1.37
4	D	20	ARG	N-CA	5.79	1.57	1.46
12	L	28	PHE	CB-CG	5.78	1.61	1.51
6	F	4	GLY	N-CA	5.77	1.54	1.46
1	N	187	SER	CA-CB	5.76	1.61	1.52
3	P	59	ARG	CZ-NH1	5.76	1.40	1.33
5	E	27	TRP	CD2-CE2	5.71	1.48	1.41
1	N	226	GLY	N-CA	5.69	1.54	1.46
4	Q	20	ARG	CZ-NH2	-5.67	1.25	1.33
13	M	32	TRP	CD2-CE2	5.67	1.48	1.41
3	P	259	TRP	CD2-CE2	5.66	1.48	1.41
2	B	192	TYR	CE1-CZ	5.63	1.45	1.38
12	L	5	GLU	CD-OE2	-5.62	1.19	1.25
1	A	129	TYR	CD1-CE1	5.62	1.47	1.39
4	D	58	GLU	CB-CG	5.61	1.62	1.52
1	A	184	PHE	CG-CD1	5.59	1.47	1.38
1	A	281	GLY	N-CA	5.58	1.54	1.46
2	O	198	GLU	CD-OE1	-5.57	1.19	1.25
4	Q	60	TYR	CE1-CZ	5.57	1.45	1.38
4	Q	48	TRP	CD2-CE2	5.56	1.48	1.41
1	A	288	TRP	CD2-CE2	5.55	1.48	1.41
5	E	39	TYR	CG-CD2	-5.55	1.31	1.39
13	M	40	TYR	CE2-CZ	5.55	1.45	1.38
11	K	29	TRP	CD2-CE2	5.54	1.48	1.41
2	B	59	GLN	CG-CD	5.53	1.63	1.51
1	N	179	TYR	CE1-CZ	5.53	1.45	1.38
1	N	270	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	307	SER	CB-OG	5.50	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	SER	CB-OG	5.50	1.49	1.42
9	I	60	PHE	CE1-CZ	5.50	1.47	1.37
1	N	305	PHE	CG-CD2	5.47	1.47	1.38
7	G	7	ASP	N-CA	5.47	1.57	1.46
1	N	244	TYR	CG-CD1	5.47	1.46	1.39
10	W	52	TRP	CD2-CE2	5.46	1.48	1.41
12	L	26	THR	CA-CB	5.46	1.67	1.53
8	U	55	TRP	CD2-CE2	5.45	1.47	1.41
1	N	396	TRP	CD2-CE2	5.44	1.47	1.41
2	O	163	TRP	CD2-CE2	5.44	1.47	1.41
3	P	116	TRP	CD2-CE2	5.44	1.47	1.41
1	N	409	TRP	CD2-CE2	5.41	1.47	1.41
1	A	266	GLU	CD-OE2	5.41	1.31	1.25
1	A	238	PHE	CG-CD2	5.41	1.46	1.38
1	N	371	TYR	CG-CD2	5.41	1.46	1.39
9	I	16	ARG	NE-CZ	5.40	1.40	1.33
7	G	17	ARG	CZ-NH1	5.37	1.40	1.33
4	D	61	ARG	CZ-NH2	5.37	1.40	1.33
2	B	65	TRP	CG-CD1	5.36	1.44	1.36
4	D	47	SER	CA-CB	5.36	1.60	1.52
1	A	305	PHE	CG-CD2	5.35	1.46	1.38
5	R	47	ILE	N-CA	5.34	1.57	1.46
1	A	242	GLU	CD-OE1	5.33	1.31	1.25
5	R	63	SER	CB-OG	5.33	1.49	1.42
1	N	324	LEU	N-CA	5.33	1.57	1.46
2	B	110	TYR	CG-CD1	5.31	1.46	1.39
5	E	78	HIS	N-CA	5.31	1.56	1.46
5	R	69	GLU	CD-OE2	-5.30	1.19	1.25
10	W	25	GLY	N-CA	5.30	1.54	1.46
1	N	505	PHE	CE2-CZ	5.30	1.47	1.37
10	J	25	GLY	N-CA	5.29	1.53	1.46
1	A	264	LYS	CD-CE	5.29	1.64	1.51
12	L	5	GLU	CD-OE1	-5.28	1.19	1.25
1	N	288	TRP	CD2-CE2	5.28	1.47	1.41
6	S	67	SER	CB-OG	5.27	1.49	1.42
1	A	238	PHE	CG-CD1	5.26	1.46	1.38
3	P	89	SER	CB-OG	5.26	1.49	1.42
1	N	355	GLY	N-CA	5.25	1.53	1.46
2	B	223	SER	CA-CB	5.24	1.60	1.52
4	D	64	PHE	CG-CD2	5.24	1.46	1.38
3	C	8	TYR	CG-CD2	5.24	1.46	1.39
2	B	53	THR	N-CA	5.23	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	5	LYS	CA-C	5.23	1.66	1.52
11	X	29	TRP	CE3-CZ3	5.21	1.47	1.38
1	A	164	PHE	CE2-CZ	5.21	1.47	1.37
2	O	132	GLU	CD-OE2	5.21	1.31	1.25
7	T	62	TRP	CD2-CE2	5.20	1.47	1.41
12	L	19	TRP	CD2-CE2	5.20	1.47	1.41
3	P	186	PHE	CG-CD1	5.20	1.46	1.38
3	C	101	PHE	CG-CD1	5.19	1.46	1.38
1	N	350	VAL	CB-CG2	5.18	1.63	1.52
2	B	43	SER	CB-OG	-5.18	1.35	1.42
6	S	18	ARG	CZ-NH1	5.17	1.39	1.33
4	D	68	PHE	CG-CD1	5.16	1.46	1.38
10	J	33	ARG	CA-CB	5.14	1.65	1.53
1	N	94	PHE	CG-CD1	5.13	1.46	1.38
11	K	31	TYR	CG-CD1	5.13	1.45	1.39
1	N	34	SER	CA-CB	5.13	1.60	1.52
3	C	34	TRP	CD2-CE2	5.13	1.47	1.41
2	B	165	VAL	CB-CG2	5.12	1.63	1.52
6	F	18	ARG	CZ-NH1	5.12	1.39	1.33
7	G	82	TYR	CE1-CZ	-5.11	1.31	1.38
2	O	94	SER	CB-OG	-5.11	1.35	1.42
1	A	81	TRP	CD2-CE2	5.10	1.47	1.41
5	E	84	TYR	CG-CD1	5.10	1.45	1.39
2	B	40	TYR	CA-CB	-5.08	1.42	1.53
3	P	259	TRP	NE1-CE2	5.08	1.44	1.37
2	B	32[A]	PHE	C-O	5.07	1.32	1.23
2	B	32[B]	PHE	C-O	5.07	1.32	1.23
2	O	147	GLU	CD-OE1	-5.07	1.20	1.25
1	N	6	TRP	CG-CD1	5.05	1.43	1.36
9	I	4	LEU	CA-CB	5.05	1.65	1.53
3	C	63	ARG	CZ-NH2	5.04	1.39	1.33
3	P	259	TRP	CG-CD1	5.04	1.43	1.36
11	K	39	GLU	CB-CG	5.04	1.61	1.52
1	N	382[A]	SER	CB-OG	-5.04	1.35	1.42
1	N	382[B]	SER	CB-OG	-5.04	1.35	1.42
1	A	334	TRP	CD2-CE2	5.03	1.47	1.41
1	N	148	PHE	CG-CD2	5.03	1.46	1.38
2	O	53	THR	N-CA	5.03	1.56	1.46
1	N	275	TRP	CD2-CE2	5.02	1.47	1.41
3	P	227	PHE	CG-CD2	5.02	1.46	1.38
3	C	65	SER	CA-CB	5.00	1.60	1.52

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	20	ARG	NE-CZ-NH2	-24.32	108.14	120.30
5	E	90	ARG	NE-CZ-NH1	23.80	132.20	120.30
4	Q	20	ARG	NE-CZ-NH1	22.14	131.37	120.30
5	E	90	ARG	NE-CZ-NH2	-21.09	109.75	120.30
1	A	71	MET	CG-SD-CE	-18.87	70.01	100.20
1	N	71	MET	CG-SD-CE	-18.73	70.24	100.20
11	K	47	ARG	NE-CZ-NH1	13.34	126.97	120.30
12	L	20	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	213	ARG	NE-CZ-NH2	-11.98	114.31	120.30
9	I	16	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	189	MET	CG-SD-CE	-10.58	83.28	100.20
2	B	151	ARG	NE-CZ-NH2	-10.48	115.06	120.30
5	R	90	ARG	NE-CZ-NH2	-10.34	115.13	120.30
5	E	90	ARG	CD-NE-CZ	10.28	137.99	123.60
4	Q	21	ASP	CB-CG-OD2	10.01	127.31	118.30
1	N	189	MET	CG-SD-CE	-9.97	84.25	100.20
3	P	63	ARG	NE-CZ-NH2	-9.90	115.35	120.30
5	E	40	ASP	CB-CG-OD1	9.81	127.13	118.30
1	A	346	PHE	CB-CG-CD2	-9.67	114.03	120.80
4	D	20	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	A	129	TYR	CB-CG-CD2	-9.33	115.40	121.00
7	G	12	GLY	N-CA-C	9.28	136.29	113.10
1	A	8	PHE	CB-CG-CD2	-8.94	114.54	120.80
12	L	20	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	N	251	PHE	CB-CG-CD2	-8.78	114.65	120.80
9	V	10	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	213	ARG	NE-CZ-NH1	8.64	124.62	120.30
2	B	151	ARG	NE-CZ-NH1	8.55	124.58	120.30
6	F	25	ARG	NE-CZ-NH2	8.27	124.44	120.30
5	E	66	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	B	82	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	N	310	MET	CG-SD-CE	-7.98	87.43	100.20
1	A	400	PHE	CB-CG-CD2	-7.95	115.23	120.80
3	P	153	GLU	OE1-CD-OE2	7.93	132.81	123.30
5	R	90	ARG	CG-CD-NE	-7.91	95.20	111.80
7	G	7	ASP	N-CA-C	7.89	132.31	111.00
5	E	90	ARG	CB-CG-CD	7.79	131.84	111.60
1	A	144	ASP	CB-CG-OD2	-7.77	111.31	118.30
8	H	73	ASP	CB-CG-OD2	-7.70	111.37	118.30
7	T	7	ASP	N-CA-C	7.68	131.72	111.00
2	O	82	ARG	NE-CZ-NH2	-7.64	116.48	120.30
5	R	60	ASP	CB-CG-OD1	7.59	125.14	118.30
6	S	43	LYS	CD-CE-NZ	-7.48	94.49	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	MET	CA-CB-CG	-7.43	100.66	113.30
1	A	310	MET	CG-SD-CE	-7.39	88.38	100.20
1	A	8	PHE	CB-CG-CD1	7.36	125.95	120.80
1	A	38	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	387	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	N	7	LEU	CB-CG-CD1	7.24	123.30	111.00
1	A	112	LEU	CD1-CG-CD2	-7.20	88.91	110.50
1	N	486	ASP	CB-CG-OD2	-7.13	111.89	118.30
3	C	102	TYR	CB-CG-CD1	-7.07	116.76	121.00
5	E	56	ARG	NE-CZ-NH2	-7.04	116.78	120.30
5	R	14	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	N	129	TYR	CB-CG-CD2	-7.03	116.78	121.00
10	W	18	LEU	CB-CG-CD1	-7.02	99.06	111.00
1	A	35	LEU	CB-CG-CD2	6.99	122.88	111.00
11	K	47	ARG	CD-NE-CZ	6.97	133.36	123.60
3	P	214	PHE	CB-CG-CD2	-6.93	115.95	120.80
2	B	139	ASP	CB-CG-OD1	6.87	124.48	118.30
2	B	42	ILE	CG1-CB-CG2	-6.86	96.31	111.40
1	A	445	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	49	GLY	N-CA-C	-6.84	96.00	113.10
7	G	64	ASP	CB-CG-OD1	6.83	124.44	118.30
1	A	127	THR	CA-CB-CG2	-6.79	102.89	112.40
12	L	20	ARG	CG-CD-NE	-6.76	97.60	111.80
5	E	107	ASP	CB-CG-OD1	6.73	124.36	118.30
3	P	93	PHE	CB-CG-CD2	-6.66	116.14	120.80
3	P	181	TYR	CG-CD1-CE1	-6.65	115.98	121.30
1	N	212	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	B	33	LEU	CB-CG-CD2	-6.62	99.74	111.00
2	B	134	ARG	NE-CZ-NH2	-6.58	117.01	120.30
5	R	40	ASP	CB-CG-OD2	-6.53	112.43	118.30
7	T	12	GLY	N-CA-C	6.51	129.37	113.10
6	S	94	HIS	N-CA-C	6.50	128.55	111.00
1	N	184	PHE	CB-CG-CD2	-6.49	116.26	120.80
1	N	486	ASP	CB-CG-OD1	6.47	124.13	118.30
2	B	73	LEU	CB-CG-CD1	-6.46	100.01	111.00
8	H	8	ILE	N-CA-C	6.46	128.43	111.00
3	P	156	ARG	NE-CZ-NH1	6.43	123.52	120.30
4	D	20	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	A	268	PHE	CB-CG-CD2	-6.35	116.36	120.80
2	O	227	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	426	PHE	CB-CG-CD1	-6.34	116.36	120.80
5	E	49	ASP	CB-CG-OD1	6.31	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	152	LEU	CB-CG-CD2	6.31	121.72	111.00
1	A	324	LEU	CB-CG-CD2	6.30	121.71	111.00
1	N	439	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	96	ARG	NE-CZ-NH2	-6.28	117.16	120.30
9	I	55	ASP	CB-CG-OD1	6.27	123.94	118.30
3	P	233	PHE	CB-CG-CD1	-6.22	116.45	120.80
8	H	61	LYS	CD-CE-NZ	6.21	125.99	111.70
3	P	35	PHE	CB-CG-CD1	6.20	125.14	120.80
7	G	44	ARG	NE-CZ-NH2	6.19	123.40	120.30
1	A	379	TYR	CB-CG-CD2	-6.18	117.29	121.00
6	S	76	LYS	CD-CE-NZ	6.17	125.89	111.70
1	N	189	MET	CB-CG-SD	-6.14	93.97	112.40
5	E	14	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	O	82	ARG	NE-CZ-NH1	6.14	123.37	120.30
3	P	214	PHE	CB-CG-CD1	6.14	125.09	120.80
3	C	80[A]	ARG	CG-CD-NE	-6.09	99.02	111.80
3	C	80[B]	ARG	CG-CD-NE	-6.09	99.02	111.80
3	P	63	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	251	PHE	CB-CG-CD2	-6.07	116.55	120.80
1	A	74	MET	CB-CG-SD	-5.99	94.44	112.40
1	N	19	TYR	CB-CG-CD1	-5.99	117.41	121.00
3	C	94	PHE	CB-CG-CD1	-5.99	116.61	120.80
1	A	393	PHE	CB-CG-CD2	-5.98	116.61	120.80
3	C	223	LEU	CB-CG-CD1	-5.96	100.88	111.00
3	P	102	TYR	CB-CG-CD1	-5.95	117.43	121.00
11	K	54	ARG	CA-C-O	-5.94	107.62	120.10
1	A	300	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	510	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	7	LEU	CB-CG-CD1	5.84	120.93	111.00
4	D	137	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	A	74	MET	CG-SD-CE	-5.80	90.91	100.20
3	P	55	TYR	CZ-CE2-CD2	-5.80	114.58	119.80
11	K	47	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
4	Q	20	ARG	CD-NE-CZ	5.79	131.71	123.60
1	N	213	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	N	513	LEU	C-N-CA	-5.78	107.24	121.70
1	A	183	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	A	372	TYR	CB-CG-CD2	-5.76	117.55	121.00
4	Q	20	ARG	CG-CD-NE	-5.75	99.73	111.80
3	C	181	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
1	N	371	TYR	CB-CG-CD2	-5.69	117.59	121.00
5	R	30	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	18	ARG	NE-CZ-NH1	5.67	123.14	120.30
7	T	44	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	C	214	PHE	CB-CG-CD2	-5.66	116.84	120.80
2	O	11	ASP	CB-CG-OD1	5.66	123.39	118.30
5	E	84	TYR	CZ-CE2-CD2	-5.65	114.71	119.80
4	D	61	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	344	PHE	CB-CG-CD2	-5.61	116.88	120.80
2	O	65	TRP	CB-CA-C	-5.59	99.22	110.40
1	N	49	GLY	N-CA-C	-5.59	99.12	113.10
3	C	86	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	A	366	VAL	CA-CB-CG2	-5.55	102.57	110.90
10	W	40	LEU	CB-CG-CD2	5.55	120.43	111.00
1	A	67	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	171	MET	CA-CB-CG	-5.53	103.89	113.30
6	F	18	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	N	35	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	A	347	LEU	CA-CB-CG	-5.51	102.62	115.30
3	P	155	ASP	CB-CG-OD1	5.50	123.25	118.30
4	D	45	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	N	302[A]	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	N	302[B]	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	152	LEU	CB-CG-CD2	5.48	120.31	111.00
4	Q	21	ASP	CB-CG-OD1	-5.48	113.37	118.30
3	P	93	PHE	CB-CG-CD1	5.47	124.63	120.80
1	A	366	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	N	35	LEU	CA-CB-CG	-5.42	102.83	115.30
7	G	18	PHE	CB-CG-CD2	-5.40	117.02	120.80
3	C	181	TYR	CB-CG-CD2	-5.40	117.76	121.00
2	B	39	LEU	CB-CG-CD1	5.39	120.16	111.00
9	I	12	LEU	CB-CG-CD1	-5.39	101.84	111.00
2	B	184	LEU	N-CA-CB	-5.38	99.64	110.40
7	T	19	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	285	PHE	CB-CG-CD1	-5.37	117.04	120.80
1	A	253	MET	CA-CB-CG	-5.37	104.18	113.30
1	N	74	MET	CB-CG-SD	-5.36	96.33	112.40
9	I	61	GLU	OE1-CD-OE2	-5.35	116.88	123.30
7	T	5	LYS	CB-CA-C	5.33	121.07	110.40
3	P	86	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	N	144	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	B	32[A]	PHE	O-C-N	5.32	131.22	122.70
2	B	32[B]	PHE	O-C-N	5.32	131.22	122.70
6	F	25	ARG	NE-CZ-NH1	-5.31	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	56	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	O	73	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	N	377	PHE	CB-CG-CD1	5.25	124.47	120.80
10	J	36	MET	CG-SD-CE	-5.24	91.81	100.20
1	N	179	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	A	470	PHE	CB-CG-CD1	-5.24	117.13	120.80
7	G	44	ARG	NE-CZ-NH1	-5.23	117.68	120.30
3	C	214	PHE	CB-CG-CD1	5.23	124.46	120.80
1	N	344	PHE	CB-CG-CD2	-5.22	117.14	120.80
7	G	5	LYS	CB-CA-C	5.21	120.82	110.40
1	N	354	THR	CA-CB-CG2	-5.21	105.11	112.40
3	C	59	ARG	NE-CZ-NH1	-5.20	117.70	120.30
13	M	35	TYR	CB-CG-CD1	-5.20	117.88	121.00
7	T	33	LEU	CA-CB-CG	5.20	127.25	115.30
1	N	8	PHE	CB-CG-CD2	-5.18	117.17	120.80
3	C	245	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	N	377	PHE	CB-CG-CD2	-5.16	117.19	120.80
6	S	9	ASP	CB-CG-OD1	5.16	122.94	118.30
4	D	58	GLU	CA-CB-CG	-5.15	102.07	113.40
1	A	296	GLY	O-C-N	-5.14	114.47	122.70
1	N	96	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	440	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	N	490	THR	CA-CB-CG2	-5.14	105.20	112.40
3	C	153	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	N	179	TYR	CD1-CE1-CZ	-5.14	115.18	119.80
6	S	22	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	129	TYR	CG-CD1-CE1	-5.12	117.21	121.30
1	A	383[A]	MET	CG-SD-CE	-5.10	92.05	100.20
1	A	383[B]	MET	CG-SD-CE	-5.10	92.05	100.20
11	K	8	ASP	CB-CG-OD1	5.09	122.88	118.30
1	N	238	PHE	CB-CG-CD1	-5.09	117.24	120.80
6	F	87	THR	OG1-CB-CG2	-5.09	98.30	110.00
1	N	438	ARG	CA-CB-CG	-5.08	102.23	113.40
2	B	59	GLN	N-CA-CB	5.07	119.73	110.60
6	S	93	PRO	C-N-CA	5.07	134.38	121.70
2	O	139	ASP	CB-CG-OD1	5.07	122.86	118.30
2	O	184	LEU	N-CA-CB	-5.06	100.28	110.40
1	A	164	PHE	CB-CG-CD1	-5.05	117.27	120.80
2	B	41[A]	ILE	C-N-CA	-5.05	109.08	121.70
2	B	41[B]	ILE	C-N-CA	-5.05	109.08	121.70
3	P	49	THR	CA-CB-CG2	-5.04	105.34	112.40
2	O	75	LEU	CB-CG-CD1	-5.03	102.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1	ALA	O-C-N	5.02	130.74	122.70
9	V	55	ASP	CB-CG-OD1	5.02	122.82	118.30
7	G	19	LEU	CB-CG-CD1	-5.02	102.47	111.00
5	R	90	ARG	NE-CZ-NH1	5.02	122.81	120.30
12	L	46	LYS	CB-CG-CD	-5.01	98.58	111.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	38	ARG	Sidechain
2	B	40	TYR	Mainchain
6	F	93	PRO	Peptide
6	F	96	LEU	Peptide
8	H	8	ILE	Peptide
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
1	N	304	TYR	Sidechain
5	R	108	LYS	Peptide
6	S	3	GLY	Peptide
6	S	94	HIS	Peptide
6	S	95	GLN	Peptide
7	T	40	GLY	Peptide
9	V	1	SAC	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	94	0
1	N	4179	0	4154	107	0
2	B	1907	0	1901	55	0
2	O	1870	0	1868	46	0
3	C	2168	0	2084	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2185	0	2097	48	0
4	D	1242	0	1235	38	1
4	Q	1224	0	1211	19	0
5	E	852	0	845	16	0
5	R	852	0	845	2	0
6	F	771	0	748	23	0
6	S	763	0	742	32	0
7	G	686	0	650	48	0
7	T	686	0	651	25	0
8	H	662	0	623	24	0
8	U	662	0	623	10	0
9	I	601	0	613	19	0
9	V	601	0	613	15	0
10	J	460	0	459	9	0
10	W	469	0	464	6	0
11	K	384	0	366	1	0
11	X	391	0	374	10	0
12	L	380	0	380	18	0
12	Y	388	0	388	20	0
13	M	335	0	352	5	0
13	Z	335	0	352	4	0
14	A	180	0	162	23	0
14	N	180	0	162	22	0
15	A	1	0	0	1	0
15	N	1	0	0	1	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	8	0
18	N	9	0	0	6	0
19	A	63	0	110	1	0
19	D	63	0	110	12	0
19	L	63	0	110	11	0
19	N	63	0	110	5	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	11	0
20	C	102	0	152	7	0
20	N	51	0	76	1	0
20	P	102	0	152	14	0
20	X	51	0	76	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	44	0	66	16	0
21	B	12	0	18	0	0
21	C	12	0	18	0	0
21	D	16	0	24	15	0
21	E	12	0	18	9	0
21	F	16	0	24	0	0
21	G	8	0	12	1	0
21	H	4	0	6	5	0
21	L	4	0	6	0	0
21	N	28	0	42	2	0
21	O	8	0	12	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	20	0	30	0	0
21	T	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	4	0
22	P	58	0	77	4	0
22	W	29	0	39	5	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	21	0
24	O	52	0	80	11	0
25	C	99	0	126	13	0
25	L	33	0	42	4	0
25	M	33	0	42	0	0
25	P	99	0	126	16	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	0	0
27	C	100	0	156	26	0
27	G	100	0	156	24	0
27	P	100	0	156	28	0
27	T	100	0	156	24	0
28	C	53	0	77	14	0
28	G	106	0	154	26	0
28	P	53	0	77	5	0
28	T	106	0	154	2	0
29	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	S	1	0	0	0	0
30	A	228	0	0	23	0
30	B	155	0	0	9	2
30	C	101	0	0	1	0
30	D	96	0	0	11	0
30	E	80	0	0	8	0
30	F	85	0	0	3	0
30	G	46	0	0	5	0
30	H	55	0	0	1	0
30	I	26	0	0	6	0
30	J	16	0	0	1	0
30	K	15	0	0	0	0
30	L	24	0	0	7	1
30	M	19	0	0	1	0
30	N	215	0	0	16	0
30	O	110	0	0	2	0
30	P	105	0	0	6	0
30	Q	37	0	0	1	0
30	R	49	0	0	0	0
30	S	79	0	0	3	0
30	T	36	0	0	0	0
30	U	38	0	0	0	0
30	V	14	0	0	1	0
30	W	13	0	0	0	0
30	X	11	0	0	3	0
30	Y	13	0	0	0	0
30	Z	12	0	0	0	0
All	All	33657	0	32632	830	2

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 13.

All (830) 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)
1:A:74:MET:CG	1:A:74:MET:CB	1.77	1.58
2:B:1:FME:CN	2:B:1:FME:N	1.71	1.50
4:D:38:LYS:HE2	30:D:303:HOH:O	1.16	1.31
24:B:303:PSC:O02	9:I:14:ALA:CB	1.80	1.28
2:B:1:FME:N	2:B:1:FME:O1	1.65	1.26
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.50	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:621:EDO:H21	30:A:770:HOH:O	1.32	1.25
2:B:29[B]:MET:SD	2:B:29[B]:MET:O	1.94	1.24
9:I:27:VAL:HG12	30:I:103:HOH:O	1.34	1.24
1:A:297[B]:MET:CB	30:A:801:HOH:O	1.77	1.23
1:N:513:LEU:O	1:N:514:LYS:CB	1.84	1.20
1:A:365:ILE:HG13	30:A:900:HOH:O	1.00	1.17
1:N:297[B]:MET:HB2	30:N:774:HOH:O	1.44	1.16
25:L:102:DMU:H26	30:L:224:HOH:O	1.43	1.15
19:D:201:TGL:HG31	30:D:355:HOH:O	1.47	1.14
5:E:90:ARG:HD2	30:E:360:HOH:O	1.43	1.14
12:L:43:GLN:CD	30:L:201:HOH:O	1.86	1.14
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.21	1.14
27:T:103:CDL:H622	27:T:103:CDL:H661	1.28	1.14
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.46	1.13
3:P:33[A]:MET:HB2	25:P:307:DMU:H9	1.24	1.12
3:C:33:MET:HE2	25:C:302:DMU:H8	1.15	1.12
24:B:303:PSC:O02	9:I:14:ALA:HB2	0.95	1.11
2:B:53:THR:HG21	30:D:323:HOH:O	1.50	1.11
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.48	1.11
1:N:297[B]:MET:CB	30:N:774:HOH:O	1.93	1.11
2:B:54:SER:HB3	21:E:202:EDO:H22	1.15	1.10
21:A:611:EDO:H22	21:A:621:EDO:H12	1.33	1.10
1:N:513:LEU:O	1:N:514:LYS:HB2	1.41	1.09
1:N:302[B]:ARG:HH11	1:N:302[B]:ARG:HB3	1.15	1.09
1:A:479:LYS:HD2	30:M:217:HOH:O	1.52	1.08
3:P:33[A]:MET:HB2	25:P:307:DMU:C19	1.83	1.08
12:Y:20:ARG:NH2	19:Y:101:TGL:HC61	1.68	1.08
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.83	1.08
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.19	1.07
4:D:19[A]:ARG:HG2	4:D:19[A]:ARG:HH21	1.05	1.07
1:A:112:LEU:HG	30:A:904:HOH:O	1.55	1.07
6:F:1:ALA:HB3	6:S:65:ASP:OD2	1.54	1.07
9:I:61:GLU:OE1	30:I:101:HOH:O	1.72	1.06
21:A:621:EDO:H22	30:A:820:HOH:O	1.55	1.06
1:A:297[B]:MET:HB3	30:A:801:HOH:O	1.45	1.05
6:F:85:CYS:SG	6:F:87:THR:HG23	1.95	1.05
12:Y:20:ARG:HH22	19:Y:101:TGL:HC61	0.90	1.05
12:L:20:ARG:HH22	19:L:101:TGL:HC32	0.93	1.05
11:X:47:ARG:HB3	11:X:47:ARG:NH1	1.71	1.05
1:A:282:PHE:HA	7:T:4:ALA:CB	1.86	1.05
2:B:29[B]:MET:SD	2:B:29[B]:MET:C	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.73	1.04
1:N:302[B]:ARG:HH11	1:N:302[B]:ARG:CB	1.70	1.04
28:C:307:PEK:C38	27:G:102:CDL:H273	1.88	1.03
9:I:61:GLU:CD	30:I:101:HOH:O	1.96	1.03
28:C:307:PEK:H382	27:G:102:CDL:H273	1.37	1.02
12:Y:20:ARG:HH22	19:Y:101:TGL:CC6	1.72	1.02
4:D:19[A]:ARG:HG2	4:D:19[A]:ARG:NH2	1.61	1.02
4:D:19[A]:ARG:HH21	4:D:19[A]:ARG:CG	1.73	1.02
1:A:312:ILE:HD12	30:A:869:HOH:O	1.58	1.01
19:L:101:TGL:OC1	19:L:101:TGL:CC4	2.08	1.00
19:L:101:TGL:OC1	19:L:101:TGL:HC42	1.19	1.00
1:N:417[A]:MET:HE2	30:N:853:HOH:O	1.61	1.00
20:P:304:PGV:H152	27:P:305:CDL:H621	1.41	1.00
1:A:297[B]:MET:HB2	30:A:801:HOH:O	1.41	0.99
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.10	0.99
1:A:417[B]:MET:CE	30:A:841:HOH:O	2.08	0.99
3:C:157:LYS:HZ1	28:C:307:PEK:H051	1.25	0.99
3:C:33:MET:CE	3:C:42:LEU:HD12	1.94	0.98
19:Y:101:TGL:HC41	19:Y:101:TGL:OC1	1.60	0.98
3:C:33:MET:HE3	3:C:42:LEU:HD12	1.43	0.98
3:C:224:LYS:CD	27:C:305:CDL:HB31	1.94	0.98
21:A:619:EDO:H22	30:A:789:HOH:O	1.64	0.97
4:Q:19[A]:ARG:CG	4:Q:21:ASP:OD1	2.13	0.97
3:C:67:PHE:HE2	27:C:305:CDL:H1	1.28	0.97
3:C:157:LYS:NZ	28:C:307:PEK:H051	1.79	0.96
1:A:74:MET:CB	1:A:74:MET:SD	2.53	0.96
21:A:611:EDO:H22	21:A:621:EDO:C1	1.94	0.96
3:P:67:PHE:HE2	27:P:305:CDL:H1	1.26	0.96
12:L:14:SER:H	19:L:101:TGL:HC31	1.27	0.96
4:D:100[B]:LYS:HE2	30:D:356:HOH:O	1.64	0.96
3:P:33[A]:MET:CB	25:P:307:DMU:H9	1.94	0.96
12:L:43:GLN:OE1	30:L:201:HOH:O	1.82	0.95
7:G:5:LYS:HG3	28:G:104:PEK:H332	1.46	0.94
12:L:20:ARG:HH22	19:L:101:TGL:CC3	1.79	0.94
1:N:365:ILE:HD11	30:N:701:HOH:O	1.68	0.94
27:T:103:CDL:OB3	27:T:103:CDL:H151	1.67	0.94
7:G:8:HIS:NE2	28:G:104:PEK:H051	1.83	0.94
8:H:9:LYS:HD3	8:H:10:ASN:H	1.29	0.94
8:H:31:GLN:HE22	21:H:101:EDO:H12	1.33	0.94
7:G:2:SER:O	28:G:104:PEK:H311	1.68	0.94
6:S:43:LYS:HE2	6:S:43:LYS:H	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:HA	21:D:202:EDO:H11	1.50	0.93
1:N:417[A]:MET:CE	30:N:853:HOH:O	2.13	0.93
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.51	0.92
2:B:54:SER:HB3	21:E:202:EDO:C2	1.99	0.92
3:P:63:ARG:HE	27:P:305:CDL:HA21	1.33	0.92
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.69	0.92
1:A:136[B]:LEU:HD11	30:A:925:HOH:O	1.71	0.91
8:U:9:LYS:HG3	8:U:10:ASN:H	1.36	0.91
30:A:916:HOH:O	19:D:201:TGL:HC31	1.71	0.91
27:T:103:CDL:H622	27:T:103:CDL:C66	1.93	0.91
4:D:19[A]:ARG:NH2	4:D:21:ASP:OD1	2.04	0.91
19:Y:101:TGL:HC62	19:Y:101:TGL:HC22	1.53	0.90
1:N:105:LEU:HD11	21:N:616:EDO:H21	1.53	0.90
3:C:63:ARG:HE	27:C:305:CDL:HA21	1.37	0.90
8:H:7:LYS:HD2	8:H:7:LYS:N	1.87	0.89
4:D:100[B]:LYS:CE	30:D:356:HOH:O	2.19	0.89
2:B:49:LYS:HE2	30:B:540:HOH:O	1.73	0.89
1:N:302[B]:ARG:NH2	30:N:701:HOH:O	2.06	0.88
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.55	0.88
24:B:303:PSC:C1	9:I:14:ALA:HB2	2.02	0.88
22:C:306:CHD:H162	22:C:306:CHD:H231	1.56	0.87
1:N:302[B]:ARG:HB3	1:N:302[B]:ARG:NH1	1.89	0.87
15:A:603:CU:CU	18:A:607[B]:AZI:N1	1.39	0.87
2:B:41[B]:ILE:HD12	9:I:21:ILE:CD1	2.05	0.86
7:G:7:ASP:HB2	1:N:178[A]:GLN:HG2	1.56	0.86
3:P:33[A]:MET:CB	25:P:307:DMU:C19	2.51	0.86
1:N:513:LEU:O	1:N:514:LYS:HB3	1.74	0.86
1:A:459:PHE:CE1	21:D:202:EDO:H12	2.11	0.85
15:N:603:CU:CU	18:N:607[B]:AZI:N1	1.38	0.85
6:S:75:HIS:H	6:S:80:GLN:HE22	1.25	0.85
1:N:302[B]:ARG:CZ	30:N:701:HOH:O	2.25	0.85
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.58	0.85
3:C:224:LYS:HD2	27:C:305:CDL:HB31	1.58	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.24	0.85
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.85
21:D:203:EDO:H11	30:E:347:HOH:O	1.77	0.84
7:G:45:PRO:O	30:G:201:HOH:O	1.95	0.84
1:A:514:LYS:N	30:A:701:HOH:O	1.68	0.84
1:N:302[B]:ARG:NH1	1:N:361:SER:OG	2.10	0.83
2:B:198:GLU:HG3	30:B:406:HOH:O	1.79	0.82
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:SER:CB	21:E:202:EDO:H22	2.04	0.82
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.62	0.82
3:P:158:HIS:CE1	6:S:2:SER:HB2	2.13	0.82
2:B:1:FME:HCN	2:B:193:TYR:H	1.45	0.82
7:G:84:LYS:NZ	7:G:84:LYS:H	1.76	0.82
20:A:610:PGV:H311	13:M:19:LEU:HD23	1.60	0.82
3:P:67:PHE:CE2	27:P:305:CDL:H1	2.15	0.82
1:N:359:ALA:HA	14:N:602[B]:HEA:OMA	1.79	0.82
7:G:8:HIS:CD2	7:G:9:GLY:H	1.97	0.82
4:D:100[B]:LYS:HE3	30:D:301:HOH:O	1.78	0.81
7:G:76:ASN:HD21	28:G:101:PEK:HN2	1.29	0.81
4:Q:19[A]:ARG:HG3	4:Q:21:ASP:OD1	1.79	0.81
24:B:303:PSC:H141	24:B:303:PSC:H343	1.62	0.80
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.16	0.80
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.45	0.80
2:B:1:FME:CN	2:B:1:FME:CA	2.59	0.80
24:B:303:PSC:H081	5:E:8:ASP:OD1	1.81	0.80
21:A:614:EDO:H12	30:A:738:HOH:O	1.82	0.79
1:N:302[B]:ARG:HH11	1:N:302[B]:ARG:CG	1.92	0.79
12:Y:46:LYS:O	12:Y:47:LYS:HB2	1.82	0.79
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.82	0.79
7:T:76:ASN:HD21	28:T:102:PEK:HN2	1.29	0.78
10:J:33:ARG:HG2	22:J:101:CHD:H152	1.65	0.78
3:C:67:PHE:CE2	27:C:305:CDL:H1	2.16	0.78
1:A:221:ASP:OD1	21:A:621:EDO:H11	1.84	0.77
20:P:304:PGV:H172	27:P:305:CDL:H632	1.66	0.77
5:E:39:TYR:HE1	21:E:202:EDO:C1	1.98	0.77
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.25	0.77
8:H:9:LYS:HD3	8:H:10:ASN:N	2.00	0.76
24:O:302:PSC:C07	9:V:10:ARG:HH21	1.98	0.76
27:T:103:CDL:H752	27:T:103:CDL:H561	1.66	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
8:H:31:GLN:HE22	21:H:101:EDO:C1	1.99	0.76
5:E:39:TYR:CE1	21:E:202:EDO:H21	2.21	0.76
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.68	0.76
27:G:102:CDL:H311	27:G:102:CDL:OA7	1.86	0.76
1:N:302[B]:ARG:HH12	1:N:361:SER:CB	1.99	0.76
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:HBD2	1.66	0.76
3:C:33:MET:CE	25:C:302:DMU:H8	2.09	0.75
2:B:160:LEU:HB2	30:B:406:HOH:O	1.86	0.75
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:45:ALA:O	8:U:47:GLY:N	2.19	0.75
24:O:302:PSC:H201	24:O:302:PSC:H22	1.67	0.75
4:D:19[A]:ARG:HG2	4:D:21:ASP:OD1	1.87	0.75
1:N:28:MET:CE	14:N:601:HEA:H271	2.17	0.75
4:D:33:LEU:O	30:D:303:HOH:O	2.05	0.75
27:G:102:CDL:H212	1:N:311[A]:ILE:CD1	2.16	0.75
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.69	0.75
7:G:84:LYS:H	7:G:84:LYS:HZ3	1.32	0.74
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.86	0.74
5:E:39:TYR:CE1	21:E:202:EDO:C1	2.70	0.74
6:S:95:GLN:HA	6:S:95:GLN:NE2	2.01	0.74
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.01	0.74
3:C:51[B]:MET:HE2	27:C:305:CDL:C39	2.17	0.74
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	1.90	0.74
2:B:52:HIS:CE1	24:B:303:PSC:H02	2.23	0.74
1:N:297[B]:MET:HB3	30:N:774:HOH:O	1.72	0.74
6:S:43:LYS:H	6:S:43:LYS:CE	2.00	0.74
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.21	0.74
11:X:47:ARG:HB3	11:X:47:ARG:CZ	2.18	0.74
2:B:41[A]:ILE:HD13	24:B:303:PSC:H342	1.69	0.73
8:U:9:LYS:HG3	8:U:10:ASN:N	2.02	0.73
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.03	0.73
3:P:63:ARG:HE	27:P:305:CDL:CA2	2.01	0.73
27:P:305:CDL:OA3	27:P:305:CDL:HB22	1.89	0.73
3:P:224:LYS:HE3	27:P:305:CDL:HB32	1.70	0.73
19:Y:101:TGL:HC62	19:Y:101:TGL:CC2	2.16	0.73
1:A:459:PHE:HE1	21:D:202:EDO:H12	1.54	0.72
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.19	0.72
27:P:305:CDL:OA3	27:P:305:CDL:CB5	2.37	0.72
20:X:101:PGV:H012	30:X:206:HOH:O	1.89	0.72
20:P:304:PGV:H172	27:P:305:CDL:H652	1.71	0.72
3:C:63:ARG:HE	27:C:305:CDL:CA2	2.02	0.72
19:N:609:TGL:H121	19:N:609:TGL:HA72	1.70	0.71
3:C:224:LYS:HD3	27:C:305:CDL:HB31	1.72	0.71
5:E:39:TYR:CE1	21:E:202:EDO:C2	2.73	0.71
7:G:38:HIS:CE1	27:G:102:CDL:H122	2.25	0.71
20:N:608:PGV:H343	28:T:102:PEK:H381	1.70	0.71
20:X:101:PGV:H031	30:X:206:HOH:O	1.91	0.71
21:A:614:EDO:C1	30:A:738:HOH:O	2.36	0.71
19:Y:101:TGL:OC1	19:Y:101:TGL:CC4	2.36	0.71
2:B:198:GLU:CG	30:B:406:HOH:O	2.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:302:PSC:H012	24:O:302:PSC:O13	1.90	0.71
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.72	0.71
1:A:417[B]:MET:HE2	30:A:841:HOH:O	1.80	0.71
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.71	0.71
2:B:41[B]:ILE:CD1	9:I:21:ILE:HD13	2.21	0.70
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.91	0.70
3:P:158:HIS:HE1	6:S:2:SER:HB2	1.53	0.70
20:A:609:PGV:H183	28:G:101:PEK:H322	1.73	0.70
19:A:608:TGL:HC22	30:I:126:HOH:O	1.90	0.70
1:A:282:PHE:CA	7:T:4:ALA:HB1	2.20	0.70
7:T:38:HIS:CE1	27:T:103:CDL:H142	2.27	0.70
3:C:51[B]:MET:HE2	27:C:305:CDL:H391	1.73	0.70
27:G:102:CDL:H352	2:O:78:LEU:HD12	1.72	0.70
20:X:101:PGV:H202	20:X:101:PGV:H42	1.73	0.70
19:Q:201:TGL:H362	9:V:20:HIS:HE1	1.57	0.69
1:N:312:ILE:HD12	30:N:725:HOH:O	1.91	0.69
7:G:5:LYS:CG	28:G:104:PEK:H332	2.22	0.69
2:B:41[B]:ILE:CD1	9:I:21:ILE:CD1	2.69	0.69
6:F:75:HIS:H	6:F:80:GLN:HE22	1.38	0.69
20:A:609:PGV:H343	28:G:101:PEK:H382	1.75	0.69
3:C:157:LYS:NZ	28:C:307:PEK:C05	2.56	0.69
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	1.91	0.69
7:G:8:HIS:CG	7:G:9:GLY:H	2.10	0.69
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.75	0.69
19:N:609:TGL:HC32	2:O:7:LEU:HD12	1.73	0.68
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE3	2.28	0.68
2:B:16[B]:ILE:HG23	30:B:495:HOH:O	1.92	0.68
3:C:33:MET:HE2	25:C:302:DMU:C19	2.09	0.68
1:A:177:SER:H	1:A:180:GLN:HE21	1.41	0.68
22:J:101:CHD:H222	22:J:101:CHD:O12	1.94	0.68
3:P:33[A]:MET:HB2	25:P:307:DMU:H8	1.73	0.68
7:T:8:HIS:O	7:T:8:HIS:CG	2.45	0.67
1:A:112:LEU:C	1:A:112:LEU:HD23	2.15	0.67
28:C:307:PEK:C38	27:G:102:CDL:C27	2.71	0.67
1:A:406:ASN:HD21	20:A:610:PGV:H22	1.59	0.67
8:H:27:ARG:HH21	21:H:101:EDO:H11	1.58	0.67
1:N:112:LEU:HD23	1:N:112:LEU:C	2.16	0.67
20:P:304:PGV:C15	27:P:305:CDL:H621	2.22	0.67
27:T:103:CDL:H111	27:T:103:CDL:H312	1.77	0.67
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	2.83	0.67
27:C:305:CDL:HB62	27:C:305:CDL:H521	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:37:THR:OG1	22:W:101:CHD:H193	1.95	0.66
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.26	0.66
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.76	0.66
20:C:308:PGV:H161	27:T:103:CDL:H621	1.78	0.66
2:O:83:ILE:O	2:O:87[A]:MET:HG3	1.95	0.66
4:D:78:TRP:N	19:D:201:TGL:HB21	2.10	0.66
1:N:28:MET:HE1	14:N:601:HEA:C27	2.25	0.66
3:P:213:THR:HG23	27:P:305:CDL:H761	1.76	0.66
6:F:96:LEU:HA	6:F:98:HIS:HB2	1.76	0.66
19:D:201:TGL:CG3	30:D:355:HOH:O	2.19	0.66
7:G:38:HIS:HE1	27:G:102:CDL:H122	1.59	0.66
6:S:43:LYS:HE2	6:S:43:LYS:N	2.10	0.66
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.77	0.66
1:N:28:MET:CE	14:N:601:HEA:C27	2.74	0.66
1:A:28:MET:CE	14:A:601:HEA:C27	2.75	0.65
3:C:33:MET:HE1	3:C:42:LEU:HD12	1.75	0.65
10:W:32:TYR:OH	22:W:101:CHD:H213	1.96	0.65
11:X:47:ARG:HB3	11:X:47:ARG:HH11	1.57	0.65
1:A:486[B]:ASP:OD1	30:A:703:HOH:O	2.13	0.65
1:N:177:SER:H	1:N:180:GLN:HE21	1.45	0.65
11:X:47:ARG:CZ	11:X:47:ARG:CB	2.75	0.65
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.35	0.65
25:C:302:DMU:H11	10:J:49:CYS:HB3	1.78	0.65
1:N:362[B]:SER:OG	30:N:702:HOH:O	2.15	0.65
2:O:92:ASN:ND2	30:O:401:HOH:O	2.30	0.65
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.27	0.64
1:N:486:ASP:OD2	4:Q:19[B]:ARG:CD	2.37	0.64
20:C:304:PGV:H12	20:C:304:PGV:H171	1.79	0.64
1:N:240:HIS:ND1	18:N:607[B]:AZI:N1	2.45	0.64
28:C:307:PEK:N	28:C:307:PEK:P	2.70	0.64
1:N:309:THR:HG22	14:N:602[B]:HEA:HMB2	1.79	0.64
1:A:365:ILE:CG1	30:A:900:HOH:O	1.85	0.64
28:C:307:PEK:H383	27:G:102:CDL:H273	1.80	0.64
6:F:64:GLU:O	6:F:65:ASP:HB2	1.96	0.64
1:A:291:HIS:CE1	18:A:607[B]:AZI:N2	2.65	0.64
14:A:602[B]:HEA:HMD1	14:A:602[B]:HEA:CBD	2.26	0.64
8:H:31:GLN:NE2	21:H:101:EDO:H12	2.10	0.64
1:A:74:MET:CG	1:A:74:MET:CA	2.72	0.64
3:C:125:ASN:HD21	27:G:102:CDL:HA22	1.63	0.63
2:B:227:LEU:HD21	30:B:496:HOH:O	1.98	0.63
5:E:39:TYR:HE1	21:E:202:EDO:H12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.63	0.63
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.63
18:A:606[B]:AZI:N3	18:A:607[B]:AZI:N1	2.46	0.63
20:A:610:PGV:H312	13:M:16:ALA:HA	1.81	0.63
8:H:9:LYS:HA	8:H:9:LYS:HZ2	1.63	0.63
7:T:38:HIS:HE1	27:T:103:CDL:H142	1.62	0.63
6:F:1:ALA:CB	6:S:65:ASP:OD2	2.39	0.63
12:Y:24[B]:MET:HG2	19:Y:101:TGL:HA22	1.80	0.63
5:E:90:ARG:CB	30:E:301:HOH:O	2.46	0.63
7:G:6:GLY:H	1:N:278[B]:MET:HE1	1.64	0.63
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.61	0.63
2:O:13:THR:HB	2:O:168:LEU:HD23	1.79	0.63
27:P:305:CDL:OB9	27:P:305:CDL:H522	1.97	0.63
3:C:224:LYS:HD3	27:C:305:CDL:CB3	2.28	0.63
1:N:178[B]:GLN:CG	1:N:186:TRP:CZ2	2.81	0.63
2:O:217:LYS:HE3	2:O:221:LYS:HZ3	1.62	0.63
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.34	0.62
7:G:4:ALA:CB	1:N:282:PHE:HA	2.29	0.62
1:A:356:ILE:HA	14:A:602[B]:HEA:HMB3	1.81	0.62
6:S:43:LYS:HE3	30:S:218:HOH:O	1.97	0.62
12:Y:24[B]:MET:HG2	19:Y:101:TGL:CA2	2.29	0.62
3:C:224:LYS:CD	27:C:305:CDL:CB3	2.76	0.62
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	2.00	0.62
28:P:308:PEK:H041	7:T:17:ARG:HH22	1.65	0.62
1:A:484:THR:HG22	30:A:911:HOH:O	2.00	0.62
1:N:178[B]:GLN:HG3	1:N:178[B]:GLN:O	1.99	0.62
4:D:17[A]:VAL:HG23	4:D:17[A]:VAL:O	1.99	0.61
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	1.99	0.61
5:E:90:ARG:CG	30:E:301:HOH:O	2.47	0.61
10:W:33:ARG:HD2	22:W:101:CHD:H152	1.82	0.61
3:P:80[B]:ARG:HG2	3:P:233:PHE:CE1	2.35	0.61
3:P:33[A]:MET:CB	25:P:307:DMU:H8	2.27	0.61
1:N:291:HIS:NE2	18:N:607[B]:AZI:N1	2.48	0.61
14:N:602[A]:HEA:HBC1	14:N:602[A]:HEA:HMC1	1.82	0.61
24:B:303:PSC:C04	30:B:413:HOH:O	2.48	0.61
9:I:61:GLU:CG	30:I:101:HOH:O	2.42	0.61
2:O:217:LYS:HE3	2:O:221:LYS:NZ	2.16	0.61
1:A:449:MET:SD	2:B:5:MET:HG2	2.41	0.61
19:Q:201:TGL:H352	9:V:16:ARG:HE	1.66	0.61
3:C:39:SER:OG	25:C:310:DMU:H2	2.01	0.60
1:N:302[B]:ARG:CB	1:N:302[B]:ARG:NH1	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:TRP:O	10:J:57:HIS:HE1	1.83	0.60
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.30	0.60
2:B:41[A]:ILE:O	2:B:42:ILE:C	2.36	0.60
22:G:103:CHD:H212	22:G:103:CHD:H12	1.83	0.60
1:N:243:VAL:HB	14:N:602[B]:HEA:HAC	1.83	0.60
1:A:328:HIS:NE2	24:B:303:PSC:H22	2.16	0.59
28:G:104:PEK:H032	3:P:80[B]:ARG:HH21	1.66	0.59
8:H:84:LYS:HZ2	8:H:84:LYS:HB2	1.67	0.59
1:N:178[B]:GLN:HG3	1:N:186:TRP:CE2	2.36	0.59
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.50	0.59
12:L:41:ARG:HH22	25:L:102:DMU:H30	1.67	0.59
1:N:356:ILE:HD13	14:N:602[B]:HEA:HMB1	1.84	0.59
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.83	0.59
21:A:611:EDO:C2	21:A:621:EDO:C1	2.77	0.59
2:B:41[B]:ILE:HD12	9:I:21:ILE:HD11	1.81	0.59
6:F:54[A]:ASN:ND2	6:F:54[A]:ASN:H	2.00	0.59
5:E:90:ARG:HB3	30:E:301:HOH:O	2.01	0.59
7:G:5:LYS:HG3	28:G:104:PEK:C33	2.25	0.59
1:A:298[A]:ASP:OD1	20:C:308:PGV:H061	2.03	0.59
22:C:306:CHD:H162	22:C:306:CHD:C23	2.27	0.59
6:S:95:GLN:HE21	6:S:95:GLN:N	2.00	0.59
24:B:303:PSC:H31	9:I:17:LEU:HD23	1.84	0.59
8:H:27:ARG:NH2	21:H:101:EDO:H11	2.18	0.59
1:A:514:LYS:HE2	30:F:216:HOH:O	2.02	0.59
6:S:76:LYS:HE2	6:S:93:PRO:CG	2.13	0.59
28:C:307:PEK:H382	27:G:102:CDL:C27	2.23	0.58
1:N:302[B]:ARG:NH1	1:N:302[B]:ARG:CG	2.64	0.58
3:P:62:ILE:HD12	27:P:305:CDL:H511	1.85	0.58
9:I:31:PHE:C	9:I:31:PHE:CD2	2.76	0.58
27:T:103:CDL:H141	27:T:103:CDL:H352	1.85	0.58
7:T:3:ALA:O	7:T:4:ALA:CB	2.51	0.58
12:L:26:THR:HG23	13:M:25:SER:HB3	1.84	0.58
25:L:102:DMU:O49	30:L:202:HOH:O	2.17	0.58
28:G:104:PEK:C03	3:P:80[B]:ARG:HH21	2.16	0.58
20:P:302:PGV:H061	30:P:448:HOH:O	2.04	0.58
27:G:102:CDL:H832	28:G:104:PEK:H372	1.86	0.58
3:C:157:LYS:HZ1	28:C:307:PEK:C05	2.09	0.58
4:D:28:ALA:H	4:D:31[B]:LYS:NZ	2.01	0.58
8:H:7:LYS:N	8:H:7:LYS:CD	2.63	0.58
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.01	0.58
8:H:43:MET:HE3	8:H:49:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:GLN:NE2	6:S:95:GLN:CA	2.66	0.57
1:A:513:LEU:O	1:A:514:LYS:HB2	2.03	0.57
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.05	0.57
27:G:102:CDL:OA7	27:G:102:CDL:H342	2.04	0.57
21:N:616:EDO:H12	30:N:786:HOH:O	2.03	0.57
25:P:307:DMU:H11	10:W:49:CYS:HB3	1.85	0.57
24:B:303:PSC:H032	5:E:40:ASP:OD2	2.04	0.57
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.57
3:P:33[A]:MET:SD	3:P:42:LEU:HD12	2.45	0.57
1:A:417[B]:MET:HE1	30:A:841:HOH:O	1.92	0.57
20:X:101:PGV:H302	13:Z:19:LEU:HD23	1.87	0.57
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.57
3:C:51[B]:MET:CE	27:C:305:CDL:H391	2.34	0.57
1:A:455:SER:HB3	21:D:202:EDO:O1	2.05	0.56
20:X:101:PGV:H311	13:Z:19:LEU:HD23	1.87	0.56
1:A:291:HIS:NE2	18:A:607[B]:AZI:N1	2.52	0.56
2:B:29[B]:MET:SD	2:B:33:LEU:HD22	2.45	0.56
4:D:100[B]:LYS:HE3	30:D:356:HOH:O	1.96	0.56
12:L:43:GLN:NE2	30:L:201:HOH:O	2.22	0.56
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.88	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.86	0.56
3:P:261:SER:OXT	25:P:309:DMU:H40	2.05	0.56
7:G:5:LYS:HB3	1:N:278[B]:MET:HE1	1.88	0.56
3:P:63:ARG:NE	27:P:305:CDL:HA21	2.14	0.56
12:L:14:SER:N	19:L:101:TGL:HC31	2.10	0.56
25:C:302:DMU:O3	25:C:310:DMU:H30	2.05	0.56
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.19	0.56
2:B:56:MET:CB	24:B:303:PSC:H221	2.36	0.56
5:E:90:ARG:NE	30:E:301:HOH:O	1.65	0.56
12:L:43:GLN:HA	30:L:201:HOH:O	2.05	0.56
7:T:31:CYS:SG	27:T:103:CDL:H542	2.46	0.56
27:T:103:CDL:H661	27:T:103:CDL:C62	2.18	0.56
1:N:291:HIS:CE1	18:N:607[B]:AZI:N2	2.73	0.55
4:D:19[A]:ARG:NH2	4:D:19[A]:ARG:CG	2.38	0.55
7:G:12:GLY:HA3	30:G:241:HOH:O	2.05	0.55
3:P:59:ARG:HA	27:P:305:CDL:H512	1.88	0.55
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.54	0.55
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.21	0.55
1:N:449:MET:SD	2:O:5:MET:HG2	2.46	0.55
27:G:102:CDL:H212	1:N:311[A]:ILE:HD13	1.88	0.55
1:N:356:ILE:HA	14:N:602[B]:HEA:HMB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:ND1	18:A:607[B]:AZI:N1	2.54	0.55
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.40	0.55
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.88	0.55
21:A:616:EDO:H22	12:L:10:ASN:HB2	1.88	0.55
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.36	0.55
19:D:201:TGL:H342	9:I:16:ARG:HE	1.71	0.55
3:P:33[A]:MET:HB3	25:P:307:DMU:C19	2.37	0.55
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.37	0.54
28:G:104:PEK:H221	3:P:81:TYR:HE1	1.72	0.54
24:O:302:PSC:H02	24:O:302:PSC:H212	1.89	0.54
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.89	0.54
6:F:87:THR:HG21	30:F:277:HOH:O	2.07	0.54
7:G:1:ALA:HB1	7:G:3:ALA:H	1.72	0.54
27:P:305:CDL:HB22	27:P:305:CDL:PA1	2.46	0.54
11:X:7:PRO:HB2	11:X:12:LYS:HE3	1.89	0.54
3:C:51[B]:MET:HE2	27:C:305:CDL:H392	1.89	0.54
8:H:8:ILE:O	8:H:8:ILE:HG22	2.08	0.54
12:Y:24[A]:MET:SD	19:Y:101:TGL:H152	2.48	0.54
3:C:33:MET:HB2	25:C:302:DMU:C19	2.37	0.54
7:G:37:LEU:HD21	27:G:102:CDL:H372	1.90	0.54
1:N:177:SER:H	1:N:180:GLN:NE2	2.04	0.54
1:N:302[B]:ARG:NH1	1:N:361:SER:CB	2.66	0.54
24:O:302:PSC:H073	9:V:10:ARG:HH21	1.71	0.54
28:P:308:PEK:H383	27:T:103:CDL:H273	1.89	0.54
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.88	0.53
12:L:26:THR:HG23	13:M:25:SER:CB	2.37	0.53
3:P:210:ILE:HD13	20:P:304:PGV:H301	1.89	0.53
1:N:112:LEU:HG	30:N:892:HOH:O	2.07	0.53
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.73	0.53
22:P:306:CHD:H183	22:P:306:CHD:H212	1.89	0.53
21:A:611:EDO:H22	21:A:621:EDO:H11	1.86	0.53
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.43	0.53
7:G:8:HIS:NE2	28:G:104:PEK:C05	2.66	0.53
8:H:9:LYS:HA	8:H:9:LYS:HZ3	1.73	0.53
2:B:1:FME:HCN	2:B:193:TYR:N	2.21	0.53
6:F:53[B]:THR:HG23	6:F:54[B]:ASN:N	2.24	0.53
6:S:95:GLN:HE21	6:S:95:GLN:CA	2.21	0.53
19:D:201:TGL:H331	9:I:16:ARG:HH21	1.73	0.53
1:N:378:HIS:O	1:N:383[B]:MET:HG2	2.09	0.53
19:Q:201:TGL:HA91	19:Q:201:TGL:H231	1.90	0.53
2:B:140:ASN:HB3	30:B:505:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:609:TGL:HA61	19:N:609:TGL:H102	1.91	0.53
2:O:116:LEU:HD13	2:O:226:MET:CG	2.36	0.52
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.09	0.52
9:V:64:ARG:NH2	9:V:65:LYS:HZ3	2.07	0.52
1:A:28:MET:HE2	14:A:601:HEA:H273	1.90	0.52
8:U:9:LYS:CG	8:U:10:ASN:H	2.16	0.52
8:U:43:MET:HE3	8:U:49:ASP:H	1.74	0.52
1:A:282:PHE:CA	7:T:4:ALA:CB	2.74	0.52
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.91	0.52
24:O:302:PSC:H231	24:O:302:PSC:H42	1.90	0.52
4:D:17[A]:VAL:O	4:D:17[A]:VAL:CG2	2.58	0.52
27:T:103:CDL:H341	27:T:103:CDL:H122	1.92	0.52
5:E:86:ILE:O	5:E:90:ARG:HG2	2.09	0.52
2:O:60:GLU:CD	2:O:60:GLU:H	2.13	0.52
20:P:304:PGV:H152	27:P:305:CDL:C62	2.26	0.52
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.91	0.52
7:G:1:ALA:HB2	30:G:245:HOH:O	2.09	0.52
3:C:62:ILE:HD12	27:C:305:CDL:H522	1.92	0.52
6:F:96:LEU:C	6:F:98:HIS:H	2.12	0.52
20:A:609:PGV:H322	28:G:101:PEK:H382	1.92	0.51
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.51
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.92	0.51
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.45	0.51
9:I:35:TYR:CD1	9:I:35:TYR:C	2.83	0.51
1:A:459:PHE:HE1	21:D:202:EDO:C1	2.21	0.51
2:O:58:ALA:O	2:O:62:GLU:HG3	2.11	0.51
12:L:46:LYS:HE3	30:L:201:HOH:O	2.10	0.51
20:A:609:PGV:C18	28:G:101:PEK:H322	2.40	0.51
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.51	0.51
1:N:321:PHE:CZ	24:O:302:PSC:H171	2.46	0.51
1:N:514:LYS:HA	6:S:38:ALA:CB	2.37	0.51
6:S:64:GLU:O	6:S:65:ASP:HB2	2.11	0.50
3:C:106:LEU:HB3	20:C:308:PGV:H22	1.93	0.50
1:A:468:MET:HG3	30:A:907:HOH:O	2.11	0.50
27:C:305:CDL:HB21	27:C:305:CDL:OB6	2.11	0.50
7:G:3:ALA:CB	28:G:104:PEK:H362	2.41	0.50
10:J:7:GLU:HG3	30:J:214:HOH:O	2.10	0.50
27:T:103:CDL:H752	27:T:103:CDL:C56	2.37	0.50
1:A:28:MET:HE2	14:A:601:HEA:C27	2.40	0.50
19:L:101:TGL:OC1	19:L:101:TGL:CC5	2.60	0.50
7:T:37:LEU:HD23	27:T:103:CDL:H371	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:8:GLN:HG2	9:V:15:ARG:CZ	2.42	0.50
1:A:377:PHE:CD2	14:A:602[A]:HEA:HAD1	2.46	0.50
4:D:28:ALA:H	4:D:31[B]:LYS:HE2	1.76	0.50
7:G:82:TYR:CE2	30:G:201:HOH:O	2.63	0.50
3:P:161[A]:GLN:NE2	28:P:308:PEK:H5	2.27	0.50
20:P:304:PGV:H172	27:P:305:CDL:C63	2.39	0.50
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.95	0.50
8:H:9:LYS:HZ2	8:H:11:TYR:H	1.60	0.50
13:M:41:LYS:O	13:M:43:SER:N	2.44	0.50
1:N:302[B]:ARG:HH12	1:N:361:SER:HG	1.53	0.50
2:O:217:LYS:CE	2:O:221:LYS:NZ	2.75	0.50
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	1.93	0.50
2:B:164:ALA:O	2:B:194:GLY:HA3	2.12	0.50
3:C:106:LEU:HD13	20:C:308:PGV:H21	1.93	0.50
6:F:96:LEU:C	6:F:98:HIS:N	2.64	0.50
1:A:278[B]:MET:HE3	7:T:5:LYS:HB3	1.93	0.49
28:C:307:PEK:P	28:C:307:PEK:HN1	2.35	0.49
1:A:347:LEU:HD11	1:A:418:PHE:CE1	2.47	0.49
30:P:414:HOH:O	6:S:2:SER:HA	2.11	0.49
21:A:611:EDO:C2	21:A:621:EDO:H11	2.41	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.93	0.49
30:P:403:HOH:O	10:W:1:PHE:HB3	2.11	0.49
20:A:609:PGV:C34	28:G:101:PEK:H382	2.40	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.47	0.49
25:C:310:DMU:H23	10:J:41:GLY:HA3	1.93	0.49
7:G:72:ASN:H	7:G:76:ASN:ND2	2.02	0.49
3:P:33[A]:MET:SD	25:P:307:DMU:H8	2.52	0.49
9:V:64:ARG:HH21	9:V:65:LYS:HZ3	1.61	0.49
30:A:916:HOH:O	19:D:201:TGL:CC3	2.46	0.49
20:A:610:PGV:O14	20:A:610:PGV:H05	2.12	0.49
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.13	0.49
27:P:305:CDL:H132	27:P:305:CDL:OA7	2.13	0.49
9:V:64:ARG:NH2	9:V:65:LYS:NZ	2.61	0.49
22:W:101:CHD:O12	22:W:101:CHD:H222	2.13	0.49
11:X:42:PRO:HG2	11:X:47:ARG:NH2	2.28	0.49
6:F:54[A]:ASN:H	6:F:54[A]:ASN:HD22	1.61	0.49
3:P:38:ASN:ND2	25:P:310:DMU:O4	2.45	0.49
7:G:5:LYS:HB2	28:G:104:PEK:H332	1.95	0.49
1:N:302[B]:ARG:CZ	2:O:84:LEU:HD11	2.43	0.49
4:Q:93:ALA:HB3	11:X:28[B]:VAL:HG12	1.94	0.49
3:C:38:ASN:HA	30:C:445:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:301:CHD:H212	22:C:301:CHD:H12	1.95	0.48
10:J:58:LYS:NZ	10:J:58:LYS:HA	2.28	0.48
1:N:54:TYR:HB2	30:N:790:HOH:O	2.12	0.48
1:N:364:ASP:OD1	14:N:602[B]:HEA:O1A	2.31	0.48
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.95	0.48
3:P:224:LYS:CE	27:P:305:CDL:HB32	2.40	0.48
27:P:305:CDL:OA8	27:P:305:CDL:H182	2.13	0.48
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.95	0.48
24:O:302:PSC:H232	24:O:302:PSC:H202	1.26	0.48
1:A:281:GLY:C	7:T:4:ALA:HB1	2.34	0.48
3:C:157:LYS:HZ2	28:C:307:PEK:C05	2.25	0.48
1:N:309:THR:HG22	14:N:602[A]:HEA:HMB2	1.94	0.48
20:C:308:PGV:C06	8:H:22:ASN:HD22	2.26	0.48
4:Q:9:GLU:O	4:Q:10:ASP:C	2.52	0.48
1:A:376:HIS:CE1	1:A:380[B]:VAL:HG11	2.49	0.48
3:C:48:THR:HG23	27:C:305:CDL:H402	1.96	0.48
3:C:175:LEU:HD21	27:C:305:CDL:H872	1.94	0.48
7:G:8:HIS:CG	7:G:9:GLY:N	2.79	0.48
7:G:9:GLY:HA3	30:G:202:HOH:O	2.13	0.48
19:L:101:TGL:H221	19:L:101:TGL:HA92	1.23	0.48
8:H:43:MET:CE	8:H:49:ASP:H	2.26	0.48
3:P:116:TRP:HA	3:P:117:PRO:C	2.33	0.48
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.48
3:C:25:LEU:HD11	25:C:302:DMU:H24	1.96	0.48
3:P:3:HIS:HB3	30:P:491:HOH:O	2.14	0.48
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.14	0.47
27:G:102:CDL:H192	1:N:311[A]:ILE:HD11	1.96	0.47
27:P:305:CDL:H211	27:P:305:CDL:H172	1.96	0.47
6:S:52:ILE:O	6:S:94:HIS:HE1	1.95	0.47
1:A:13:LYS:CD	21:A:616:EDO:H12	2.44	0.47
1:A:28:MET:CE	14:A:601:HEA:H271	2.43	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.47
3:C:226:HIS:CE1	27:C:305:CDL:HB32	2.49	0.47
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.47
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.96	0.47
5:E:39:TYR:CE1	21:E:202:EDO:H11	2.50	0.47
27:G:102:CDL:H522	27:G:102:CDL:H712	1.97	0.47
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.49	0.47
2:O:217:LYS:CE	2:O:221:LYS:HZ1	2.27	0.47
1:A:13:LYS:HD2	21:A:616:EDO:H12	1.96	0.47
12:L:2:HIS:CG	12:L:3:TYR:H	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:609:TGL:H251	19:N:609:TGL:H282	1.55	0.47
12:Y:2:HIS:CD2	12:Y:3:TYR:H	2.31	0.47
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.49	0.47
4:Q:5:VAL:O	4:Q:6:VAL:HG22	2.15	0.47
2:B:52:HIS:ND1	24:B:303:PSC:H02	2.28	0.47
21:D:203:EDO:C1	30:E:347:HOH:O	2.48	0.47
10:J:32:TYR:OH	22:J:101:CHD:H213	2.14	0.47
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.63	0.47
3:P:33[B]:MET:HA	25:P:307:DMU:H9	1.95	0.47
4:D:104:TYR:OH	21:D:202:EDO:H21	2.14	0.47
20:X:101:PGV:H302	13:Z:19:LEU:CD2	2.44	0.47
1:A:355:GLY:C	14:A:602[B]:HEA:HMB3	2.35	0.47
4:Q:7:LYS:O	4:Q:8:SER:HB3	2.14	0.47
6:S:64:GLU:HA	30:S:201:HOH:O	2.14	0.47
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.46
7:G:84:LYS:H	7:G:84:LYS:HZ2	1.57	0.46
6:S:76:LYS:CE	6:S:93:PRO:CG	2.75	0.46
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.33	0.46
3:C:63:ARG:NE	27:C:305:CDL:HA21	2.16	0.46
28:G:104:PEK:H221	3:P:81:TYR:CE1	2.49	0.46
6:S:52:ILE:O	6:S:94:HIS:CE1	2.67	0.46
6:S:94:HIS:O	6:S:95:GLN:HB2	2.14	0.46
27:T:103:CDL:H231	27:T:103:CDL:H531	1.97	0.46
19:Y:101:TGL:HA91	19:Y:101:TGL:H222	1.26	0.46
1:N:136[B]:LEU:HG	30:N:894:HOH:O	2.15	0.46
1:N:302[B]:ARG:CZ	2:O:84:LEU:CD1	2.93	0.46
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC3	3.04	0.46
27:G:102:CDL:H171	27:G:102:CDL:H392	1.96	0.46
1:N:356:ILE:HD13	14:N:602[B]:HEA:CMB	2.45	0.46
20:P:304:PGV:C17	27:P:305:CDL:H632	2.42	0.46
19:Q:201:TGL:HG12	19:Q:201:TGL:HC31	1.98	0.46
3:C:33:MET:CB	25:C:302:DMU:H9	2.46	0.46
1:N:383[B]:MET:SD	1:N:421:VAL:HG11	2.55	0.46
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.63	0.46
24:B:303:PSC:C06	9:I:10:ARG:HH21	2.28	0.46
8:H:45:ALA:HB1	8:H:46:LYS:HE2	1.96	0.46
28:P:308:PEK:C38	27:T:103:CDL:H273	2.46	0.46
27:T:103:CDL:H402	27:T:103:CDL:H431	1.72	0.46
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.45	0.46
6:F:64:GLU:O	6:F:65:ASP:CB	2.60	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:OD1	21:A:621:EDO:C1	2.59	0.46
3:C:16:TRP:N	3:C:17:PRO:CD	2.79	0.46
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.60	0.45
20:P:302:PGV:C06	30:P:448:HOH:O	2.62	0.45
3:C:51[B]:MET:HG2	27:C:305:CDL:H612	1.99	0.45
3:C:54[A]:MET:HE3	27:C:305:CDL:H611	1.98	0.45
14:N:601:HEA:H262	14:N:601:HEA:H122	1.99	0.45
14:N:602[B]:HEA:HMD1	14:N:602[B]:HEA:CBD	2.42	0.45
20:X:101:PGV:H02	20:X:101:PGV:H05	1.99	0.45
12:Y:46:LYS:O	12:Y:47:LYS:CB	2.59	0.45
4:D:28:ALA:H	4:D:31[B]:LYS:CE	2.29	0.45
7:G:59:PRO:O	21:G:106:EDO:H12	2.16	0.45
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.64	0.45
1:A:328:HIS:NE2	24:B:303:PSC:C2	2.79	0.45
3:C:156:ARG:HE	22:C:306:CHD:C24	2.29	0.45
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.63	0.45
4:D:121:LYS:HZ3	21:D:205:EDO:H22	1.82	0.45
1:N:415:ALA:HB1	19:Q:201:TGL:H112	1.99	0.45
7:G:6:GLY:N	1:N:278[B]:MET:HE1	2.31	0.45
1:N:359:ALA:CA	14:N:602[B]:HEA:OMA	2.59	0.45
19:N:609:TGL:HC42	19:N:609:TGL:HC72	1.68	0.45
24:B:303:PSC:P	30:B:413:HOH:O	2.75	0.45
6:F:85:CYS:SG	6:F:87:THR:CG2	2.87	0.45
2:O:47:THR:HB	19:Q:201:TGL:H181	1.99	0.45
3:P:95:THR:HG21	20:P:302:PGV:H302	1.97	0.45
20:P:304:PGV:C17	27:P:305:CDL:H652	2.43	0.45
2:B:83:ILE:O	2:B:87[A]:MET:HG3	2.17	0.45
3:C:62:ILE:CD1	27:C:305:CDL:H522	2.47	0.45
5:E:90:ARG:CD	30:E:301:HOH:O	2.36	0.45
20:X:101:PGV:C01	30:X:206:HOH:O	2.59	0.45
27:G:102:CDL:H362	27:G:102:CDL:H121	1.99	0.45
1:N:488:THR:HB	1:N:495:LEU:HD13	1.99	0.45
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.47	0.45
1:A:240:HIS:C	1:A:240:HIS:CD2	2.90	0.44
2:B:217:LYS:HA	2:B:217:LYS:HD3	1.81	0.44
2:O:42:ILE:HG21	19:Q:201:TGL:H232	1.98	0.44
22:P:301:CHD:H162	20:P:302:PGV:H231	1.99	0.44
27:P:305:CDL:H421	27:P:305:CDL:H452	1.71	0.44
1:N:439:ARG:HD3	2:O:199:ILE:HB	1.99	0.44
8:U:9:LYS:O	8:U:10:ASN:HB2	2.18	0.44
1:A:372:TYR:N	1:A:432:GLY:HA3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:308:PGV:H151	20:C:308:PGV:H11	1.99	0.44
9:V:61:GLU:HG3	9:V:65:LYS:NZ	2.32	0.44
2:B:56:MET:HA	24:B:303:PSC:H221	1.99	0.44
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.44
8:H:37:HIS:HE1	30:H:204:HOH:O	2.00	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.18	0.44
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.86	0.44
1:A:291:HIS:CE1	18:A:607[B]:AZI:N1	2.84	0.44
1:A:311[A]:ILE:HD12	27:T:103:CDL:H221	1.99	0.44
7:G:2:SER:O	28:G:104:PEK:C31	2.54	0.44
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.44
2:O:39:LEU:CD1	19:Q:201:TGL:H221	2.47	0.44
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.99	0.44
20:X:101:PGV:H202	20:X:101:PGV:C4	2.45	0.44
7:G:3:ALA:O	7:G:4:ALA:HB2	2.17	0.44
30:A:900:HOH:O	2:B:87[B]:MET:HE1	2.17	0.44
2:B:60:GLU:H	2:B:60:GLU:CD	2.21	0.44
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.18	0.44
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.98	0.44
3:P:259:TRP:CD1	25:P:309:DMU:H30	2.53	0.44
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.99	0.44
3:C:149:HIS:CE1	7:G:11:TPO:HG22	2.53	0.44
6:S:65:ASP:N	30:S:201:HOH:O	1.92	0.44
22:C:306:CHD:C23	22:C:306:CHD:C16	2.96	0.43
6:F:96:LEU:CA	6:F:98:HIS:HB2	2.44	0.43
10:J:29:ASN:HD22	10:J:29:ASN:H	1.64	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.52	0.43
8:U:43:MET:HE3	8:U:49:ASP:N	2.33	0.43
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.16	0.43
8:H:37:HIS:HD2	8:H:40:GLU:OE2	2.00	0.43
2:O:67:ILE:HD11	30:O:505:HOH:O	2.19	0.43
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.81	0.43
6:F:43:LYS:HE2	6:F:43:LYS:HB2	1.79	0.43
28:G:104:PEK:H132	3:P:247:VAL:HG11	1.99	0.43
2:O:53:THR:HG21	30:Q:319:HOH:O	2.18	0.43
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.99	0.43
22:C:306:CHD:H183	22:C:306:CHD:H20	1.85	0.43
28:C:307:PEK:C05	28:C:307:PEK:O14	2.67	0.43
4:D:109:HIS:HD2	30:D:366:HOH:O	2.00	0.43
1:N:297[B]:MET:O	1:N:302[B]:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:PHE:CD1	22:P:306:CHD:H192	2.53	0.43
6:S:2:SER:O	6:S:2:SER:OG	2.32	0.43
7:T:84:LYS:HA	7:T:84:LYS:HD3	1.66	0.43
27:T:103:CDL:H581	27:T:103:CDL:H782	2.01	0.43
7:G:5:LYS:CB	28:G:104:PEK:H332	2.48	0.43
1:N:110:LEU:HG	25:P:307:DMU:H24	1.99	0.43
1:A:42:GLY:HA3	21:D:202:EDO:H21	2.00	0.43
25:C:302:DMU:H20	10:J:50:LEU:HB2	2.01	0.43
6:F:94:HIS:O	6:F:95:GLN:HB2	2.19	0.43
7:G:3:ALA:HB1	28:G:104:PEK:H362	2.00	0.43
1:N:302[B]:ARG:NH1	1:N:361:SER:HB2	2.33	0.43
2:O:41:ILE:HG21	24:O:302:PSC:H332	2.01	0.43
3:P:54[A]:MET:HE3	27:P:305:CDL:H591	2.00	0.43
14:A:601:HEA:HHC	14:A:601:HEA:H122	1.99	0.43
4:D:104:TYR:OH	21:D:202:EDO:C2	2.66	0.43
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.54	0.43
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.85	0.43
1:A:240:HIS:HE1	18:A:606[B]:AZI:N2	2.17	0.43
19:Y:101:TGL:CC6	19:Y:101:TGL:CC2	2.92	0.43
1:A:459:PHE:CE1	21:D:202:EDO:C1	2.92	0.43
2:B:16[A]:ILE:CD1	2:B:87[A]:MET:HG2	2.44	0.43
2:B:26:HIS:O	2:B:29[B]:MET:HB3	2.19	0.43
27:T:103:CDL:OB6	27:T:103:CDL:H191	2.18	0.43
10:W:33:ARG:HD2	22:W:101:CHD:O7	2.18	0.43
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.19	0.43
1:A:356:ILE:HD13	14:A:602[B]:HEA:CMB	2.48	0.42
27:G:102:CDL:H401	2:O:77:ALA:CB	2.49	0.42
4:Q:4:SER:HB3	4:Q:5:VAL:H	1.61	0.42
1:A:485:VAL:CG2	21:A:619:EDO:H12	2.49	0.42
12:Y:24[B]:MET:HG2	19:Y:101:TGL:HA21	2.00	0.42
28:G:104:PEK:H132	3:P:247:VAL:CG1	2.49	0.42
20:P:304:PGV:H172	27:P:305:CDL:C65	2.43	0.42
5:R:41:LEU:HA	30:V:110:HOH:O	2.20	0.42
6:S:54:ASN:HD22	6:S:54:ASN:C	2.21	0.42
6:F:87:THR:HG21	30:F:216:HOH:O	2.19	0.42
1:A:240:HIS:CE1	18:A:606[B]:AZI:N2	2.88	0.42
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.02	0.42
12:L:20:ARG:HH21	19:L:101:TGL:HC32	1.67	0.42
25:L:102:DMU:H36	25:L:102:DMU:H2	1.90	0.42
3:C:33:MET:HE1	3:C:42:LEU:CD1	2.46	0.42
27:G:102:CDL:H522	27:G:102:CDL:H241	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:2:HIS:CD2	12:Y:3:TYR:N	2.87	0.42
2:B:47:THR:HB	19:D:201:TGL:H161	2.01	0.42
1:N:380[A]:VAL:HG21	14:N:602[A]:HEA:C3C	2.50	0.42
11:X:42:PRO:HG2	11:X:47:ARG:HH21	1.84	0.42
12:L:20:ARG:NH2	19:L:101:TGL:CC3	2.46	0.42
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.19	0.42
1:A:417[A]:MET:CE	14:A:601:HEA:H263	2.49	0.42
3:C:224:LYS:HD3	27:C:305:CDL:OB5	2.19	0.42
7:G:42:ARG:HD3	7:G:42:ARG:HA	1.73	0.42
1:N:243:VAL:HG11	14:N:602[B]:HEA:HMD2	2.02	0.42
20:A:610:PGV:H202	20:A:610:PGV:H231	1.35	0.42
4:D:121:LYS:NZ	21:D:205:EDO:H22	2.34	0.42
7:G:3:ALA:HB3	28:G:104:PEK:H331	2.01	0.42
27:G:102:CDL:H212	1:N:311[A]:ILE:HD12	1.97	0.42
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.42
2:O:41:ILE:HD13	24:O:302:PSC:H342	2.02	0.42
3:P:246:ASP:HB2	30:P:490:HOH:O	2.20	0.42
8:H:43:MET:CE	8:H:49:ASP:N	2.82	0.41
1:N:110:LEU:CD2	25:P:307:DMU:H24	2.50	0.41
1:N:291:HIS:NE2	18:N:607[B]:AZI:N2	2.68	0.41
14:N:601:HEA:H122	14:N:601:HEA:HHC	2.02	0.41
2:B:1:FME:CN	2:B:1:FME:HA	2.46	0.41
1:N:417[A]:MET:HE1	30:N:853:HOH:O	2.01	0.41
1:N:514:LYS:NZ	30:N:711:HOH:O	2.53	0.41
2:O:108:TYR:O	2:O:117:SER:HA	2.20	0.41
1:A:383[B]:MET:HE1	14:A:601:HEA:H262	2.02	0.41
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.41
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.56	0.41
8:U:84:LYS:NZ	8:U:84:LYS:HB2	2.35	0.41
2:B:32[A]:PHE:HD1	2:B:32[A]:PHE:HA	1.55	0.41
1:N:409:TRP:HB3	1:N:471:ILE:HG12	2.02	0.41
27:T:103:CDL:H352	27:T:103:CDL:C14	2.51	0.41
1:A:282:PHE:N	7:T:4:ALA:HB1	2.34	0.41
3:C:149:HIS:HE1	7:G:11:TPO:HG22	1.84	0.41
27:C:305:CDL:H812	27:C:305:CDL:H842	1.82	0.41
1:N:302[B]:ARG:NH1	2:O:84:LEU:CD1	2.83	0.41
28:P:308:PEK:C04	7:T:17:ARG:HH22	2.33	0.41
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.20	0.41
2:B:56:MET:HB3	24:B:303:PSC:H221	2.02	0.41
2:B:56:MET:CA	24:B:303:PSC:H221	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.56	0.41
2:O:111:THR:HA	2:O:114:GLU:O	2.21	0.41
8:U:9:LYS:CG	8:U:10:ASN:N	2.77	0.41
20:A:609:PGV:H343	28:G:101:PEK:C38	2.47	0.41
6:S:94:HIS:HB3	6:S:95:GLN:H	1.26	0.41
27:T:103:CDL:H161	27:T:103:CDL:H372	2.03	0.41
1:A:172:LYS:NZ	1:A:178[A]:GLN:NE2	2.65	0.41
25:C:309:DMU:H23	27:G:102:CDL:H622	2.02	0.41
14:A:602[B]:HEA:HMB1	14:A:602[B]:HEA:H11	1.81	0.41
2:B:56:MET:HG2	24:B:303:PSC:H221	2.02	0.41
3:P:3:HIS:CD2	3:P:4:GLN:H	2.38	0.41
3:P:33[A]:MET:HE1	3:P:41:THR:HB	2.01	0.41
1:A:377:PHE:CB	14:A:602[A]:HEA:C2D	2.99	0.41
2:B:28:LEU:HG	2:B:32[A]:PHE:CE2	2.56	0.41
7:G:8:HIS:CD2	7:G:9:GLY:N	2.77	0.41
14:N:602[B]:HEA:HMB1	14:N:602[B]:HEA:H11	1.92	0.41
27:T:103:CDL:H112	27:T:103:CDL:OA4	2.21	0.41
1:A:309:THR:HG22	14:A:602[A]:HEA:HMB2	2.02	0.40
3:C:37:PHE:CG	25:C:302:DMU:H6	2.56	0.40
7:G:84:LYS:HZ3	7:G:84:LYS:N	2.11	0.40
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.08	0.40
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.36	0.40
11:X:9:PHE:HB2	20:X:101:PGV:H201	2.03	0.40
11:X:47:ARG:NH1	11:X:47:ARG:CB	2.60	0.40
2:O:82:ARG:HH11	2:O:86:MET:CE	2.31	0.40
12:Y:27:LEU:HD23	12:Y:27:LEU:HA	1.89	0.40
22:J:101:CHD:H111	22:J:101:CHD:H193	1.68	0.40
1:N:25:TRP:CE3	19:Y:101:TGL:HB91	2.57	0.40
4:Q:17[B]:VAL:HG22	4:Q:19[B]:ARG:HG3	2.03	0.40
9:V:35:TYR:CD1	9:V:35:TYR:C	2.94	0.40
3:C:155:ASP:OD2	6:F:2:SER:HA	2.21	0.40
3:C:157:LYS:HZ2	28:C:307:PEK:H051	1.73	0.40
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.22	0.40
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.04	0.40
1:N:302[B]:ARG:NH1	2:O:84:LEU:HD11	2.36	0.40
24:O:302:PSC:H201	24:O:302:PSC:C2	2.43	0.40
24:B:303:PSC:H51	30:I:115:HOH:O	2.20	0.40
3:C:226:HIS:HE1	27:C:305:CDL:HB32	1.85	0.40
27:G:102:CDL:CB5	27:G:102:CDL:H201	2.52	0.40
1:N:110:LEU:HD21	25:P:307:DMU:H24	2.04	0.40
1:N:243:VAL:HG11	18:N:607[A]:AZI:N3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.40
22:P:301:CHD:H212	22:P:301:CHD:H12	2.03	0.40
5:R:7:THR:HB	5:R:9:GLU:OE2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:541:HOH:O	30:L:219:HOH:O[2_584]	2.09	0.11
4:D:7:LYS:CD	30:B:405:HOH:O[2_585]	2.11	0.09

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%)	518 (97%)	16 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
3	C	264/261 (101%)	259 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	137 (94%)	4 (3%)	4 (3%)	5	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	3
6	F	99/98 (101%)	93 (94%)	3 (3%)	3 (3%)	4	0
6	S	98/98 (100%)	93 (95%)	3 (3%)	2 (2%)	7	0
7	G	82/85 (96%)	69 (84%)	9 (11%)	4 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	82/85 (96%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	2	0
8	U	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	45 (100%)	0	0	100	100
13	M	41/46 (89%)	38 (93%)	1 (2%)	2 (5%)	2	0
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3595/3614 (100%)	3465 (96%)	103 (3%)	27 (1%)	19	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
8	H	45	ALA
4	Q	7	LYS
4	Q	8	SER
5	R	6	GLU
6	S	95	GLN
7	T	5	LYS
7	T	8	HIS
8	U	46	LYS
7	G	41	HIS
13	M	42	LYS
6	S	94	HIS
7	T	3	ALA
7	T	4	ALA

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Mol	Chain	Res	Type
8	U	8	ILE
8	U	45	ALA
7	G	5	LYS
8	H	46	LYS
8	H	48	GLY
13	M	41	LYS
4	Q	5	VAL
4	Q	6	VAL

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%)	441 (99%)	6 (1%)	69	50
1	N	445/426 (104%)	438 (98%)	7 (2%)	62	41
2	B	220/210 (105%)	210 (96%)	10 (4%)	27	7
2	O	215/210 (102%)	205 (95%)	10 (5%)	26	6
3	C	231/226 (102%)	228 (99%)	3 (1%)	69	50
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	29
4	D	133/129 (103%)	128 (96%)	5 (4%)	33	10
4	Q	131/129 (102%)	122 (93%)	9 (7%)	15	2
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	12
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	7
6	F	84/81 (104%)	81 (96%)	3 (4%)	35	11
6	S	83/81 (102%)	76 (92%)	7 (8%)	11	1
7	G	68/68 (100%)	60 (88%)	8 (12%)	5	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	2
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	2
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	32
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	9
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	22
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	21
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	22
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	19
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	4
All	All	3129/3082 (102%)	3017 (96%)	112 (4%)	35	11

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	338	MET
1	A	369	ASP
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	110	PRO
3	C	159	MET
4	D	19[A]	ARG
4	D	19[B]	ARG
4	D	31[A]	LYS
4	D	31[B]	LYS
4	D	147	LYS
5	E	70	VAL

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Mol	Chain	Res	Type
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS
6	F	80	GLN
6	F	96	LEU
7	G	2	SER
7	G	5	LYS
7	G	7	ASP
7	G	18	PHE
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	2	THR
10	J	58	LYS
12	L	47	LYS
13	M	38	ASP
1	N	38	ARG
1	N	109	PHE
1	N	178[A]	GLN
1	N	178[B]	GLN
1	N	180	GLN
1	N	369	ASP
1	N	514	LYS
2	O	15	PRO
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
2	O	221	LYS
2	O	227	LEU
3	P	3	HIS
3	P	17	PRO
3	P	159	MET

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Mol	Chain	Res	Type
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	5	VAL
4	Q	7	LYS
4	Q	20	ARG
4	Q	31	LYS
4	Q	51	LEU
4	Q	58	GLU
4	Q	142	LYS
4	Q	147	LYS
5	R	5	HIS
5	R	79	LYS
5	R	83	PRO
5	R	108	LYS
6	S	2	SER
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	93	PRO
6	S	95	GLN
7	T	2	SER
7	T	7	ASP
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	29	LEU
9	V	37	PHE
9	V	65	LYS
9	V	70	GLN
10	W	50	LEU
10	W	57	HIS
11	X	47	ARG

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Mol	Chain	Res	Type
12	Y	47	LYS
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
6	F	80	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
8	H	22	ASN
8	H	31	GLN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	99	ASN
1	N	180	GLN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	38	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
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	$\#\|Z\| > 2$
7	TPO	T	11	7	8,10,11	2.06	2 (25%)	10,14,16	1.88	4 (40%)
1	FME	A	1	1	8,9,10	0.94	1 (12%)	7,9,11	2.16	5 (71%)
2	FME	B	1	2	8,9,10	5.13	6 (75%)	7,9,11	9.46	3 (42%)
9	SAC	I	1	9	7,8,9	1.11	1 (14%)	8,9,11	2.33	1 (12%)
2	FME	O	1	2	8,9,10	1.45	2 (25%)	7,9,11	1.59	1 (14%)
7	TPO	G	11	7	8,10,11	1.98	2 (25%)	10,14,16	1.70	2 (20%)
9	SAC	V	1	9	7,8,9	2.00	1 (14%)	8,9,11	2.36	3 (37%)
1	FME	N	1	1	8,9,10	1.22	1 (12%)	7,9,11	1.27	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	11.20	1.71	1.33
2	B	1	FME	CA-N	5.36	1.53	1.46
9	V	1	SAC	CA-N	5.06	1.53	1.46
2	B	1	FME	CB-CG	4.89	1.70	1.51
2	B	1	FME	CG-SD	-3.59	1.62	1.81
7	G	11	TPO	P-OG1	3.50	1.65	1.59
7	T	11	TPO	P-OG1	3.20	1.65	1.59
7	T	11	TPO	P-O1P	3.12	1.60	1.50
2	B	1	FME	CB-CA	3.08	1.58	1.53
2	B	1	FME	O-C	2.83	1.31	1.19
7	G	11	TPO	P-O1P	2.65	1.59	1.50
1	N	1	FME	CA-N	2.59	1.50	1.46
9	I	1	SAC	CA-N	2.50	1.49	1.46
2	O	1	FME	CG-SD	-2.41	1.68	1.81
2	O	1	FME	CB-CG	2.29	1.60	1.51
1	A	1	FME	O-C	2.21	1.28	1.19

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	O1-CN-N	-22.22	66.76	125.27
2	B	1	FME	CA-N-CN	-10.90	106.06	122.82
9	I	1	SAC	OG-CB-CA	-5.84	96.06	110.97
9	V	1	SAC	CA-N-C1A	4.86	132.10	123.15
7	T	11	TPO	CG2-CB-CA	3.82	120.71	113.16
1	A	1	FME	C-CA-N	3.33	115.74	109.73
7	G	11	TPO	CG2-CB-CA	3.08	119.24	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	C-CA-N	2.90	114.97	109.73
2	O	1	FME	CG-CB-CA	-2.61	105.70	112.95
1	A	1	FME	CE-SD-CG	2.55	109.15	100.40
7	T	11	TPO	O3P-P-O2P	2.49	117.17	107.64
7	G	11	TPO	O2P-P-OG1	2.46	117.00	105.99
2	B	1	FME	C-CA-N	2.39	114.04	109.73
1	N	1	FME	O-C-CA	-2.38	118.53	124.78
9	V	1	SAC	CB-CA-N	-2.22	105.57	110.55
7	T	11	TPO	O-C-CA	-2.16	119.13	124.78
1	A	1	FME	O1-CN-N	-2.15	119.62	125.27
7	T	11	TPO	O3P-P-O1P	-2.10	102.46	110.68
1	A	1	FME	CA-N-CN	2.07	126.01	122.82
1	A	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	N-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
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
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	CA-CB-CG-SD
9	V	1	SAC	CB-CA-N-C1A
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	CG2-CB-OG1-P

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Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
9	V	1	SAC	C-CA-N-C1A
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
2	B	1	FME	6	0
7	G	11	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 118 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 108 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	$\#\|Z\| > 2$
28	PEK	T	102	-	52,52,52	0.95	3 (5%)	55,57,57	1.27	5 (9%)
21	EDO	A	616	-	3,3,3	1.06	0	2,2,2	2.70	2 (100%)
21	EDO	F	104	-	3,3,3	1.59	0	2,2,2	0.63	0
21	EDO	B	306	-	3,3,3	0.56	0	2,2,2	0.03	0
21	EDO	A	618	-	3,3,3	1.10	0	2,2,2	1.10	0
21	EDO	S	102	-	3,3,3	0.86	0	2,2,2	0.43	0
14	HEA	N	601	1	57,67,67	1.64	15 (26%)	61,103,103	2.71	22 (36%)
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	T	104	-	3,3,3	1.14	0	2,2,2	0.72	0
21	EDO	D	204	-	3,3,3	0.58	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	F	103	-	3,3,3	0.79	0	2,2,2	0.19	0
20	PGV	A	609	-	50,50,50	1.11	4 (8%)	53,56,56	1.28	5 (9%)
21	EDO	D	202	-	3,3,3	0.76	0	2,2,2	1.03	0
20	PGV	N	608	-	50,50,50	1.15	5 (10%)	53,56,56	1.53	8 (15%)
20	PGV	C	308	-	50,50,50	1.40	3 (6%)	53,56,56	1.62	7 (13%)
21	EDO	D	205	-	3,3,3	0.26	0	2,2,2	1.60	1 (50%)
25	DMU	C	302	-	34,34,34	0.98	1 (2%)	45,45,45	1.57	5 (11%)
21	EDO	G	105	-	3,3,3	0.97	0	2,2,2	0.58	0
27	CDL	P	305	-	99,99,99	1.73	21 (21%)	105,111,111	1.57	18 (17%)
21	EDO	H	101	-	3,3,3	0.30	0	2,2,2	2.28	2 (100%)
21	EDO	B	305	-	3,3,3	0.55	0	2,2,2	0.77	0
14	HEA	A	602[A]	18,1	57,67,67	1.56	9 (15%)	61,103,103	2.04	17 (27%)
21	EDO	A	617	-	3,3,3	1.23	0	2,2,2	0.34	0
28	PEK	G	104	-	52,52,52	1.32	3 (5%)	55,57,57	1.47	8 (14%)
22	CHD	P	306	-	32,32,32	1.63	7 (21%)	51,51,51	2.88	20 (39%)
21	EDO	A	620	-	3,3,3	0.62	0	2,2,2	0.41	0
21	EDO	C	312	-	3,3,3	0.44	0	2,2,2	0.79	0
24	PSC	B	303	-	51,51,51	1.54	7 (13%)	57,59,59	2.16	12 (21%)
21	EDO	S	103	-	3,3,3	0.47	0	2,2,2	0.27	0
21	EDO	B	304	-	3,3,3	0.88	0	2,2,2	0.78	0
22	CHD	G	103	-	32,32,32	2.05	13 (40%)	51,51,51	2.38	22 (43%)
21	EDO	C	313	-	3,3,3	1.05	0	2,2,2	0.80	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.59	0
27	CDL	T	103	-	99,99,99	1.58	15 (15%)	105,111,111	1.62	17 (16%)
21	EDO	A	612	-	3,3,3	1.74	1 (33%)	2,2,2	0.97	0
20	PGV	C	304	-	50,50,50	0.82	0	53,56,56	1.31	6 (11%)
21	EDO	N	612	-	3,3,3	0.68	0	2,2,2	0.77	0
21	EDO	P	311	-	3,3,3	0.99	0	2,2,2	0.39	0
14	HEA	A	602[B]	18,1	57,67,67	1.49	9 (15%)	61,103,103	2.34	23 (37%)
21	EDO	P	312	-	3,3,3	1.12	0	2,2,2	2.42	2 (100%)
25	DMU	C	310	-	34,34,34	1.76	8 (23%)	45,45,45	3.10	18 (40%)
19	TGL	L	101	-	62,62,62	1.61	7 (11%)	65,65,65	2.71	21 (32%)
21	EDO	A	619	-	3,3,3	0.39	0	2,2,2	0.70	0
25	DMU	Z	101	-	34,34,34	0.85	3 (8%)	45,45,45	1.43	5 (11%)
20	PGV	P	304	-	50,50,50	0.93	1 (2%)	53,56,56	1.32	5 (9%)
21	EDO	L	103	-	3,3,3	0.59	0	2,2,2	0.29	0
21	EDO	O	304	-	3,3,3	0.82	0	2,2,2	0.54	0
27	CDL	C	305	-	99,99,99	1.64	18 (18%)	105,111,111	1.64	21 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	S	105	-	3,3,3	1.04	0	2,2,2	1.61	1 (50%)
22	CHD	J	101	-	32,32,32	1.23	3 (9%)	51,51,51	3.23	24 (47%)
21	EDO	A	615	-	3,3,3	0.93	0	2,2,2	0.72	0
22	CHD	W	101	-	32,32,32	1.18	2 (6%)	51,51,51	3.62	24 (47%)
21	EDO	A	611	-	3,3,3	0.47	0	2,2,2	0.21	0
25	DMU	C	309	-	34,34,34	0.80	1 (2%)	45,45,45	2.56	12 (26%)
25	DMU	P	307	-	34,34,34	1.20	1 (2%)	45,45,45	1.38	6 (13%)
23	CUA	B	302	2	0,1,1	-	-	-		
21	EDO	N	615	-	3,3,3	0.45	0	2,2,2	1.04	0
18	AZI	A	607[A]	14,15	0,2,2	-	-	0,1,1	-	-
25	DMU	P	309	-	34,34,34	0.84	2 (5%)	45,45,45	2.27	12 (26%)
25	DMU	L	102	-	34,34,34	1.11	4 (11%)	45,45,45	1.75	12 (26%)
28	PEK	P	308	-	52,52,52	1.31	3 (5%)	55,57,57	1.42	8 (14%)
14	HEA	N	602[A]	18,1	57,67,67	1.67	12 (21%)	61,103,103	2.00	16 (26%)
21	EDO	C	311	-	3,3,3	1.03	0	2,2,2	0.27	0
14	HEA	A	601	1	57,67,67	1.78	17 (29%)	61,103,103	2.86	29 (47%)
19	TGL	Y	101	-	62,62,62	1.64	7 (11%)	65,65,65	2.16	19 (29%)
20	PGV	P	302	-	50,50,50	1.22	2 (4%)	53,56,56	1.34	4 (7%)
21	EDO	Y	102	-	3,3,3	0.63	0	2,2,2	0.15	0
22	CHD	P	301	-	32,32,32	1.76	9 (28%)	51,51,51	2.35	16 (31%)
27	CDL	G	102	-	99,99,99	1.57	16 (16%)	105,111,111	1.72	22 (20%)
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.56	9 (15%)
22	CHD	C	306	-	32,32,32	1.26	4 (12%)	51,51,51	3.31	21 (41%)
21	EDO	F	102	-	3,3,3	0.99	0	2,2,2	0.31	0
18	AZI	N	606[B]	14	0,2,2	-	-	0,1,1	-	-
19	TGL	A	608	-	62,62,62	1.36	5 (8%)	65,65,65	1.87	11 (16%)
18	AZI	N	607[A]	14,15	0,2,2	-	-	0,1,1	-	-
21	EDO	N	616	-	3,3,3	1.35	1 (33%)	2,2,2	1.66	0
21	EDO	G	106	-	3,3,3	0.53	0	2,2,2	0.94	0
21	EDO	N	611	-	3,3,3	0.70	0	2,2,2	1.02	0
25	DMU	M	101	-	34,34,34	0.97	2 (5%)	45,45,45	1.36	7 (15%)
19	TGL	Q	201	-	62,62,62	1.60	4 (6%)	65,65,65	1.44	9 (13%)
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	E	203	-	3,3,3	0.50	0	2,2,2	0.93	0
21	EDO	A	613	-	3,3,3	0.80	0	2,2,2	0.71	0
21	EDO	N	614	-	3,3,3	1.34	0	2,2,2	0.57	0
21	EDO	R	201	-	3,3,3	0.66	0	2,2,2	0.81	0
21	EDO	A	614	-	3,3,3	1.10	0	2,2,2	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	HEA	N	602[B]	18,1	57,67,67	1.57	11 (19%)	61,103,103	1.94	18 (29%)
21	EDO	N	610	-	3,3,3	1.33	1 (33%)	2,2,2	0.34	0
21	EDO	N	613	-	3,3,3	0.73	0	2,2,2	0.24	0
19	TGL	N	609	-	62,62,62	1.10	4 (6%)	65,65,65	1.91	10 (15%)
20	PGV	X	101	-	50,50,50	1.35	3 (6%)	53,56,56	1.59	8 (15%)
28	PEK	C	307	-	52,52,52	1.37	5 (9%)	55,57,57	1.54	7 (12%)
21	EDO	F	105	-	3,3,3	1.15	0	2,2,2	0.70	0
22	CHD	C	301	-	32,32,32	1.88	8 (25%)	51,51,51	2.37	17 (33%)
28	PEK	T	101	-	52,52,52	1.34	2 (3%)	55,57,57	1.62	9 (16%)
20	PGV	A	610	-	50,50,50	1.86	4 (8%)	53,56,56	2.74	10 (18%)
22	CHD	B	301	-	32,32,32	1.98	14 (43%)	51,51,51	2.64	26 (50%)
28	PEK	G	101	-	52,52,52	1.02	3 (5%)	55,57,57	1.34	8 (14%)
21	EDO	D	203	-	3,3,3	0.41	0	2,2,2	0.88	0
18	AZI	N	607[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.60	0
25	DMU	P	310	-	34,34,34	1.06	1 (2%)	45,45,45	1.49	5 (11%)
21	EDO	S	104	-	3,3,3	1.36	0	2,2,2	0.40	0
19	TGL	D	201	-	62,62,62	2.27	6 (9%)	65,65,65	2.97	16 (24%)
21	EDO	A	621	-	3,3,3	0.38	0	2,2,2	1.22	0
23	CUA	O	301	2	0,1,1	-	-	-		
21	EDO	E	202	-	3,3,3	0.91	0	2,2,2	0.57	0
21	EDO	S	106	-	3,3,3	1.15	0	2,2,2	0.83	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
28	PEK	T	102	-	-	16/56/56/56	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
14	HEA	N	601	1	-	4/32/76/76	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
21	EDO	F	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	A	609	-	-	7/55/55/55	-
21	EDO	D	202	-	-	0/1/1/1	-
20	PGV	N	608	-	-	7/55/55/55	-
20	PGV	C	308	-	-	37/55/55/55	-
21	EDO	D	205	-	-	1/1/1/1	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
21	EDO	G	105	-	-	0/1/1/1	-
27	CDL	P	305	-	-	59/110/110/110	-
21	EDO	H	101	-	-	1/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
14	HEA	A	602[A]	18,1	-	4/32/76/76	-
21	EDO	A	617	-	-	1/1/1/1	-
28	PEK	G	104	-	-	27/56/56/56	-
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
21	EDO	A	620	-	-	1/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
24	PSC	B	303	-	-	21/55/55/55	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
21	EDO	C	313	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
27	CDL	T	103	-	-	51/110/110/110	-
21	EDO	A	612	-	-	0/1/1/1	-
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
14	HEA	A	602[B]	18,1	-	5/32/76/76	-
21	EDO	P	312	-	-	1/1/1/1	-
25	DMU	C	310	-	-	11/19/59/59	0/2/2/2
19	TGL	L	101	-	-	39/65/65/65	-
21	EDO	A	619	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
20	PGV	P	304	-	-	11/55/55/55	-
21	EDO	L	103	-	-	0/1/1/1	-
21	EDO	O	304	-	-	0/1/1/1	-
27	CDL	C	305	-	-	58/110/110/110	-
21	EDO	S	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
21	EDO	A	615	-	-	1/1/1/1	-
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
21	EDO	A	611	-	-	0/1/1/1	-
25	DMU	C	309	-	-	6/19/59/59	0/2/2/2
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
21	EDO	N	615	-	-	1/1/1/1	-
25	DMU	P	309	-	-	6/19/59/59	0/2/2/2
25	DMU	L	102	-	-	14/19/59/59	0/2/2/2
28	PEK	P	308	-	-	32/56/56/56	-
14	HEA	N	602[A]	18,1	-	4/32/76/76	-
21	EDO	C	311	-	-	0/1/1/1	-
14	HEA	A	601	1	-	5/32/76/76	-
19	TGL	Y	101	-	-	40/65/65/65	-
20	PGV	P	302	-	-	27/55/55/55	-
21	EDO	Y	102	-	-	1/1/1/1	-
22	CHD	P	301	-	-	3/9/74/74	0/4/4/4
27	CDL	G	102	-	-	71/110/110/110	-
24	PSC	O	302	-	-	28/55/55/55	-
22	CHD	C	306	-	-	7/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	N	616	-	-	1/1/1/1	-
21	EDO	G	106	-	-	1/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
25	DMU	M	101	-	-	2/19/59/59	0/2/2/2
19	TGL	Q	201	-	-	34/65/65/65	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
14	HEA	N	602[B]	18,1	-	5/32/76/76	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	613	-	-	1/1/1/1	-
19	TGL	N	609	-	-	33/65/65/65	-
20	PGV	X	101	-	-	31/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEK	C	307	-	-	23/56/56/56	-
21	EDO	F	105	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
28	PEK	T	101	-	-	31/56/56/56	-
20	PGV	A	610	-	-	26/55/55/55	-
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
28	PEK	G	101	-	-	17/56/56/56	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-
25	DMU	P	310	-	-	7/19/59/59	0/2/2/2
21	EDO	S	104	-	-	0/1/1/1	-
19	TGL	D	201	-	-	39/65/65/65	-
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	S	106	-	-	0/1/1/1	-

All (313) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	11.00	1.55	1.22
19	D	201	TGL	OG2-CB1	8.23	1.57	1.34
20	A	610	PGV	O02-C1	8.05	1.46	1.22
19	L	101	TGL	OG2-CB1	7.02	1.54	1.34
20	A	610	PGV	O01-C1	6.83	1.53	1.34
19	Y	101	TGL	OG3-CC1	6.83	1.53	1.33
19	Y	101	TGL	OG2-CB1	6.80	1.53	1.34
19	D	201	TGL	OG1-CA1	6.69	1.52	1.33
20	X	101	PGV	O03-C19	6.68	1.52	1.33
20	C	308	PGV	O01-C1	6.66	1.53	1.34
19	Q	201	TGL	OG2-CB1	6.46	1.52	1.34
27	G	102	CDL	OB6-CB5	6.29	1.52	1.34
19	Q	201	TGL	OB1-CB1	6.16	1.40	1.22
27	C	305	CDL	OB8-CB7	6.13	1.51	1.33
19	L	101	TGL	OG3-CC1	6.07	1.51	1.33
28	T	101	PEK	O01-C1	6.06	1.51	1.34
27	P	305	CDL	OB8-CB7	5.98	1.50	1.33
27	T	103	CDL	OB8-CB7	5.97	1.50	1.33
28	G	104	PEK	O03-C21	5.79	1.50	1.33
20	A	610	PGV	O03-C19	5.77	1.50	1.33
27	P	305	CDL	OA8-CA7	5.76	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	307	PEK	O03-C21	5.72	1.50	1.33
19	A	608	TGL	OG1-CA1	5.62	1.49	1.33
27	G	102	CDL	OB8-CB7	5.58	1.49	1.33
28	G	104	PEK	O01-C1	5.58	1.50	1.34
28	T	101	PEK	O03-C21	5.57	1.49	1.33
24	O	302	PSC	O01-C1	5.56	1.50	1.34
27	P	305	CDL	OA6-CA5	5.55	1.49	1.34
27	T	103	CDL	OA6-CA5	5.53	1.49	1.34
22	C	301	CHD	C11-C12	5.51	1.62	1.53
28	P	308	PEK	O01-C1	5.48	1.49	1.34
27	C	305	CDL	OA8-CA7	5.47	1.49	1.33
28	C	307	PEK	O01-C1	5.43	1.49	1.34
28	P	308	PEK	O03-C21	5.41	1.49	1.33
25	C	310	DMU	O16-C6	5.39	1.49	1.40
24	B	303	PSC	O01-C1	5.33	1.49	1.34
27	T	103	CDL	OB6-CB5	5.23	1.49	1.34
19	Y	101	TGL	OG1-CA1	5.20	1.48	1.33
20	P	302	PGV	O03-C19	5.11	1.48	1.33
27	T	103	CDL	OA8-CA7	5.02	1.48	1.33
19	L	101	TGL	OG1-CA1	4.99	1.47	1.33
27	G	102	CDL	OA6-CA5	4.98	1.48	1.34
25	P	307	DMU	O16-C6	4.94	1.48	1.40
20	P	302	PGV	O01-C1	4.84	1.47	1.34
27	G	102	CDL	OA8-CA7	4.79	1.47	1.33
19	D	201	TGL	OC1-CC1	4.76	1.36	1.22
24	O	302	PSC	O03-C19	4.68	1.47	1.33
24	B	303	PSC	O03-C19	4.68	1.47	1.33
19	Q	201	TGL	OG1-CA1	4.59	1.46	1.33
19	N	609	TGL	OG1-CA1	4.57	1.46	1.33
24	B	303	PSC	O01-C02	4.51	1.57	1.46
19	Q	201	TGL	OG3-CC1	4.49	1.46	1.33
27	C	305	CDL	PB2-OB3	4.49	1.66	1.50
20	C	308	PGV	O03-C19	4.39	1.46	1.33
25	P	310	DMU	O16-C6	4.37	1.47	1.40
20	X	101	PGV	O01-C1	4.37	1.46	1.34
27	P	305	CDL	OB6-CB5	4.30	1.46	1.34
14	N	602[A]	HEA	O11-C11	4.29	1.52	1.42
19	D	201	TGL	OG3-CC1	4.29	1.45	1.33
27	C	305	CDL	OA6-CA5	4.21	1.46	1.34
14	A	601	HEA	C12-C11	-4.19	1.45	1.52
27	C	305	CDL	OB6-CB5	4.17	1.46	1.34
14	A	602[B]	HEA	CHD-C1D	4.17	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHD-C1D	4.15	1.45	1.35
14	N	602[A]	HEA	CHC-C4B	4.11	1.45	1.35
27	P	305	CDL	PB2-OB3	4.09	1.65	1.50
19	A	608	TGL	OG2-CG2	4.07	1.56	1.46
14	N	601	HEA	CHD-C1D	4.05	1.45	1.35
22	P	306	CHD	C8-C9	4.03	1.61	1.53
22	B	301	CHD	C11-C9	4.01	1.60	1.53
14	A	601	HEA	C20-C19	3.98	1.59	1.51
22	G	103	CHD	C18-C13	3.96	1.60	1.54
19	A	608	TGL	OC1-CC1	-3.94	1.10	1.22
24	B	303	PSC	C13-C12	3.94	1.54	1.31
14	A	602[B]	HEA	CHC-C4B	3.88	1.44	1.35
14	N	602[B]	HEA	CHD-C1D	3.83	1.44	1.35
24	O	302	PSC	C13-C12	3.76	1.53	1.31
22	P	301	CHD	C11-C12	3.74	1.59	1.53
22	J	101	CHD	C20-C17	3.71	1.60	1.54
19	A	608	TGL	OG3-CC1	3.70	1.44	1.33
19	N	609	TGL	OG3-CC1	3.68	1.44	1.33
25	C	302	DMU	O16-C6	3.68	1.46	1.40
14	N	602[B]	HEA	C4B-C3B	-3.60	1.38	1.44
14	N	601	HEA	CMD-C2D	3.59	1.58	1.50
14	A	602[A]	HEA	CMC-C2C	3.57	1.59	1.51
14	A	602[A]	HEA	CHD-C1D	3.57	1.44	1.35
22	G	103	CHD	C8-C7	3.55	1.59	1.53
14	N	602[A]	HEA	C3C-C2C	-3.55	1.35	1.40
27	P	305	CDL	O1-C1	3.54	1.54	1.43
14	A	601	HEA	C1D-ND	-3.53	1.34	1.40
14	A	601	HEA	C12-C13	3.53	1.65	1.53
14	N	602[B]	HEA	C1B-C2B	-3.50	1.37	1.44
22	G	103	CHD	C11-C9	3.50	1.59	1.53
14	A	602[A]	HEA	C4D-C3D	-3.49	1.39	1.45
22	B	301	CHD	C8-C7	3.49	1.59	1.53
19	N	609	TGL	OG2-CB1	3.48	1.44	1.34
22	C	301	CHD	C22-C20	3.47	1.63	1.54
14	N	601	HEA	CHC-C4B	3.45	1.43	1.35
25	C	310	DMU	C10-C5	3.43	1.62	1.52
25	C	310	DMU	O3-C5	3.39	1.51	1.43
22	G	103	CHD	C1-C2	3.33	1.60	1.53
27	P	305	CDL	PA1-OA5	3.32	1.72	1.59
14	A	602[A]	HEA	C3C-C2C	-3.31	1.35	1.40
14	N	602[A]	HEA	C4D-C3D	-3.26	1.39	1.45
27	C	305	CDL	C82-C81	-3.25	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	305	CDL	CB2-C1	3.25	1.62	1.51
14	N	601	HEA	O11-C11	3.25	1.49	1.42
22	P	301	CHD	C8-C7	3.23	1.59	1.53
14	N	602[A]	HEA	CHD-C1D	3.23	1.43	1.35
14	A	601	HEA	CAA-C2A	3.22	1.57	1.52
22	P	306	CHD	C10-C5	3.21	1.60	1.55
27	C	305	CDL	C59-C58	-3.21	1.33	1.51
22	C	301	CHD	C2-C3	3.19	1.59	1.51
27	T	103	CDL	C59-C58	-3.17	1.33	1.51
22	G	103	CHD	C13-C12	-3.15	1.49	1.54
27	T	103	CDL	C62-C61	-3.14	1.33	1.51
27	C	305	CDL	O1-C1	3.11	1.52	1.43
22	P	301	CHD	C11-C9	3.08	1.58	1.53
14	A	602[A]	HEA	CHC-C4B	3.06	1.42	1.35
14	N	602[B]	HEA	CHC-C4B	3.04	1.42	1.35
14	N	602[B]	HEA	C1D-ND	-3.02	1.35	1.40
20	N	608	PGV	O01-C1	3.01	1.42	1.34
27	T	103	CDL	C42-C41	-3.00	1.34	1.51
27	P	305	CDL	C19-C18	-2.99	1.34	1.51
22	P	306	CHD	C11-C9	2.98	1.58	1.53
27	C	305	CDL	C62-C61	-2.98	1.34	1.51
25	C	310	DMU	O5-C6	2.98	1.49	1.41
14	A	602[B]	HEA	C18-C19	2.97	1.40	1.33
27	C	305	CDL	C79-C78	-2.97	1.34	1.51
27	P	305	CDL	C22-C21	-2.93	1.35	1.51
19	A	608	TGL	OG2-CB1	2.93	1.42	1.34
20	N	608	PGV	C3-C2	2.93	1.63	1.52
22	G	103	CHD	O12-C12	2.91	1.48	1.43
22	B	301	CHD	C18-C13	2.90	1.59	1.54
27	P	305	CDL	C59-C58	-2.90	1.35	1.51
22	B	301	CHD	O7-C7	2.90	1.49	1.43
22	W	101	CHD	C13-C17	2.90	1.60	1.55
27	G	102	CDL	C59-C58	-2.89	1.35	1.51
27	C	305	CDL	C22-C21	-2.89	1.35	1.51
19	L	101	TGL	CG3-CG2	2.89	1.59	1.50
27	G	102	CDL	C19-C18	-2.89	1.35	1.51
27	P	305	CDL	C79-C78	-2.88	1.35	1.51
25	L	102	DMU	O16-C6	2.88	1.45	1.40
27	G	102	CDL	C62-C61	-2.87	1.35	1.51
20	A	609	PGV	C3-C2	2.87	1.62	1.52
14	A	601	HEA	CAD-C3D	2.84	1.58	1.51
22	G	103	CHD	C20-C17	2.83	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[B]	HEA	C4B-C3B	-2.81	1.39	1.44
19	L	101	TGL	CC2-CC1	2.81	1.58	1.50
27	G	102	CDL	C82-C81	-2.81	1.35	1.51
27	G	102	CDL	C39-C38	-2.80	1.35	1.51
19	Y	101	TGL	CG3-CG2	2.79	1.59	1.50
27	P	305	CDL	C62-C61	-2.79	1.35	1.51
27	C	305	CDL	C19-C18	-2.79	1.35	1.51
25	Z	101	DMU	O16-C6	2.78	1.44	1.40
27	P	305	CDL	C39-C38	-2.78	1.36	1.51
27	T	103	CDL	C79-C78	-2.78	1.36	1.51
27	T	103	CDL	C39-C38	-2.77	1.36	1.51
27	G	102	CDL	C22-C21	-2.74	1.36	1.51
14	A	601	HEA	CBD-CAD	2.74	1.60	1.52
27	C	305	CDL	CA2-C1	2.74	1.60	1.51
27	P	305	CDL	C42-C41	-2.74	1.36	1.51
14	N	601	HEA	CBD-CAD	2.73	1.60	1.52
22	G	103	CHD	C6-C7	2.72	1.57	1.52
27	T	103	CDL	C22-C21	-2.71	1.36	1.51
19	N	609	TGL	OC1-CC1	-2.71	1.14	1.22
27	C	305	CDL	C39-C38	-2.70	1.36	1.51
14	A	601	HEA	C4B-C3B	-2.70	1.40	1.44
27	P	305	CDL	CA3-CA4	2.69	1.58	1.50
27	P	305	CDL	C82-C81	-2.68	1.36	1.51
14	N	602[B]	HEA	FE-NB	2.67	2.10	1.96
20	N	608	PGV	C01-C02	2.67	1.58	1.50
27	T	103	CDL	C19-C18	-2.66	1.36	1.51
14	A	602[A]	HEA	C1D-C2D	-2.66	1.39	1.44
27	G	102	CDL	C42-C41	-2.65	1.36	1.51
14	A	601	HEA	C16-C17	-2.65	1.44	1.53
27	P	305	CDL	CB2-C1	2.64	1.60	1.51
25	C	310	DMU	O7-C10	2.64	1.49	1.41
25	C	310	DMU	O1-C10	2.64	1.48	1.41
24	B	303	PSC	C03-C02	2.63	1.58	1.50
14	N	602[A]	HEA	C3A-CMA	2.62	1.52	1.46
27	G	102	CDL	C79-C78	-2.61	1.36	1.51
20	A	609	PGV	C01-C02	2.61	1.58	1.50
19	D	201	TGL	CC2-CC1	2.59	1.58	1.50
22	G	103	CHD	O7-C7	2.59	1.48	1.43
27	C	305	CDL	C42-C41	-2.59	1.37	1.51
24	B	303	PSC	C01-C02	2.59	1.58	1.50
14	N	602[B]	HEA	C4B-NB	-2.59	1.35	1.40
14	N	602[A]	HEA	FE-NB	2.58	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[A]	HEA	C3B-C2B	2.57	1.40	1.34
27	T	103	CDL	C82-C81	-2.56	1.37	1.51
22	P	306	CHD	C8-C14	2.56	1.58	1.53
20	C	308	PGV	C01-C02	2.56	1.58	1.50
25	M	101	DMU	O16-C6	2.56	1.44	1.40
27	P	305	CDL	PA1-OA2	2.56	1.69	1.59
22	B	301	CHD	C20-C17	2.56	1.58	1.54
22	P	301	CHD	C13-C12	2.54	1.58	1.54
22	C	301	CHD	C18-C13	2.54	1.58	1.54
22	G	103	CHD	C19-C10	2.54	1.58	1.54
22	B	301	CHD	C19-C10	2.54	1.58	1.54
22	B	301	CHD	C11-C12	2.52	1.57	1.53
27	C	305	CDL	PA1-OA5	2.50	1.69	1.59
22	C	301	CHD	C23-C24	2.50	1.56	1.50
22	P	301	CHD	C23-C24	2.49	1.56	1.50
22	C	306	CHD	C16-C17	2.49	1.59	1.54
27	T	103	CDL	CB6-CB4	2.48	1.58	1.50
22	G	103	CHD	O25-C24	2.48	1.30	1.22
14	A	601	HEA	CHC-C4B	2.47	1.41	1.35
22	B	301	CHD	C21-C20	2.47	1.59	1.53
20	N	608	PGV	C06-C05	2.46	1.61	1.51
14	A	602[B]	HEA	C1B-NB	-2.46	1.33	1.38
22	W	101	CHD	C20-C17	2.43	1.58	1.54
14	N	601	HEA	C1D-ND	-2.43	1.36	1.40
14	A	602[B]	HEA	C4D-ND	-2.43	1.33	1.38
27	P	305	CDL	PB2-OB2	2.42	1.69	1.59
25	P	309	DMU	O16-C6	2.40	1.44	1.40
19	L	101	TGL	CB2-CB1	2.39	1.57	1.50
28	G	101	PEK	O01-C1	2.39	1.41	1.34
22	J	101	CHD	C23-C24	2.38	1.56	1.50
28	G	104	PEK	C01-C02	2.37	1.58	1.50
25	L	102	DMU	O7-C10	2.37	1.48	1.41
22	B	301	CHD	C16-C15	2.36	1.60	1.54
22	P	306	CHD	C11-C12	2.36	1.57	1.53
19	L	101	TGL	OG2-CG2	2.35	1.52	1.46
28	T	102	PEK	O11-C03	2.35	1.53	1.44
19	Y	101	TGL	CC2-CC1	2.34	1.57	1.50
27	P	305	CDL	C51-CB5	-2.34	1.43	1.50
14	A	601	HEA	CMB-C2B	2.32	1.55	1.50
14	N	602[A]	HEA	C4C-NC	-2.32	1.31	1.36
22	B	301	CHD	C10-C9	-2.32	1.51	1.56
22	C	306	CHD	C8-C9	2.31	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	C16-C17	-2.30	1.46	1.53
14	N	602[B]	HEA	FE-ND	2.30	2.08	1.96
28	C	307	PEK	C22-C21	2.30	1.57	1.50
28	G	101	PEK	P-O14	2.30	1.59	1.50
14	A	601	HEA	C18-C19	-2.30	1.27	1.33
25	C	309	DMU	O16-C6	2.30	1.44	1.40
22	C	301	CHD	C8-C7	2.30	1.57	1.53
14	N	602[B]	HEA	C2A-C1A	-2.29	1.37	1.42
25	L	102	DMU	O7-C3	2.29	1.49	1.43
14	N	601	HEA	C4B-NB	-2.29	1.36	1.40
28	C	307	PEK	C03-C02	2.27	1.57	1.50
27	T	103	CDL	CA3-CA4	2.27	1.57	1.50
19	Y	101	TGL	CC3-CC2	2.26	1.60	1.52
14	A	602[B]	HEA	C3C-C2C	2.26	1.43	1.40
22	B	301	CHD	O25-C24	2.25	1.29	1.22
14	N	601	HEA	CBA-CGA	2.25	1.55	1.50
22	C	301	CHD	O26-C24	-2.25	1.23	1.30
27	C	305	CDL	PB2-OB2	2.22	1.68	1.59
27	G	102	CDL	CB3-CB4	2.22	1.57	1.50
14	A	602[B]	HEA	C3A-CMA	2.22	1.51	1.46
25	M	101	DMU	C2-C1	2.21	1.58	1.52
21	N	610	EDO	O2-C2	2.21	1.53	1.42
28	T	102	PEK	C6-C5	2.21	1.44	1.31
27	G	102	CDL	C51-CB5	2.21	1.57	1.50
27	G	102	CDL	CB6-CB4	2.20	1.57	1.50
22	P	306	CHD	C13-C12	2.19	1.58	1.54
14	A	601	HEA	CBD-CGD	2.17	1.55	1.50
28	C	307	PEK	C01-C02	2.17	1.57	1.50
22	P	301	CHD	C16-C15	2.15	1.59	1.54
21	A	612	EDO	O2-C2	2.15	1.53	1.42
20	A	609	PGV	C21-C20	2.15	1.60	1.52
25	C	310	DMU	O16-C18	2.15	1.48	1.43
14	N	601	HEA	C12-C13	2.15	1.60	1.53
20	X	101	PGV	C01-C02	2.15	1.57	1.50
20	A	609	PGV	O03-C01	2.15	1.50	1.45
20	N	608	PGV	O03-C01	2.14	1.50	1.45
24	B	303	PSC	C3-C2	2.13	1.60	1.52
28	T	102	PEK	O03-C21	2.13	1.39	1.33
14	N	602[A]	HEA	C1D-ND	-2.12	1.36	1.40
22	P	301	CHD	C15-C14	2.12	1.58	1.54
28	G	101	PEK	O01-C02	2.12	1.51	1.46
22	P	301	CHD	O26-C24	-2.12	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	101	TGL	OG3-CG3	2.11	1.50	1.45
20	A	610	PGV	P-O13	2.10	1.58	1.50
25	L	102	DMU	O1-C10	2.10	1.47	1.41
14	A	601	HEA	C1B-NB	-2.10	1.34	1.38
25	C	310	DMU	O7-C3	2.10	1.49	1.43
22	G	103	CHD	C16-C17	2.09	1.58	1.54
21	N	616	EDO	O2-C2	2.09	1.52	1.42
22	C	301	CHD	C8-C14	2.09	1.57	1.53
20	P	304	PGV	O03-C19	2.08	1.39	1.33
14	N	602[B]	HEA	C3A-CMA	2.08	1.51	1.46
27	P	305	CDL	CA2-C1	2.07	1.58	1.51
25	P	309	DMU	C8-C9	2.07	1.57	1.53
14	N	601	HEA	C4B-C3B	-2.07	1.41	1.44
14	A	602[A]	HEA	C24-C23	2.07	1.55	1.50
22	P	301	CHD	C16-C17	2.06	1.58	1.54
25	Z	101	DMU	C2-C1	2.06	1.57	1.52
14	A	602[A]	HEA	C18-C19	2.06	1.37	1.33
22	B	301	CHD	O3-C3	2.06	1.49	1.43
14	N	602[A]	HEA	C12-C13	2.06	1.60	1.53
27	T	103	CDL	PB2-OB5	2.05	1.67	1.59
22	C	306	CHD	O25-C24	2.05	1.29	1.22
14	N	602[B]	HEA	C14-C15	2.05	1.37	1.33
22	C	306	CHD	C4-C3	2.05	1.55	1.51
22	G	103	CHD	C11-C12	2.04	1.56	1.53
28	P	308	PEK	C22-C21	2.04	1.56	1.50
14	N	602[A]	HEA	C1C-CHC	2.04	1.46	1.41
14	N	601	HEA	C27-C19	2.04	1.55	1.50
27	G	102	CDL	PB2-OB5	2.03	1.67	1.59
22	P	306	CHD	C1-C10	2.03	1.57	1.54
14	A	601	HEA	C4D-C3D	-2.03	1.41	1.45
14	N	601	HEA	C3A-C2A	-2.03	1.37	1.40
25	Z	101	DMU	O1-C10	2.02	1.47	1.41
22	B	301	CHD	C13-C17	-2.02	1.52	1.55
14	A	601	HEA	O1A-CGA	2.02	1.28	1.22
14	N	601	HEA	CBD-CGD	2.02	1.55	1.50
14	A	602[A]	HEA	CMB-C2B	2.01	1.55	1.50
14	N	601	HEA	C18-C19	-2.01	1.28	1.33
14	A	602[B]	HEA	C14-C15	2.01	1.37	1.33
22	J	101	CHD	C21-C20	2.00	1.58	1.53
22	B	301	CHD	O12-C12	2.00	1.46	1.43

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	201	TGL	OG2-CB1-CB2	-13.46	82.48	111.50
19	D	201	TGL	OG2-CB1-OB1	12.52	153.95	123.70
22	C	306	CHD	C23-C22-C20	-12.09	92.43	114.52
22	W	101	CHD	C17-C13-C12	11.12	127.81	117.67
20	A	610	PGV	O01-C1-O02	10.68	149.52	123.70
22	W	101	CHD	C13-C17-C20	10.51	132.04	119.50
19	L	101	TGL	OG2-CB1-CB2	10.37	133.86	111.50
25	C	310	DMU	C18-O16-C6	10.24	130.83	113.84
20	A	610	PGV	O01-C1-C2	-9.55	90.92	111.50
25	C	310	DMU	O16-C6-C1	8.90	122.19	108.30
22	P	306	CHD	C18-C13-C12	-8.89	100.02	109.07
22	J	101	CHD	C13-C17-C20	8.84	130.04	119.50
22	J	101	CHD	C17-C13-C12	8.65	125.56	117.67
22	W	101	CHD	C11-C12-C13	8.60	120.07	111.24
22	W	101	CHD	C18-C13-C12	-8.51	100.40	109.07
22	C	306	CHD	C6-C7-C8	8.09	120.11	111.48
19	Y	101	TGL	OG2-CB1-CB2	7.91	128.56	111.50
24	B	303	PSC	O01-C1-C2	7.87	128.47	111.50
25	C	310	DMU	O7-C10-C5	7.85	128.44	108.10
25	C	309	DMU	C10-O1-C9	-7.61	98.76	113.69
22	J	101	CHD	C15-C14-C8	7.58	128.92	118.33
19	L	101	TGL	CG2-OG2-CB1	7.56	136.41	117.79
14	N	601	HEA	C13-C14-C15	-7.52	109.55	127.66
28	T	101	PEK	O01-C1-C2	7.52	127.70	111.50
24	B	303	PSC	C02-O01-C1	-7.23	99.99	117.79
14	A	601	HEA	C20-C19-C18	7.09	135.47	121.12
22	P	306	CHD	C6-C7-C8	7.07	119.02	111.48
14	N	601	HEA	C1D-ND-C4D	-7.05	97.80	105.07
20	A	610	PGV	C02-O01-C1	7.03	135.11	117.79
22	J	101	CHD	C14-C8-C7	6.95	121.03	111.81
19	D	201	TGL	CB3-CB2-CB1	6.89	138.68	113.62
22	C	306	CHD	C21-C20-C17	6.88	123.45	112.92
19	A	608	TGL	OG2-CG2-CG3	6.86	133.26	108.40
27	G	102	CDL	OB6-CB5-C51	6.83	126.23	111.50
19	Y	101	TGL	CG2-OG2-CB1	6.62	134.10	117.79
25	C	309	DMU	O7-C10-C5	6.60	125.21	108.10
22	J	101	CHD	C10-C9-C8	6.58	118.89	111.82
19	L	101	TGL	CC4-CC3-CC2	-6.50	89.83	113.19
24	O	302	PSC	O01-C1-C2	6.45	125.41	111.50
25	C	309	DMU	O16-C6-C1	6.45	118.38	108.30
22	P	301	CHD	C6-C7-C8	-6.44	104.61	111.48
25	C	309	DMU	C10-C5-C7	-6.36	96.75	110.00
22	C	301	CHD	C18-C13-C12	6.31	115.49	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	301	CHD	C17-C13-C12	6.27	123.39	117.67
19	N	609	TGL	OG2-CB1-CB2	6.21	124.89	111.50
14	N	601	HEA	C26-C15-C16	-6.19	104.85	115.27
27	T	103	CDL	OA6-CA5-C11	6.17	124.80	111.50
25	P	309	DMU	C10-O1-C9	-6.13	101.66	113.69
24	B	303	PSC	C03-C02-C01	-6.12	97.30	111.79
22	P	306	CHD	C15-C14-C8	6.10	126.85	118.33
19	A	608	TGL	OG2-CB1-CB2	6.09	124.62	111.50
25	C	310	DMU	O3-C5-C10	6.08	124.82	110.05
25	P	309	DMU	O16-C6-C1	6.07	117.78	108.30
14	A	602[B]	HEA	CMB-C2B-C1B	6.05	134.26	125.04
22	B	301	CHD	C11-C9-C10	-6.01	107.52	113.73
20	P	302	PGV	O03-C19-C20	6.01	130.78	111.91
22	W	101	CHD	C14-C8-C7	5.87	119.60	111.81
20	A	610	PGV	C3-C2-C1	5.86	134.95	113.62
22	P	306	CHD	C19-C10-C9	-5.86	103.11	111.18
19	L	101	TGL	OG3-CC1-CC2	5.85	130.25	111.91
14	N	601	HEA	C3D-C4D-ND	5.84	116.02	110.36
22	C	306	CHD	C14-C13-C12	5.84	112.84	107.40
22	G	103	CHD	C1-C10-C9	5.82	120.51	111.35
14	A	601	HEA	C4B-NB-C1B	-5.81	99.07	105.07
20	C	308	PGV	O01-C1-C2	5.75	123.89	111.50
14	A	601	HEA	C13-C14-C15	-5.64	114.08	127.66
14	A	601	HEA	C27-C19-C20	-5.59	105.87	115.27
22	W	101	CHD	C17-C13-C14	-5.57	94.47	100.09
14	A	601	HEA	C2B-C1B-NB	5.56	116.54	109.88
22	P	301	CHD	C21-C20-C22	-5.56	101.65	110.36
25	P	310	DMU	O16-C6-C1	5.54	116.96	108.30
14	A	601	HEA	C2D-C1D-ND	5.52	116.37	109.84
27	G	102	CDL	CB4-OB6-CB5	5.50	131.33	117.79
14	N	602[A]	HEA	CAD-CBD-CGD	-5.48	101.80	113.60
14	N	601	HEA	C2D-C1D-ND	5.46	116.31	109.84
19	N	609	TGL	OG1-CA1-CA2	5.43	128.96	111.91
20	X	101	PGV	C02-O01-C1	-5.41	104.48	117.79
22	P	306	CHD	C16-C17-C13	5.39	108.84	103.55
14	N	602[A]	HEA	C26-C15-C16	5.37	124.31	115.27
22	B	301	CHD	C16-C17-C20	-5.35	103.87	112.15
25	P	309	DMU	C18-O16-C6	-5.33	105.00	113.84
28	P	308	PEK	O01-C1-C2	5.33	122.98	111.50
14	A	602[A]	HEA	CMC-C2C-C3C	5.32	134.64	124.68
14	A	602[B]	HEA	C20-C19-C18	-5.31	110.37	121.12
19	N	609	TGL	OG3-CC1-OC1	-5.29	110.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C3D-C4D-ND	5.28	115.47	110.36
22	P	301	CHD	C22-C20-C17	-5.24	99.45	110.28
22	B	301	CHD	C16-C17-C13	5.24	108.69	103.55
14	N	602[B]	HEA	C3D-C4D-ND	5.17	115.37	110.36
20	C	308	PGV	O03-C19-C20	5.12	127.98	111.91
27	T	103	CDL	OB6-CB5-C51	5.09	122.46	111.50
22	J	101	CHD	C11-C12-C13	5.07	116.45	111.24
19	N	609	TGL	CG3-CG2-CG1	-5.06	99.82	111.79
19	Y	101	TGL	OG3-CC1-CC2	5.06	127.77	111.91
20	A	610	PGV	C03-C02-C01	-5.02	99.92	111.79
22	J	101	CHD	C14-C8-C9	-5.01	102.83	109.71
19	Y	101	TGL	OG3-CG3-CG2	5.00	122.98	108.43
14	N	602[A]	HEA	CBA-CAA-C2A	-4.98	104.20	112.60
25	C	302	DMU	C22-C19-C18	-4.98	91.42	113.49
22	P	306	CHD	C5-C4-C3	-4.98	105.44	112.76
14	A	602[A]	HEA	CAD-CBD-CGD	-4.98	102.89	113.60
14	N	602[B]	HEA	C13-C12-C11	-4.97	106.88	114.35
22	C	306	CHD	C17-C13-C12	-4.96	113.14	117.67
28	T	101	PEK	C2-C3-C4	4.95	122.06	113.23
28	C	307	PEK	O01-C1-C2	4.94	122.14	111.50
22	W	101	CHD	C9-C11-C12	4.91	120.79	114.30
22	C	306	CHD	C13-C17-C20	-4.90	113.64	119.50
14	A	601	HEA	C1D-ND-C4D	-4.90	100.01	105.07
14	A	602[B]	HEA	C27-C19-C20	4.89	123.50	115.27
20	N	608	PGV	O01-C1-O02	-4.88	111.90	123.70
19	N	609	TGL	OG2-CB1-OB1	-4.88	111.91	123.70
14	A	602[B]	HEA	CMB-C2B-C3B	-4.85	121.09	130.34
22	G	103	CHD	C16-C17-C20	-4.84	104.65	112.15
27	C	305	CDL	OA6-CA5-C11	4.80	121.85	111.50
25	P	309	DMU	O7-C10-C5	4.80	120.53	108.10
27	T	103	CDL	OB8-CB6-CB4	4.75	122.26	108.43
27	P	305	CDL	OA6-CA5-C11	4.75	121.73	111.50
22	G	103	CHD	C11-C9-C10	-4.74	108.84	113.73
27	P	305	CDL	OB8-CB7-C71	4.72	126.72	111.91
25	L	102	DMU	O5-C4-C3	4.72	119.70	109.75
19	D	201	TGL	CG1-OG1-CA1	4.71	134.56	117.12
27	P	305	CDL	OA8-CA7-C31	4.70	126.66	111.91
22	C	306	CHD	O7-C7-C6	-4.69	98.31	109.94
22	C	301	CHD	C23-C22-C20	-4.65	106.03	114.52
22	J	101	CHD	C1-C10-C5	4.63	114.62	107.77
22	G	103	CHD	C21-C20-C17	-4.60	105.87	112.92
27	P	305	CDL	OA8-CA6-CA4	4.59	121.81	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C2B-C1B-NB	4.57	115.36	109.88
27	G	102	CDL	CB6-OB8-CB7	4.55	133.98	117.12
25	C	302	DMU	C18-O16-C6	4.54	121.36	113.84
22	C	301	CHD	C1-C10-C5	4.53	114.47	107.77
22	W	101	CHD	C14-C13-C12	4.52	111.61	107.40
22	G	103	CHD	C10-C9-C8	4.52	116.67	111.82
19	N	609	TGL	OG1-CA1-OA1	-4.51	112.20	123.59
22	P	301	CHD	C23-C22-C20	-4.50	106.30	114.52
14	A	602[B]	HEA	C13-C12-C11	-4.49	107.60	114.35
28	G	104	PEK	O03-C21-C22	4.47	125.93	111.91
27	C	305	CDL	OA8-CA7-C31	4.46	125.90	111.91
14	A	602[A]	HEA	C26-C15-C16	4.46	122.77	115.27
22	C	306	CHD	C16-C17-C20	4.42	118.99	112.15
19	A	608	TGL	OG3-CC1-OC1	-4.42	112.44	123.59
22	C	306	CHD	C4-C5-C10	4.41	117.34	112.66
22	C	301	CHD	C1-C2-C3	-4.41	104.81	110.47
19	A	608	TGL	OG3-CG3-CG2	4.40	121.25	108.43
19	A	608	TGL	CG3-OG3-CC1	4.39	133.38	117.12
22	W	101	CHD	C4-C5-C10	4.39	117.31	112.66
28	G	104	PEK	O03-C01-C02	4.38	121.19	108.43
14	A	602[A]	HEA	C4D-CHA-C1A	4.37	128.33	122.56
22	P	301	CHD	C1-C10-C5	4.37	114.22	107.77
22	C	301	CHD	C22-C20-C17	-4.35	101.30	110.28
20	P	304	PGV	C03-C02-C01	-4.34	101.52	111.79
14	A	601	HEA	CBA-CAA-C2A	-4.34	105.29	112.60
28	G	104	PEK	O01-C1-C2	4.33	120.84	111.50
14	A	602[A]	HEA	OMA-CMA-C3A	-4.33	115.47	124.91
28	T	102	PEK	C8-C7-C6	4.29	133.17	112.02
22	G	103	CHD	C18-C13-C12	-4.29	104.70	109.07
19	D	201	TGL	OG1-CA1-CA2	4.26	125.26	111.91
28	G	104	PEK	C02-O01-C1	4.23	128.21	117.79
25	C	310	DMU	C8-C7-C5	-4.22	103.45	110.82
22	P	306	CHD	C1-C10-C9	4.22	117.98	111.35
27	C	305	CDL	OA8-CA6-CA4	4.22	120.70	108.43
22	G	103	CHD	C2-C1-C10	-4.21	105.57	112.78
20	N	608	PGV	O02-C1-C2	4.21	140.14	123.73
14	N	601	HEA	C4B-NB-C1B	-4.21	100.73	105.07
27	C	305	CDL	OB8-CB7-C71	4.20	125.07	111.91
19	D	201	TGL	OC1-CC1-CC2	4.19	140.08	123.73
14	N	601	HEA	C27-C19-C18	-4.17	112.98	123.68
28	T	102	PEK	O03-C21-C22	4.15	124.94	111.91
25	P	309	DMU	C10-C5-C7	-4.15	101.35	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	101	TGL	OG1-CA1-CA2	4.14	124.91	111.91
27	G	102	CDL	OA6-CA5-C11	4.13	120.41	111.50
19	L	101	TGL	OG3-CC1-OC1	-4.11	113.22	123.59
25	P	309	DMU	O49-C1-C2	-4.11	100.85	110.35
14	A	602[B]	HEA	C2B-C1B-NB	4.10	114.79	109.88
27	G	102	CDL	OB8-CB7-C71	4.09	124.74	111.91
25	C	310	DMU	O16-C18-C19	4.09	123.89	109.56
14	N	602[A]	HEA	OMA-CMA-C3A	-4.07	116.04	124.91
19	L	101	TGL	CB3-CB2-CB1	4.07	128.42	113.62
14	N	602[B]	HEA	CMB-C2B-C3B	-4.05	122.62	130.34
22	P	301	CHD	C14-C13-C12	4.04	111.17	107.40
19	Q	201	TGL	OG3-CC1-OC1	-4.04	113.39	123.59
19	Q	201	TGL	OG2-CB1-CB2	-4.04	102.79	111.50
22	P	306	CHD	O7-C7-C6	-4.04	99.92	109.94
25	C	309	DMU	C8-C7-C5	-4.02	103.81	110.82
14	N	601	HEA	C27-C19-C20	4.01	122.02	115.27
19	D	201	TGL	CG3-OG3-CC1	3.99	131.91	117.12
19	L	101	TGL	C20-CA9-CA8	-3.99	94.15	114.42
28	C	307	PEK	O03-C21-C22	3.96	124.35	111.91
25	L	102	DMU	O7-C3-C2	3.95	117.79	107.28
19	L	101	TGL	OG2-CB1-OB1	-3.95	114.16	123.70
22	B	301	CHD	O26-C24-O25	-3.92	113.52	123.30
28	G	101	PEK	C02-O01-C1	-3.92	108.14	117.79
19	Q	201	TGL	OG3-CC1-CC2	3.90	124.16	111.91
14	A	601	HEA	C4A-CHB-C1B	3.89	127.70	122.56
20	C	308	PGV	C02-O01-C1	3.89	127.37	117.79
22	C	301	CHD	C9-C11-C12	-3.88	109.18	114.30
19	N	609	TGL	CG3-OG3-CC1	3.87	131.44	117.12
22	C	306	CHD	C22-C23-C24	-3.87	102.25	112.51
20	X	101	PGV	C01-O03-C19	3.86	131.43	117.12
27	C	305	CDL	OA2-PA1-OA3	3.86	124.16	109.07
19	A	608	TGL	OG3-CC1-CC2	3.86	124.01	111.91
28	C	307	PEK	O03-C21-O04	-3.85	113.87	123.59
14	N	602[A]	HEA	O2A-CGA-CBA	3.85	126.41	114.03
14	A	601	HEA	C13-C12-C11	-3.85	108.57	114.35
22	P	301	CHD	C5-C6-C7	3.85	118.70	114.46
19	D	201	TGL	CG3-CG2-CG1	3.83	120.85	111.79
22	B	301	CHD	O12-C12-C13	-3.83	104.55	111.03
19	L	101	TGL	C25-C24-C23	-3.81	95.07	114.42
14	N	602[B]	HEA	C20-C19-C18	-3.81	113.40	121.12
14	N	601	HEA	OMA-CMA-C3A	-3.81	116.61	124.91
22	C	306	CHD	C5-C6-C7	3.80	118.65	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	303	PSC	O01-C02-C01	3.79	122.13	108.40
27	T	103	CDL	CA4-OA6-CA5	3.79	127.12	117.79
14	A	602[B]	HEA	C4B-NB-C1B	-3.79	101.16	105.07
14	A	601	HEA	CHA-C4D-C3D	-3.78	119.29	124.84
19	L	101	TGL	C26-C25-C24	-3.77	95.28	114.42
22	W	101	CHD	C19-C10-C5	-3.76	103.99	110.36
22	C	301	CHD	C4-C5-C10	-3.75	108.67	112.66
25	P	309	DMU	O5-C4-C57	3.73	115.71	106.44
25	P	307	DMU	C6-O5-C4	3.72	121.00	113.69
14	A	602[A]	HEA	CHC-C4B-NB	3.72	128.98	124.38
20	A	610	PGV	O05-C05-C06	3.71	125.46	109.12
19	N	609	TGL	OG3-CC1-CC2	3.71	123.55	111.91
22	C	301	CHD	C2-C1-C10	3.69	119.12	112.78
22	C	306	CHD	C15-C14-C8	3.69	123.50	118.33
22	C	306	CHD	C11-C9-C8	3.68	116.26	110.88
22	P	306	CHD	C15-C14-C13	3.67	107.16	103.55
14	N	601	HEA	C16-C15-C14	3.67	128.55	121.12
14	A	602[A]	HEA	C20-C19-C18	-3.65	113.72	121.12
20	A	609	PGV	O01-C1-O02	-3.65	114.88	123.70
24	B	303	PSC	O01-C02-C03	3.65	121.62	108.40
14	A	601	HEA	C1B-C2B-C3B	-3.65	102.44	106.80
22	G	103	CHD	C14-C13-C12	3.64	110.79	107.40
19	D	201	TGL	OG3-CC1-OC1	-3.64	114.40	123.59
22	W	101	CHD	C11-C9-C10	3.63	117.47	113.73
22	W	101	CHD	C5-C6-C7	-3.61	110.48	114.46
25	P	307	DMU	O16-C18-C19	3.60	122.17	109.56
22	P	301	CHD	C5-C4-C3	-3.59	107.48	112.76
14	A	602[A]	HEA	C13-C12-C11	-3.58	108.98	114.35
22	B	301	CHD	C19-C10-C1	-3.56	102.52	108.26
14	N	601	HEA	C4A-CHB-C1B	3.53	127.22	122.56
22	B	301	CHD	C10-C9-C8	3.53	115.61	111.82
14	A	602[B]	HEA	O1A-CGA-CBA	-3.51	111.79	123.08
25	C	302	DMU	O55-C2-C3	3.51	119.24	109.94
28	P	308	PEK	O03-C21-O04	-3.50	114.77	123.59
19	Y	101	TGL	CC4-CC3-CC2	-3.49	100.65	113.19
27	G	102	CDL	OA8-CA7-C31	3.48	122.84	111.91
22	J	101	CHD	C4-C5-C10	3.47	116.34	112.66
20	P	302	PGV	O04-C19-C20	-3.47	110.19	123.73
20	X	101	PGV	O03-C19-C20	3.47	122.79	111.91
22	C	301	CHD	C22-C23-C24	-3.46	103.32	112.51
19	Y	101	TGL	OG2-CG2-CG3	3.45	120.91	108.40
22	C	306	CHD	C1-C10-C5	3.45	112.87	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	103	CDL	OA8-CA7-C31	3.44	122.71	111.91
25	C	310	DMU	O7-C3-C4	3.44	118.87	109.45
22	G	103	CHD	O12-C12-C11	-3.43	102.14	109.12
22	B	301	CHD	C1-C10-C9	3.42	116.73	111.35
19	Q	201	TGL	CB3-CB2-CB1	3.42	126.04	113.62
22	P	306	CHD	C14-C13-C12	3.41	110.58	107.40
22	C	301	CHD	C11-C9-C10	-3.41	110.21	113.73
14	N	602[B]	HEA	CMB-C2B-C1B	3.40	130.22	125.04
22	J	101	CHD	C22-C20-C17	3.40	117.31	110.28
14	A	601	HEA	C16-C17-C18	-3.39	100.73	111.88
25	C	310	DMU	O5-C4-C3	3.38	116.88	109.75
24	O	302	PSC	C02-O01-C1	3.38	126.11	117.79
20	P	302	PGV	O01-C1-C2	3.37	118.77	111.50
14	N	601	HEA	C1B-C2B-C3B	-3.37	102.77	106.80
24	B	303	PSC	O03-C19-C20	3.37	122.48	111.91
19	L	101	TGL	CG3-OG3-CC1	3.37	129.60	117.12
27	C	305	CDL	PA1-OA2-CA2	3.36	141.40	121.68
14	N	602[B]	HEA	C27-C19-C20	3.36	120.93	115.27
22	P	301	CHD	C11-C9-C10	-3.36	110.27	113.73
20	N	608	PGV	O03-C19-O04	-3.35	115.15	123.59
20	A	610	PGV	O03-C19-C20	3.35	122.41	111.91
22	B	301	CHD	C18-C13-C12	-3.34	105.67	109.07
14	A	601	HEA	CHD-C1D-C2D	-3.33	117.51	126.72
28	P	308	PEK	O03-C21-C22	3.32	122.34	111.91
19	A	608	TGL	CC3-CC2-CC1	-3.32	101.55	113.62
22	J	101	CHD	C9-C8-C7	3.31	115.83	111.88
22	P	306	CHD	C16-C17-C20	3.29	117.24	112.15
14	A	602[A]	HEA	CMC-C2C-C1C	-3.28	123.42	128.46
20	X	101	PGV	O03-C01-C02	3.28	117.97	108.43
19	Q	201	TGL	OG2-CB1-OB1	3.28	131.62	123.70
27	G	102	CDL	OB8-CB7-OB9	-3.27	115.34	123.59
27	C	305	CDL	OA5-PA1-OA3	-3.26	96.33	109.07
22	C	301	CHD	C6-C7-C8	-3.26	108.01	111.48
27	G	102	CDL	C80-C79-C78	3.25	130.94	114.42
27	C	305	CDL	C83-C82-C81	3.25	130.93	114.42
24	B	303	PSC	O01-C1-O02	-3.24	115.87	123.70
20	P	304	PGV	O01-C1-O02	-3.24	115.87	123.70
19	L	101	TGL	OG1-CG1-CG2	3.23	117.85	108.43
19	A	608	TGL	OG2-CB1-OB1	-3.23	115.89	123.70
14	A	602[B]	HEA	CAA-CBA-CGA	-3.23	104.71	113.76
20	N	608	PGV	C3-C2-C1	-3.22	101.89	113.62
25	P	307	DMU	C22-C19-C18	-3.22	99.24	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	103	CDL	OA6-CA5-OA7	-3.22	115.93	123.70
19	L	101	TGL	OB1-CB1-CB2	-3.20	111.24	123.73
25	M	101	DMU	C18-O16-C6	-3.19	108.55	113.84
22	B	301	CHD	C2-C1-C10	-3.18	107.33	112.78
22	J	101	CHD	C1-C10-C9	-3.17	106.36	111.35
27	P	305	CDL	OB6-CB5-C51	3.17	118.33	111.50
21	A	616	EDO	O2-C2-C1	-3.16	89.15	111.91
20	X	101	PGV	C3-C2-C1	-3.16	102.14	113.62
27	T	103	CDL	CB6-OB8-CB7	3.15	128.77	117.12
14	N	601	HEA	CHA-C4D-ND	-3.14	121.02	124.43
14	A	601	HEA	C1D-C2D-C3D	-3.14	103.65	106.96
24	O	302	PSC	O03-C19-C20	3.13	121.72	111.91
14	N	602[B]	HEA	CHA-C4D-ND	-3.13	121.03	124.43
14	A	602[A]	HEA	CBA-CAA-C2A	-3.13	107.34	112.60
14	A	601	HEA	C3C-C4C-NC	3.12	113.25	109.21
28	C	307	PEK	C36-C35-C34	-3.11	98.64	114.42
22	W	101	CHD	C21-C20-C22	3.11	115.23	110.36
14	N	601	HEA	C20-C21-C22	-3.11	101.68	111.88
14	A	602[B]	HEA	C3B-C4B-NB	3.10	113.51	109.84
25	M	101	DMU	C22-C19-C18	-3.10	99.75	113.49
19	D	201	TGL	OG1-CG1-CG2	-3.10	99.42	108.43
25	Z	101	DMU	C6-O5-C4	3.10	119.77	113.69
14	A	602[B]	HEA	CHA-C4D-C3D	-3.09	120.29	124.84
24	O	302	PSC	O01-C1-O02	-3.08	116.26	123.70
22	C	301	CHD	C17-C13-C12	-3.08	114.86	117.67
22	W	101	CHD	C4-C3-C2	3.07	114.22	110.55
14	A	601	HEA	CAD-CBD-CGD	-3.07	106.99	113.60
27	P	305	CDL	C52-C51-CB5	-3.07	102.47	113.62
22	W	101	CHD	C6-C5-C4	-3.06	107.66	111.19
25	C	309	DMU	O2-C8-C7	3.04	117.37	110.35
25	M	101	DMU	O5-C4-C3	-3.03	103.36	109.75
27	T	103	CDL	OA6-CA4-CA3	3.03	119.36	108.40
14	A	601	HEA	C26-C15-C16	-3.02	110.19	115.27
22	P	301	CHD	C14-C8-C7	-3.02	107.80	111.81
22	B	301	CHD	C21-C20-C17	-3.02	108.30	112.92
19	Q	201	TGL	CG2-OG2-CB1	-3.01	110.37	117.79
22	G	103	CHD	C19-C10-C1	-3.01	103.41	108.26
22	B	301	CHD	C19-C10-C5	-3.01	105.26	110.36
14	A	602[B]	HEA	C17-C18-C19	-3.00	120.44	127.66
22	C	301	CHD	C1-C10-C9	-3.00	106.64	111.35
27	P	305	CDL	C54-C53-C52	-2.99	99.23	114.42
14	A	601	HEA	CHB-C1B-NB	-2.99	121.18	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[A]	HEA	C26-C15-C14	-2.99	116.02	123.68
14	A	602[B]	HEA	CAD-CBD-CGD	-2.98	107.18	113.60
22	J	101	CHD	O26-C24-C23	2.98	123.61	114.03
25	C	309	DMU	O1-C9-C8	-2.97	104.30	109.69
25	C	310	DMU	O5-C6-O16	2.97	117.01	109.97
24	B	303	PSC	O03-C01-C02	2.96	117.05	108.43
22	J	101	CHD	C14-C13-C12	-2.96	104.65	107.40
19	Y	101	TGL	CG3-OG3-CC1	2.96	128.07	117.12
28	C	307	PEK	O03-C01-C02	2.95	117.01	108.43
20	N	608	PGV	C4-C3-C2	-2.94	102.61	113.19
22	J	101	CHD	C22-C23-C24	2.94	120.30	112.51
25	C	309	DMU	O55-C2-C1	2.93	117.13	110.35
19	A	608	TGL	CG1-OG1-CA1	2.93	127.97	117.12
22	G	103	CHD	O26-C24-O25	-2.93	116.01	123.30
27	P	305	CDL	OB2-PB2-OB3	2.92	120.47	109.07
14	N	601	HEA	CHD-C1D-C2D	-2.92	118.65	126.72
20	X	101	PGV	O01-C1-C2	2.92	117.79	111.50
25	P	310	DMU	O3-C5-C7	-2.90	103.65	110.35
27	T	103	CDL	C44-C43-C42	2.90	129.12	114.42
22	C	306	CHD	O26-C24-O25	2.90	130.51	123.30
25	P	309	DMU	O7-C3-C4	-2.89	101.52	109.45
14	N	602[A]	HEA	O2A-CGA-O1A	-2.89	116.09	123.30
22	B	301	CHD	O3-C3-C4	-2.89	104.10	109.85
28	G	101	PEK	C24-C23-C22	-2.89	102.81	113.19
22	C	301	CHD	C13-C17-C20	-2.88	116.05	119.50
22	C	306	CHD	C19-C10-C9	-2.88	107.21	111.18
25	C	310	DMU	C10-C5-C7	2.88	115.99	110.00
14	A	602[B]	HEA	CBA-CAA-C2A	-2.87	107.76	112.60
22	J	101	CHD	C18-C13-C12	-2.87	106.14	109.07
20	C	304	PGV	C30-C29-C28	-2.86	99.88	114.42
28	C	307	PEK	C01-O03-C21	2.86	127.73	117.12
25	L	102	DMU	C1-C2-C3	2.86	116.22	109.68
22	P	306	CHD	C11-C9-C8	2.86	115.06	110.88
14	A	601	HEA	CMB-C2B-C3B	2.85	135.78	130.34
27	P	305	CDL	OB8-CB7-OB9	-2.85	116.39	123.59
28	T	101	PEK	C01-O03-C21	2.85	127.68	117.12
20	X	101	PGV	C6-C5-C4	-2.85	99.96	114.42
14	A	602[B]	HEA	C12-C13-C14	-2.85	104.71	112.23
28	T	101	PEK	O01-C1-O02	-2.84	116.83	123.70
14	N	602[B]	HEA	C4D-CHA-C1A	2.84	126.31	122.56
14	N	602[A]	HEA	CHA-C4D-C3D	-2.83	120.67	124.84
27	G	102	CDL	OA8-CA7-OA9	-2.83	116.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Z	101	DMU	C18-O16-C6	-2.83	109.14	113.84
25	C	310	DMU	C10-O1-C9	2.83	119.25	113.69
19	Y	101	TGL	C26-C25-C24	-2.83	100.04	114.42
24	O	302	PSC	C28-C27-C26	-2.83	100.05	114.42
14	N	601	HEA	O2A-CGA-CBA	2.83	123.12	114.03
22	W	101	CHD	C13-C14-C8	2.83	118.35	114.74
19	A	608	TGL	CG3-CG2-CG1	-2.83	105.11	111.79
19	Q	201	TGL	OG1-CA1-CA2	2.81	120.74	111.91
22	B	301	CHD	C4-C3-C2	2.81	113.91	110.55
22	P	306	CHD	C6-C5-C10	2.81	115.64	112.66
25	C	310	DMU	O7-C3-C2	2.81	114.75	107.28
25	P	310	DMU	C18-O16-C6	2.81	118.49	113.84
19	Y	101	TGL	CA4-CA3-CA2	-2.79	103.15	113.19
27	C	305	CDL	C57-C56-C55	-2.79	100.28	114.42
20	C	304	PGV	C23-C22-C21	2.78	128.56	114.42
25	Z	101	DMU	C10-O7-C3	-2.78	111.08	117.96
27	T	103	CDL	OB8-CB7-C71	2.78	120.62	111.91
20	A	610	PGV	C4-C3-C2	-2.77	103.22	113.19
22	C	306	CHD	C15-C14-C13	2.77	106.27	103.55
22	C	306	CHD	C14-C8-C9	-2.77	105.91	109.71
22	W	101	CHD	C15-C14-C8	2.76	122.19	118.33
25	L	102	DMU	C57-C4-C3	-2.76	105.29	113.33
22	C	306	CHD	C4-C3-C2	2.76	113.84	110.55
22	P	301	CHD	C10-C9-C8	-2.75	108.87	111.82
22	B	301	CHD	C23-C22-C20	-2.75	109.50	114.52
22	B	301	CHD	C9-C8-C7	-2.75	108.59	111.88
22	J	101	CHD	C6-C5-C4	-2.74	108.03	111.19
20	N	608	PGV	O03-C19-C20	2.74	120.51	111.91
22	B	301	CHD	C22-C23-C24	-2.74	105.23	112.51
25	C	309	DMU	O3-C5-C10	2.74	116.70	110.05
14	A	602[A]	HEA	C16-C15-C14	-2.73	115.59	121.12
25	C	309	DMU	O4-C7-C8	2.73	116.66	110.35
19	N	609	TGL	CC3-CC2-CC1	2.73	123.54	113.62
20	C	304	PGV	C25-C24-C23	2.73	128.28	114.42
28	T	101	PEK	C02-O01-C1	2.73	124.50	117.79
22	J	101	CHD	O26-C24-O25	-2.72	116.51	123.30
22	W	101	CHD	C22-C20-C17	2.72	115.91	110.28
19	D	201	TGL	C22-C21-C20	2.72	128.23	114.42
24	B	303	PSC	C4-C3-C2	2.72	122.96	113.19
27	C	305	CDL	OA6-CA5-OA7	-2.71	117.15	123.70
19	Y	101	TGL	OB1-CB1-CB2	-2.71	113.17	123.73
27	G	102	CDL	C82-C81-C80	2.70	128.15	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	304	PGV	O03-C19-O04	-2.70	116.78	123.59
19	Q	201	TGL	OG1-CA1-OA1	-2.69	116.79	123.59
22	W	101	CHD	C16-C17-C20	-2.69	107.98	112.15
22	P	306	CHD	C17-C13-C12	2.69	120.12	117.67
25	L	102	DMU	C10-O1-C9	2.69	118.96	113.69
22	B	301	CHD	C1-C2-C3	-2.67	107.04	110.47
14	N	602[B]	HEA	CMC-C2C-C3C	2.67	129.67	124.68
21	P	312	EDO	O2-C2-C1	2.66	131.05	111.91
25	C	310	DMU	O3-C5-C7	2.66	116.49	110.35
27	C	305	CDL	OB4-PB2-OB5	-2.66	95.41	107.75
25	C	309	DMU	O7-C10-O1	2.65	118.08	110.67
20	C	308	PGV	O04-C19-C20	-2.65	113.39	123.73
14	N	602[A]	HEA	CHA-C4D-ND	2.65	127.31	124.43
14	A	602[A]	HEA	CHB-C1B-C2B	-2.65	120.84	124.98
25	L	102	DMU	O1-C9-C11	2.64	113.00	106.44
20	A	610	PGV	C01-O03-C19	2.63	126.88	117.12
19	Y	101	TGL	CG3-CG2-CG1	-2.63	105.56	111.79
19	Y	101	TGL	OG3-CC1-OC1	-2.63	116.95	123.59
25	L	102	DMU	O49-C1-C2	-2.63	104.28	110.35
19	D	201	TGL	CB4-CB3-CB2	-2.62	103.75	113.19
27	C	305	CDL	C39-C38-C37	2.62	127.72	114.42
27	G	102	CDL	C60-C59-C58	2.61	127.69	114.42
14	A	601	HEA	CBD-CAD-C3D	-2.61	105.37	112.63
20	A	609	PGV	C30-C29-C28	2.61	127.66	114.42
22	P	306	CHD	C14-C8-C9	-2.61	106.14	109.71
28	C	307	PEK	C24-C23-C22	2.60	122.55	113.19
14	N	601	HEA	C3B-C4B-NB	2.60	112.92	109.84
19	Y	101	TGL	OG1-CA1-CA2	2.59	120.05	111.91
19	L	101	TGL	OG2-CG2-CG3	2.59	117.79	108.40
27	C	305	CDL	CB6-CB4-CB3	-2.59	105.66	111.79
19	L	101	TGL	OG3-CG3-CG2	2.59	115.97	108.43
28	G	101	PEK	C25-C24-C23	-2.58	101.33	114.42
14	N	601	HEA	CHB-C1B-NB	-2.58	121.63	124.43
20	A	609	PGV	C34-C33-C32	-2.58	93.87	113.42
19	N	609	TGL	OG1-CG1-CG2	2.58	115.93	108.43
27	G	102	CDL	C23-C22-C21	2.57	127.48	114.42
14	A	602[B]	HEA	O2A-CGA-O1A	2.57	129.71	123.30
22	W	101	CHD	O12-C12-C13	2.56	115.36	111.03
14	A	601	HEA	C27-C19-C18	-2.55	117.14	123.68
20	C	308	PGV	C22-C21-C20	-2.54	104.05	113.19
24	O	302	PSC	O04-C19-C20	-2.54	113.83	123.73
22	P	301	CHD	C16-C17-C20	-2.54	108.22	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[B]	HEA	CAA-CBA-CGA	-2.52	106.71	113.76
27	P	305	CDL	OB7-CB5-C51	-2.51	113.93	123.73
25	C	310	DMU	C2-C3-C4	-2.51	105.17	110.93
14	A	602[A]	HEA	C27-C19-C20	2.51	119.49	115.27
14	N	602[B]	HEA	CMC-C2C-C1C	-2.51	124.61	128.46
22	C	301	CHD	C5-C6-C7	2.50	117.22	114.46
19	Y	101	TGL	CC3-CC2-CC1	2.49	122.69	113.62
22	W	101	CHD	C9-C10-C5	2.48	112.06	108.58
14	N	602[A]	HEA	CMC-C2C-C3C	2.48	129.32	124.68
27	C	305	CDL	OA8-CA7-OA9	-2.48	117.33	123.59
25	P	309	DMU	C7-C8-C9	2.48	114.66	110.24
14	A	602[A]	HEA	C2B-C1B-NB	2.48	112.85	109.88
27	C	305	CDL	C54-C53-C52	-2.47	101.86	114.42
14	N	602[B]	HEA	C4D-C3D-C2D	-2.47	103.29	106.90
22	J	101	CHD	C21-C20-C22	2.47	114.24	110.36
25	C	310	DMU	C57-C4-C3	-2.47	106.15	113.33
22	B	301	CHD	O12-C12-C11	2.46	114.14	109.12
14	A	601	HEA	CHC-C4B-NB	-2.46	121.34	124.38
25	C	309	DMU	O5-C6-O16	-2.46	104.16	109.97
28	G	101	PEK	C23-C22-C21	2.45	122.55	113.62
22	P	306	CHD	C19-C10-C1	-2.45	104.31	108.26
19	L	101	TGL	C23-C22-C21	-2.45	101.99	114.42
22	C	306	CHD	C6-C5-C4	-2.45	108.37	111.19
14	A	601	HEA	CAA-CBA-CGA	-2.45	106.89	113.76
14	N	602[A]	HEA	C13-C12-C11	-2.45	110.67	114.35
22	P	301	CHD	O3-C3-C2	-2.45	103.94	110.16
27	G	102	CDL	C40-C39-C38	2.45	126.84	114.42
14	N	602[B]	HEA	C12-C13-C14	-2.45	105.78	112.23
14	A	602[B]	HEA	CMC-C2C-C1C	-2.45	124.71	128.46
27	C	305	CDL	C42-C41-C40	2.44	126.83	114.42
25	P	310	DMU	O1-C9-C11	2.44	112.50	106.44
27	G	102	CDL	CA6-OA8-CA7	2.44	126.14	117.12
21	H	101	EDO	O2-C2-C1	-2.43	94.41	111.91
25	L	102	DMU	O55-C2-C1	-2.43	104.73	110.35
14	A	602[B]	HEA	CHA-C4D-ND	2.43	127.07	124.43
14	A	601	HEA	C3B-C4B-NB	2.43	112.71	109.84
25	Z	101	DMU	O1-C9-C8	-2.42	105.30	109.69
19	A	608	TGL	OG1-CA1-CA2	2.42	119.50	111.91
22	B	301	CHD	C5-C4-C3	-2.42	109.20	112.76
25	M	101	DMU	O3-C5-C10	-2.42	104.17	110.05
22	W	101	CHD	C1-C10-C5	2.42	111.34	107.77
27	P	305	CDL	C42-C41-C40	2.42	126.69	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602[B]	HEA	C4A-CHB-C1B	-2.42	119.37	122.56
28	G	104	PEK	C01-O03-C21	2.42	126.06	117.12
24	B	303	PSC	C01-O03-C19	2.41	126.05	117.12
25	L	102	DMU	C10-O7-C3	2.41	123.92	117.96
27	P	305	CDL	C20-C19-C18	2.40	126.63	114.42
22	C	306	CHD	C6-C5-C10	2.40	115.21	112.66
22	P	306	CHD	O3-C3-C4	-2.40	105.07	109.85
20	C	308	PGV	C3-C2-C1	2.40	122.34	113.62
20	P	304	PGV	O02-C1-C2	2.40	133.09	123.73
27	G	102	CDL	OA6-CA5-OA7	-2.40	117.91	123.70
19	L	101	TGL	OG2-CG2-CG1	2.40	117.08	108.40
20	X	101	PGV	O01-C02-C01	2.40	117.08	108.40
20	N	608	PGV	C03-C02-C01	-2.39	106.14	111.79
14	A	602[B]	HEA	O2D-CGD-CBD	2.39	121.70	114.03
25	C	310	DMU	O2-C8-C7	2.38	115.86	110.35
25	L	102	DMU	O5-C6-O16	2.38	115.61	109.97
27	T	103	CDL	C23-C22-C21	2.38	126.51	114.42
14	A	602[A]	HEA	C20-C21-C22	-2.38	104.07	111.88
22	J	101	CHD	C6-C7-C8	2.37	114.01	111.48
27	P	305	CDL	OA8-CA7-OA9	-2.37	117.62	123.59
28	T	102	PEK	O03-C21-O04	-2.36	117.63	123.59
14	N	602[B]	HEA	C2D-C1D-ND	2.36	112.64	109.84
14	A	602[B]	HEA	C1D-C2D-C3D	-2.36	104.47	106.96
25	C	310	DMU	O4-C7-C8	-2.36	104.89	110.35
22	W	101	CHD	O26-C24-O25	-2.36	117.42	123.30
27	C	305	CDL	OB2-PB2-OB3	2.36	118.28	109.07
27	T	103	CDL	CA6-OA8-CA7	2.36	125.85	117.12
14	N	602[A]	HEA	CHC-C4B-NB	2.36	127.29	124.38
14	A	601	HEA	O2A-CGA-CBA	2.35	121.59	114.03
27	P	305	CDL	C39-C38-C37	2.35	126.36	114.42
28	G	101	PEK	O04-C21-C22	2.34	132.87	123.73
28	G	101	PEK	O11-P-O14	-2.34	99.93	109.07
22	G	103	CHD	C1-C2-C3	-2.34	107.47	110.47
27	G	102	CDL	C39-C38-C37	2.34	126.29	114.42
27	G	102	CDL	OB7-CB5-C51	-2.33	114.63	123.73
22	G	103	CHD	O7-C7-C6	2.33	115.72	109.94
25	P	309	DMU	C8-C7-C5	-2.32	106.77	110.82
24	B	303	PSC	C27-C26-C25	-2.32	102.63	114.42
19	D	201	TGL	CC4-CC3-CC2	2.32	121.54	113.19
22	P	301	CHD	C11-C12-C13	-2.32	108.86	111.24
22	G	103	CHD	C19-C10-C5	-2.31	106.44	110.36
25	C	310	DMU	C7-C8-C9	2.31	114.37	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	301	CHD	C19-C10-C9	-2.31	108.00	111.18
27	T	103	CDL	C83-C82-C81	2.30	126.10	114.42
22	P	306	CHD	C16-C15-C14	2.30	109.69	105.13
24	O	302	PSC	O03-C01-C02	2.30	115.12	108.43
28	T	102	PEK	O11-P-O14	-2.29	100.11	109.07
14	N	602[B]	HEA	C3C-C4C-NC	2.29	112.17	109.21
28	T	101	PEK	C11-C10-C9	2.28	123.27	112.02
27	P	305	CDL	CB4-OB6-CB5	-2.28	112.17	117.79
14	N	602[B]	HEA	O1D-CGD-CBD	-2.28	115.75	123.08
19	Y	101	TGL	OG2-CB1-OB1	-2.28	118.19	123.70
19	L	101	TGL	CB9-CB8-CB7	-2.28	102.85	114.42
25	Z	101	DMU	C34-C31-C28	-2.27	102.89	114.42
22	G	103	CHD	C17-C13-C12	-2.27	115.59	117.67
25	P	309	DMU	O4-C7-C8	2.27	115.60	110.35
20	P	304	PGV	C24-C23-C22	-2.27	102.89	114.42
28	P	308	PEK	C35-C34-C33	2.27	125.96	114.42
20	C	308	PGV	O02-C1-C2	-2.27	114.89	123.73
25	M	101	DMU	O49-C1-C6	-2.26	104.54	110.05
25	M	101	DMU	C28-C25-C22	-2.26	102.96	114.42
22	G	103	CHD	C23-C22-C20	-2.25	110.40	114.52
19	Y	101	TGL	CG1-OG1-CA1	2.25	125.46	117.12
27	G	102	CDL	C44-C43-C42	2.25	125.84	114.42
14	A	602[B]	HEA	C3D-C4D-ND	2.24	112.53	110.36
22	W	101	CHD	C10-C9-C8	2.24	114.22	111.82
14	A	602[B]	HEA	C2D-C1D-ND	2.24	112.49	109.84
27	C	305	CDL	OB5-PB2-OB3	2.23	117.79	109.07
14	N	602[A]	HEA	CAA-CBA-CGA	-2.23	107.50	113.76
25	P	307	DMU	C10-O1-C9	2.22	118.05	113.69
22	J	101	CHD	C2-C1-C10	2.22	116.59	112.78
27	P	305	CDL	C83-C82-C81	2.21	125.65	114.42
25	L	102	DMU	C6-C1-C2	2.21	114.60	110.00
22	P	306	CHD	C18-C13-C14	2.21	114.67	111.21
27	P	305	CDL	C63-C62-C61	2.20	125.61	114.42
14	A	601	HEA	CMB-C2B-C1B	-2.20	121.69	125.04
19	Q	201	TGL	CB5-CB4-CB3	2.19	125.56	114.42
22	G	103	CHD	O26-C24-C23	2.19	121.06	114.03
28	P	308	PEK	C02-O01-C1	2.18	123.17	117.79
22	B	301	CHD	C15-C14-C13	2.18	105.69	103.55
27	G	102	CDL	C20-C19-C18	2.18	125.50	114.42
14	N	601	HEA	C4D-C3D-C2D	-2.18	103.72	106.90
22	J	101	CHD	C9-C10-C5	2.18	111.64	108.58
14	N	602[A]	HEA	C27-C19-C20	2.18	118.93	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	602[A]	HEA	C1B-C2B-C3B	-2.17	104.20	106.80
25	C	302	DMU	C2-C3-C4	-2.17	105.94	110.93
25	M	101	DMU	C6-C1-C2	-2.17	105.47	110.00
19	Y	101	TGL	OC1-CC1-CC2	-2.17	115.28	123.73
20	A	609	PGV	C15-C14-C13	-2.17	104.36	113.79
14	A	602[A]	HEA	C13-C14-C15	-2.16	122.45	127.66
27	T	103	CDL	OA4-PA1-OA3	2.16	122.94	112.24
28	T	101	PEK	O03-C21-C22	2.16	118.69	111.91
22	J	101	CHD	C13-C14-C8	-2.16	111.98	114.74
22	B	301	CHD	C13-C17-C20	-2.16	116.92	119.50
19	L	101	TGL	CA3-CA2-CA1	-2.16	105.78	113.62
27	T	103	CDL	C80-C79-C78	2.15	125.36	114.42
24	O	302	PSC	C23-C22-C21	-2.15	103.49	114.42
22	J	101	CHD	C18-C13-C14	-2.15	107.85	111.21
21	P	312	EDO	O1-C1-C2	-2.15	96.46	111.91
28	G	104	PEK	C2-C3-C4	2.15	117.05	113.23
14	N	601	HEA	C13-C12-C11	-2.14	111.13	114.35
19	L	101	TGL	OG1-CA1-OA1	-2.14	118.19	123.59
28	P	308	PEK	O12-C04-C05	-2.14	101.09	109.10
20	P	304	PGV	C3-C2-C1	-2.14	105.84	113.62
21	A	616	EDO	O1-C1-C2	2.14	127.27	111.91
25	P	310	DMU	O5-C4-C57	2.13	111.74	106.44
22	G	103	CHD	C13-C17-C20	-2.13	116.95	119.50
20	C	304	PGV	C24-C23-C22	2.13	125.22	114.42
20	C	304	PGV	C28-C27-C26	-2.13	103.63	114.42
28	T	101	PEK	O02-C1-C2	-2.12	115.46	123.73
28	G	104	PEK	O03-C21-O04	-2.12	118.25	123.59
19	Y	101	TGL	CA7-CA6-CA5	-2.11	103.70	114.42
21	H	101	EDO	O1-C1-C2	-2.11	96.71	111.91
21	S	105	EDO	O1-C1-C2	-2.11	96.75	111.91
22	B	301	CHD	C9-C11-C12	-2.11	111.52	114.30
22	B	301	CHD	C18-C13-C14	-2.10	107.92	111.21
19	D	201	TGL	OG2-CG2-CG1	2.10	116.01	108.40
19	D	201	TGL	OG1-CA1-OA1	-2.10	118.29	123.59
14	N	602[A]	HEA	CHD-C1D-ND	2.10	126.97	124.38
25	P	309	DMU	O1-C10-C5	2.10	114.79	110.35
20	A	610	PGV	C6-C5-C4	-2.10	103.79	114.42
27	C	305	CDL	CB6-OB8-CB7	2.09	124.88	117.12
25	P	307	DMU	C1-C2-C3	2.09	114.45	109.68
24	B	303	PSC	O02-C1-C2	-2.08	115.60	123.73
22	G	103	CHD	C15-C14-C13	-2.08	101.51	103.55
24	O	302	PSC	C22-C21-C20	-2.08	105.71	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T	102	PEK	O01-C02-C03	-2.08	100.87	108.40
14	A	601	HEA	C20-C21-C22	-2.08	105.05	111.88
19	D	201	TGL	OG3-CC1-CC2	-2.08	105.38	111.91
28	T	101	PEK	O03-C01-C02	2.08	114.48	108.43
27	C	305	CDL	C62-C61-C60	2.08	124.97	114.42
25	L	102	DMU	O3-C5-C10	2.07	115.09	110.05
22	G	103	CHD	C9-C8-C7	-2.07	109.39	111.88
21	D	205	EDO	O2-C2-C1	-2.07	96.99	111.91
20	N	608	PGV	C26-C25-C24	2.07	124.95	114.42
25	C	302	DMU	C34-C31-C28	2.07	124.95	114.42
28	G	101	PEK	O03-C21-O04	-2.06	118.39	123.59
14	A	602[B]	HEA	C4A-CHB-C1B	2.06	125.28	122.56
28	P	308	PEK	C29-C28-C27	2.06	124.88	114.42
28	P	308	PEK	O03-C01-C02	2.06	114.42	108.43
14	N	602[B]	HEA	C1D-ND-C4D	-2.05	102.95	105.07
27	T	103	CDL	C63-C62-C61	2.05	124.85	114.42
28	G	101	PEK	C01-O03-C21	2.05	124.72	117.12
27	P	305	CDL	OA9-CA7-C31	-2.05	115.72	123.73
22	G	103	CHD	C13-C14-C8	-2.05	112.12	114.74
22	B	301	CHD	C1-C10-C5	2.04	110.79	107.77
22	P	301	CHD	C15-C14-C13	2.04	105.55	103.55
22	C	301	CHD	C11-C12-C13	2.04	113.34	111.24
27	T	103	CDL	C22-C21-C20	2.03	124.75	114.42
20	P	302	PGV	O03-C01-C02	2.03	114.35	108.43
14	N	602[A]	HEA	C21-C20-C19	2.03	119.66	112.98
20	A	609	PGV	C4-C3-C2	-2.03	105.89	113.19
28	G	104	PEK	O04-C21-C22	-2.03	115.82	123.73
25	P	307	DMU	O5-C4-C57	2.02	111.47	106.44
22	G	103	CHD	C22-C20-C17	2.02	114.46	110.28
27	C	305	CDL	OB6-CB4-CB3	-2.02	101.09	108.40
27	G	102	CDL	C52-C51-CB5	2.02	120.96	113.62
22	C	301	CHD	C16-C17-C20	-2.02	109.02	112.15
19	Y	101	TGL	CB3-CB2-CB1	2.02	120.95	113.62
27	G	102	CDL	C22-C21-C20	2.01	124.64	114.42
14	N	601	HEA	C16-C17-C18	-2.00	105.29	111.88
22	P	306	CHD	C11-C9-C10	2.00	115.79	113.73
27	G	102	CDL	OA4-PA1-OA5	-2.00	98.45	107.75

There are no chirality outliers.

All (957) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	602[B]	HEA	C2D-C3D-CAD-CBD
19	D	201	TGL	CG2-CG1-OG1-CA1
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	Y	101	TGL	CB2-CB1-OG2-CG2
20	A	610	PGV	C03-O11-P-O14
20	A	610	PGV	C04-O12-P-O13
20	C	308	PGV	C03-O11-P-O14
20	C	308	PGV	O03-C01-C02-O01
20	C	308	PGV	O12-C04-C05-C06
20	C	308	PGV	C04-C05-C06-O06
20	P	302	PGV	C04-C05-C06-O06
20	X	101	PGV	C03-O11-P-O13
20	X	101	PGV	C03-O11-P-O14
20	X	101	PGV	C02-C03-O11-P
20	X	101	PGV	C04-C05-C06-O06
20	X	101	PGV	O02-C1-O01-C02
20	X	101	PGV	C2-C1-O01-C02
22	J	101	CHD	C13-C17-C20-C21
22	J	101	CHD	C13-C17-C20-C22
22	J	101	CHD	C16-C17-C20-C21
22	J	101	CHD	C16-C17-C20-C22
22	W	101	CHD	C13-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
24	O	302	PSC	O12-C04-C05-N
24	O	302	PSC	O02-C1-O01-C02
24	O	302	PSC	O04-C19-O03-C01
24	O	302	PSC	C20-C19-O03-C01
24	O	302	PSC	C11-C12-C13-C14
25	C	310	DMU	C1-C6-O16-C18
25	C	310	DMU	O5-C6-O16-C18
25	P	307	DMU	O5-C6-O16-C18
25	P	310	DMU	O5-C6-O16-C18
27	C	305	CDL	CA3-OA5-PA1-OA2
27	C	305	CDL	C11-CA5-OA6-CA4
27	C	305	CDL	CB2-OB2-PB2-OB3
27	C	305	CDL	CB2-OB2-PB2-OB4
27	G	102	CDL	O1-C1-CB2-OB2
27	G	102	CDL	C1-CA2-OA2-PA1
27	G	102	CDL	CA2-OA2-PA1-OA3
27	G	102	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
27	G	102	CDL	CA2-OA2-PA1-OA5
27	G	102	CDL	CA3-OA5-PA1-OA3
27	G	102	CDL	OA5-CA3-CA4-OA6
27	G	102	CDL	CB2-OB2-PB2-OB3
27	G	102	CDL	CB2-OB2-PB2-OB4
27	G	102	CDL	CB2-OB2-PB2-OB5
27	G	102	CDL	CB3-OB5-PB2-OB3
27	P	305	CDL	C1-CA2-OA2-PA1
27	P	305	CDL	CA2-OA2-PA1-OA3
27	P	305	CDL	CA2-OA2-PA1-OA4
27	P	305	CDL	CA2-OA2-PA1-OA5
27	P	305	CDL	CA3-OA5-PA1-OA3
27	P	305	CDL	CA4-CA3-OA5-PA1
27	P	305	CDL	CB2-OB2-PB2-OB3
27	P	305	CDL	CB2-OB2-PB2-OB4
27	P	305	CDL	CB2-OB2-PB2-OB5
27	P	305	CDL	CB3-OB5-PB2-OB3
27	P	305	CDL	CB3-OB5-PB2-OB4
27	T	103	CDL	CA3-OA5-PA1-OA4
27	T	103	CDL	OA5-CA3-CA4-OA6
27	T	103	CDL	OA7-CA5-OA6-CA4
27	T	103	CDL	C11-CA5-OA6-CA4
27	T	103	CDL	CB3-OB5-PB2-OB2
27	T	103	CDL	CB3-OB5-PB2-OB3
27	T	103	CDL	C51-CB5-OB6-CB4
28	C	307	PEK	C04-O12-P-O11
28	C	307	PEK	C04-O12-P-O13
28	C	307	PEK	C04-O12-P-O14
28	C	307	PEK	O12-C04-C05-N
28	C	307	PEK	C05-C04-O12-P
28	C	307	PEK	C2-C1-O01-C02
28	C	307	PEK	C10-C11-C12-C13
28	P	308	PEK	O03-C01-C02-O01
28	P	308	PEK	C2-C1-O01-C02
28	P	308	PEK	C12-C13-C14-C15
28	T	101	PEK	C03-O11-P-O13
28	T	101	PEK	C04-O12-P-O14
28	T	101	PEK	O12-C04-C05-N
28	T	101	PEK	O02-C1-O01-C02
28	T	102	PEK	C6-C7-C8-C9
28	T	102	PEK	C11-C12-C13-C14
28	T	102	PEK	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OC1-CC1-OG3-CG3
19	Y	101	TGL	OA1-CA1-OG1-CG1
20	X	101	PGV	O04-C19-O03-C01
27	G	102	CDL	OA9-CA7-OA8-CA6
19	L	101	TGL	CG2-CG1-OG1-CA1
25	P	309	DMU	C5-C10-O7-C3
20	X	101	PGV	C20-C19-O03-C01
27	G	102	CDL	C31-CA7-OA8-CA6
25	L	102	DMU	C2-C3-O7-C10
19	A	608	TGL	OC1-CC1-OG3-CG3
19	N	609	TGL	OC1-CC1-OG3-CG3
20	A	610	PGV	O04-C19-O03-C01
25	C	309	DMU	C5-C10-O7-C3
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	610	PGV	O02-C1-O01-C02
27	C	305	CDL	OA7-CA5-OA6-CA4
27	C	305	CDL	OB7-CB5-OB6-CB4
27	G	102	CDL	OB7-CB5-OB6-CB4
27	T	103	CDL	OB7-CB5-OB6-CB4
28	C	307	PEK	O02-C1-O01-C02
28	P	308	PEK	O02-C1-O01-C02
25	L	102	DMU	C3-C4-C57-O61
19	D	201	TGL	CA2-CA1-OG1-CG1
19	D	201	TGL	CC2-CC1-OG3-CG3
19	Y	101	TGL	CA2-CA1-OG1-CG1
20	A	610	PGV	C20-C19-O03-C01
24	O	302	PSC	C2-C1-O01-C02
27	C	305	CDL	C51-CB5-OB6-CB4
28	T	101	PEK	C2-C1-O01-C02
22	W	101	CHD	C16-C17-C20-C22
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
25	C	310	DMU	C3-C4-C57-O61
19	A	608	TGL	CC2-CC1-OG3-CG3
20	A	610	PGV	C10-C11-C12-C13
28	C	307	PEK	C4-C5-C6-C7
28	C	307	PEK	C13-C14-C15-C16
28	G	101	PEK	C7-C8-C9-C10
28	G	101	PEK	C13-C14-C15-C16
28	G	104	PEK	C7-C8-C9-C10
28	T	102	PEK	C7-C8-C9-C10
14	N	602[B]	HEA	C4D-C3D-CAD-CBD
19	N	609	TGL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	M	101	DMU	C28-C31-C34-C37
27	P	305	CDL	C38-C39-C40-C41
19	Q	201	TGL	OC1-CC1-OG3-CG3
27	C	305	CDL	C38-C39-C40-C41
19	N	609	TGL	CC2-CC1-OG3-CG3
19	Q	201	TGL	CC2-CC1-OG3-CG3
24	B	303	PSC	C20-C19-O03-C01
27	P	305	CDL	C42-C43-C44-C45
19	D	201	TGL	OA1-CA1-OG1-CG1
25	P	307	DMU	O6-C11-C9-C8
20	C	308	PGV	C2-C1-O01-C02
27	G	102	CDL	C11-CA5-OA6-CA4
27	G	102	CDL	C51-CB5-OB6-CB4
19	L	101	TGL	CC1-CC2-CC3-CC4
25	P	307	DMU	O6-C11-C9-O1
19	L	101	TGL	CA9-C20-C21-C22
27	T	103	CDL	C62-C63-C64-C65
19	Y	101	TGL	CC3-CC4-CC5-CC6
27	T	103	CDL	C79-C80-C81-C82
19	Y	101	TGL	CC1-CC2-CC3-CC4
19	A	608	TGL	CA9-C20-C21-C22
27	G	102	CDL	OA7-CA5-OA6-CA4
20	A	610	PGV	C20-C21-C22-C23
24	O	302	PSC	C20-C21-C22-C23
27	T	103	CDL	C1-CA2-OA2-PA1
27	C	305	CDL	C81-C82-C83-C84
25	C	310	DMU	O5-C4-C57-O61
25	L	102	DMU	O5-C4-C57-O61
24	B	303	PSC	O04-C19-O03-C01
27	G	102	CDL	OB9-CB7-OB8-CB6
27	G	102	CDL	C23-C24-C25-C26
27	G	102	CDL	C71-CB7-OB8-CB6
22	C	306	CHD	C17-C20-C22-C23
19	A	608	TGL	C22-C23-C24-C25
27	C	305	CDL	CB2-C1-CA2-OA2
27	G	102	CDL	CA2-C1-CB2-OB2
27	P	305	CDL	CB2-C1-CA2-OA2
20	C	308	PGV	O02-C1-O01-C02
20	C	308	PGV	C20-C21-C22-C23
27	T	103	CDL	C31-CA7-OA8-CA6
27	T	103	CDL	C71-CB7-OB8-CB6
27	P	305	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
28	P	308	PEK	C21-C22-C23-C24
25	L	102	DMU	O6-C11-C9-C8
24	O	302	PSC	C22-C23-C24-C25
25	L	102	DMU	O6-C11-C9-O1
20	C	308	PGV	O12-C04-C05-O05
20	P	302	PGV	O12-C04-C05-O05
20	X	101	PGV	O12-C04-C05-O05
27	C	305	CDL	O1-C1-CB2-OB2
27	P	305	CDL	O1-C1-CA2-OA2
28	P	308	PEK	C1-C2-C3-C4
25	P	310	DMU	C1-C6-O16-C18
27	P	305	CDL	C13-C14-C15-C16
27	T	103	CDL	OA9-CA7-OA8-CA6
27	T	103	CDL	OB9-CB7-OB8-CB6
27	P	305	CDL	C51-CB5-OB6-CB4
19	Y	101	TGL	CA9-C20-C21-C22
20	X	101	PGV	C19-C20-C21-C22
22	W	101	CHD	C17-C20-C22-C23
19	Y	101	TGL	CA1-CA2-CA3-CA4
20	C	308	PGV	C1-C2-C3-C4
28	G	101	PEK	C10-C11-C12-C13
28	G	104	PEK	C4-C5-C6-C7
28	T	102	PEK	C13-C14-C15-C16
28	P	308	PEK	C33-C34-C35-C36
19	A	608	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	CA1-CA2-CA3-CA4
19	N	609	TGL	CC1-CC2-CC3-CC4
27	C	305	CDL	C18-C19-C20-C21
25	C	302	DMU	O16-C18-C19-C22
25	P	310	DMU	O16-C18-C19-C22
20	X	101	PGV	C05-C04-O12-P
19	Q	201	TGL	CB1-CB2-CB3-CB4
20	A	610	PGV	C19-C20-C21-C22
27	C	305	CDL	CB5-C51-C52-C53
21	H	101	EDO	O1-C1-C2-O2
21	N	615	EDO	O1-C1-C2-O2
20	A	610	PGV	C2-C1-O01-C02
22	C	306	CHD	C21-C20-C22-C23
27	C	305	CDL	O1-C1-CA2-OA2
27	G	102	CDL	O1-C1-CA2-OA2
27	P	305	CDL	O1-C1-CB2-OB2
19	A	608	TGL	CB1-CB2-CB3-CB4

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C10-C11-C12-C13
20	X	101	PGV	C10-C11-C12-C13
24	O	302	PSC	C11-C10-C9-C8
24	O	302	PSC	C29-C30-C31-C32
20	A	610	PGV	C04-O12-P-O11
20	X	101	PGV	C03-O11-P-O12
27	C	305	CDL	CB2-OB2-PB2-OB5
27	T	103	CDL	CA3-OA5-PA1-OA2
28	C	307	PEK	C03-O11-P-O12
28	P	308	PEK	C03-O11-P-O12
28	P	308	PEK	C04-O12-P-O11
28	T	101	PEK	C03-O11-P-O12
27	G	102	CDL	CB7-C71-C72-C73
27	G	102	CDL	CB2-C1-CA2-OA2
19	A	608	TGL	OB1-CB1-OG2-CG2
25	C	309	DMU	O6-C11-C9-C8
19	N	609	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	C21-C22-C23-C24
24	O	302	PSC	C3-C4-C5-C6
27	P	305	CDL	C77-C78-C79-C80
19	N	609	TGL	CC6-CC7-CC8-CC9
19	Q	201	TGL	CA6-CA7-CA8-CA9
28	T	102	PEK	C26-C27-C28-C29
19	D	201	TGL	C19-C33-C34-C35
27	G	102	CDL	C72-C73-C74-C75
27	P	305	CDL	C16-C17-C18-C19
28	T	101	PEK	C25-C26-C27-C28
19	L	101	TGL	CG1-CG2-OG2-CB1
20	X	101	PGV	C01-C02-O01-C1
27	P	305	CDL	OB7-CB5-OB6-CB4
19	Q	201	TGL	CC1-CC2-CC3-CC4
20	C	304	PGV	C7-C8-C9-C10
24	O	302	PSC	C24-C25-C26-C27
27	G	102	CDL	C77-C78-C79-C80
27	P	305	CDL	C43-C44-C45-C46
27	P	305	CDL	C56-C57-C58-C59
27	P	305	CDL	C78-C79-C80-C81
27	T	103	CDL	C51-C52-C53-C54
28	C	307	PEK	C25-C26-C27-C28
20	P	304	PGV	C10-C11-C12-C13
24	B	303	PSC	C11-C10-C9-C8
19	D	201	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
20	C	304	PGV	C27-C28-C29-C30
20	C	308	PGV	C23-C24-C25-C26
20	P	304	PGV	C7-C8-C9-C10
25	C	309	DMU	C25-C28-C31-C34
27	C	305	CDL	C57-C58-C59-C60
27	T	103	CDL	C59-C60-C61-C62
19	L	101	TGL	C16-C15-CC9-CC8
19	Y	101	TGL	CB5-CB6-CB7-CB8
20	P	304	PGV	C24-C25-C26-C27
25	P	309	DMU	C28-C31-C34-C37
28	G	104	PEK	C21-C22-C23-C24
19	D	201	TGL	CB9-C10-C11-C12
19	D	201	TGL	C13-C14-C29-C30
19	Y	101	TGL	CB6-CB7-CB8-CB9
27	G	102	CDL	C56-C57-C58-C59
28	T	101	PEK	C23-C24-C25-C26
19	A	608	TGL	C16-C15-CC9-CC8
20	A	610	PGV	C22-C23-C24-C25
20	P	302	PGV	C27-C28-C29-C30
27	C	305	CDL	C58-C59-C60-C61
27	C	305	CDL	C75-C76-C77-C78
27	G	102	CDL	C35-C36-C37-C38
19	A	608	TGL	CC5-CC6-CC7-CC8
19	A	608	TGL	C20-C21-C22-C23
19	D	201	TGL	CC9-C15-C16-C17
19	L	101	TGL	C21-C22-C23-C24
19	N	609	TGL	C24-C25-C26-C27
19	Q	201	TGL	C19-C33-C34-C35
20	C	304	PGV	C13-C14-C15-C16
20	C	308	PGV	C3-C4-C5-C6
20	C	308	PGV	C22-C23-C24-C25
27	C	305	CDL	C80-C81-C82-C83
27	C	305	CDL	C82-C83-C84-C85
27	G	102	CDL	C17-C18-C19-C20
27	P	305	CDL	C23-C24-C25-C26
27	T	103	CDL	C31-C32-C33-C34
27	T	103	CDL	C80-C81-C82-C83
28	G	101	PEK	C25-C26-C27-C28
19	D	201	TGL	C11-C12-C13-C14
19	Y	101	TGL	C16-C15-CC9-CC8
20	X	101	PGV	C28-C29-C30-C31
20	X	101	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C2-C1-O01-C02
19	A	608	TGL	C16-C17-C18-C19
20	P	302	PGV	C30-C31-C32-C33
27	C	305	CDL	C56-C57-C58-C59
27	P	305	CDL	C82-C83-C84-C85
28	C	307	PEK	C1-C2-C3-C4
19	A	608	TGL	CC7-CC8-CC9-C15
19	D	201	TGL	C21-C22-C23-C24
19	D	201	TGL	C14-C29-C30-C31
19	L	101	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CB2-CB3-CB4-CB5
19	Y	101	TGL	CC6-CC7-CC8-CC9
20	A	609	PGV	C28-C29-C30-C31
25	P	309	DMU	C19-C22-C25-C28
27	P	305	CDL	C41-C42-C43-C44
27	T	103	CDL	C75-C76-C77-C78
28	T	101	PEK	C31-C32-C33-C34
19	L	101	TGL	CC2-CC3-CC4-CC5
27	T	103	CDL	C20-C21-C22-C23
28	G	101	PEK	C23-C24-C25-C26
19	Q	201	TGL	CC6-CC7-CC8-CC9
19	Y	101	TGL	CC4-CC5-CC6-CC7
27	G	102	CDL	C20-C21-C22-C23
27	G	102	CDL	C38-C39-C40-C41
19	N	609	TGL	CA1-CA2-CA3-CA4
28	G	104	PEK	C1-C2-C3-C4
19	A	608	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	C17-C18-C19-C33
19	D	201	TGL	C23-C24-C25-C26
25	L	102	DMU	C4-C3-O7-C10
25	C	310	DMU	C18-C19-C22-C25
19	Y	101	TGL	CA2-CA3-CA4-CA5
25	M	101	DMU	C19-C22-C25-C28
27	P	305	CDL	C37-C38-C39-C40
28	G	104	PEK	C34-C35-C36-C37
19	D	201	TGL	C16-C17-C18-C19
19	L	101	TGL	C22-C23-C24-C25
19	N	609	TGL	CC5-CC6-CC7-CC8
20	C	308	PGV	C30-C31-C32-C33
28	P	308	PEK	C10-C11-C12-C13
19	A	608	TGL	C13-C14-C29-C30

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Mol	Chain	Res	Type	Atoms
20	X	101	PGV	C3-C4-C5-C6
24	B	303	PSC	C24-C25-C26-C27
27	C	305	CDL	C77-C78-C79-C80
27	G	102	CDL	C57-C58-C59-C60
19	Q	201	TGL	CB9-C10-C11-C12
19	A	608	TGL	CB2-CB1-OG2-CG2
19	N	609	TGL	CB2-CB1-OG2-CG2
19	Q	201	TGL	CB2-CB1-OG2-CG2
20	C	308	PGV	O05-C05-C06-O06
20	P	302	PGV	O05-C05-C06-O06
20	X	101	PGV	O05-C05-C06-O06
19	Y	101	TGL	C11-C12-C13-C14
25	L	102	DMU	C19-C22-C25-C28
27	G	102	CDL	C63-C64-C65-C66
28	G	101	PEK	C16-C17-C18-C19
20	C	308	PGV	C12-C13-C14-C15
20	C	304	PGV	C22-C23-C24-C25
27	P	305	CDL	C11-C12-C13-C14
27	G	102	CDL	C52-C53-C54-C55
27	G	102	CDL	C43-C44-C45-C46
27	G	102	CDL	C61-C62-C63-C64
28	T	101	PEK	C32-C33-C34-C35
19	L	101	TGL	C23-C24-C25-C26
27	T	103	CDL	C61-C62-C63-C64
27	T	103	CDL	C76-C77-C78-C79
19	N	609	TGL	OB1-CB1-OG2-CG2
24	B	303	PSC	O02-C1-O01-C02
19	N	609	TGL	C13-C14-C29-C30
24	B	303	PSC	C3-C4-C5-C6
19	A	608	TGL	C24-C25-C26-C27
19	N	609	TGL	CA6-CA7-CA8-CA9
20	P	302	PGV	C6-C7-C8-C9
21	A	615	EDO	O1-C1-C2-O2
21	A	618	EDO	O1-C1-C2-O2
21	D	205	EDO	O1-C1-C2-O2
21	G	106	EDO	O1-C1-C2-O2
21	P	312	EDO	O1-C1-C2-O2
19	N	609	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	C12-C13-C14-C29
27	C	305	CDL	C23-C24-C25-C26
27	T	103	CDL	C12-C13-C14-C15
27	T	103	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	CA6-CA7-CA8-CA9
19	N	609	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	C11-C10-CB9-CB8
20	X	101	PGV	C20-C21-C22-C23
19	N	609	TGL	OA1-CA1-OG1-CG1
19	L	101	TGL	CB2-CB3-CB4-CB5
20	P	302	PGV	C13-C14-C15-C16
27	C	305	CDL	C14-C15-C16-C17
27	G	102	CDL	C31-C32-C33-C34
28	T	101	PEK	C22-C23-C24-C25
20	P	304	PGV	C12-C13-C14-C15
28	G	104	PEK	C2-C3-C4-C5
28	P	308	PEK	C2-C3-C4-C5
27	P	305	CDL	OA7-CA5-OA6-CA4
19	A	608	TGL	CA2-CA1-OG1-CG1
20	C	308	PGV	C20-C19-O03-C01
19	A	608	TGL	CC4-CC5-CC6-CC7
19	N	609	TGL	CC9-C15-C16-C17
27	C	305	CDL	C83-C84-C85-C86
28	G	101	PEK	C26-C27-C28-C29
28	G	104	PEK	C33-C34-C35-C36
28	T	102	PEK	C22-C23-C24-C25
19	Q	201	TGL	CA2-CA3-CA4-CA5
28	G	104	PEK	C22-C23-C24-C25
19	L	101	TGL	C19-C33-C34-C35
27	T	103	CDL	C33-C34-C35-C36
19	Q	201	TGL	CC9-C15-C16-C17
20	A	609	PGV	C30-C31-C32-C33
25	C	310	DMU	C31-C34-C37-C40
19	A	608	TGL	CB3-CB4-CB5-CB6
19	A	608	TGL	C10-C11-C12-C13
19	D	201	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	C17-C18-C19-C33
19	Q	201	TGL	C22-C23-C24-C25
20	P	302	PGV	C25-C26-C27-C28
24	B	303	PSC	C25-C26-C27-C28
27	P	305	CDL	C11-CA5-OA6-CA4
28	C	307	PEK	O01-C02-C03-O11
19	D	201	TGL	C10-C11-C12-C13
19	N	609	TGL	CA5-CA6-CA7-CA8
28	G	104	PEK	C31-C32-C33-C34
25	C	310	DMU	O1-C10-O7-C3

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C13-C14-C15-C16
19	Q	201	TGL	OB1-CB1-OG2-CG2
19	Y	101	TGL	C22-C23-C24-C25
25	P	310	DMU	C31-C34-C37-C40
27	P	305	CDL	C59-C60-C61-C62
27	T	103	CDL	C32-C33-C34-C35
19	Q	201	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	CA3-CA4-CA5-CA6
20	P	304	PGV	C22-C23-C24-C25
27	C	305	CDL	C60-C61-C62-C63
28	T	101	PEK	C2-C3-C4-C5
20	A	609	PGV	C26-C27-C28-C29
19	A	608	TGL	C21-C20-CA9-CA8
19	D	201	TGL	C15-C16-C17-C18
20	X	101	PGV	C30-C31-C32-C33
27	C	305	CDL	C51-C52-C53-C54
27	T	103	CDL	C11-C12-C13-C14
28	T	102	PEK	C10-C11-C12-C13
19	Q	201	TGL	CB4-CB5-CB6-CB7
27	P	305	CDL	C36-C37-C38-C39
27	C	305	CDL	CA5-C11-C12-C13
19	L	101	TGL	C11-C12-C13-C14
19	L	101	TGL	C20-C21-C22-C23
19	A	608	TGL	OA1-CA1-OG1-CG1
19	Q	201	TGL	C17-C18-C19-C33
20	A	610	PGV	C03-O11-P-O12
27	G	102	CDL	CB3-OB5-PB2-OB2
27	C	305	CDL	C12-C13-C14-C15
19	N	609	TGL	CB1-CB2-CB3-CB4
27	G	102	CDL	OA5-CA3-CA4-CA6
27	P	305	CDL	OA5-CA3-CA4-CA6
20	C	308	PGV	C13-C14-C15-C16
20	C	304	PGV	C23-C24-C25-C26
24	B	303	PSC	C26-C27-C28-C29
27	G	102	CDL	C83-C84-C85-C86
27	T	103	CDL	C83-C84-C85-C86
20	N	608	PGV	C12-C13-C14-C15
19	L	101	TGL	CC5-CC6-CC7-CC8
19	A	608	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	C21-C20-CA9-CA8
19	N	609	TGL	CB7-CB8-CB9-C10
27	C	305	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C28-C29-C30-C31
19	Y	101	TGL	C10-C11-C12-C13
19	D	201	TGL	OG1-CG1-CG2-CG3
19	L	101	TGL	OG1-CG1-CG2-CG3
19	Q	201	TGL	OG1-CG1-CG2-CG3
20	C	308	PGV	O03-C01-C02-C03
27	C	305	CDL	CB3-CB4-CB6-OB8
27	C	305	CDL	C78-C79-C80-C81
28	G	101	PEK	C28-C29-C30-C31
28	P	308	PEK	O03-C01-C02-C03
20	C	304	PGV	C10-C11-C12-C13
27	P	305	CDL	C60-C61-C62-C63
28	C	307	PEK	C35-C36-C37-C38
19	D	201	TGL	C11-C10-CB9-CB8
19	N	609	TGL	C21-C20-CA9-CA8
27	C	305	CDL	C32-C33-C34-C35
28	G	101	PEK	C17-C18-C19-C20
19	Y	101	TGL	C18-C19-C33-C34
20	C	308	PGV	C31-C32-C33-C34
20	P	302	PGV	C28-C29-C30-C31
27	G	102	CDL	C78-C79-C80-C81
28	G	101	PEK	C27-C28-C29-C30
19	Y	101	TGL	C33-C34-C35-C36
20	A	609	PGV	C31-C32-C33-C34
20	P	302	PGV	C24-C25-C26-C27
27	G	102	CDL	C59-C60-C61-C62
27	T	103	CDL	C58-C59-C60-C61
20	P	302	PGV	C31-C32-C33-C34
25	P	307	DMU	O16-C18-C19-C22
25	P	309	DMU	C34-C37-C40-C43
27	P	305	CDL	CB5-C51-C52-C53
19	D	201	TGL	C29-C30-C31-C32
27	G	102	CDL	C64-C65-C66-C67
19	D	201	TGL	CG3-CG2-OG2-CB1
24	O	302	PSC	C01-C02-O01-C1
25	L	102	DMU	C25-C28-C31-C34
28	P	308	PEK	C35-C36-C37-C38
19	Q	201	TGL	C15-C16-C17-C18
27	T	103	CDL	C84-C85-C86-C87
20	A	610	PGV	O01-C02-C03-O11
19	L	101	TGL	C10-C11-C12-C13
19	N	609	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	C25-C26-C27-C28
19	Y	101	TGL	C29-C30-C31-C32
20	X	101	PGV	C11-C10-C9-C8
20	A	610	PGV	C1-C2-C3-C4
19	D	201	TGL	C16-C15-CC9-CC8
19	Y	101	TGL	OG1-CG1-CG2-OG2
20	X	101	PGV	O03-C01-C02-O01
27	P	305	CDL	OA6-CA4-CA6-OA8
19	Y	101	TGL	CC7-CC8-CC9-C15
20	C	308	PGV	O04-C19-O03-C01
28	T	101	PEK	C33-C34-C35-C36
19	D	201	TGL	CB1-CB2-CB3-CB4
19	L	101	TGL	OG1-CA1-CA2-CA3
27	T	103	CDL	C55-C56-C57-C58
19	L	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	C24-C25-C26-C27
27	C	305	CDL	C39-C40-C41-C42
19	Y	101	TGL	CC9-C15-C16-C17
25	L	102	DMU	C34-C37-C40-C43
27	C	305	CDL	C24-C25-C26-C27
27	P	305	CDL	C61-C62-C63-C64
27	T	103	CDL	CB2-C1-CA2-OA2
25	L	102	DMU	C28-C31-C34-C37
28	T	102	PEK	C4-C5-C6-C7
19	A	608	TGL	C29-C30-C31-C32
19	Y	101	TGL	CA6-CA7-CA8-CA9
20	P	302	PGV	C23-C24-C25-C26
27	C	305	CDL	C43-C44-C45-C46
20	A	610	PGV	C01-C02-C03-O11
20	X	101	PGV	C01-C02-C03-O11
27	C	305	CDL	OA5-CA3-CA4-CA6
28	C	307	PEK	C01-C02-C03-O11
28	P	308	PEK	C01-C02-C03-O11
19	N	609	TGL	CC7-CC8-CC9-C15
19	Q	201	TGL	C11-C12-C13-C14
22	W	101	CHD	C20-C22-C23-C24
19	D	201	TGL	CC5-CC6-CC7-CC8
19	D	201	TGL	CC7-CC8-CC9-C15
28	G	101	PEK	C32-C33-C34-C35
20	A	610	PGV	C05-C04-O12-P
20	P	304	PGV	C02-C03-O11-P
20	P	302	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	T	102	PEK	C33-C34-C35-C36
25	C	310	DMU	C19-C18-O16-C6
25	L	102	DMU	C19-C18-O16-C6
27	T	103	CDL	C54-C55-C56-C57
19	A	608	TGL	C11-C12-C13-C14
19	A	608	TGL	OG1-CG1-CG2-CG3
20	A	610	PGV	O03-C01-C02-C03
24	B	303	PSC	O03-C01-C02-C03
24	O	302	PSC	O03-C01-C02-C03
27	G	102	CDL	CA3-CA4-CA6-OA8
27	P	305	CDL	CB3-CB4-CB6-OB8
27	G	102	CDL	C19-C20-C21-C22
28	P	308	PEK	C4-C5-C6-C7
22	P	306	CHD	C13-C17-C20-C21
25	C	310	DMU	C34-C37-C40-C43
28	T	101	PEK	C35-C36-C37-C38
19	Y	101	TGL	OG1-CA1-CA2-CA3
19	N	609	TGL	C23-C24-C25-C26
28	T	101	PEK	C30-C31-C32-C33
19	Q	201	TGL	CB5-CB6-CB7-CB8
25	C	309	DMU	C19-C22-C25-C28
25	L	102	DMU	C31-C34-C37-C40
24	O	302	PSC	C9-C10-C11-C12
28	C	307	PEK	C9-C10-C11-C12
28	G	101	PEK	C9-C10-C11-C12
28	G	104	PEK	C5-C6-C7-C8
28	G	104	PEK	C6-C7-C8-C9
28	G	104	PEK	C11-C10-C9-C8
28	G	104	PEK	C9-C10-C11-C12
28	P	308	PEK	C5-C6-C7-C8
28	P	308	PEK	C6-C7-C8-C9
28	P	308	PEK	C11-C10-C9-C8
28	P	308	PEK	C9-C10-C11-C12
28	T	101	PEK	C5-C6-C7-C8
28	T	101	PEK	C11-C10-C9-C8
28	T	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C12-C13-C14-C15
28	T	102	PEK	C11-C10-C9-C8
20	C	308	PGV	O01-C02-C03-O11
20	P	302	PGV	O01-C02-C03-O11
28	P	308	PEK	O01-C02-C03-O11
19	D	201	TGL	CB2-CB3-CB4-CB5

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C25-C26-C27-C28
19	L	101	TGL	CC4-CC5-CC6-CC7
20	A	610	PGV	C31-C32-C33-C34
19	L	101	TGL	CA6-CA7-CA8-CA9
28	T	101	PEK	O03-C01-C02-O01
22	P	301	CHD	C16-C17-C20-C22
20	A	610	PGV	C15-C16-C17-C18
25	P	309	DMU	O16-C18-C19-C22
28	G	101	PEK	C31-C32-C33-C34
25	P	310	DMU	C18-C19-C22-C25
20	P	302	PGV	O12-C04-C05-C06
19	Q	201	TGL	CB2-CB3-CB4-CB5
20	C	304	PGV	C21-C22-C23-C24
25	Z	101	DMU	C34-C37-C40-C43
24	O	302	PSC	C31-C32-C33-C34
20	A	610	PGV	C02-C03-O11-P
20	C	308	PGV	C02-C03-O11-P
24	O	302	PSC	C02-C03-O11-P
19	A	608	TGL	CA2-CA3-CA4-CA5
20	N	608	PGV	C14-C15-C16-C17
20	C	308	PGV	C15-C16-C17-C18
25	C	302	DMU	C22-C25-C28-C31
25	P	307	DMU	C34-C37-C40-C43
27	G	102	CDL	C76-C77-C78-C79
21	A	620	EDO	O1-C1-C2-O2
21	F	103	EDO	O1-C1-C2-O2
28	G	104	PEK	C25-C26-C27-C28
25	L	102	DMU	O16-C18-C19-C22
22	C	306	CHD	C16-C17-C20-C22
19	N	609	TGL	C11-C10-CB9-CB8
27	G	102	CDL	C16-C17-C18-C19
28	T	101	PEK	C28-C29-C30-C31
27	G	102	CDL	C62-C63-C64-C65
20	C	308	PGV	C01-C02-C03-O11
20	P	302	PGV	C01-C02-C03-O11
27	T	103	CDL	OA5-CA3-CA4-CA6
22	C	306	CHD	C20-C22-C23-C24
20	P	304	PGV	C1-C2-C3-C4
27	G	102	CDL	C75-C76-C77-C78
20	P	302	PGV	C9-C10-C11-C12
20	C	304	PGV	C15-C16-C17-C18
27	G	102	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	C	307	PEK	C32-C33-C34-C35
27	C	305	CDL	C42-C43-C44-C45
28	G	104	PEK	C26-C27-C28-C29
28	P	308	PEK	C15-C16-C17-C18
20	C	304	PGV	C02-C03-O11-P
20	P	302	PGV	C02-C03-O11-P
27	P	305	CDL	CB4-CB6-OB8-CB7
27	C	305	CDL	OA5-CA3-CA4-OA6
19	A	608	TGL	CA5-CA6-CA7-CA8
27	C	305	CDL	C59-C60-C61-C62
28	G	101	PEK	C34-C35-C36-C37
28	T	102	PEK	C34-C35-C36-C37
19	D	201	TGL	CC2-CC3-CC4-CC5
19	L	101	TGL	C29-C30-C31-C32
27	C	305	CDL	C76-C77-C78-C79
19	L	101	TGL	OG1-CG1-CG2-OG2
20	A	610	PGV	O03-C01-C02-O01
27	C	305	CDL	OB6-CB4-CB6-OB8
27	G	102	CDL	OA6-CA4-CA6-OA8
27	P	305	CDL	OB6-CB4-CB6-OB8
19	Q	201	TGL	OG2-CB1-CB2-CB3
20	X	101	PGV	C27-C28-C29-C30
27	C	305	CDL	C11-C12-C13-C14
27	T	103	CDL	C74-C75-C76-C77
24	O	302	PSC	C13-C14-C15-C16
27	G	102	CDL	CB5-C51-C52-C53
27	C	305	CDL	C40-C41-C42-C43
27	T	103	CDL	C22-C23-C24-C25
24	O	302	PSC	C21-C22-C23-C24
25	Z	101	DMU	O16-C18-C19-C22
19	Y	101	TGL	CC2-CC1-OG3-CG3
20	C	308	PGV	C04-O12-P-O11
27	G	102	CDL	CA3-OA5-PA1-OA2
27	P	305	CDL	CA3-OA5-PA1-OA2
27	P	305	CDL	CB3-OB5-PB2-OB2
27	T	103	CDL	CA2-OA2-PA1-OA5
28	T	101	PEK	C04-O12-P-O11
19	L	101	TGL	C24-C25-C26-C27
28	C	307	PEK	C26-C27-C28-C29
14	A	601	HEA	C26-C15-C16-C17
19	L	101	TGL	CB3-CB4-CB5-CB6
25	C	309	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C03-O11-P-O13
27	G	102	CDL	CB3-OB5-PB2-OB4
28	C	307	PEK	C03-O11-P-O14
28	P	308	PEK	C03-O11-P-O13
28	P	308	PEK	C03-O11-P-O14
28	P	308	PEK	C04-O12-P-O14
28	G	101	PEK	O12-C04-C05-N
21	N	616	EDO	O1-C1-C2-O2
21	Y	102	EDO	O1-C1-C2-O2
20	C	308	PGV	C7-C8-C9-C10
19	Y	101	TGL	C11-C10-CB9-CB8
27	G	102	CDL	C39-C40-C41-C42
27	P	305	CDL	C57-C58-C59-C60
27	G	102	CDL	C15-C16-C17-C18
19	A	608	TGL	C12-C13-C14-C29
19	Y	101	TGL	C16-C17-C18-C19
27	P	305	CDL	OA5-CA3-CA4-OA6
28	G	104	PEK	O01-C02-C03-O11
28	P	308	PEK	C29-C30-C31-C32
20	N	608	PGV	C27-C28-C29-C30
19	L	101	TGL	C18-C19-C33-C34
27	G	102	CDL	C82-C83-C84-C85
28	P	308	PEK	C28-C29-C30-C31
28	P	308	PEK	C26-C27-C28-C29
28	T	102	PEK	O03-C21-C22-C23
19	D	201	TGL	CG1-CG2-CG3-OG3
20	X	101	PGV	O03-C01-C02-C03
24	B	303	PSC	O12-C04-C05-N
27	P	305	CDL	C80-C81-C82-C83
28	G	104	PEK	O03-C01-C02-C03
28	T	101	PEK	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-OG2
24	O	302	PSC	O03-C01-C02-O01
28	G	104	PEK	O03-C01-C02-O01
19	Q	201	TGL	CA5-CA6-CA7-CA8
28	T	102	PEK	C30-C31-C32-C33
24	B	303	PSC	C6-C7-C8-C9
19	Y	101	TGL	OC1-CC1-OG3-CG3
27	C	305	CDL	OB9-CB7-OB8-CB6
27	G	102	CDL	CA4-CA3-OA5-PA1
20	C	308	PGV	C21-C22-C23-C24
20	P	302	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	X	101	PGV	C31-C32-C33-C34
27	P	305	CDL	C35-C36-C37-C38
20	C	304	PGV	C28-C29-C30-C31
24	B	303	PSC	C20-C21-C22-C23
20	A	609	PGV	C10-C11-C12-C13
19	L	101	TGL	CC6-CC7-CC8-CC9
27	T	103	CDL	O1-C1-CB2-OB2
14	N	601	HEA	C26-C15-C16-C17
27	P	305	CDL	C84-C85-C86-C87
19	Q	201	TGL	C16-C17-C18-C19
28	G	104	PEK	C24-C25-C26-C27
27	T	103	CDL	C24-C25-C26-C27
24	B	303	PSC	C01-C02-O01-C1
20	C	304	PGV	C1-C2-C3-C4
27	P	305	CDL	OA9-CA7-OA8-CA6
24	O	302	PSC	C1-C2-C3-C4
27	G	102	CDL	C14-C15-C16-C17
20	C	308	PGV	C14-C15-C16-C17
20	X	101	PGV	O01-C02-C03-O11
20	C	308	PGV	C27-C28-C29-C30
27	C	305	CDL	C73-C74-C75-C76
21	D	203	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
27	P	305	CDL	C31-CA7-OA8-CA6
19	Y	101	TGL	CB3-CB4-CB5-CB6
27	G	102	CDL	C60-C61-C62-C63
19	L	101	TGL	CA2-CA1-OG1-CG1
20	C	308	PGV	C03-O11-P-O12
20	P	302	PGV	C03-O11-P-O12
20	P	302	PGV	C04-O12-P-O11
24	B	303	PSC	C03-O11-P-O12
24	O	302	PSC	C03-O11-P-O12
24	O	302	PSC	C04-O12-P-O11
27	C	305	CDL	CA2-OA2-PA1-OA5
27	T	103	CDL	CB2-OB2-PB2-OB5
19	A	608	TGL	CC2-CC3-CC4-CC5
28	C	307	PEK	C30-C31-C32-C33
20	P	302	PGV	C2-C3-C4-C5
27	G	102	CDL	C58-C59-C60-C61
20	A	610	PGV	C21-C22-C23-C24
27	G	102	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C2-C3-C4-C5
27	T	103	CDL	C36-C37-C38-C39
20	P	304	PGV	C31-C32-C33-C34
28	G	104	PEK	C28-C29-C30-C31
20	C	304	PGV	C05-C04-O12-P
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
27	C	305	CDL	C31-CA7-OA8-CA6
27	C	305	CDL	C71-CB7-OB8-CB6
28	C	307	PEK	C7-C8-C9-C10
28	G	104	PEK	C10-C11-C12-C13
19	D	201	TGL	CB7-CB8-CB9-C10
20	P	304	PGV	C11-C12-C13-C14
14	N	602[B]	HEA	CAA-CBA-CGA-O1A
19	Q	201	TGL	CC4-CC5-CC6-CC7
22	J	101	CHD	C22-C23-C24-O26
28	P	308	PEK	C27-C28-C29-C30
27	C	305	CDL	C22-C23-C24-C25
19	N	609	TGL	OG1-CA1-CA2-CA3
20	P	302	PGV	C7-C8-C9-C10
22	C	306	CHD	C22-C23-C24-O26
20	C	304	PGV	C24-C25-C26-C27
20	P	304	PGV	C05-C04-O12-P
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
22	G	103	CHD	C22-C23-C24-O26
25	P	310	DMU	C34-C37-C40-C43
27	G	102	CDL	C13-C14-C15-C16
24	B	303	PSC	C27-C28-C29-C30
27	G	102	CDL	C37-C38-C39-C40
27	T	103	CDL	C17-C18-C19-C20
14	A	601	HEA	CAD-CBD-CGD-O1D
21	A	621	EDO	O1-C1-C2-O2
21	E	202	EDO	O1-C1-C2-O2
22	B	301	CHD	C22-C23-C24-O26
27	G	102	CDL	C71-C72-C73-C74
20	A	610	PGV	C29-C30-C31-C32
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
22	B	301	CHD	C22-C23-C24-O25
22	G	103	CHD	C22-C23-C24-O25
22	P	306	CHD	C22-C23-C24-O25
22	W	101	CHD	C22-C23-C24-O25
19	Q	201	TGL	C20-C21-C22-C23
20	A	610	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
27	P	305	CDL	CA6-CA4-OA6-CA5
27	T	103	CDL	CA6-CA4-OA6-CA5
14	A	601	HEA	C14-C15-C16-C17
20	C	308	PGV	C6-C7-C8-C9
24	O	302	PSC	C4-C5-C6-C7
22	P	306	CHD	C22-C23-C24-O26
19	L	101	TGL	C33-C34-C35-C36
28	G	101	PEK	C6-C7-C8-C9
28	G	104	PEK	C12-C13-C14-C15
28	T	101	PEK	C9-C10-C11-C12
19	A	608	TGL	C17-C18-C19-C33
19	Q	201	TGL	OG1-CA1-CA2-CA3
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
22	J	101	CHD	C22-C23-C24-O25
22	C	306	CHD	C13-C17-C20-C22
20	P	302	PGV	C26-C27-C28-C29
27	T	103	CDL	C56-C57-C58-C59
28	T	101	PEK	C01-C02-C03-O11
27	G	102	CDL	C42-C43-C44-C45
27	P	305	CDL	C19-C20-C21-C22
28	C	307	PEK	C29-C30-C31-C32
20	P	302	PGV	C19-C20-C21-C22
19	N	609	TGL	CC4-CC5-CC6-CC7
27	P	305	CDL	C32-C33-C34-C35
14	N	602[B]	HEA	CAA-CBA-CGA-O2A
25	C	309	DMU	O16-C18-C19-C22
14	N	601	HEA	CAD-CBD-CGD-O2D
20	N	608	PGV	C31-C32-C33-C34
19	Q	201	TGL	OG2-CG2-CG3-OG3
27	P	305	CDL	C14-C15-C16-C17
28	T	101	PEK	C4-C5-C6-C7
27	P	305	CDL	C20-C21-C22-C23
14	A	601	HEA	C15-C16-C17-C18
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
22	C	306	CHD	C22-C23-C24-O25
14	N	601	HEA	C14-C15-C16-C17
27	G	102	CDL	C24-C25-C26-C27
27	C	305	CDL	OA9-CA7-OA8-CA6
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
20	A	609	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	C22-C23-C24-C25
19	Y	101	TGL	OG2-CB1-CB2-CB3
28	T	102	PEK	C15-C16-C17-C18
24	O	302	PSC	C23-C24-C25-C26
14	N	601	HEA	CAD-CBD-CGD-O1D
19	L	101	TGL	OA1-CA1-OG1-CG1
28	T	101	PEK	O04-C21-O03-C01
19	L	101	TGL	CA5-CA6-CA7-CA8
19	N	609	TGL	CB2-CB3-CB4-CB5
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
20	X	101	PGV	C21-C22-C23-C24
27	T	103	CDL	C39-C40-C41-C42
20	P	302	PGV	C5-C6-C7-C8
25	L	102	DMU	C18-C19-C22-C25
20	C	308	PGV	C25-C26-C27-C28
19	Q	201	TGL	C13-C14-C29-C30
25	C	302	DMU	O5-C6-O16-C18
28	G	104	PEK	C01-C02-C03-O11
19	Y	101	TGL	C23-C24-C25-C26
25	C	310	DMU	O16-C18-C19-C22
19	A	608	TGL	CB7-CB8-CB9-C10
14	A	602[B]	HEA	C26-C15-C16-C17
14	N	602[B]	HEA	C26-C15-C16-C17
19	L	101	TGL	CC9-C15-C16-C17
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
25	C	302	DMU	C28-C31-C34-C37
19	D	201	TGL	C33-C34-C35-C36
20	C	304	PGV	C9-C10-C11-C12
20	C	304	PGV	C11-C12-C13-C14
28	T	101	PEK	C3-C4-C5-C6
14	A	601	HEA	CAD-CBD-CGD-O2D
22	W	101	CHD	C22-C23-C24-O26
28	T	101	PEK	C26-C27-C28-C29
28	P	308	PEK	C3-C4-C5-C6
27	G	102	CDL	C11-C12-C13-C14
27	C	305	CDL	CA3-CA4-CA6-OA8
27	P	305	CDL	CA3-CA4-CA6-OA8
24	B	303	PSC	O01-C02-C03-O11
28	T	101	PEK	O01-C02-C03-O11
28	G	104	PEK	O01-C1-C2-C3
19	L	101	TGL	CB4-CB5-CB6-CB7
22	C	301	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
22	C	301	CHD	C22-C23-C24-O26
19	A	608	TGL	C15-C16-C17-C18
19	A	608	TGL	CB9-C10-C11-C12
21	A	617	EDO	O1-C1-C2-O2
21	C	313	EDO	O1-C1-C2-O2
21	S	103	EDO	O1-C1-C2-O2
20	A	609	PGV	C11-C12-C13-C14
24	B	303	PSC	C12-C13-C14-C15
19	L	101	TGL	OA1-CA1-CA2-CA3
28	T	102	PEK	O04-C21-C22-C23
19	D	201	TGL	OG1-CA1-CA2-CA3
27	T	103	CDL	C32-C31-CA7-OA8
19	Q	201	TGL	OG3-CC1-CC2-CC3
22	P	301	CHD	C22-C23-C24-O25
19	N	609	TGL	CA7-CA8-CA9-C20
20	P	304	PGV	C13-C14-C15-C16
20	N	608	PGV	O03-C19-C20-C21
28	P	308	PEK	O01-C1-C2-C3
25	P	310	DMU	C19-C22-C25-C28
22	P	301	CHD	C22-C23-C24-O26
19	Y	101	TGL	OA1-CA1-CA2-CA3
25	C	310	DMU	C22-C25-C28-C31
19	Q	201	TGL	C16-C15-CC9-CC8
24	B	303	PSC	C31-C32-C33-C34
25	Z	101	DMU	C22-C25-C28-C31
28	G	104	PEK	O02-C1-C2-C3
19	N	609	TGL	CC2-CC3-CC4-CC5
20	N	608	PGV	C11-C12-C13-C14
19	Y	101	TGL	CA4-CA5-CA6-CA7
20	C	308	PGV	C24-C25-C26-C27
19	N	609	TGL	OC1-CC1-CC2-CC3
19	Y	101	TGL	OG1-CG1-CG2-CG3
20	X	101	PGV	O03-C19-C20-C21
20	N	608	PGV	C23-C24-C25-C26
27	T	103	CDL	C32-C31-CA7-OA9
25	P	309	DMU	C31-C34-C37-C40
20	C	308	PGV	C03-O11-P-O13
20	P	302	PGV	C04-O12-P-O13
24	B	303	PSC	C03-O11-P-O14
24	O	302	PSC	C04-O12-P-O14
27	C	305	CDL	CA2-OA2-PA1-OA3
27	C	305	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
27	T	103	CDL	CB2-OB2-PB2-OB3
27	G	102	CDL	C74-C75-C76-C77
28	G	101	PEK	C35-C36-C37-C38
21	B	304	EDO	O1-C1-C2-O2
21	P	311	EDO	O1-C1-C2-O2
19	N	609	TGL	OG3-CC1-CC2-CC3
28	P	308	PEK	C25-C26-C27-C28
19	D	201	TGL	OA1-CA1-CA2-CA3
19	D	201	TGL	CB4-CB5-CB6-CB7
20	X	101	PGV	O04-C19-C20-C21
27	T	103	CDL	C40-C41-C42-C43
25	C	302	DMU	C18-C19-C22-C25
28	T	101	PEK	C22-C21-O03-C01
19	D	201	TGL	OG3-CC1-CC2-CC3
27	C	305	CDL	C12-C11-CA5-OA6
25	Z	101	DMU	C25-C28-C31-C34
24	B	303	PSC	O03-C19-C20-C21
27	C	305	CDL	C12-C11-CA5-OA7
19	D	201	TGL	OG2-CB1-CB2-CB3
28	G	104	PEK	O03-C21-C22-C23
20	X	101	PGV	C9-C10-C11-C12
19	D	201	TGL	OC1-CC1-CC2-CC3
19	Q	201	TGL	OC1-CC1-CC2-CC3
27	C	305	CDL	C13-C14-C15-C16
27	C	305	CDL	C44-C45-C46-C47
27	G	102	CDL	C41-C42-C43-C44
19	A	608	TGL	CC3-CC4-CC5-CC6
27	G	102	CDL	C52-C51-CB5-OB6
27	P	305	CDL	C52-C53-C54-C55
28	G	104	PEK	O04-C21-C22-C23
20	C	308	PGV	C11-C12-C13-C14
28	P	308	PEK	O02-C1-C2-C3

There are no ring outliers.

61 monomers are involved in 418 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	T	102	PEK	2	0
21	A	616	EDO	3	0
14	N	601	HEA	7	0
18	A	606[B]	AZI	3	0
20	A	609	PGV	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	D	202	EDO	11	0
20	N	608	PGV	1	0
20	C	308	PGV	6	0
21	D	205	EDO	2	0
25	C	302	DMU	10	0
27	P	305	CDL	28	0
21	H	101	EDO	5	0
14	A	602[A]	HEA	4	0
28	G	104	PEK	19	0
22	P	306	CHD	2	0
24	B	303	PSC	21	0
22	G	103	CHD	1	0
27	T	103	CDL	24	0
20	C	304	PGV	1	0
14	A	602[B]	HEA	10	0
25	C	310	DMU	3	0
19	L	101	TGL	11	0
21	A	619	EDO	2	0
20	P	304	PGV	10	0
27	C	305	CDL	26	0
22	J	101	CHD	4	0
22	W	101	CHD	5	0
21	A	611	EDO	5	0
25	C	309	DMU	1	0
25	P	307	DMU	13	0
25	P	309	DMU	2	0
25	L	102	DMU	4	0
28	P	308	PEK	5	0
14	N	602[A]	HEA	3	0
14	A	601	HEA	9	0
19	Y	101	TGL	20	0
20	P	302	PGV	4	0
22	P	301	CHD	2	0
27	G	102	CDL	24	0
24	O	302	PSC	11	0
22	C	306	CHD	5	0
19	A	608	TGL	1	0
18	N	607[A]	AZI	1	0
21	N	616	EDO	2	0
21	G	106	EDO	1	0
19	Q	201	TGL	12	0
18	A	607[B]	AZI	6	0

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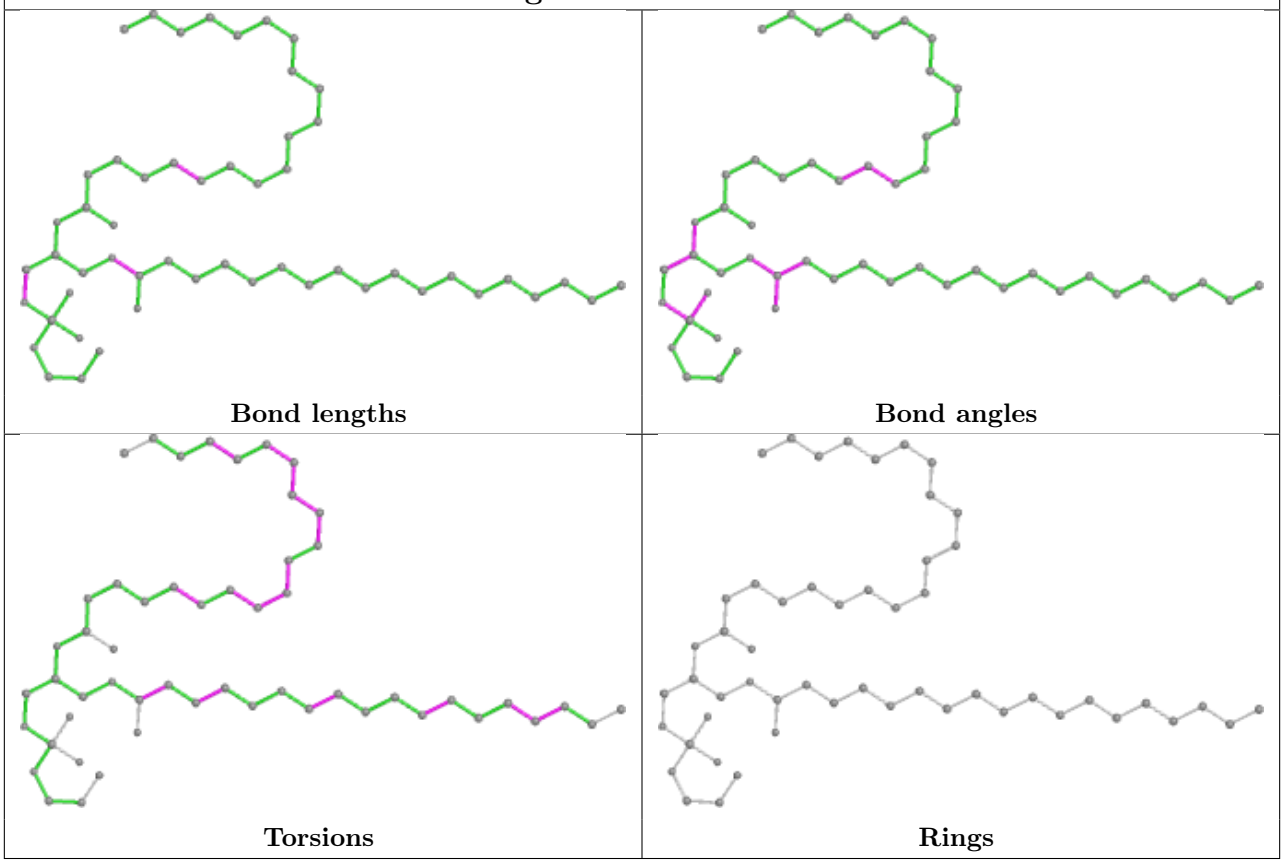
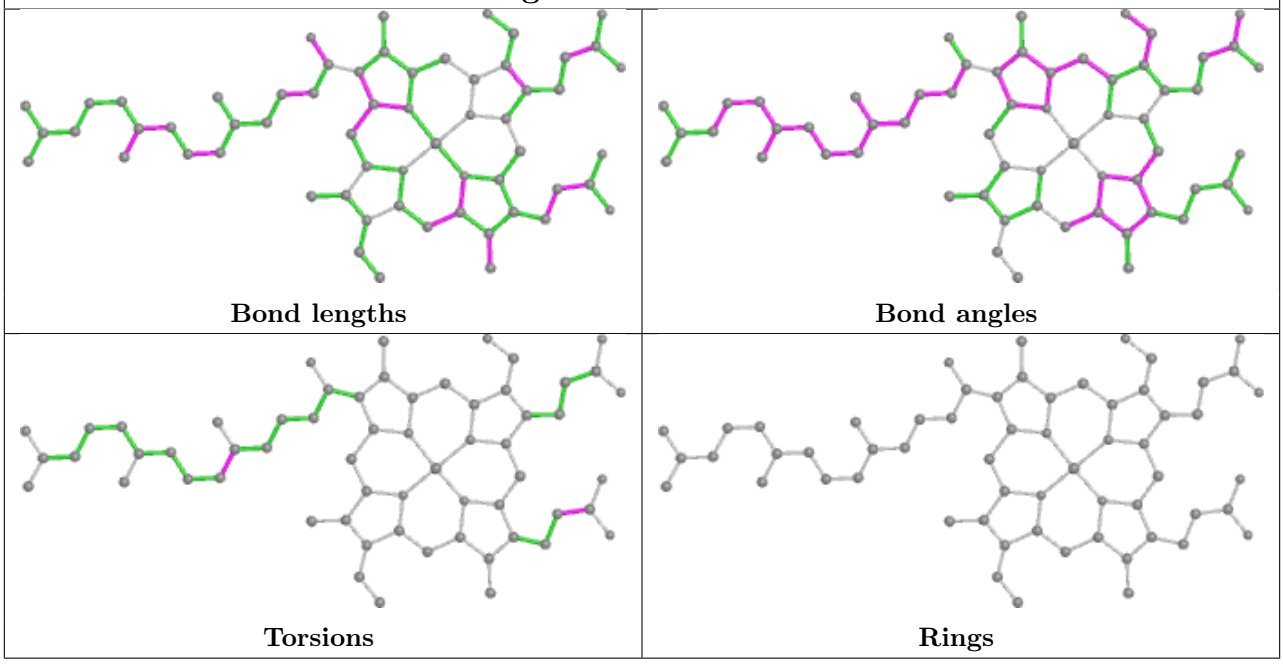
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	614	EDO	2	0
14	N	602[B]	HEA	12	0
19	N	609	TGL	5	0
20	X	101	PGV	10	0
28	C	307	PEK	14	0
22	C	301	CHD	1	0
20	A	610	PGV	5	0
28	G	101	PEK	7	0
21	D	203	EDO	2	0
18	N	607[B]	AZI	5	0
25	P	310	DMU	1	0
19	D	201	TGL	12	0
21	A	621	EDO	9	0
21	E	202	EDO	9	0

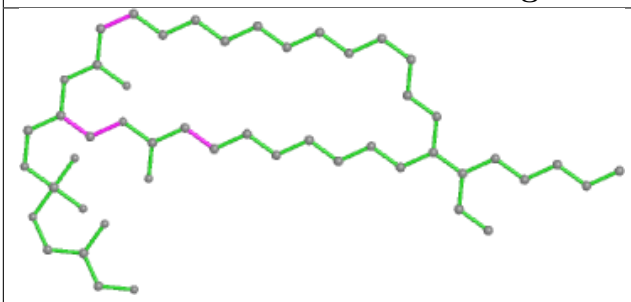
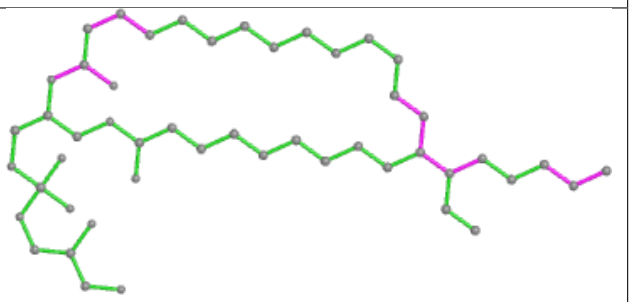
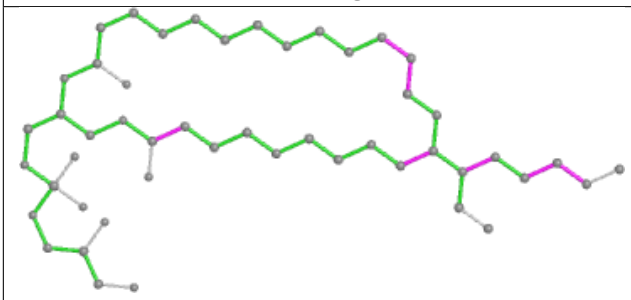
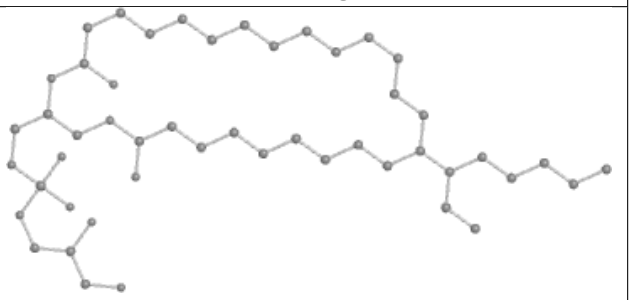
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

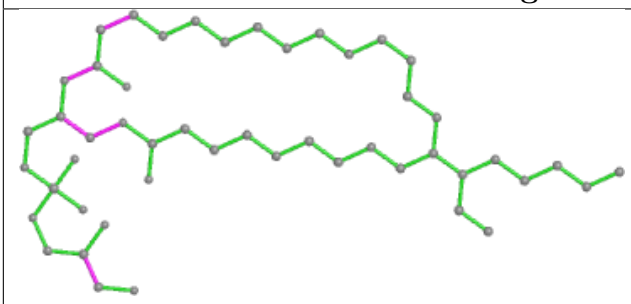
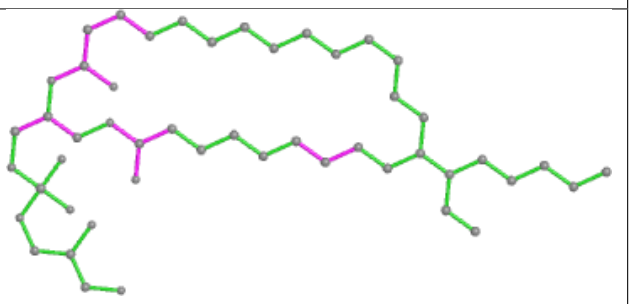
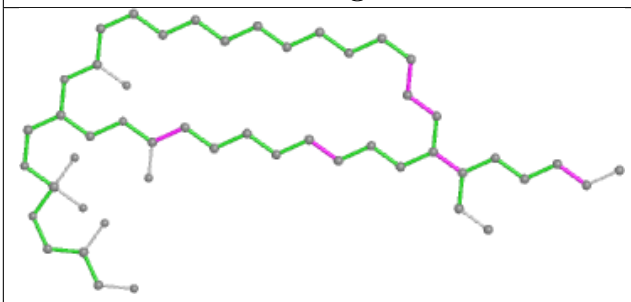
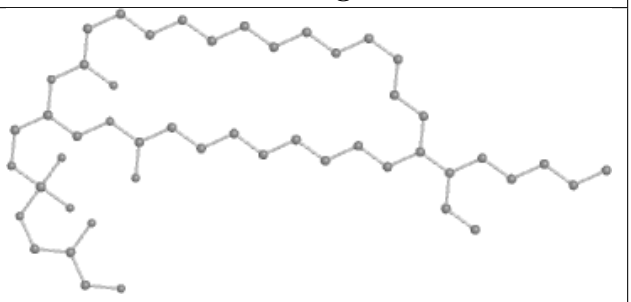
Ligand PEK T 102



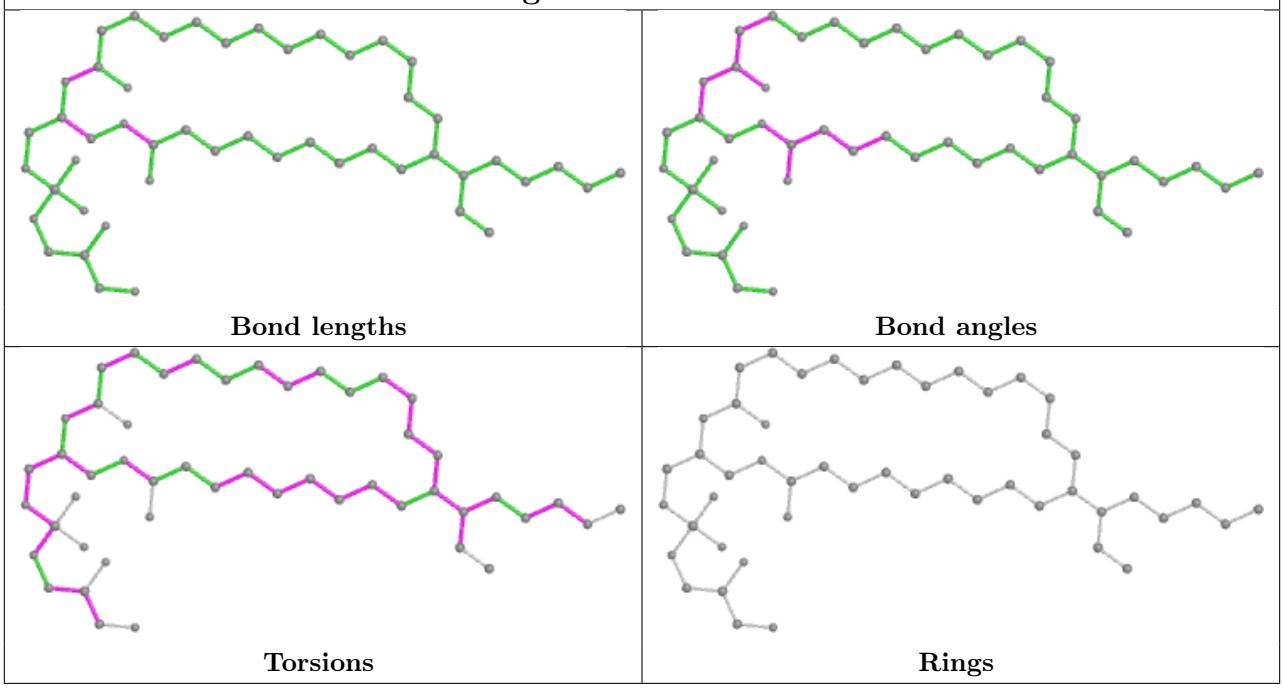
Ligand HEA N 601



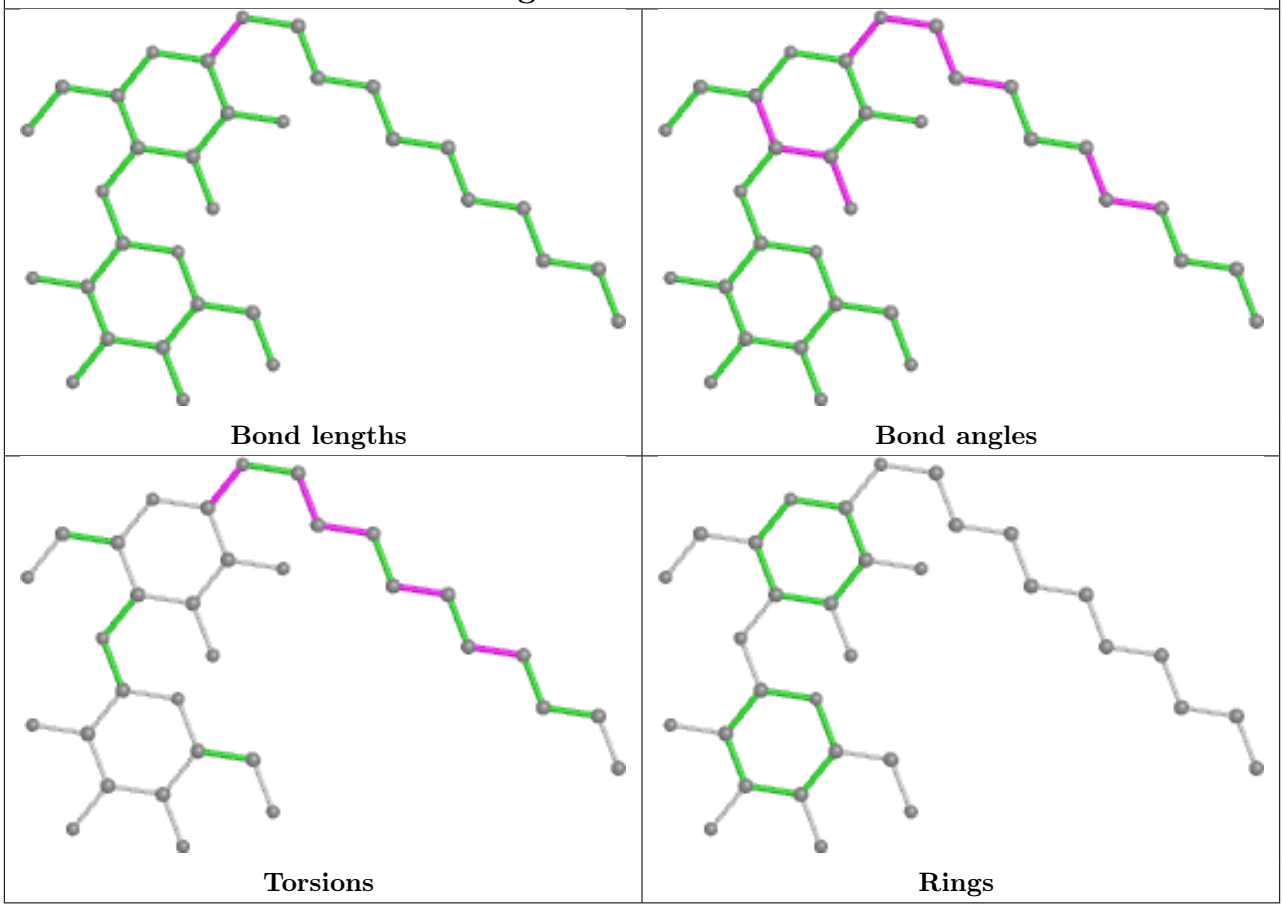
Ligand PGV A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV N 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

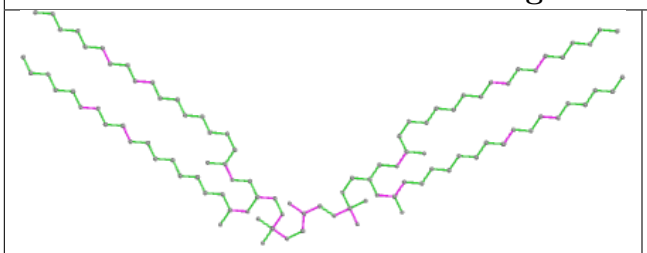
Ligand PGV C 308



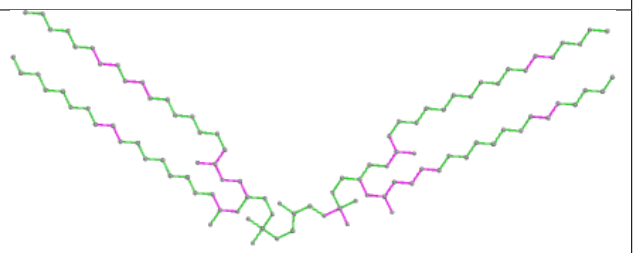
Ligand DMU C 302



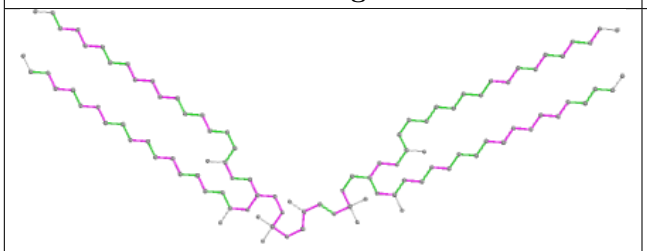
Ligand CDL P 305



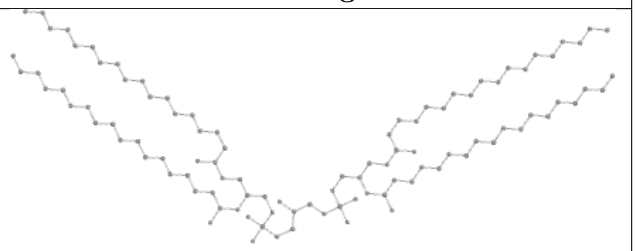
Bond lengths



Bond angles

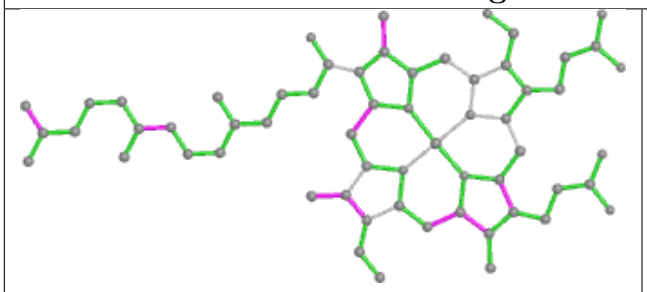


Torsions

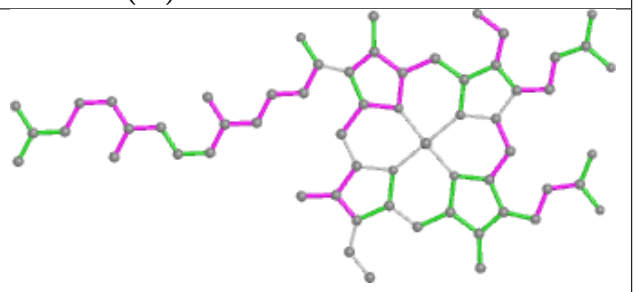


Rings

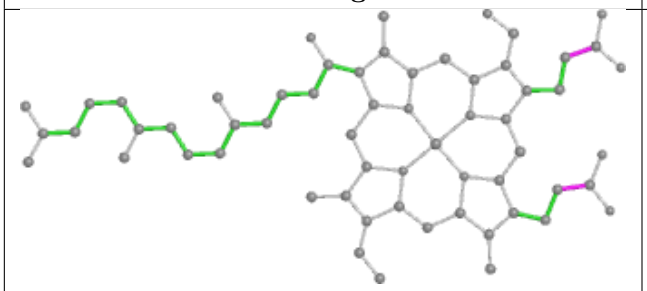
Ligand HEA A 602 (A)



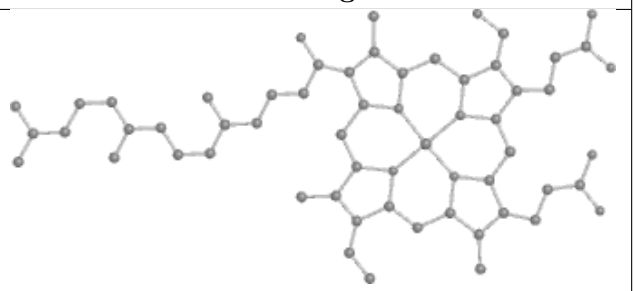
Bond lengths



Bond angles

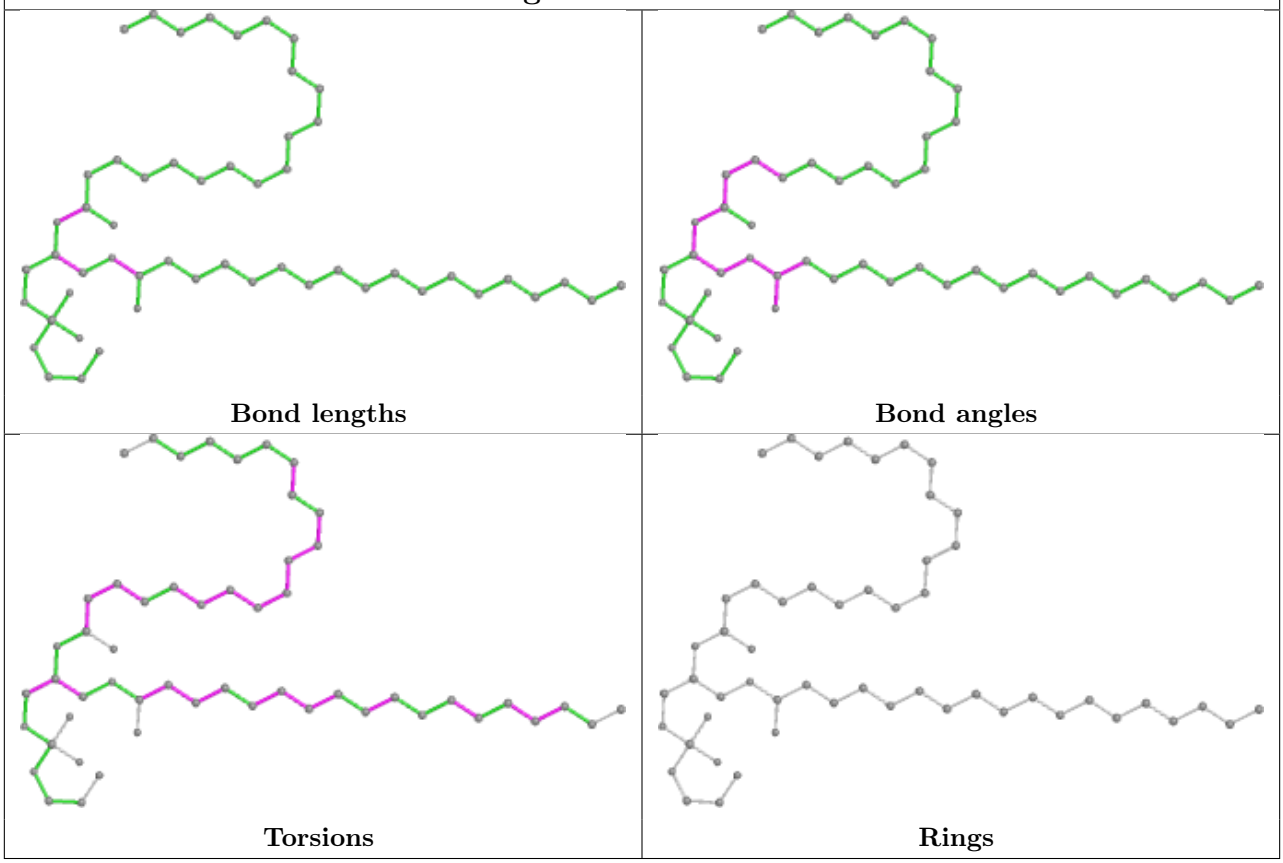


Torsions

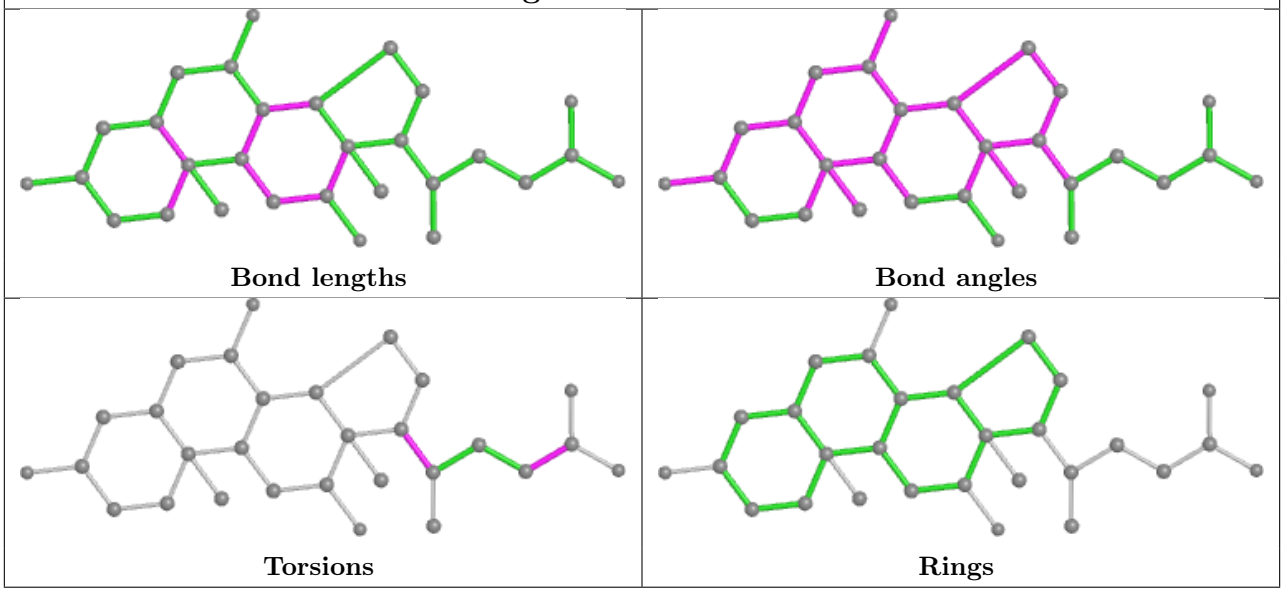


Rings

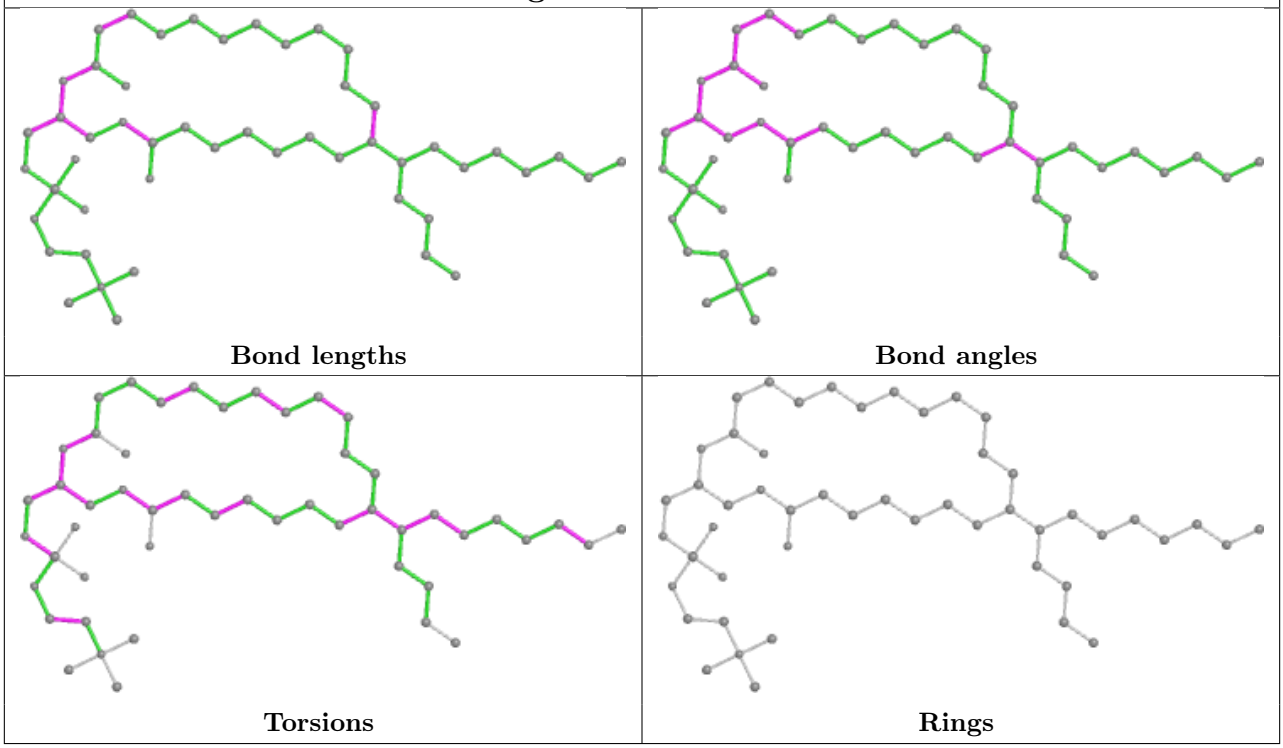
Ligand PEK G 104



Ligand CHD P 306



Ligand PSC B 303



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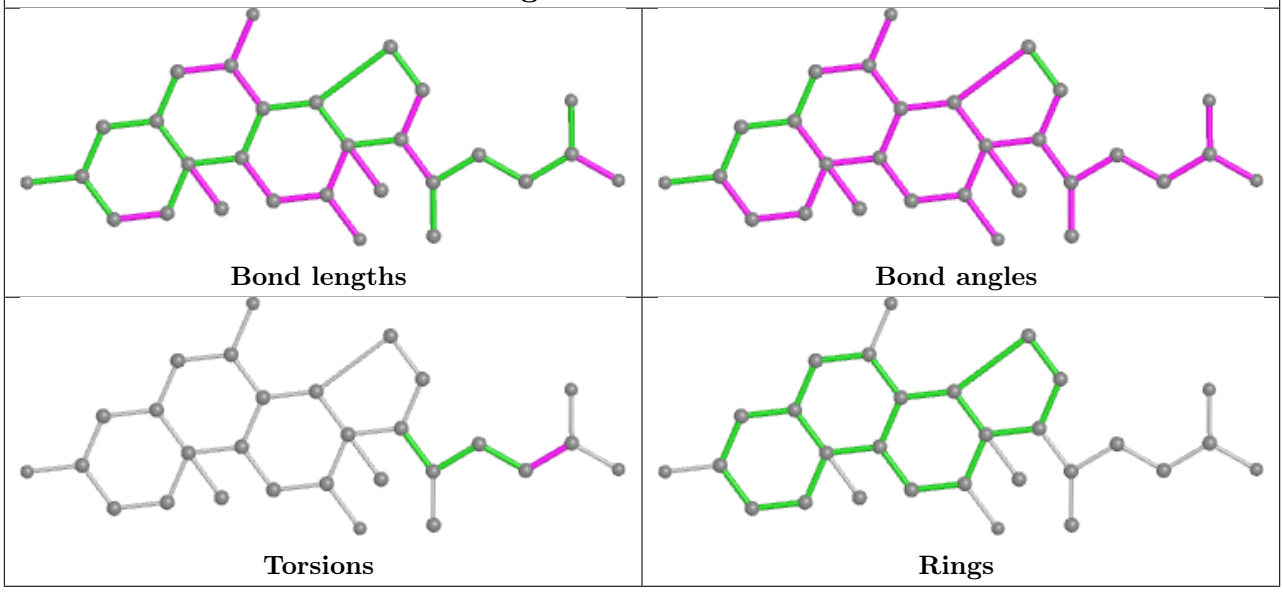
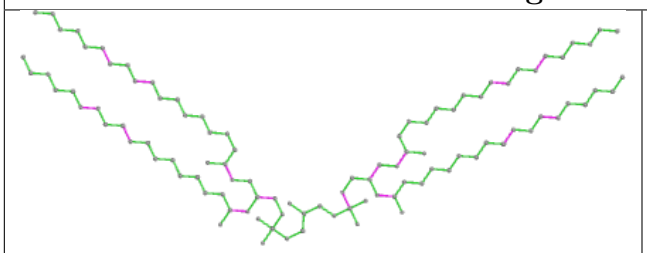
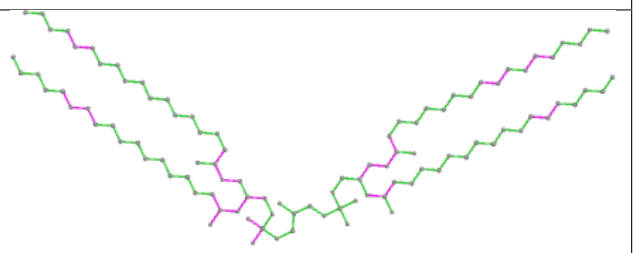


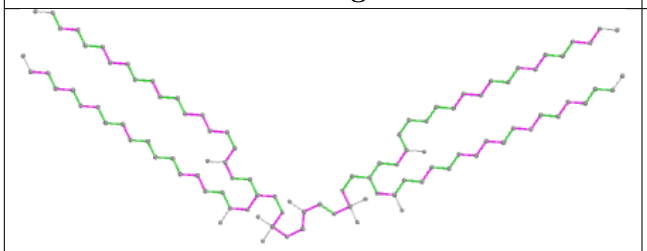
Ligand CDL T 103



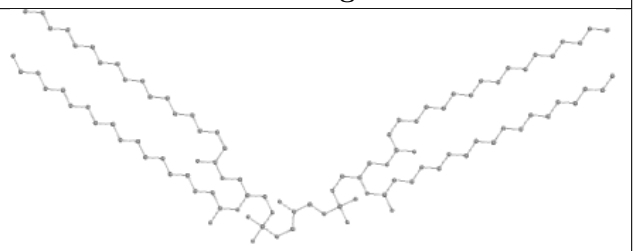
Bond lengths



Bond angles

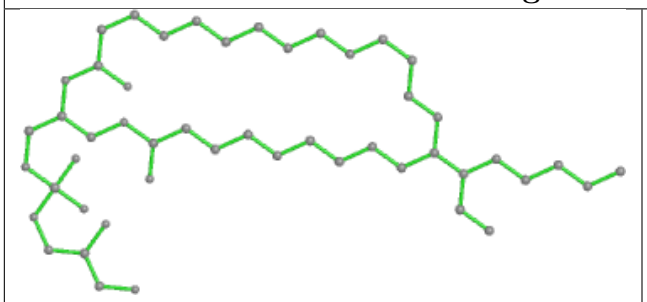


Torsions

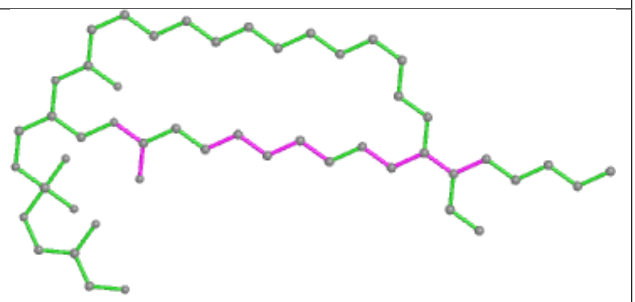


Rings

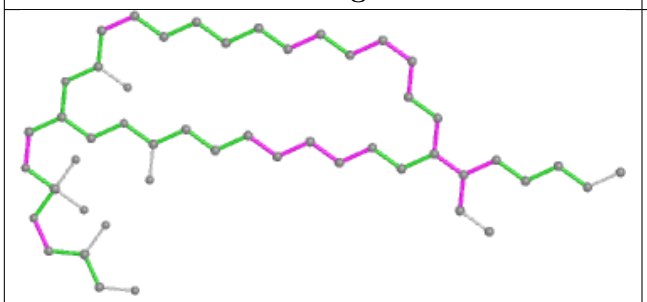
Ligand PGV C 304



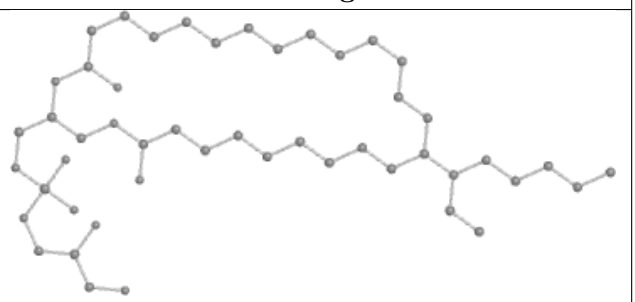
Bond lengths



Bond angles

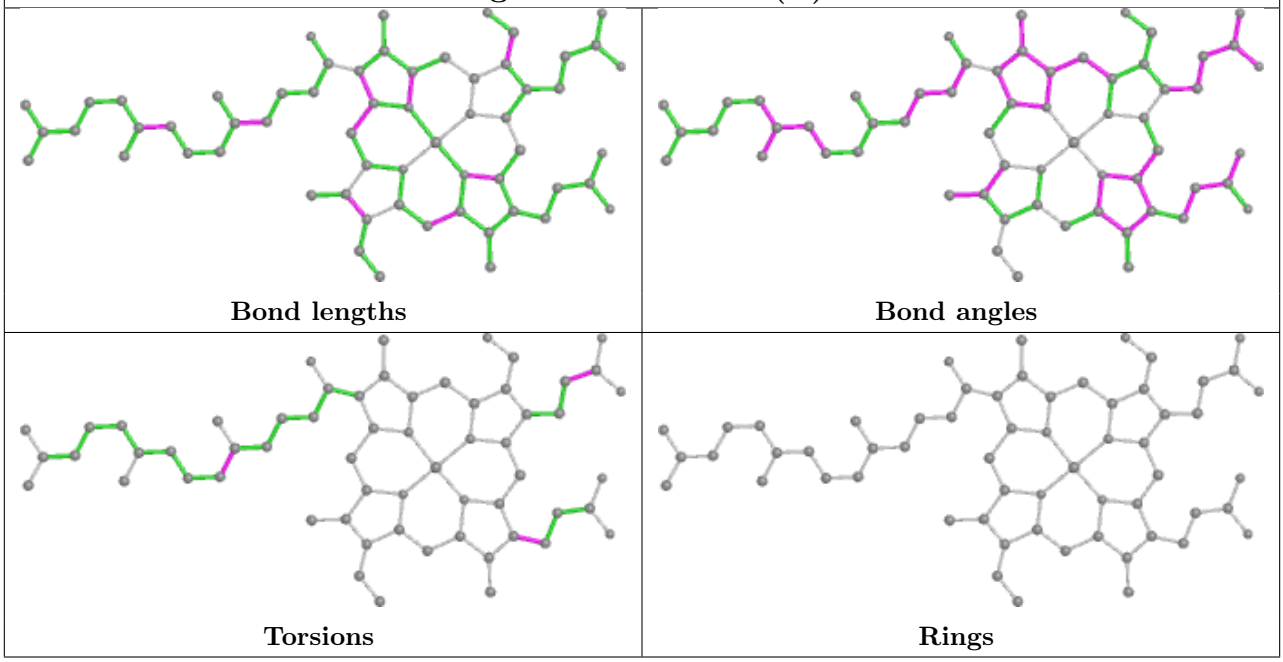


Torsions

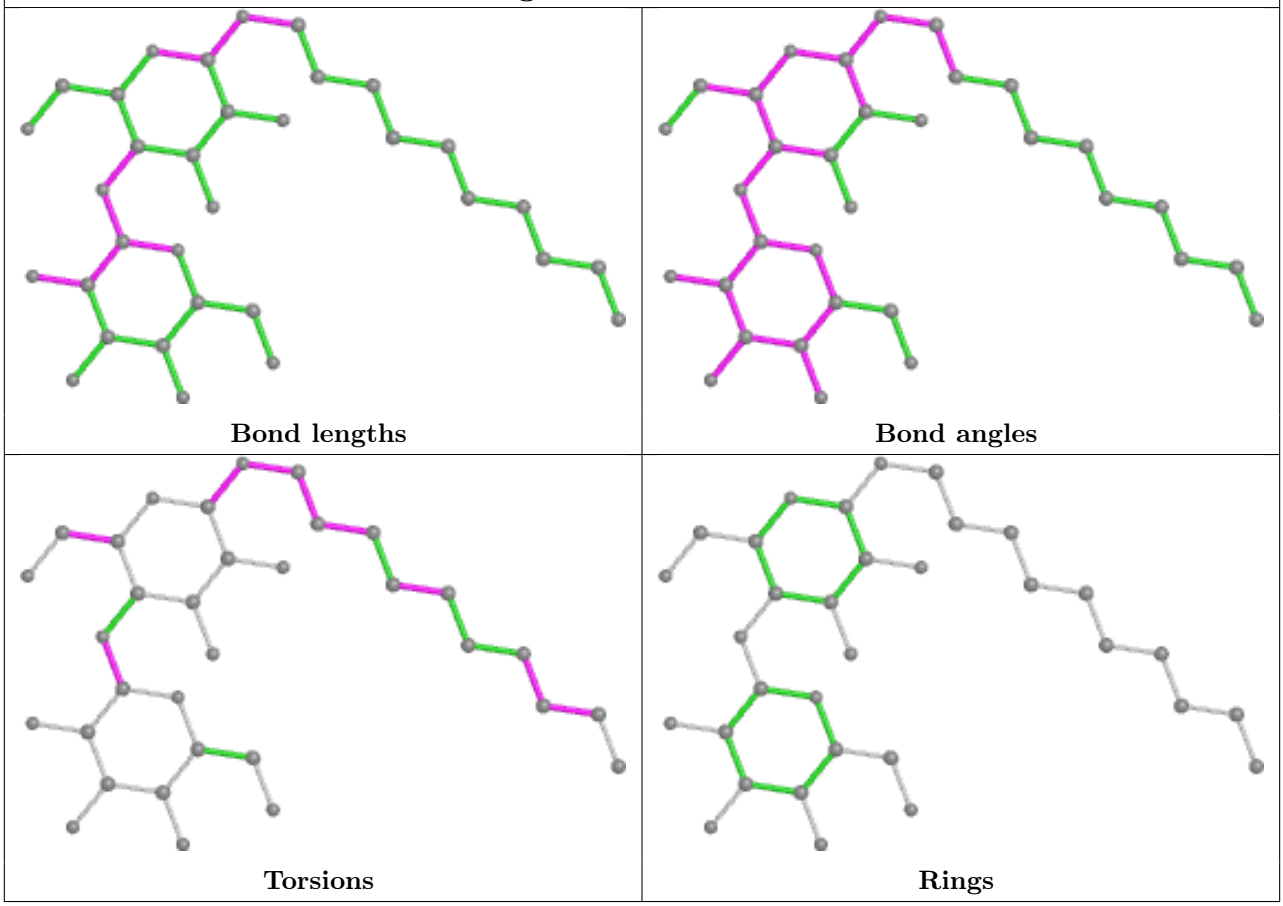


Rings

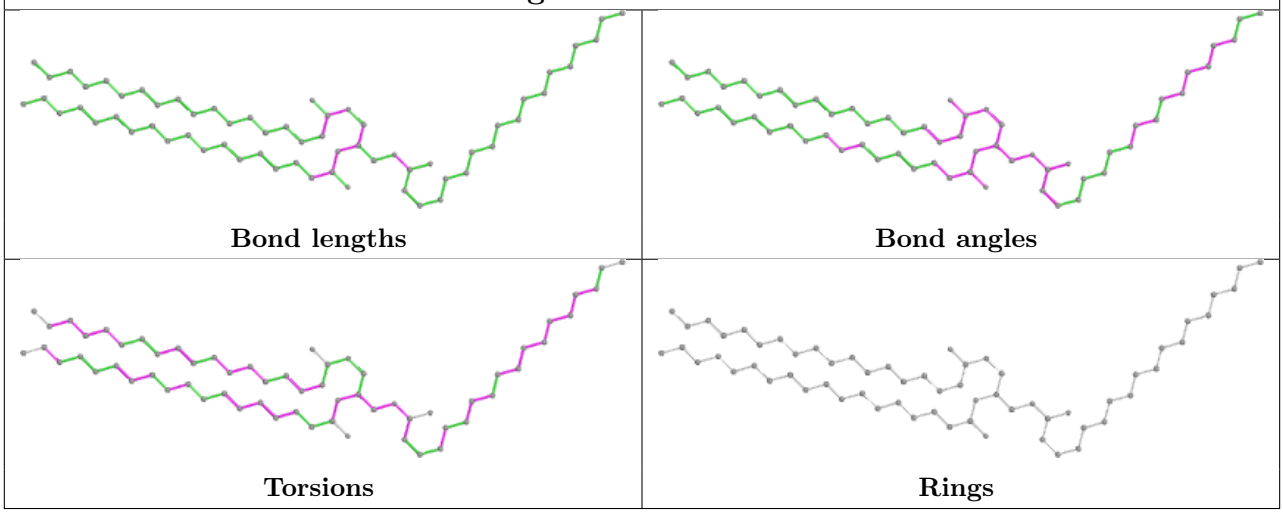
Ligand HEA A 602 (B)



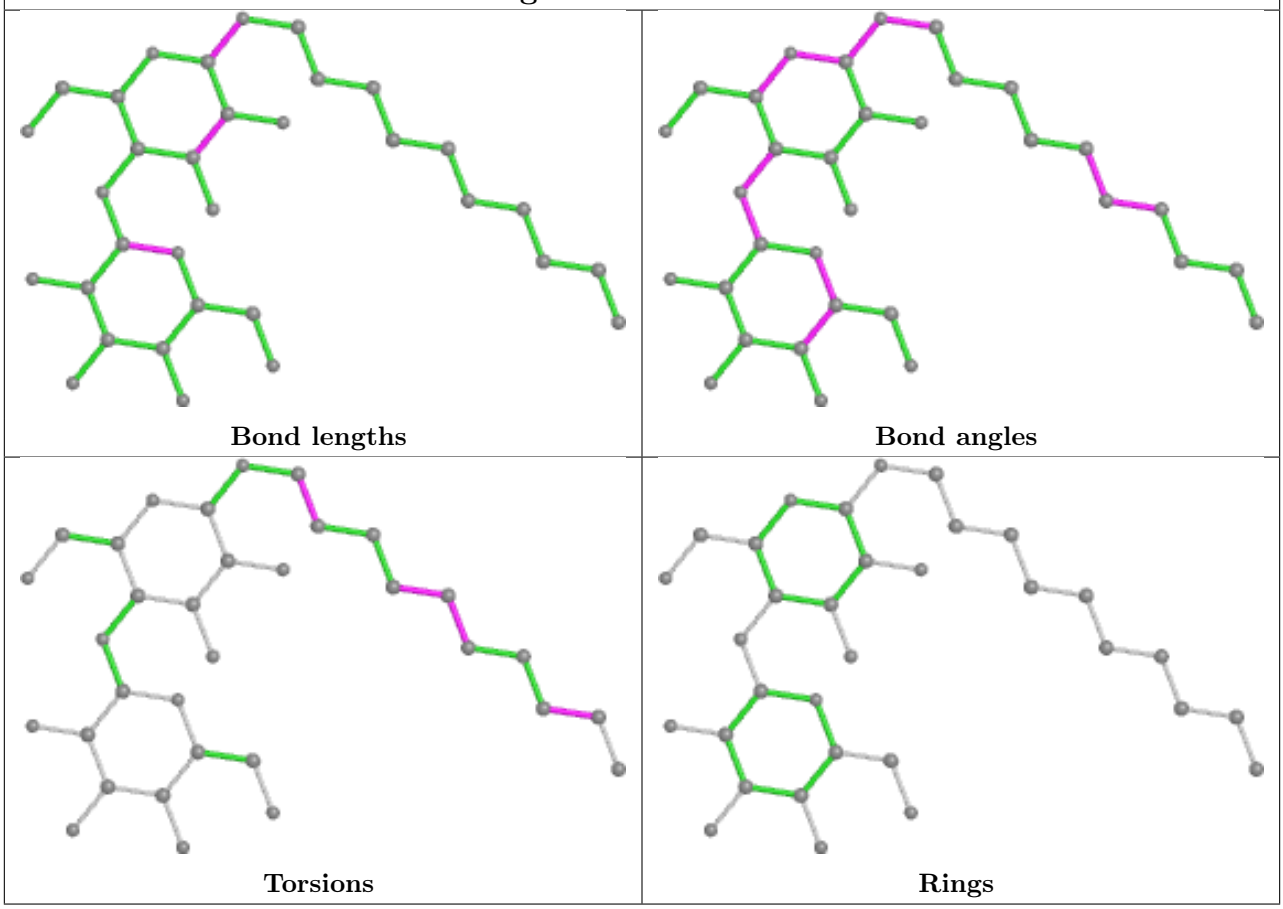
Ligand DMU C 310



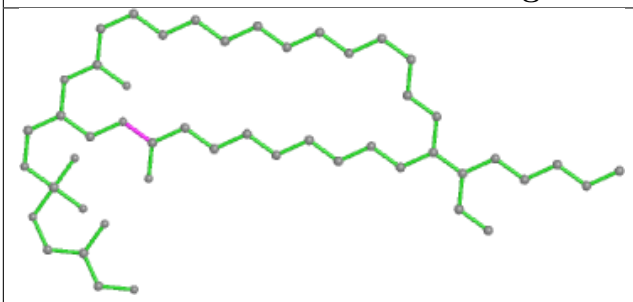
Ligand TGL L 101



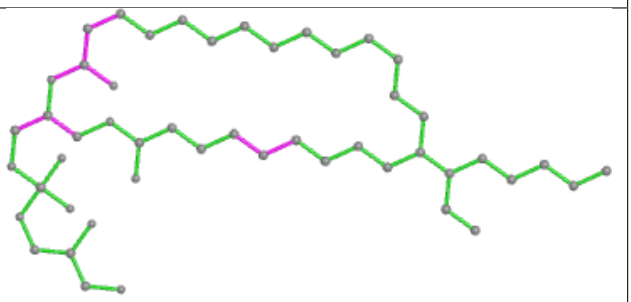
Ligand DMU Z 101



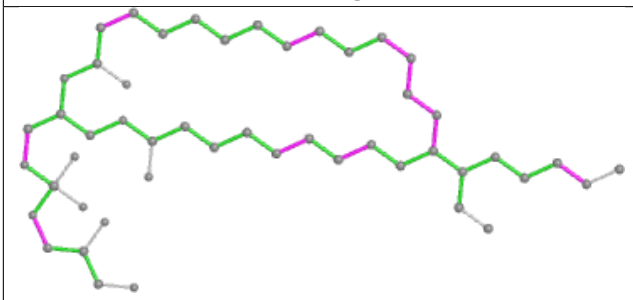
Ligand PGV P 304



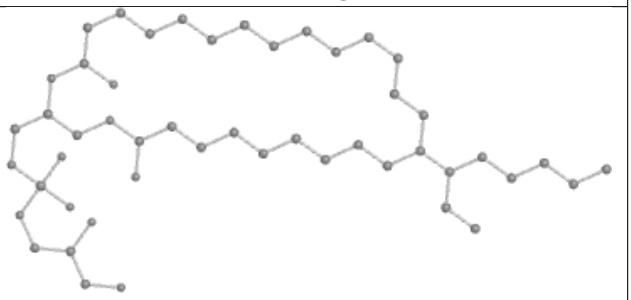
Bond lengths



Bond angles

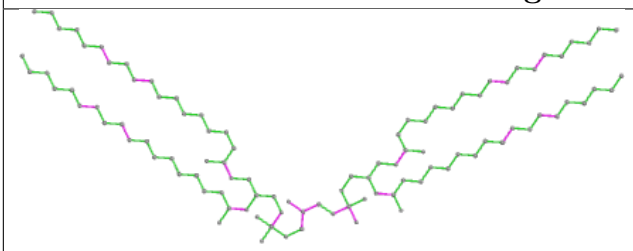


Torsions

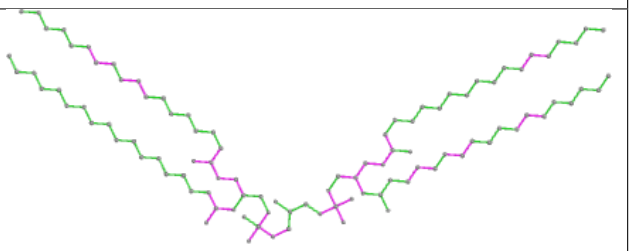


Rings

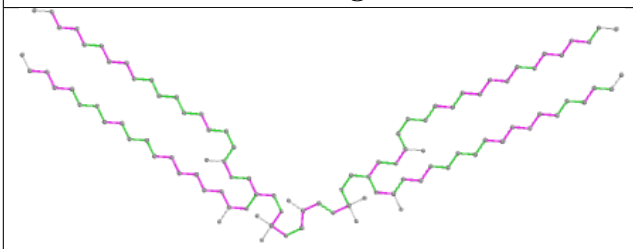
Ligand CDL C 305



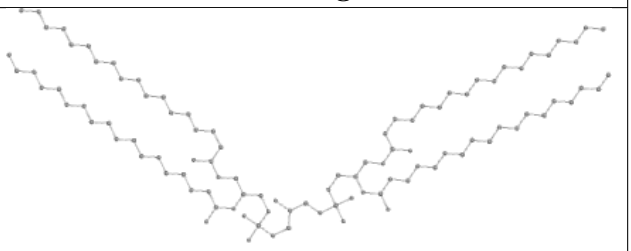
Bond lengths



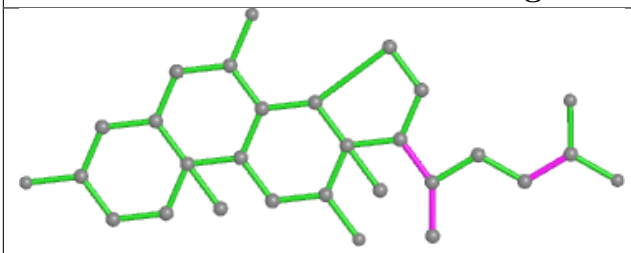
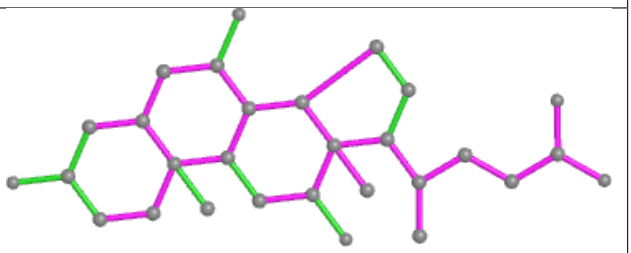
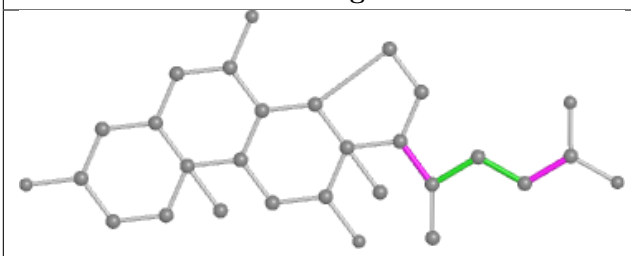
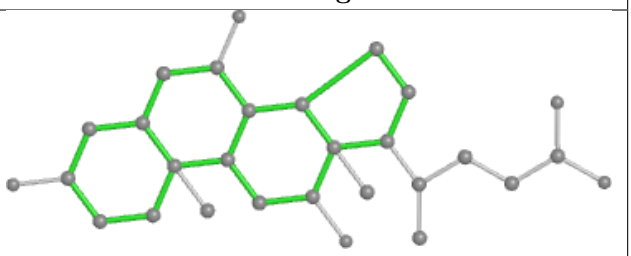
Bond angles

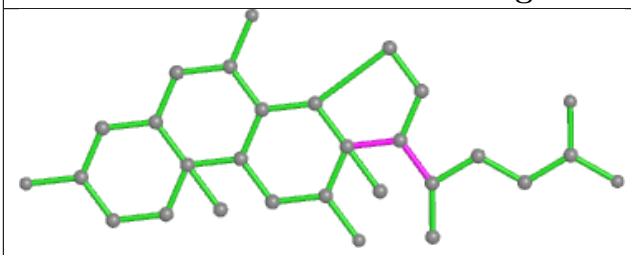
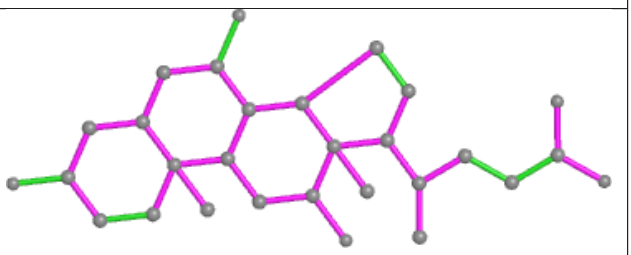
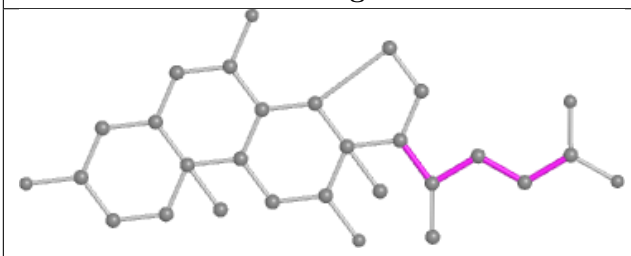
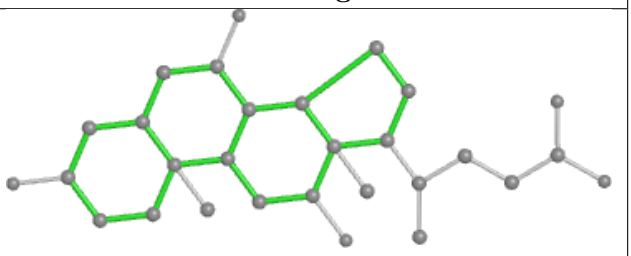


Torsions

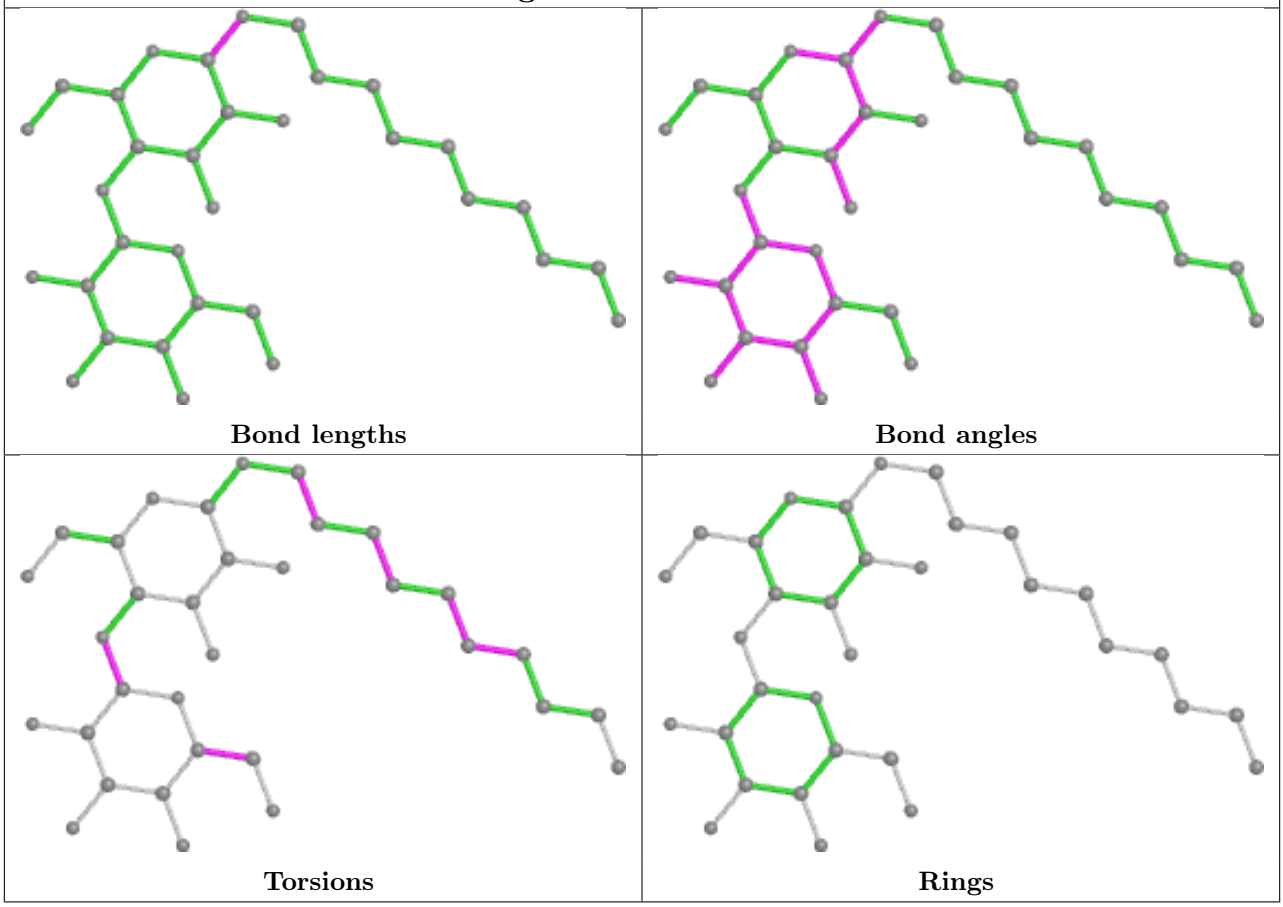


Rings

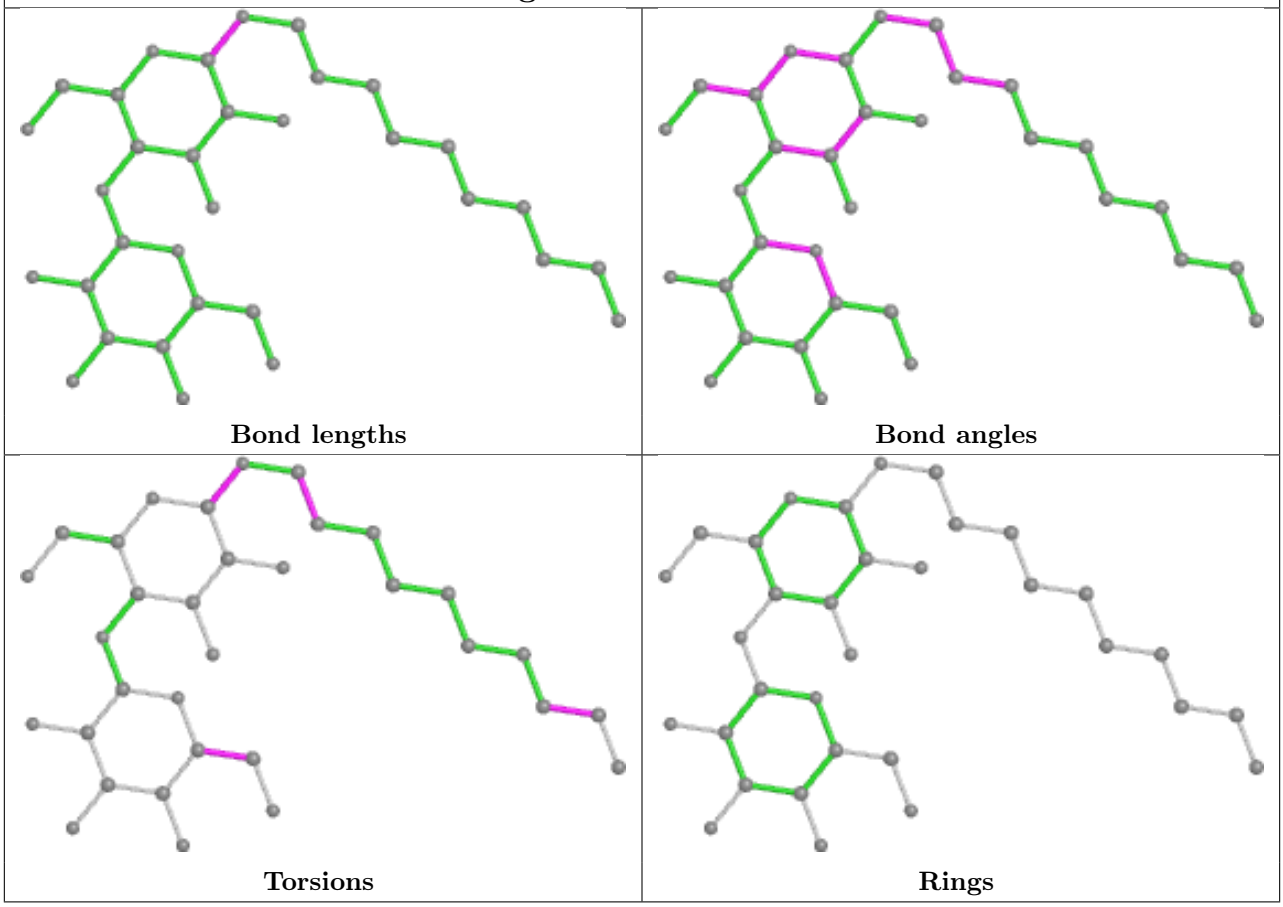
Ligand CHD J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

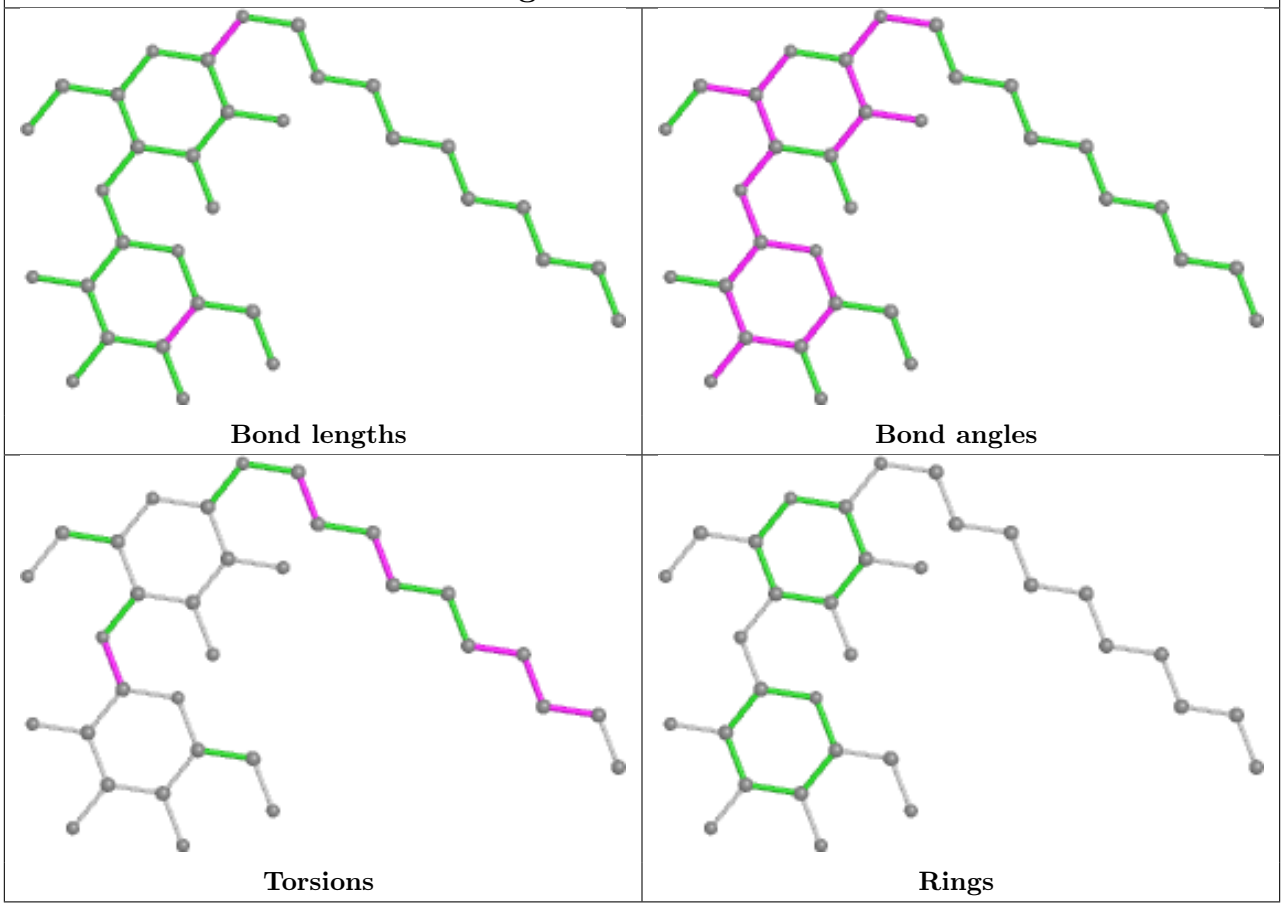
Ligand DMU C 309

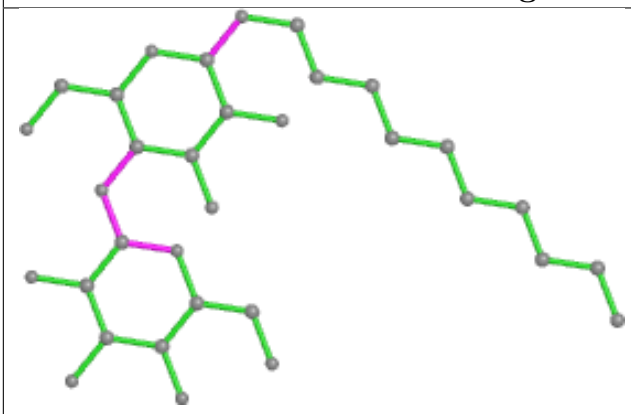
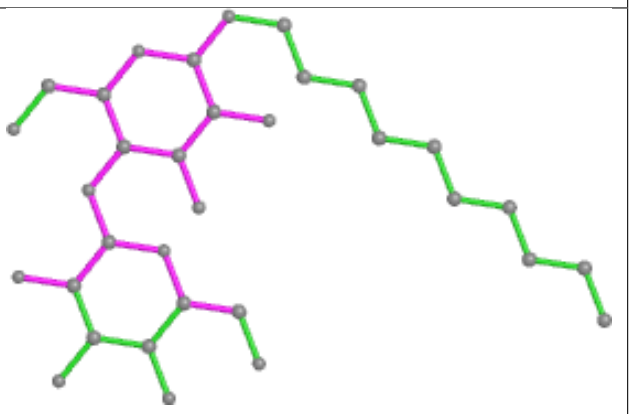
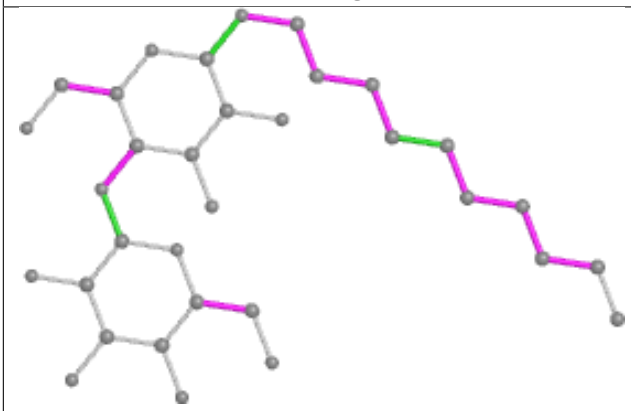
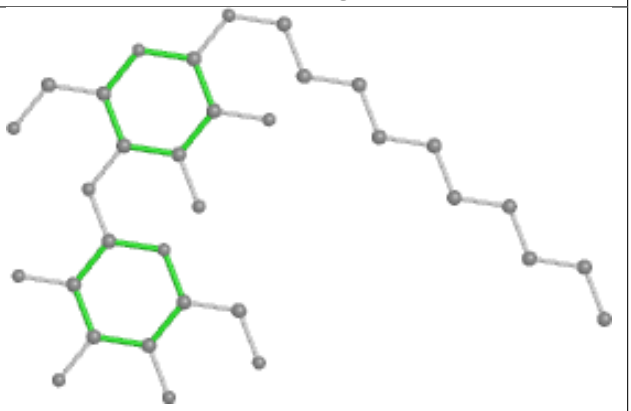


Ligand DMU P 307

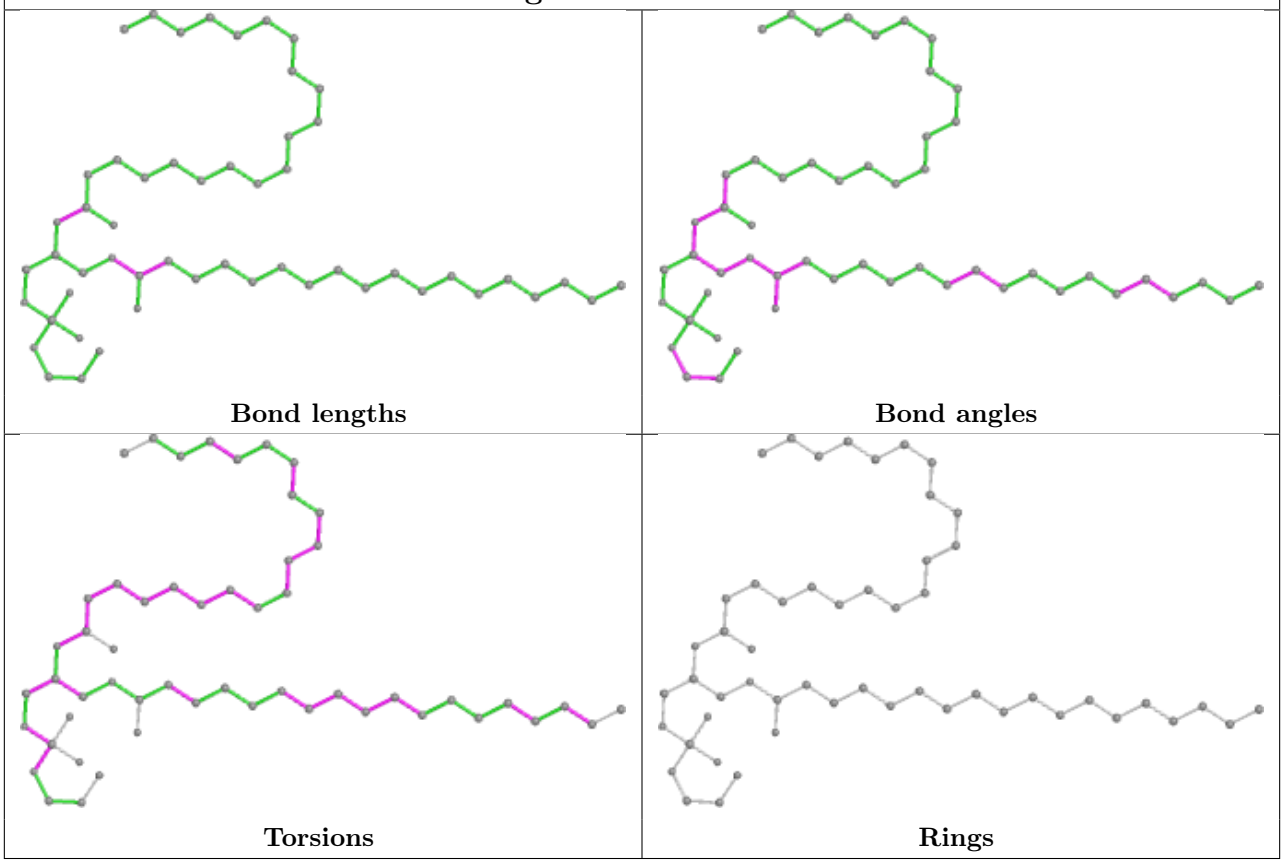


Ligand DMU P 309

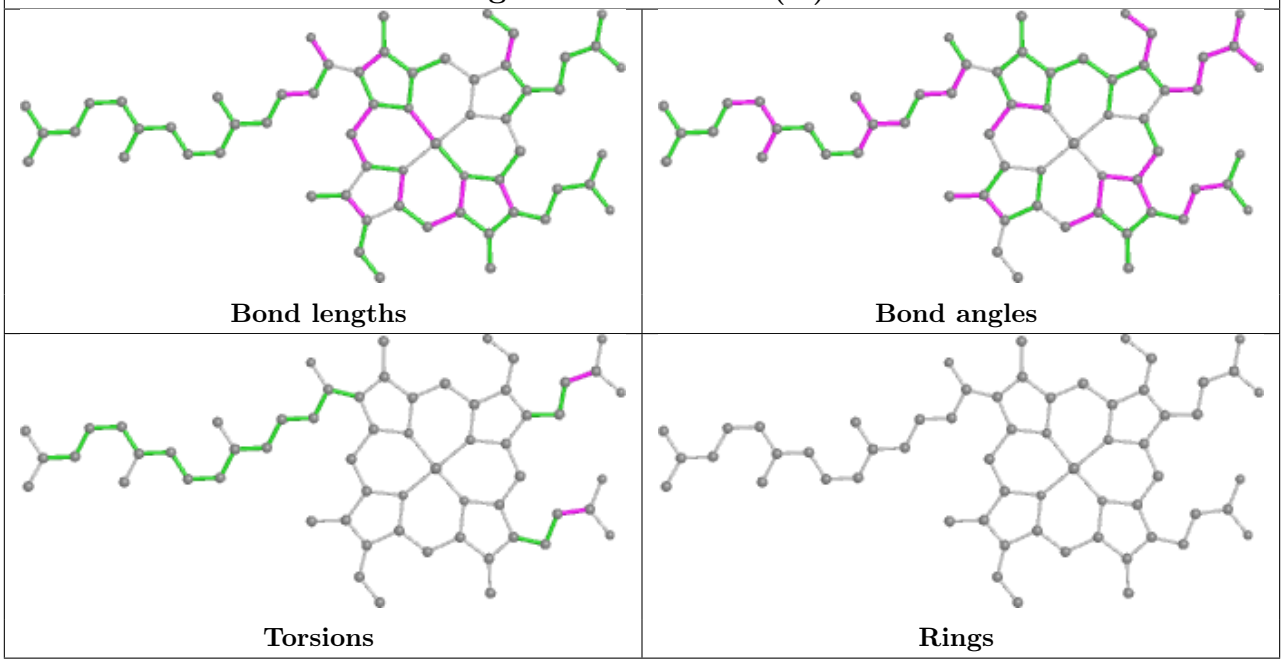


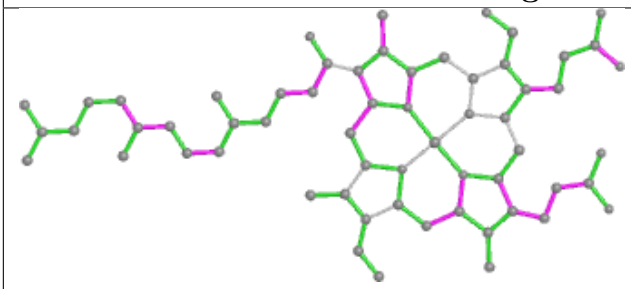
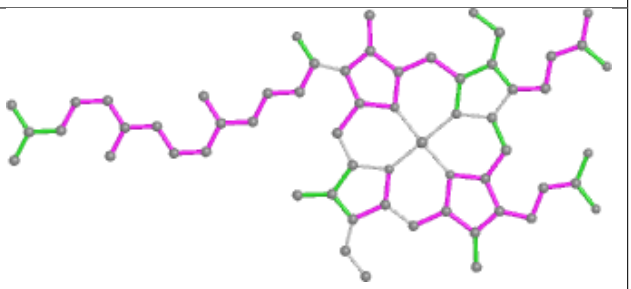
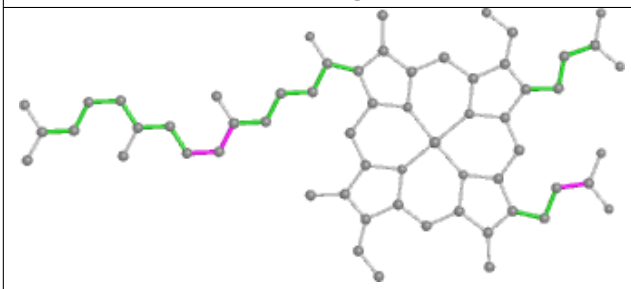
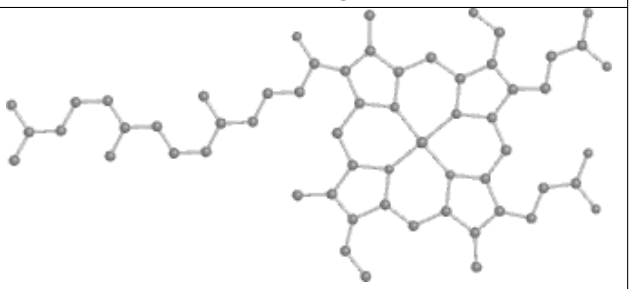
Ligand DMU L 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

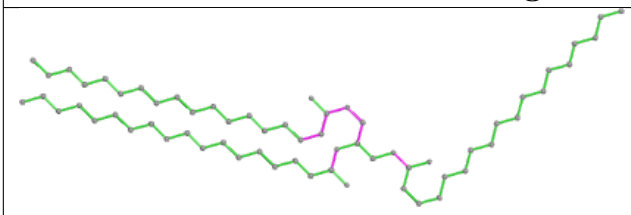
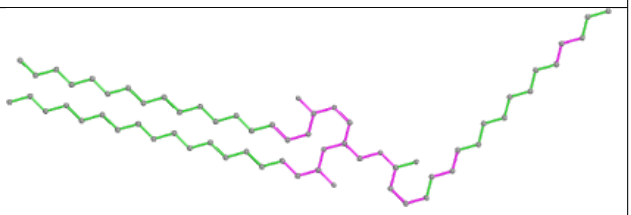
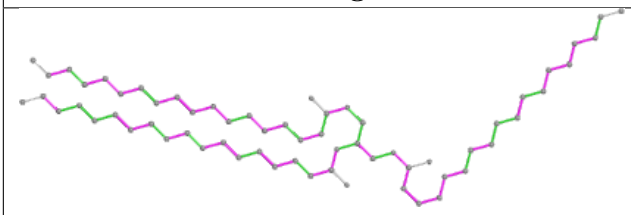
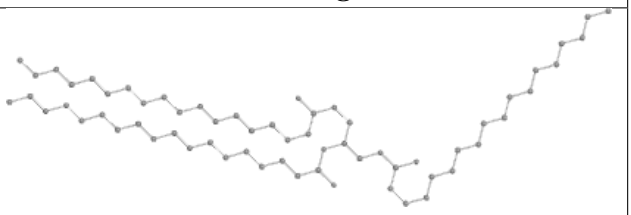
Ligand PEK P 308



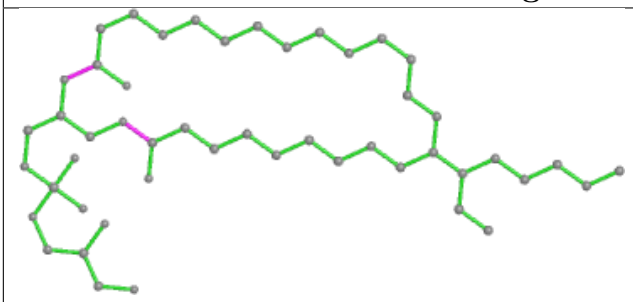
Ligand HEA N 602 (A)



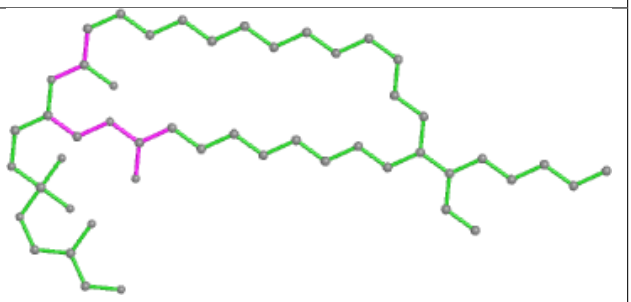
Ligand HEA A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TGL Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

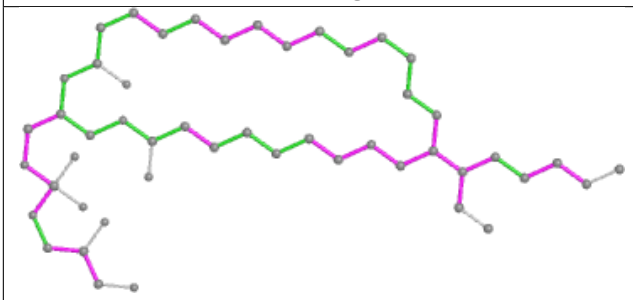
Ligand PGV P 302



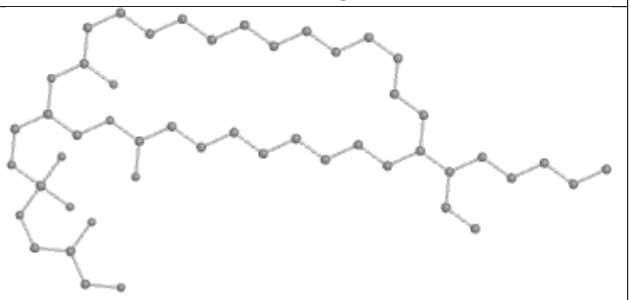
Bond lengths



Bond angles

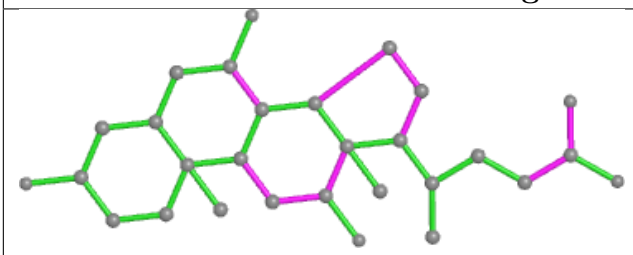


Torsions

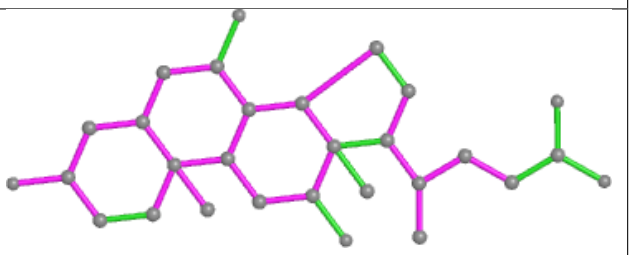


Rings

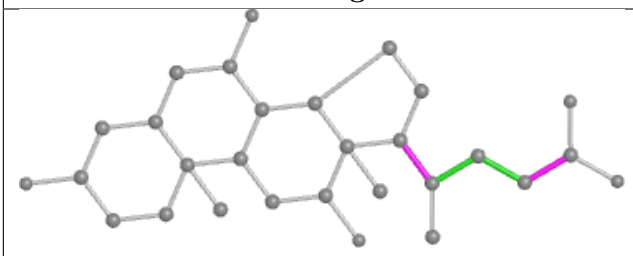
Ligand CHD P 301



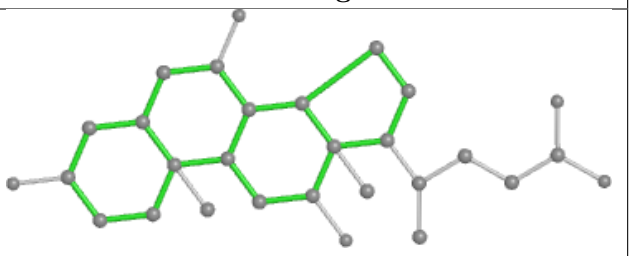
Bond lengths



Bond angles

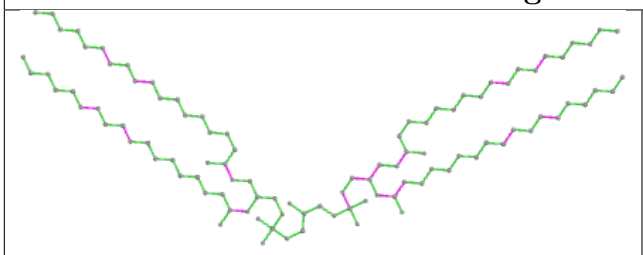


Torsions

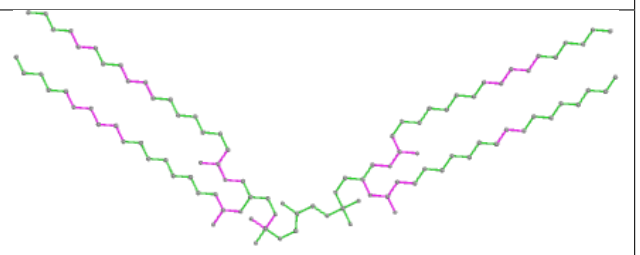


Rings

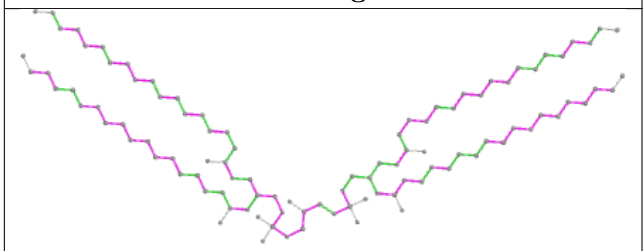
Ligand CDL G 102



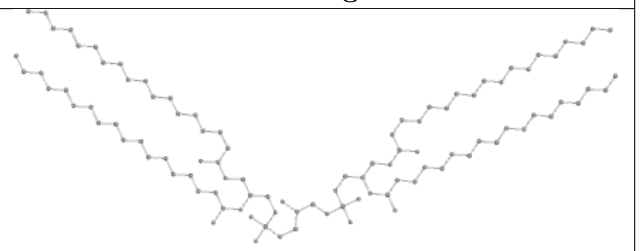
Bond lengths



Bond angles

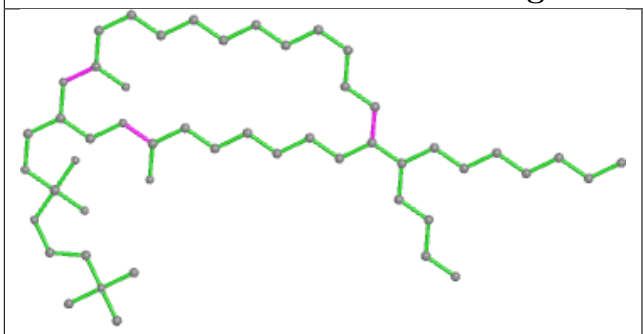


Torsions

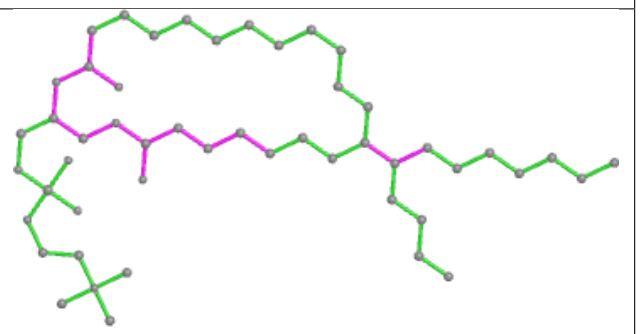


Rings

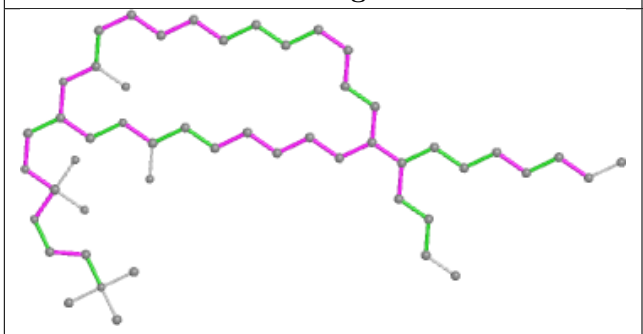
Ligand PSC O 302



Bond lengths



Bond angles



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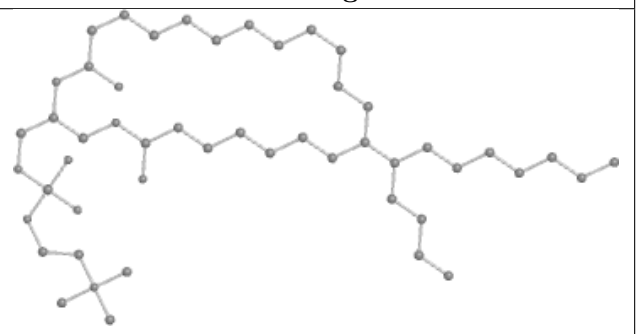
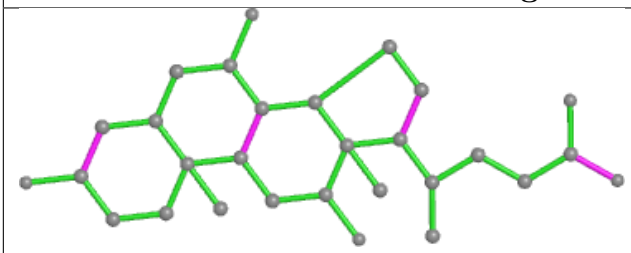


Rings

Ligand CHD C 306



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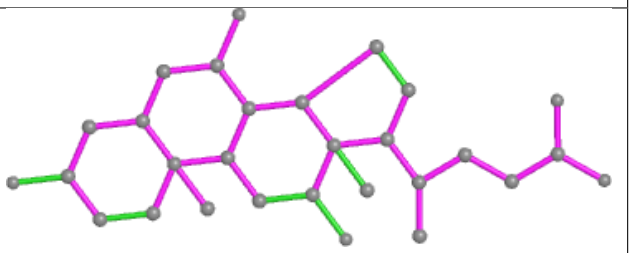

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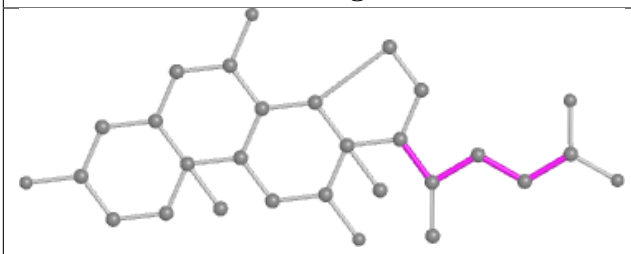

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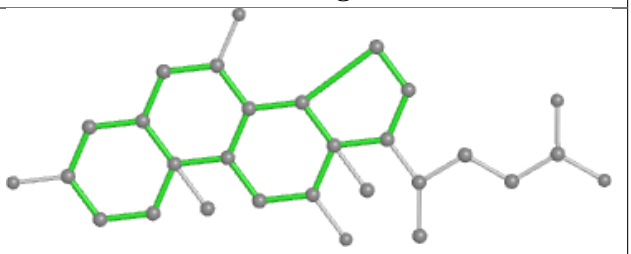
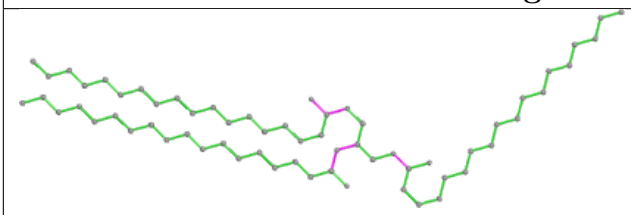


Rings

Ligand TGL A 608



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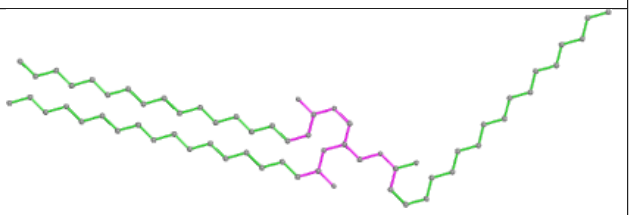
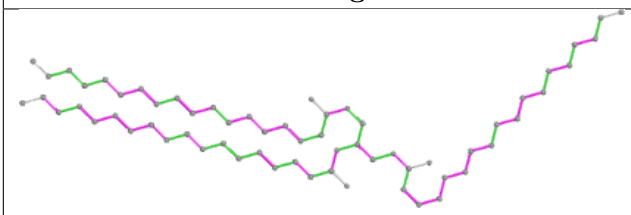


Bond angles



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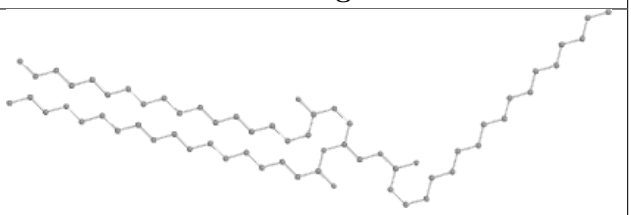
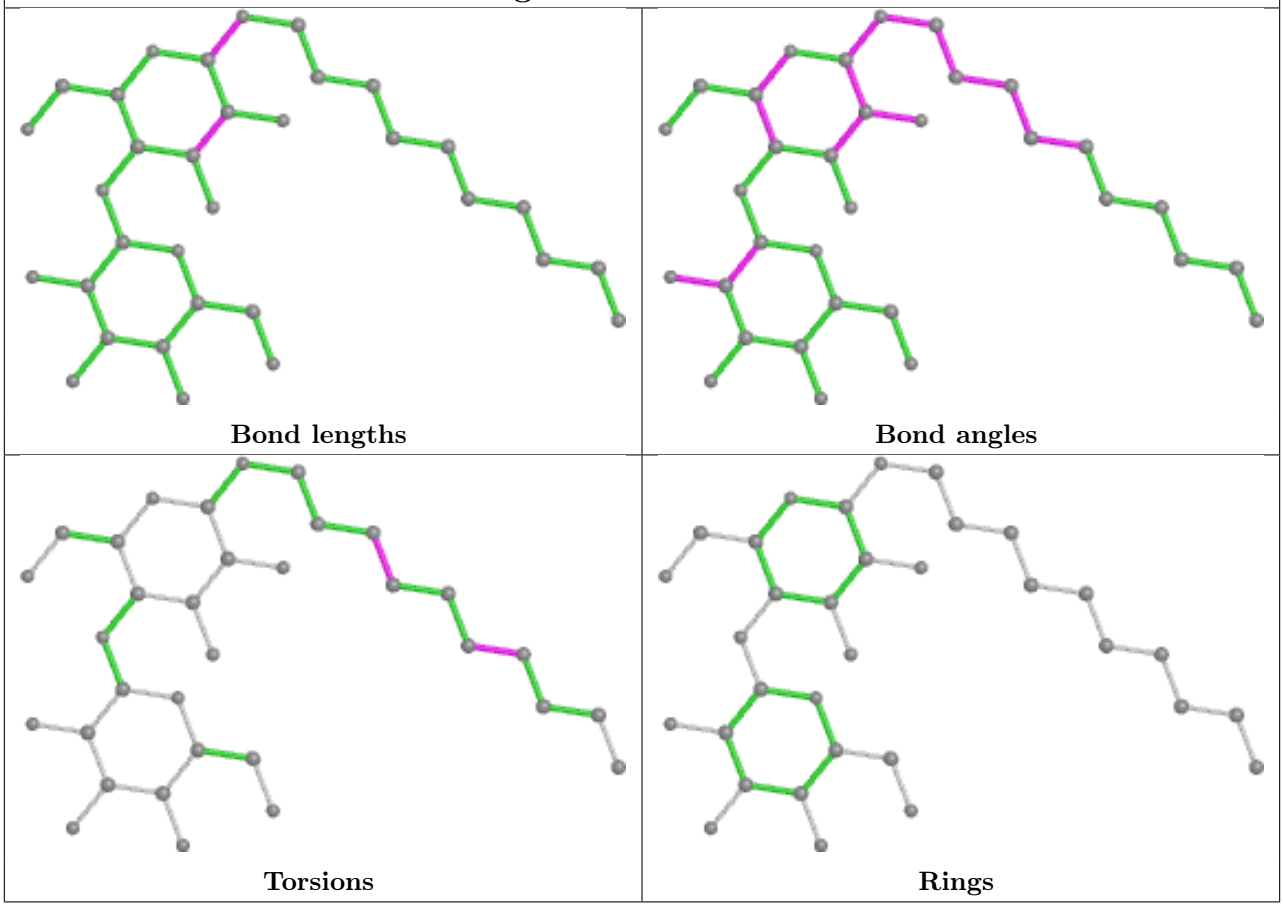
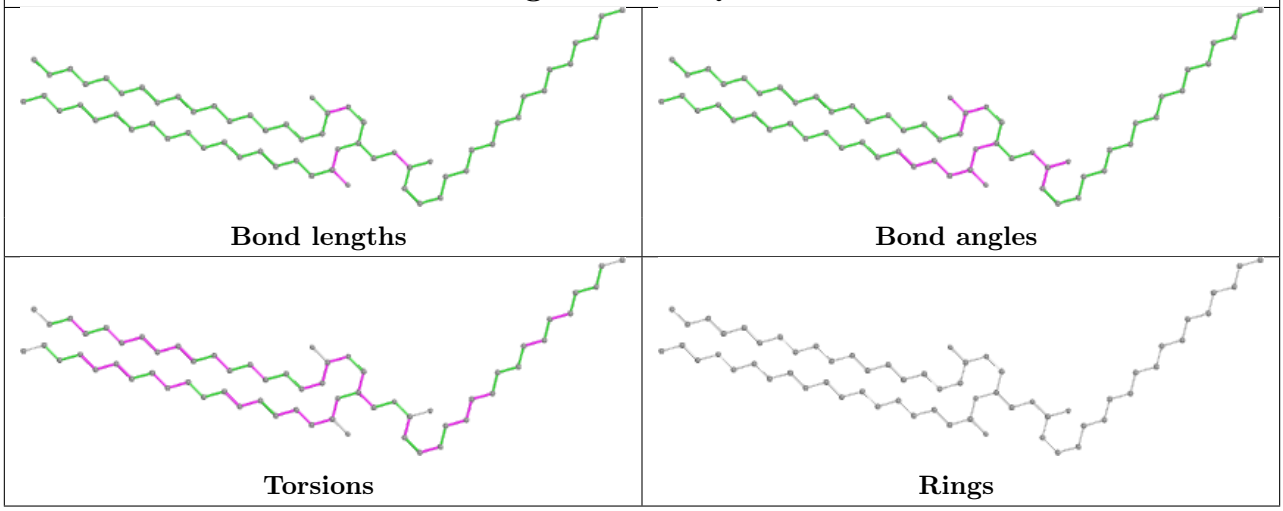


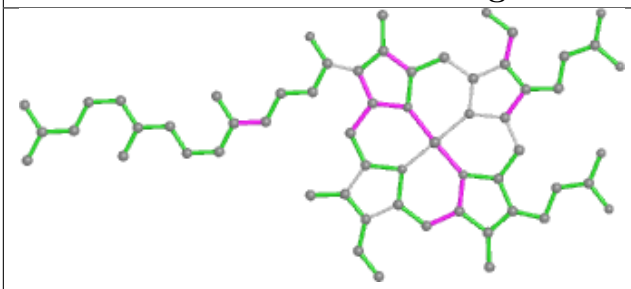
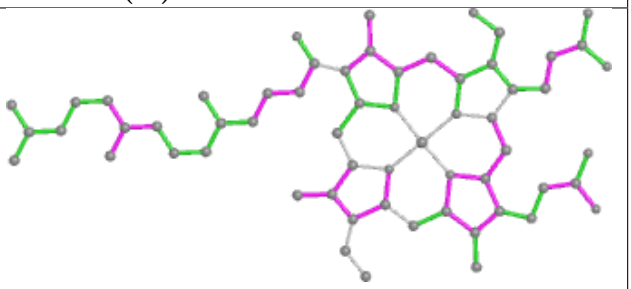
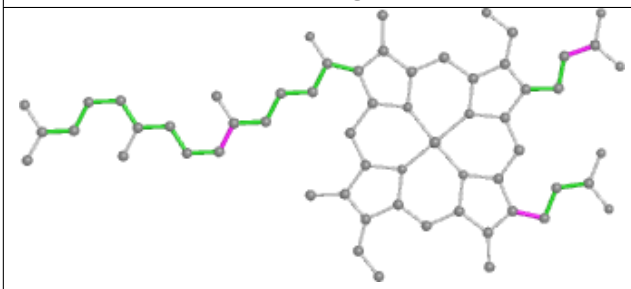
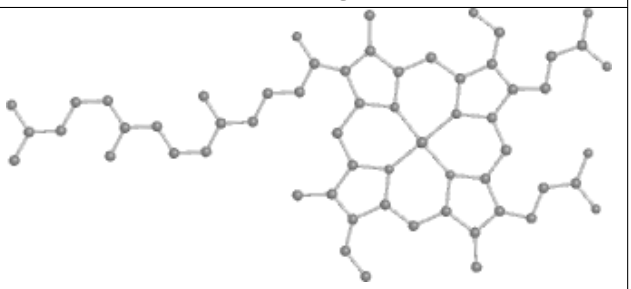
Rings

Ligand DMU M 101



Ligand TGL Q 201



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

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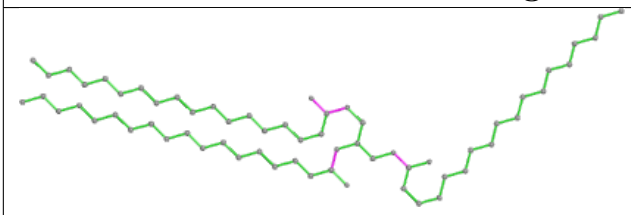
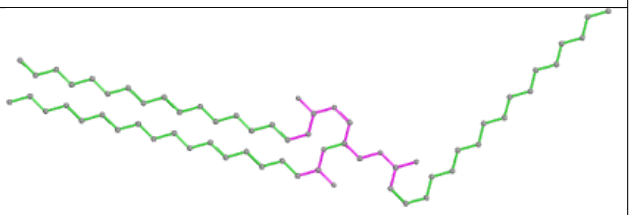
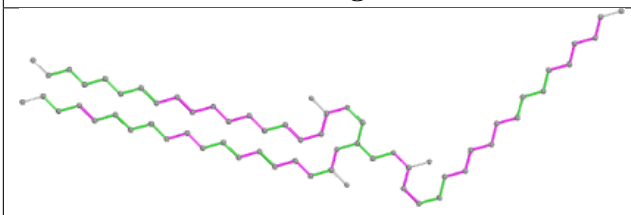
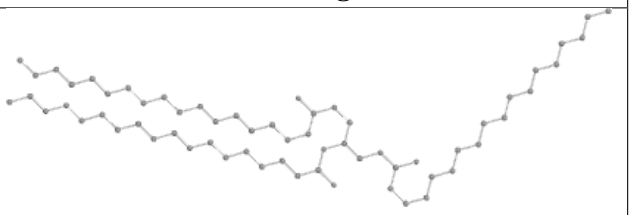
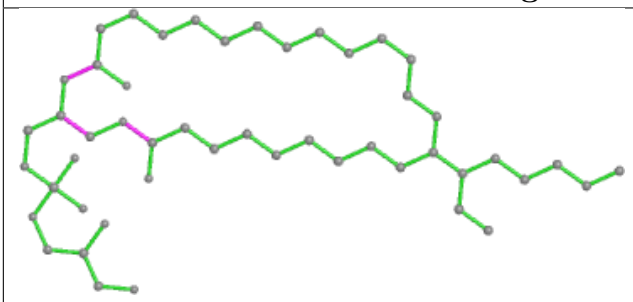
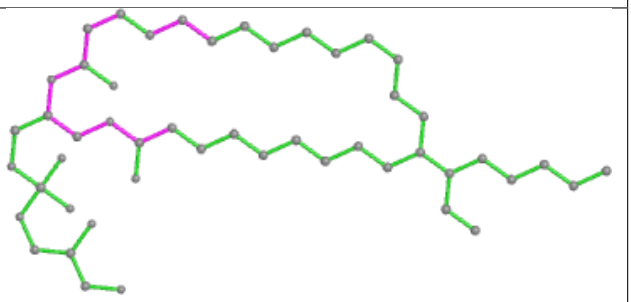
 Bond lengths	 Bond angles
 Torsions	 Rings

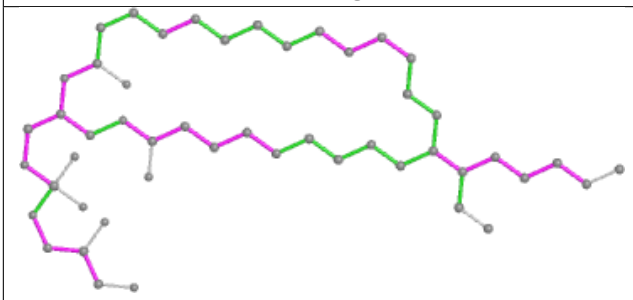
Ligand PGV X 101



Bond lengths



Bond angles



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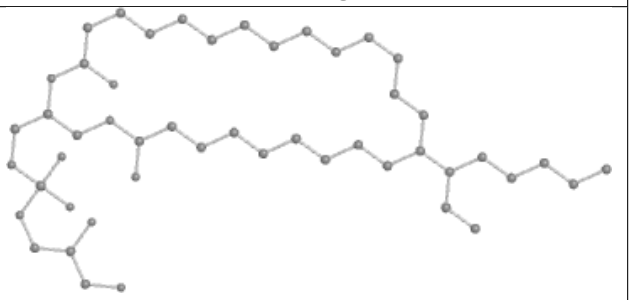
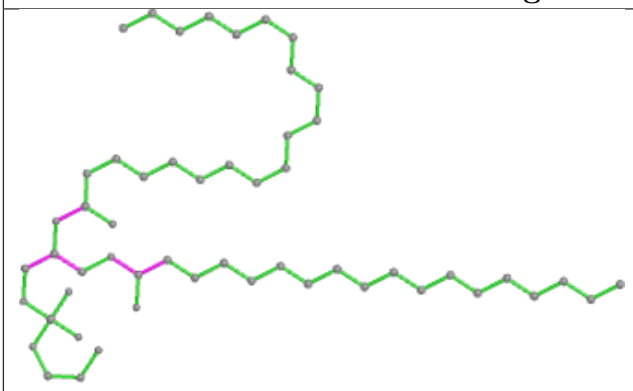


Rings

Ligand PEK C 307



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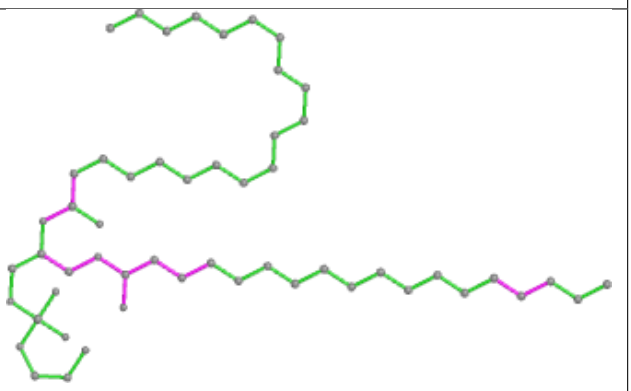
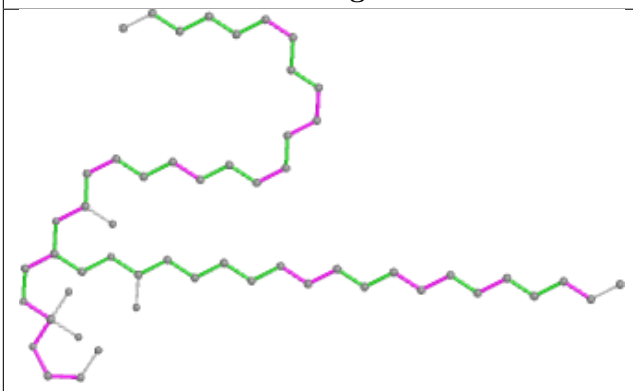


Bond angles



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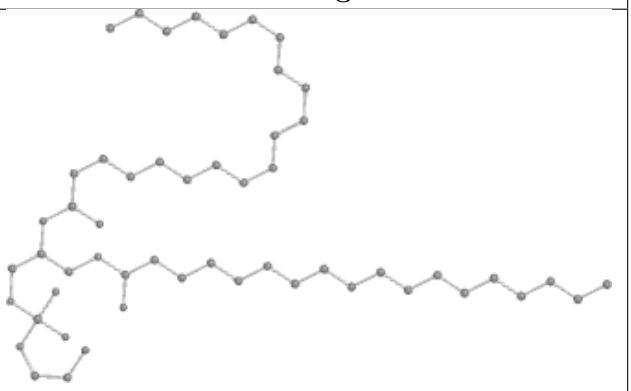
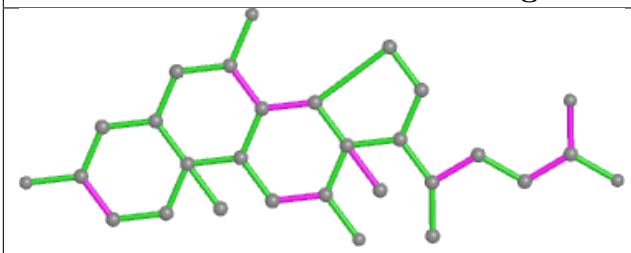


Rings

Ligand CHD C 301



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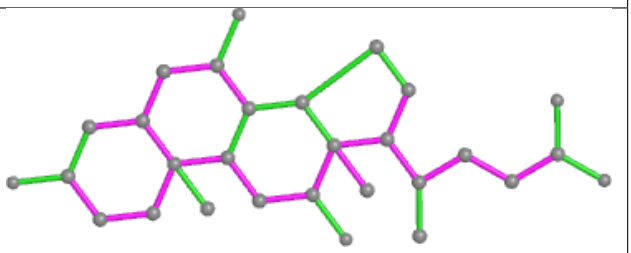
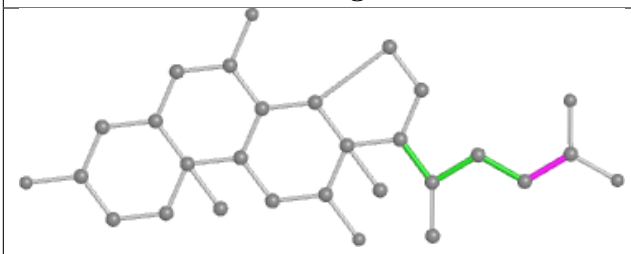


Bond angles



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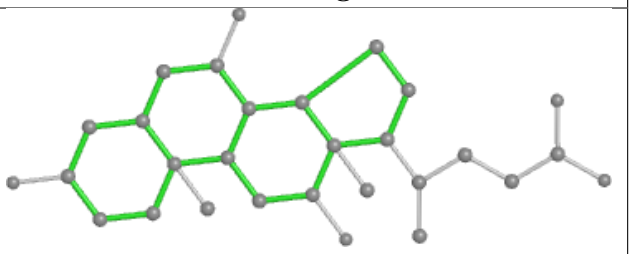
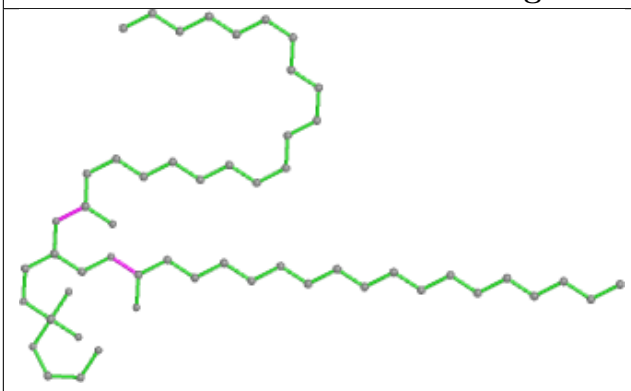


Rings

Ligand PEK T 101



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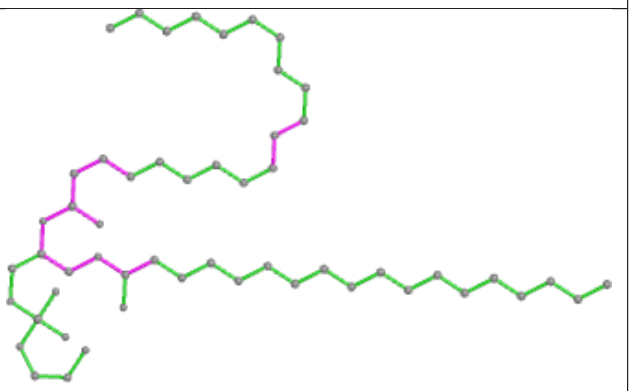
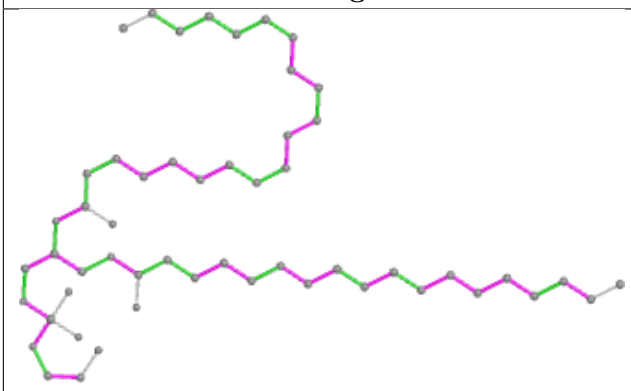
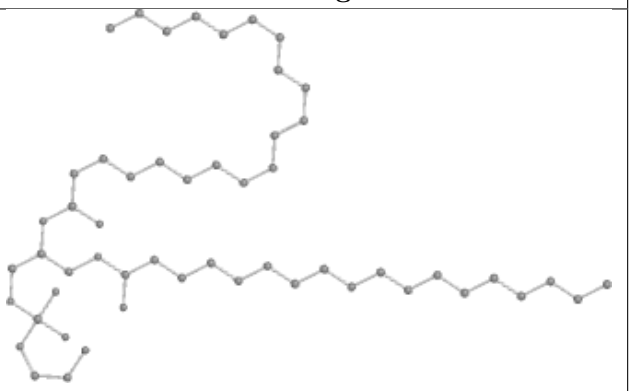


Bond angles

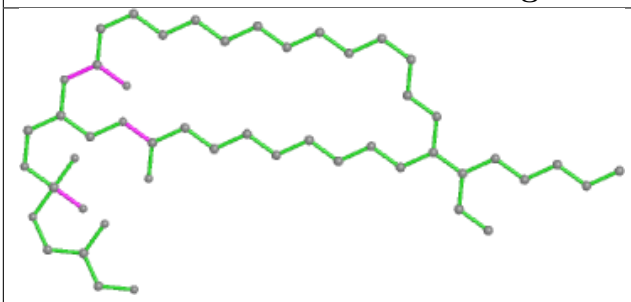


Torsions



Rings

Ligand PGV A 610



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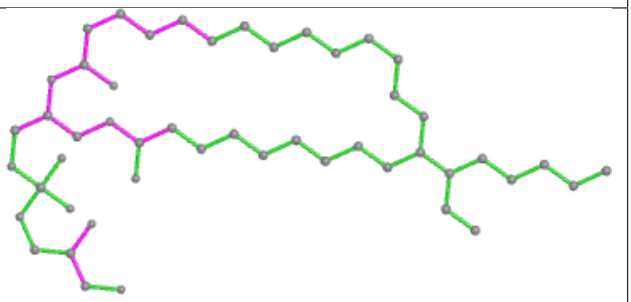
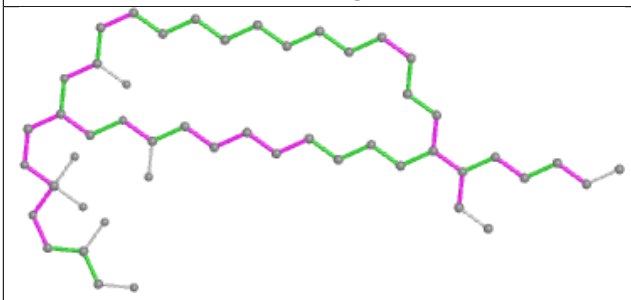


Bond angles



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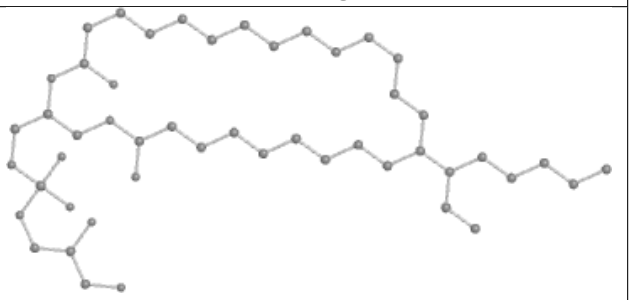
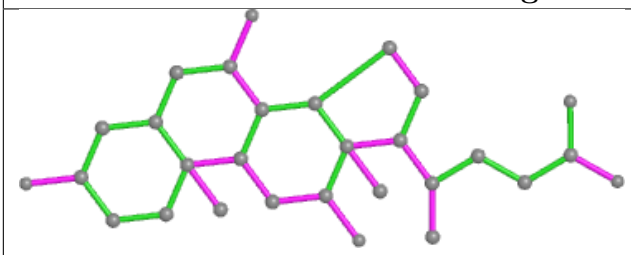


Rings

Ligand CHD B 301



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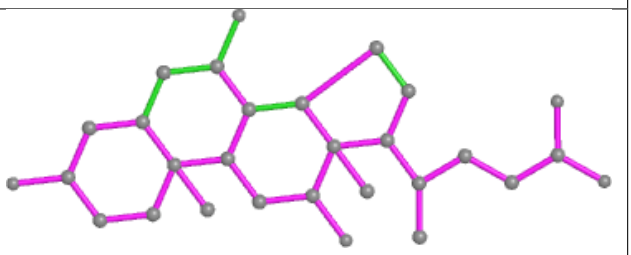
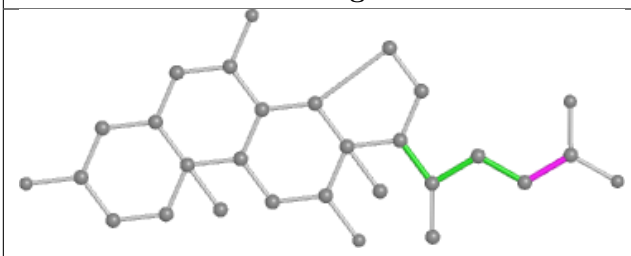
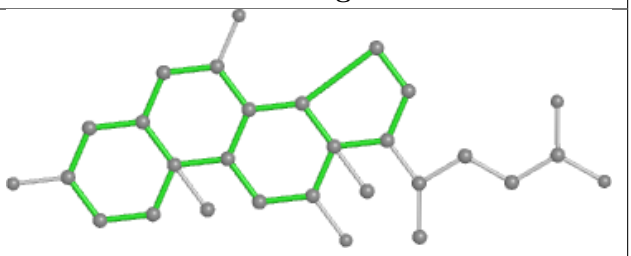


Bond angles

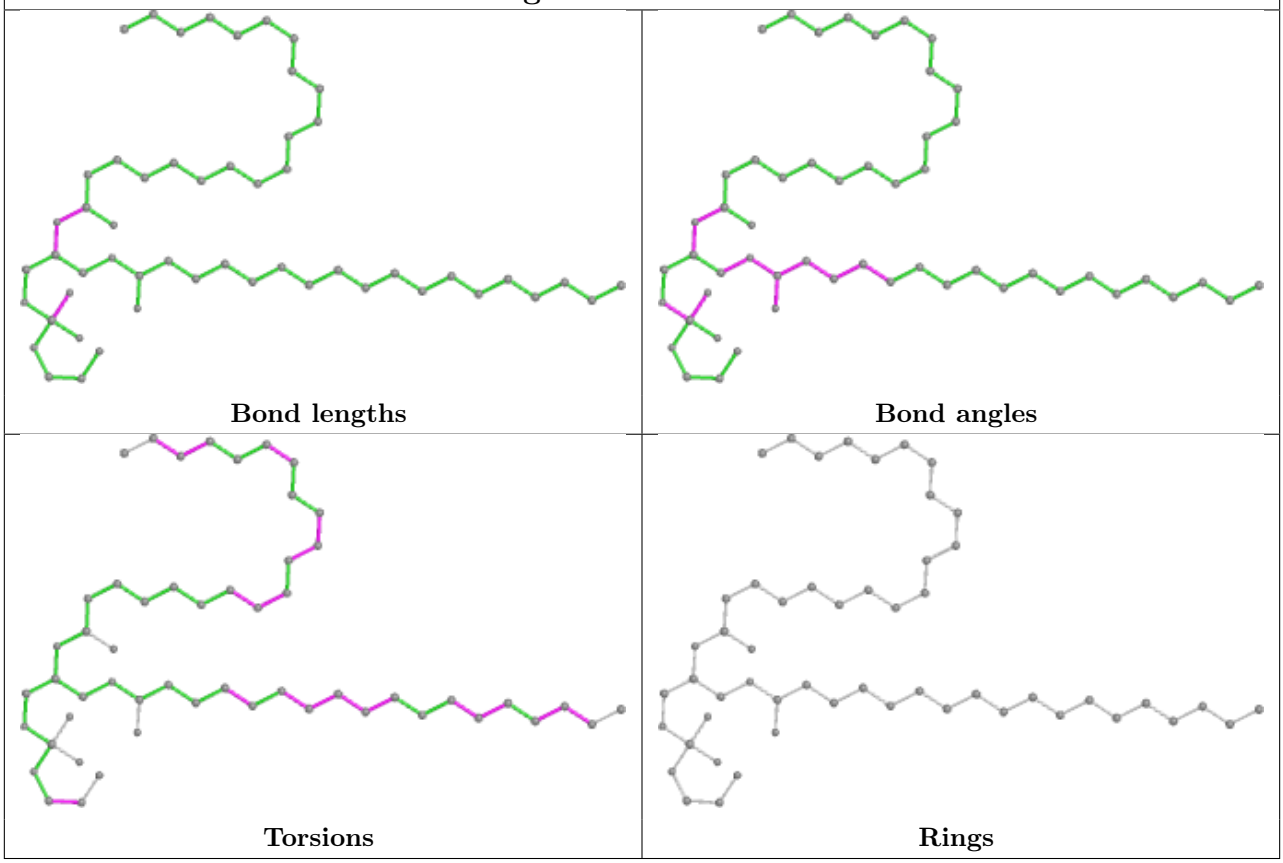


Torsions

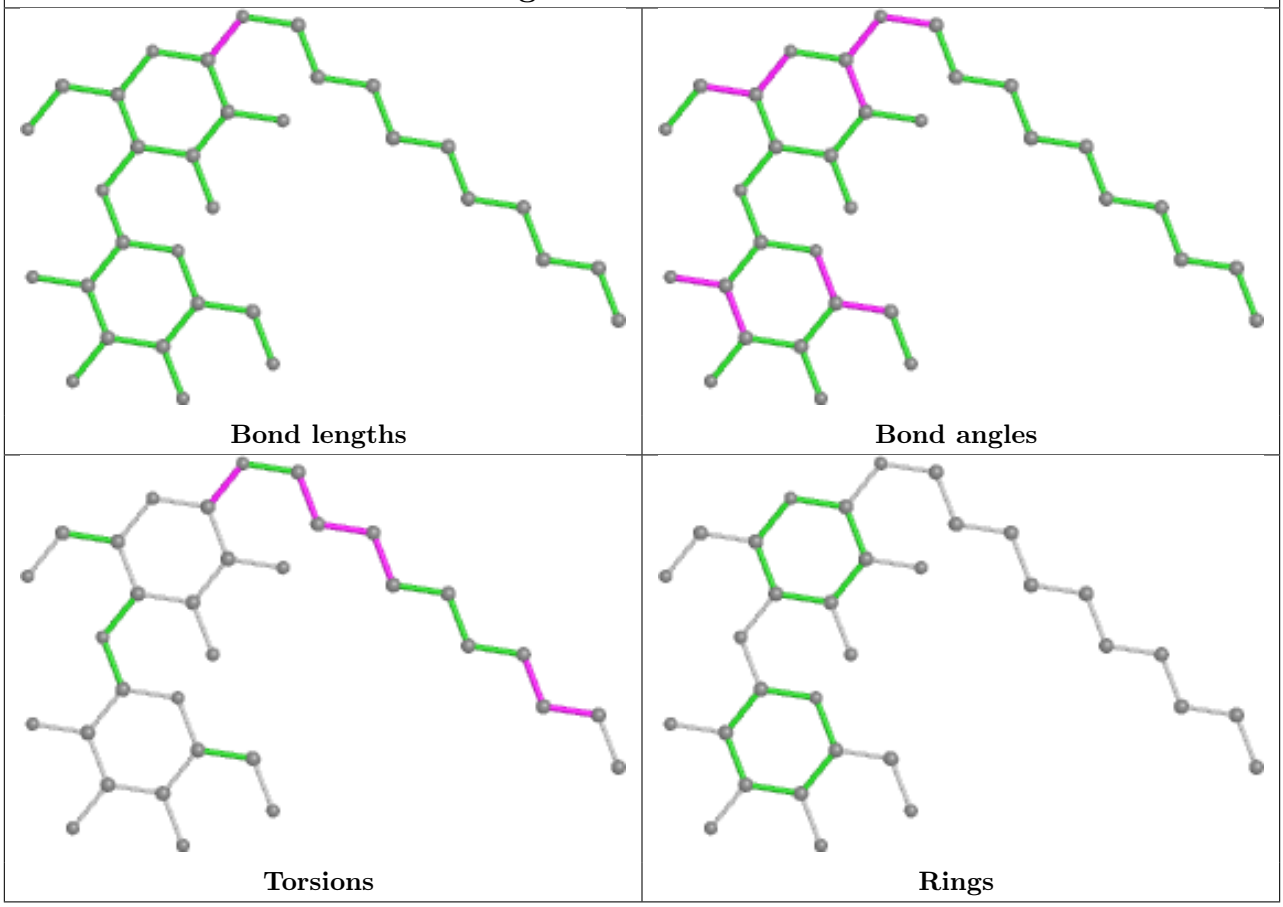


Rings

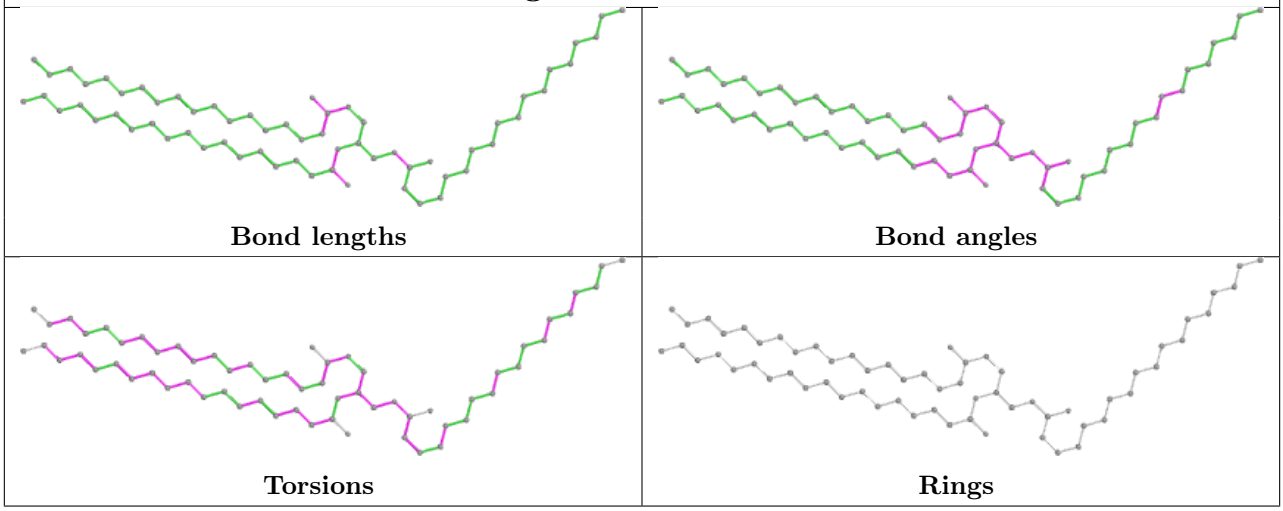
Ligand PEK G 101



Ligand DMU P 310



Ligand TGL D 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.16	0	100	100	19, 23, 31, 69	0
1	N	513/514 (99%)	-0.24	0	100	100	21, 27, 36, 68	0
2	B	226/227 (99%)	-0.13	5 (2%)	62	63	22, 30, 48, 64	0
2	O	226/227 (99%)	-0.15	5 (2%)	62	63	28, 37, 59, 78	0
3	C	259/261 (99%)	-0.23	1 (0%)	92	93	21, 27, 38, 74	0
3	P	259/261 (99%)	-0.25	3 (1%)	79	81	22, 28, 39, 57	0
4	D	144/147 (97%)	-0.32	2 (1%)	75	79	25, 31, 46, 73	0
4	Q	144/147 (97%)	0.49	9 (6%)	20	19	32, 44, 69, 141	0
5	E	105/109 (96%)	-0.29	2 (1%)	66	69	24, 31, 53, 103	0
5	R	105/109 (96%)	-0.24	2 (1%)	66	69	28, 38, 57, 103	0
6	F	98/98 (100%)	0.34	8 (8%)	11	11	23, 33, 88, 139	0
6	S	98/98 (100%)	0.33	9 (9%)	9	8	23, 33, 84, 114	0
7	G	83/85 (97%)	0.81	17 (20%)	1	1	26, 34, 100, 127	0
7	T	83/85 (97%)	0.78	17 (20%)	1	1	25, 37, 93, 135	0
8	H	79/85 (92%)	0.22	8 (10%)	7	6	27, 37, 83, 101	0
8	U	79/85 (92%)	0.33	9 (11%)	5	4	34, 42, 93, 103	0
9	I	72/73 (98%)	0.45	8 (11%)	5	4	28, 40, 75, 85	0
9	V	72/73 (98%)	0.46	7 (9%)	7	6	28, 51, 74, 90	0
10	J	58/59 (98%)	0.15	4 (6%)	16	15	26, 36, 63, 99	0
10	W	58/59 (98%)	0.32	5 (8%)	10	10	29, 39, 68, 115	0
11	K	49/56 (87%)	-0.25	0	100	100	30, 37, 50, 57	0
11	X	49/56 (87%)	0.28	3 (6%)	21	19	39, 46, 65, 76	0
12	L	46/47 (97%)	-0.05	1 (2%)	62	63	24, 29, 47, 83	0
12	Y	46/47 (97%)	-0.03	1 (2%)	62	63	30, 37, 55, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.18	4 (9%)	8	7	26, 29, 61, 107	0
13	Z	43/46 (93%)	0.27	4 (9%)	8	7	33, 40, 75, 116	0
All	All	3550/3614 (98%)	-0.02	134 (3%)	40	40	19, 31, 61, 141	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	26.0
4	Q	6	VAL	16.1
4	Q	8	SER	14.9
6	S	97	ALA	14.5
6	F	97	ALA	11.5
6	F	2	SER	11.2
4	Q	4	SER	10.2
7	G	10	GLY	9.2
6	S	1	ALA	8.7
10	W	58	LYS	8.7
6	S	94	HIS	8.7
10	J	58	LYS	8.3
6	F	1	ALA	7.9
6	F	98	HIS	7.7
7	T	10	GLY	7.6
6	F	96	LEU	7.5
6	S	98	HIS	7.4
5	R	109	VAL	7.3
7	G	3	ALA	6.9
7	T	3	ALA	6.9
7	G	41	HIS	6.8
10	W	57	HIS	6.8
9	I	29	LEU	6.8
8	U	8	ILE	6.8
13	Z	42	LYS	6.7
4	Q	7	LYS	6.7
6	F	95	GLN	6.5
13	Z	43	SER	6.5
9	I	25	PHE	6.3
12	Y	47	LYS	6.0
8	U	7	LYS	5.9
9	I	37	PHE	5.7
13	M	42	LYS	5.7
6	S	2	SER	5.5

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Mol	Chain	Res	Type	RSRZ
5	R	5	HIS	5.4
7	T	8	HIS	5.3
13	M	43	SER	5.3
7	T	40	GLY	5.3
11	X	6	ALA	5.2
9	V	37	PHE	5.2
8	U	10	ASN	5.0
7	T	42	ARG	4.9
8	H	46	LYS	4.8
6	S	95	GLN	4.8
7	G	40	GLY	4.8
9	I	30	GLY	4.8
5	E	109	VAL	4.7
7	G	42	ARG	4.7
6	F	94	HIS	4.6
6	S	96	LEU	4.6
7	G	2	SER	4.6
2	O	90	ILE	4.5
2	O	113	TYR	4.5
10	W	1	PHE	4.5
7	T	36	TRP	4.5
7	T	1	ALA	4.4
7	T	6	GLY	4.4
10	J	1	PHE	4.3
7	T	39	SER	4.3
7	G	36	TRP	4.3
7	G	37	LEU	4.2
7	T	2	SER	4.2
9	V	29	LEU	4.2
8	H	47	GLY	4.2
5	E	5	HIS	4.1
2	O	91	ASN	4.0
7	G	9	GLY	4.0
8	H	7	LYS	4.0
7	G	8	HIS	3.9
7	T	5	LYS	3.9
6	S	93	PRO	3.9
9	V	2	THR	3.8
2	O	227	LEU	3.8
7	T	9	GLY	3.8
9	V	33	THR	3.7
12	L	2	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
7	G	6	GLY	3.5
7	G	5	LYS	3.5
9	I	33	THR	3.5
11	X	7	PRO	3.4
7	G	84	LYS	3.4
9	V	25	PHE	3.4
9	V	34	PHE	3.3
13	Z	39	ASN	3.3
6	S	3	GLY	3.3
8	U	44	THR	3.2
8	U	46	LYS	3.2
8	H	45	ALA	3.2
6	F	3	GLY	3.2
7	T	7	ASP	3.1
8	H	48	GLY	3.1
8	U	48	GLY	3.1
7	G	4	ALA	3.0
9	V	30	GLY	3.0
7	T	41	HIS	2.9
8	U	9	LYS	2.9
13	Z	40	TYR	2.9
8	H	8	ILE	2.9
7	G	7	ASP	2.8
4	Q	147	LYS	2.7
9	I	26	MET	2.7
10	W	52	TRP	2.7
2	B	90	ILE	2.7
2	B	59	GLN	2.7
9	I	32	ALA	2.6
10	W	55	PHE	2.6
7	T	4	ALA	2.6
8	U	45	ALA	2.6
8	H	10	ASN	2.6
10	J	52	TRP	2.5
2	B	60	GLU	2.5
8	H	44	THR	2.5
9	I	34	PHE	2.5
7	G	43	GLU	2.4
13	M	40	TYR	2.4
2	B	91	ASN	2.4
7	T	43	GLU	2.4
7	T	38	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
4	Q	140	TYR	2.4
4	Q	10	ASP	2.3
3	P	33[A]	MET	2.3
4	Q	33	LEU	2.3
8	U	47	GLY	2.3
3	C	33	MET	2.2
10	J	57	HIS	2.2
7	G	1	ALA	2.2
4	D	4	SER	2.2
13	M	39	ASN	2.2
3	P	37	PHE	2.1
3	P	3	HIS	2.1
2	B	55	THR	2.1
4	D	87[A]	PHE	2.1
2	O	87[A]	MET	2.0
11	X	13	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	T	11	11/12	0.45	0.41	76,101,117,121	0
7	TPO	G	11	11/12	0.56	0.44	84,110,125,127	0
9	SAC	V	1	9/10	0.63	0.64	107,118,124,126	0
9	SAC	I	1	9/10	0.85	0.25	59,70,74,74	0
1	FME	A	1	10/11	0.95	0.11	33,43,67,83	0
2	FME	B	1	10/11	0.95	0.12	20,28,45,61	0
1	FME	N	1	10/11	0.97	0.11	36,44,71,76	0
2	FME	O	1	10/11	0.98	0.09	36,36,43,57	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CHD	W	101	29/29	0.49	0.43	58,114,135,143	0
24	PSC	B	303	52/52	0.57	0.30	31,74,150,157	0
25	DMU	C	310	33/33	0.59	0.26	46,72,105,111	0
25	DMU	L	102	33/33	0.63	0.23	47,83,107,120	0
27	CDL	G	102	100/100	0.64	0.22	49,86,117,152	0
21	EDO	F	103	4/4	0.65	0.49	52,76,77,81	0
22	CHD	J	101	29/29	0.67	0.43	50,112,133,141	0
20	PGV	C	308	51/51	0.69	0.22	42,72,109,132	0
27	CDL	T	103	100/100	0.69	0.22	51,84,123,146	0
21	EDO	N	615	4/4	0.70	0.17	66,67,67,72	0
28	PEK	G	104	53/53	0.70	0.29	44,88,153,155	0
19	TGL	Q	201	63/63	0.71	0.19	47,72,92,103	0
28	PEK	P	308	53/53	0.71	0.25	37,69,131,149	0
28	PEK	T	101	53/53	0.71	0.26	43,93,153,154	0
28	PEK	C	307	53/53	0.72	0.23	39,79,139,146	0
25	DMU	P	309	33/33	0.73	0.20	53,72,93,94	0
25	DMU	C	302	33/33	0.73	0.35	30,61,103,109	0
27	CDL	P	305	100/100	0.73	0.25	35,80,118,122	0
25	DMU	P	307	33/33	0.73	0.30	38,61,96,102	0
27	CDL	C	305	100/100	0.75	0.21	30,70,103,110	0
25	DMU	P	310	33/33	0.75	0.23	61,74,92,94	0
20	PGV	X	101	51/51	0.76	0.24	42,70,129,151	0
24	PSC	O	302	52/52	0.76	0.25	39,78,148,161	0
22	CHD	P	306	29/29	0.78	0.24	48,58,64,66	0
25	DMU	C	309	33/33	0.78	0.24	51,70,95,98	0
21	EDO	D	203	4/4	0.78	0.35	45,50,64,66	0
20	PGV	P	302	51/51	0.79	0.19	50,77,127,132	0
20	PGV	A	610	51/51	0.80	0.20	30,59,101,112	0
19	TGL	Y	101	63/63	0.81	0.23	39,66,108,129	0
21	EDO	A	618	4/4	0.82	0.17	41,47,51,58	0
22	CHD	C	306	29/29	0.82	0.23	50,61,66,68	0
21	EDO	A	620	4/4	0.83	0.16	54,57,62,64	0
21	EDO	C	313	4/4	0.83	0.24	46,58,62,63	0
19	TGL	N	609	63/63	0.83	0.15	44,70,96,112	0
26	UNX	C	303	1/1	0.83	0.14	24,24,24,24	0
19	TGL	L	101	63/63	0.84	0.17	30,58,91,103	0
21	EDO	E	202	4/4	0.84	0.34	39,41,54,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	TGL	D	201	63/63	0.85	0.15	27,58,80,93	0
25	DMU	Z	101	33/33	0.86	0.16	44,50,65,65	0
21	EDO	Y	102	4/4	0.86	0.26	59,62,66,70	0
21	EDO	H	101	4/4	0.87	0.14	54,54,59,66	0
21	EDO	S	105	4/4	0.87	0.16	41,47,48,57	0
21	EDO	O	303	4/4	0.88	0.18	49,51,51,57	0
21	EDO	B	305	4/4	0.89	0.16	45,50,51,54	0
21	EDO	G	106	4/4	0.89	0.14	47,58,62,69	0
25	DMU	M	101	33/33	0.89	0.10	36,40,53,57	0
21	EDO	A	615	4/4	0.89	0.14	43,43,47,61	0
19	TGL	A	608	63/63	0.90	0.15	33,66,93,101	0
21	EDO	A	614	4/4	0.90	0.15	45,49,54,83	0
21	EDO	L	103	4/4	0.91	0.19	43,56,67,73	0
21	EDO	N	612	4/4	0.91	0.17	51,51,59,60	0
21	EDO	D	205	4/4	0.91	0.13	44,47,49,58	0
21	EDO	N	616	4/4	0.92	0.23	26,33,42,59	0
21	EDO	A	617	4/4	0.92	0.11	39,42,42,45	0
21	EDO	F	104	4/4	0.93	0.09	35,39,40,45	0
21	EDO	D	202	4/4	0.93	0.53	31,40,46,85	0
21	EDO	T	104	4/4	0.94	0.10	33,33,41,43	0
21	EDO	C	312	4/4	0.94	0.11	54,56,58,68	0
22	CHD	C	301	29/29	0.94	0.08	24,29,33,35	0
21	EDO	A	619	4/4	0.95	0.31	34,48,49,55	0
21	EDO	O	304	4/4	0.95	0.09	34,35,35,35	0
21	EDO	P	312	4/4	0.95	0.10	29,34,43,47	0
26	UNX	P	303	1/1	0.95	0.15	24,24,24,24	0
21	EDO	A	612	4/4	0.95	0.14	28,28,30,35	0
21	EDO	B	304	4/4	0.95	0.11	36,42,48,49	0
28	PEK	T	102	53/53	0.95	0.12	27,43,78,91	0
21	EDO	F	105	4/4	0.96	0.09	32,33,36,36	0
21	EDO	N	613	4/4	0.96	0.13	34,42,44,45	0
21	EDO	N	614	4/4	0.96	0.11	36,37,42,45	0
28	PEK	G	101	53/53	0.96	0.12	25,43,71,86	0
21	EDO	S	103	4/4	0.96	0.14	35,58,59,60	0
21	EDO	S	104	4/4	0.96	0.10	35,38,42,44	0
21	EDO	A	621	4/4	0.96	0.24	41,45,46,59	0
21	EDO	N	610	4/4	0.96	0.10	29,30,32,38	0
21	EDO	A	611	4/4	0.97	0.12	31,40,44,46	0
20	PGV	P	304	51/51	0.97	0.10	24,33,75,82	0
22	CHD	B	301	29/29	0.97	0.07	23,26,30,37	0
21	EDO	N	611	4/4	0.97	0.09	24,27,31,32	0
21	EDO	B	306	4/4	0.97	0.09	25,26,31,31	0

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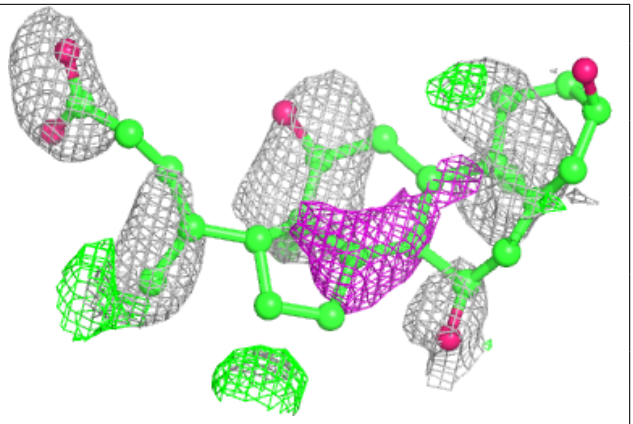
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CHD	G	103	29/29	0.97	0.08	24,27,30,34	0
21	EDO	G	105	4/4	0.97	0.08	29,30,37,39	0
22	CHD	P	301	29/29	0.97	0.07	26,30,34,38	0
21	EDO	C	311	4/4	0.97	0.08	34,35,36,37	0
20	PGV	C	304	51/51	0.97	0.10	24,32,80,88	0
21	EDO	S	106	4/4	0.97	0.07	32,33,33,34	0
14	HEA	N	602[A]	60/60	0.98	0.11	19,23,26,27	60
14	HEA	N	602[B]	60/60	0.98	0.11	22,25,38,39	60
21	EDO	A	613	4/4	0.98	0.12	23,24,25,26	0
20	PGV	A	609	51/51	0.98	0.10	21,29,60,64	0
16	MG	N	604	1/1	0.98	0.07	28,28,28,28	0
21	EDO	A	616	4/4	0.98	0.09	32,36,40,45	0
18	AZI	N	606[B]	3/3	0.98	0.15	21,21,23,24	3
21	EDO	D	204	4/4	0.98	0.13	35,35,50,57	0
14	HEA	A	601	60/60	0.98	0.09	19,21,43,47	0
21	EDO	E	201	4/4	0.98	0.08	36,37,39,41	0
20	PGV	N	608	51/51	0.98	0.09	23,32,61,63	0
21	EDO	E	203	4/4	0.98	0.06	34,37,43,45	0
14	HEA	A	602[A]	60/60	0.98	0.11	17,20,25,28	60
21	EDO	P	311	4/4	0.98	0.16	39,40,40,43	0
14	HEA	A	602[B]	60/60	0.98	0.11	17,21,28,31	60
21	EDO	R	201	4/4	0.98	0.10	38,40,42,43	0
21	EDO	S	102	4/4	0.98	0.08	25,25,25,26	0
14	HEA	N	601	60/60	0.98	0.09	23,26,45,50	0
16	MG	A	604	1/1	0.99	0.07	23,23,23,23	0
18	AZI	N	607[A]	3/3	0.99	0.14	25,25,26,29	3
18	AZI	N	607[B]	3/3	0.99	0.14	19,19,20,27	3
18	AZI	A	606[B]	3/3	0.99	0.18	20,20,20,21	3
18	AZI	A	607[A]	3/3	0.99	0.12	20,20,21,24	3
21	EDO	F	102	4/4	0.99	0.08	23,24,26,26	0
18	AZI	A	607[B]	3/3	0.99	0.12	16,16,17,26	3
23	CUA	O	301	2/2	1.00	0.12	29,29,29,30	0
17	NA	N	605	1/1	1.00	0.06	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.13	23,23,23,23	0
15	CU	N	603	1/1	1.00	0.14	26,26,26,26	0
17	NA	A	605	1/1	1.00	0.07	25,25,25,25	0
23	CUA	B	302	2/2	1.00	0.14	23,23,23,23	0
29	ZN	F	101	1/1	1.00	0.12	28,28,28,28	0
29	ZN	S	101	1/1	1.00	0.11	29,29,29,29	0

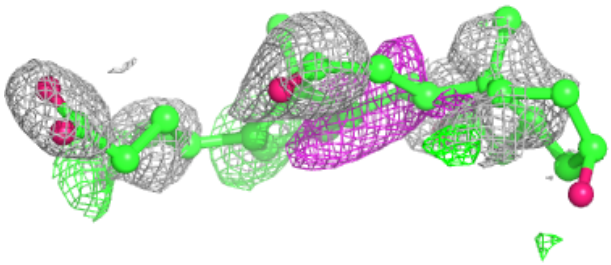
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

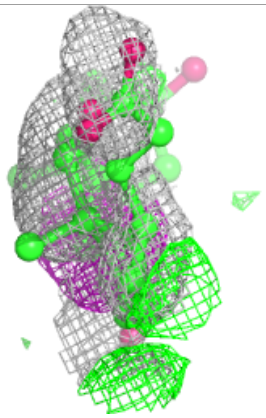
orientation to approximate a three-dimensional view.

Electron density around 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)

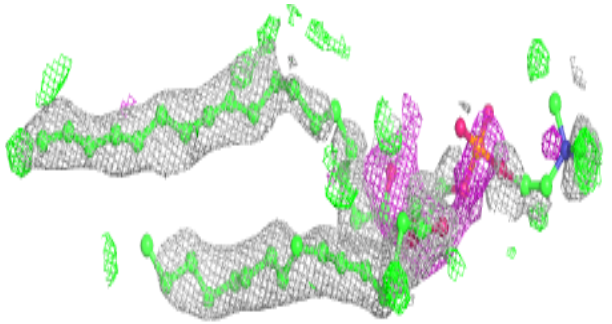


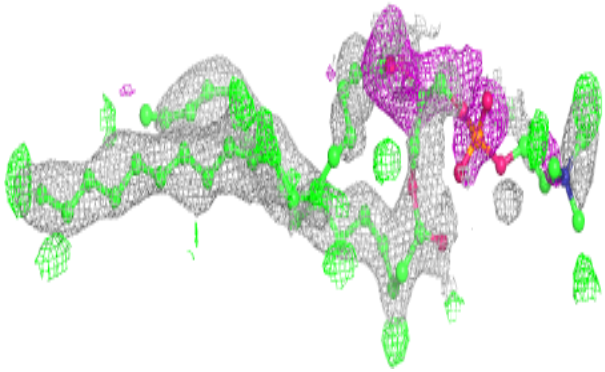


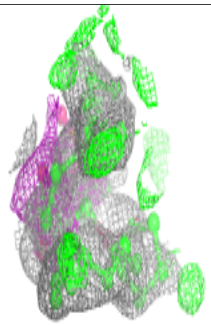


Electron density around PSC B 303:

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

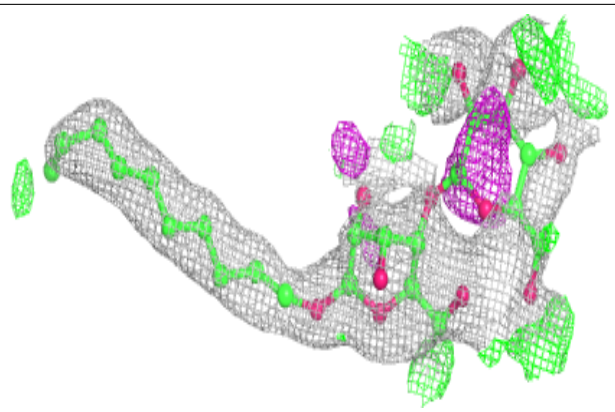


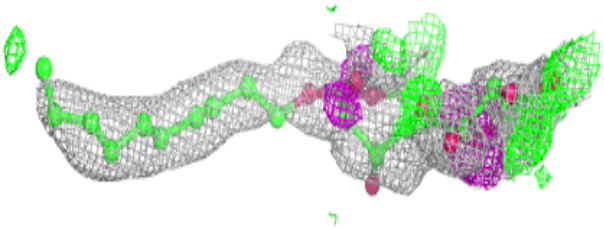


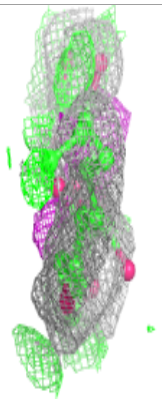


Electron density around DMU C 310:

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

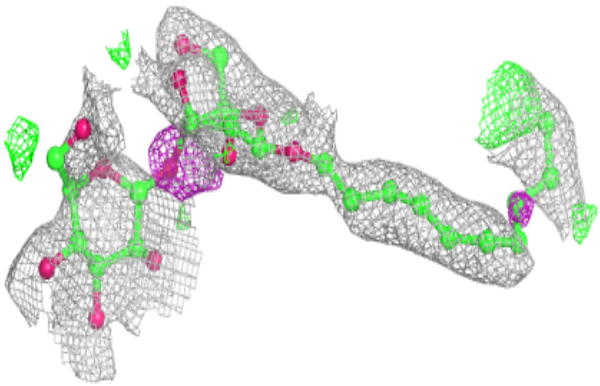


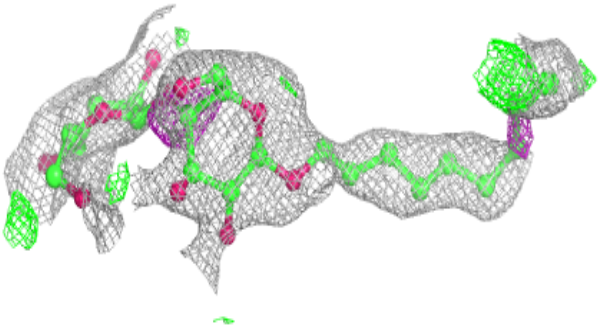


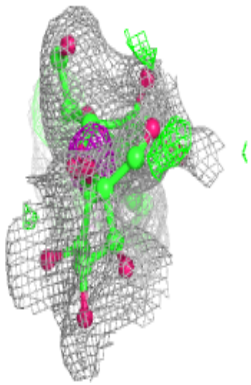


Electron density around DMU L 102:

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

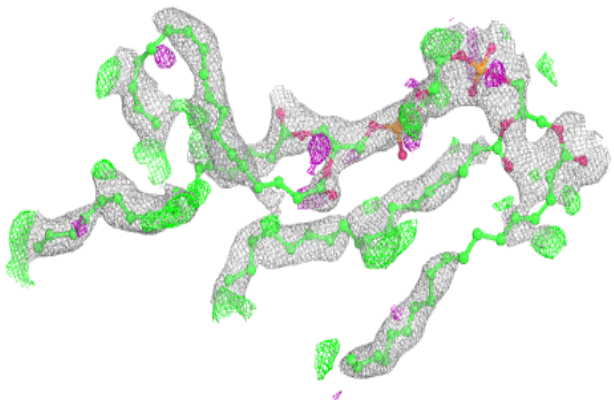


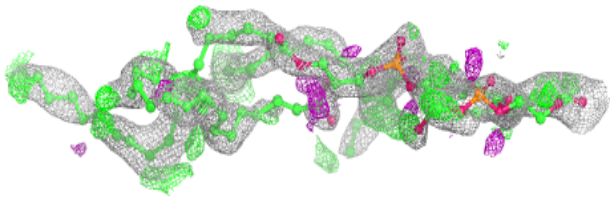


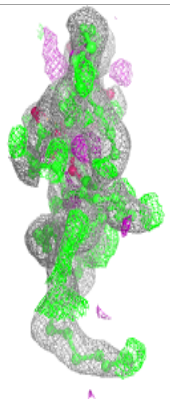


Electron density around CDL G 102:

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

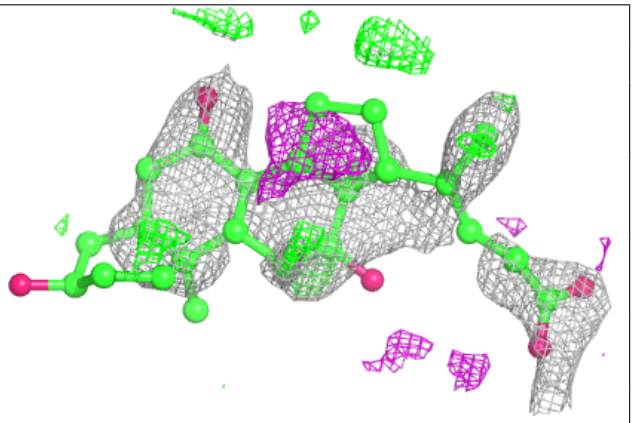


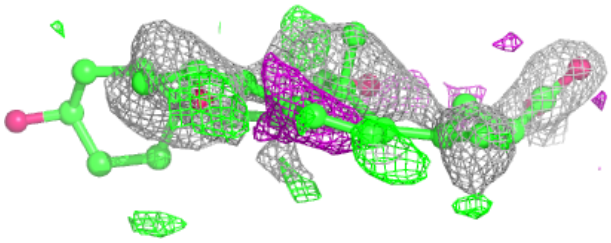


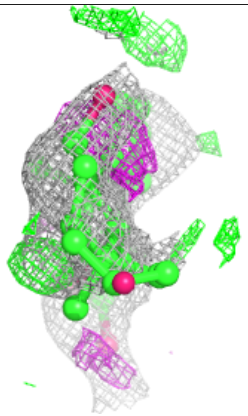


Electron density around CHD J 101:

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

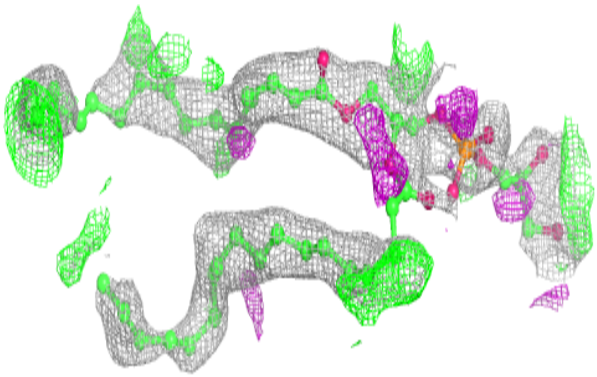


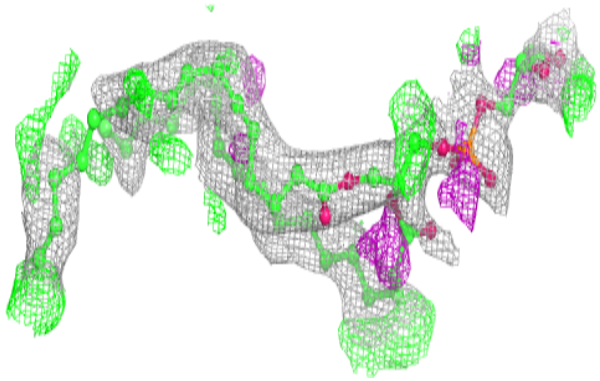


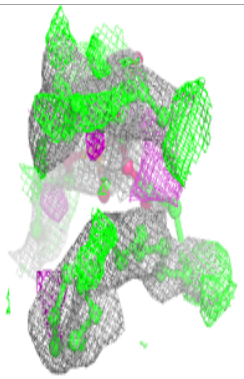


Electron density around PGV C 308:

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

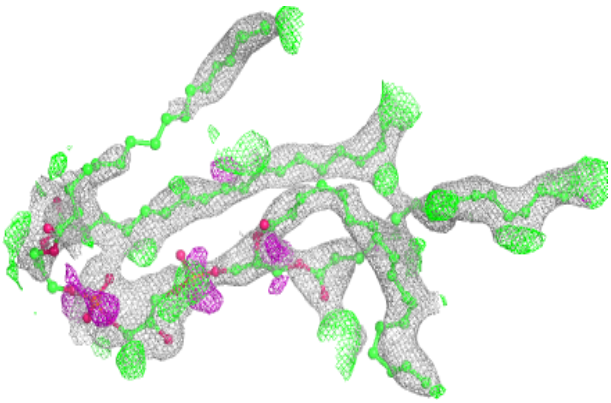


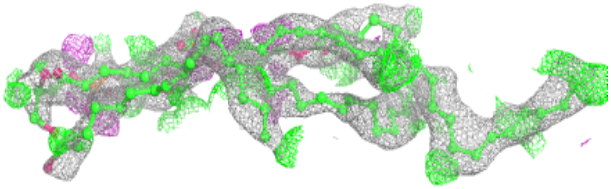


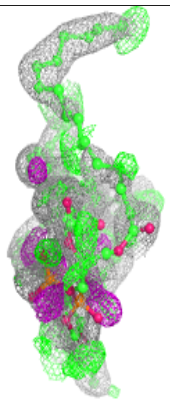


Electron density around CDL T 103:

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

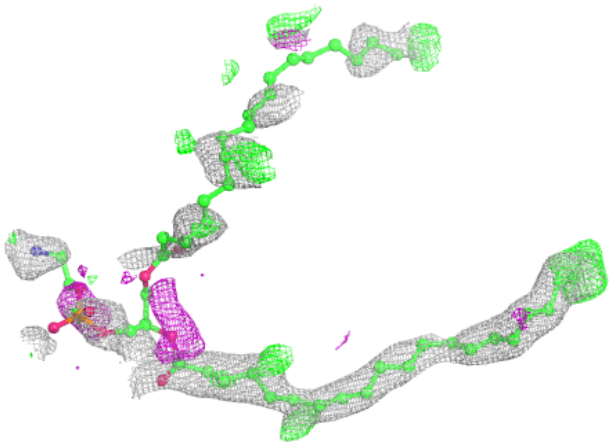


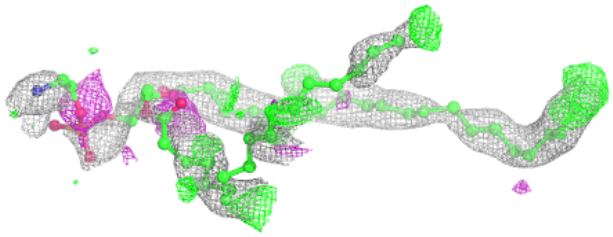


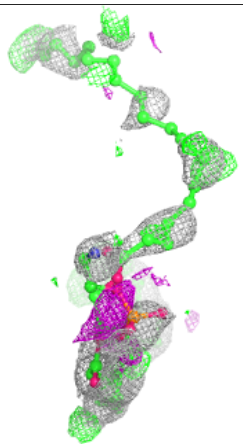


Electron density around PEK G 104:

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

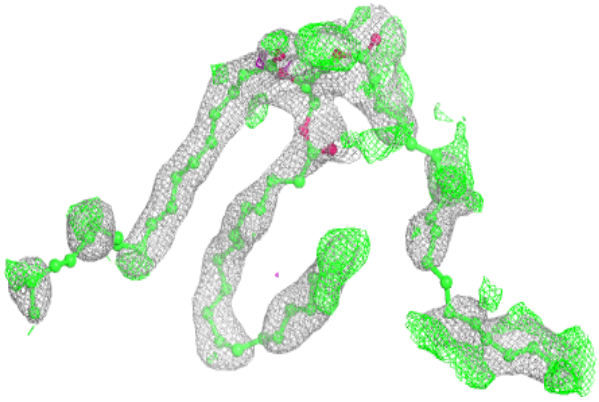


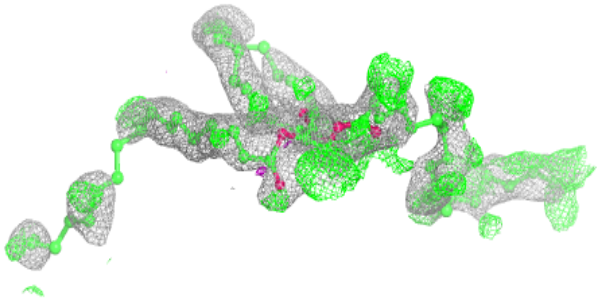


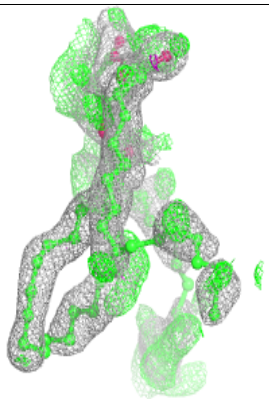


Electron density around TGL Q 201:

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

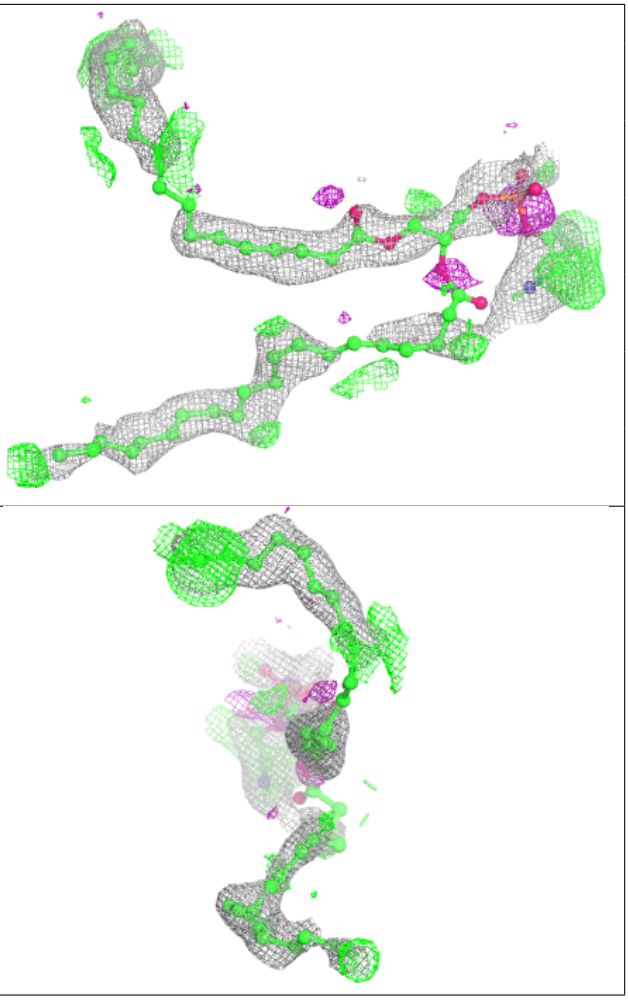






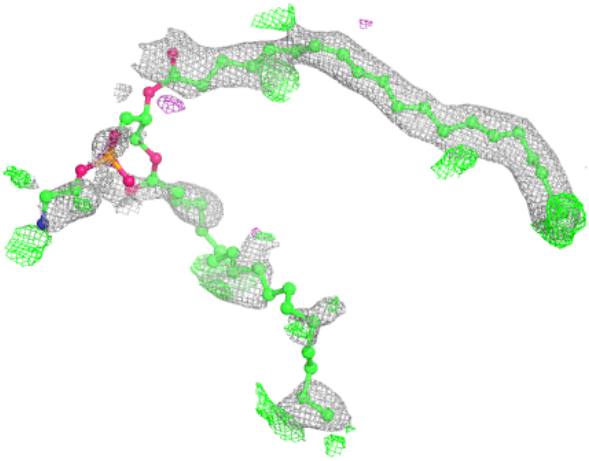
Electron density around PEK P 308:

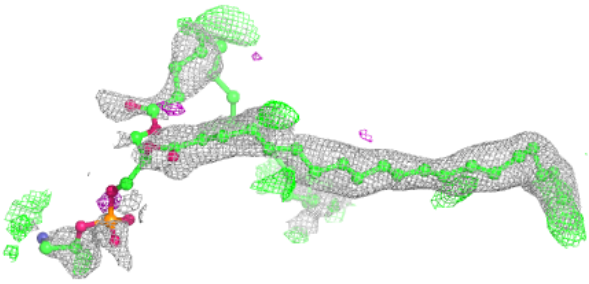
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

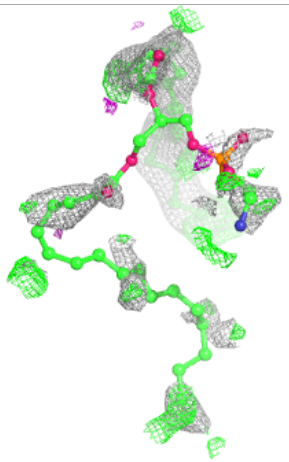


Electron density around PEK T 101:

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

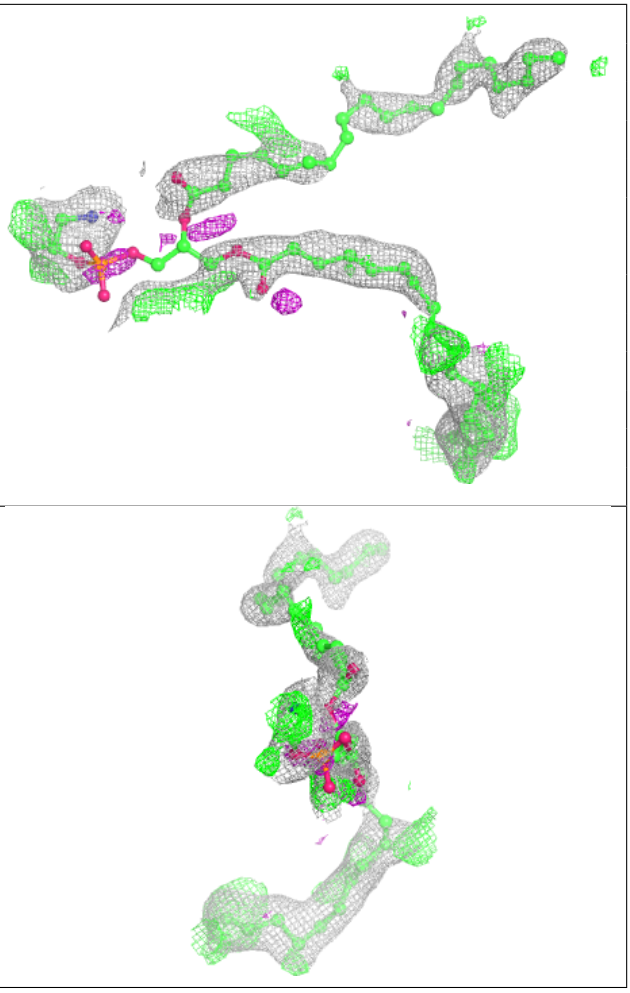






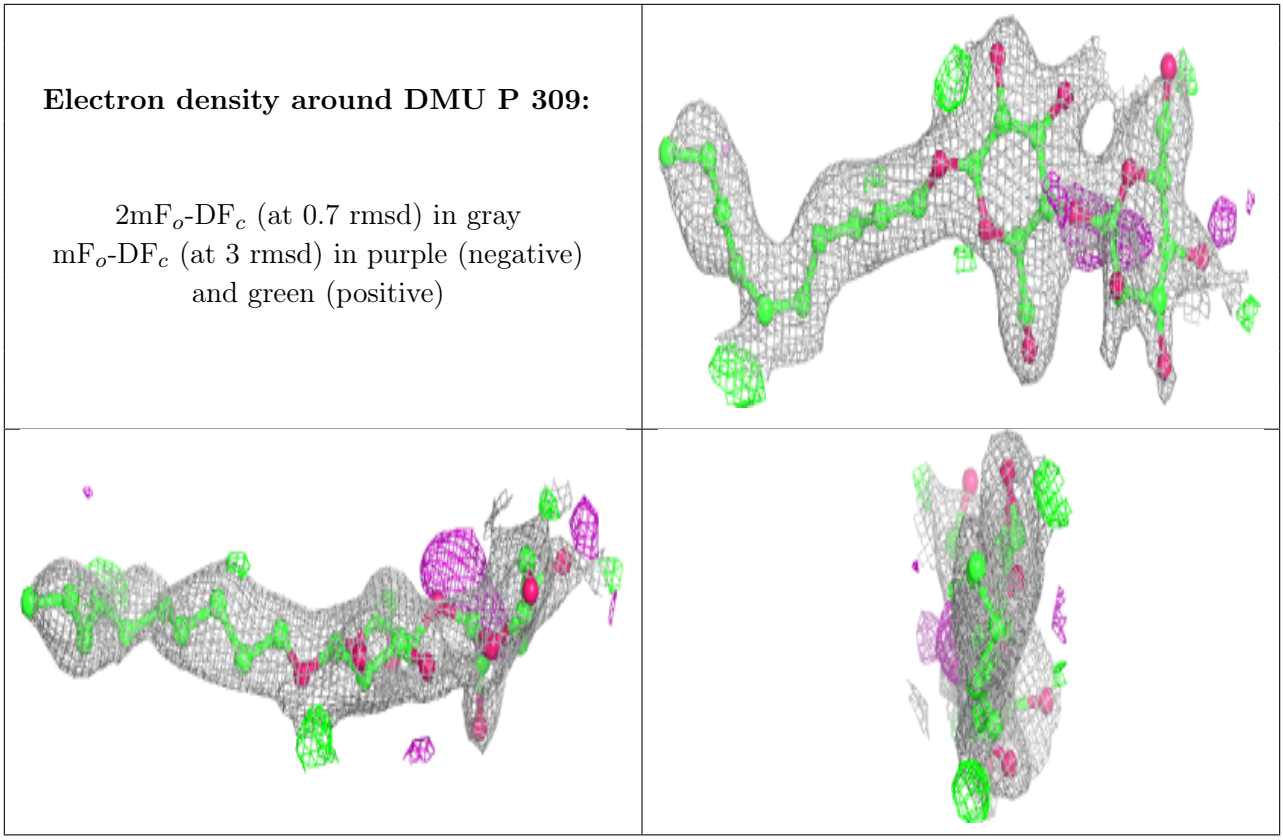
Electron density around PEK C 307:

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



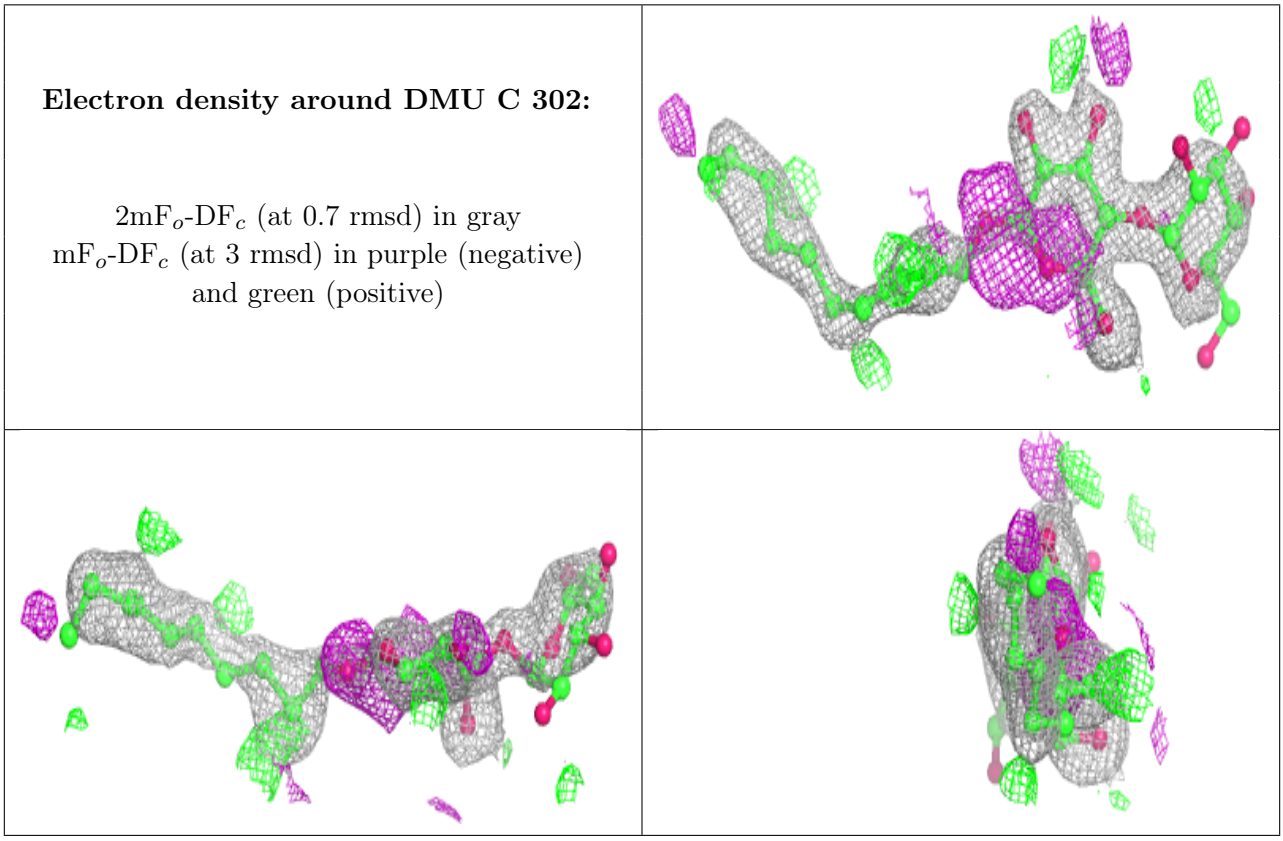
Electron density around DMU P 309:

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



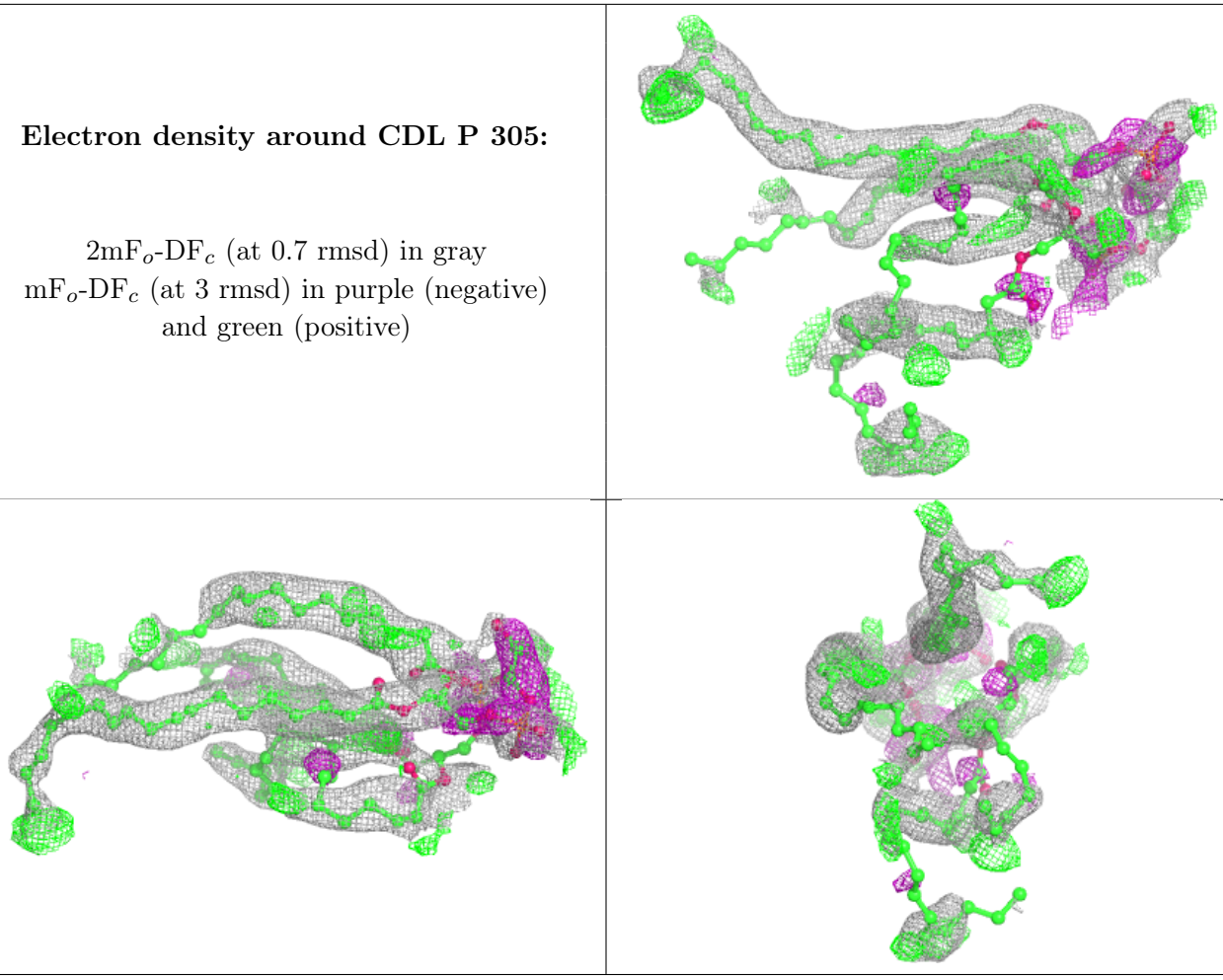
Electron density around DMU C 302:

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



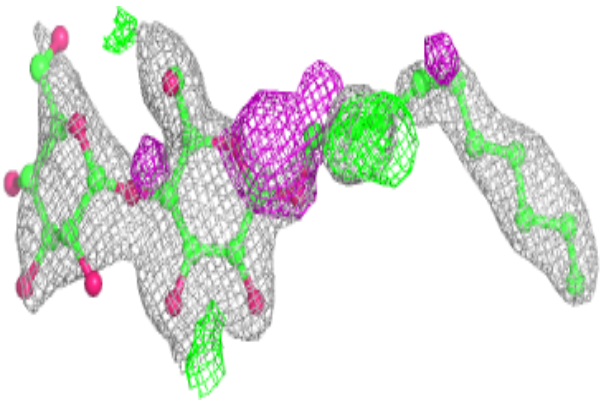
Electron density around CDL P 305:

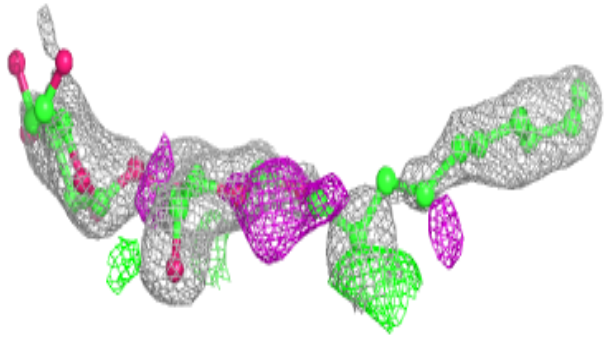
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

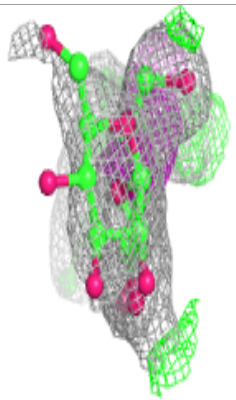


Electron density around DMU P 307:

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

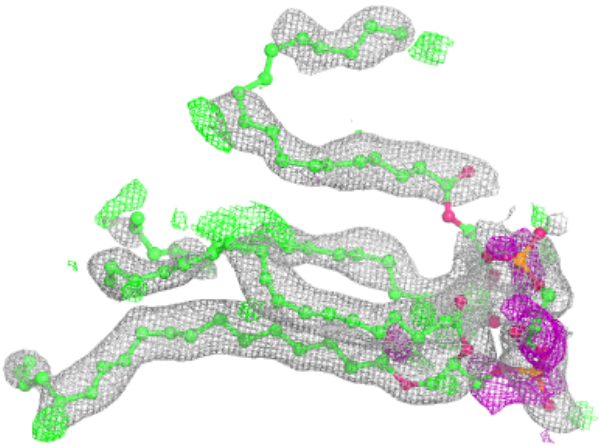


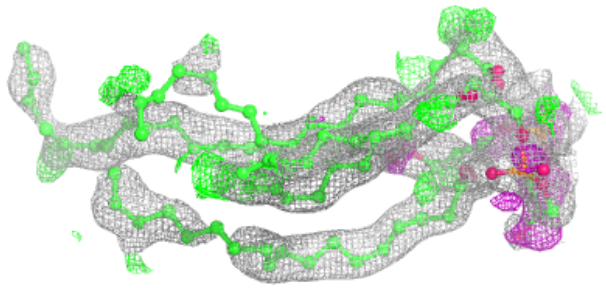


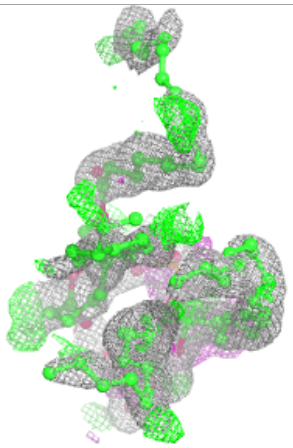


Electron density around CDL C 305:

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

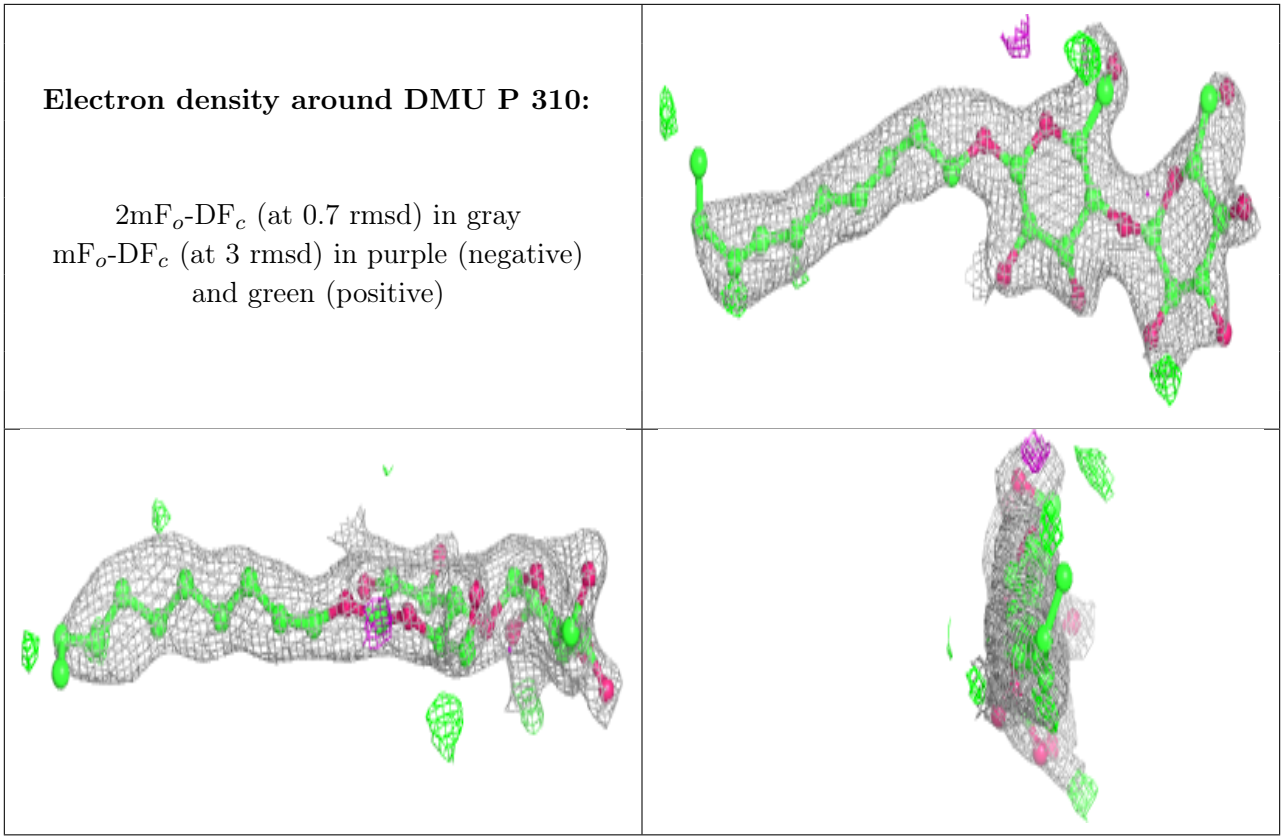






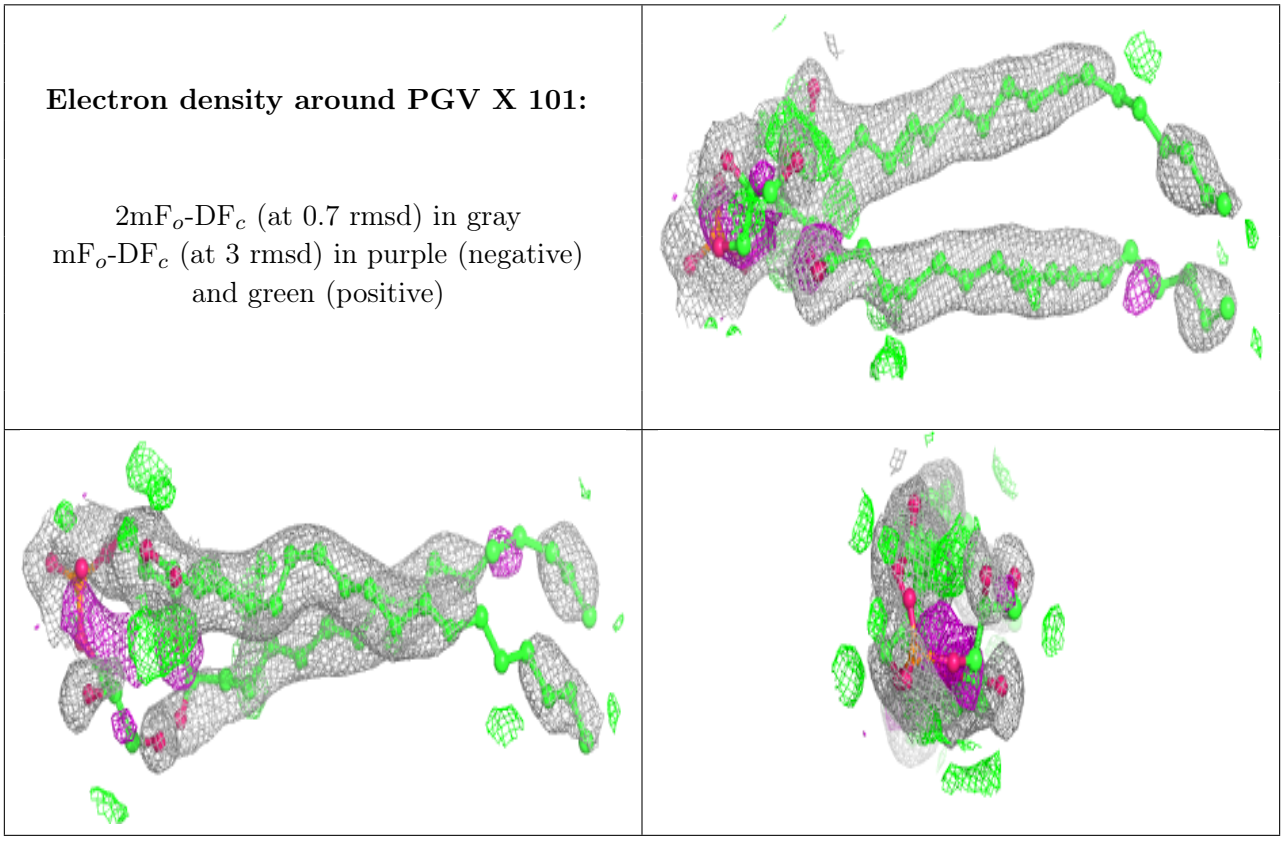
Electron density around DMU P 310:

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



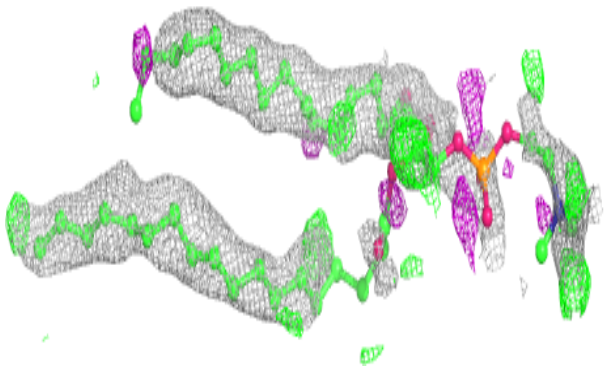
Electron density around PGV X 101:

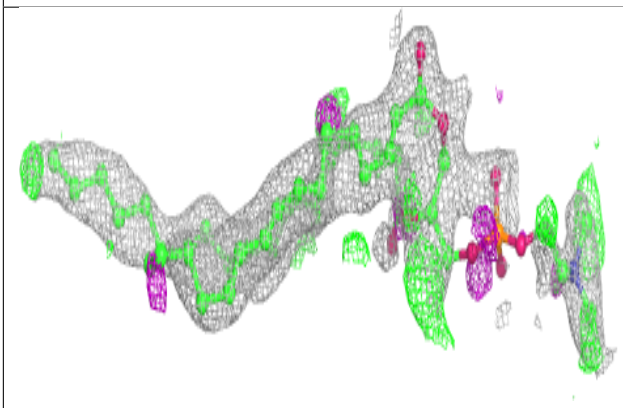
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

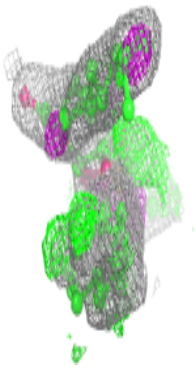


Electron density around PSC O 302:

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

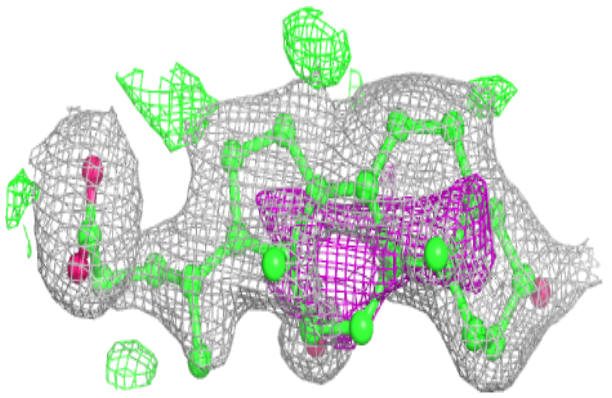


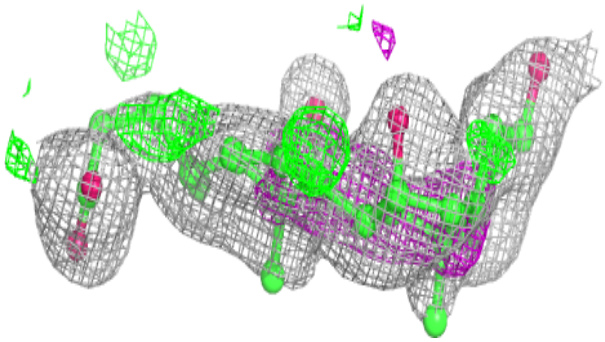


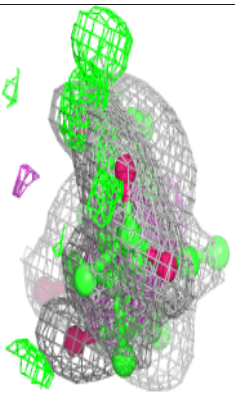


Electron density around CHD P 306:

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

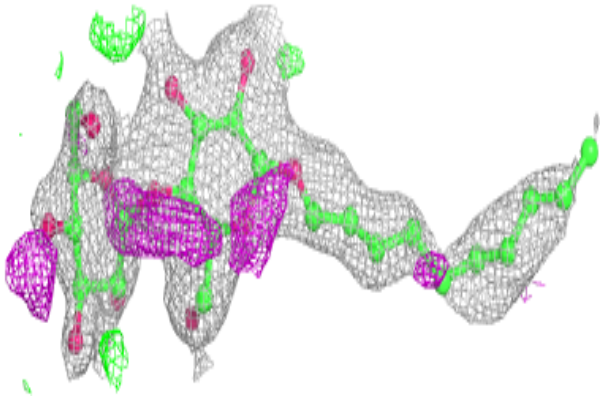


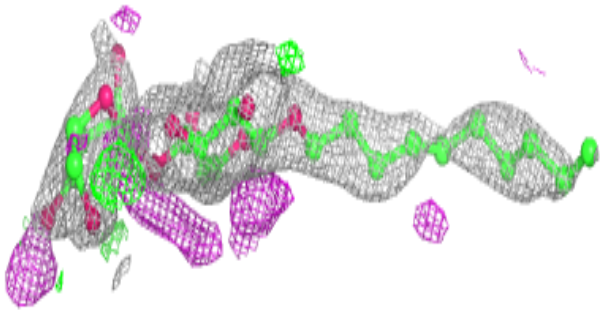


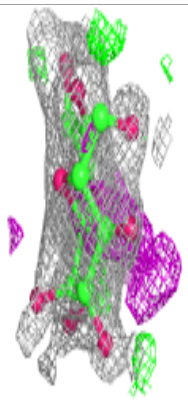


Electron density around DMU C 309:

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

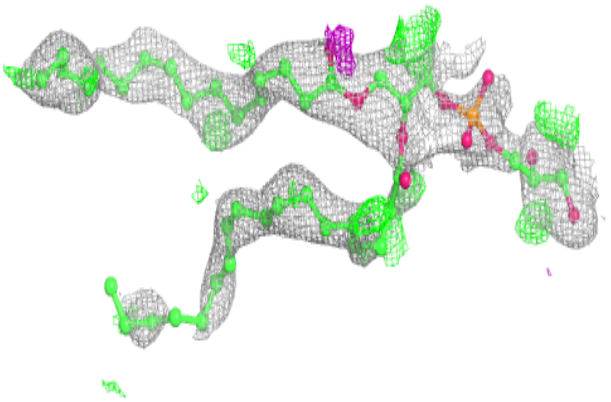


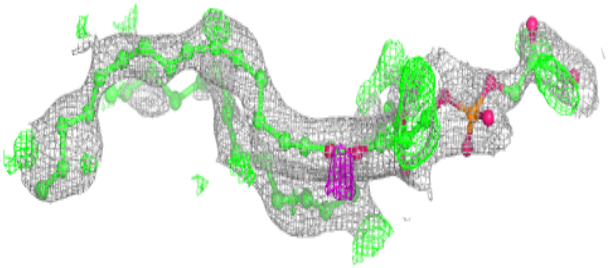


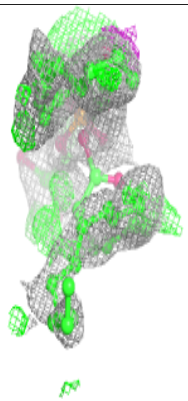


Electron density around PGV P 302:

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

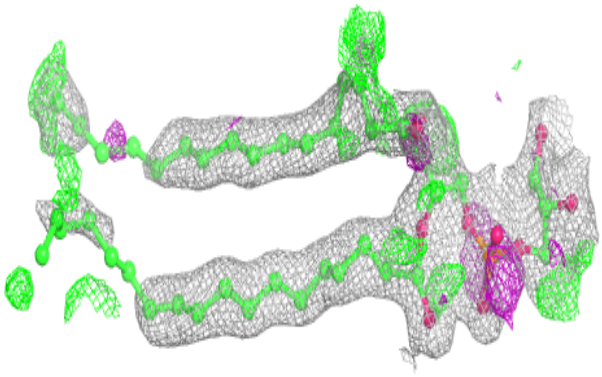


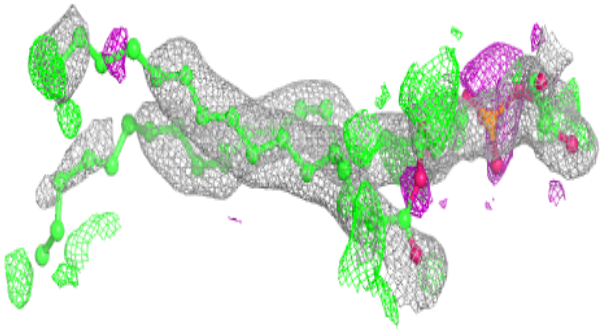


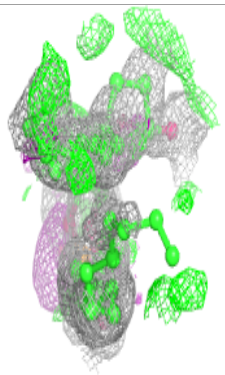


Electron density around PGV A 610:

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

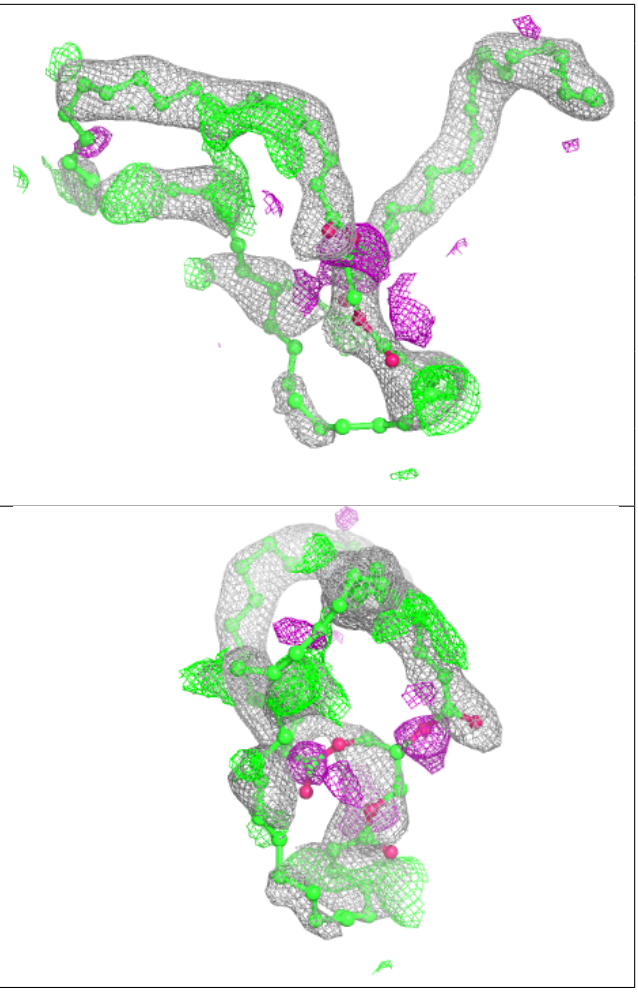






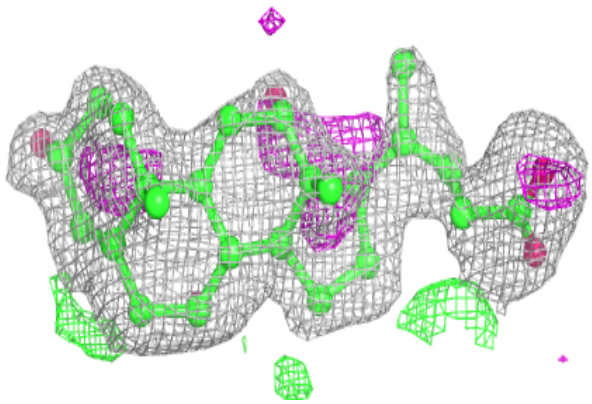
Electron density around TGL Y 101:

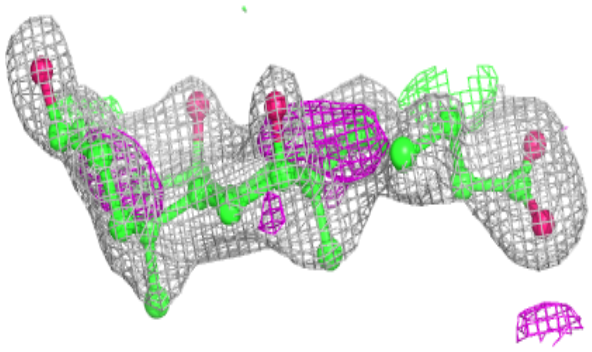
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

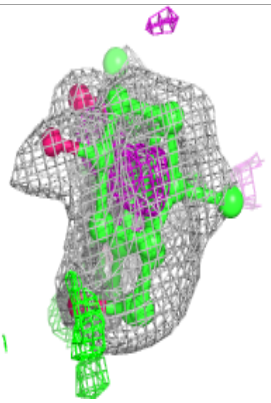


Electron density around CHD C 306:

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

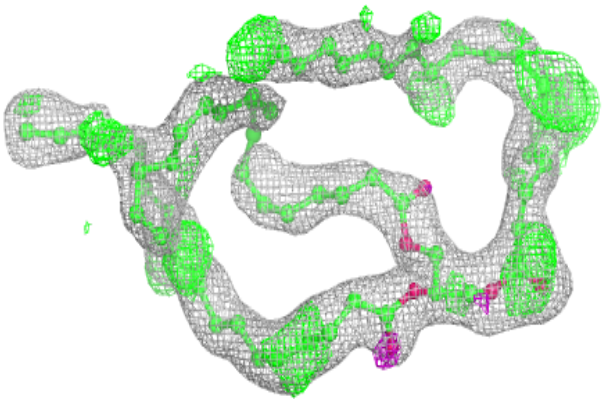


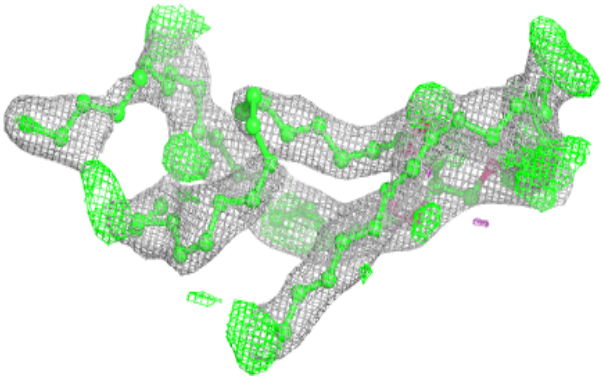


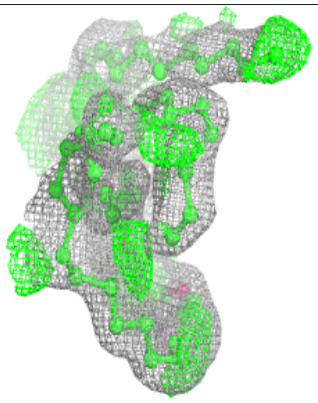


Electron density around TGL N 609:

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

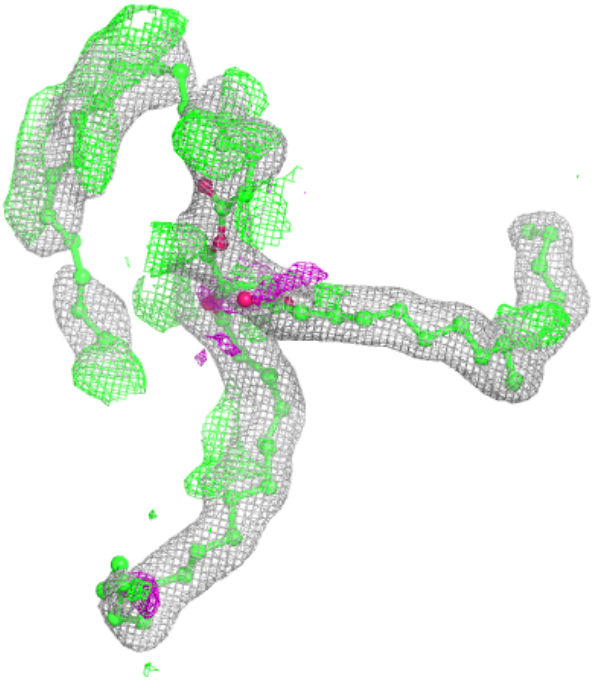


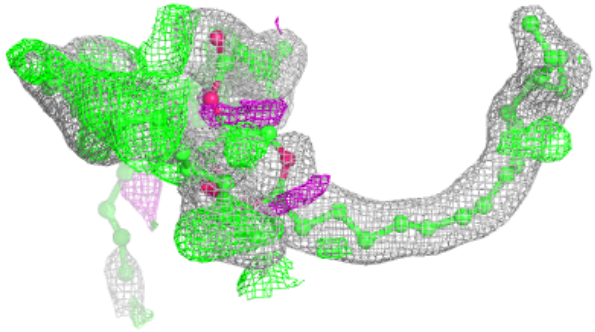


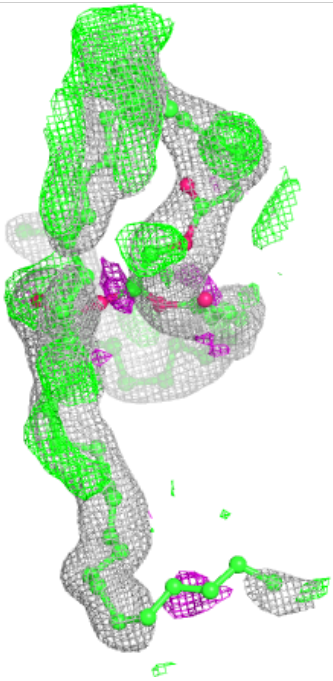


Electron density around TGL L 101:

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

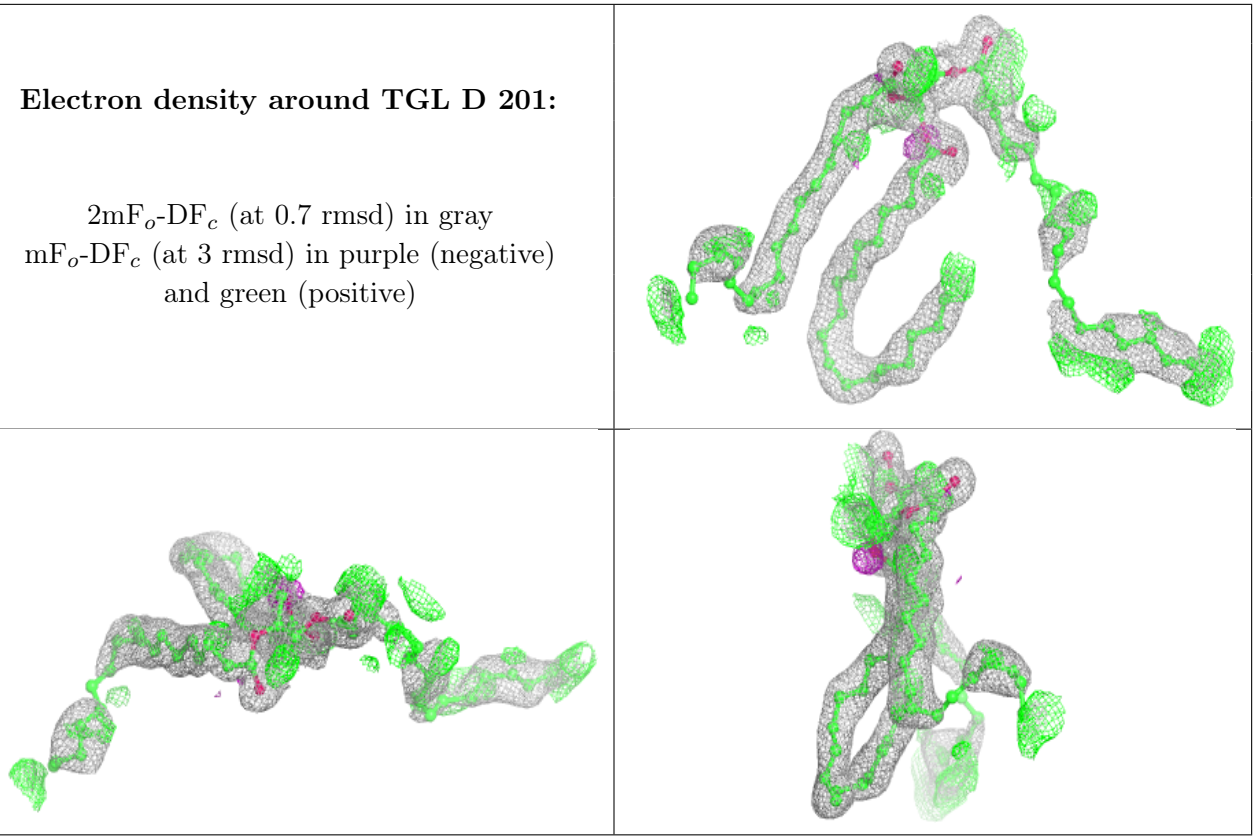






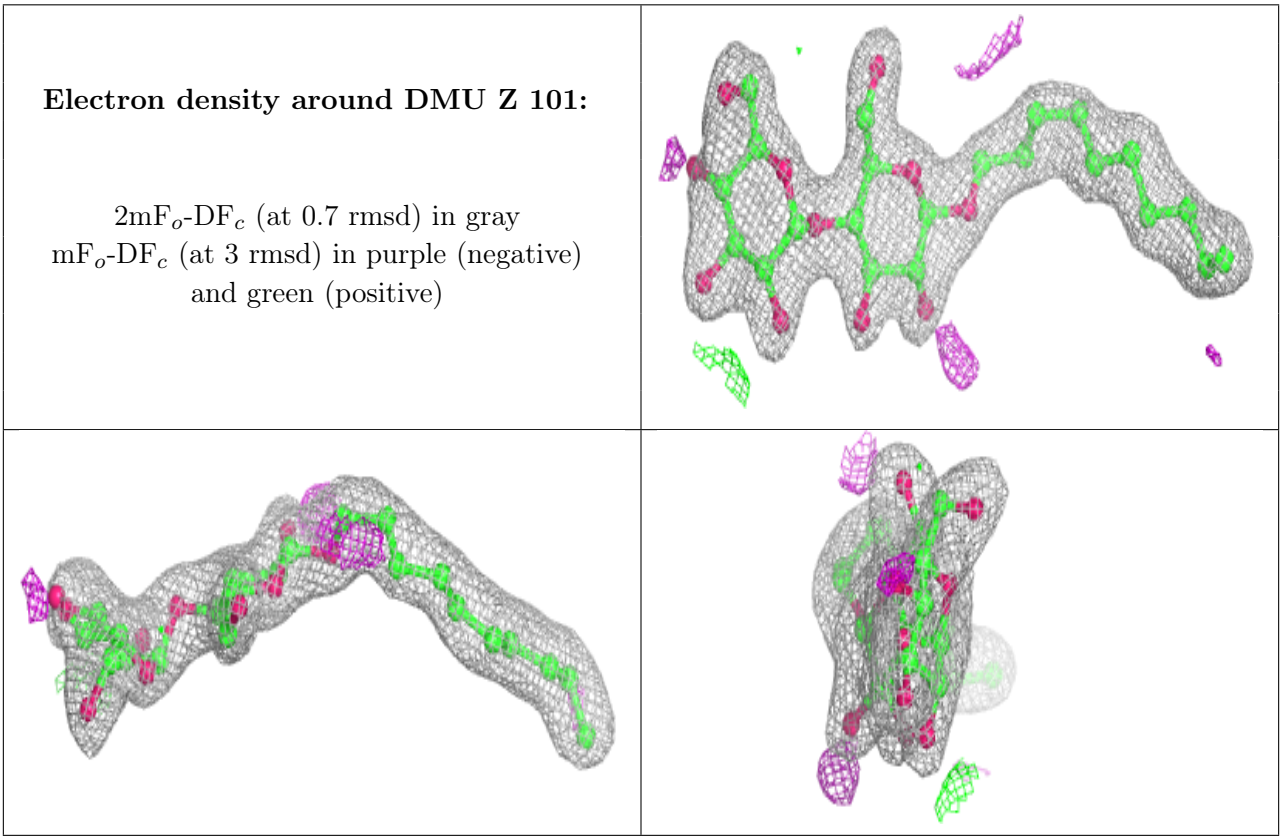
Electron density around TGL D 201:

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



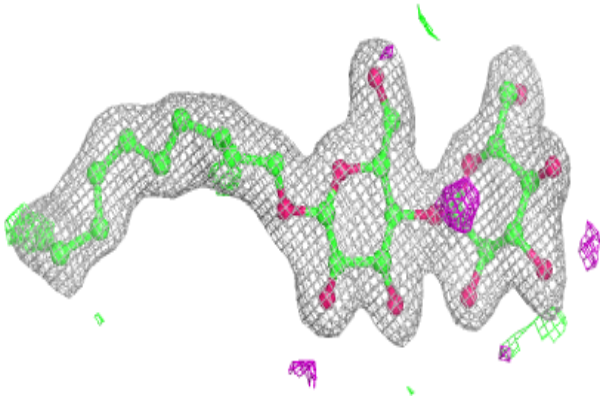
Electron density around DMU Z 101:

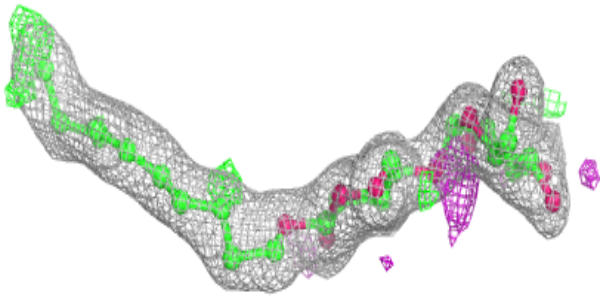
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

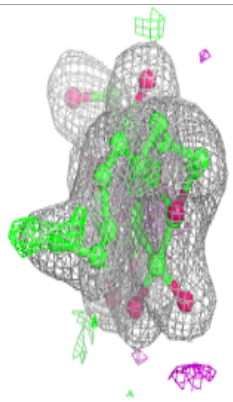


Electron density around DMU M 101:

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

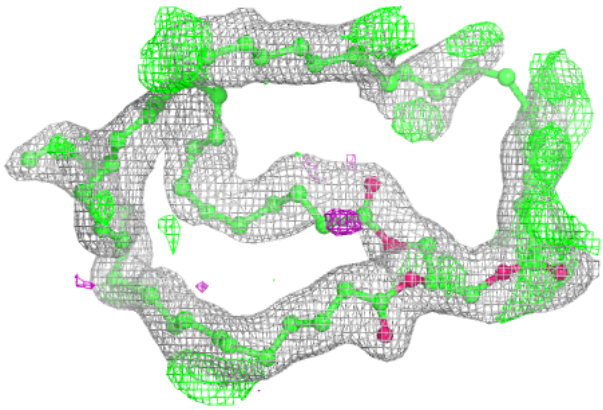


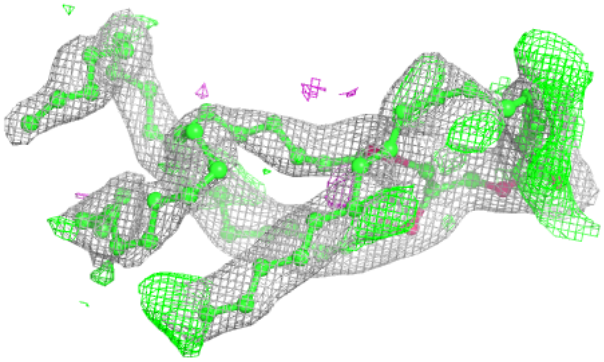


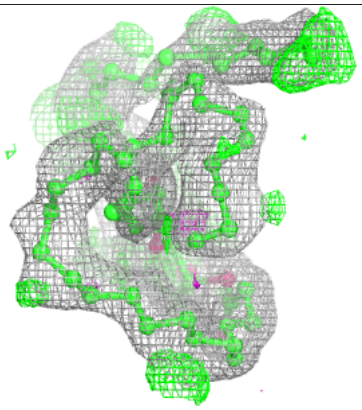


Electron density around TGL A 608:

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

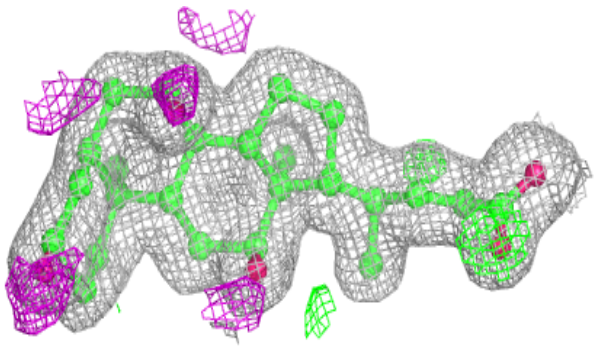


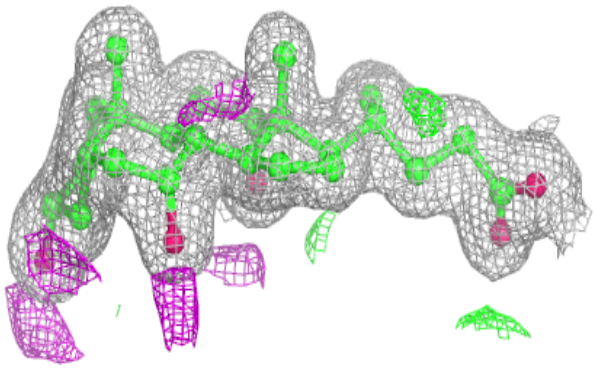


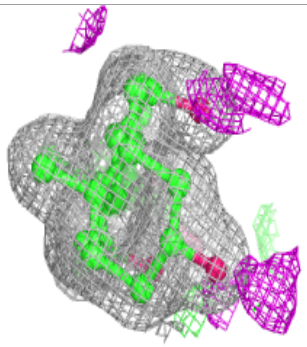


Electron density around CHD C 301:

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

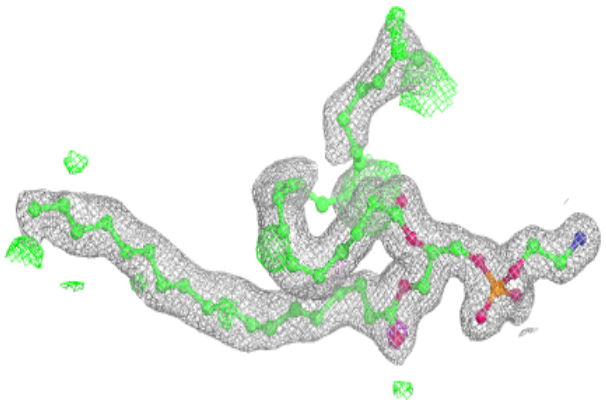


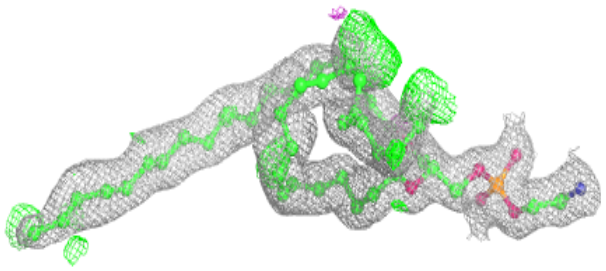


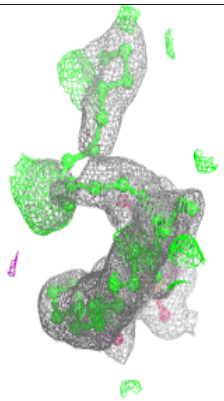


Electron density around PEK T 102:

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

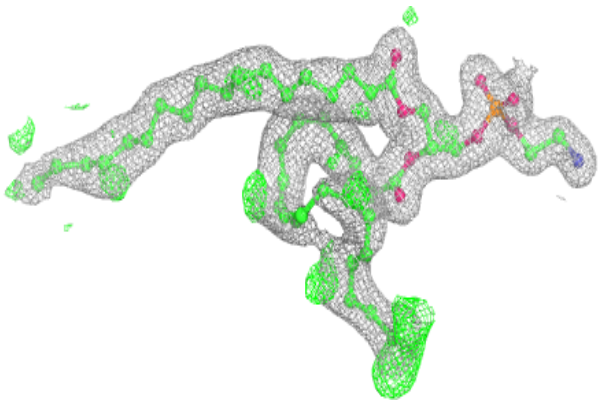


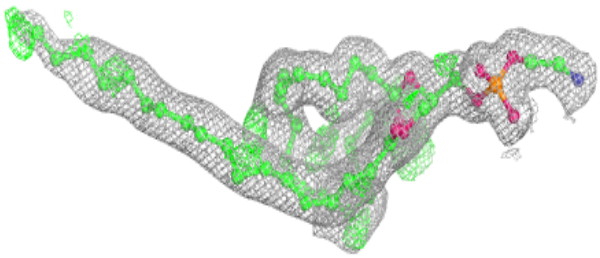


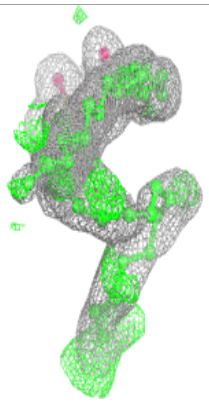


Electron density around PEK G 101:

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

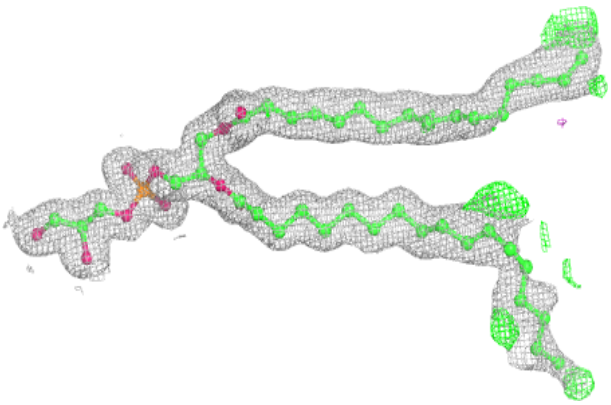


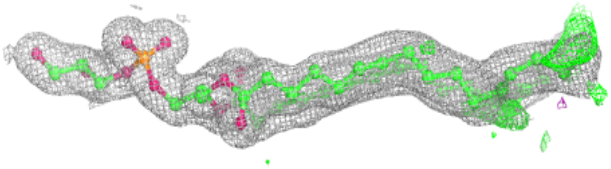


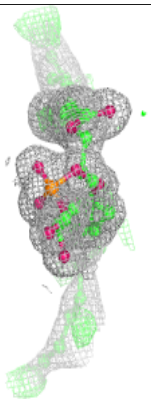


Electron density around PGV P 304:

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

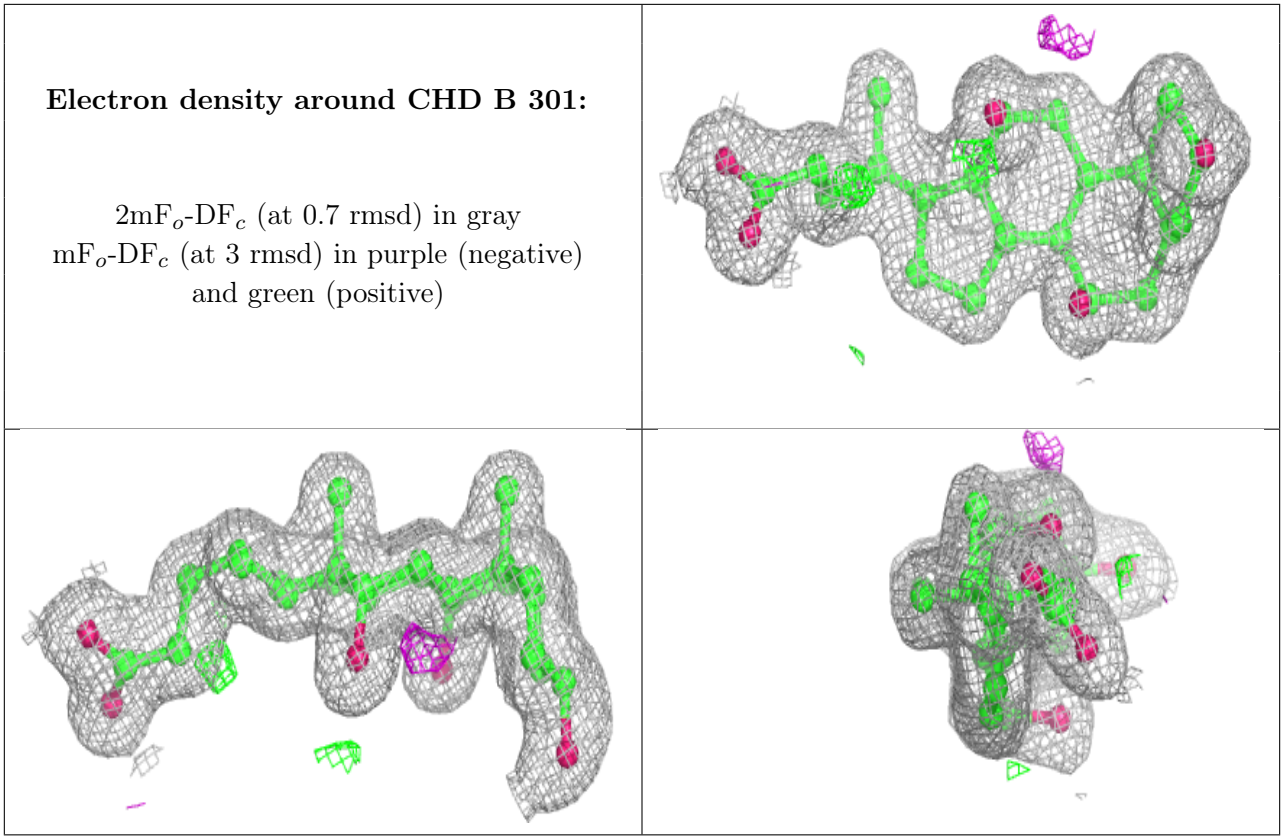






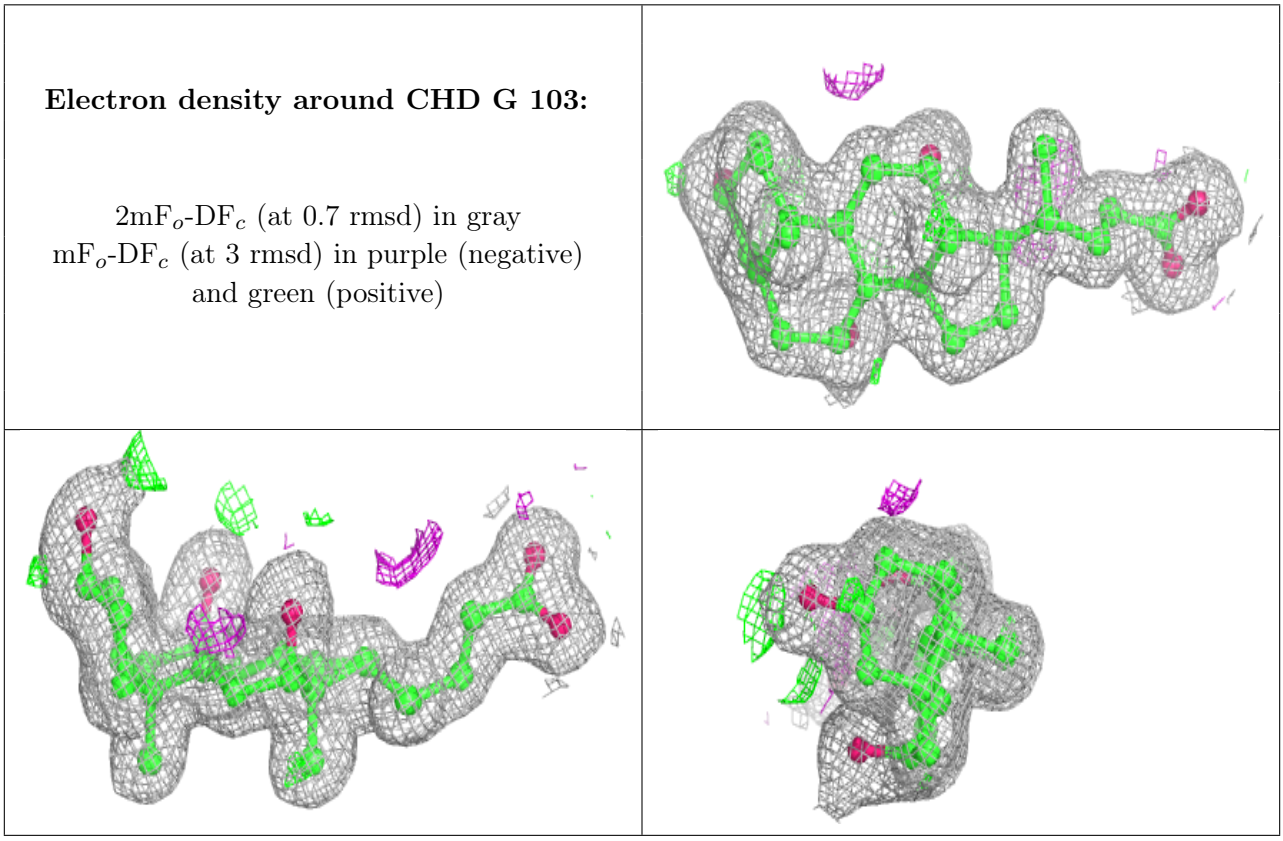
Electron density around CHD B 301:

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



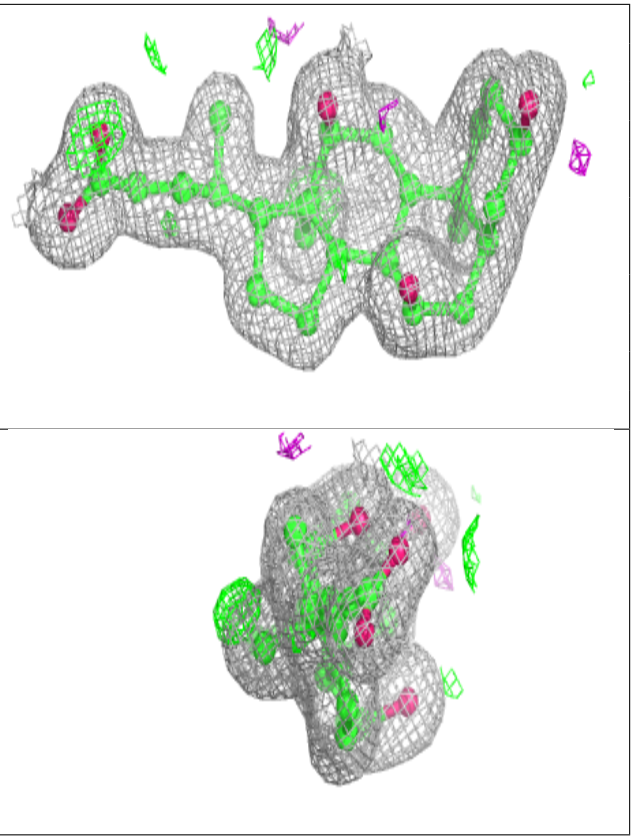
Electron density around CHD G 103:

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



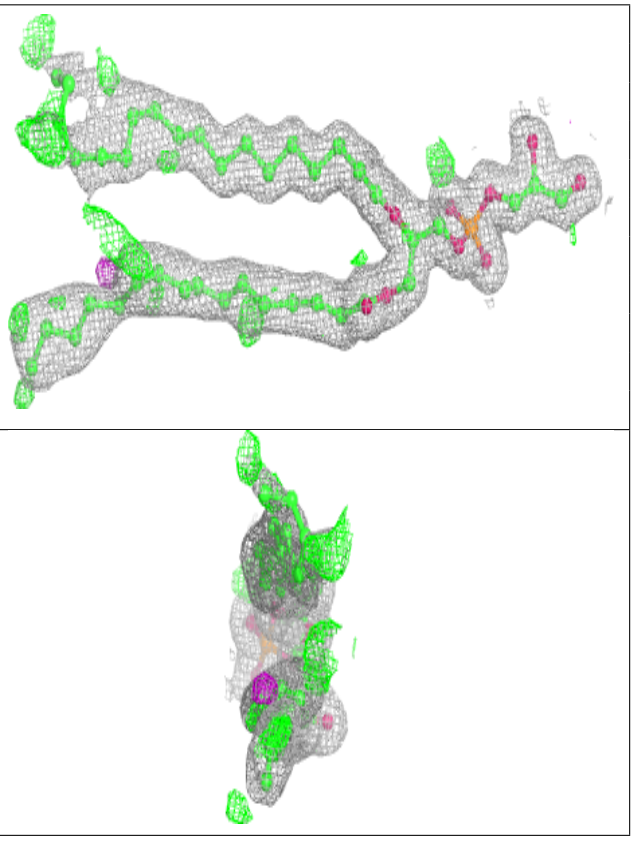
Electron density around CHD P 301:

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



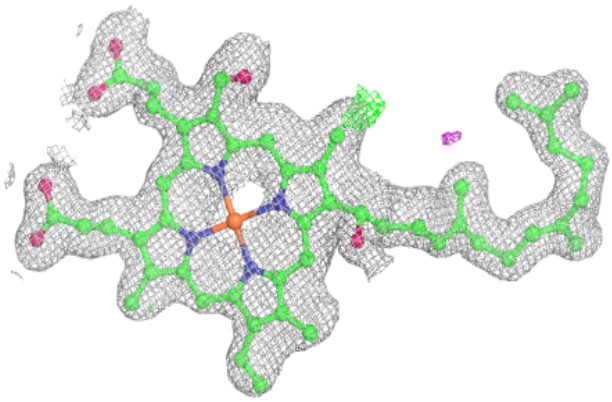
Electron density around PGV C 304:

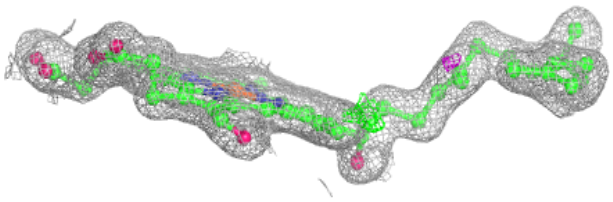
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

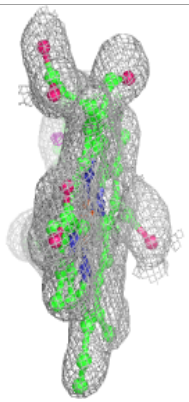


Electron density around HEA N 602 (A):

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

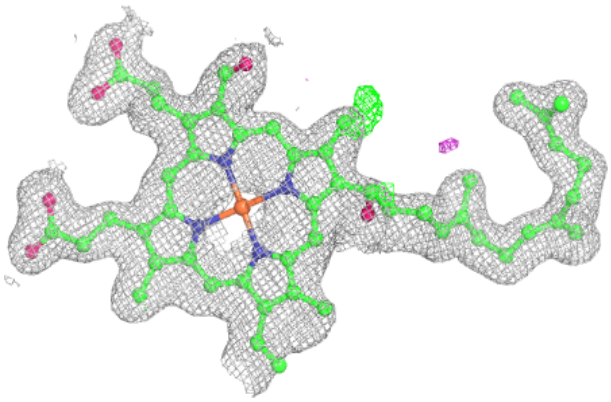


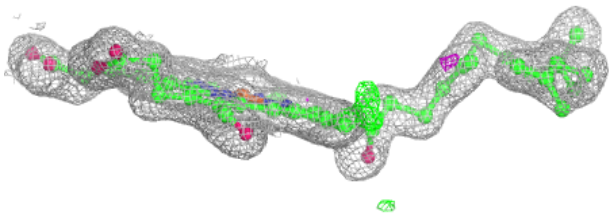


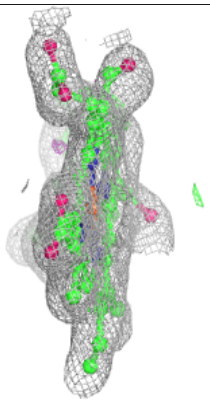


Electron density around HEA N 602 (B):

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

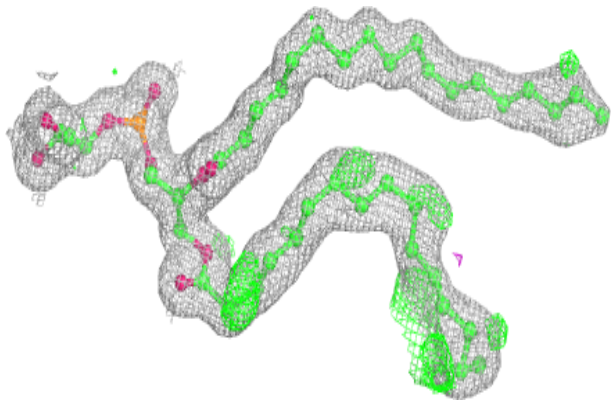


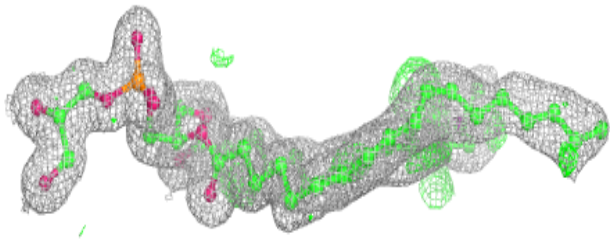


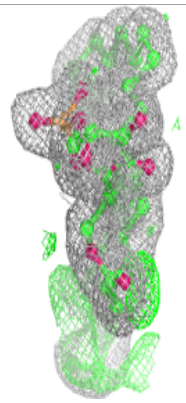


Electron density around PGV A 609:

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

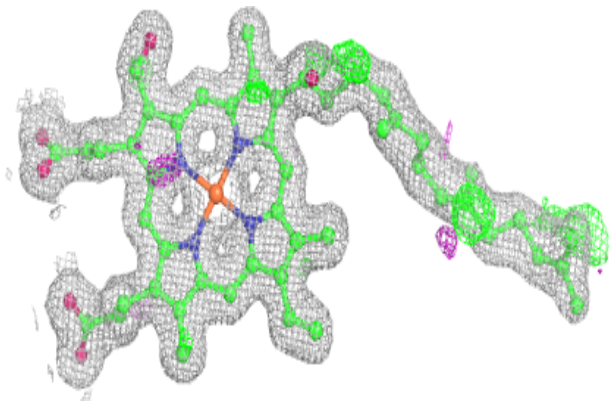


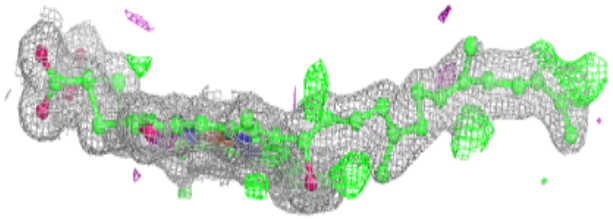


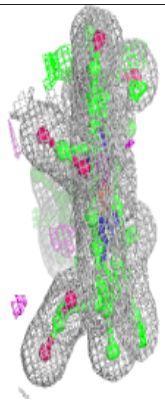


Electron density around HEA A 601:

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

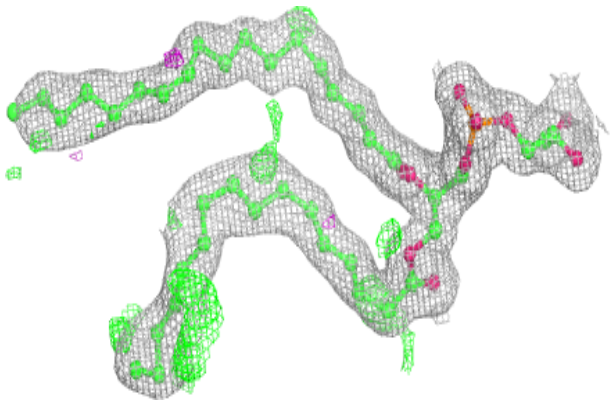


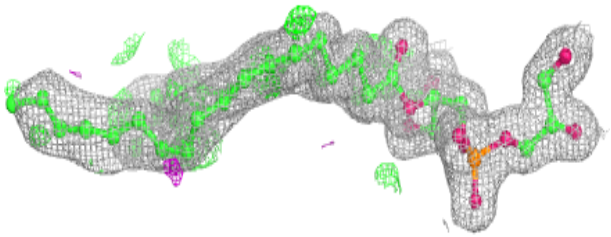




Electron density around PGV N 608:

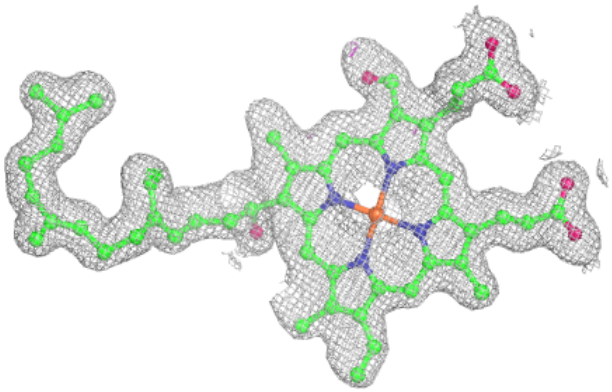
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

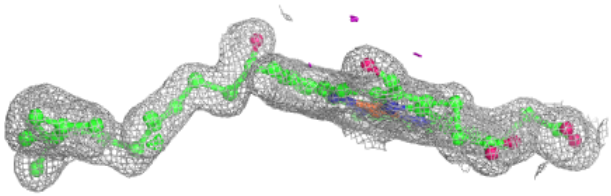


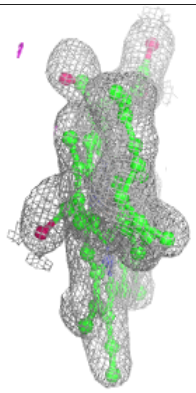


Electron density around HEA A 602 (A):

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

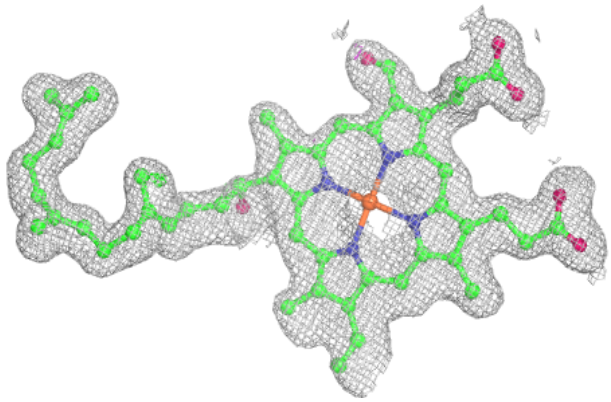


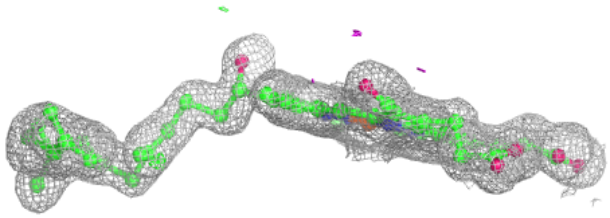


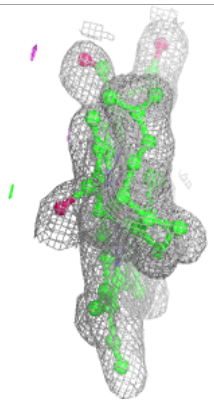


Electron density around HEA A 602 (B):

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

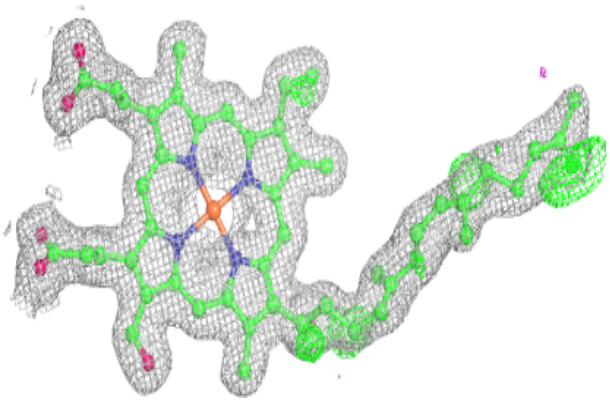


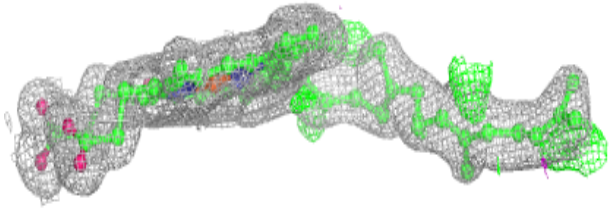


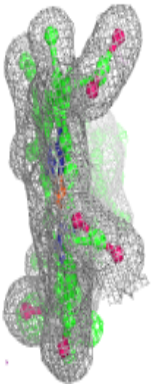


Electron density around HEA N 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.