Full wwPDB EM Validation Report (i)

Jan 16, 2023 – 01:04 pm GMT

PDB ID	:	8AB8
EMDB ID	:	EMD-15314
Title	:	Complex III2, b-position, with decylubiquinone and ascorbate-reduced
Authors	:	Wieferig, J.P.; Kuhlbrandt, W.
Deposited on	:	2022-07-04
Resolution	:	2.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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 (1)) were used in the production of this report:

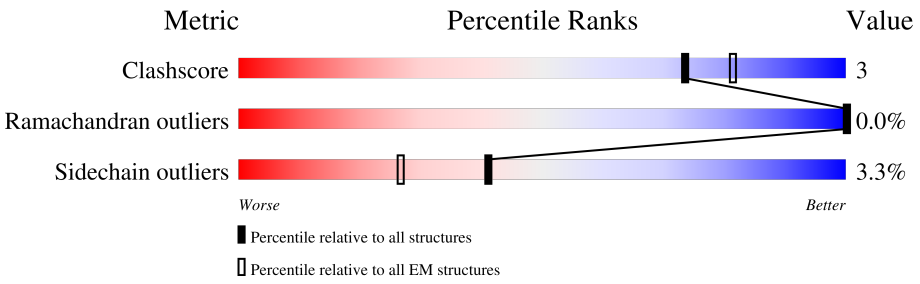
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	385	90% 9% ••
1	N	385	93% 6% ••
2	E	225	23% • 74%
2	P	225	14% 61% 19% • 17%
3	G	128	90% 6% • •
3	R	128	93% • • •
4	F	137	• 49% • 48%
4	Q	137	• 49% • 48%

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Mol	Chain	Length	Quality of chain
5	A	474	87% 5% 8%
5	L	474	88% 5% 8%
6	B	417	89% 6%
6	M	417	89% 7%
7	D	330	68% 6% 26%
7	O	330	68% 5% 26%
8	H	93	87% 9%
8	S	93	88% 9%
9	I	69	75% 22%
9	T	69	75% 22%
10	J	82	84% 6% 9%
10	U	82	85% 6% 9%

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
16	DCQ	C	507	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 32550 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	383	3052	2064	474	496	18	0	0
1	N	383	3052	2064	474	496	18	0	0

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	186	1445	920	248	268	9	0	0
2	E	59	452	288	74	87	3	0	0

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	124	994	640	162	190	2	0	0
3	R	124	994	640	162	190	2	0	0

- Molecule 4 is a protein called YALI0F24673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	71	579	361	99	115	4	0	0
4	Q	71	579	361	99	115	4	0	0

- Molecule 5 is a protein called YALI0A14806p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	438	3446	2154	603	682	7	0	0
5	L	438	3446	2154	603	682	7	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	402	3008	1907	516	583	2	0	0
6	M	402	3008	1907	516	583	2	0	0

- Molecule 7 is a protein called YALI0A17468p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	244	1893	1210	323	352	8	0	0
7	O	244	1893	1210	323	352	8	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	85	690	459	118	111	2	0	0
8	S	85	690	459	118	111	2	0	0

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	54	452	297	76	78	1	0	0
9	T	54	452	297	76	78	1	0	0

- Molecule 10 is a protein called YALI0C12210p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	75	598	403	99	96	0	0

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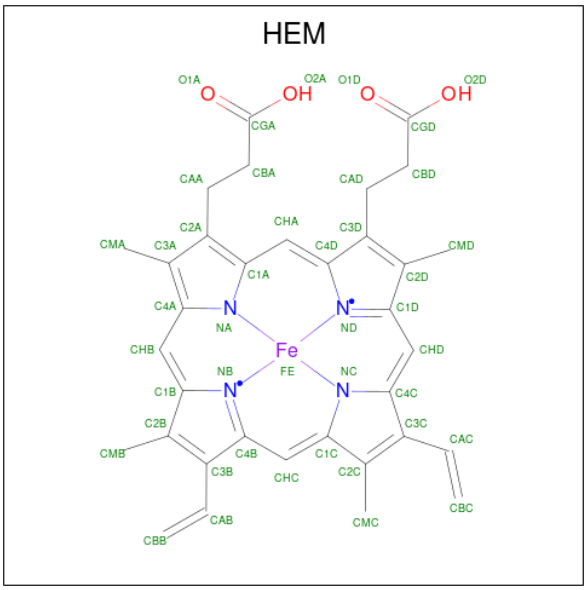
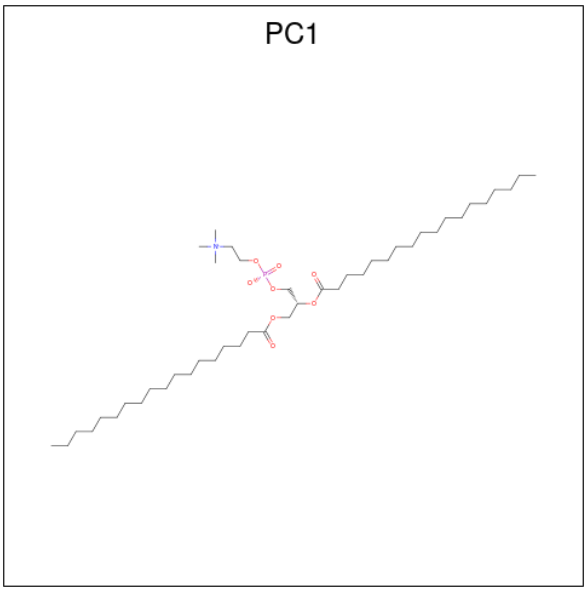
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	75	598	403	99	96	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



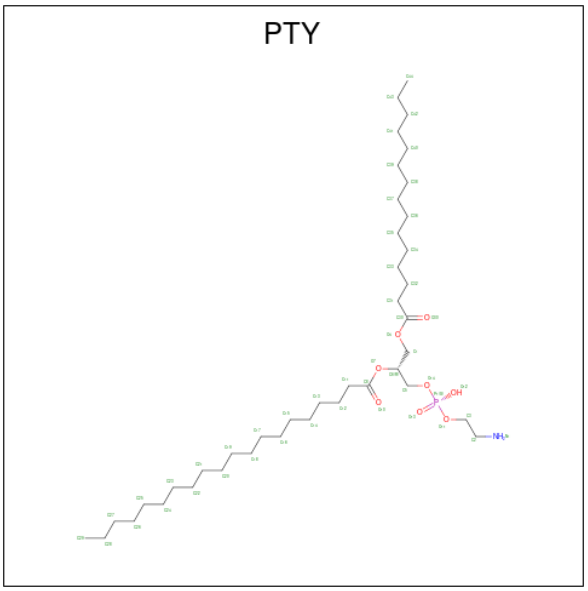
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
11	C	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	C	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	N	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	N	1	86	68	2	8	8	0

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



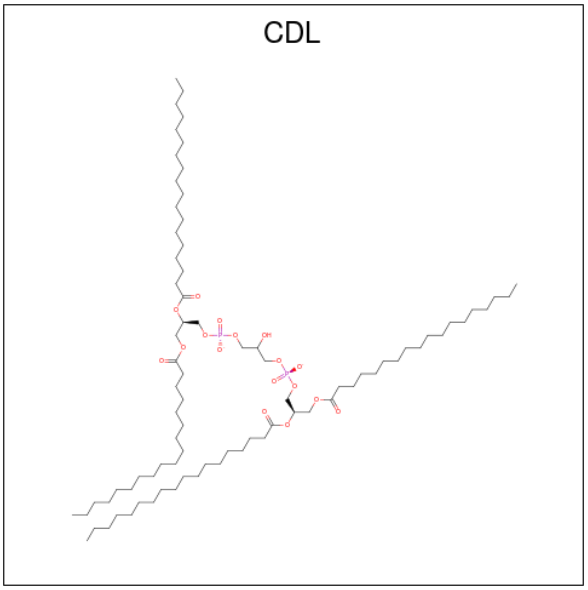
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	I	1	32	22	1	8	1	0
			Total	C	N	O	P	
12	N	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	T	1	32	22	1	8	1	0

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	E	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	A	1	Total	C	O	P	0
			89	55	30	4	
14	A	1	Total	C	O	P	0
			89	55	30	4	
14	H	1	Total	C	O	P	0
			89	51	34	4	
14	H	1	Total	C	O	P	0
			89	51	34	4	
14	N	1	Total	C	O	P	0
			48	29	17	2	
14	L	1	Total	C	O	P	0
			89	55	30	4	
14	L	1	Total	C	O	P	0
			89	55	30	4	

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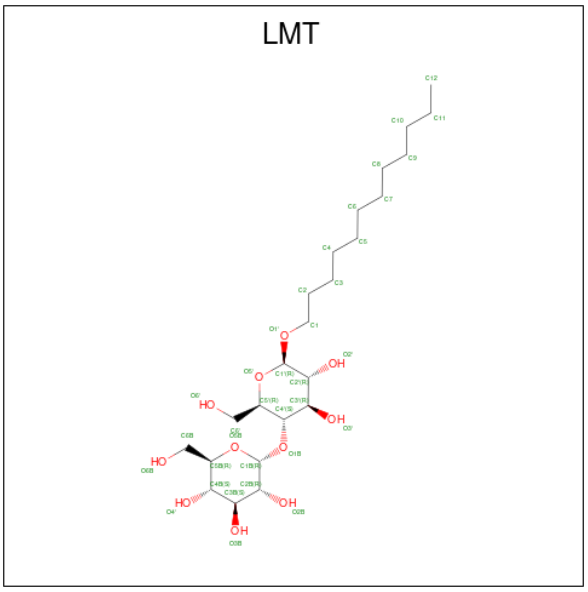
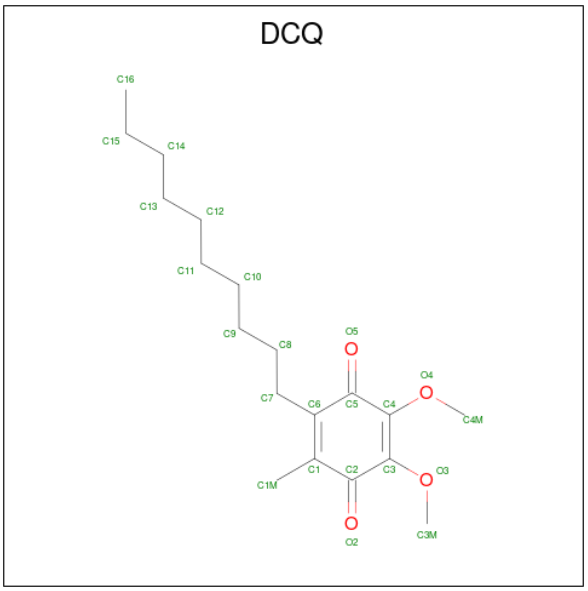
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	S	1	89	51	34	4	0
			Total	C	O	P	
14	S	1	89	51	34	4	0

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



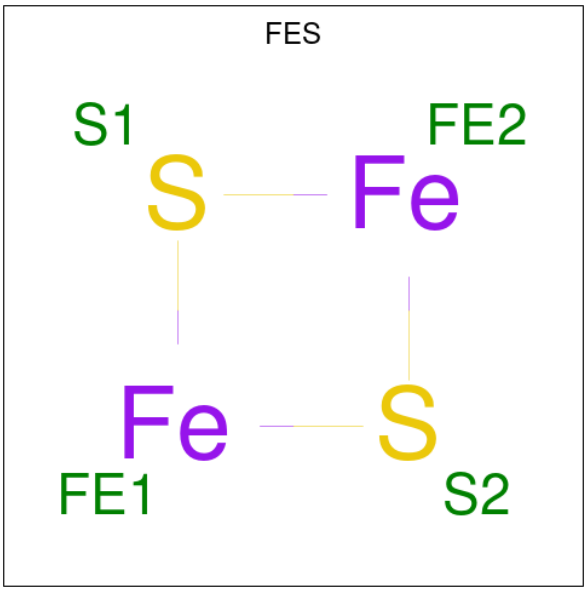
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	C	1	35	24	11	0
			Total	C	O	
15	P	1	35	24	11	0
			Total	C	O	
15	J	1	35	24	11	0
			Total	C	O	
15	N	1	35	24	11	0

- Molecule 16 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



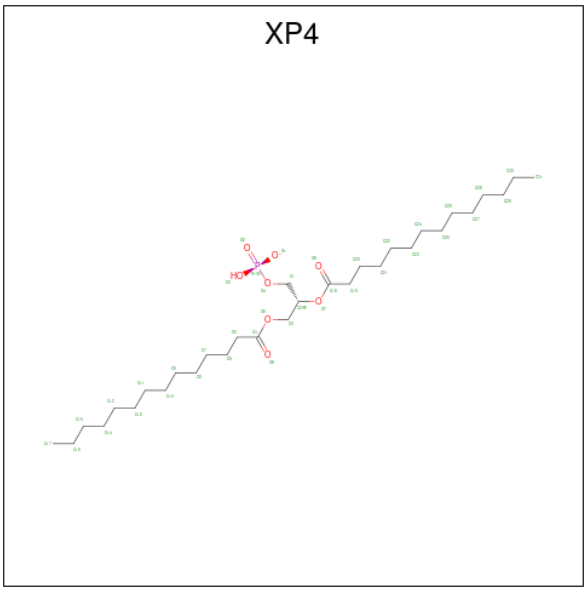
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	C	1	23	19	4	0

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



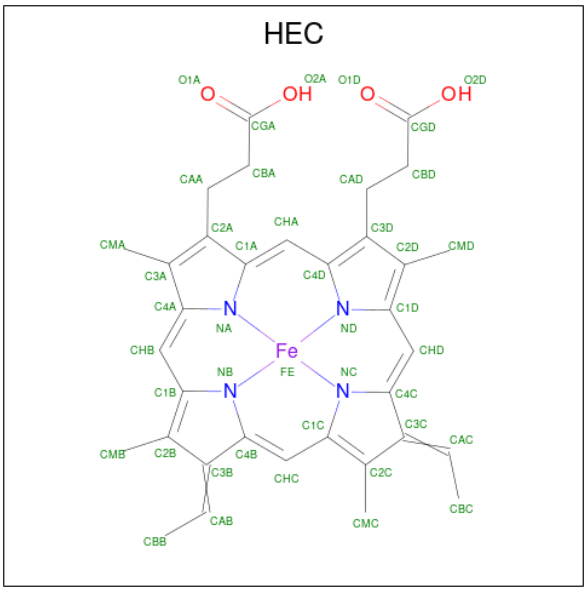
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	P	1	4	2	2	0

- Molecule 18 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: $C_{31}H_{60}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			24	15	8	1	
18	L	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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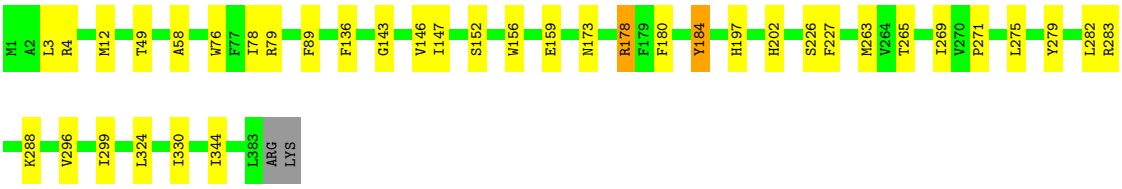
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
19	O	1	43	34	1	4	4	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 b

Chain C:

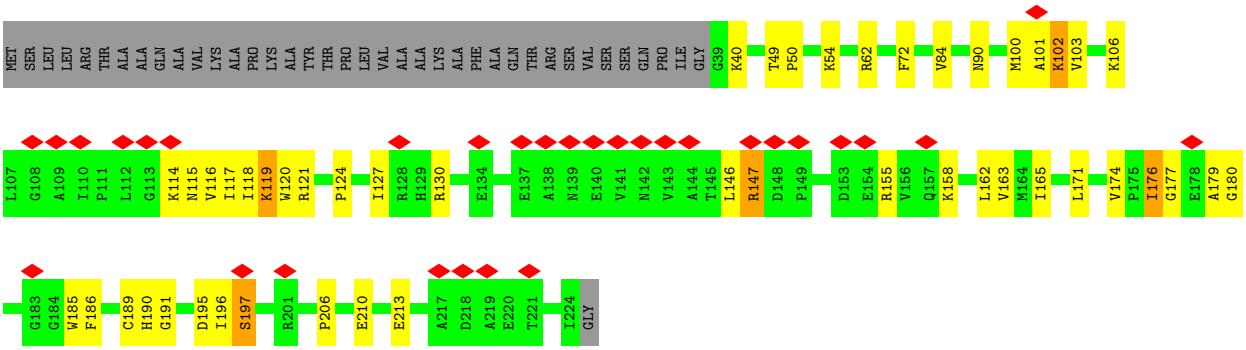


• Molecule 1: Cytochrome b

Chain N:

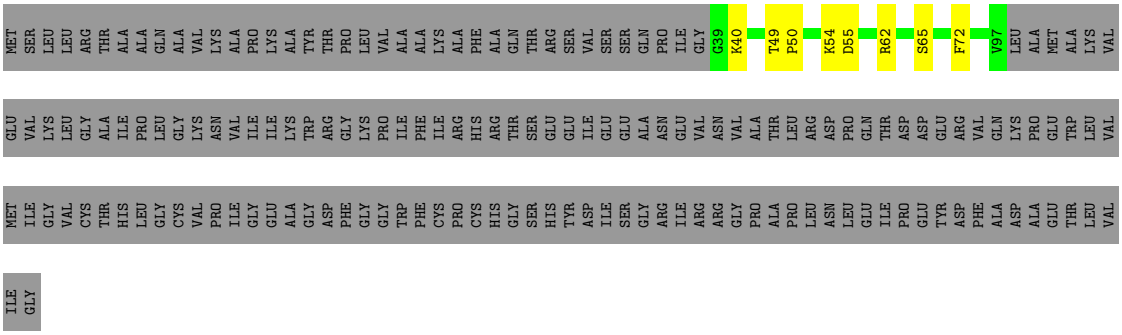
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



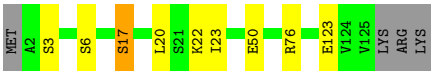
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



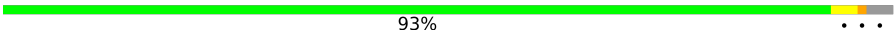
- Molecule 3: Cytochrome b-c1 complex subunit 7

Chain G:



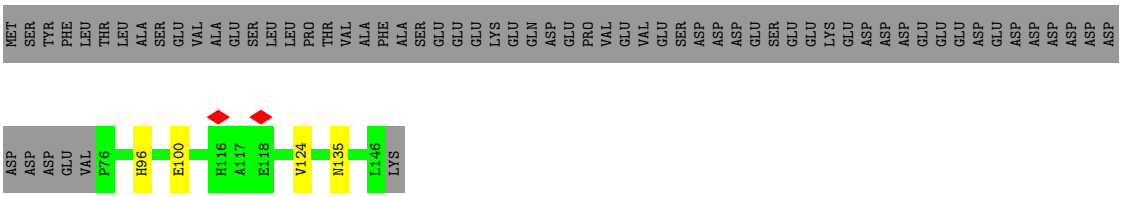
- Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:



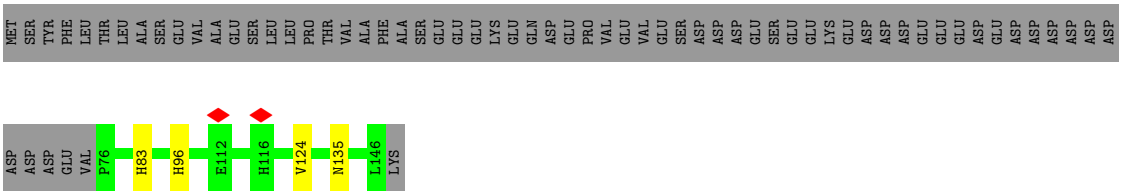
- Molecule 4: YALI0F24673p

Chain F:



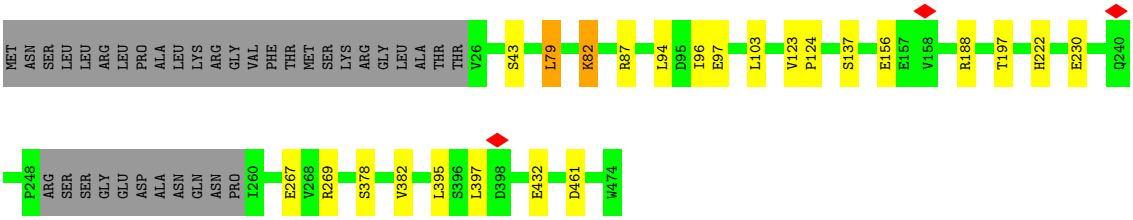
- Molecule 4: YALI0F24673p

Chain Q:



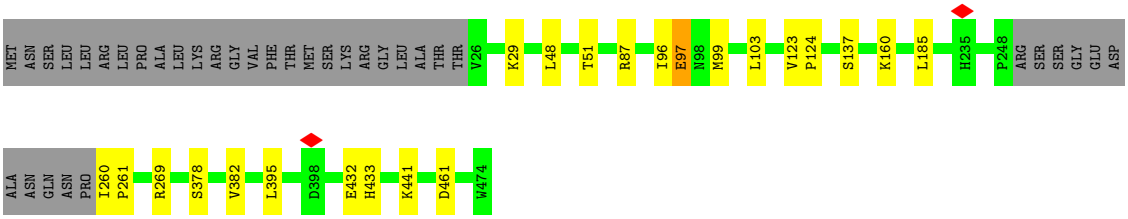
- Molecule 5: YALI0A14806p

Chain A:



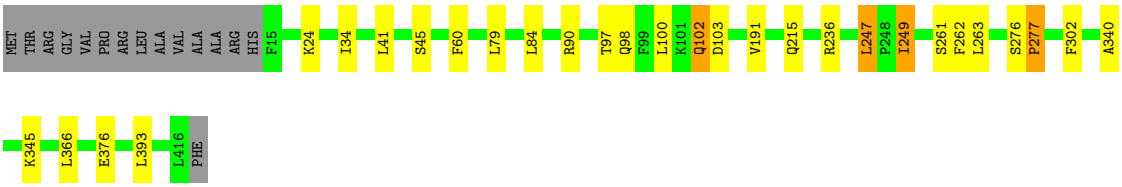
- Molecule 5: YALI0A14806p

Chain L:



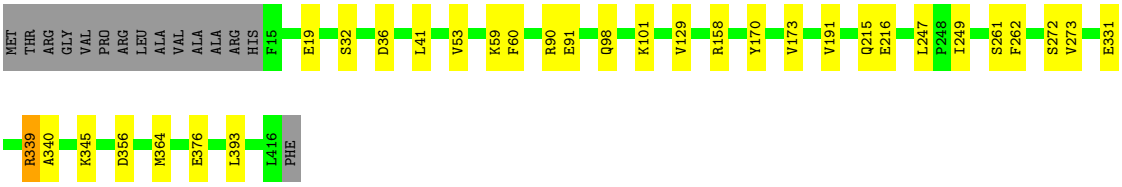
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



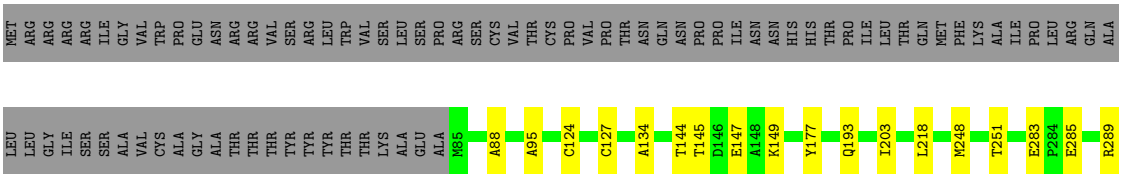
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

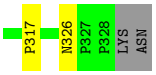
Chain M:



- Molecule 7: YALI0A17468p

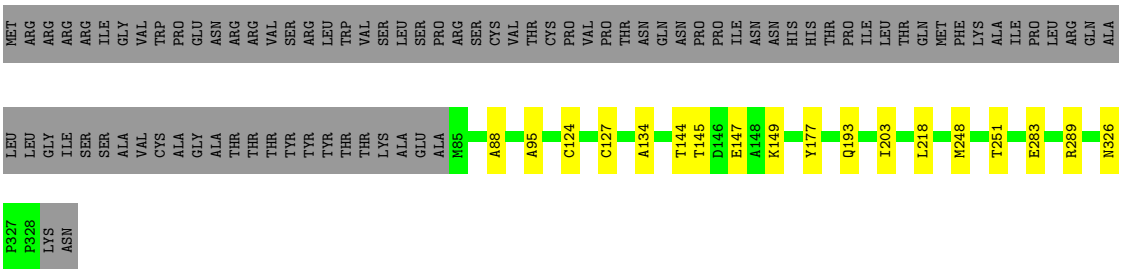
Chain D:





• Molecule 7: YALI0A17468p

Chain O:



• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:

• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:

• Molecule 9: Complex III subunit 9

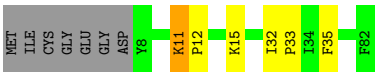
Chain I:

• Molecule 9: Complex III subunit 9

Chain T:

• Molecule 10: YALI0C12210p

Chain J:



• Molecule 10: YALI0C12210p

Chain U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	301.32, 301.32, 301.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

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: LMT, PTY, CDL, HEM, HEC, XP4, DCQ, PC1, FES

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	C	0.37	0/3153	0.67	3/4305 (0.1%)
1	N	0.36	0/3153	0.66	1/4305 (0.0%)
2	E	0.41	0/461	0.73	1/619 (0.2%)
2	P	0.34	0/1479	0.73	1/2003 (0.0%)
3	G	0.36	0/1012	0.70	1/1373 (0.1%)
3	R	0.36	0/1012	0.69	1/1373 (0.1%)
4	F	0.28	0/595	0.63	0/805
4	Q	0.29	0/595	0.67	1/805 (0.1%)
5	A	0.35	0/3510	0.70	1/4768 (0.0%)
5	L	0.35	0/3510	0.72	3/4768 (0.1%)
6	B	0.34	0/3069	0.73	2/4178 (0.0%)
6	M	0.34	0/3069	0.73	3/4178 (0.1%)
7	D	0.34	0/1950	0.75	2/2656 (0.1%)
7	O	0.34	0/1950	0.74	1/2656 (0.0%)
8	H	0.35	0/717	0.64	0/975
8	S	0.35	0/717	0.64	0/975
9	I	0.35	0/465	0.58	0/629
9	T	0.34	0/465	0.58	0/629
10	J	0.34	0/620	0.62	0/846
10	U	0.34	0/620	0.62	0/846
All	All	0.35	0/32122	0.70	21/43692 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	90	ARG	CG-CD-NE	-8.96	92.98	111.80
6	M	215	GLN	CB-CA-C	-8.87	92.66	110.40
6	B	215	GLN	CB-CA-C	-8.82	92.76	110.40
6	M	90	ARG	CG-CD-NE	-8.66	93.62	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	283	GLU	CB-CA-C	-7.21	95.98	110.40
3	G	76	ARG	NE-CZ-NH1	-6.92	116.84	120.30
7	D	283	GLU	CB-CA-C	-6.82	96.76	110.40
3	R	76	ARG	NE-CZ-NH1	-6.81	116.89	120.30
2	P	62	ARG	CB-CG-CD	-6.80	93.93	111.60
5	L	269	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	E	62	ARG	CB-CG-CD	-5.68	96.82	111.60
7	D	283	GLU	CB-CG-CD	-5.65	98.95	114.20
5	A	269	ARG	CG-CD-NE	-5.55	100.14	111.80
1	N	4	ARG	CG-CD-NE	-5.51	100.23	111.80
1	C	4	ARG	CG-CD-NE	-5.45	100.35	111.80
5	L	269	ARG	CG-CD-NE	-5.41	100.44	111.80
1	C	178	ARG	CB-CA-C	5.31	121.02	110.40
4	Q	96	HIS	CB-CA-C	-5.24	99.92	110.40
1	C	283	ARG	CG-CD-NE	5.12	122.56	111.80
5	L	269	ARG	NE-CZ-NH1	5.12	122.86	120.30
6	M	158	ARG	CG-CD-NE	-5.03	101.25	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3052	0	3113	32	0
1	N	3052	0	3113	15	0
2	E	452	0	443	3	0
2	P	1445	0	1426	35	0
3	G	994	0	1022	1	0
3	R	994	0	1022	2	0
4	F	579	0	511	2	0
4	Q	579	0	511	2	0
5	A	3446	0	3369	13	0
5	L	3446	0	3369	6	0
6	B	3008	0	2991	16	0
6	M	3008	0	2991	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1893	0	1834	21	0
7	O	1893	0	1834	21	0
8	H	690	0	673	4	0
8	S	690	0	673	3	0
9	I	452	0	435	1	0
9	T	452	0	435	1	0
10	J	598	0	615	4	0
10	U	598	0	615	3	0
11	C	86	0	60	5	0
11	N	86	0	60	5	0
12	C	38	0	50	1	0
12	I	32	0	38	2	0
12	N	38	0	50	1	0
12	T	32	0	38	3	0
13	C	41	0	58	5	0
13	E	41	0	58	3	0
13	N	41	0	58	9	0
13	P	41	0	58	13	0
14	A	89	0	85	4	0
14	C	48	0	40	1	0
14	H	89	0	66	6	0
14	L	89	0	85	0	0
14	N	48	0	40	2	0
14	S	89	0	66	7	0
15	C	35	0	46	2	0
15	J	35	0	46	2	0
15	N	35	0	46	1	0
15	P	35	0	46	1	0
16	C	23	0	30	16	0
17	P	4	0	0	0	0
18	A	24	0	22	1	0
18	L	24	0	22	1	0
19	D	43	0	32	12	0
19	O	43	0	32	14	0
All	All	32550	0	32227	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (215) 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)
2:P:84:VAL:CG2	13:P:303:PTY:H441	1.44	1.45
16:C:507:DCQ:O4	16:C:507:DCQ:C4M	1.69	1.38
7:D:124:CYS:SG	19:D:401:HEC:HBB3	1.65	1.37
7:O:124:CYS:SG	19:O:401:HEC:HBB3	1.73	1.27
7:O:127:CYS:SG	19:O:401:HEC:HBC3	1.86	1.15
7:D:124:CYS:SG	19:D:401:HEC:CBB	2.37	1.12
7:D:127:CYS:SG	19:D:401:HEC:HBC3	1.91	1.11
7:O:127:CYS:SG	19:O:401:HEC:CAC	2.40	1.09
7:D:127:CYS:SG	19:D:401:HEC:CAC	2.40	1.08
7:O:127:CYS:SG	19:O:401:HEC:CBC	2.41	1.08
2:P:84:VAL:HG23	13:P:303:PTY:C44	1.82	1.07
7:D:127:CYS:SG	19:D:401:HEC:CBC	2.44	1.04
2:P:84:VAL:CG2	13:P:303:PTY:C44	2.35	1.04
7:O:124:CYS:SG	19:O:401:HEC:CBB	2.44	1.04
2:P:84:VAL:HG22	13:P:303:PTY:H441	1.38	1.02
16:C:507:DCQ:C4M	16:C:507:DCQ:C4	2.38	1.02
5:A:395:LEU:HD23	6:B:34:ILE:HD12	1.42	1.00
2:P:84:VAL:HG23	13:P:303:PTY:H441	0.99	0.99
7:D:124:CYS:SG	19:D:401:HEC:CAB	2.56	0.94
7:O:124:CYS:SG	19:O:401:HEC:CAB	2.58	0.91
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.55	0.88
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.07	0.87
1:C:265:THR:OG1	2:P:174:VAL:HG22	1.74	0.87
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.59	0.84
1:C:58:ALA:H	1:C:173:ASN:HD22	1.27	0.82
1:C:344:ILE:HD12	2:P:190:HIS:HA	1.62	0.82
1:C:296:VAL:HA	16:C:507:DCQ:H16	1.62	0.80
1:C:269:ILE:HD12	2:P:189:CYS:SG	2.22	0.80
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.64	0.79
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.65	0.78
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.65	0.76
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.71	0.73
2:P:84:VAL:HG22	13:P:303:PTY:C44	2.11	0.72
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.71	0.71
5:A:395:LEU:CD2	6:B:34:ILE:HD12	2.20	0.69
14:S:702:CDL:CB6	14:S:702:CDL:C72	2.71	0.69
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	1.91	0.68
1:C:146:VAL:HG21	16:C:507:DCQ:H3MB	1.76	0.67
7:D:251:THR:HG21	19:D:401:HEC:HMC2	1.74	0.67
7:O:251:THR:HG21	19:O:401:HEC:HMC2	1.76	0.67
5:A:395:LEU:HD23	6:B:34:ILE:CD1	2.22	0.67
1:C:146:VAL:HG11	16:C:507:DCQ:C3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:702:CDL:C72	14:H:702:CDL:HB61	2.27	0.65
1:C:299:ILE:HD12	16:C:507:DCQ:H16B	1.79	0.65
8:H:51:ARG:HH21	14:H:701:CDL:HA22	1.62	0.65
14:H:702:CDL:C72	14:H:702:CDL:CB6	2.74	0.64
14:S:702:CDL:C72	14:S:702:CDL:HB61	2.27	0.64
1:C:58:ALA:H	1:C:173:ASN:ND2	1.94	0.62
2:P:155:ARG:NH1	2:P:197:SER:O	2.32	0.62
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.24	0.61
7:D:218:LEU:HD11	19:D:401:HEC:HMB2	1.82	0.61
8:S:47:ASN:O	8:S:51:ARG:HG2	2.01	0.61
6:M:91:GLU:HG2	6:M:364:MET:HE1	1.83	0.61
7:O:218:LEU:HD11	19:O:401:HEC:HMB2	1.83	0.61
8:S:51:ARG:HH21	14:S:701:CDL:HA21	1.65	0.60
1:C:344:ILE:CD1	2:P:190:HIS:HA	2.32	0.59
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.36	0.59
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.38	0.59
8:H:47:ASN:O	8:H:51:ARG:HG2	2.02	0.59
1:C:143:GLY:HA2	16:C:507:DCQ:H4M	1.83	0.59
7:D:127:CYS:SG	19:D:401:HEC:C3C	2.92	0.58
6:B:236:ARG:HD3	6:M:170:TYR:CE1	2.39	0.58
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.30	0.58
14:S:701:CDL:OB3	14:S:702:CDL:O1	2.22	0.57
2:P:180:GLY:HA2	2:P:186:PHE:HB2	1.87	0.57
5:A:378:SER:HA	5:A:432:GLU:OE1	2.06	0.56
1:C:143:GLY:HA2	16:C:507:DCQ:C4M	2.34	0.56
2:P:186:PHE:CE1	2:P:191:GLY:HA2	2.39	0.56
7:O:127:CYS:SG	19:O:401:HEC:C3C	2.92	0.56
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.87	0.56
7:D:145:THR:O	7:D:149:LYS:HG3	2.06	0.56
9:T:19:VAL:HG22	12:T:201:PC1:H332	1.87	0.56
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.88	0.55
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.36	0.55
7:O:203:ILE:HG12	19:O:401:HEC:HMA3	1.87	0.55
2:P:84:VAL:HG23	13:P:303:PTY:C43	2.37	0.55
7:D:124:CYS:SG	19:D:401:HEC:C3B	2.94	0.55
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.89	0.55
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.87	0.55
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.36	0.54
1:C:146:VAL:HG13	2:P:171:LEU:HD13	1.90	0.54
7:O:124:CYS:HG	19:O:401:HEC:HBB3	1.65	0.54
11:C:502:HEM:HBC2	11:C:502:HEM:HMC2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:124:CYS:SG	19:O:401:HEC:C3B	2.96	0.54
11:N:501:HEM:HHD	11:N:501:HEM:CBC	2.36	0.54
5:A:43:SER:CB	5:A:222:HIS:HD2	2.21	0.53
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.88	0.53
6:M:91:GLU:HG2	6:M:364:MET:CE	2.38	0.53
1:C:3:LEU:HD11	14:N:505:CDL:HB32	1.90	0.53
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.91	0.53
1:N:229:ASP:HB2	13:N:504:PTY:H382	1.90	0.53
7:D:203:ILE:HG12	19:D:401:HEC:HMA3	1.91	0.53
6:M:59:LYS:HB3	6:M:129:VAL:HG13	1.91	0.52
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.57	0.52
6:M:53:VAL:HG12	6:M:173:VAL:HG13	1.92	0.52
13:P:303:PTY:H141	13:P:303:PTY:H311	1.92	0.52
4:F:124:VAL:HG11	7:D:88:ALA:HB2	1.92	0.52
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.92	0.51
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.09	0.51
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.74	0.51
11:C:501:HEM:HHD	11:C:501:HEM:CBC	2.41	0.50
5:A:395:LEU:HD22	6:B:98:GLN:HG2	1.92	0.50
5:A:96:ILE:HG12	5:A:103:LEU:HD13	1.93	0.50
6:B:249:ILE:HD11	6:B:302:PHE:HB2	1.94	0.50
2:P:177:GLY:HA2	2:P:185:TRP:CD1	2.46	0.49
6:B:236:ARG:HD3	6:M:170:TYR:CD1	2.47	0.49
13:N:504:PTY:H111	12:T:201:PC1:O31	2.13	0.49
9:I:22:ILE:HG21	12:I:201:PC1:H331	1.95	0.49
2:P:124:PRO:HG2	2:P:174:VAL:HG11	1.93	0.49
5:L:97:GLU:HB3	6:M:339:ARG:HD3	1.94	0.49
1:C:146:VAL:HG11	16:C:507:DCQ:C2	2.42	0.49
13:C:504:PTY:H361	14:A:3001:CDL:H362	1.95	0.48
4:Q:124:VAL:HG11	7:O:88:ALA:HB2	1.93	0.48
5:L:96:ILE:HG12	5:L:103:LEU:HD13	1.95	0.48
18:L:3003:XP4:H8	10:U:35:PHE:HE1	1.78	0.48
2:P:118:ILE:HD13	2:P:127:ILE:HD12	1.96	0.48
1:C:275:LEU:HD13	16:C:507:DCQ:H10A	1.96	0.48
16:C:507:DCQ:H7A	16:C:507:DCQ:H1M	1.28	0.48
6:M:249:ILE:HD11	6:M:393:LEU:HD21	1.95	0.48
10:J:11:LYS:HD2	10:J:12:PRO:HD2	1.97	0.47
13:N:504:PTY:H112	12:T:201:PC1:H242	1.96	0.47
6:M:247:LEU:HD13	6:M:393:LEU:HB3	1.96	0.47
1:C:279:TYR:CE1	16:C:507:DCQ:C2	2.98	0.47
2:P:72:PHE:HE2	13:N:504:PTY:H152	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:103:VAL:HG22	2:P:120:TRP:CD1	2.49	0.47
13:P:303:PTY:H352	13:P:303:PTY:H381	1.69	0.47
14:H:702:CDL:HA62	14:H:702:CDL:H311	1.65	0.47
2:P:49:THR:N	2:P:50:PRO:HD2	2.29	0.47
14:C:505:CDL:HB32	1:N:3:LEU:HD11	1.96	0.47
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.97	0.47
15:P:302:LMT:H32	15:P:302:LMT:H62	1.50	0.46
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.98	0.46
1:C:282:LEU:HD22	16:C:507:DCQ:H1MA	1.97	0.46
2:P:101:ALA:HA	2:P:121:ARG:HE	1.80	0.46
12:I:201:PC1:H351	12:I:201:PC1:H322	1.59	0.46
14:S:702:CDL:HA62	14:S:702:CDL:H311	1.58	0.46
7:D:326:ASN:OD1	2:E:40:LYS:HA	2.16	0.46
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.96	0.46
5:A:82:LYS:HA	5:A:82:LYS:HD3	1.61	0.46
6:B:247:LEU:HD13	6:B:393:LEU:HB3	1.96	0.46
7:O:144:THR:OG1	7:O:147:GLU:HG3	2.16	0.46
2:P:116:VAL:HG23	2:P:127:ILE:O	2.16	0.46
14:A:3002:CDL:H132	14:A:3002:CDL:H522	1.98	0.46
7:D:144:THR:OG1	7:D:147:GLU:HG3	2.16	0.45
14:H:701:CDL:OB3	14:H:702:CDL:O1	2.34	0.45
6:M:249:ILE:CD1	6:M:393:LEU:HD21	2.47	0.45
15:J:101:LMT:H42	15:J:101:LMT:H71	1.47	0.45
8:H:56:ALA:HA	14:H:701:CDL:H132	1.99	0.45
13:N:504:PTY:H331	13:N:504:PTY:H362	1.54	0.45
1:C:271:PRO:HB3	16:C:507:DCQ:O5	2.17	0.45
13:C:504:PTY:H112	13:C:504:PTY:HC12	1.99	0.45
2:P:103:VAL:HG22	2:P:120:TRP:HD1	1.82	0.45
7:O:248:MET:HB2	19:O:401:HEC:C1D	2.47	0.44
13:N:504:PTY:H402	13:N:504:PTY:H372	1.73	0.44
1:C:147:ILE:HD11	16:C:507:DCQ:O5	2.18	0.44
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.51	0.44
7:D:248:MET:HB2	19:D:401:HEC:C1D	2.47	0.44
13:E:401:PTY:H132	13:E:401:PTY:H161	1.54	0.44
2:P:130:ARG:HD2	2:P:162:LEU:HB2	1.99	0.44
13:E:401:PTY:H352	13:E:401:PTY:H381	1.40	0.44
2:P:40:LYS:HA	7:O:326:ASN:OD1	2.17	0.43
2:P:102:LYS:HB2	2:P:102:LYS:HE2	1.52	0.43
10:J:11:LYS:HB3	10:J:11:LYS:HE3	1.88	0.43
1:N:226:SER:HB3	13:N:504:PTY:H331	2.00	0.43
13:P:303:PTY:H331	13:P:303:PTY:H361	1.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:101:LMT:H22	15:J:101:LMT:H51	1.65	0.43
2:P:176:ILE:H	2:P:176:ILE:HG12	1.66	0.43
1:C:271:PRO:HG3	16:C:507:DCQ:O5	2.18	0.43
1:N:49:THR:HG21	1:N:78:ILE:HD13	2.01	0.43
7:O:127:CYS:HG	19:O:401:HEC:HBC3	1.75	0.43
18:A:3003:XP4:H8	10:J:35:PHE:HE1	1.83	0.43
5:A:79:LEU:HD12	5:A:79:LEU:HA	1.89	0.43
6:B:102:GLN:H	6:B:102:GLN:HG3	1.51	0.43
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.54	0.43
1:N:227:PHE:HZ	13:N:504:PTY:HC6	1.84	0.43
2:P:147:ARG:HD2	2:P:206:PRO:HA	2.01	0.42
1:N:108:THR:HA	14:N:505:CDL:OA4	2.20	0.42
2:P:171:LEU:HD12	2:P:190:HIS:CE1	2.54	0.42
6:B:100:LEU:HB2	6:B:103:ASP:OD2	2.18	0.42
1:N:226:SER:HB3	13:N:504:PTY:H321	2.01	0.42
7:O:145:THR:HG22	7:O:149:LYS:HD2	2.02	0.42
13:C:504:PTY:H132	2:E:72:PHE:CE2	2.54	0.42
6:B:263:LEU:HA	6:B:277:PRO:HG2	2.01	0.42
1:C:227:PHE:CZ	13:C:504:PTY:H322	2.55	0.42
1:C:12:MET:HB3	15:C:506:LMT:H41	2.02	0.42
7:D:317:PRO:HG3	8:H:31:PRO:HD3	2.02	0.42
6:B:262:PHE:HB2	6:B:340:ALA:HB2	2.02	0.42
1:C:263:MET:CE	2:P:119:LYS:HB3	2.50	0.41
2:P:84:VAL:CG2	13:P:303:PTY:C43	2.94	0.41
7:O:134:ALA:HA	7:O:177:TYR:HA	2.02	0.41
1:C:202:HIS:HD2	15:C:506:LMT:O3'	2.03	0.41
7:D:134:ALA:HA	7:D:177:TYR:HA	2.02	0.41
2:P:177:GLY:C	2:P:179:ALA:H	2.24	0.41
5:L:160:LYS:HA	5:L:160:LYS:HD2	1.93	0.41
13:P:303:PTY:H161	13:P:303:PTY:H132	1.88	0.41
5:A:123:VAL:N	5:A:124:PRO:CD	2.84	0.41
2:P:165:ILE:HD12	2:P:210:GLU:HB2	2.02	0.41
2:E:49:THR:N	2:E:50:PRO:HD2	2.35	0.41
3:R:20:LEU:HD23	3:R:20:LEU:HA	1.91	0.41
5:L:123:VAL:N	5:L:124:PRO:CD	2.84	0.41
8:S:56:ALA:HA	14:S:701:CDL:H132	2.03	0.41
1:N:202:HIS:HD2	15:N:506:LMT:O3'	2.04	0.41
1:N:324:LEU:HD23	1:N:324:LEU:HA	1.96	0.41
10:U:29:SER:HA	10:U:32:ILE:HG12	2.03	0.41
13:P:303:PTY:H412	13:P:303:PTY:H443	1.64	0.41
1:N:27:ASN:HB2	14:S:701:CDL:OB4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:THR:HG21	1:C:78:ILE:HD13	2.02	0.40
1:C:226:SER:HB3	13:C:504:PTY:H331	2.02	0.40
13:E:401:PTY:H141	13:E:401:PTY:H311	2.03	0.40
1:C:76:TRP:CG	7:D:285:GLU:HG3	2.56	0.40
10:J:32:ILE:HB	10:J:33:PRO:HD3	2.02	0.40
1:N:276:LEU:N	1:N:277:PRO:CD	2.84	0.40
2:P:127:ILE:HG12	2:P:163:VAL:HG22	2.04	0.40
6:M:262:PHE:HB2	6:M:340:ALA:HB2	2.03	0.40
5:L:260:ILE:HA	5:L:261:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	C	381/385 (99%)	374 (98%)	6 (2%)	1 (0%)	41	64
1	N	381/385 (99%)	374 (98%)	7 (2%)	0	100	100
2	E	57/225 (25%)	56 (98%)	1 (2%)	0	100	100
2	P	184/225 (82%)	169 (92%)	15 (8%)	0	100	100
3	G	122/128 (95%)	122 (100%)	0	0	100	100
3	R	122/128 (95%)	122 (100%)	0	0	100	100
4	F	69/137 (50%)	67 (97%)	2 (3%)	0	100	100
4	Q	69/137 (50%)	67 (97%)	2 (3%)	0	100	100
5	A	434/474 (92%)	424 (98%)	10 (2%)	0	100	100
5	L	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
6	B	400/417 (96%)	384 (96%)	16 (4%)	0	100	100
6	M	400/417 (96%)	387 (97%)	13 (3%)	0	100	100
7	D	242/330 (73%)	238 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	242/330 (73%)	238 (98%)	4 (2%)	0	100	100
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
9	I	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
9	T	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
10	J	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
10	U	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
All	All	3953/4680 (84%)	3853 (98%)	99 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	156	TRP

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 PDB entries followed by that with respect to all EM entries.

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	C	331/333 (99%)	321 (97%)	10 (3%)	41	67
1	N	331/333 (99%)	320 (97%)	11 (3%)	38	64
2	E	48/182 (26%)	45 (94%)	3 (6%)	18	36
2	P	154/182 (85%)	137 (89%)	17 (11%)	6	11
3	G	113/117 (97%)	106 (94%)	7 (6%)	18	37
3	R	113/117 (97%)	110 (97%)	3 (3%)	44	71
4	F	61/123 (50%)	59 (97%)	2 (3%)	38	64
4	Q	61/123 (50%)	60 (98%)	1 (2%)	62	82
5	A	377/407 (93%)	366 (97%)	11 (3%)	42	68
5	L	377/407 (93%)	364 (97%)	13 (3%)	37	63
6	B	311/322 (97%)	300 (96%)	11 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	311/322 (97%)	298 (96%)	13 (4%)	30	55
7	D	192/268 (72%)	191 (100%)	1 (0%)	88	96
7	O	192/268 (72%)	191 (100%)	1 (0%)	88	96
8	H	67/71 (94%)	66 (98%)	1 (2%)	65	83
8	S	67/71 (94%)	66 (98%)	1 (2%)	65	83
9	I	46/57 (81%)	45 (98%)	1 (2%)	52	76
9	T	46/57 (81%)	45 (98%)	1 (2%)	52	76
10	J	63/68 (93%)	61 (97%)	2 (3%)	39	65
10	U	63/68 (93%)	63 (100%)	0	100	100
All	All	3324/3896 (85%)	3214 (97%)	110 (3%)	41	64

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ARG
1	C	89	PHE
1	C	136	PHE
1	C	152	SER
1	C	159	GLU
1	C	178	ARG
1	C	184	TYR
1	C	197	HIS
1	C	288	LYS
1	C	324	LEU
2	P	54	LYS
2	P	90	ASN
2	P	100	MET
2	P	102	LYS
2	P	106	LYS
2	P	114	LYS
2	P	115	ASN
2	P	117	ILE
2	P	119	LYS
2	P	146	LEU
2	P	147	ARG
2	P	158	LYS
2	P	176	ILE
2	P	195	ASP
2	P	196	ILE

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Mol	Chain	Res	Type
2	P	197	SER
2	P	213	GLU
3	G	3	SER
3	G	6	SER
3	G	17	SER
3	G	22	LYS
3	G	23	ILE
3	G	50	GLU
3	G	123	GLU
4	F	96	HIS
4	F	100	GLU
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	137	SER
5	A	197	THR
5	A	230	GLU
5	A	267	GLU
5	A	397	LEU
5	A	461	ASP
6	B	45	SER
6	B	60	PHE
6	B	79	LEU
6	B	102	GLN
6	B	247	LEU
6	B	249	ILE
6	B	261	SER
6	B	276	SER
6	B	277	PRO
6	B	345	LYS
6	B	376	GLU
7	D	193	GLN
8	H	51	ARG
9	I	27	PHE
10	J	11	LYS
10	J	15	LYS
1	N	79	ARG
1	N	89	PHE
1	N	136	PHE
1	N	178	ARG

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Mol	Chain	Res	Type
1	N	184	TYR
1	N	197	HIS
1	N	250	LYS
1	N	255	ASP
1	N	270	VAL
1	N	288	LYS
1	N	324	LEU
2	E	54	LYS
2	E	55	ASP
2	E	65	SER
3	R	17	SER
3	R	22	LYS
3	R	23	ILE
4	Q	83	HIS
5	L	29	LYS
5	L	48	LEU
5	L	51	THR
5	L	87	ARG
5	L	97	GLU
5	L	99	MET
5	L	137	SER
5	L	185	LEU
5	L	378	SER
5	L	395	LEU
5	L	433	HIS
5	L	441	LYS
5	L	461	ASP
6	M	19	GLU
6	M	32	SER
6	M	60	PHE
6	M	101	LYS
6	M	216	GLU
6	M	261	SER
6	M	272	SER
6	M	273	VAL
6	M	331	GLU
6	M	339	ARG
6	M	345	LYS
6	M	356	ASP
6	M	376	GLU
7	O	193	GLN
8	S	51	ARG

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Mol	Chain	Res	Type
9	T	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	11	ASN
1	C	14	ASN
1	C	173	ASN
1	C	202	HIS
1	C	332	ASN
2	P	90	ASN
3	G	54	ASN
5	A	222	HIS
6	B	215	GLN
10	J	70	HIS
1	N	14	ASN
1	N	202	HIS
1	N	332	ASN
2	E	90	ASN
6	M	92	HIS
6	M	184	GLN
6	M	215	GLN
10	U	70	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 ligands 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	$\#\|Z\| > 2$
14	CDL	A	3002	-	46,46,99	0.36	0	51,56,111	0.82	3 (5%)
13	PTY	E	401	-	40,40,49	0.39	0	43,45,54	0.50	0
11	HEM	N	502	1	41,50,50	1.36	6 (14%)	45,82,82	2.32	19 (42%)
14	CDL	C	505	-	47,47,99	0.42	0	53,59,111	0.78	2 (3%)
19	HEC	D	401	7	32,50,50	2.02	9 (28%)	24,82,82	2.79	6 (25%)
17	FES	P	301	2	0,4,4	-	-	-		
11	HEM	C	502	1	41,50,50	1.30	5 (12%)	45,82,82	2.29	17 (37%)
15	LMT	C	506	-	36,36,36	0.45	0	47,47,47	1.08	4 (8%)
14	CDL	L	3002	-	46,46,99	0.33	0	51,56,111	0.77	3 (5%)
13	PTY	P	303	-	40,40,49	0.39	0	43,45,54	0.61	0
18	XP4	L	3003	-	23,23,39	1.43	2 (8%)	27,28,44	1.91	5 (18%)
14	CDL	S	702	-	38,38,99	0.40	0	44,50,111	1.12	3 (6%)
12	PC1	C	503	-	37,37,53	0.63	0	43,45,61	0.95	2 (4%)
14	CDL	H	701	-	49,49,99	0.36	0	55,61,111	0.74	1 (1%)
12	PC1	N	503	-	37,37,53	0.65	1 (2%)	43,45,61	0.92	3 (6%)
14	CDL	N	505	-	47,47,99	0.42	0	53,59,111	0.73	2 (3%)
14	CDL	L	3001	-	41,41,99	0.40	0	45,51,111	0.69	1 (2%)
14	CDL	S	701	-	49,49,99	0.37	0	55,61,111	0.72	0
15	LMT	J	101	-	36,36,36	0.38	0	47,47,47	1.05	4 (8%)
19	HEC	O	401	7	32,50,50	2.00	8 (25%)	24,82,82	2.99	5 (20%)
11	HEM	N	501	1	41,50,50	1.36	8 (19%)	45,82,82	2.09	10 (22%)
16	DCQ	C	507	-	23,23,23	2.99	6 (26%)	26,29,29	2.26	7 (26%)
11	HEM	C	501	1	41,50,50	1.34	8 (19%)	45,82,82	1.97	10 (22%)
15	LMT	N	506	-	36,36,36	0.43	0	47,47,47	1.11	6 (12%)
13	PTY	N	504	-	40,40,49	0.32	0	43,45,54	0.68	1 (2%)
14	CDL	H	702	-	38,38,99	0.39	0	44,50,111	1.10	3 (6%)
12	PC1	I	201	-	31,31,53	0.36	0	37,39,61	0.72	0
12	PC1	T	201	-	31,31,53	0.35	0	37,39,61	0.49	0
13	PTY	C	504	-	40,40,49	0.33	0	43,45,54	0.65	0
15	LMT	P	302	-	36,36,36	0.39	0	47,47,47	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	XP4	A	3003	-	23,23,39	1.43	2 (8%)	27,28,44	1.93	5 (18%)
14	CDL	A	3001	-	41,41,99	0.44	0	45,51,111	0.66	1 (2%)

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
14	CDL	A	3002	-	-	30/54/54/110	-
13	PTY	E	401	-	-	28/44/44/53	-
11	HEM	N	502	1	-	4/12/54/54	-
14	CDL	C	505	-	-	30/57/57/110	-
19	HEC	D	401	7	-	4/10/54/54	-
17	FES	P	301	2	-	-	0/1/1/1
11	HEM	C	502	1	-	4/12/54/54	-
15	LMT	C	506	-	-	16/21/61/61	0/2/2/2
14	CDL	L	3002	-	-	31/54/54/110	-
13	PTY	P	303	-	-	25/44/44/53	-
18	XP4	L	3003	-	-	1/24/24/41	-
14	CDL	S	702	-	-	26/48/48/110	-
12	PC1	C	503	-	-	12/41/41/57	-
14	CDL	H	701	-	-	33/59/59/110	-
12	PC1	N	503	-	-	13/41/41/57	-
14	CDL	N	505	-	-	29/57/57/110	-
14	CDL	L	3001	-	-	22/48/48/110	-
14	CDL	S	701	-	-	34/59/59/110	-
15	LMT	J	101	-	-	13/21/61/61	0/2/2/2
19	HEC	O	401	7	-	4/10/54/54	-
11	HEM	N	501	1	-	5/12/54/54	-
16	DCQ	C	507	-	-	5/14/38/38	0/1/1/1
11	HEM	C	501	1	-	5/12/54/54	-
15	LMT	N	506	-	-	12/21/61/61	0/2/2/2
13	PTY	N	504	-	-	29/44/44/53	-
14	CDL	H	702	-	-	26/48/48/110	-
12	PC1	I	201	-	-	17/35/35/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PC1	T	201	-	-	11/35/35/57	-
13	PTY	C	504	-	-	30/44/44/53	-
15	LMT	P	302	-	-	11/21/61/61	0/2/2/2
18	XP4	A	3003	-	-	3/24/24/41	-
14	CDL	A	3001	-	-	16/48/48/110	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	507	DCQ	O4-C4M	10.43	1.69	1.45
19	D	401	HEC	C3C-C2C	5.74	1.46	1.40
19	O	401	HEC	C2B-C3B	5.64	1.46	1.40
18	L	3003	XP4	O7-C18	5.23	1.47	1.35
19	O	401	HEC	C3C-C2C	5.15	1.46	1.40
16	C	507	DCQ	O3-C3M	-5.11	1.33	1.45
19	D	401	HEC	C2B-C3B	4.97	1.45	1.40
18	A	3003	XP4	O7-C18	4.88	1.46	1.35
16	C	507	DCQ	C7-C6	-4.76	1.39	1.51
16	C	507	DCQ	C6-C1	-4.17	1.27	1.35
11	N	502	HEM	C1B-NB	-4.10	1.33	1.40
16	C	507	DCQ	O4-C4	-3.93	1.27	1.36
18	A	3003	XP4	O5-C4	3.90	1.44	1.33
11	C	502	HEM	C1B-NB	-3.49	1.34	1.40
18	L	3003	XP4	O5-C4	3.44	1.43	1.33
11	C	501	HEM	C1B-NB	-3.35	1.34	1.40
11	N	501	HEM	C1B-NB	-3.18	1.34	1.40
11	C	502	HEM	FE-NB	3.10	2.12	1.96
19	D	401	HEC	CAA-C2A	-3.09	1.46	1.52
11	C	502	HEM	C4D-ND	-3.03	1.35	1.40
19	D	401	HEC	CAD-C3D	-3.02	1.47	1.52
11	C	501	HEM	C3C-C2C	-2.91	1.36	1.40
11	N	501	HEM	C4B-NB	-2.91	1.32	1.38
19	O	401	HEC	CAD-C3D	-2.85	1.47	1.52
11	N	502	HEM	C4D-ND	-2.82	1.35	1.40
19	D	401	HEC	C3D-C2D	2.77	1.45	1.37
11	N	501	HEM	FE-NB	2.77	2.10	1.96
19	O	401	HEC	CAA-C2A	-2.75	1.47	1.52
11	C	501	HEM	C4B-NB	-2.73	1.33	1.38
19	D	401	HEC	C2A-C3A	2.69	1.45	1.37
19	O	401	HEC	C3D-C2D	2.66	1.45	1.37
11	C	501	HEM	FE-NB	2.64	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	502	HEM	C4B-NB	-2.53	1.33	1.38
19	O	401	HEC	C2A-C3A	2.45	1.44	1.37
19	D	401	HEC	C4D-CHA	2.44	1.47	1.41
11	N	501	HEM	CHB-C1B	2.39	1.41	1.35
16	C	507	DCQ	O5-C5	-2.29	1.18	1.23
11	C	502	HEM	CHB-C1B	2.26	1.40	1.35
19	O	401	HEC	C3A-C4A	2.26	1.47	1.42
11	N	501	HEM	O2D-CGD	-2.23	1.23	1.30
11	N	502	HEM	FE-NB	2.20	2.07	1.96
11	C	501	HEM	C1D-C2D	2.20	1.48	1.44
19	D	401	HEC	C2A-C1A	2.16	1.47	1.42
11	N	501	HEM	C4D-ND	-2.15	1.36	1.40
11	C	501	HEM	O2D-CGD	-2.15	1.23	1.30
19	D	401	HEC	C3A-C4A	2.13	1.47	1.42
11	N	502	HEM	CHB-C1B	2.12	1.40	1.35
11	N	501	HEM	C1D-C2D	2.12	1.48	1.44
11	C	502	HEM	CHA-C4D	2.11	1.40	1.35
12	N	503	PC1	C22-C21	2.10	1.56	1.50
11	N	502	HEM	C1D-ND	-2.08	1.34	1.38
19	O	401	HEC	C1B-NB	-2.07	1.31	1.36
11	N	501	HEM	C3C-C2C	-2.05	1.37	1.40
11	C	501	HEM	C4D-ND	-2.02	1.36	1.40
11	C	501	HEM	CHB-C1B	2.00	1.40	1.35

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	O	401	HEC	CMB-C2B-C3B	8.71	136.06	125.82
19	D	401	HEC	CMB-C2B-C3B	7.47	134.60	125.82
11	N	502	HEM	CHC-C4B-NB	6.83	131.85	124.43
18	L	3003	XP4	O7-C18-C19	6.78	123.56	111.09
18	A	3003	XP4	O7-C18-C19	6.61	123.26	111.09
19	O	401	HEC	C1D-C2D-C3D	-6.59	102.41	107.00
16	C	507	DCQ	C8-C7-C6	6.37	131.63	113.12
19	D	401	HEC	C1D-C2D-C3D	-6.17	102.70	107.00
11	C	501	HEM	CBA-CAA-C2A	-5.52	103.19	112.62
19	O	401	HEC	CMC-C2C-C3C	5.41	132.18	125.82
11	C	501	HEM	CHC-C4B-NB	5.40	130.29	124.43
11	N	501	HEM	CBA-CAA-C2A	-5.37	103.46	112.62
11	N	501	HEM	CHC-C4B-NB	5.23	130.11	124.43
11	C	502	HEM	CHC-C4B-NB	5.20	130.08	124.43
19	D	401	HEC	CAA-CBA-CGA	-5.19	99.20	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	O	401	HEC	CAA-CBA-CGA	-5.01	99.71	113.76
11	N	501	HEM	CHD-C1D-ND	5.00	129.86	124.43
16	C	507	DCQ	C1-C6-C5	4.78	124.08	119.58
19	D	401	HEC	CMC-C2C-C3C	4.64	131.28	125.82
11	C	502	HEM	CHA-C4D-ND	4.63	130.10	124.38
11	N	501	HEM	C1B-NB-C4B	4.39	109.61	105.07
19	D	401	HEC	CBD-CAD-C3D	-4.37	105.16	112.62
11	C	502	HEM	CHD-C1D-ND	4.36	129.17	124.43
11	C	501	HEM	C1B-NB-C4B	4.23	109.44	105.07
11	C	502	HEM	C4C-CHD-C1D	-4.23	116.98	122.56
11	C	502	HEM	C1B-NB-C4B	4.22	109.44	105.07
11	N	501	HEM	CHA-C4D-ND	4.18	129.54	124.38
11	N	502	HEM	C1B-NB-C4B	4.15	109.36	105.07
11	N	502	HEM	CHD-C1D-ND	4.12	128.90	124.43
11	N	502	HEM	CHA-C4D-ND	4.10	129.45	124.38
11	C	501	HEM	CHD-C1D-ND	4.10	128.88	124.43
11	C	502	HEM	C2C-C3C-C4C	4.02	109.71	106.90
19	O	401	HEC	CBD-CAD-C3D	-4.00	105.80	112.62
18	A	3003	XP4	O7-C18-O8	-3.96	115.10	122.96
11	C	502	HEM	CHD-C1D-C2D	-3.82	119.00	124.98
16	C	507	DCQ	C1M-C1-C6	-3.78	118.23	124.40
16	C	507	DCQ	C7-C6-C5	3.73	123.11	117.00
11	N	502	HEM	CHD-C1D-C2D	-3.50	119.52	124.98
18	L	3003	XP4	O7-C18-O8	-3.50	116.02	122.96
11	N	501	HEM	CHA-C4D-C3D	-3.33	119.07	125.33
15	J	101	LMT	C1-O1'-C1'	-3.30	108.36	113.84
11	C	501	HEM	CAD-CBD-CGD	-3.30	106.51	113.60
11	N	502	HEM	C4C-CHD-C1D	-3.27	118.24	122.56
11	C	501	HEM	CHA-C4D-ND	3.27	128.43	124.38
14	S	702	CDL	CB4-OB6-CB5	3.26	123.98	117.90
11	N	502	HEM	CHB-C1B-NB	3.23	128.37	124.38
11	N	502	HEM	CHC-C4B-C3B	-3.15	119.74	124.57
11	N	501	HEM	CHD-C1D-C2D	-3.07	120.18	124.98
11	C	501	HEM	CHD-C1D-C2D	-3.01	120.28	124.98
11	C	502	HEM	C3C-C4C-NC	-3.00	105.27	110.94
16	C	507	DCQ	C4M-O4-C4	-3.00	105.82	116.47
11	N	501	HEM	CAD-CBD-CGD	-3.00	107.16	113.60
15	C	506	LMT	C1B-O5B-C5B	2.94	119.45	113.69
12	C	503	PC1	O22-C21-C22	2.93	135.15	123.73
15	N	506	LMT	C3B-C4B-C5B	2.91	115.43	110.24
14	H	702	CDL	CB4-OB6-CB5	2.91	123.32	117.90
14	H	702	CDL	OB6-CB4-CB6	2.87	118.78	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	502	HEM	CBA-CAA-C2A	-2.86	107.73	112.62
11	C	502	HEM	CHB-C1B-NB	2.86	127.91	124.38
11	N	502	HEM	O2D-CGD-CBD	2.85	123.17	114.03
11	C	502	HEM	CHA-C4D-C3D	-2.81	120.06	125.33
11	C	502	HEM	O2D-CGD-CBD	2.75	122.87	114.03
14	A	3002	CDL	OA6-CA4-CA6	2.73	118.30	108.40
12	N	503	PC1	O22-C21-C22	2.71	134.31	123.73
16	C	507	DCQ	C3M-O3-C3	2.70	126.04	116.47
15	N	506	LMT	O5B-C5B-C4B	2.69	114.59	109.69
11	N	502	HEM	C2C-C3C-C4C	2.68	108.77	106.90
12	C	503	PC1	O21-C21-C22	-2.67	105.75	111.50
14	C	505	CDL	OB6-CB4-CB3	2.67	118.05	108.40
18	L	3003	XP4	O5-C4-C5	2.65	120.21	111.91
14	L	3001	CDL	OB6-CB4-CB3	-2.64	100.29	109.56
11	N	502	HEM	CHA-C4D-C3D	-2.64	120.37	125.33
15	C	506	LMT	O5B-C5B-C4B	2.63	114.48	109.69
14	H	702	CDL	OA5-PA1-OA3	-2.62	98.83	109.07
14	S	702	CDL	OA5-PA1-OA3	-2.60	98.90	109.07
14	S	702	CDL	OB6-CB4-CB6	2.60	117.81	108.40
15	C	506	LMT	C3B-C4B-C5B	2.57	114.82	110.24
15	N	506	LMT	C1B-O5B-C5B	2.57	118.72	113.69
11	N	502	HEM	CBD-CAD-C3D	-2.56	105.50	112.63
18	L	3003	XP4	O5-C4-O6	-2.50	117.28	123.59
11	C	502	HEM	CBD-CAD-C3D	-2.49	105.71	112.63
18	A	3003	XP4	O5-C4-C5	2.48	119.70	111.91
11	C	501	HEM	CHA-C4D-C3D	-2.47	120.69	125.33
11	C	502	HEM	CMD-C2D-C1D	2.44	128.75	125.04
15	J	101	LMT	O1'-C1'-C2'	2.43	112.10	108.30
14	A	3002	CDL	OA2-PA1-OA3	2.43	118.54	109.07
18	L	3003	XP4	O5-C3-C2	-2.39	101.46	108.43
19	D	401	HEC	CMA-C3A-C2A	2.39	129.45	124.94
11	N	502	HEM	C3C-C4C-NC	-2.39	106.44	110.94
11	N	502	HEM	C4A-C3A-C2A	-2.36	105.35	107.00
15	N	506	LMT	O1'-C1'-C2'	-2.36	104.62	108.30
14	C	505	CDL	CB4-OB6-CB5	2.34	123.56	117.79
11	N	501	HEM	CHB-C1B-NB	2.33	127.26	124.38
11	C	502	HEM	C1D-C2D-C3D	-2.33	104.51	106.96
14	A	3002	CDL	OA5-PA1-OA3	-2.32	100.00	109.07
14	L	3002	CDL	OA5-PA1-OA3	-2.31	100.03	109.07
14	A	3001	CDL	OB8-CB6-CB4	2.31	116.93	105.77
15	J	101	LMT	C4B-C3B-C2B	2.29	114.83	110.82
14	L	3002	CDL	OA2-PA1-OA3	2.28	117.99	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	507	DCQ	C6-C1-C2	2.27	120.98	119.18
11	C	502	HEM	O1D-CGD-CBD	-2.27	115.80	123.08
15	N	506	LMT	O4'-C4B-C3B	-2.25	105.16	110.35
14	L	3002	CDL	OA6-CA4-CA6	2.24	116.50	108.40
18	A	3003	XP4	O5-C4-O6	-2.22	117.99	123.59
11	C	502	HEM	O2A-CGA-O1A	-2.22	117.78	123.30
15	C	506	LMT	C4B-C3B-C2B	2.21	114.68	110.82
15	N	506	LMT	C4B-C3B-C2B	2.20	114.66	110.82
11	N	502	HEM	C3B-C2B-C1B	-2.20	104.86	106.49
11	C	502	HEM	CBA-CAA-C2A	-2.18	108.90	112.62
11	N	502	HEM	C4B-CHC-C1C	-2.18	119.69	122.56
11	N	502	HEM	O2A-CGA-O1A	-2.15	117.93	123.30
13	N	504	PTY	O14-P1-O13	-2.14	100.70	109.07
11	N	502	HEM	CHB-C1B-C2B	-2.14	120.81	126.72
12	N	503	PC1	O21-C21-O22	-2.13	118.56	123.70
14	N	505	CDL	CB4-OB6-CB5	2.12	123.00	117.79
14	N	505	CDL	OB6-CB4-CB3	2.09	115.98	108.40
11	N	501	HEM	O2D-CGD-O1D	-2.07	118.13	123.30
14	H	701	CDL	OB6-CB4-CB6	2.05	115.82	108.40
12	N	503	PC1	O21-C21-C22	-2.04	107.10	111.50
18	A	3003	XP4	O7-C2-C3	-2.04	101.03	108.40
15	J	101	LMT	C2'-C3'-C4'	2.02	114.31	109.68
11	C	501	HEM	O2D-CGD-O1D	-2.01	118.28	123.30
11	C	501	HEM	CHB-C1B-NB	2.00	126.85	124.38

There are no chirality outliers.

All (529) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	I	201	PC1	C11-O13-P-O14
12	I	201	PC1	C11-O13-P-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	C11-O13-P-O14
12	T	201	PC1	C11-O13-P-O11
12	T	201	PC1	O21-C2-C3-O31
13	C	504	PTY	N1-C2-C3-O11
13	C	504	PTY	C11-C8-O7-C6
13	C	504	PTY	C3-O11-P1-O13
13	C	504	PTY	C3-O11-P1-O14
13	P	303	PTY	C5-O14-P1-O11
13	P	303	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
13	N	504	PTY	C11-C8-O7-C6
13	N	504	PTY	C3-O11-P1-O12
13	N	504	PTY	C3-O11-P1-O13
13	N	504	PTY	C5-O14-P1-O13
13	E	401	PTY	N1-C2-C3-O11
13	E	401	PTY	C3-O11-P1-O13
13	E	401	PTY	C5-O14-P1-O12
14	C	505	CDL	O1-C1-CA2-OA2
14	C	505	CDL	CA3-OA5-PA1-OA3
14	C	505	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	CB2-OB2-PB2-OB3
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB3-OB5-PB2-OB3
14	C	505	CDL	CB3-OB5-PB2-OB4
14	A	3001	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	CA2-OA2-PA1-OA3
14	A	3002	CDL	CA2-OA2-PA1-OA4
14	A	3002	CDL	CA2-OA2-PA1-OA5
14	A	3002	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	CA2-OA2-PA1-OA4
14	H	702	CDL	CB2-OB2-PB2-OB3
14	H	702	CDL	CB3-OB5-PB2-OB4
14	N	505	CDL	O1-C1-CA2-OA2
14	N	505	CDL	CA3-OA5-PA1-OA3
14	N	505	CDL	C11-CA5-OA6-CA4
14	N	505	CDL	CB2-OB2-PB2-OB3
14	N	505	CDL	CB2-OB2-PB2-OB4
14	N	505	CDL	CB2-OB2-PB2-OB5
14	N	505	CDL	CB3-OB5-PB2-OB3
14	N	505	CDL	CB3-OB5-PB2-OB4
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	L	3001	CDL	CB3-CB4-CB6-OB8
14	L	3002	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	CA2-OA2-PA1-OA3
14	L	3002	CDL	CA2-OA2-PA1-OA4
14	L	3002	CDL	CA2-OA2-PA1-OA5
14	L	3002	CDL	CB2-OB2-PB2-OB3
14	L	3002	CDL	CB3-OB5-PB2-OB3
14	L	3002	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
14	S	701	CDL	CA2-OA2-PA1-OA3
14	S	701	CDL	CA2-OA2-PA1-OA4
14	S	702	CDL	CA2-OA2-PA1-OA4
14	S	702	CDL	C31-CA7-OA8-CA6
14	S	702	CDL	CB2-OB2-PB2-OB3
14	S	702	CDL	CB3-OB5-PB2-OB4
14	S	702	CDL	C51-CB5-OB6-CB4
15	P	302	LMT	O5'-C1'-O1'-C1
14	H	702	CDL	C51-CB5-OB6-CB4
14	H	702	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	OB9-CB7-OB8-CB6
14	S	702	CDL	OA9-CA7-OA8-CA6
14	A	3001	CDL	CB4-CB6-OB8-CB7
12	T	201	PC1	C32-C31-O31-C3
14	H	702	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	C71-CB7-OB8-CB6
14	H	702	CDL	OB7-CB5-OB6-CB4
12	T	201	PC1	O32-C31-O31-C3
14	A	3001	CDL	OA9-CA7-OA8-CA6
14	H	701	CDL	OB9-CB7-OB8-CB6
14	S	701	CDL	OB9-CB7-OB8-CB6
14	S	702	CDL	OB9-CB7-OB8-CB6
14	S	702	CDL	OB7-CB5-OB6-CB4
13	C	504	PTY	O10-C8-O7-C6
13	N	504	PTY	O10-C8-O7-C6
14	C	505	CDL	OA7-CA5-OA6-CA4
14	S	701	CDL	OB7-CB5-OB6-CB4
14	L	3001	CDL	OA9-CA7-OA8-CA6
14	A	3001	CDL	C31-CA7-OA8-CA6
14	H	701	CDL	C71-CB7-OB8-CB6
14	S	701	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	OA9-CA7-OA8-CA6
14	S	702	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	C31-CA7-OA8-CA6
12	I	201	PC1	C32-C33-C34-C35
14	N	505	CDL	OA7-CA5-OA6-CA4
14	L	3001	CDL	OB9-CB7-OB8-CB6
13	N	504	PTY	C31-C32-C33-C34
14	A	3001	CDL	OA5-CA3-CA4-OA6
14	A	3002	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
14	L	3002	CDL	O1-C1-CB2-OB2
14	S	702	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	C31-CA7-OA8-CA6
14	L	3001	CDL	C71-CB7-OB8-CB6
15	C	506	LMT	O5'-C5'-C6'-O6'
14	A	3001	CDL	OB6-CB4-CB6-OB8
14	A	3002	CDL	C11-CA5-OA6-CA4
14	L	3002	CDL	C11-CA5-OA6-CA4
14	S	701	CDL	C51-CB5-OB6-CB4
13	P	303	PTY	C37-C38-C39-C40
14	S	701	CDL	OA9-CA7-OA8-CA6
13	N	504	PTY	C33-C34-C35-C36
15	J	101	LMT	C2-C3-C4-C5
15	N	506	LMT	O5'-C5'-C6'-O6'
13	P	303	PTY	C33-C34-C35-C36
13	E	401	PTY	C13-C14-C15-C16
16	C	507	DCQ	C6-C7-C8-C9
15	C	506	LMT	O5B-C5B-C6B-O6B
15	N	506	LMT	O5B-C5B-C6B-O6B
14	A	3002	CDL	OA7-CA5-OA6-CA4
13	C	504	PTY	C31-C32-C33-C34
15	J	101	LMT	C4-C5-C6-C7
13	N	504	PTY	C37-C38-C39-C40
15	P	302	LMT	C3-C4-C5-C6
14	C	505	CDL	CB2-C1-CA2-OA2
14	N	505	CDL	CB2-C1-CA2-OA2
14	N	505	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-CA6
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	S	701	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	OA7-CA5-OA6-CA4
13	C	504	PTY	C35-C36-C37-C38
13	P	303	PTY	C31-C30-O4-C1
13	P	303	PTY	C35-C36-C37-C38
14	S	701	CDL	C31-CA7-OA8-CA6
13	E	401	PTY	C35-C36-C37-C38
13	E	401	PTY	O14-C5-C6-O7
15	C	506	LMT	C4'-C5'-C6'-O6'
15	N	506	LMT	C4'-C5'-C6'-O6'
14	H	702	CDL	O1-C1-CA2-OA2
14	N	505	CDL	O1-C1-CB2-OB2
13	N	504	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	A	3001	CDL	CB7-C71-C72-C73
14	L	3002	CDL	CA7-C31-C32-C33
14	L	3001	CDL	OB6-CB4-CB6-OB8
12	C	503	PC1	C32-C31-O31-C3
12	T	201	PC1	C21-C22-C23-C24
13	P	303	PTY	C30-C31-C32-C33
13	E	401	PTY	C30-C31-C32-C33
14	C	505	CDL	CA7-C31-C32-C33
14	H	701	CDL	CA5-C11-C12-C13
14	H	701	CDL	CB7-C71-C72-C73
14	S	701	CDL	CA5-C11-C12-C13
14	S	701	CDL	CB7-C71-C72-C73
12	N	503	PC1	C32-C31-O31-C3
12	T	201	PC1	C31-C32-C33-C34
14	N	505	CDL	CA7-C31-C32-C33
12	C	503	PC1	O32-C31-O31-C3
13	P	303	PTY	O30-C30-O4-C1
12	I	201	PC1	C21-C22-C23-C24
14	H	702	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	S	701	CDL	O1-C1-CB2-OB2
14	S	702	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	C51-CB5-OB6-CB4
12	N	503	PC1	O32-C31-O31-C3
13	E	401	PTY	C40-C41-C42-C43
13	N	504	PTY	C3-O11-P1-O14
13	E	401	PTY	C5-O14-P1-O11
14	C	505	CDL	CB2-OB2-PB2-OB5
14	C	505	CDL	CB3-OB5-PB2-OB2
14	A	3002	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CA2-OA2-PA1-OA5
14	H	702	CDL	CB3-OB5-PB2-OB2
14	N	505	CDL	CB3-OB5-PB2-OB2
14	L	3002	CDL	CB3-OB5-PB2-OB2
14	S	701	CDL	CA2-OA2-PA1-OA5
14	S	702	CDL	CA2-OA2-PA1-OA5
14	S	702	CDL	CB3-OB5-PB2-OB2
15	J	101	LMT	O5B-C5B-C6B-O6B
12	I	201	PC1	C32-C31-O31-C3
15	C	506	LMT	C4B-C5B-C6B-O6B
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
14	H	702	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	CA2-C1-CB2-OB2
14	S	702	CDL	CB2-C1-CA2-OA2
14	S	702	CDL	CA2-C1-CB2-OB2
13	C	504	PTY	C8-C11-C12-C13
13	E	401	PTY	C38-C39-C40-C41
14	L	3002	CDL	C12-C13-C14-C15
15	P	302	LMT	C7-C8-C9-C10
15	N	506	LMT	C7-C8-C9-C10
13	C	504	PTY	C14-C15-C16-C17
13	P	303	PTY	C16-C17-C18-C19
15	J	101	LMT	C5-C6-C7-C8
15	J	101	LMT	C6-C7-C8-C9
15	N	506	LMT	C4B-C5B-C6B-O6B
13	C	504	PTY	C13-C14-C15-C16
13	N	504	PTY	C32-C33-C34-C35
14	A	3002	CDL	O1-C1-CA2-OA2
14	S	701	CDL	O1-C1-CA2-OA2
14	H	701	CDL	CB5-C51-C52-C53
13	P	303	PTY	C40-C41-C42-C43
15	C	506	LMT	C4-C5-C6-C7
15	C	506	LMT	C6-C7-C8-C9
13	E	401	PTY	C16-C17-C18-C19
14	L	3001	CDL	CB7-C71-C72-C73
14	A	3002	CDL	C12-C13-C14-C15
14	H	701	CDL	C71-C72-C73-C74
14	H	701	CDL	C73-C74-C75-C76
14	S	701	CDL	C74-C75-C76-C77
15	C	506	LMT	C5-C6-C7-C8
12	I	201	PC1	O32-C31-O31-C3
14	H	701	CDL	C11-C12-C13-C14
12	I	201	PC1	C31-C32-C33-C34
13	E	401	PTY	C8-C11-C12-C13
13	C	504	PTY	C37-C38-C39-C40
13	P	303	PTY	C34-C35-C36-C37
13	E	401	PTY	C11-C12-C13-C14
13	C	504	PTY	C38-C39-C40-C41
14	A	3002	CDL	OB7-CB5-OB6-CB4
14	S	701	CDL	C71-C72-C73-C74
15	C	506	LMT	C3-C4-C5-C6
14	H	701	CDL	C74-C75-C76-C77
12	C	503	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
14	H	702	CDL	CB3-CB4-CB6-OB8
15	C	506	LMT	C11-C10-C9-C8
14	H	701	CDL	C51-CB5-OB6-CB4
12	N	503	PC1	C28-C29-C2A-C2B
14	S	701	CDL	C11-C12-C13-C14
15	P	302	LMT	C2-C3-C4-C5
14	L	3001	CDL	C32-C33-C34-C35
14	A	3001	CDL	OB5-CB3-CB4-CB6
14	L	3001	CDL	CB2-C1-CA2-OA2
13	P	303	PTY	C38-C39-C40-C41
14	A	3001	CDL	C71-C72-C73-C74
14	L	3002	CDL	C31-C32-C33-C34
15	N	506	LMT	C1-C2-C3-C4
13	N	504	PTY	C14-C15-C16-C17
15	J	101	LMT	C3-C4-C5-C6
14	A	3002	CDL	CA7-C31-C32-C33
13	E	401	PTY	C31-C30-O4-C1
15	P	302	LMT	C4'-C5'-C6'-O6'
13	P	303	PTY	C31-C32-C33-C34
15	C	506	LMT	C7-C8-C9-C10
14	C	505	CDL	OB7-CB5-OB6-CB4
14	H	701	CDL	OB7-CB5-OB6-CB4
15	C	506	LMT	C1-C2-C3-C4
13	N	504	PTY	C30-C31-C32-C33
14	A	3002	CDL	C33-C34-C35-C36
15	J	101	LMT	C1-C2-C3-C4
14	A	3001	CDL	C72-C73-C74-C75
15	N	506	LMT	C5-C6-C7-C8
14	C	505	CDL	C51-CB5-OB6-CB4
14	N	505	CDL	C51-CB5-OB6-CB4
13	N	504	PTY	C16-C17-C18-C19
15	N	506	LMT	C6-C7-C8-C9
12	T	201	PC1	C33-C34-C35-C36
14	N	505	CDL	OB7-CB5-OB6-CB4
14	L	3001	CDL	C71-C72-C73-C74
14	L	3002	CDL	C33-C34-C35-C36
12	C	503	PC1	O21-C2-C3-O31
12	N	503	PC1	O21-C2-C3-O31
13	E	401	PTY	C12-C13-C14-C15
15	P	302	LMT	C4-C5-C6-C7
14	N	505	CDL	C11-C12-C13-C14
13	E	401	PTY	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
13	N	504	PTY	C34-C35-C36-C37
13	C	504	PTY	C5-O14-P1-O11
13	N	504	PTY	C5-O14-P1-O11
14	N	505	CDL	CA3-OA5-PA1-OA2
13	N	504	PTY	O14-C5-C6-C1
13	E	401	PTY	O14-C5-C6-C1
14	A	3002	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA5-CA3-CA4-CA6
14	S	702	CDL	OB5-CB3-CB4-CB6
13	N	504	PTY	C36-C37-C38-C39
12	I	201	PC1	C34-C35-C36-C37
13	E	401	PTY	O30-C30-O4-C1
14	L	3002	CDL	O1-C1-CA2-OA2
13	C	504	PTY	O4-C1-C6-C5
13	N	504	PTY	O4-C1-C6-C5
12	I	201	PC1	C33-C34-C35-C36
13	P	303	PTY	C11-C12-C13-C14
13	E	401	PTY	C14-C15-C16-C17
12	C	503	PC1	C22-C23-C24-C25
12	C	503	PC1	C26-C27-C28-C29
13	N	504	PTY	C41-C42-C43-C44
15	N	506	LMT	C9-C10-C11-C12
13	C	504	PTY	C17-C18-C19-C20
13	E	401	PTY	C41-C42-C43-C44
14	A	3002	CDL	C34-C35-C36-C37
13	P	303	PTY	C41-C42-C43-C44
13	C	504	PTY	C41-C42-C43-C44
14	L	3002	CDL	C13-C14-C15-C16
14	C	505	CDL	C13-C14-C15-C16
15	N	506	LMT	C2-C3-C4-C5
14	A	3002	CDL	CA6-CA4-OA6-CA5
14	H	702	CDL	CB6-CB4-OB6-CB5
14	L	3002	CDL	CA6-CA4-OA6-CA5
13	C	504	PTY	C33-C34-C35-C36
12	N	503	PC1	C22-C23-C24-C25
14	H	701	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OA5-CA3-CA4-OA6
14	S	701	CDL	OA5-CA3-CA4-OA6
13	P	303	PTY	C8-C11-C12-C13
14	S	701	CDL	CB5-C51-C52-C53
13	E	401	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
15	N	506	LMT	C3-C4-C5-C6
14	A	3002	CDL	C13-C14-C15-C16
14	S	701	CDL	C75-C76-C77-C78
14	C	505	CDL	OB6-CB4-CB6-OB8
13	N	504	PTY	C38-C39-C40-C41
14	S	701	CDL	OA7-CA5-OA6-CA4
13	C	504	PTY	C40-C41-C42-C43
14	L	3002	CDL	C51-CB5-OB6-CB4
13	C	504	PTY	C39-C40-C41-C42
14	H	701	CDL	C75-C76-C77-C78
14	A	3002	CDL	CB2-C1-CA2-OA2
14	S	701	CDL	CB2-C1-CA2-OA2
14	C	505	CDL	C11-C12-C13-C14
15	C	506	LMT	C9-C10-C11-C12
15	J	101	LMT	C9-C10-C11-C12
14	H	701	CDL	OB5-CB3-CB4-CB6
14	S	701	CDL	C73-C74-C75-C76
15	P	302	LMT	O5'-C5'-C6'-O6'
12	C	503	PC1	C27-C28-C29-C2A
14	L	3002	CDL	C34-C35-C36-C37
14	H	701	CDL	CB3-CB4-CB6-OB8
14	S	702	CDL	CB3-CB4-CB6-OB8
13	N	504	PTY	C17-C18-C19-C20
12	N	503	PC1	C26-C27-C28-C29
13	C	504	PTY	C12-C13-C14-C15
14	A	3001	CDL	CB3-OB5-PB2-OB2
14	H	701	CDL	OB5-CB3-CB4-OB6
14	S	701	CDL	OB5-CB3-CB4-OB6
14	A	3002	CDL	CB5-C51-C52-C53
14	A	3001	CDL	OB5-CB3-CB4-OB6
14	L	3001	CDL	O1-C1-CA2-OA2
14	A	3001	CDL	C73-C74-C75-C76
15	J	101	LMT	O1'-C1-C2-C3
13	P	303	PTY	C15-C16-C17-C18
13	N	504	PTY	O4-C1-C6-O7
14	H	702	CDL	OB6-CB4-CB6-OB8
14	S	702	CDL	OB6-CB4-CB6-OB8
15	N	506	LMT	C11-C10-C9-C8
14	L	3002	CDL	CB2-C1-CA2-OA2
16	C	507	DCQ	C10-C11-C12-C13
14	C	505	CDL	CA4-CA3-OA5-PA1
14	N	505	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
13	P	303	PTY	C14-C15-C16-C17
14	N	505	CDL	C13-C14-C15-C16
11	N	501	HEM	C3D-CAD-CBD-CGD
14	S	701	CDL	C11-CA5-OA6-CA4
13	C	504	PTY	C11-C12-C13-C14
14	H	702	CDL	OA5-CA3-CA4-CA6
14	S	701	CDL	OA5-CA3-CA4-CA6
13	N	504	PTY	C12-C13-C14-C15
13	E	401	PTY	C31-C32-C33-C34
13	E	401	PTY	C36-C37-C38-C39
18	L	3003	XP4	C5-C6-C7-C8
15	J	101	LMT	C11-C10-C9-C8
14	S	702	CDL	CB6-CB4-OB6-CB5
14	N	505	CDL	C31-C32-C33-C34
12	C	503	PC1	C1-C2-C3-O31
12	T	201	PC1	C1-C2-C3-O31
14	S	701	CDL	CA3-CA4-CA6-OA8
14	S	701	CDL	CB3-CB4-CB6-OB8
13	N	504	PTY	O14-C5-C6-O7
14	N	505	CDL	OA5-CA3-CA4-OA6
14	S	702	CDL	OA5-CA3-CA4-OA6
12	N	503	PC1	C27-C28-C29-C2A
14	L	3002	CDL	OB7-CB5-OB6-CB4
14	C	505	CDL	C31-C32-C33-C34
13	C	504	PTY	O4-C1-C6-O7
14	H	701	CDL	OA6-CA4-CA6-OA8
14	H	701	CDL	OB6-CB4-CB6-OB8
14	S	701	CDL	OA6-CA4-CA6-OA8
15	P	302	LMT	C1-C2-C3-C4
12	I	201	PC1	C22-C21-O21-C2
15	P	302	LMT	O5B-C5B-C6B-O6B
14	H	701	CDL	OA7-CA5-OA6-CA4
14	L	3002	CDL	CA5-C11-C12-C13
15	C	506	LMT	O1'-C1-C2-C3
13	E	401	PTY	C34-C35-C36-C37
13	E	401	PTY	C3-O11-P1-O14
14	C	505	CDL	CA3-OA5-PA1-OA2
14	H	702	CDL	CB2-OB2-PB2-OB5
14	S	702	CDL	CB2-OB2-PB2-OB5
13	C	504	PTY	C5-O14-P1-O12
13	C	504	PTY	C5-O14-P1-O13
13	P	303	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
13	N	504	PTY	C5-O14-P1-O12
14	C	505	CDL	CA3-OA5-PA1-OA4
14	A	3002	CDL	CB3-OB5-PB2-OB4
14	H	701	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB3-OB5-PB2-OB3
14	N	505	CDL	CA3-OA5-PA1-OA4
14	L	3001	CDL	CB2-OB2-PB2-OB4
14	L	3002	CDL	CB3-OB5-PB2-OB4
14	S	702	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	CA5-C11-C12-C13
14	H	701	CDL	OA5-CA3-CA4-CA6
14	S	702	CDL	OA5-CA3-CA4-CA6
13	C	504	PTY	C30-C31-C32-C33
13	P	303	PTY	O14-C5-C6-O7
14	C	505	CDL	OA5-CA3-CA4-OA6
13	N	504	PTY	C13-C14-C15-C16
16	C	507	DCQ	C11-C10-C9-C8
12	N	503	PC1	C1-C2-C3-O31
13	P	303	PTY	C13-C14-C15-C16
14	H	701	CDL	CA3-CA4-CA6-OA8
14	N	505	CDL	OB6-CB4-CB6-OB8
18	A	3003	XP4	C5-C6-C7-C8
13	C	504	PTY	C32-C33-C34-C35
14	S	701	CDL	C51-C52-C53-C54
14	L	3001	CDL	C34-C35-C36-C37
16	C	507	DCQ	C2-C3-O3-C3M
16	C	507	DCQ	C7-C8-C9-C10
13	C	504	PTY	C15-C16-C17-C18
15	C	506	LMT	C2'-C1'-O1'-C1
13	P	303	PTY	C3-O11-P1-O14
14	A	3002	CDL	CB2-OB2-PB2-OB5
14	L	3002	CDL	CB2-OB2-PB2-OB5
12	I	201	PC1	C22-C23-C24-C25
11	C	501	HEM	C3D-CAD-CBD-CGD
15	C	506	LMT	O5'-C1'-O1'-C1
14	S	701	CDL	OB5-CB3-CB4-CB6
13	C	504	PTY	O14-C5-C6-O7
11	C	502	HEM	CAD-CBD-CGD-O2D
11	N	501	HEM	CAA-CBA-CGA-O2A
15	P	302	LMT	C5-C6-C7-C8
14	S	702	CDL	CB4-CB3-OB5-PB2
11	C	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	C	501	HEM	CAA-CBA-CGA-O2A
11	C	502	HEM	CAD-CBD-CGD-O1D
14	H	701	CDL	C51-C52-C53-C54
14	N	505	CDL	C32-C33-C34-C35
15	C	506	LMT	C2-C3-C4-C5
11	N	502	HEM	CAA-CBA-CGA-O1A
12	N	503	PC1	C23-C24-C25-C26
14	C	505	CDL	CA2-C1-CB2-OB2
12	I	201	PC1	O22-C21-O21-C2
14	L	3002	CDL	C11-C12-C13-C14
11	C	502	HEM	CAA-CBA-CGA-O2A
11	N	502	HEM	CAD-CBD-CGD-O2D
14	L	3002	CDL	C52-C53-C54-C55
11	N	501	HEM	CAA-CBA-CGA-O1A
19	D	401	HEC	CAA-CBA-CGA-O1A
15	J	101	LMT	C4B-C5B-C6B-O6B
15	P	302	LMT	C6-C7-C8-C9
11	N	502	HEM	CAA-CBA-CGA-O2A
19	O	401	HEC	CAA-CBA-CGA-O2A
11	C	502	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAD-CBD-CGD-O1D
14	C	505	CDL	O1-C1-CB2-OB2
13	N	504	PTY	C11-C12-C13-C14
13	P	303	PTY	C12-C13-C14-C15
19	O	401	HEC	CAA-CBA-CGA-O1A
14	A	3002	CDL	C31-CA7-OA8-CA6
14	C	505	CDL	C32-C33-C34-C35
19	D	401	HEC	CAA-CBA-CGA-O2A
14	H	701	CDL	C11-CA5-OA6-CA4
14	A	3002	CDL	OA9-CA7-OA8-CA6
14	L	3002	CDL	CB5-C51-C52-C53
14	L	3002	CDL	OA5-CA3-CA4-OA6
13	C	504	PTY	O14-C5-C6-C1
14	C	505	CDL	OA5-CA3-CA4-CA6
12	C	503	PC1	C23-C24-C25-C26
14	H	702	CDL	C72-C71-CB7-OB8
14	H	701	CDL	C72-C71-CB7-OB8
14	L	3002	CDL	CA3-OA5-PA1-OA2
14	H	702	CDL	C32-C31-CA7-OA9
11	C	501	HEM	CAD-CBD-CGD-O2D
11	N	501	HEM	CAD-CBD-CGD-O2D
12	N	503	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
12	I	201	PC1	O21-C21-C22-C23
14	A	3001	CDL	C72-C71-CB7-OB8
14	N	505	CDL	OA5-CA3-CA4-CA6
11	N	501	HEM	CAD-CBD-CGD-O1D
19	O	401	HEC	CAD-CBD-CGD-O1D
12	C	503	PC1	O31-C31-C32-C33
13	P	303	PTY	O4-C30-C31-C32
14	S	701	CDL	C72-C71-CB7-OB8
12	I	201	PC1	O21-C2-C3-O31
14	A	3002	CDL	OA6-CA4-CA6-OA8
14	H	701	CDL	C72-C73-C74-C75
12	N	503	PC1	O31-C31-C32-C33
14	C	505	CDL	C32-C31-CA7-OA8
14	N	505	CDL	C32-C31-CA7-OA8
15	J	101	LMT	C4'-C5'-C6'-O6'
13	C	504	PTY	C6-C5-O14-P1
14	H	702	CDL	C32-C31-CA7-OA8
19	D	401	HEC	CAD-CBD-CGD-O1D
14	A	3001	CDL	C33-C34-C35-C36
14	C	505	CDL	CA5-C11-C12-C13
14	H	701	CDL	C72-C71-CB7-OB9
14	H	701	CDL	C12-C13-C14-C15
11	C	501	HEM	CAD-CBD-CGD-O1D
18	A	3003	XP4	C10-C11-C12-C13
14	S	702	CDL	C32-C31-CA7-OA9
12	C	503	PC1	C33-C34-C35-C36
12	I	201	PC1	O22-C21-C22-C23
15	J	101	LMT	C7-C8-C9-C10
14	H	701	CDL	CB3-OB5-PB2-OB2
13	P	303	PTY	O30-C30-C31-C32
14	A	3002	CDL	C52-C53-C54-C55
12	I	201	PC1	C1-O11-P-O14
12	T	201	PC1	C11-C12-N-C14
14	A	3002	CDL	CB2-OB2-PB2-OB3
13	E	401	PTY	C39-C40-C41-C42
14	C	505	CDL	CB6-CB4-OB6-CB5
14	H	701	CDL	CA3-CA4-OA6-CA5
14	N	505	CDL	CB6-CB4-OB6-CB5
14	S	701	CDL	C72-C73-C74-C75
19	D	401	HEC	CAD-CBD-CGD-O2D
14	N	505	CDL	C32-C31-CA7-OA9
14	L	3001	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
13	E	401	PTY	O4-C30-C31-C32
19	O	401	HEC	CAD-CBD-CGD-O2D
18	A	3003	XP4	C6-C7-C8-C9
12	N	503	PC1	C33-C34-C35-C36
12	N	503	PC1	O32-C31-C32-C33
14	C	505	CDL	C32-C31-CA7-OA9
14	S	701	CDL	C72-C71-CB7-OB9
12	C	503	PC1	O32-C31-C32-C33
14	S	702	CDL	C32-C31-CA7-OA8
13	E	401	PTY	O30-C30-C31-C32
13	N	504	PTY	C31-C30-O4-C1
14	L	3001	CDL	C72-C71-CB7-OB8

There are no ring outliers.

29 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	3002	CDL	2	0
13	E	401	PTY	3	0
11	N	502	HEM	1	0
14	C	505	CDL	1	0
19	D	401	HEC	12	0
11	C	502	HEM	1	0
15	C	506	LMT	2	0
13	P	303	PTY	13	0
18	L	3003	XP4	1	0
14	S	702	CDL	4	0
12	C	503	PC1	1	0
14	H	701	CDL	3	0
12	N	503	PC1	1	0
14	N	505	CDL	2	0
14	S	701	CDL	4	0
15	J	101	LMT	2	0
19	O	401	HEC	14	0
11	N	501	HEM	4	0
16	C	507	DCQ	16	0
11	C	501	HEM	4	0
15	N	506	LMT	1	0
13	N	504	PTY	9	0
14	H	702	CDL	4	0
12	I	201	PC1	2	0
12	T	201	PC1	3	0

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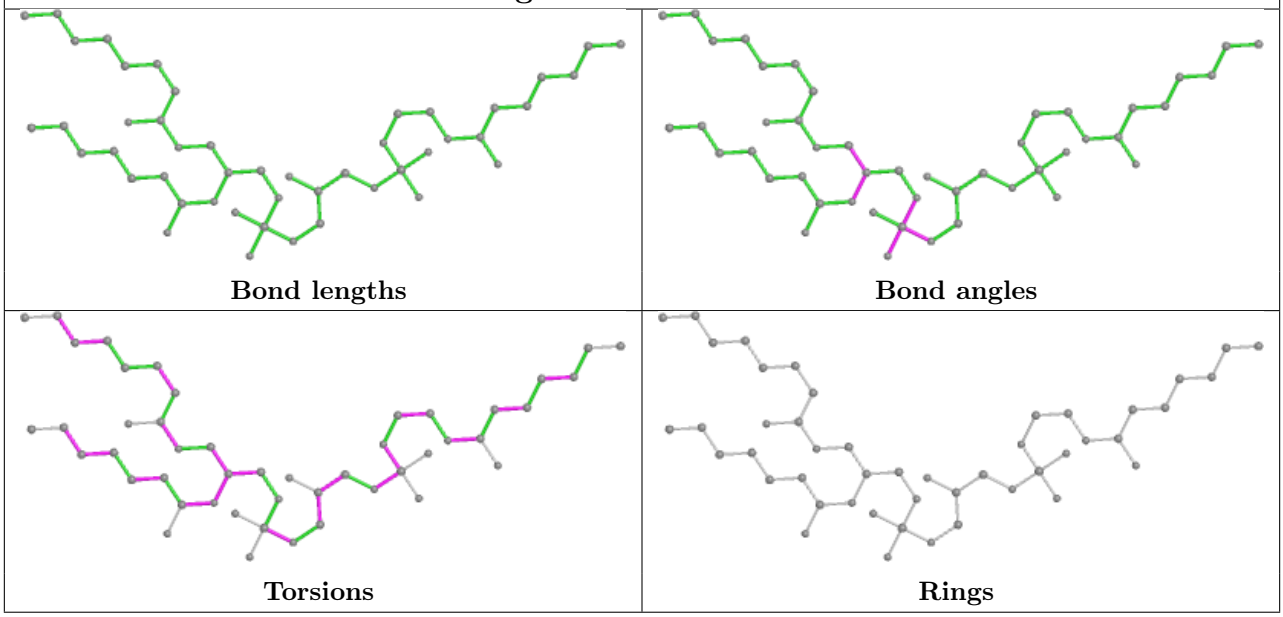
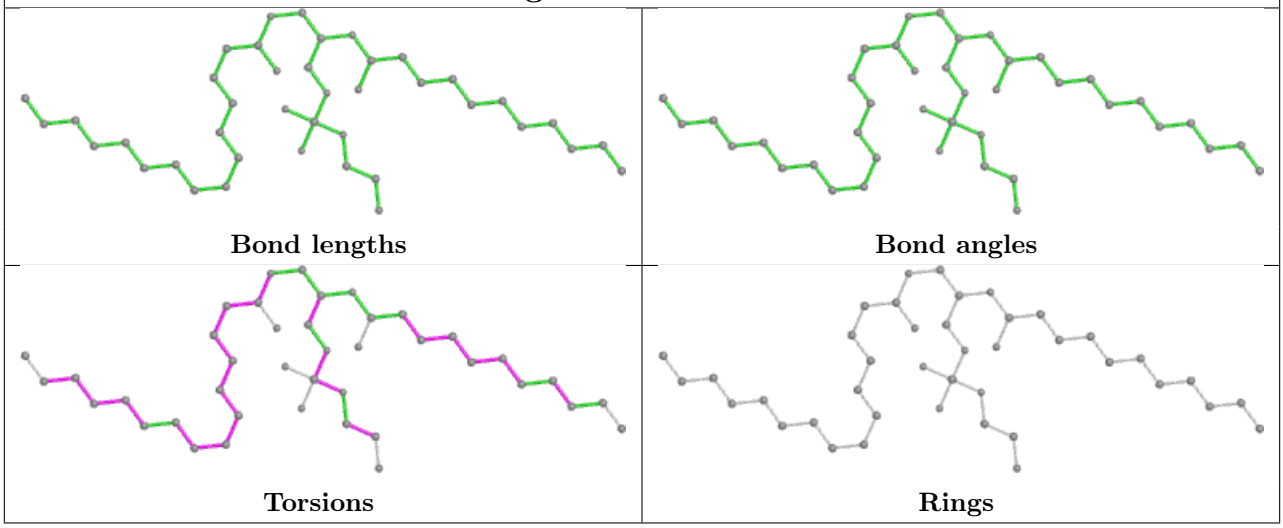
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	504	PTY	5	0
15	P	302	LMT	1	0
18	A	3003	XP4	1	0
14	A	3001	CDL	3	0

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.

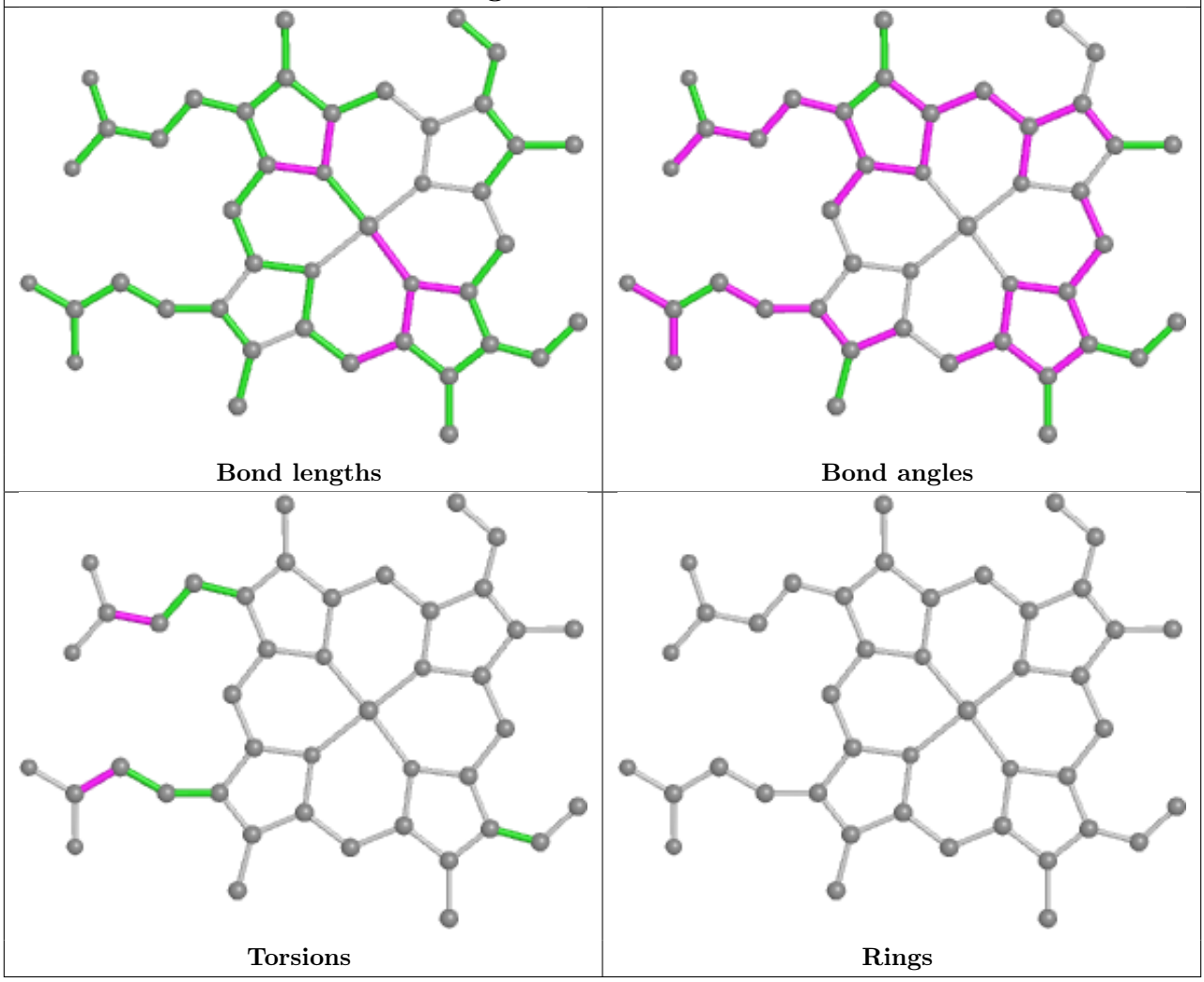
Ligand CDL A 3002

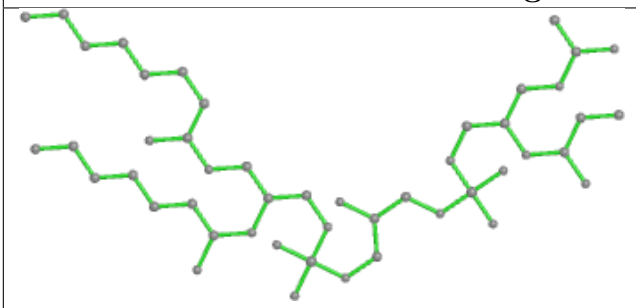
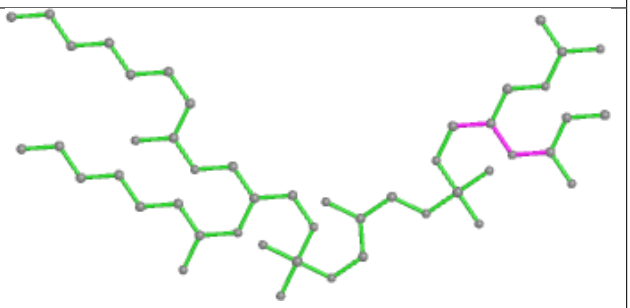
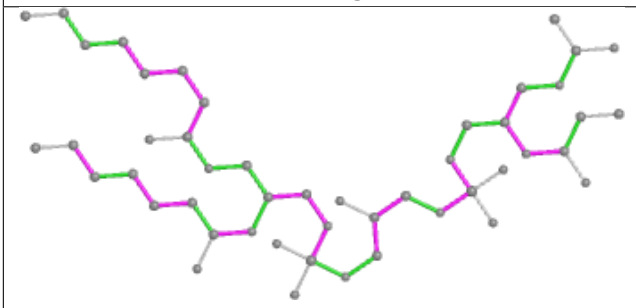
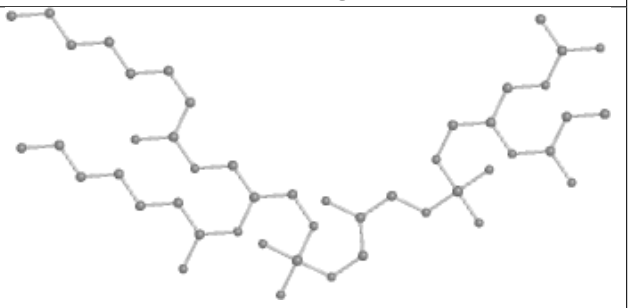


Ligand PTY E 401

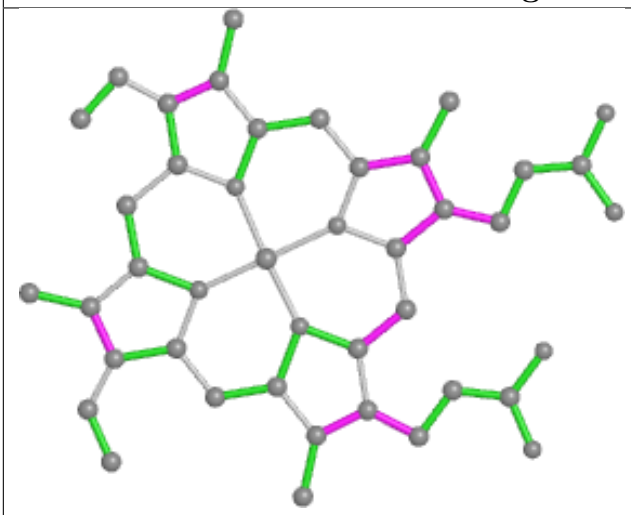


Ligand HEM N 502

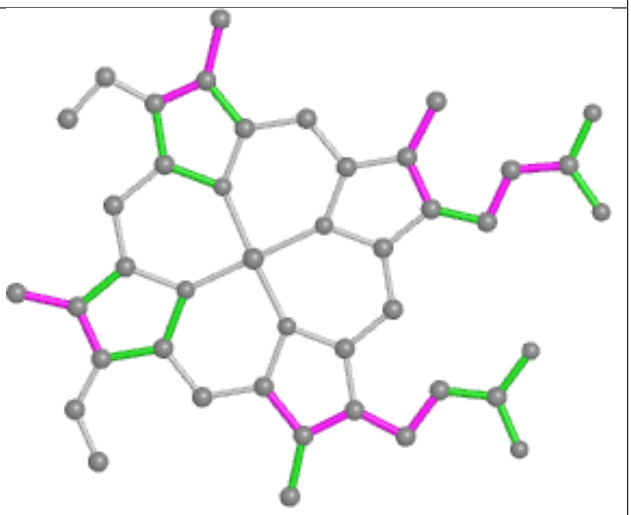


Ligand CDL C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC D 401



Bond lengths



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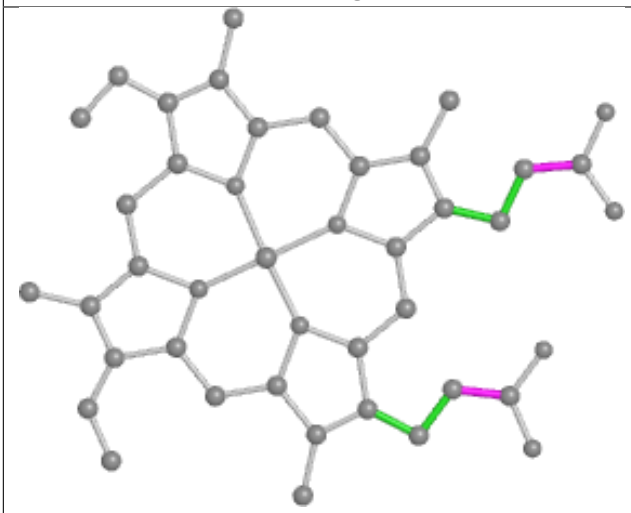
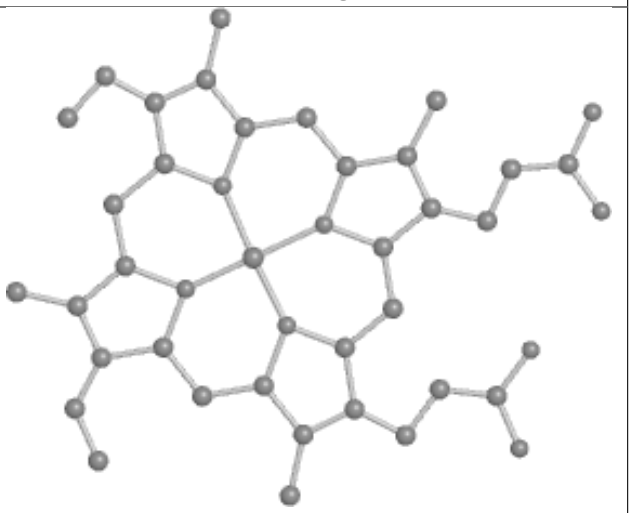
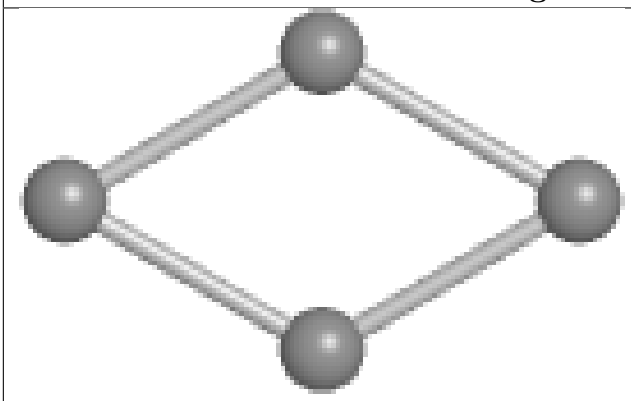
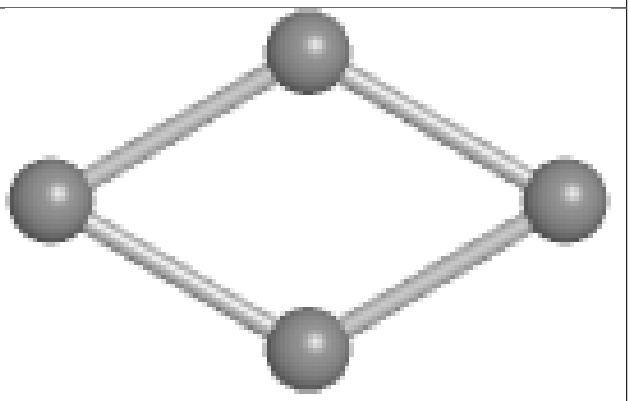
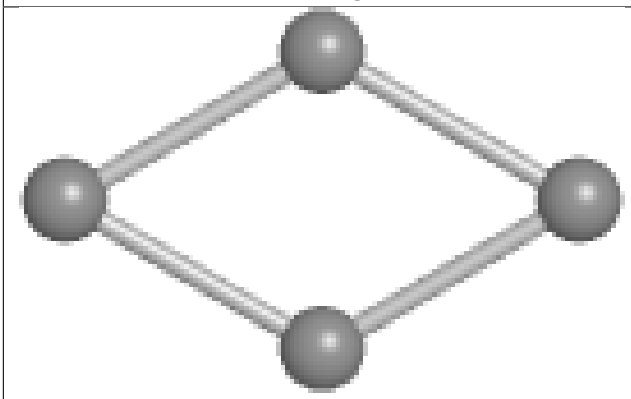
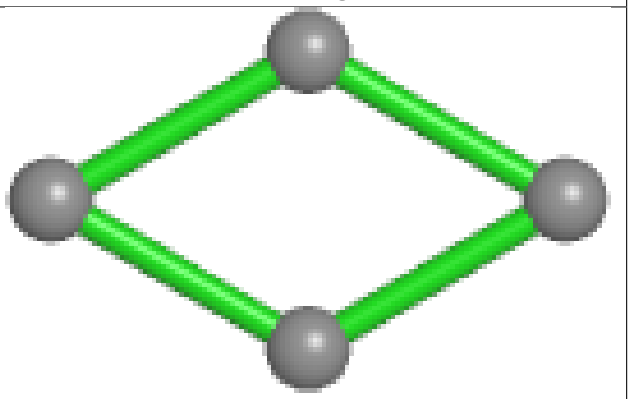


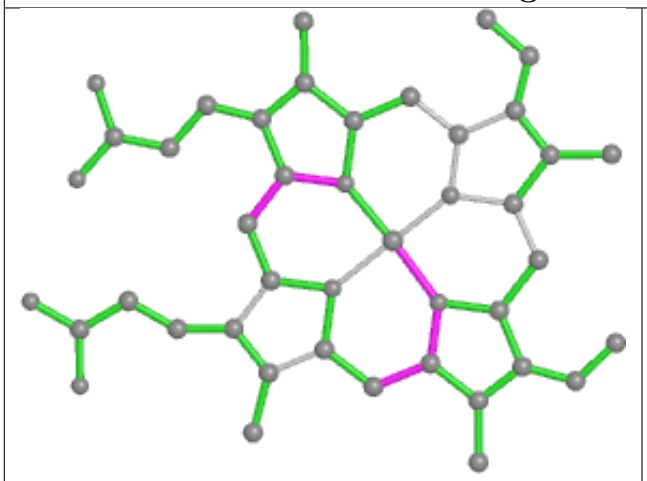
Torsions



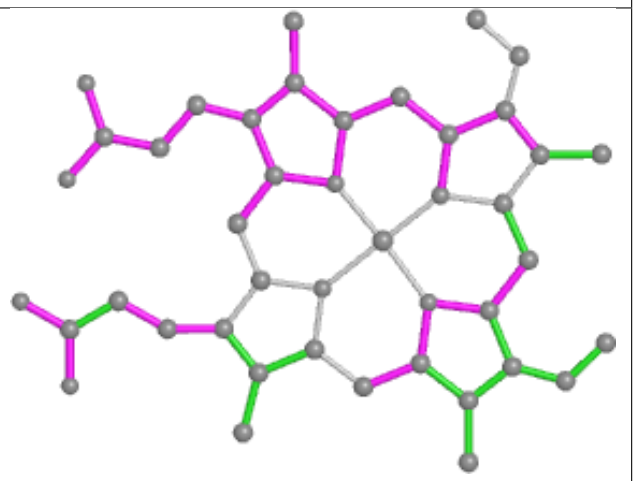
Rings

Ligand FES P 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM C 502



Bond lengths



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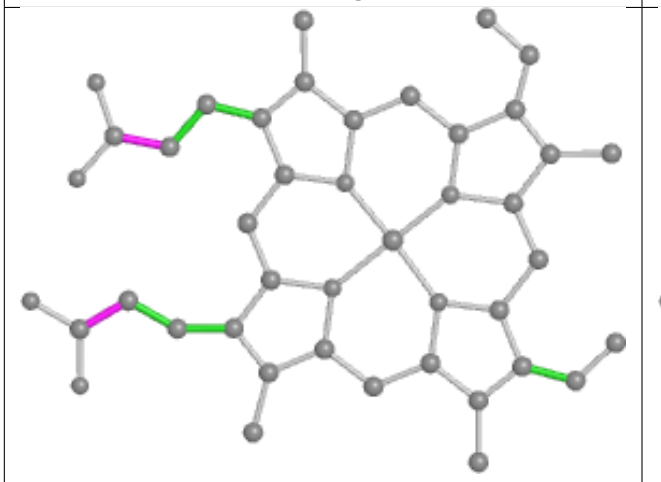

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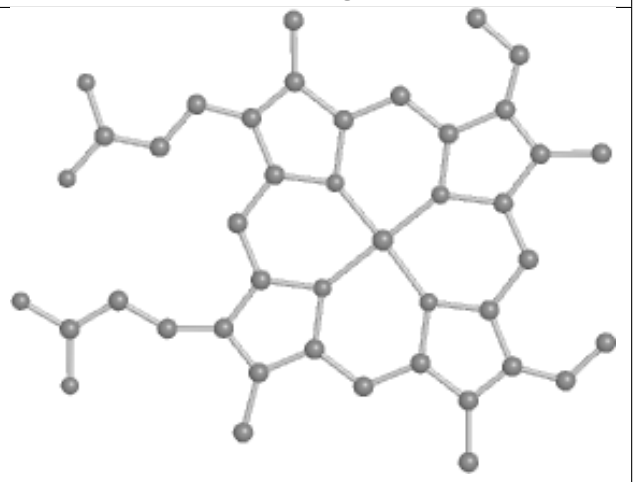

Rings

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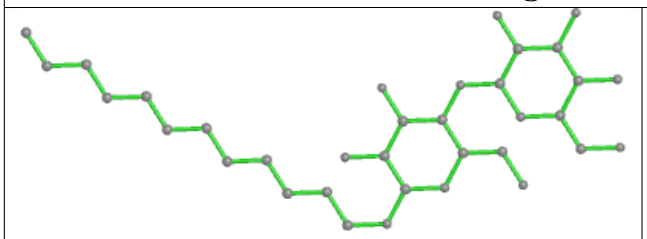

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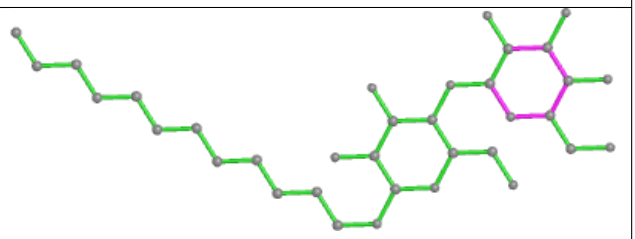

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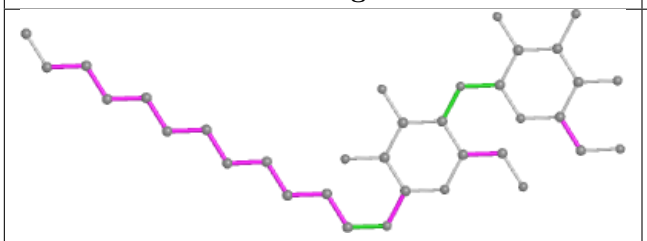

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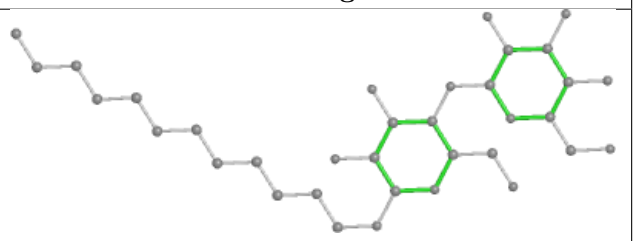
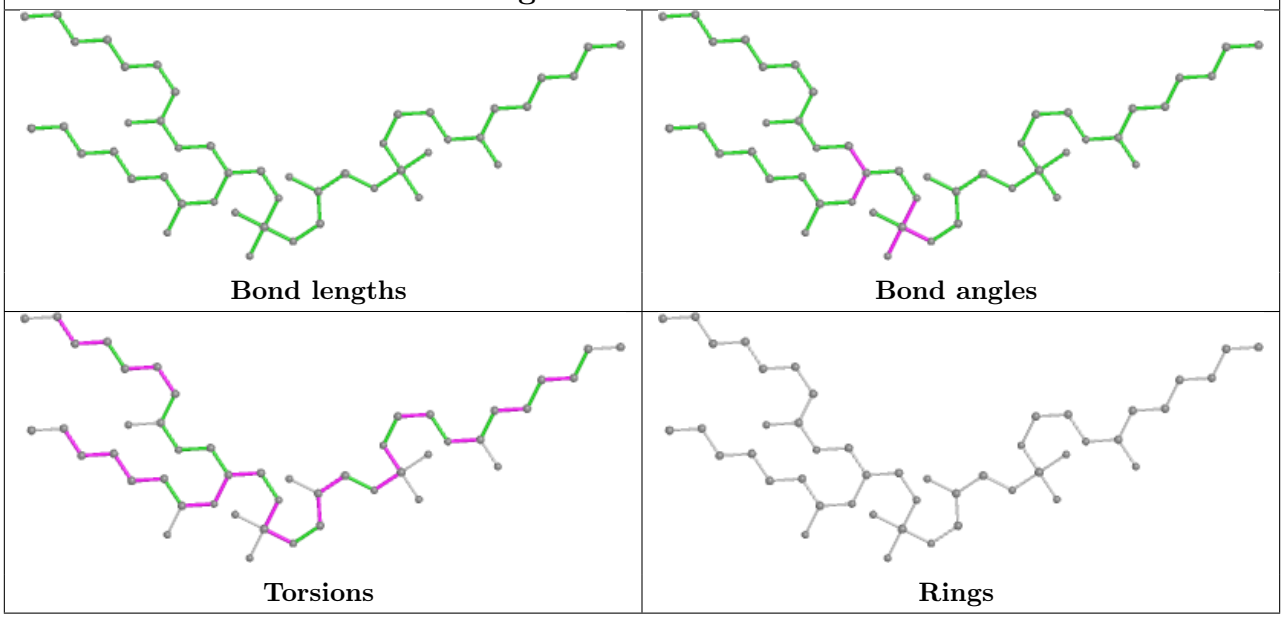
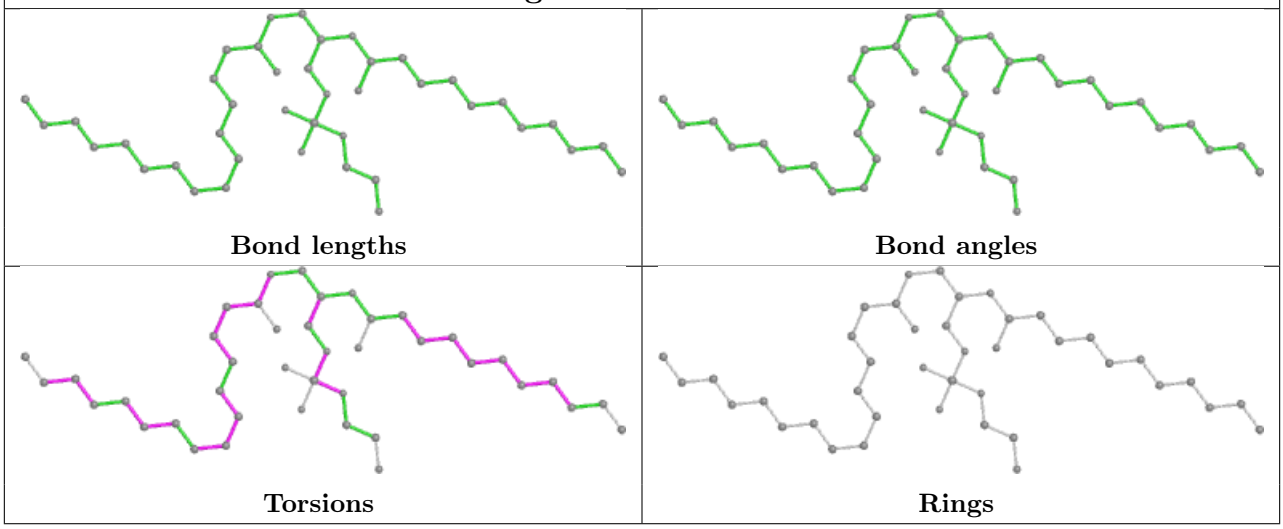


Rings

Ligand CDL L 3002



Ligand PTY P 303



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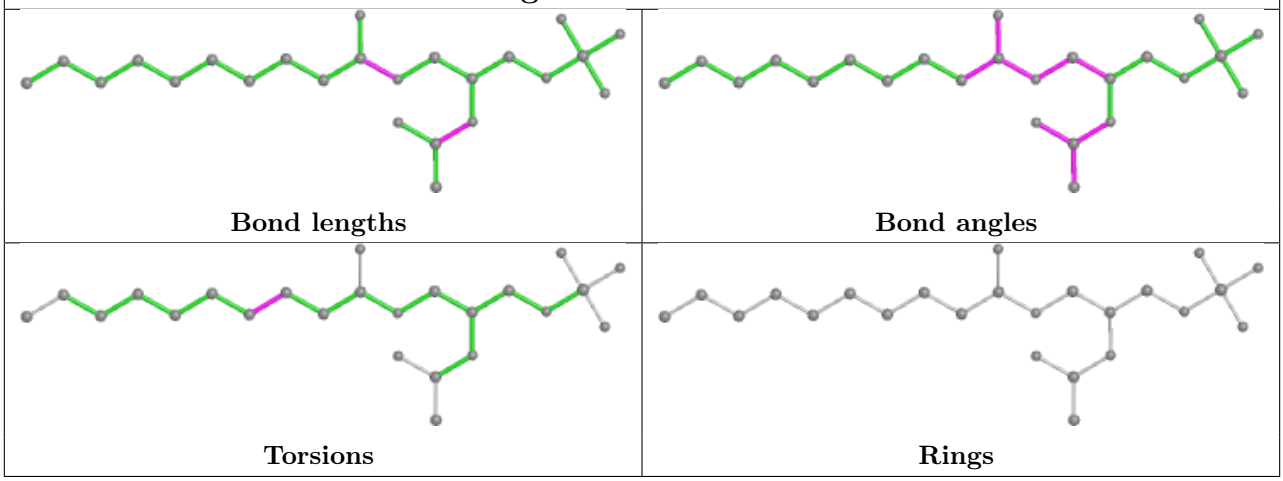
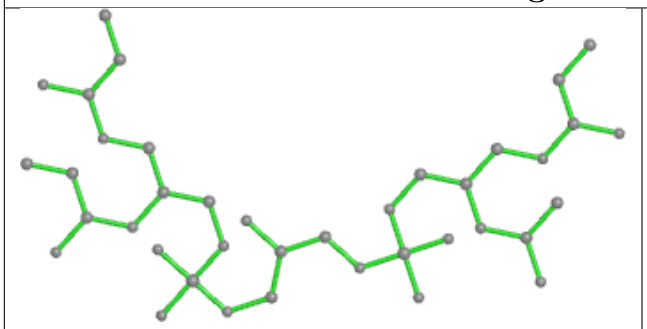


Ligand CDL S 702



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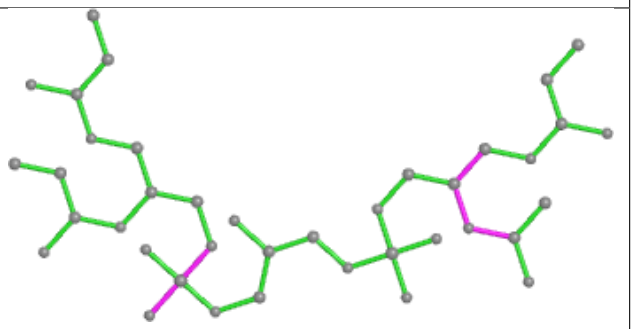
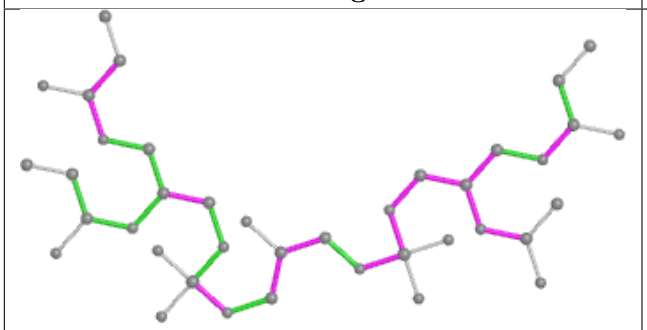
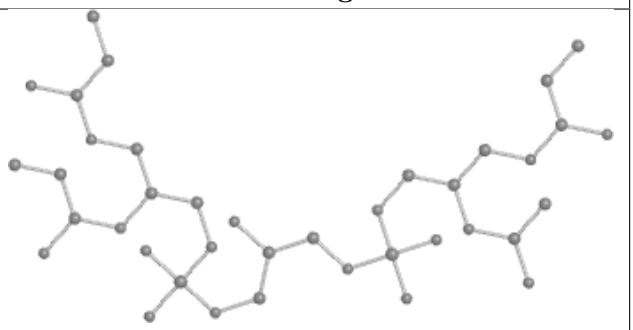


Bond angles

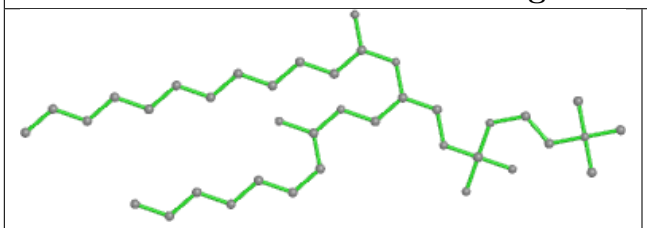


Torsions



Rings

Ligand PC1 C 503



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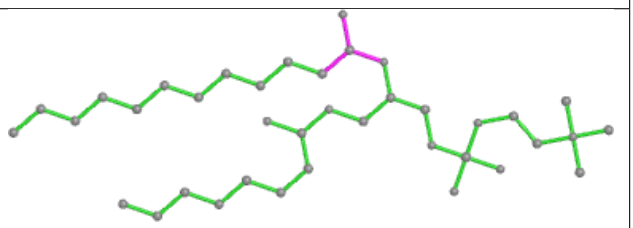
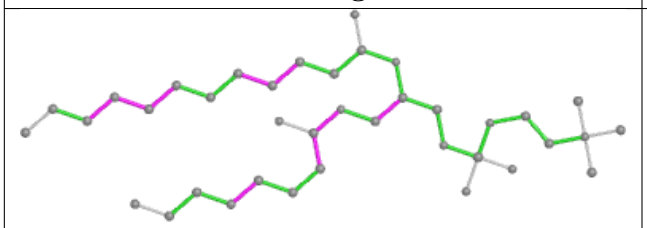


Bond angles



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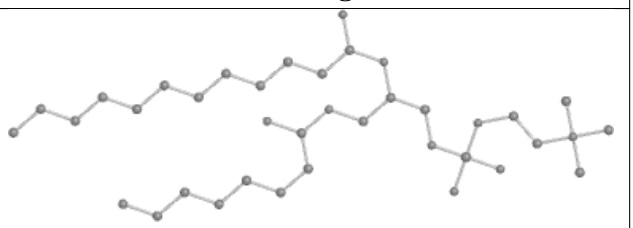
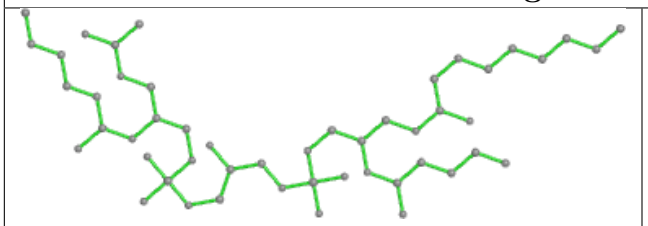


Rings

Ligand CDL H 701



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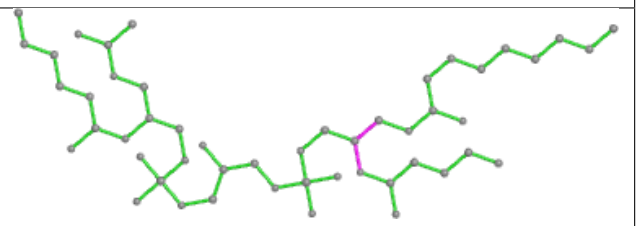

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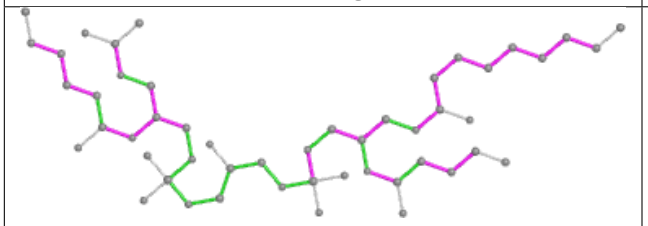

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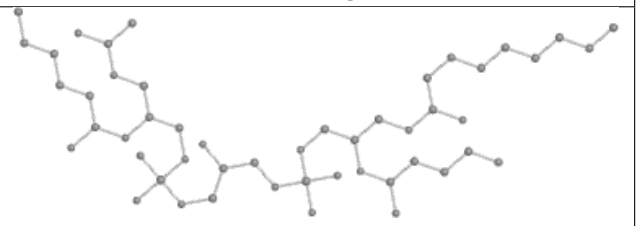
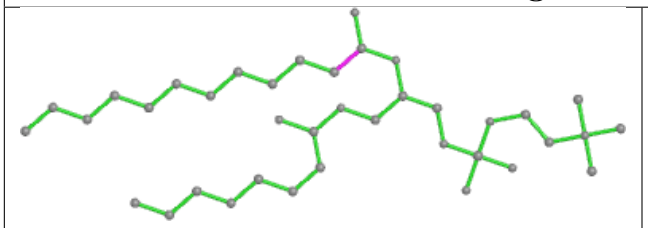


Rings

Ligand PC1 N 503



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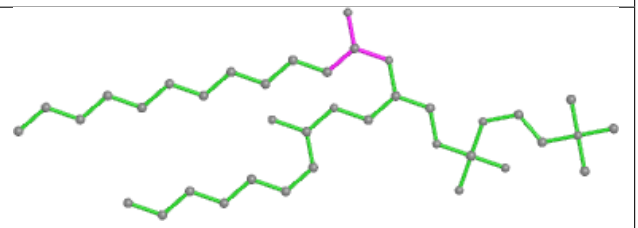
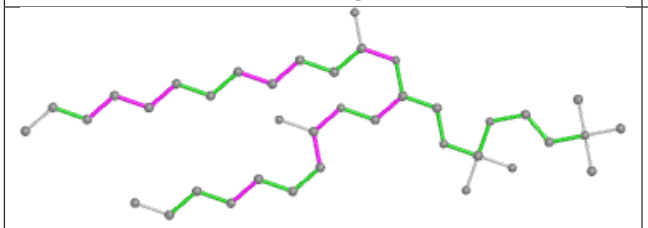


Bond angles



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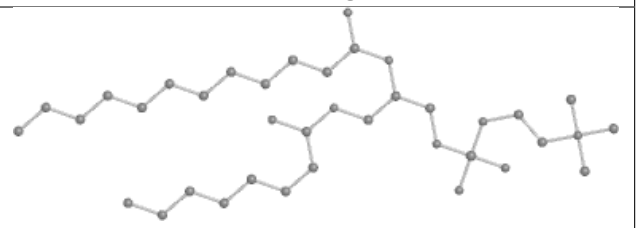

Rings

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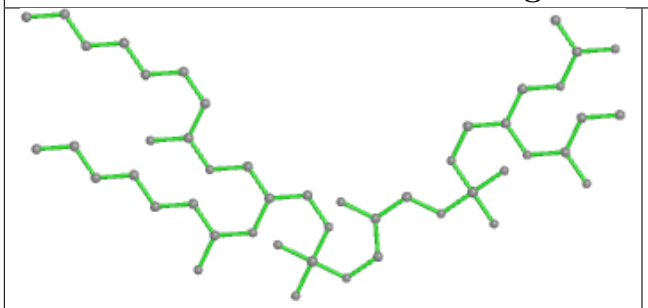

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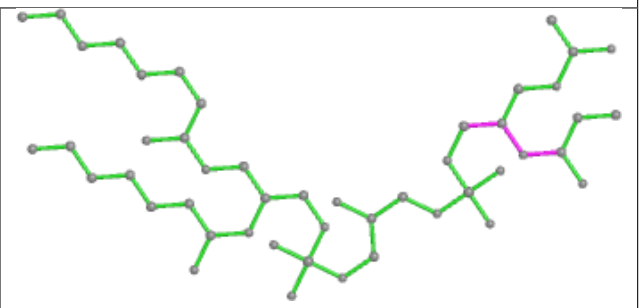
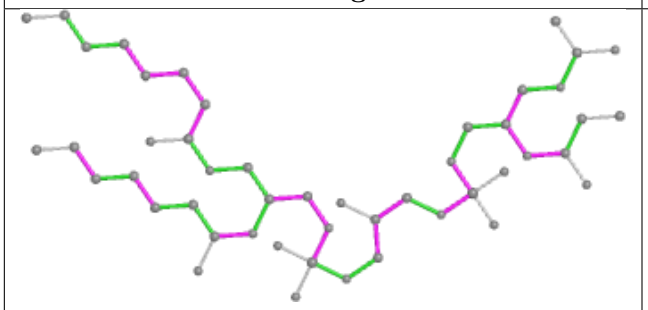
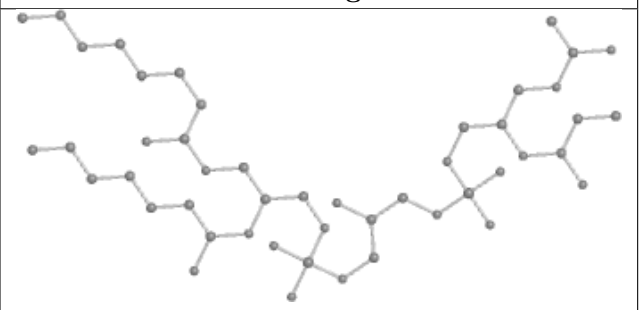


Bond angles

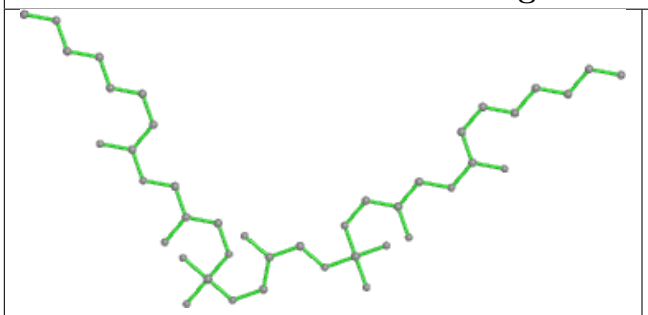


Torsions

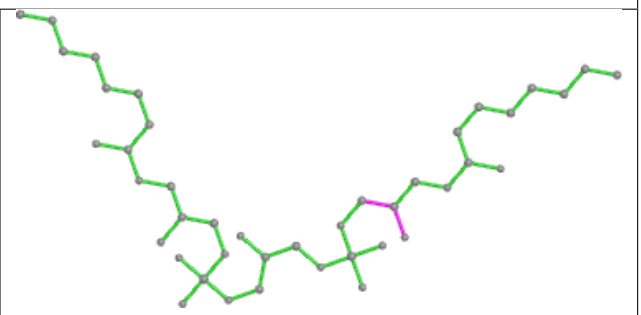


Rings

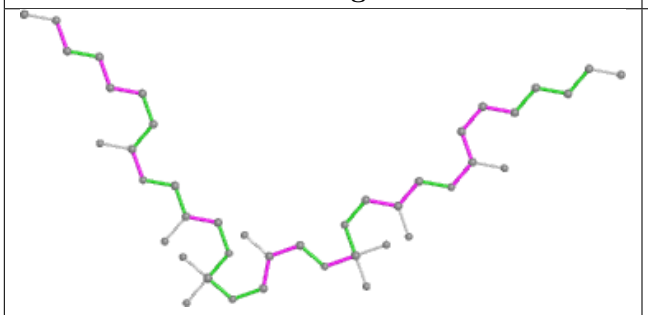
Ligand CDL L 3001



Bond lengths



Bond angles



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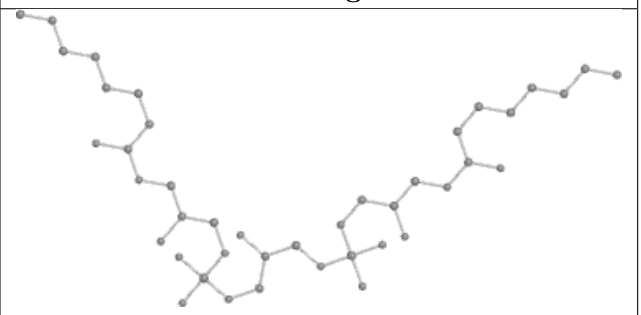
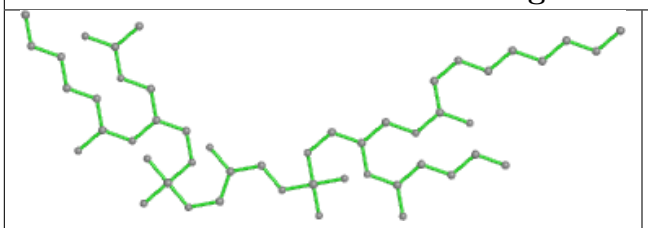
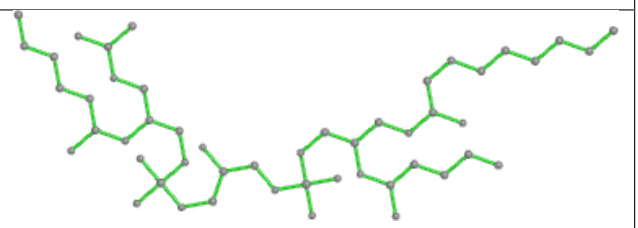


Rings

Ligand CDL S 701



Bond lengths



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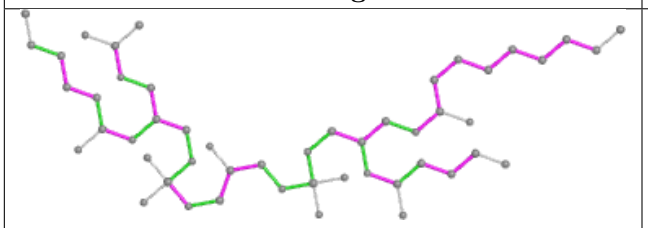

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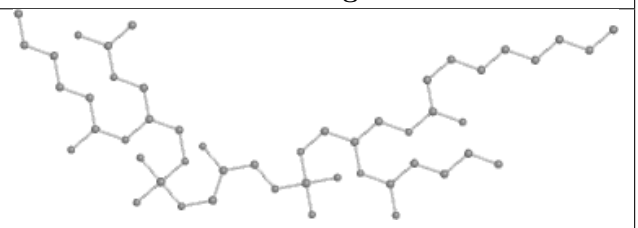
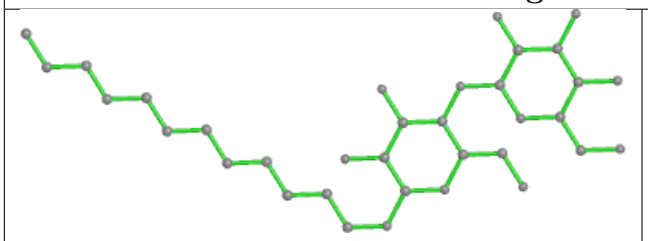


Rings

Ligand LMT J 101



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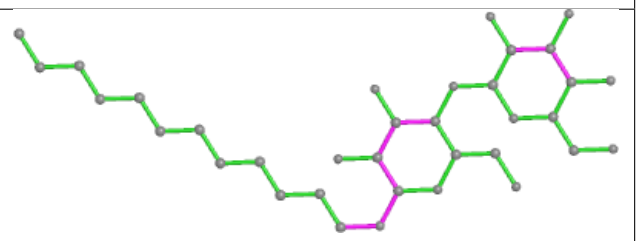
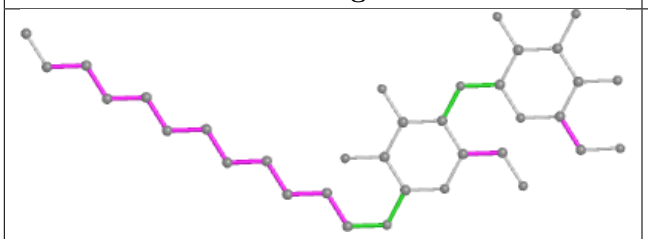


Bond angles



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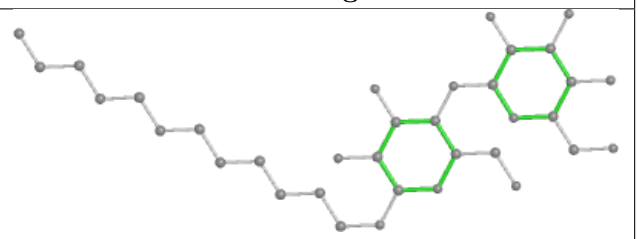
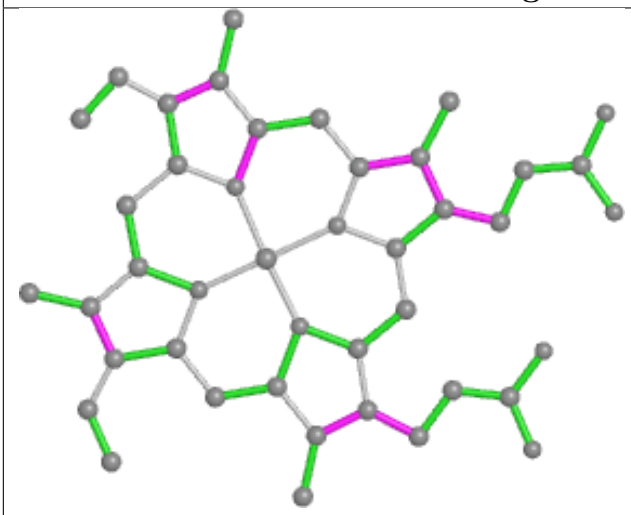
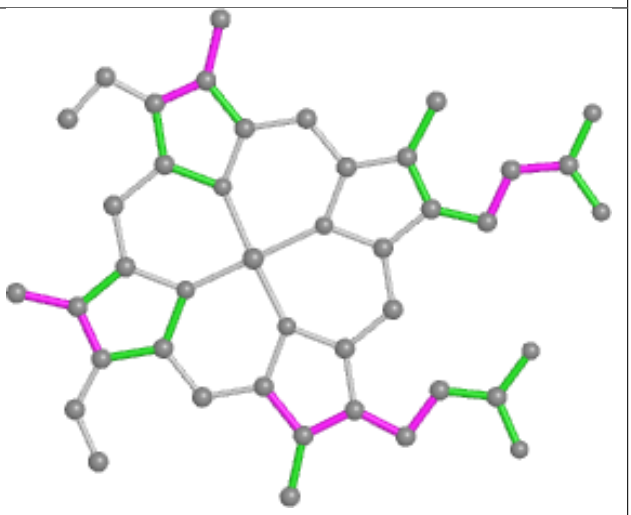


Rings

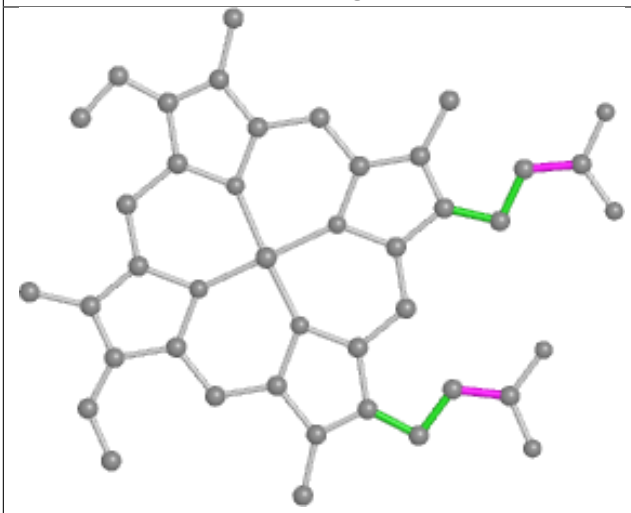
Ligand HEC O 401



Bond lengths



Bond angles



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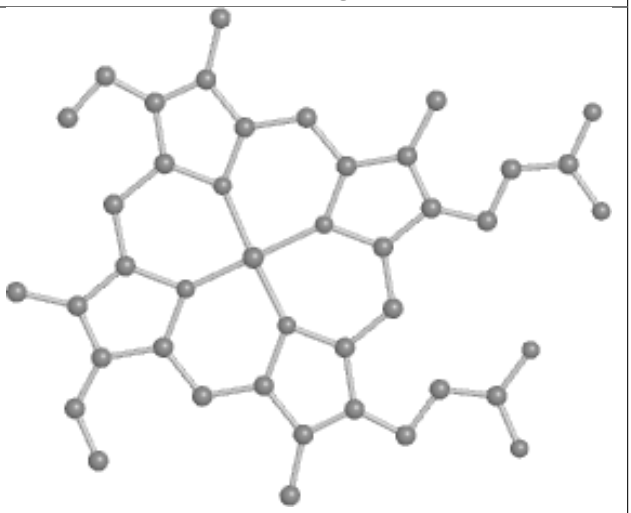
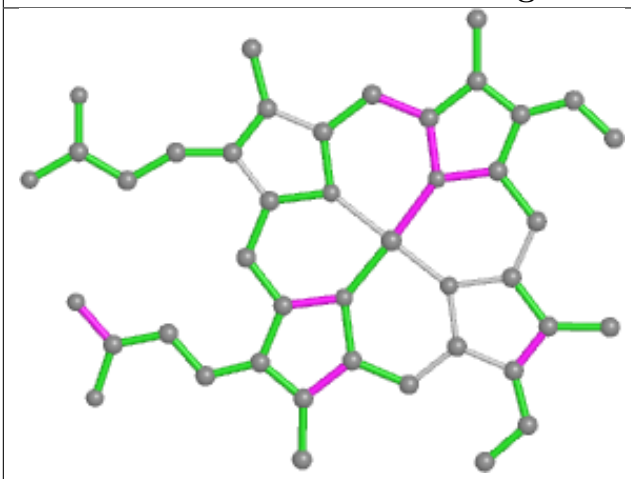
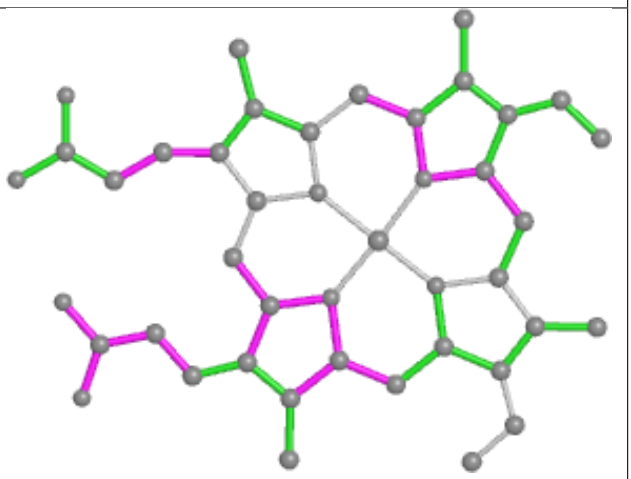


Rings

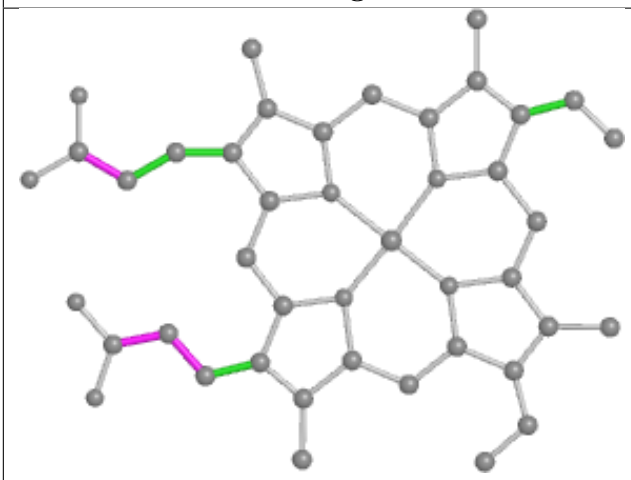
Ligand HEM N 501



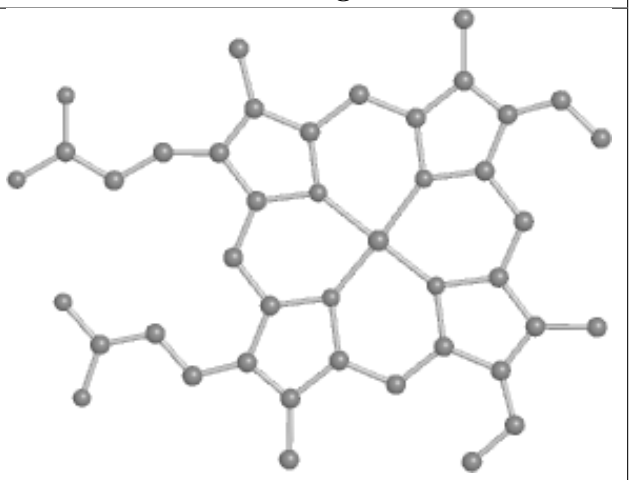
Bond lengths



Bond angles

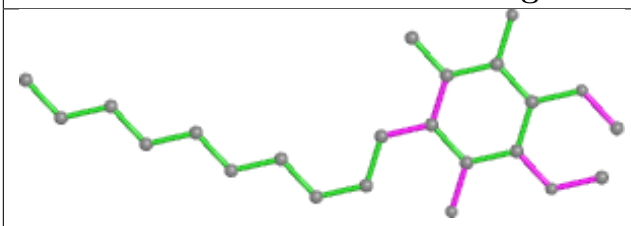


Torsions



Rings

Ligand DCQ C 507



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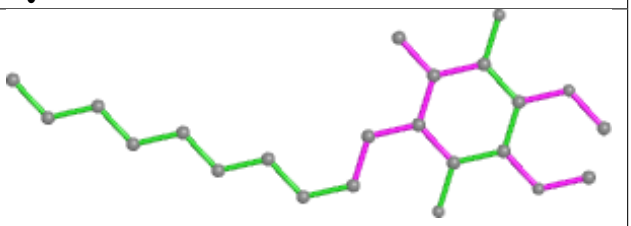
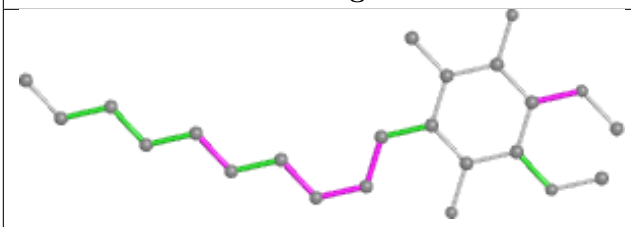


Bond angles



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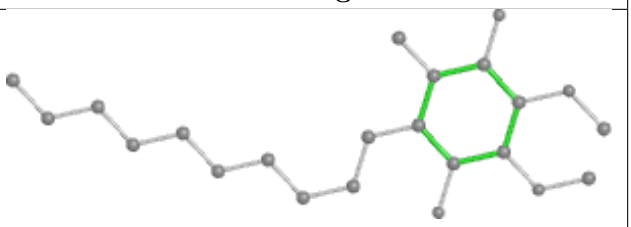

Rings

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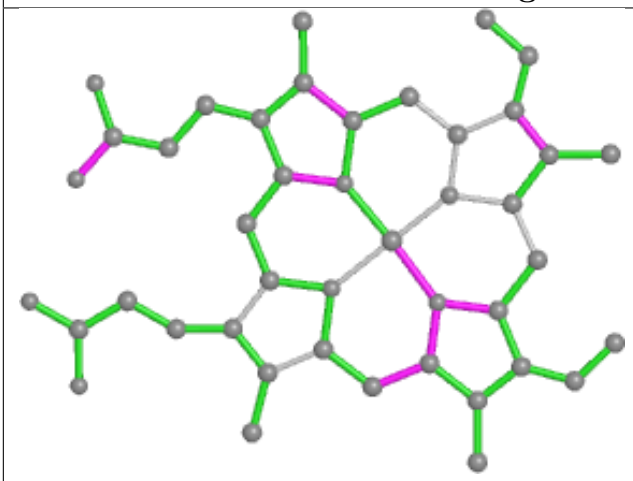

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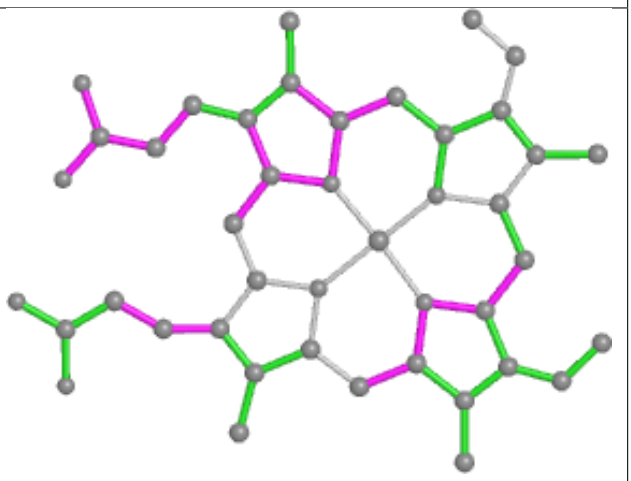
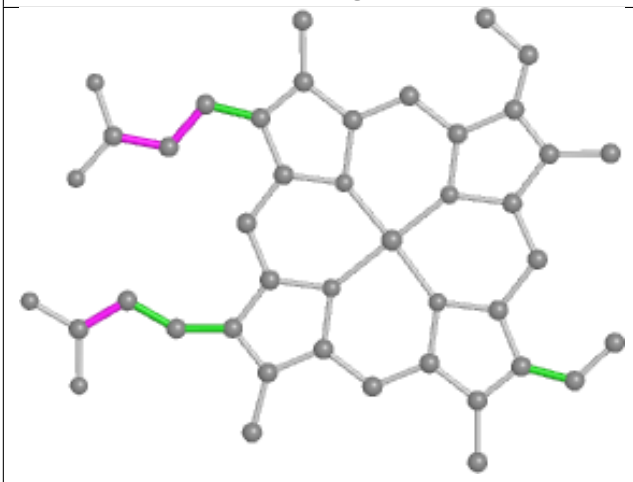


Bond angles



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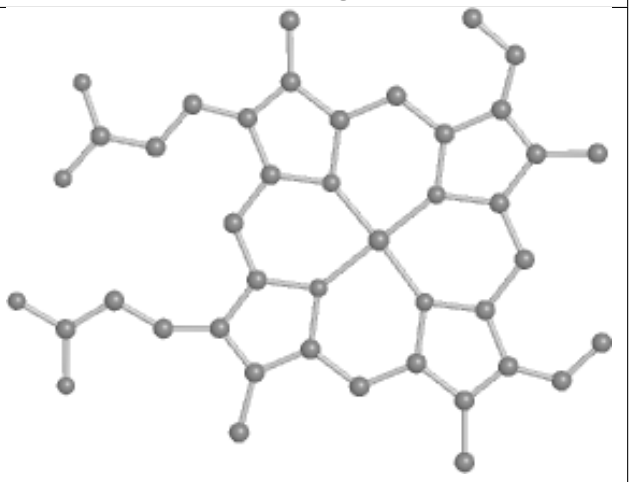
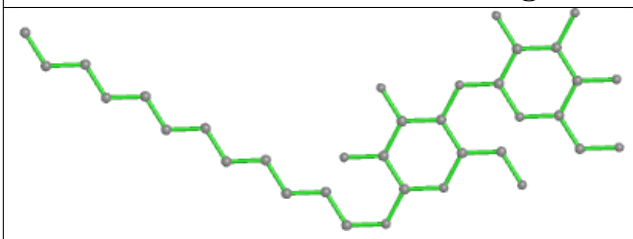
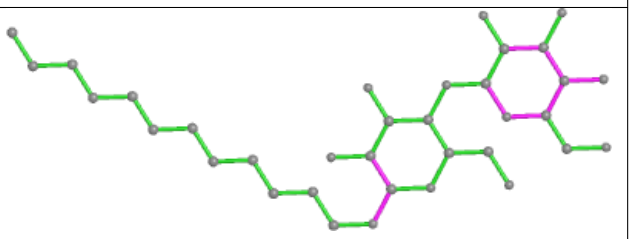


Rings

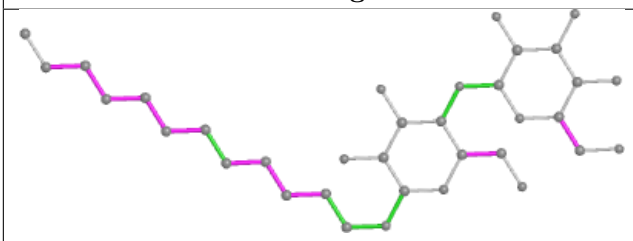
Ligand LMT N 506



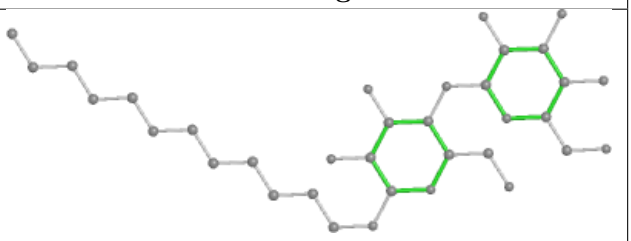
Bond lengths



Bond angles

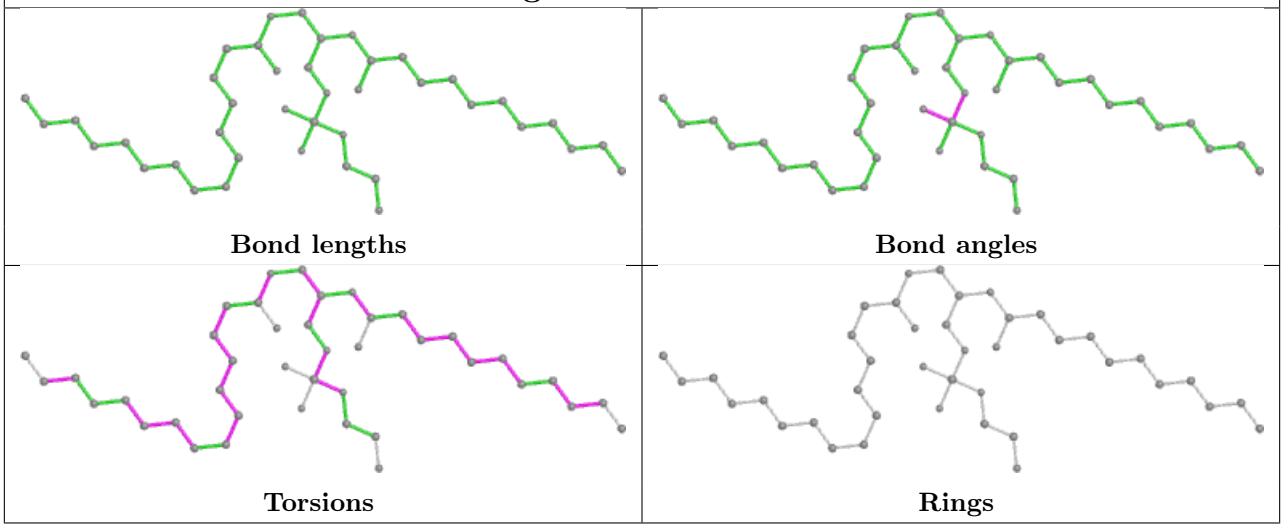


Torsions

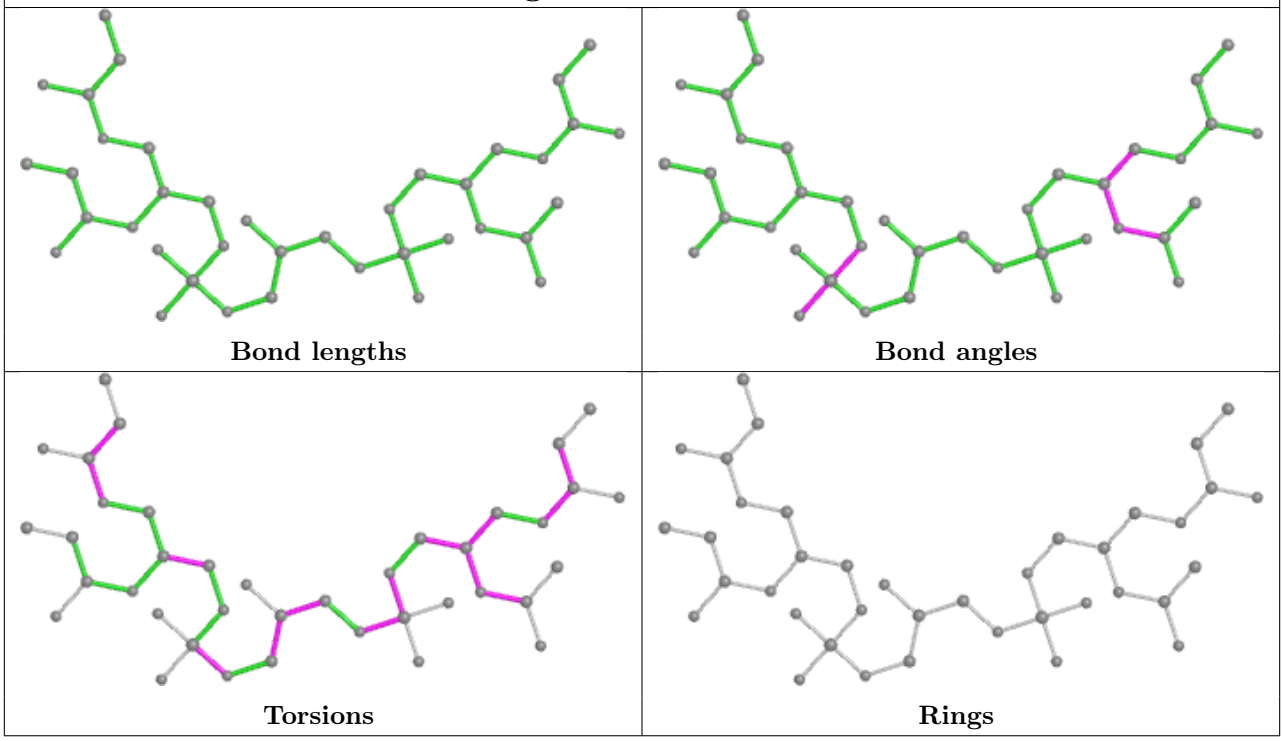


Rings

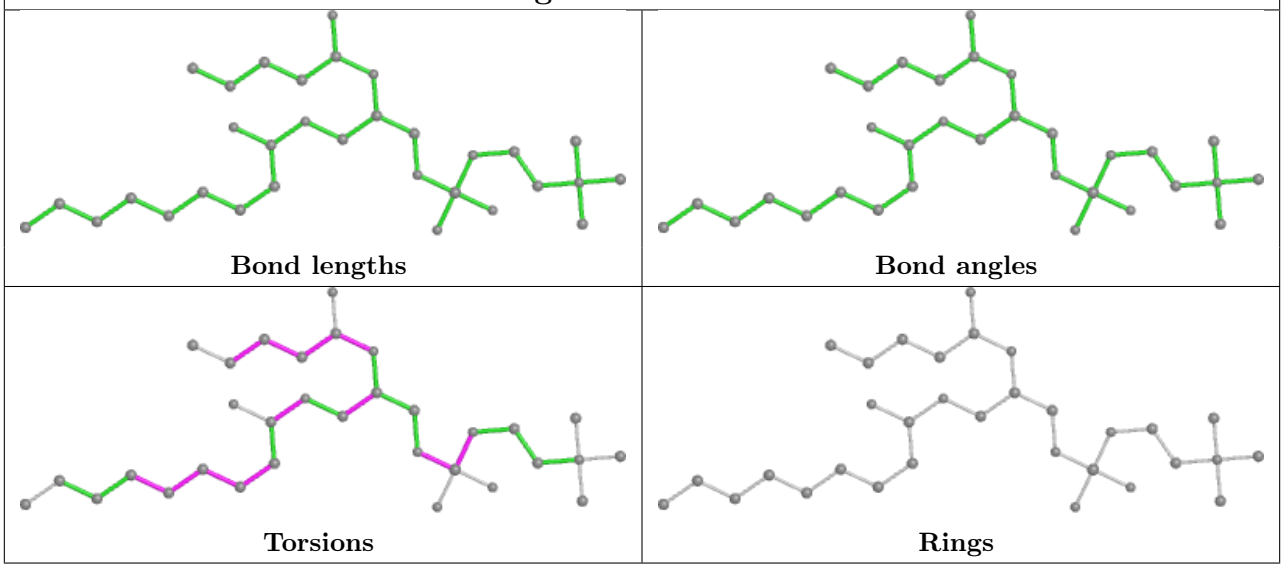
Ligand PTY N 504



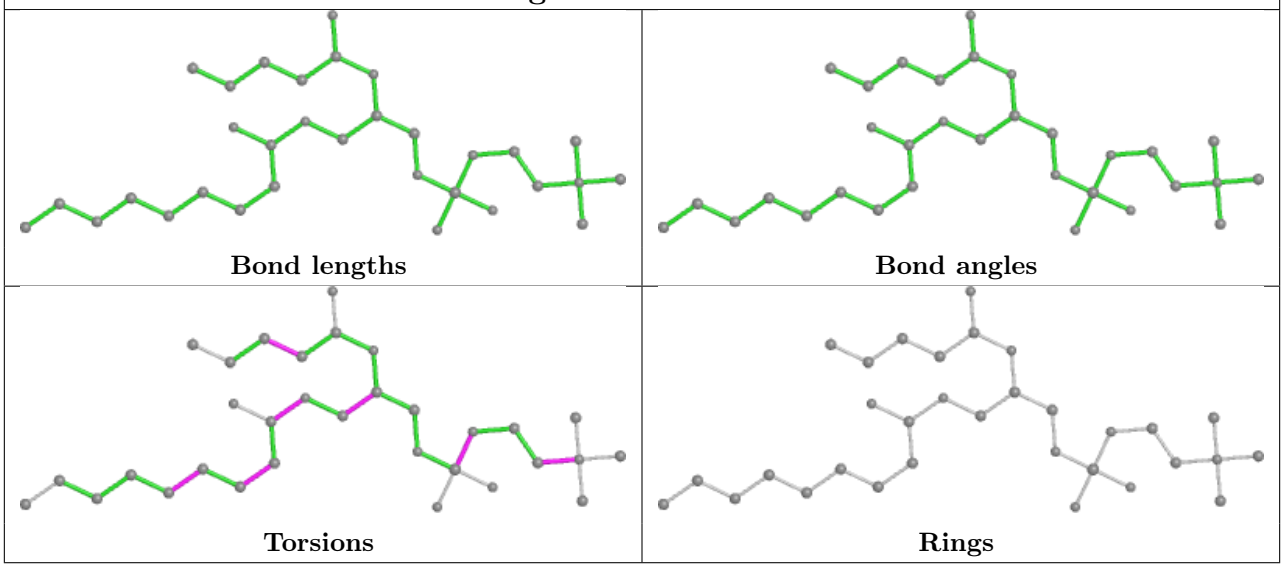
Ligand CDL H 702



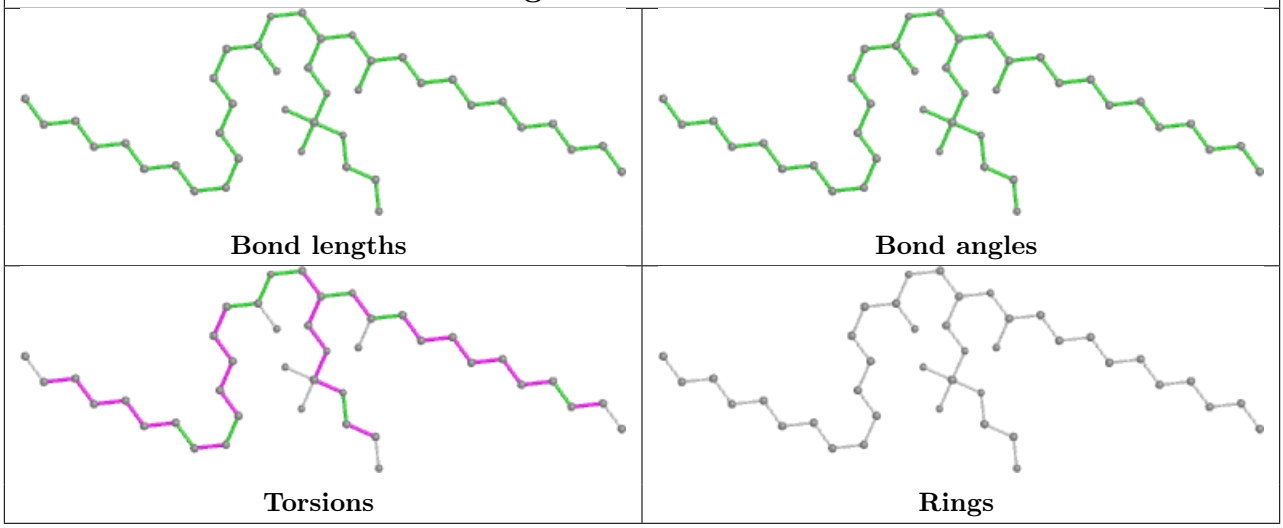
Ligand PC1 I 201



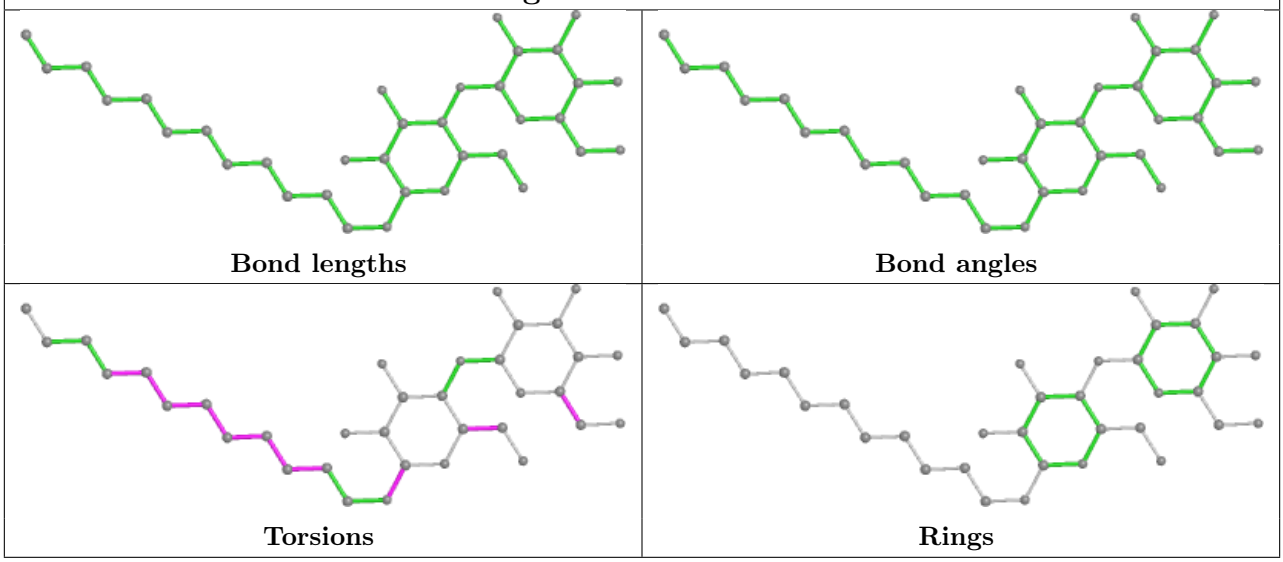
Ligand PC1 T 201



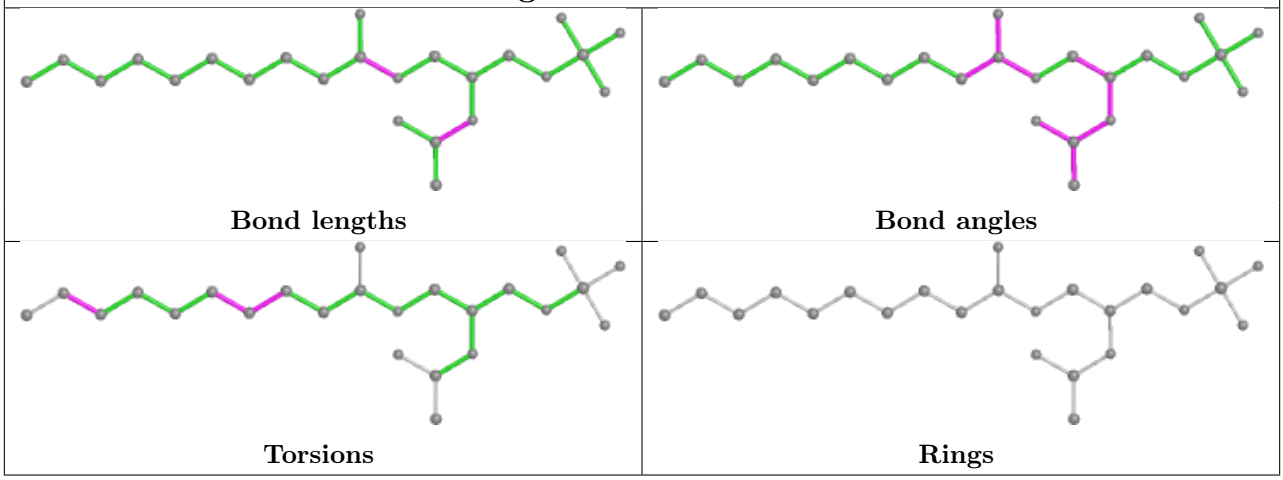
Ligand PTY C 504

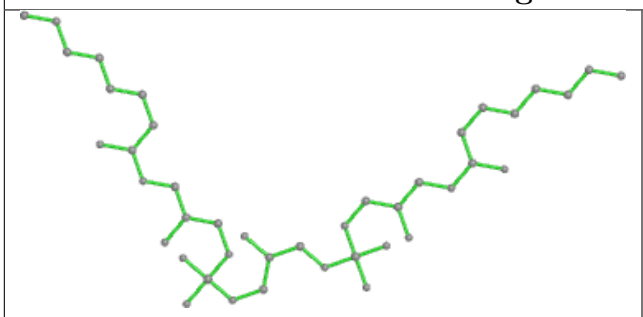
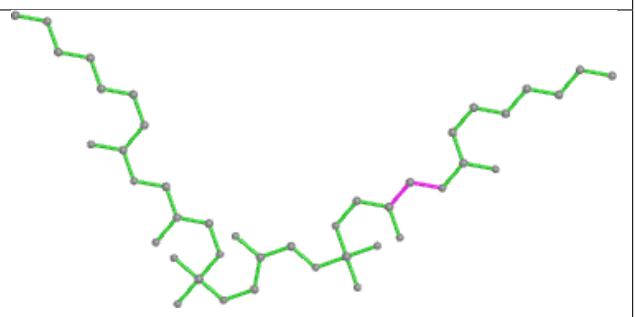
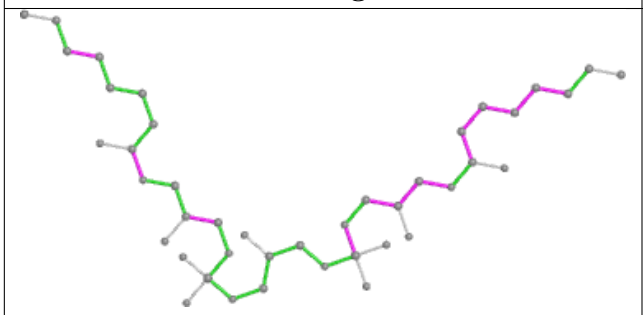
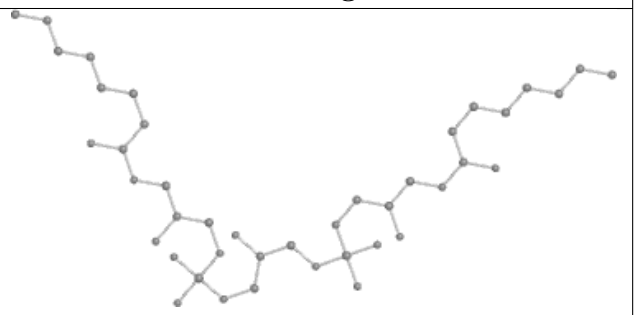


Ligand LMT P 302



Ligand XP4 A 3003



Ligand CDL A 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

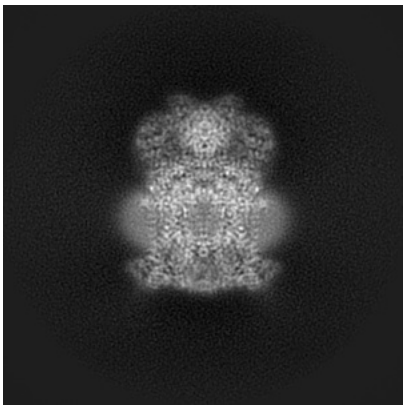
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15314. These allow visual inspection of the internal detail of the map and identification of artifacts.

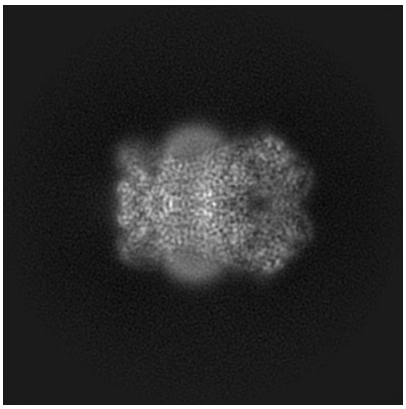
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

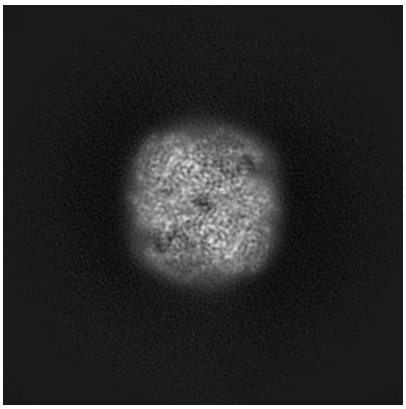
6.1.1 Primary map



X

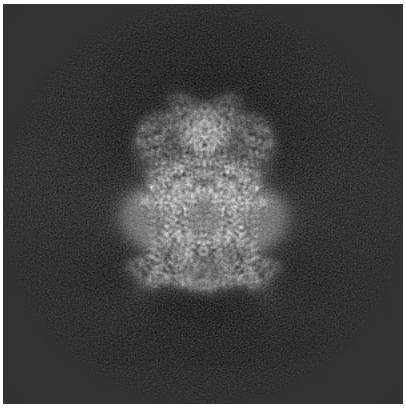


Y

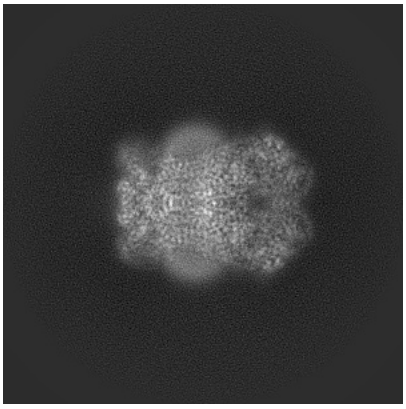


Z

6.1.2 Raw map



X



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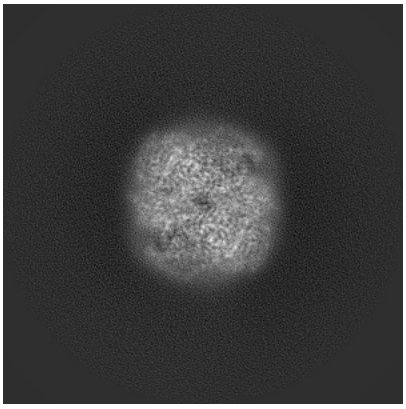
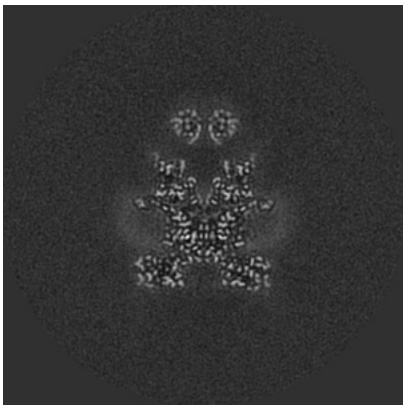


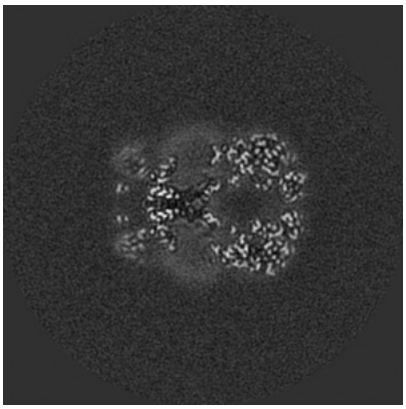
Z

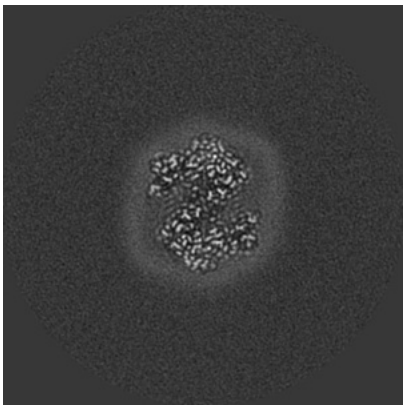
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

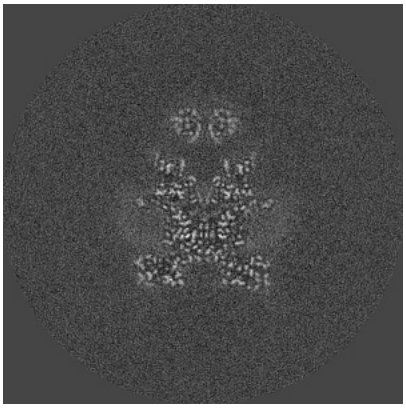
6.2.1 Primary map

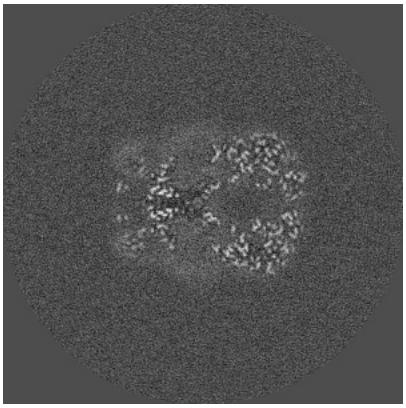

X Index: 180

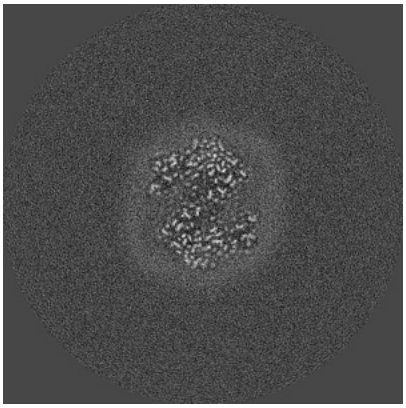

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

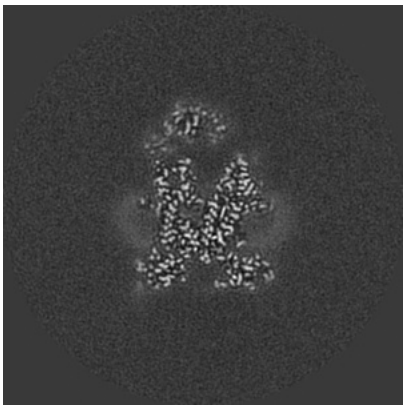

Y Index: 180

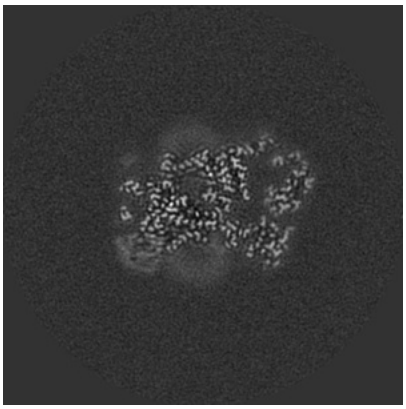

Z Index: 180

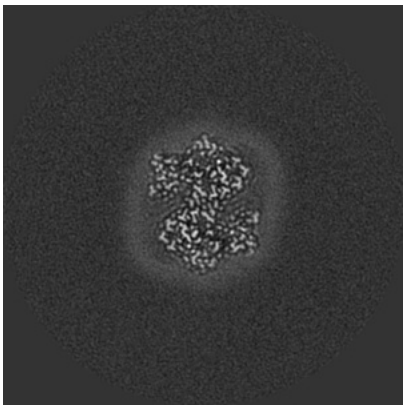
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

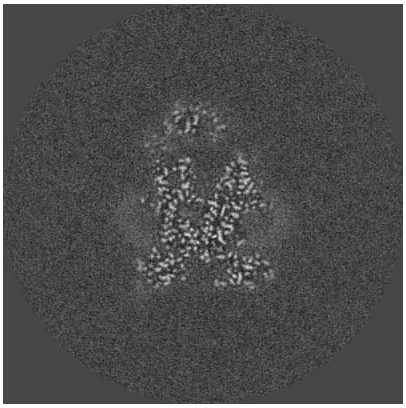
6.3.1 Primary map

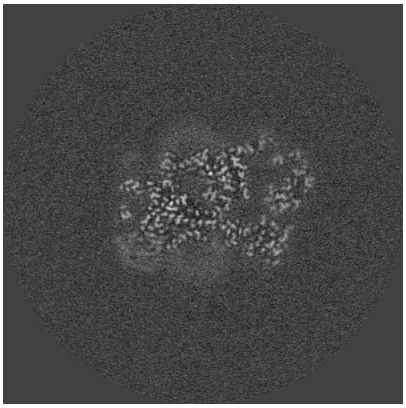

X Index: 186

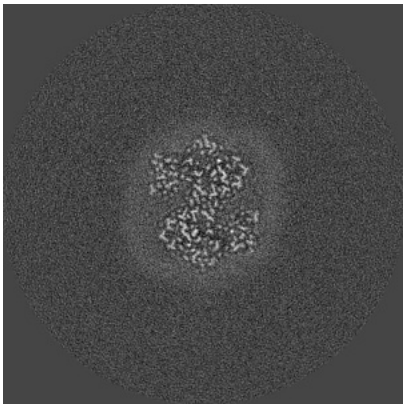

Y Index: 166


Z Index: 182

6.3.2 Raw map


X Index: 186

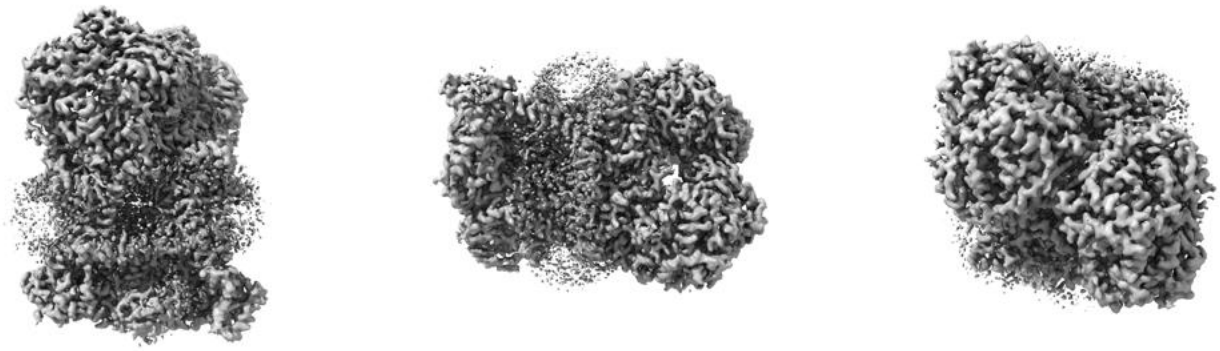

Y Index: 166


Z Index: 182

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

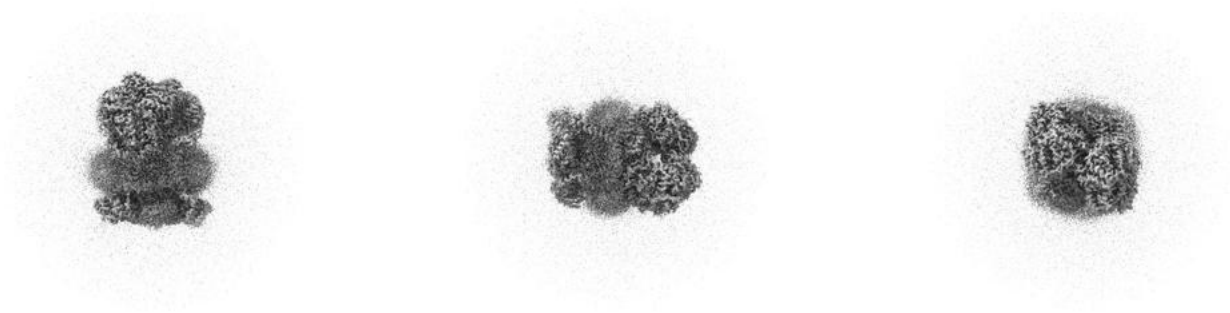
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

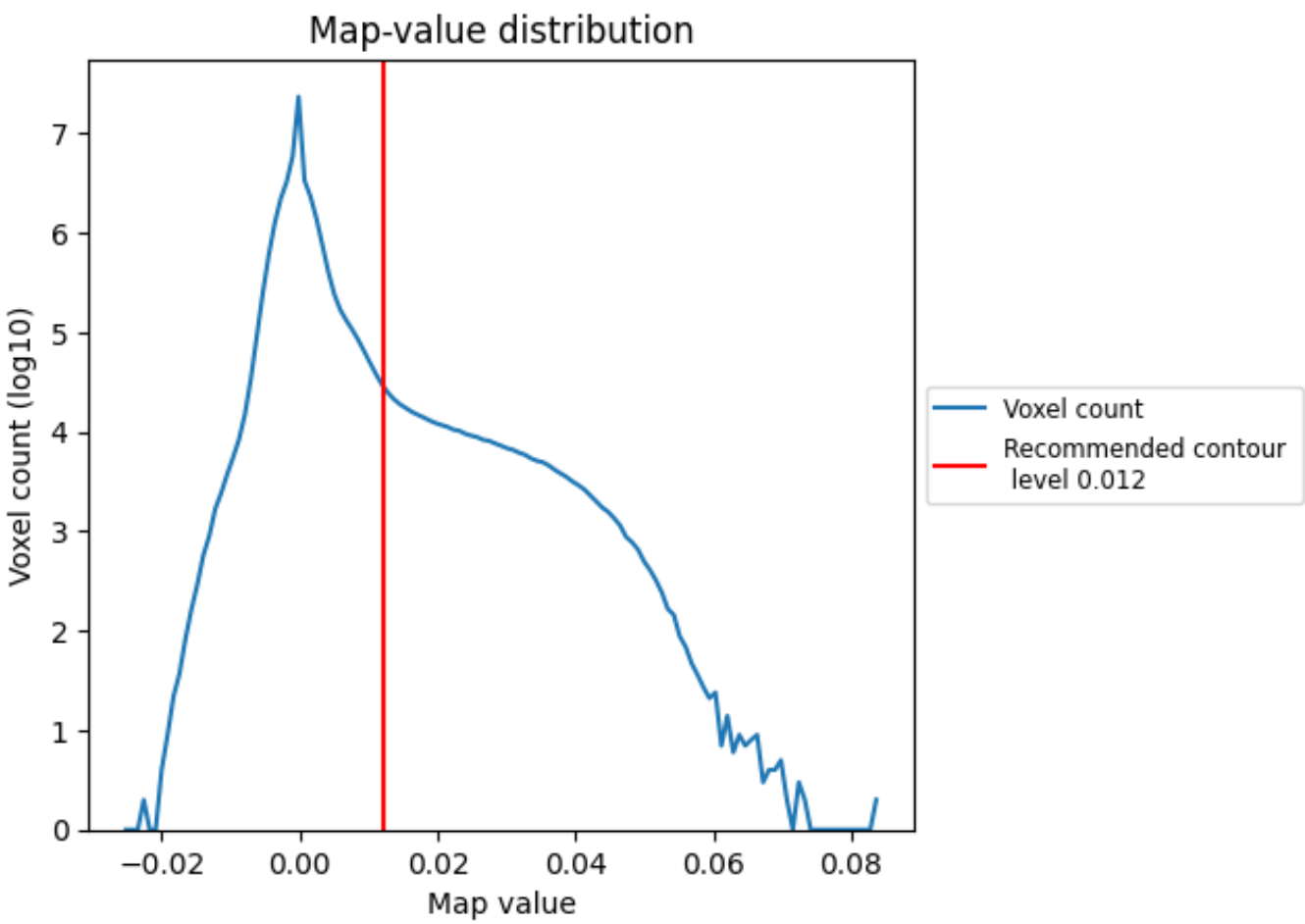
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

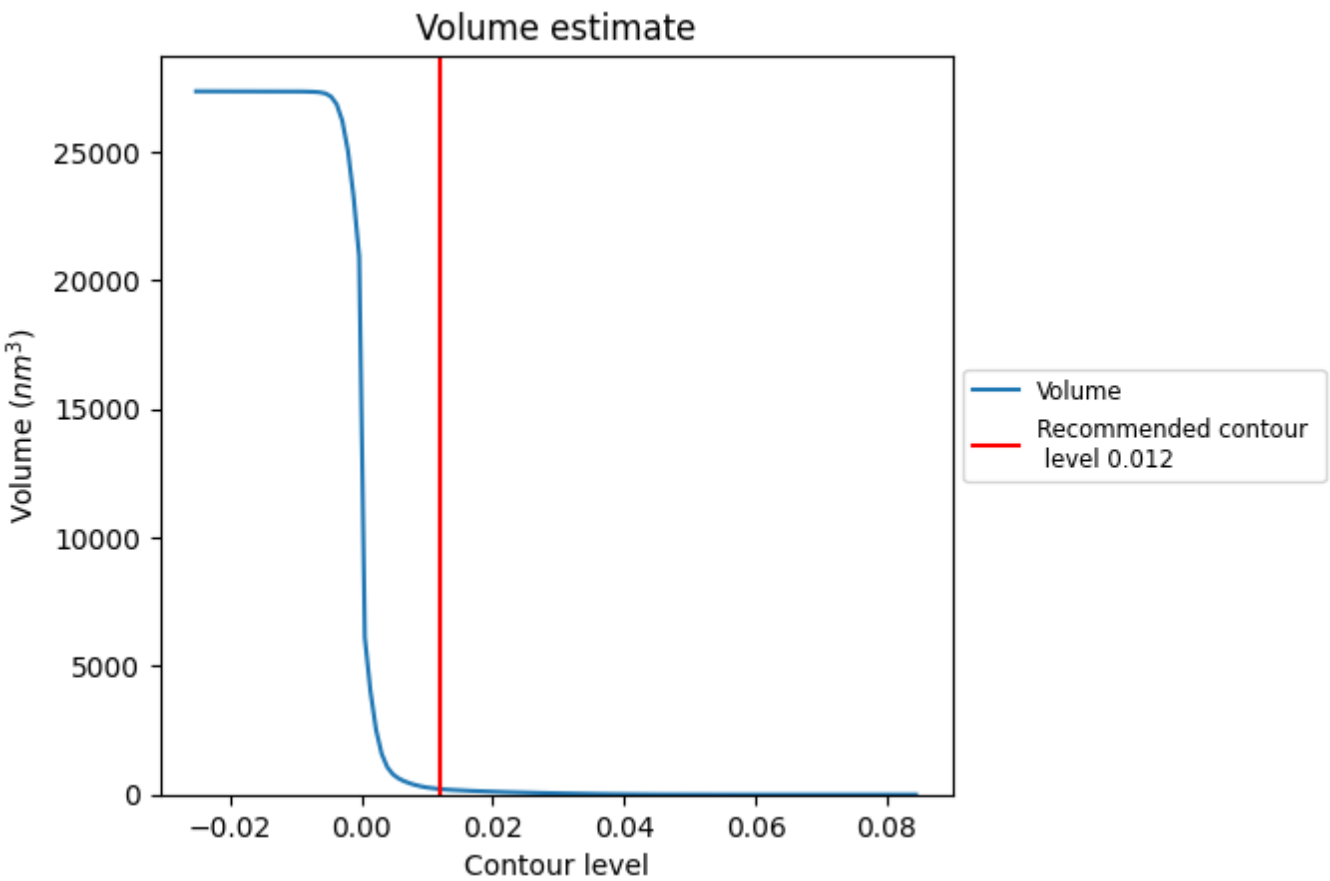
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

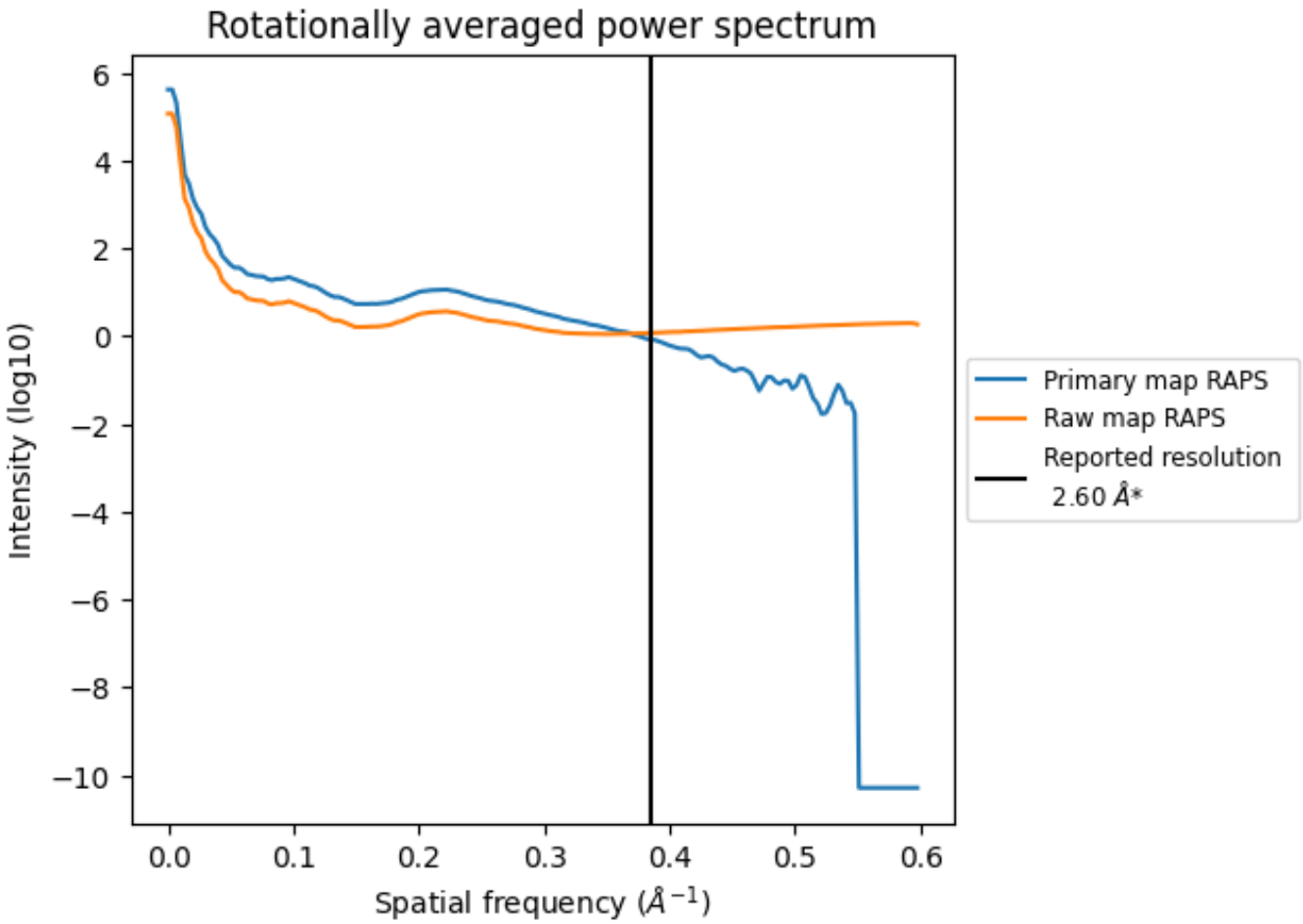
7.2 Volume estimate (i)



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

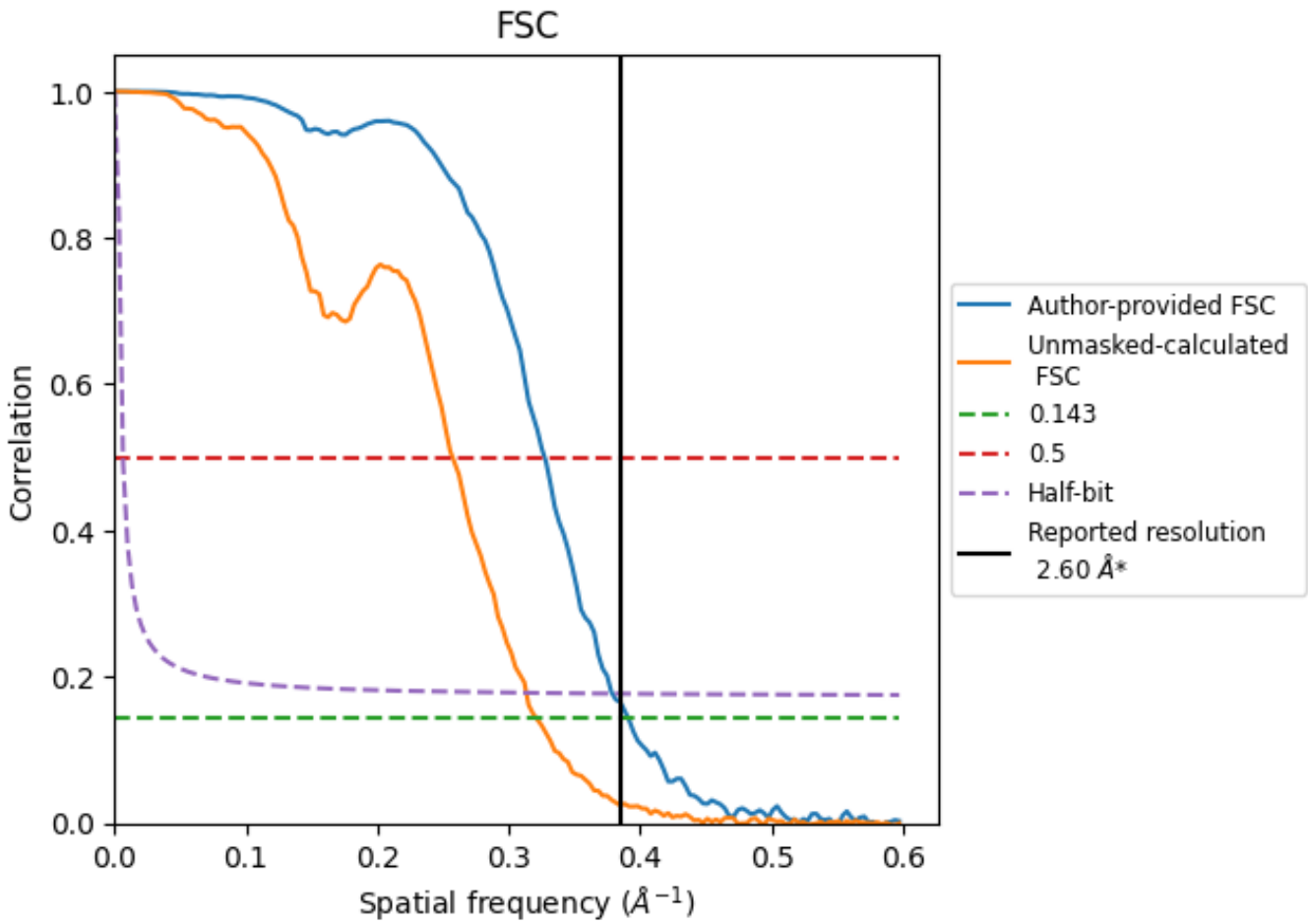


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

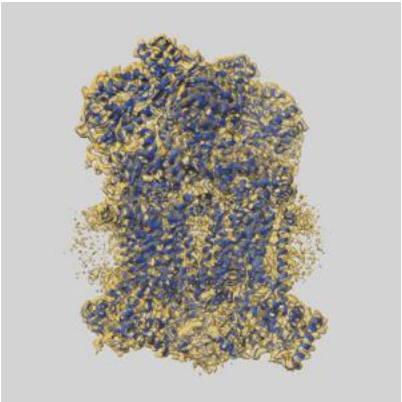
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.56	3.06	2.64
Unmasked-calculated*	3.11	3.89	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.6 by more than 10 %

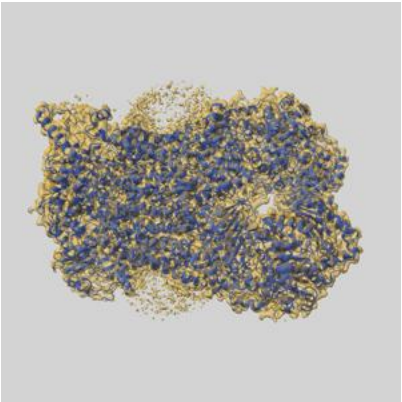
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15314 and PDB model 8AB8. Per-residue inclusion information can be found in section 3 on page 13.

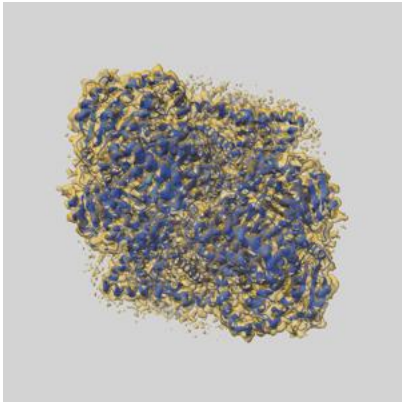
9.1 Map-model overlay (i)



X



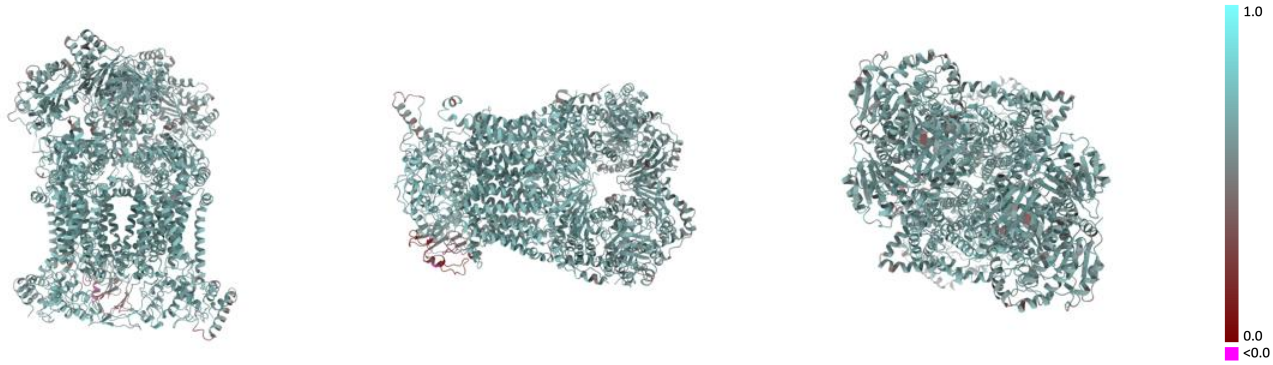
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

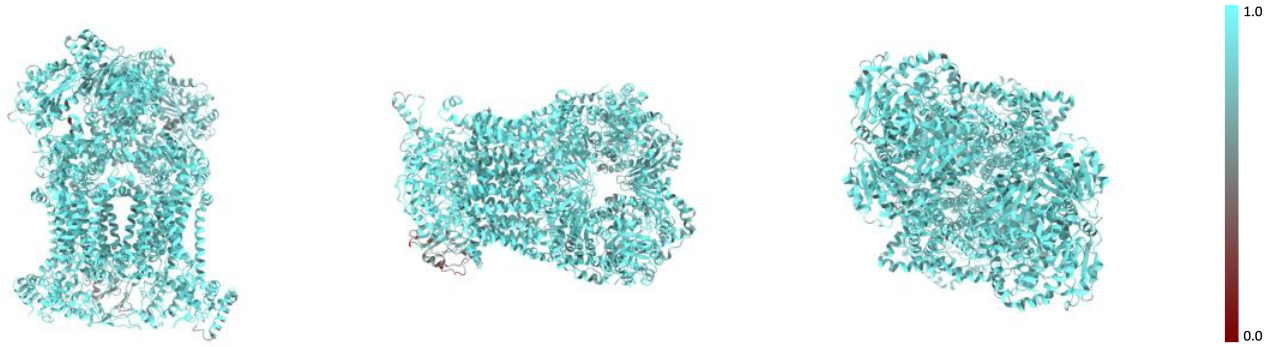
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

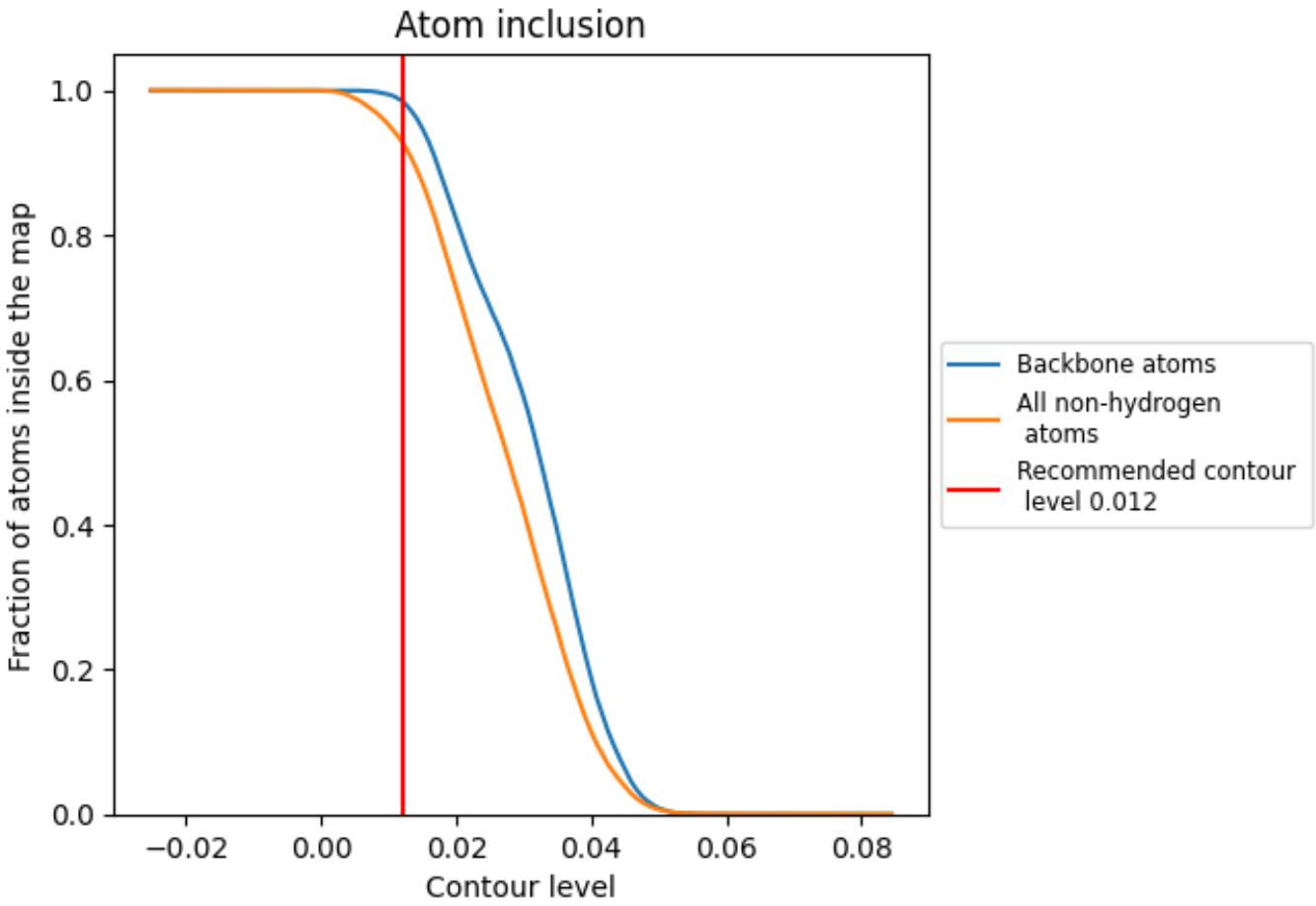
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9290	0.6250
A	0.9234	0.6240
B	0.9225	0.6130
C	0.9700	0.6630
D	0.9572	0.6520
E	0.9568	0.6500
F	0.8394	0.5630
G	0.9334	0.6420
H	0.9541	0.6430
I	0.9705	0.6570
J	0.9051	0.6110
L	0.9203	0.6240
M	0.9178	0.6110
N	0.9781	0.6660
O	0.9572	0.6500
P	0.7422	0.4330
Q	0.8464	0.5590
R	0.9385	0.6460
S	0.9567	0.6420
T	0.9662	0.6500
U	0.9114	0.6230