wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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:

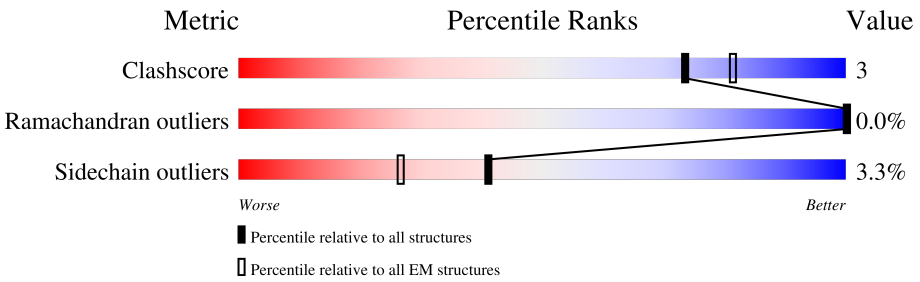
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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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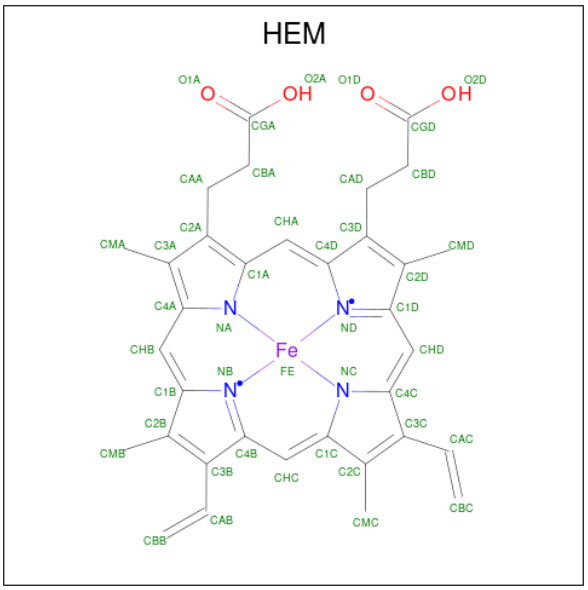
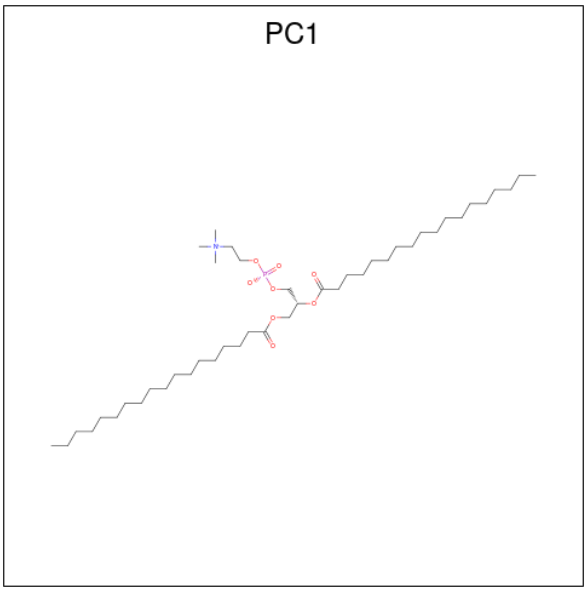
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	75	598	403	99	96	0	0

- 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).



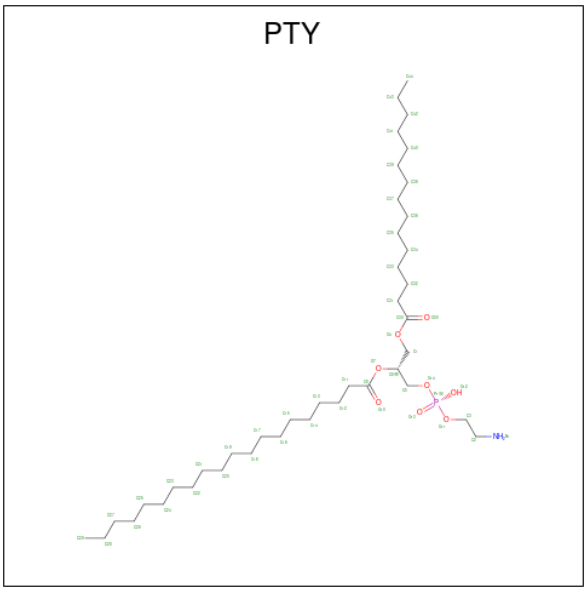
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
11	C	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	C	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	N	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
11	N	1	86	68	2	8	8	0

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



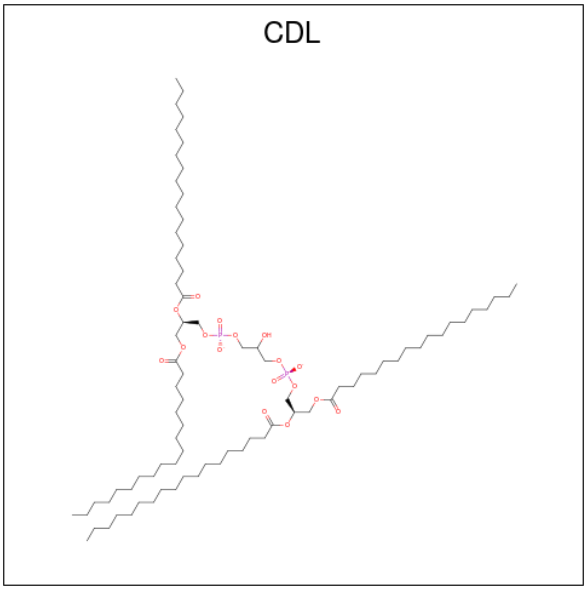
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	I	1	32	22	1	8	1	0
			Total	C	N	O	P	
12	N	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	T	1	32	22	1	8	1	0

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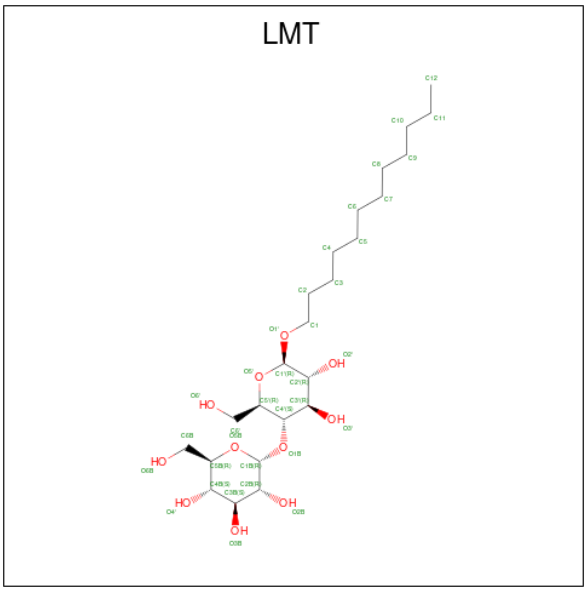
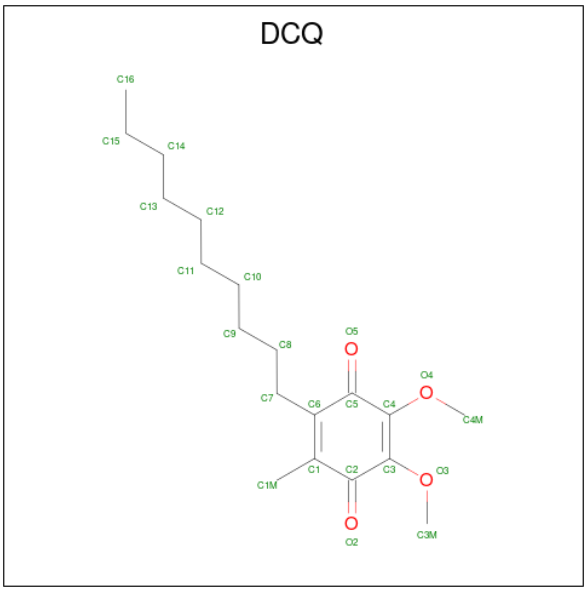
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	S	1	89	51	34	4	0
			Total	C	O	P	
14	S	1	89	51	34	4	0

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



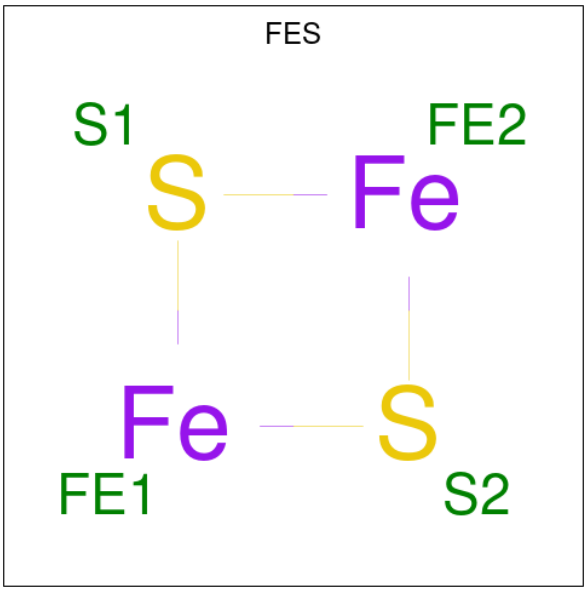
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	C	1	35	24	11	0
			Total	C	O	
15	P	1	35	24	11	0
			Total	C	O	
15	J	1	35	24	11	0
			Total	C	O	
15	N	1	35	24	11	0

- 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).



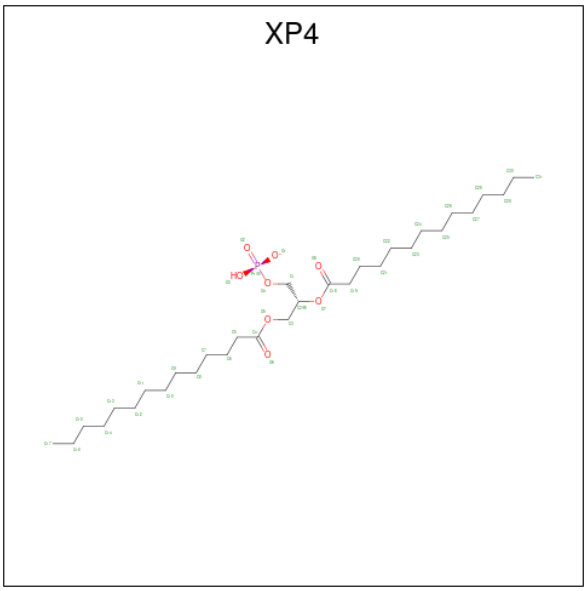
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	C	1	23	19	4	0

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



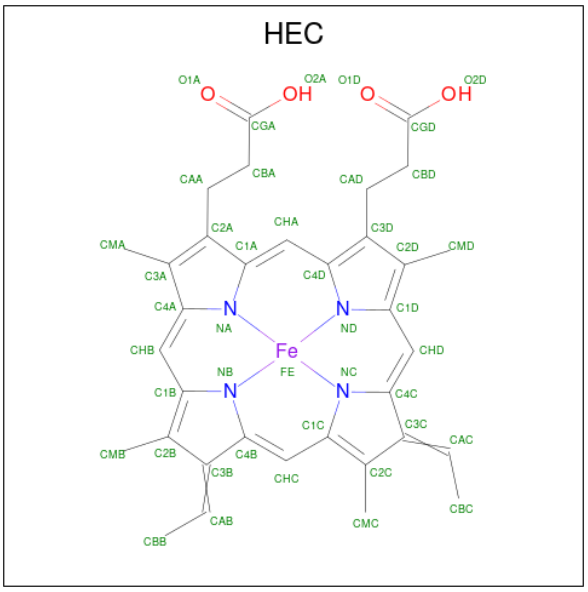
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	P	1	4	2	2	0

- 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 24	C 15	O 8	P 1	0
18	L	1	Total 24	C 15	O 8	P 1	0

- 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 43	C 34	Fe 1	N 4	O 4	0

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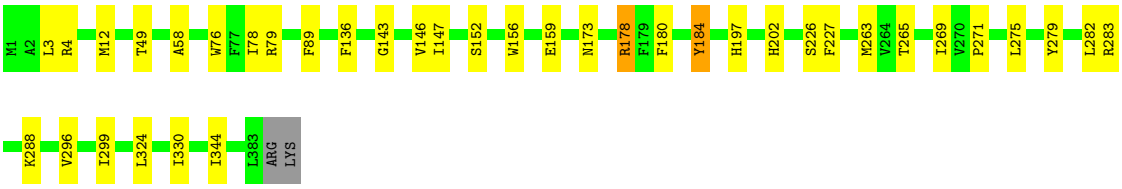
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
19	O	1	43	34	1	4	4	0

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:

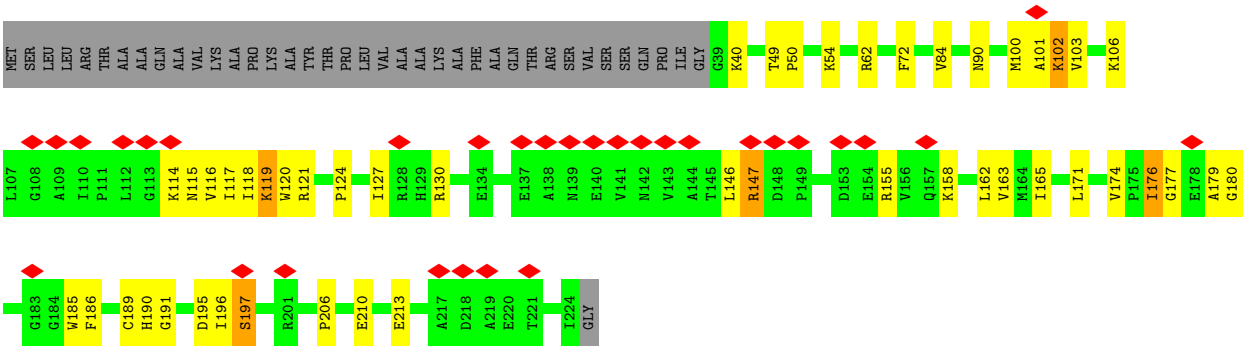


• Molecule 1: Cytochrome b

Chain N:

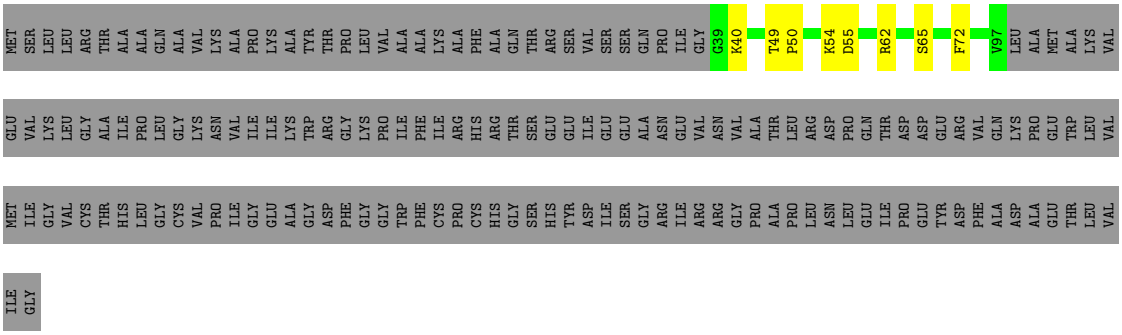
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



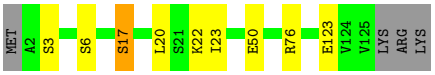
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



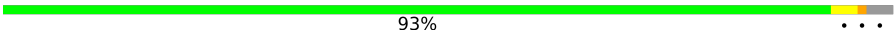
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain G:



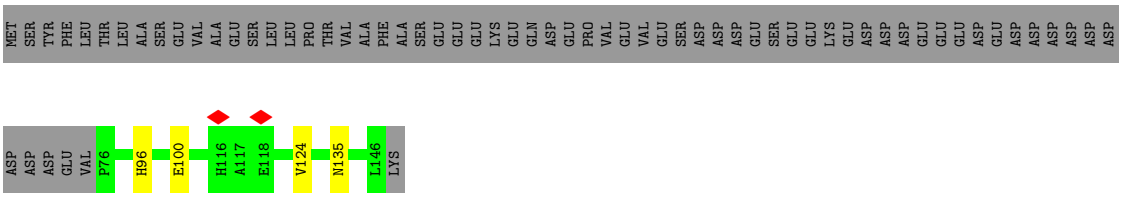
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:



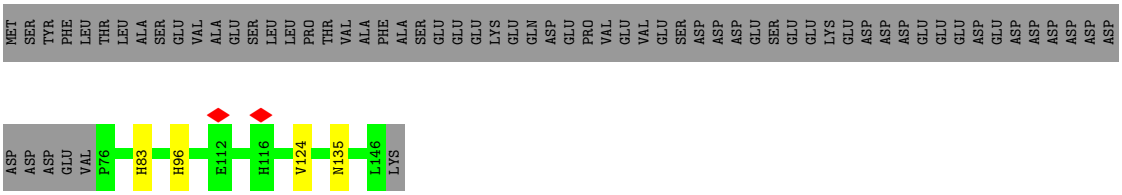
• Molecule 4: YALI0F24673p

Chain F:



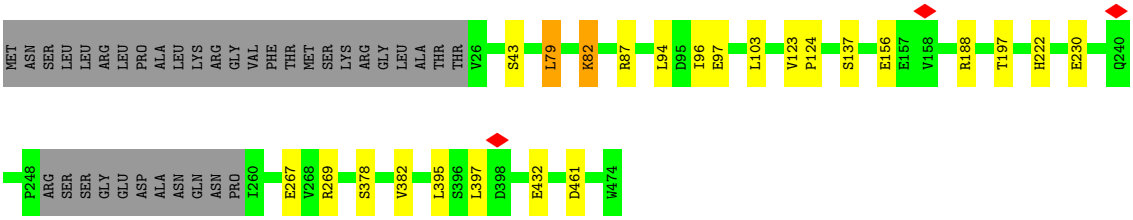
• Molecule 4: YALI0F24673p

Chain Q:



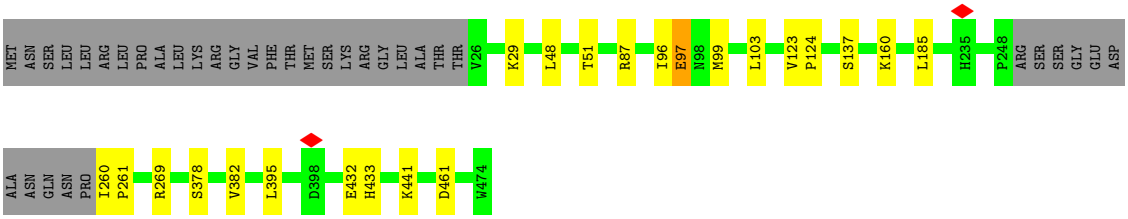
• Molecule 5: YALI0A14806p

Chain A:



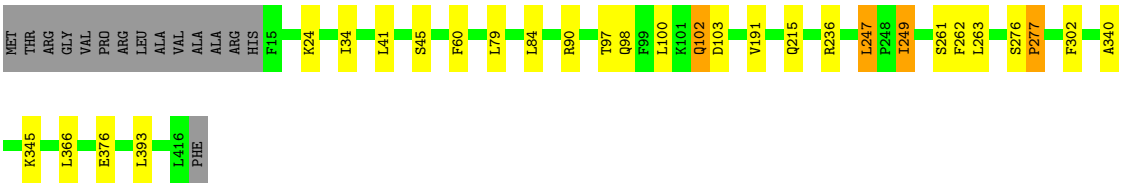
- Molecule 5: YALI0A14806p

Chain L:



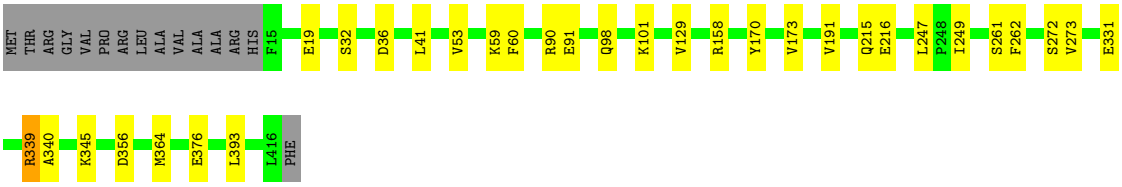
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



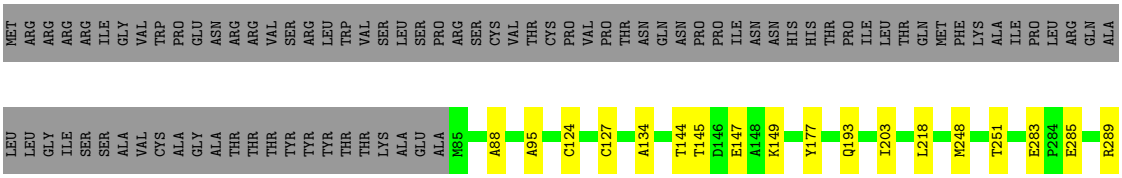
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

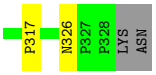
Chain M:



- Molecule 7: YALI0A17468p

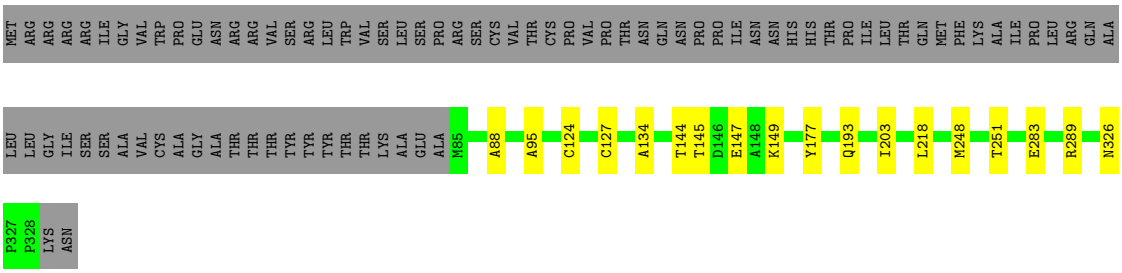
Chain D:





• 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

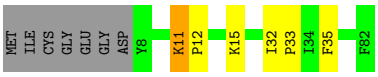
Chain I:

• 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.

The worst 5 of 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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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
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
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

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	376	GLU
1	N	270	VAL
9	T	27	PHE
6	M	261	SER
8	H	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	M	92	HIS
10	U	70	HIS
6	M	215	GLN
6	B	215	GLN
2	E	90	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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

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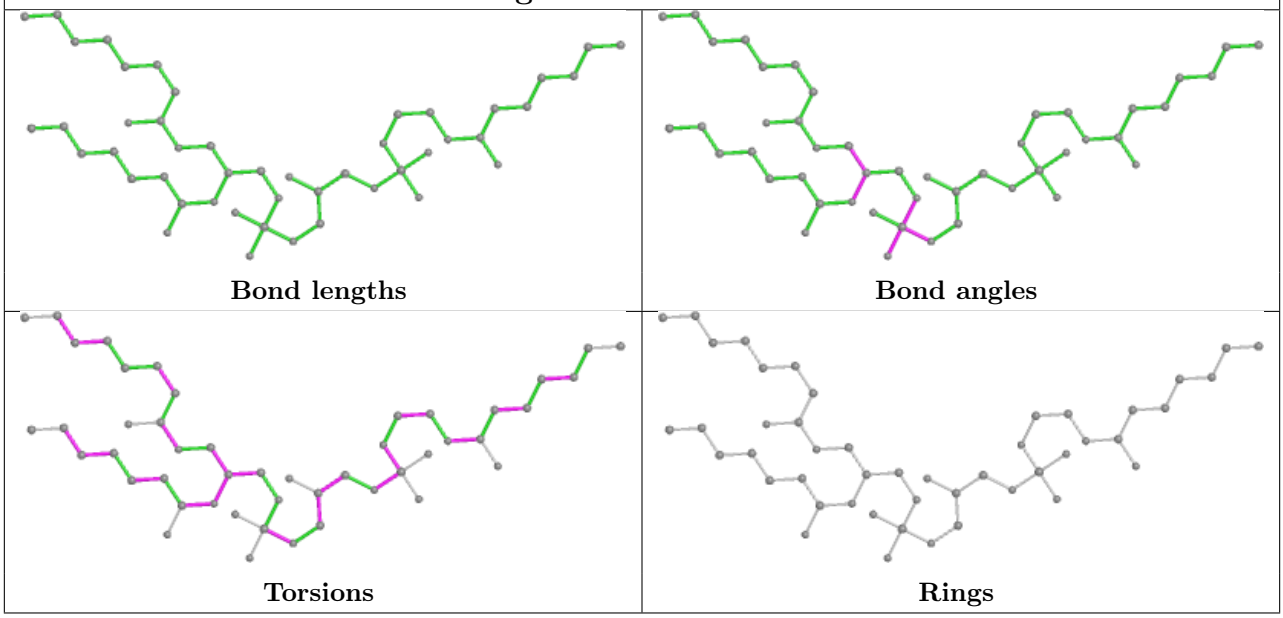
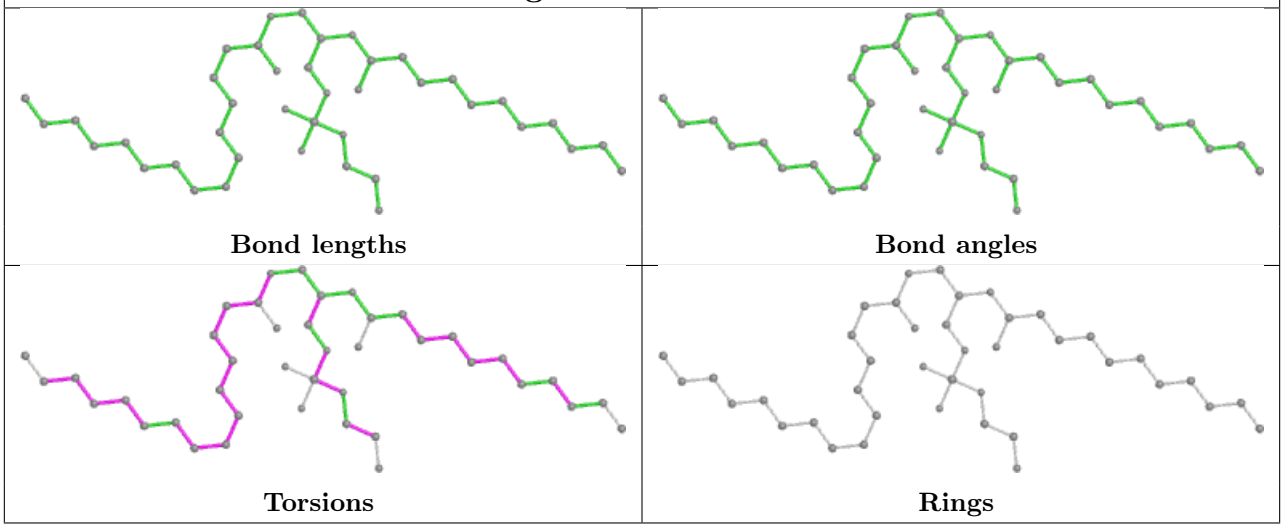
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	702	CDL	4	0
12	I	201	PC1	2	0
12	T	201	PC1	3	0
13	C	504	PTY	5	0
15	P	302	LMT	1	0
18	A	3003	XP4	1	0
14	A	3001	CDL	3	0

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.

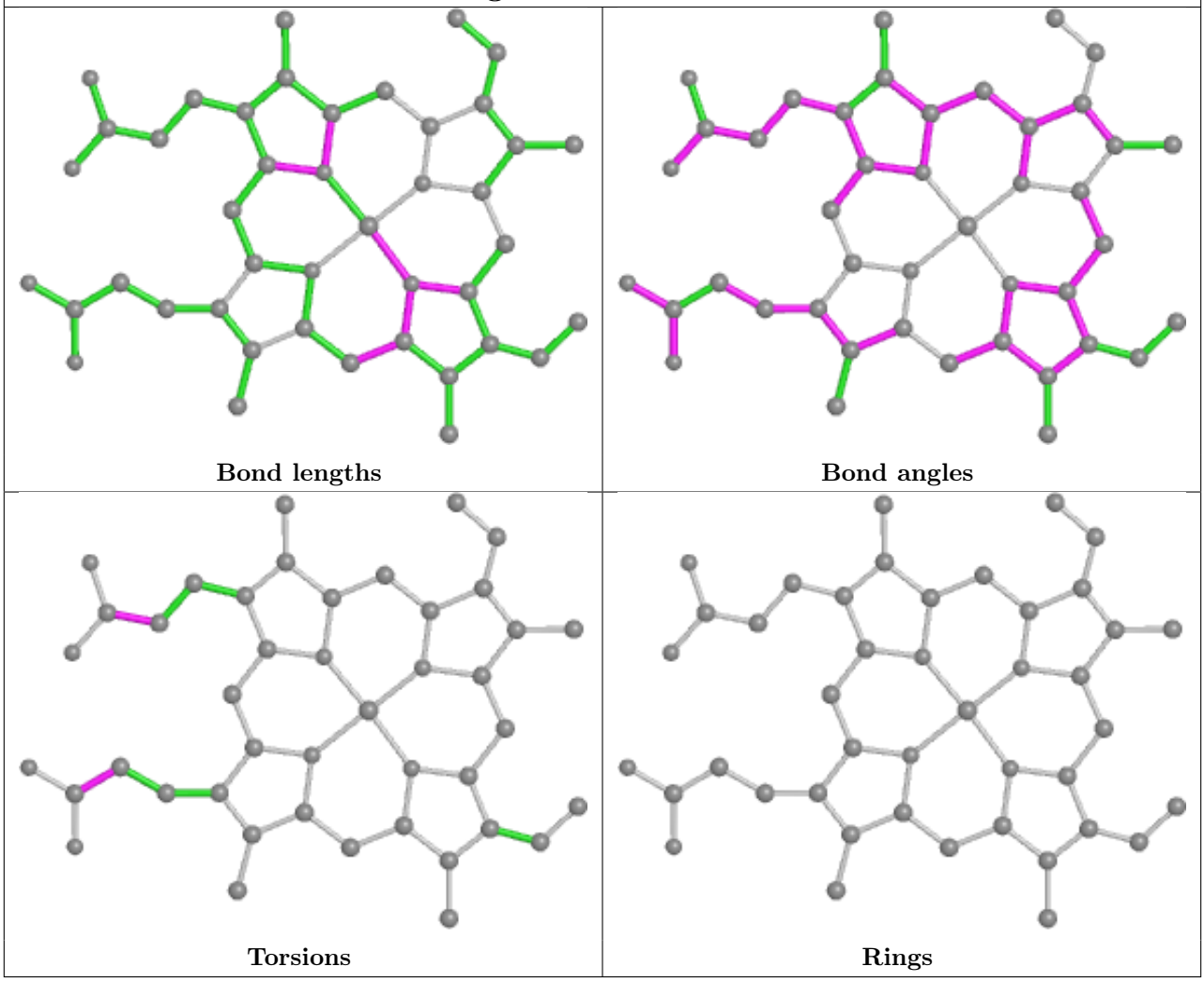
Ligand CDL A 3002

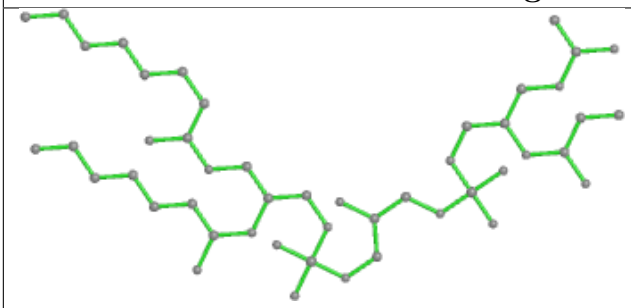
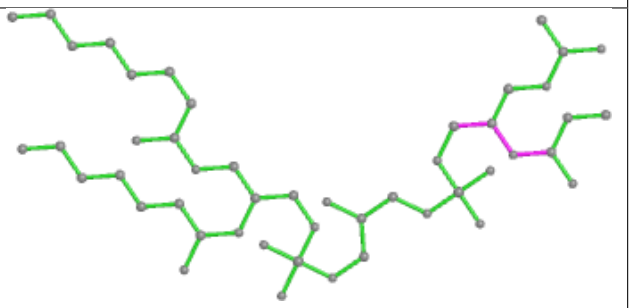
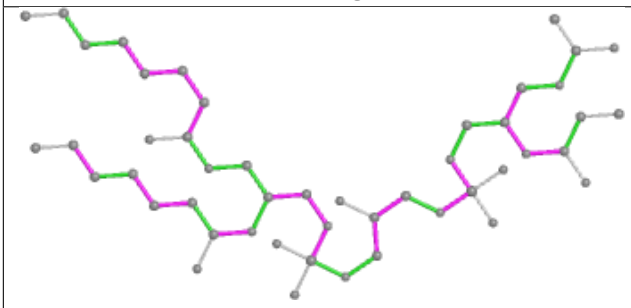
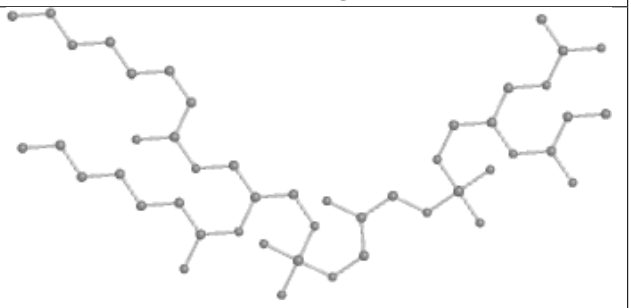


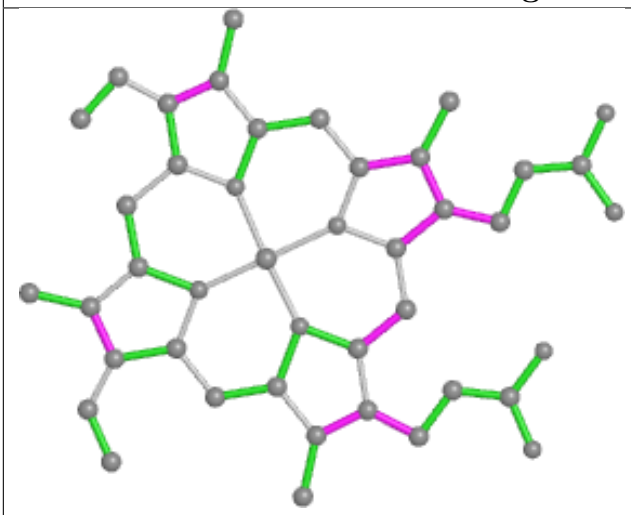
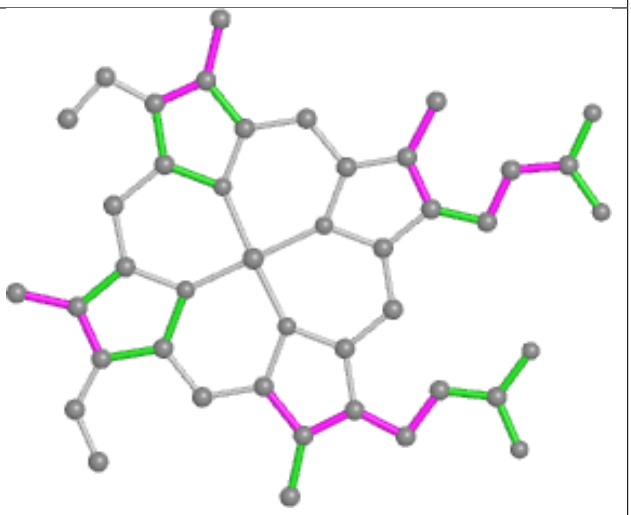
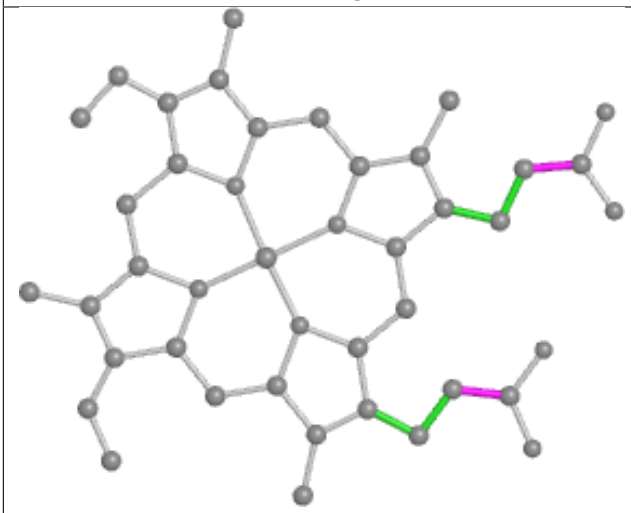
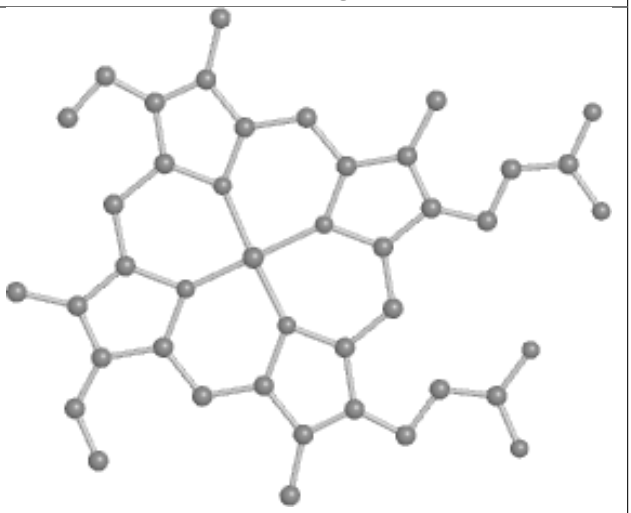
Ligand PTY E 401

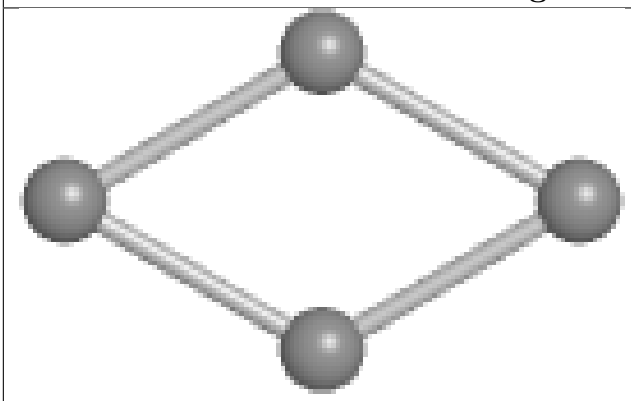
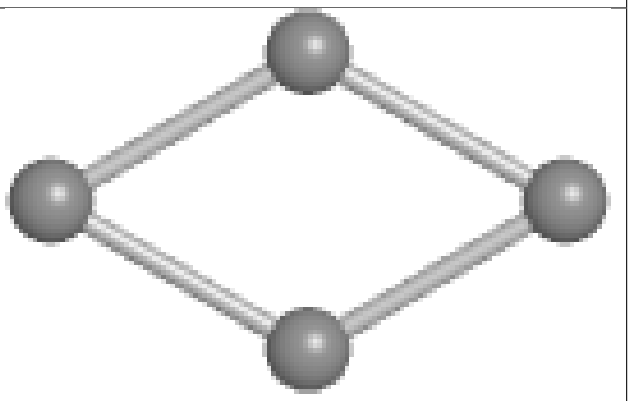
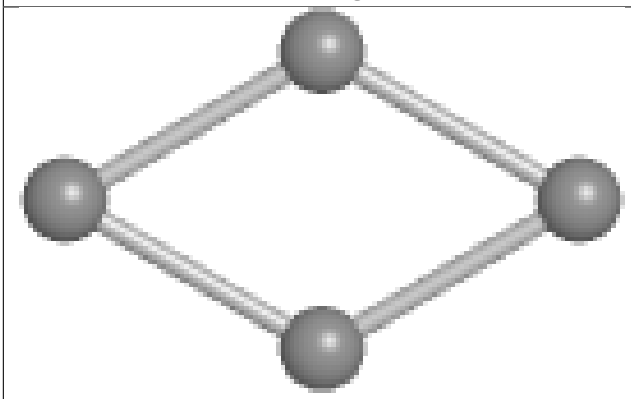
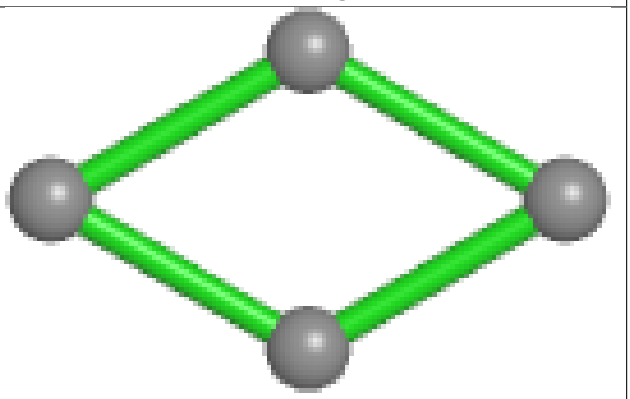


Ligand HEM N 502

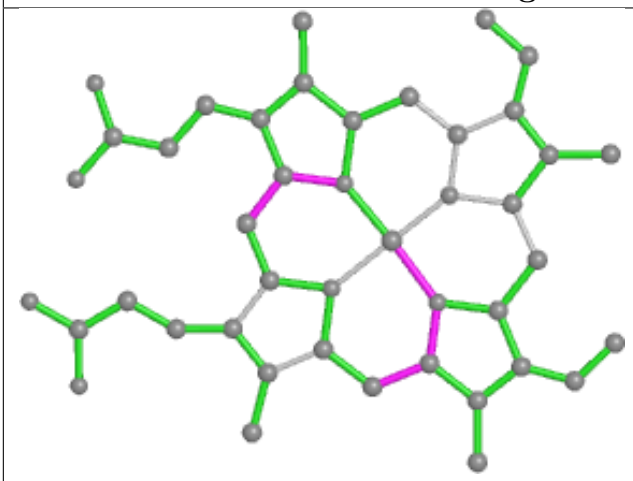


Ligand CDL C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

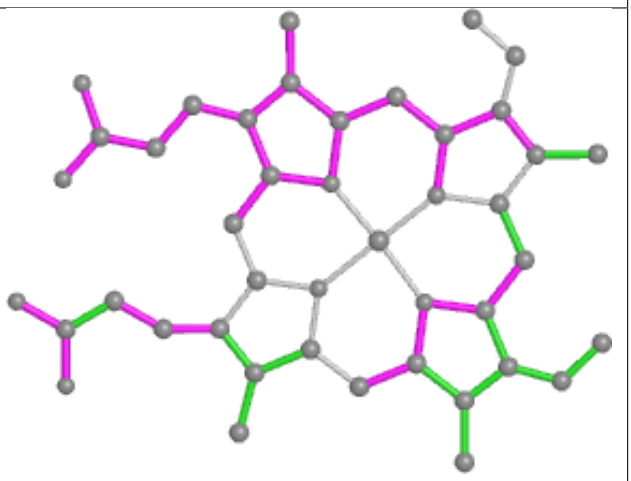
Ligand HEC D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES P 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

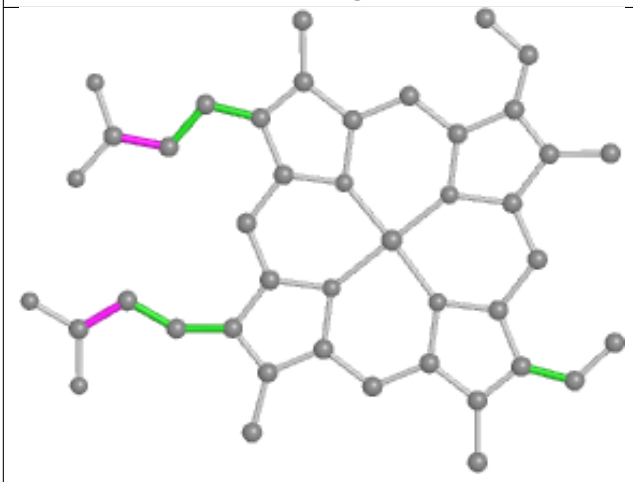
Ligand HEM C 502



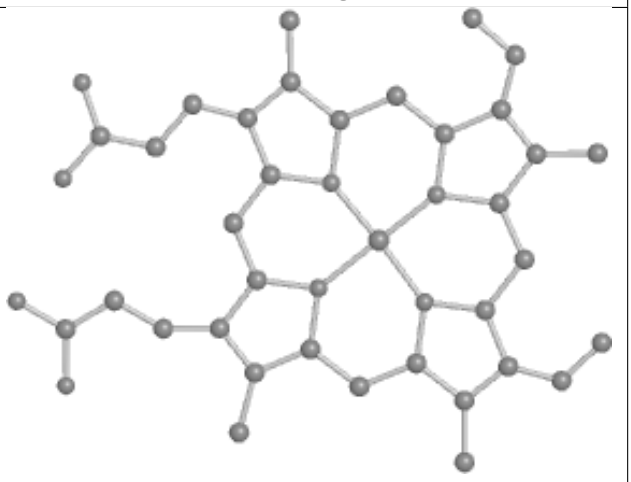
Bond lengths



Bond angles

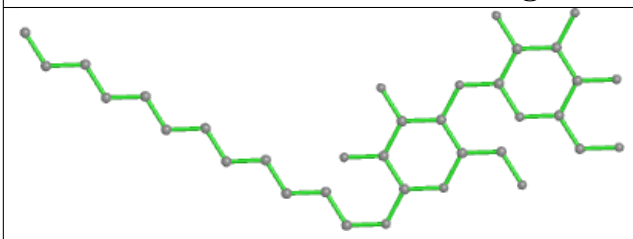


Torsions

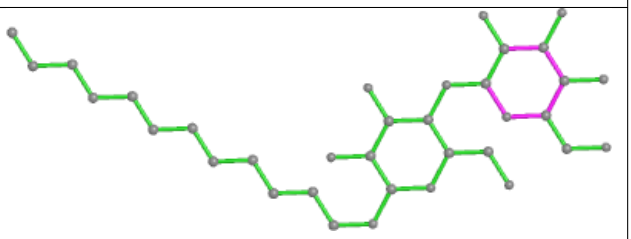


Rings

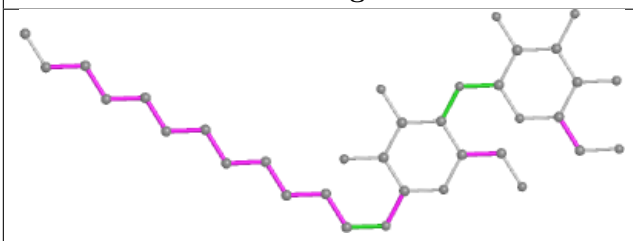
Ligand LMT C 506



Bond lengths



Bond angles



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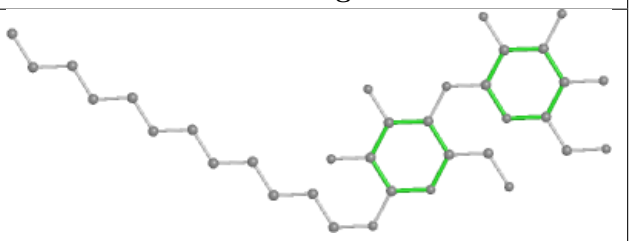
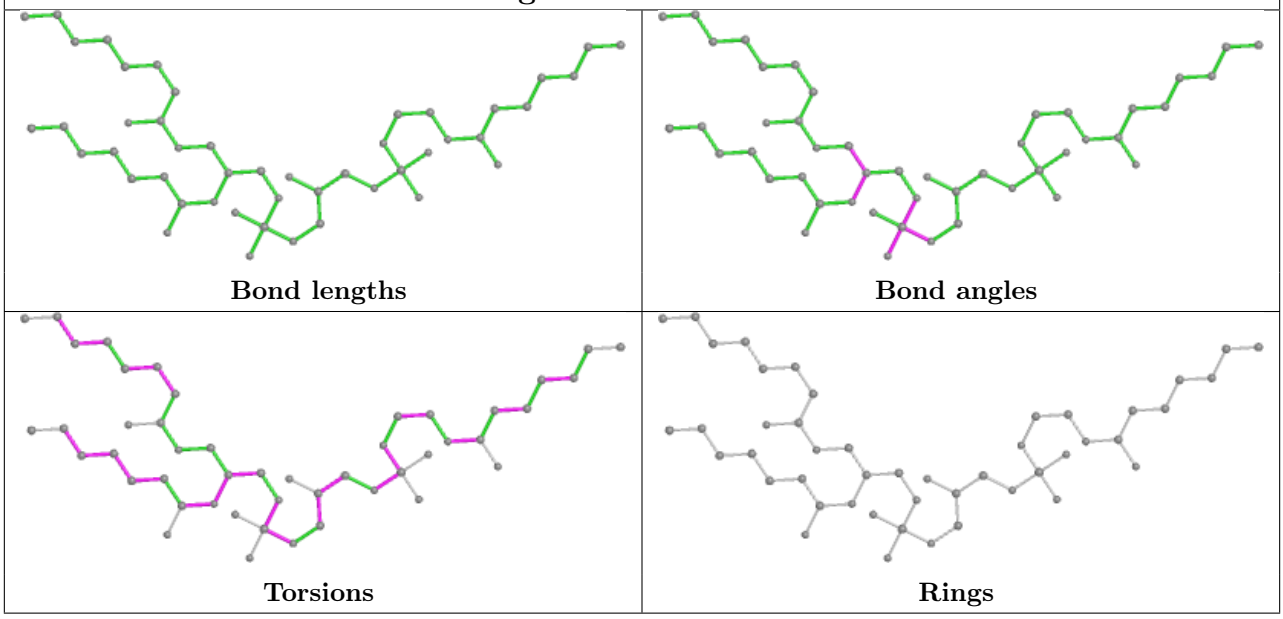
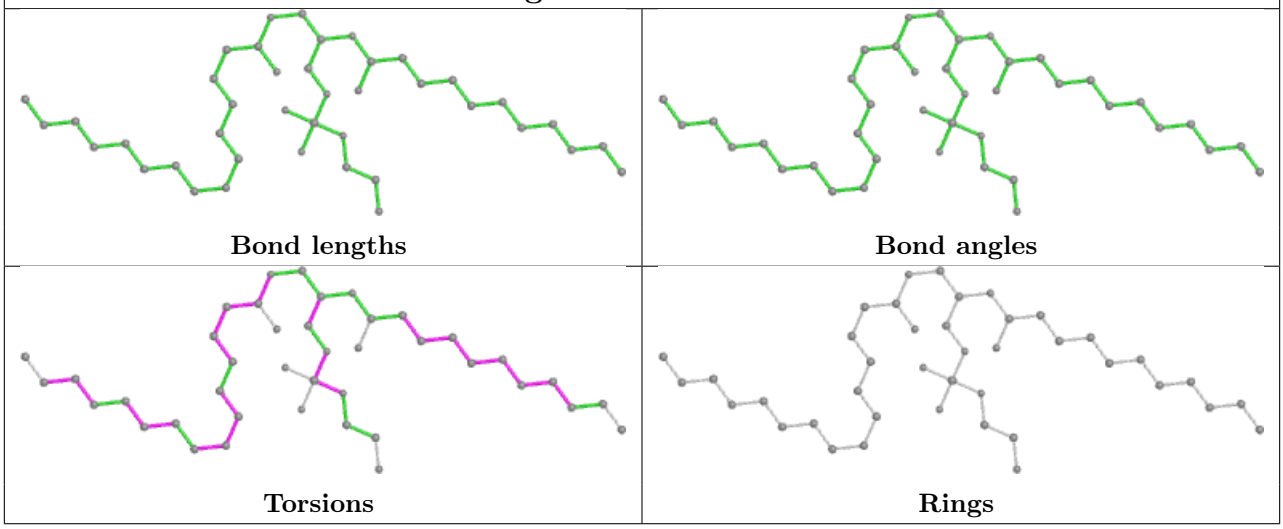


Rings

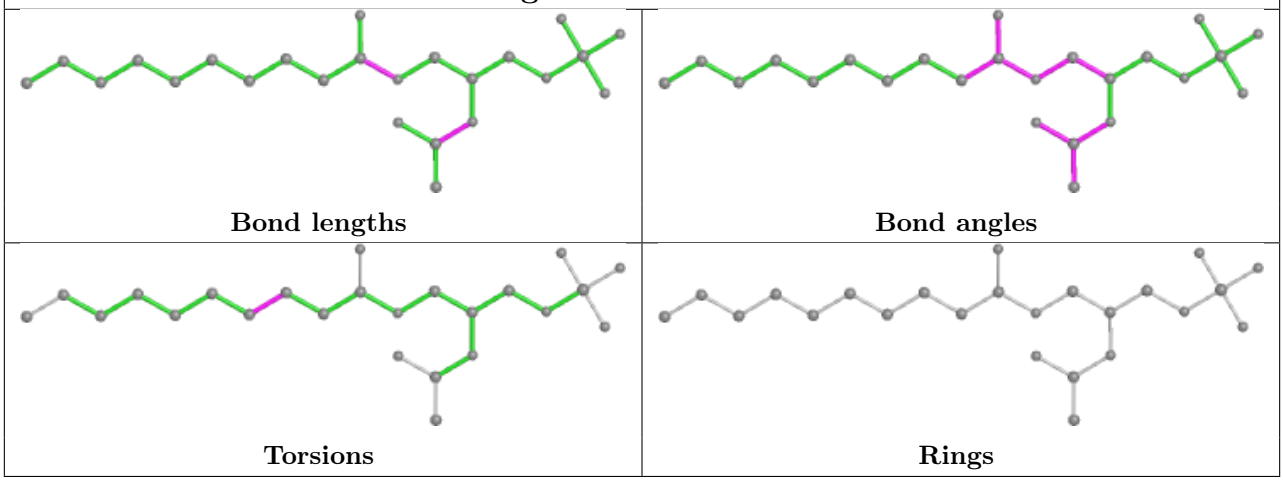
Ligand CDL L 3002

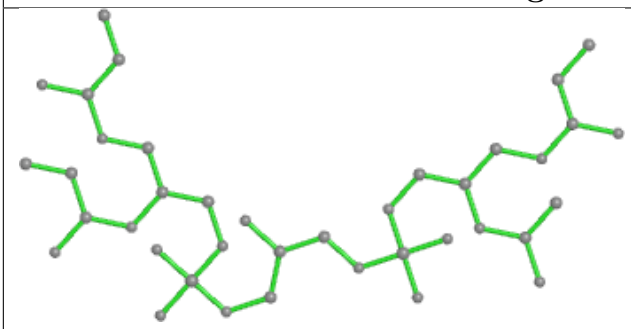
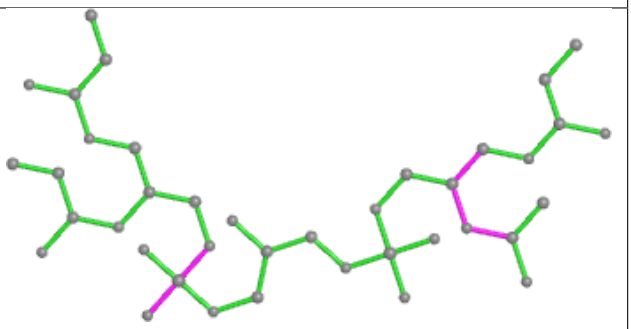
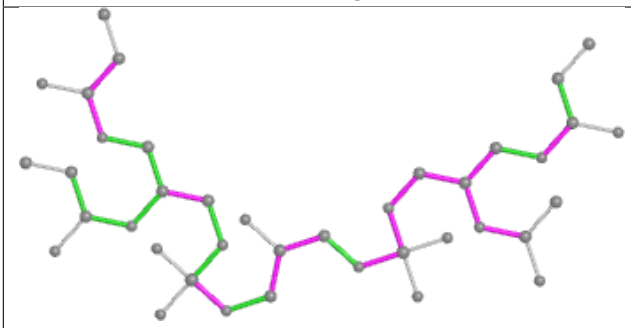
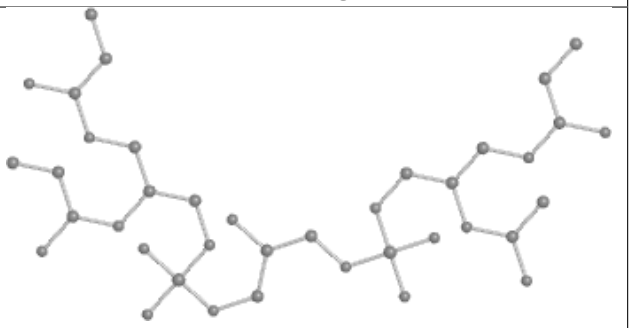


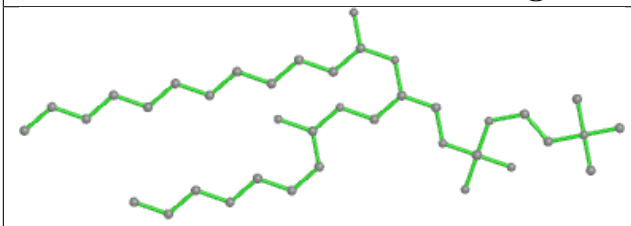
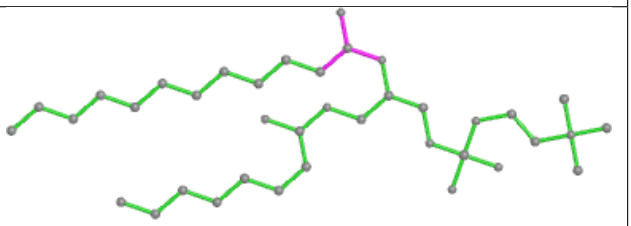
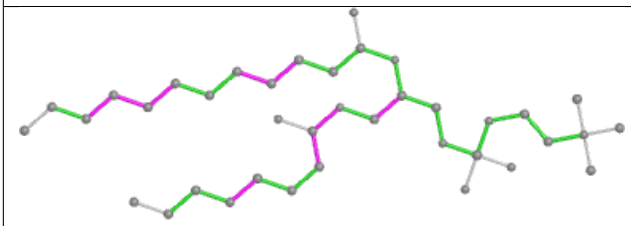
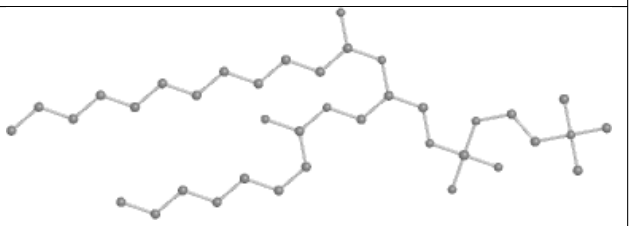
Ligand PTY P 303



Ligand XP4 L 3003



Ligand CDL S 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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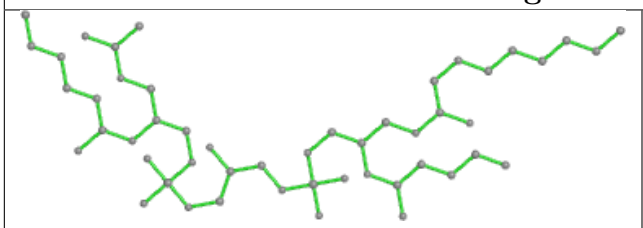
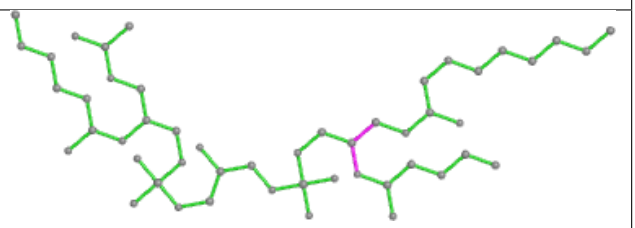
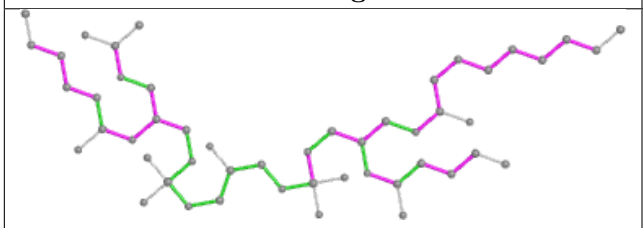
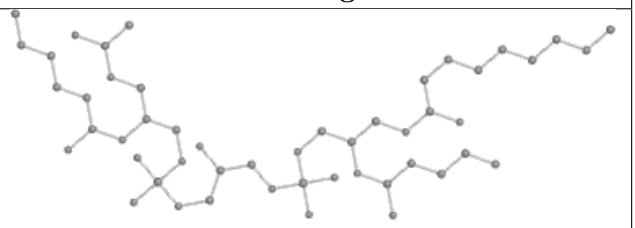
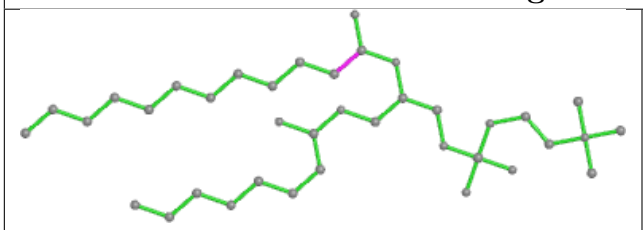
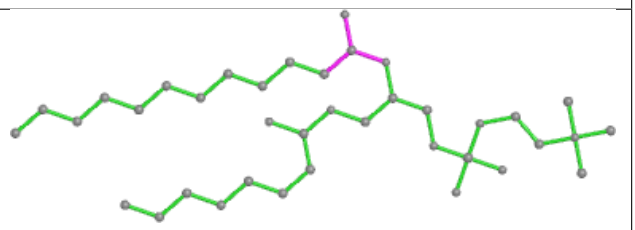
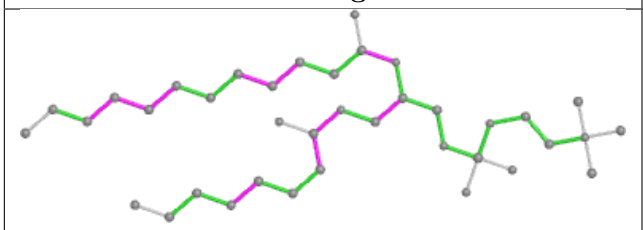
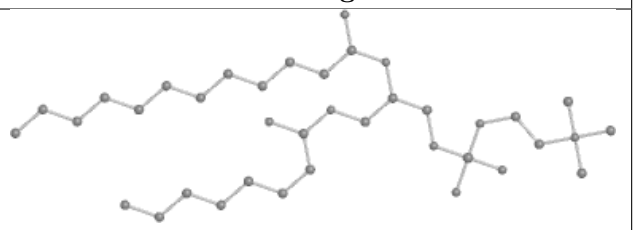
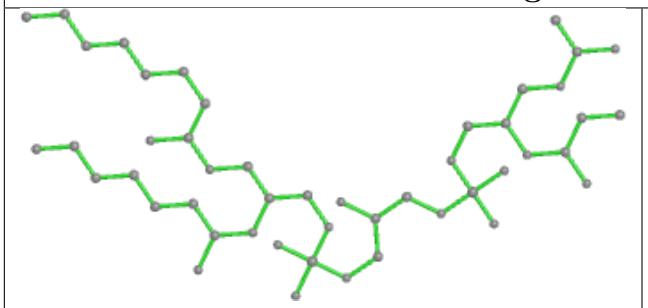
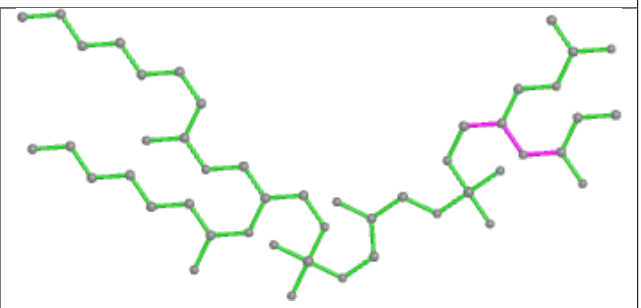
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 N 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

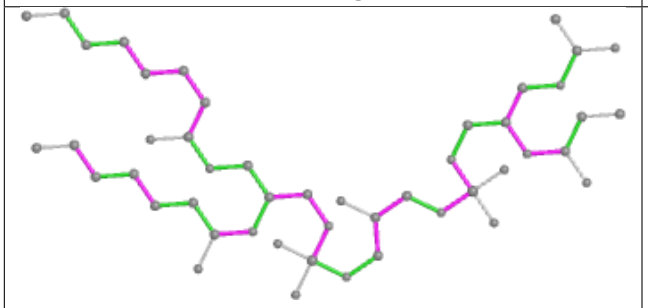
Ligand CDL N 505



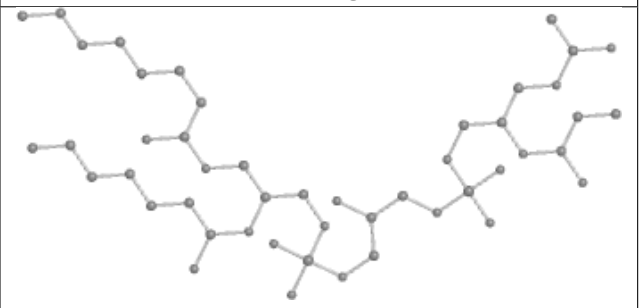
Bond lengths



Bond angles

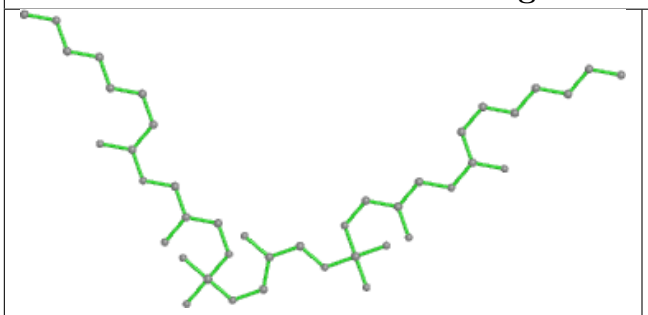


Torsions



Rings

Ligand CDL L 3001



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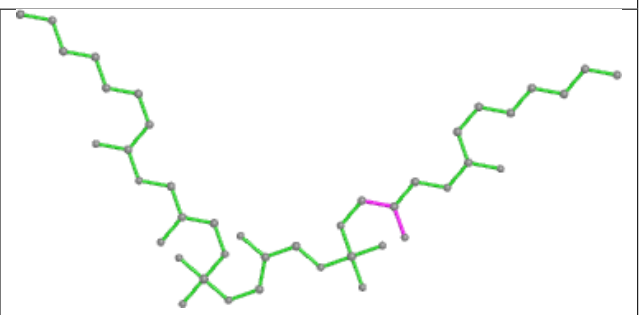
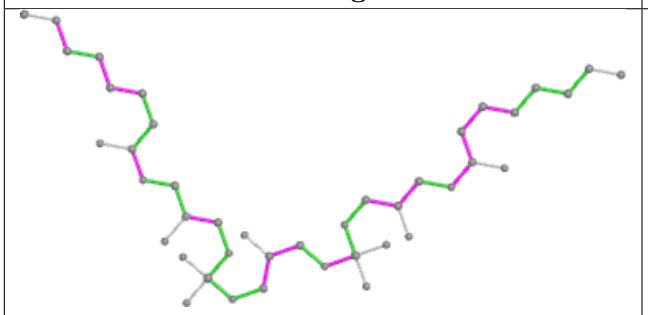


Bond angles



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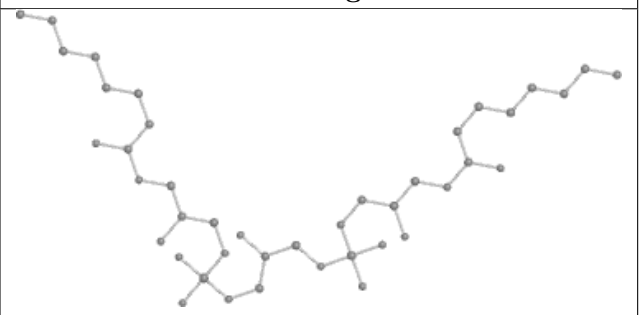
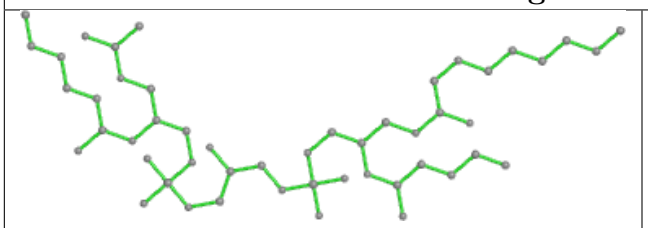


Rings

Ligand CDL S 701



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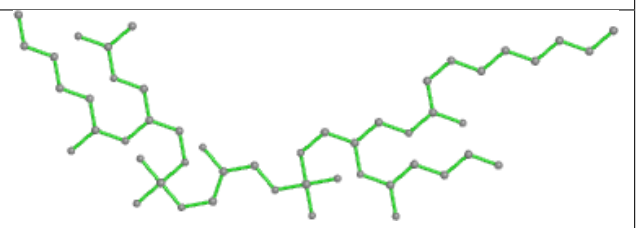
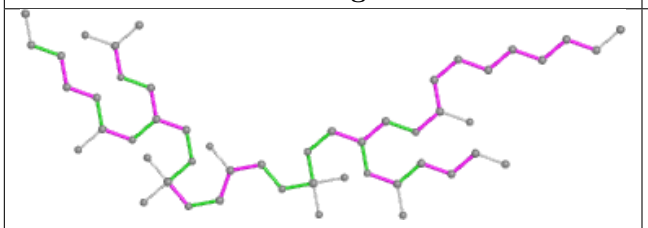


Bond angles



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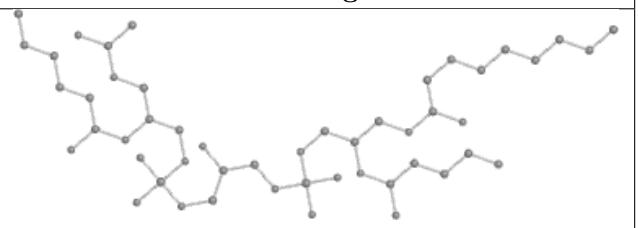
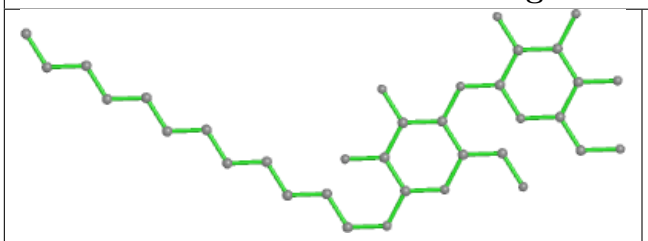
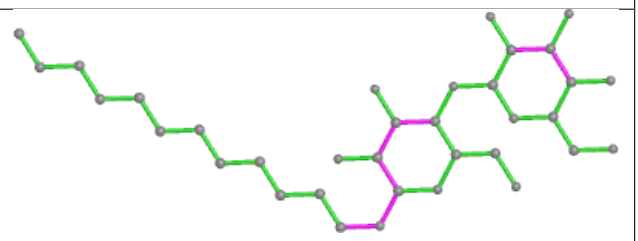


Rings

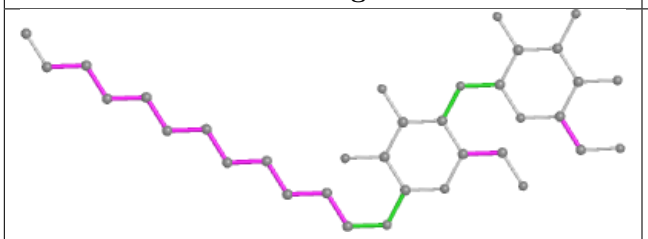
Ligand LMT J 101



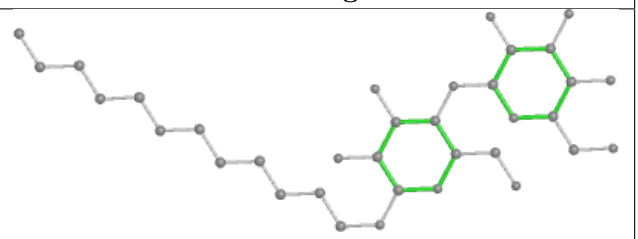
Bond lengths



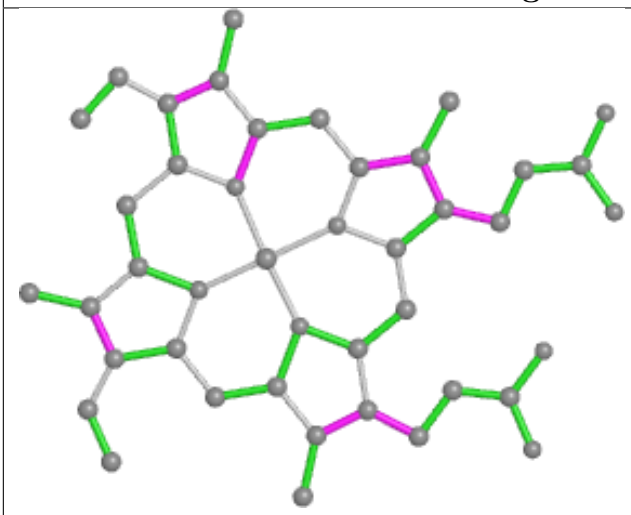
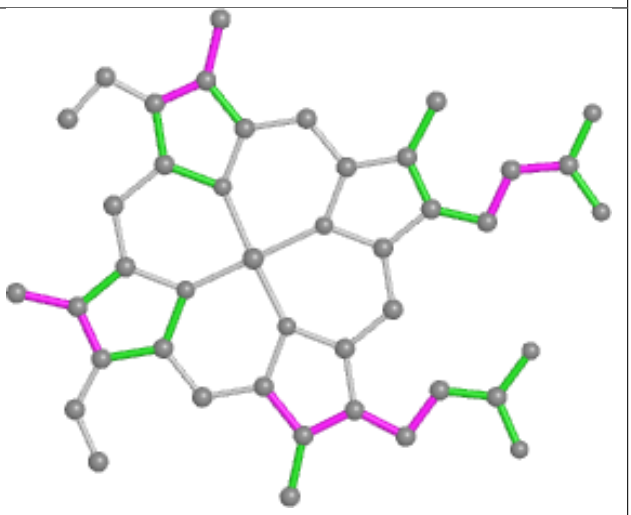
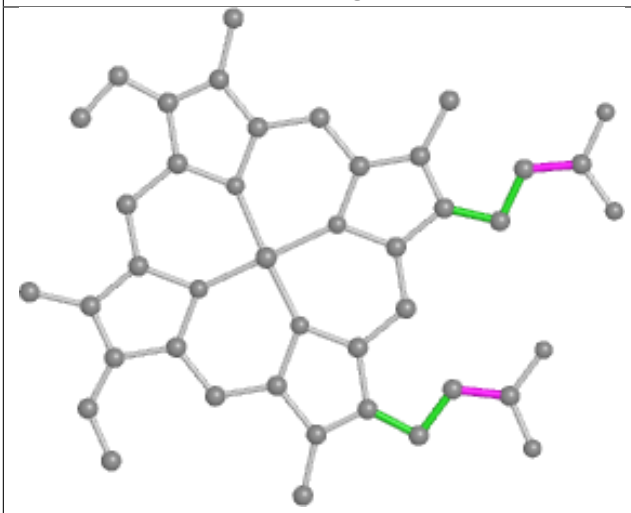
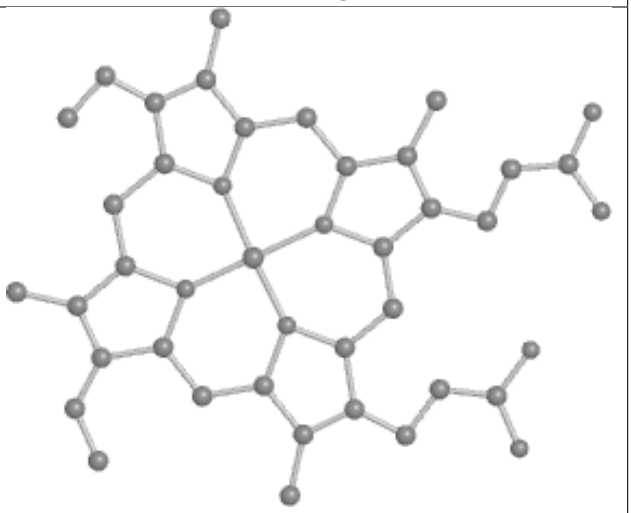
Bond angles



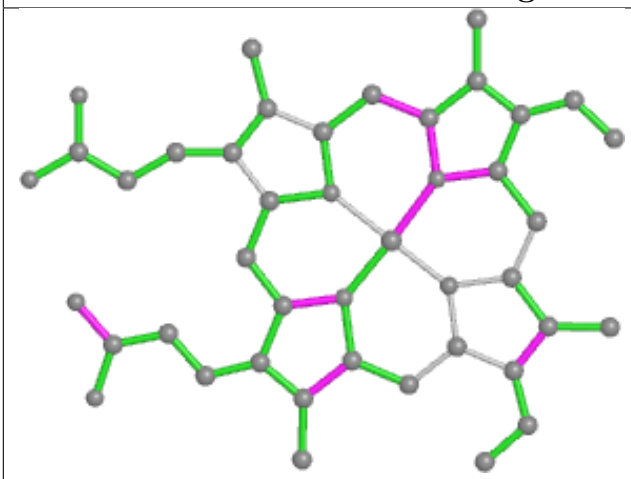
Torsions



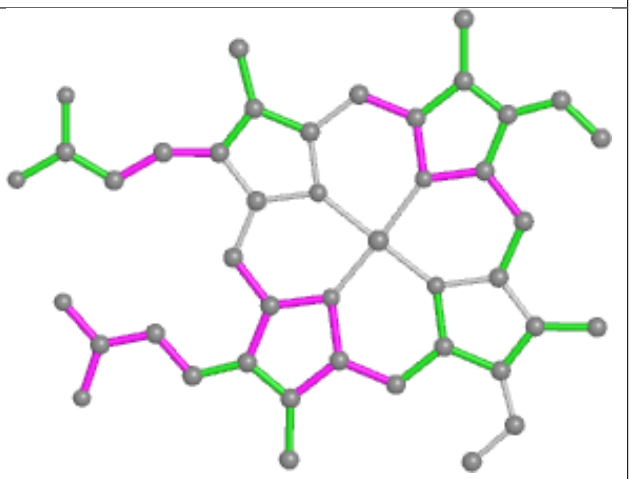
Rings

Ligand HEC O 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

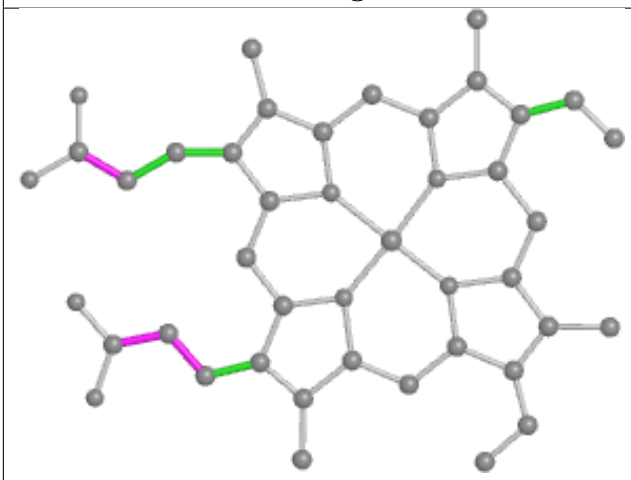
Ligand HEM N 501



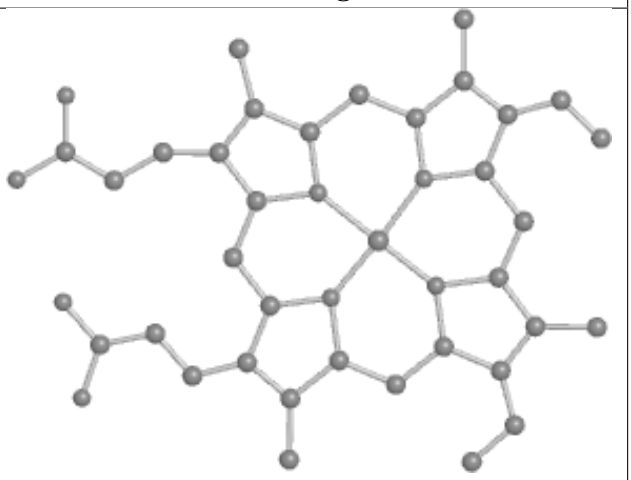
Bond lengths



Bond angles

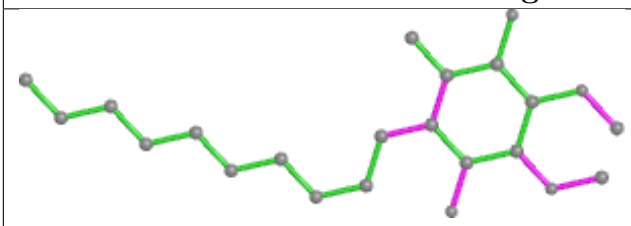


Torsions

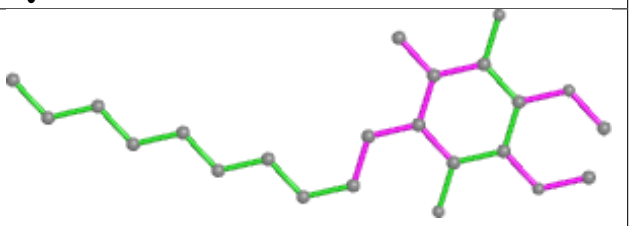


Rings

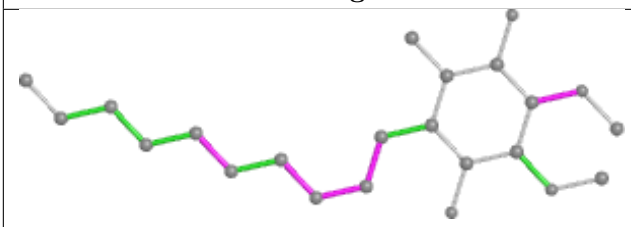
Ligand DCQ C 507



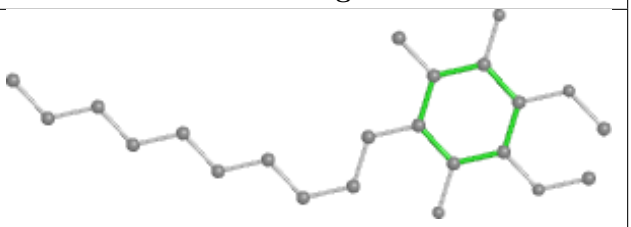
Bond lengths



Bond angles

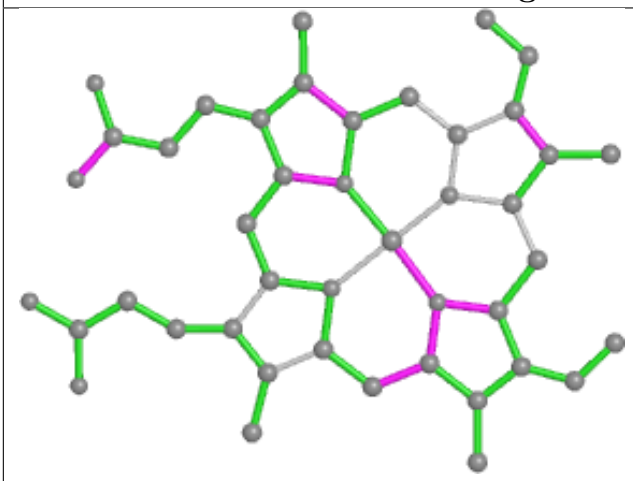


Torsions

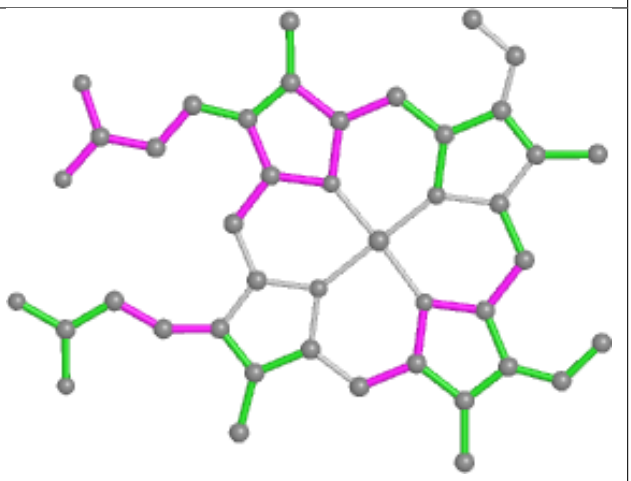


Rings

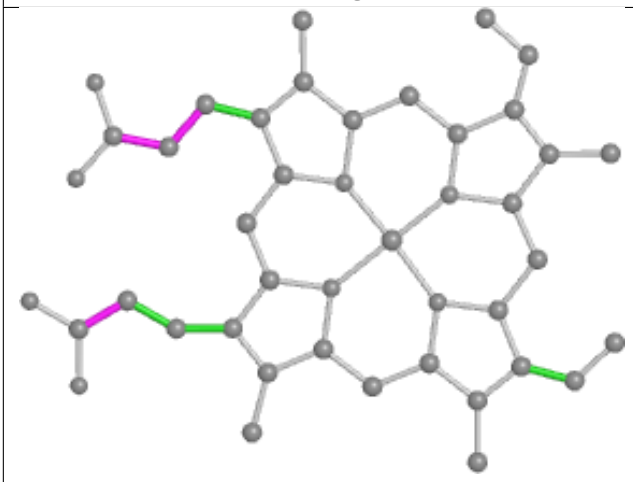
Ligand HEM C 501



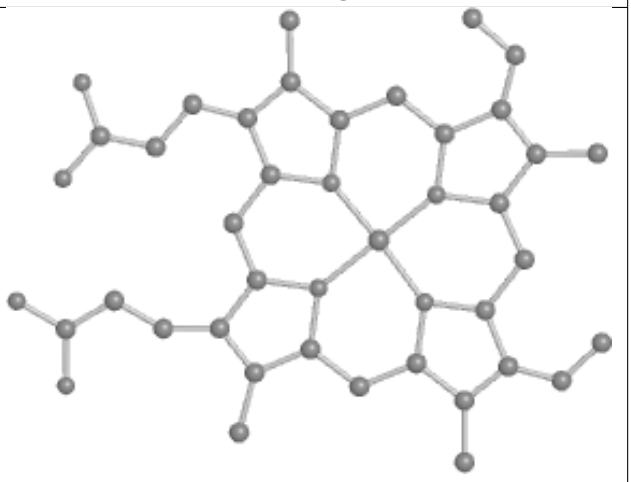
Bond lengths



Bond angles

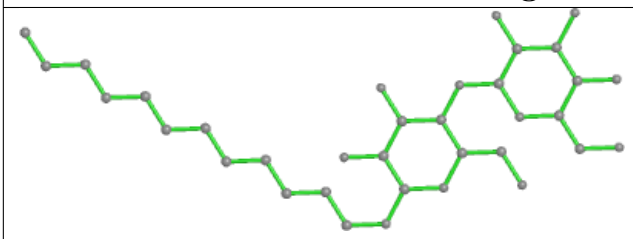


Torsions

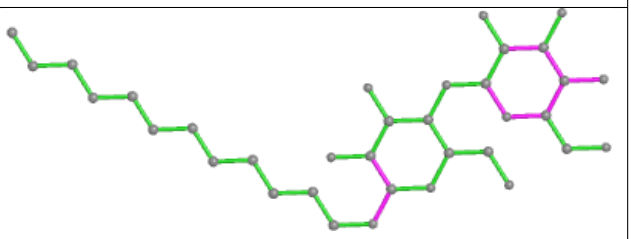


Rings

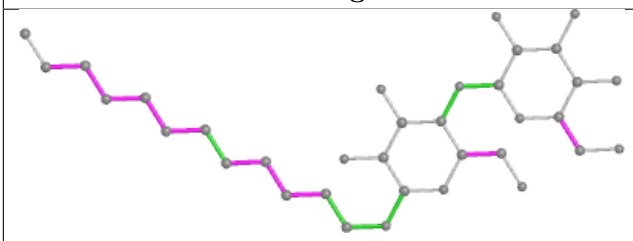
Ligand LMT N 506



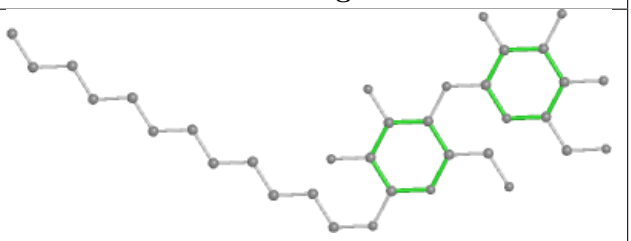
Bond lengths



Bond angles

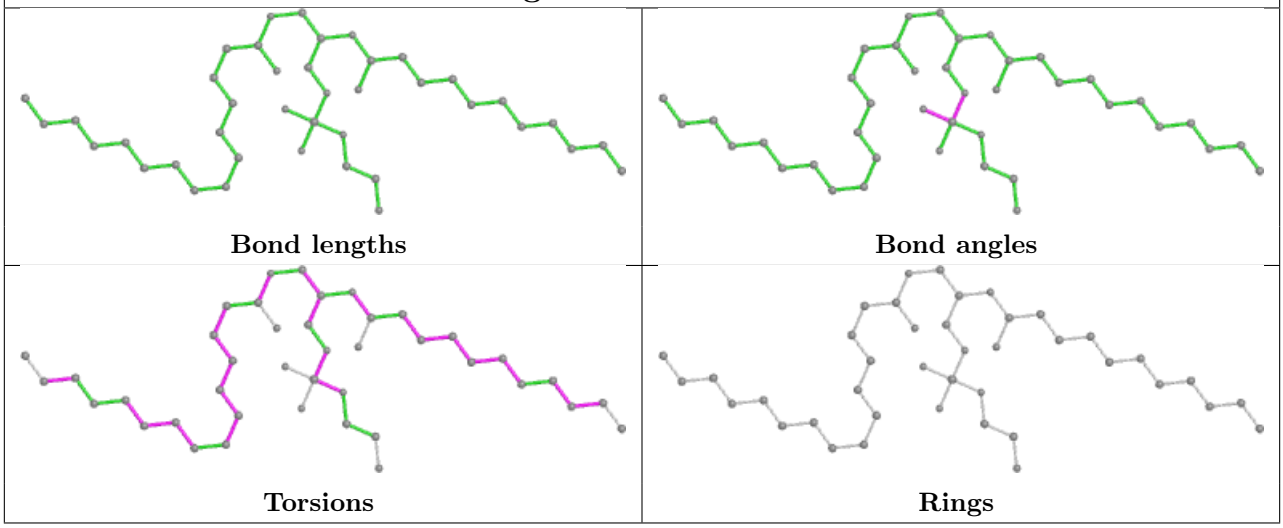


Torsions

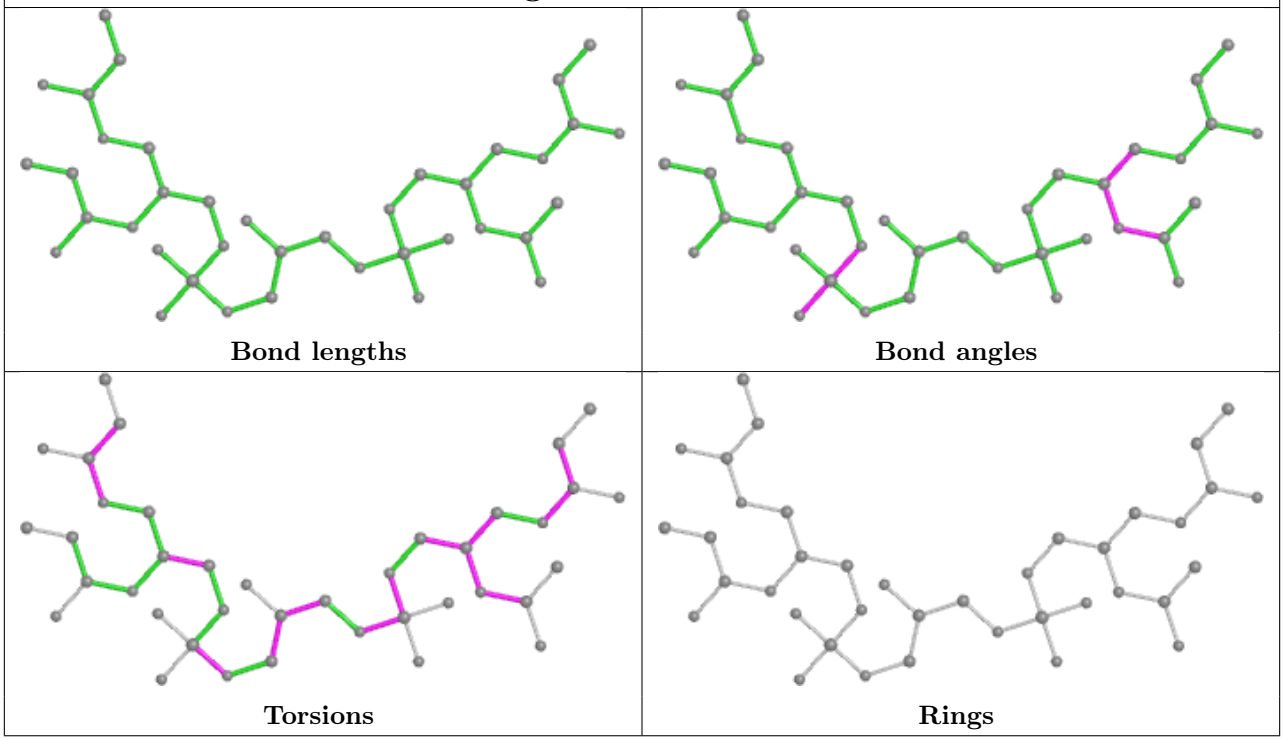


Rings

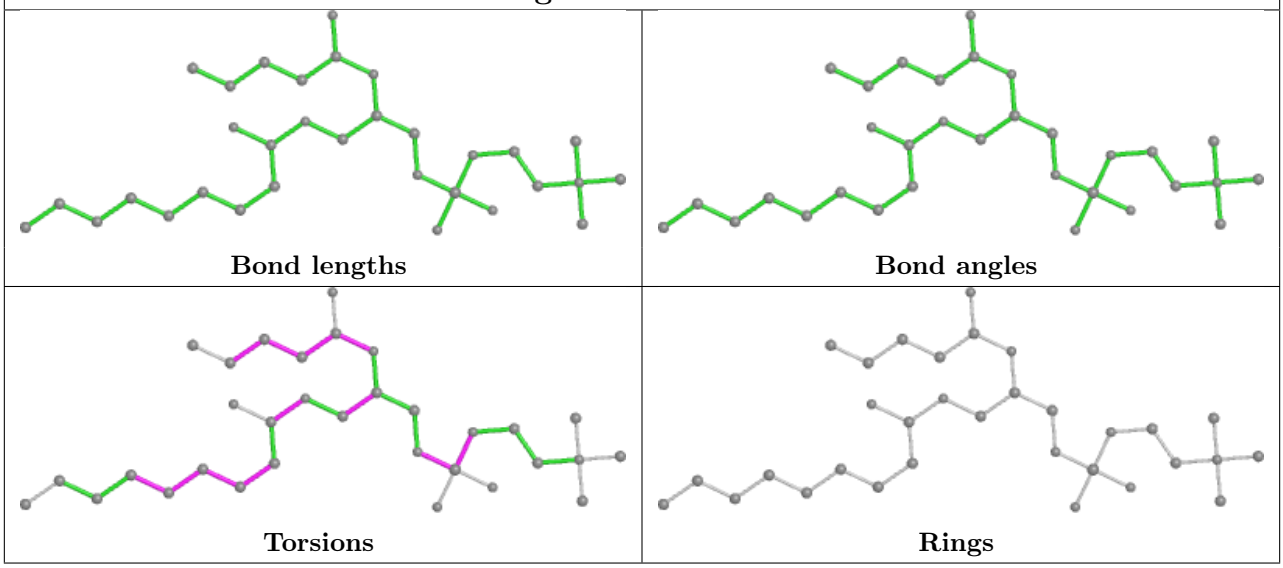
Ligand PTY N 504



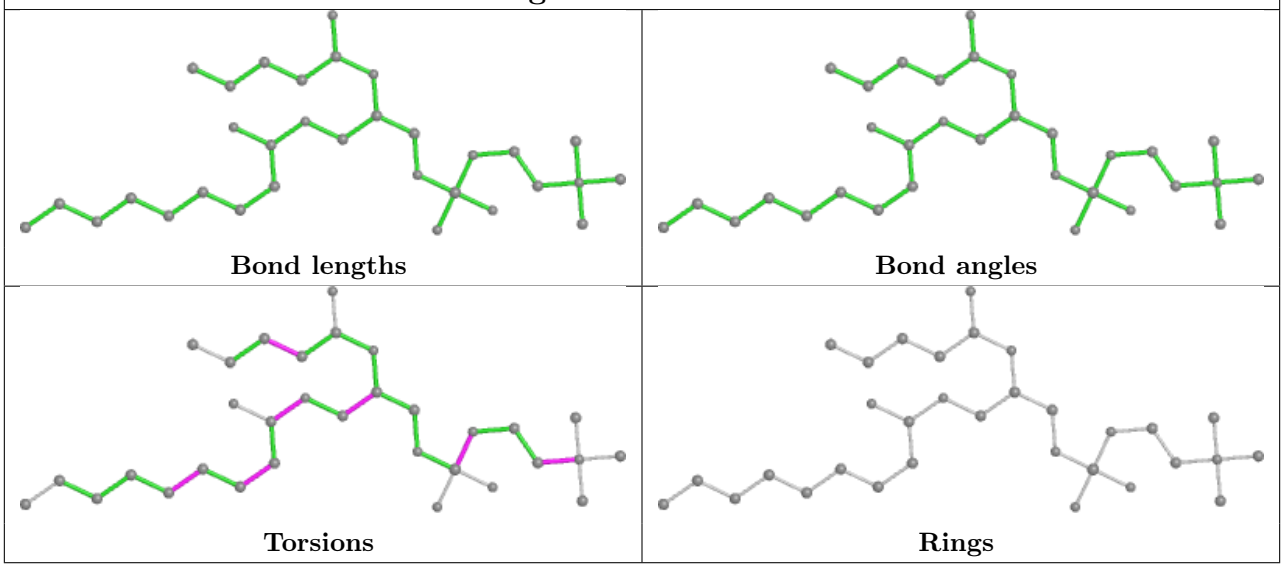
Ligand CDL H 702



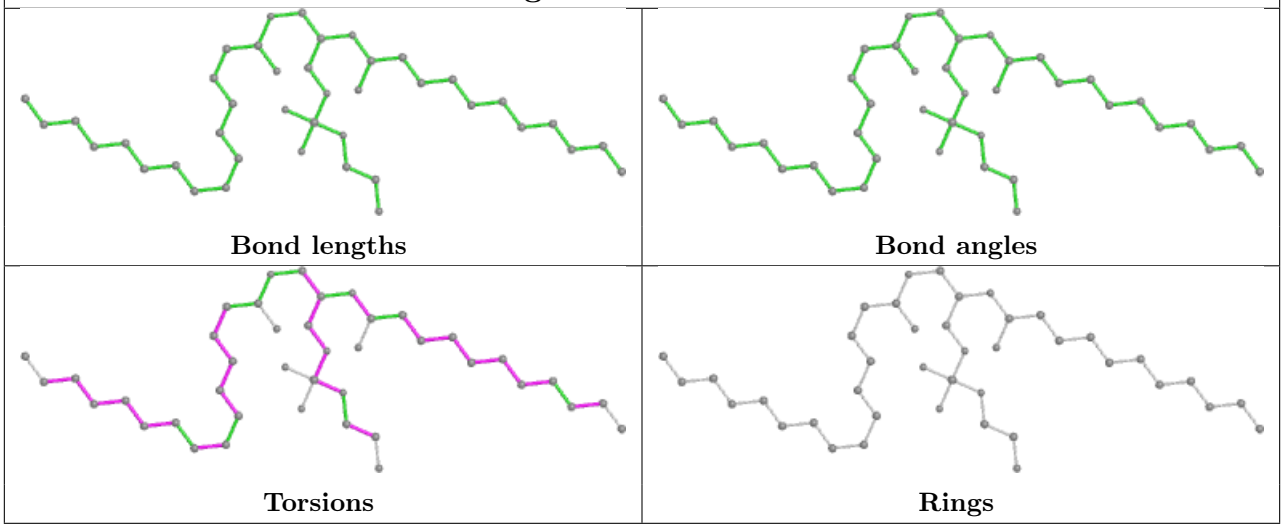
Ligand PC1 I 201

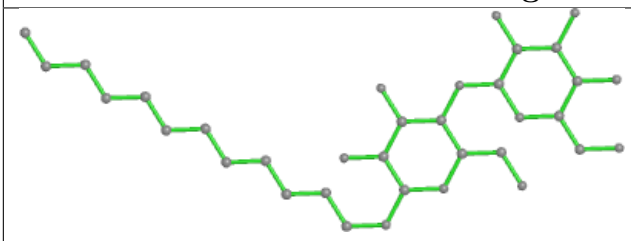
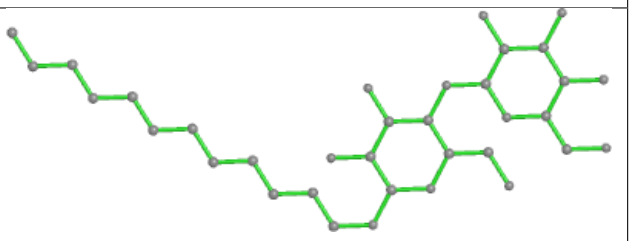
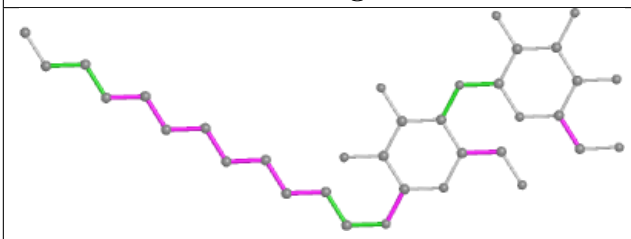
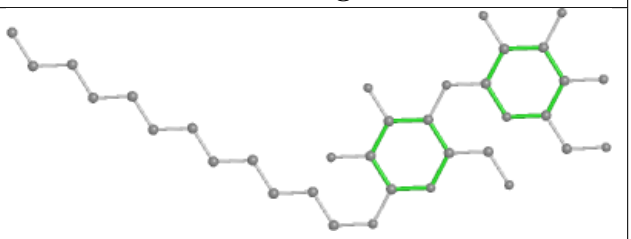


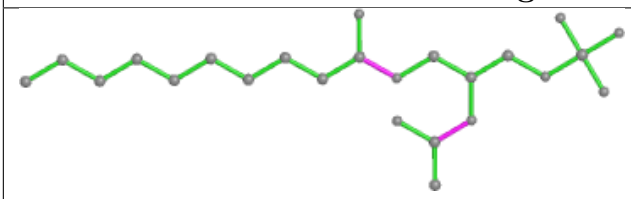
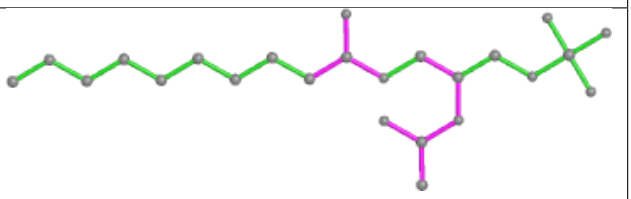
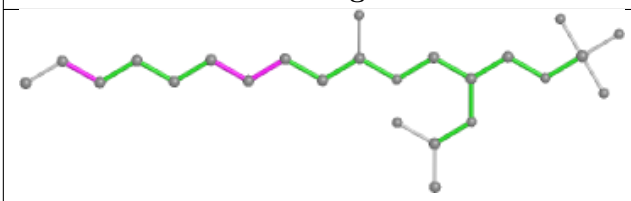
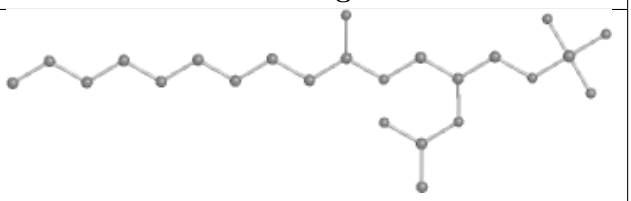
Ligand PC1 T 201

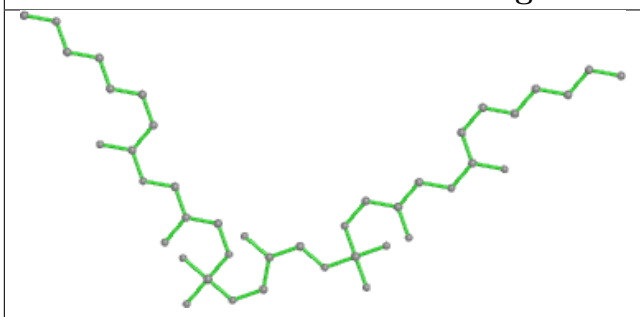
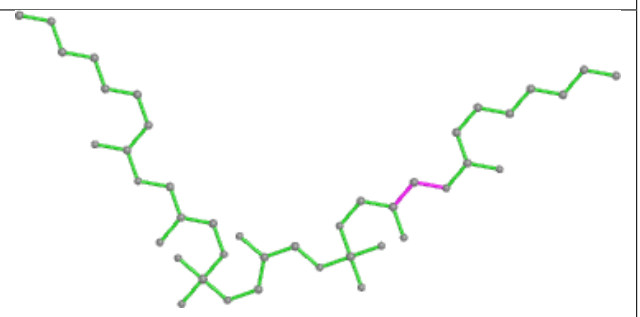
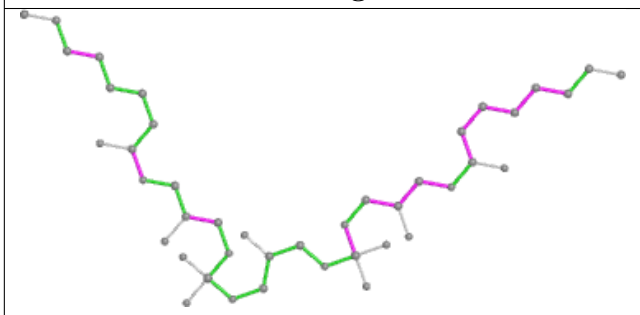
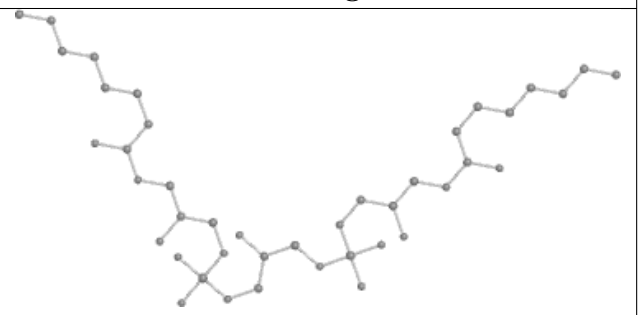


Ligand PTY C 504



Ligand LMT P 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XP4 A 3003	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

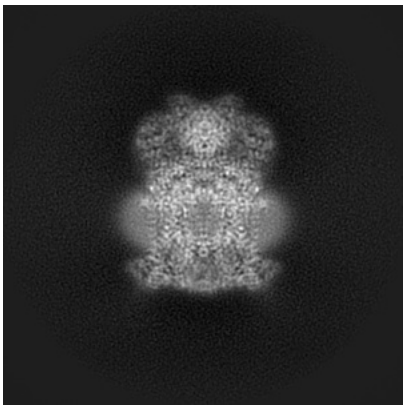
6 Map visualisation (i)

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.

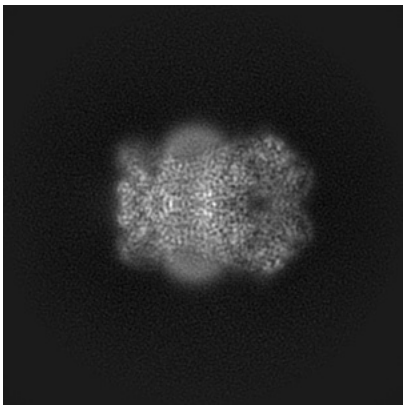
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

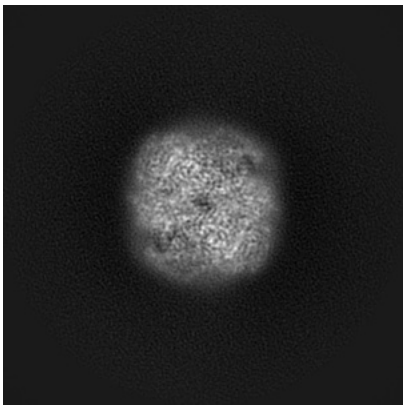
6.1.1 Primary map



X

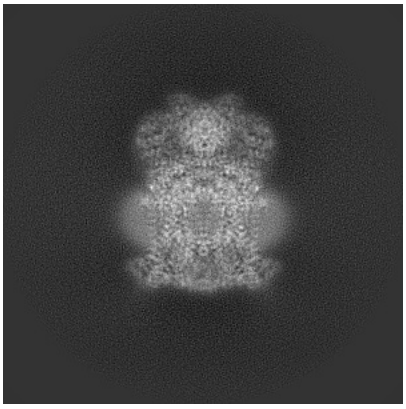


Y

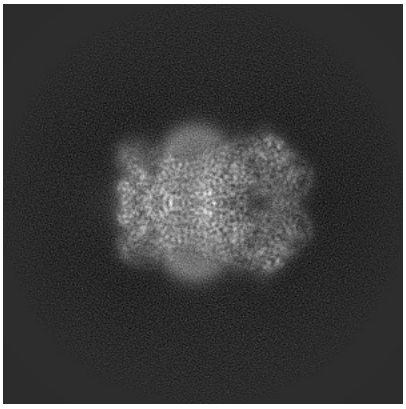


Z

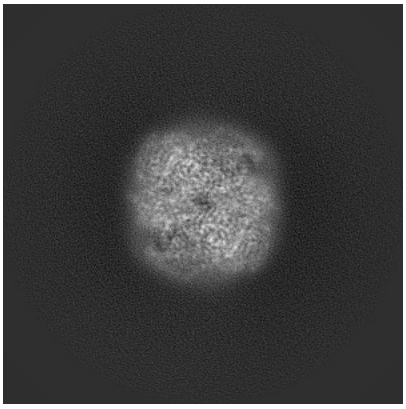
6.1.2 Raw map



X



Y

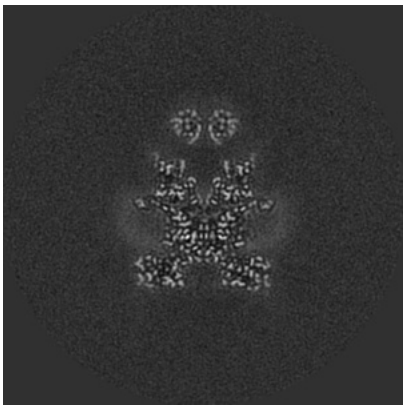


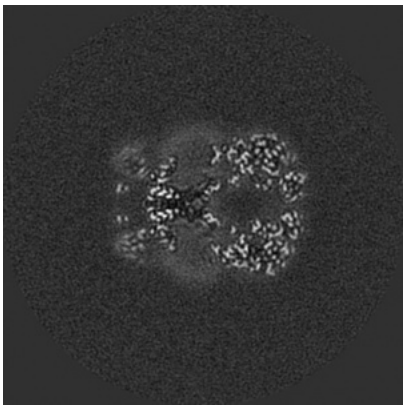
Z

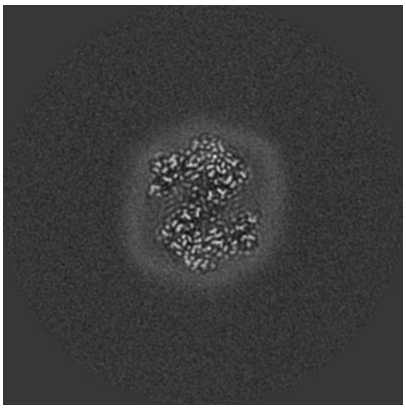
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

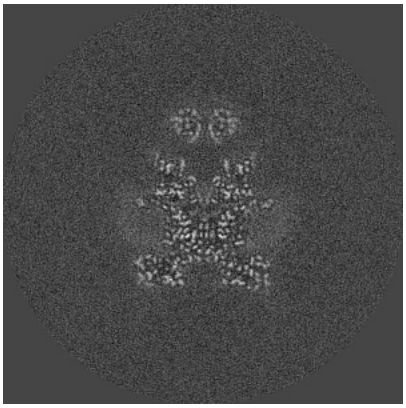
6.2.1 Primary map

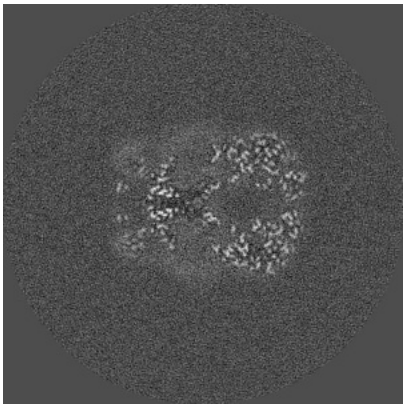

X Index: 180

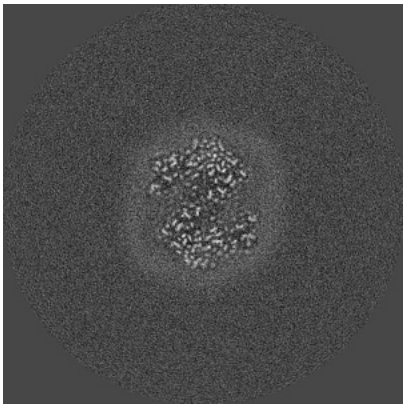

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

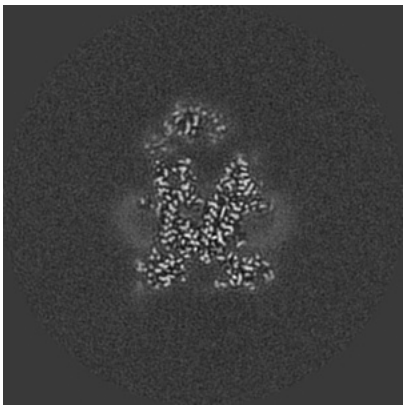

Y Index: 180

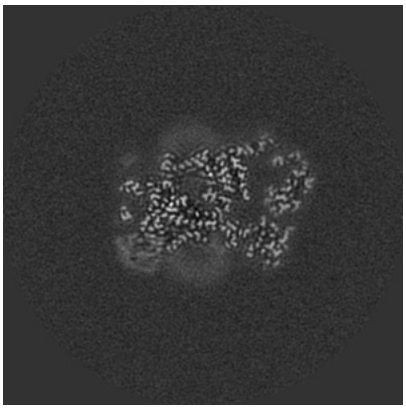

Z Index: 180

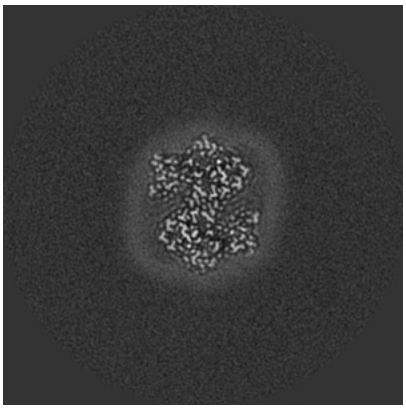
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

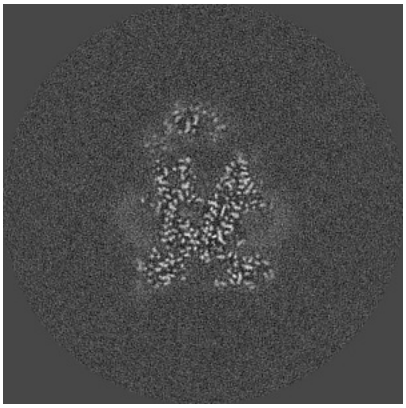
6.3.1 Primary map

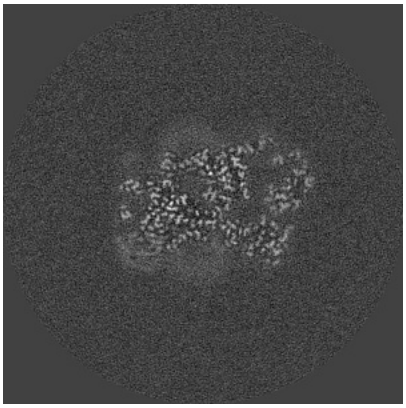

X Index: 186

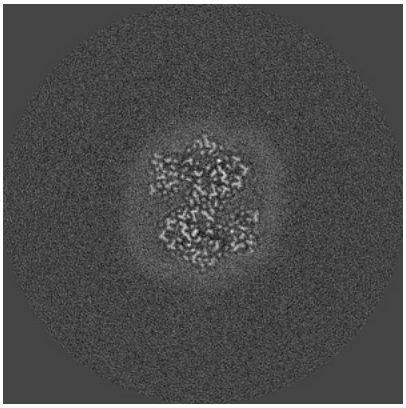

Y Index: 166


Z Index: 182

6.3.2 Raw map


X Index: 186

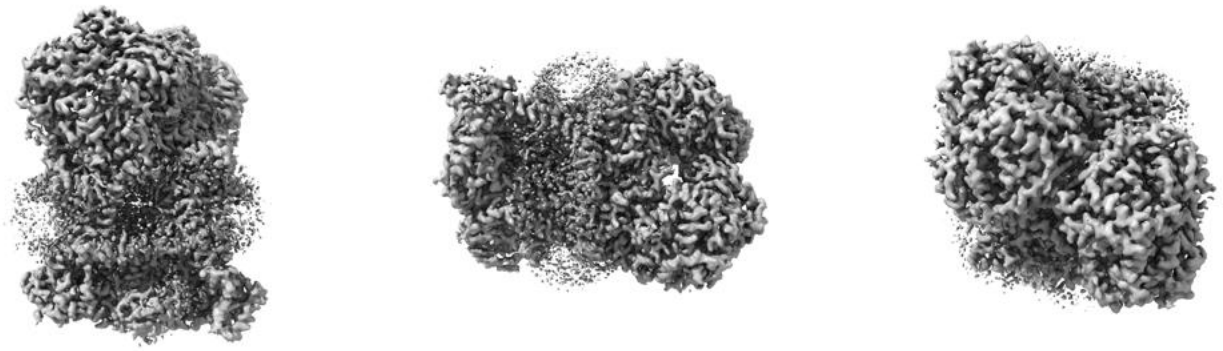

Y Index: 166


Z Index: 182

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

6.4 Orthogonal surface views (i)

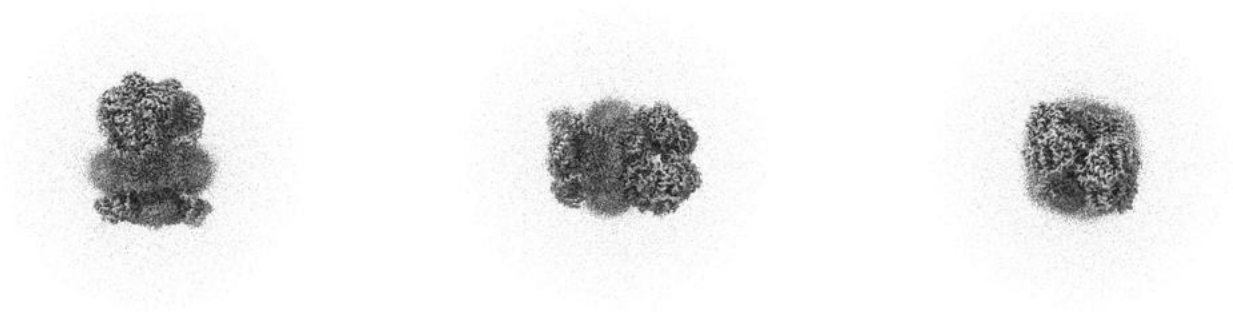
6.4.1 Primary map



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.

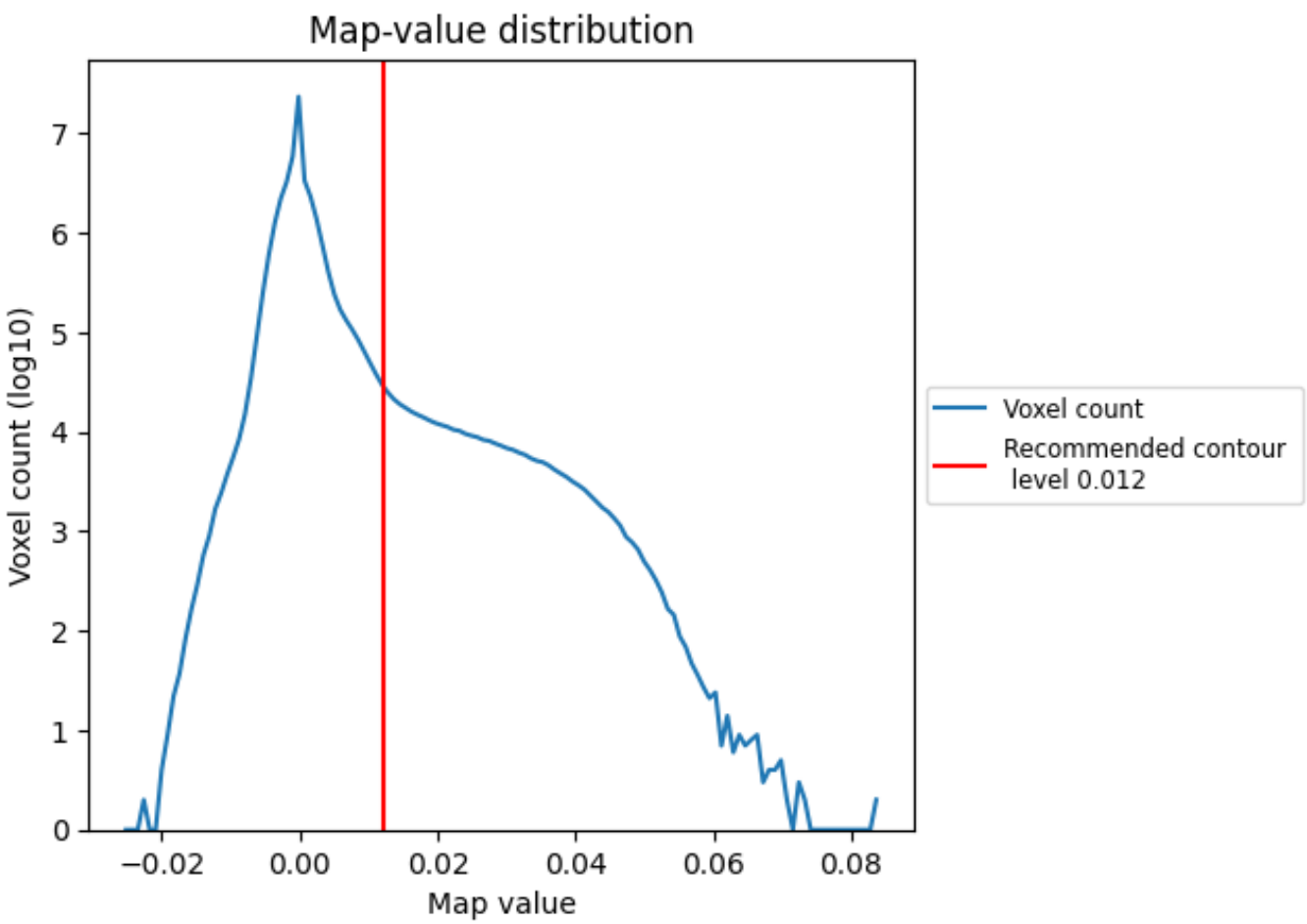
6.5 Mask visualisation (i)

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

7 Map analysis (i)

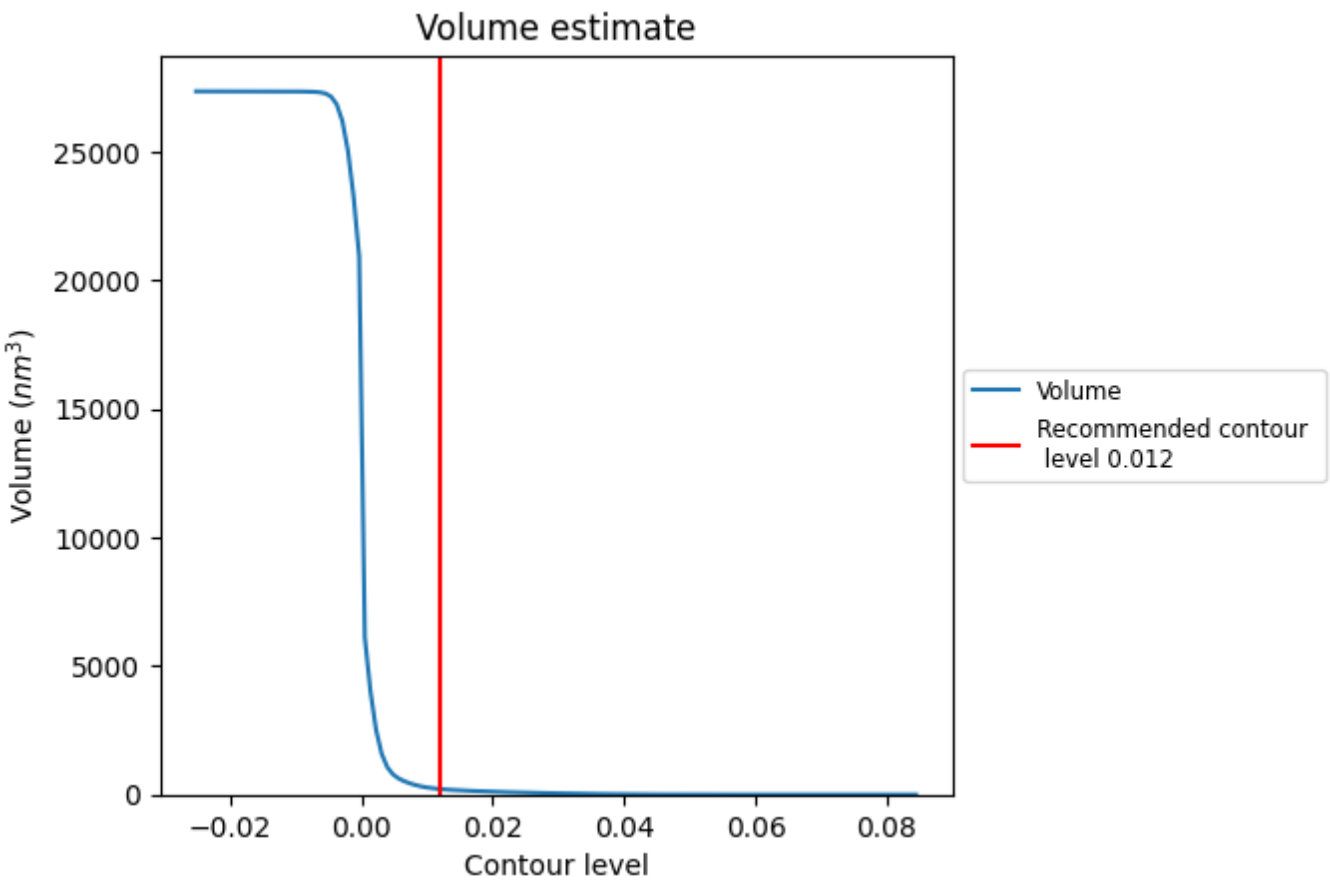
This section contains the results of statistical analysis of the map.

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.

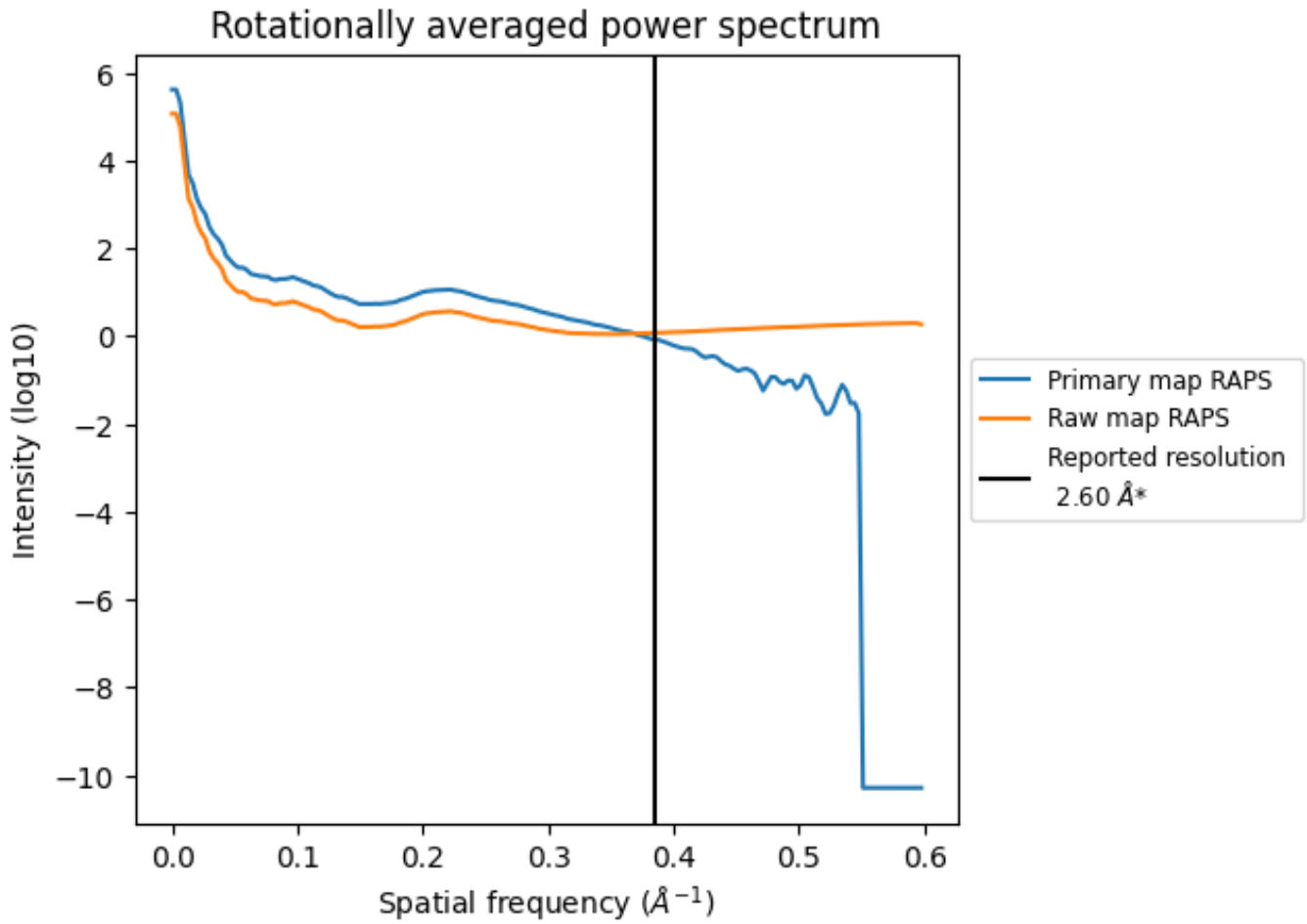
7.2 Volume estimate (i)



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)

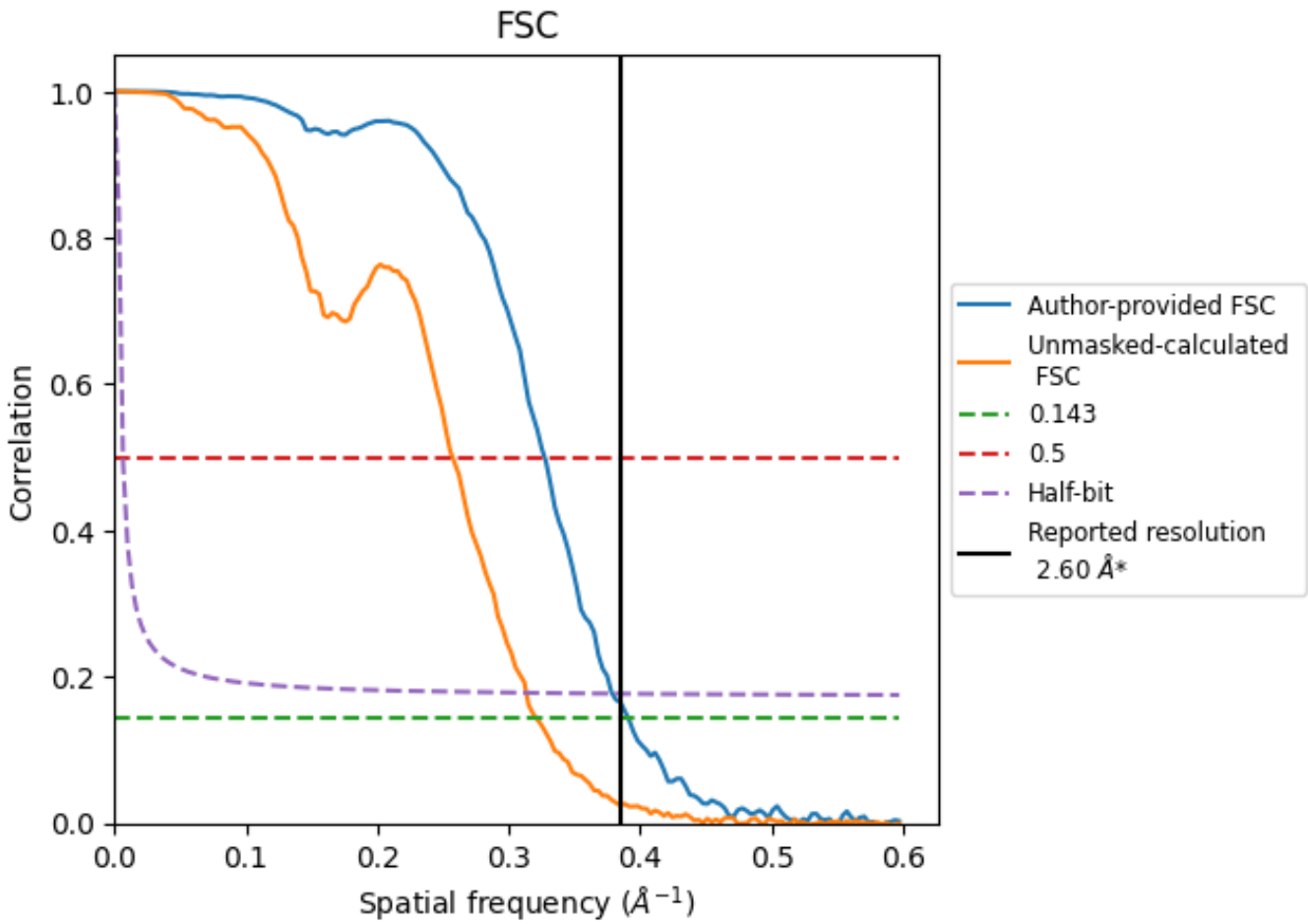


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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)

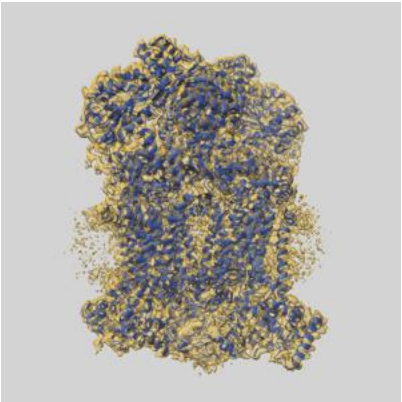
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.56	3.06	2.64
Unmasked-calculated*	3.11	3.89	3.19

*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 %

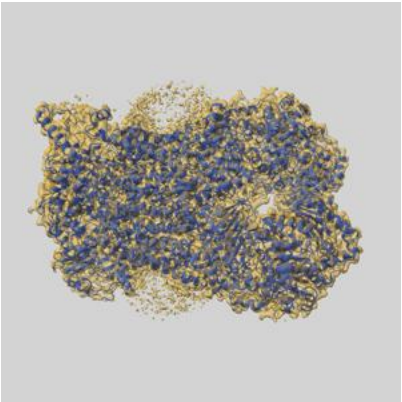
9 Map-model fit (i)

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.

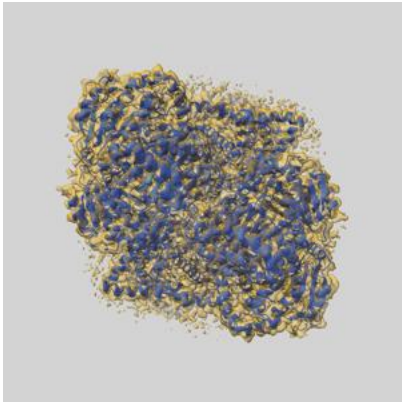
9.1 Map-model overlay (i)



X



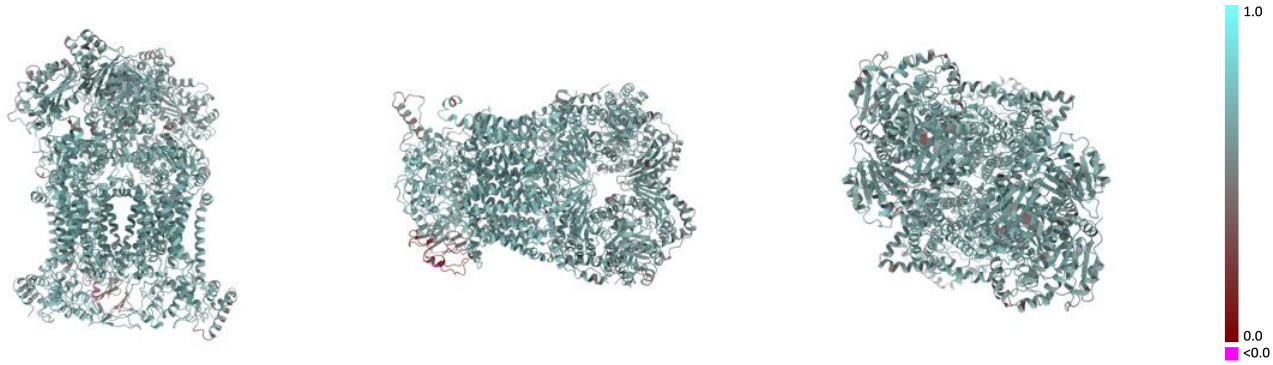
Y



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.

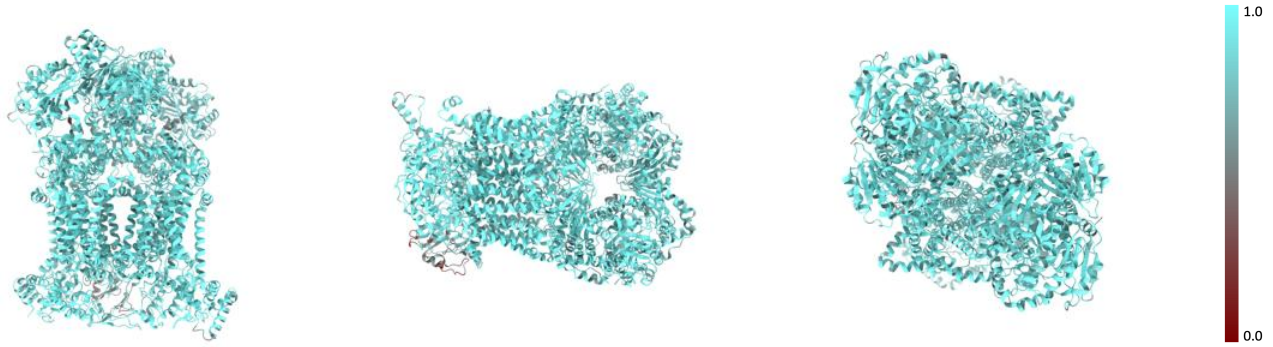
9.2 Q-score mapped to coordinate model (i)



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.

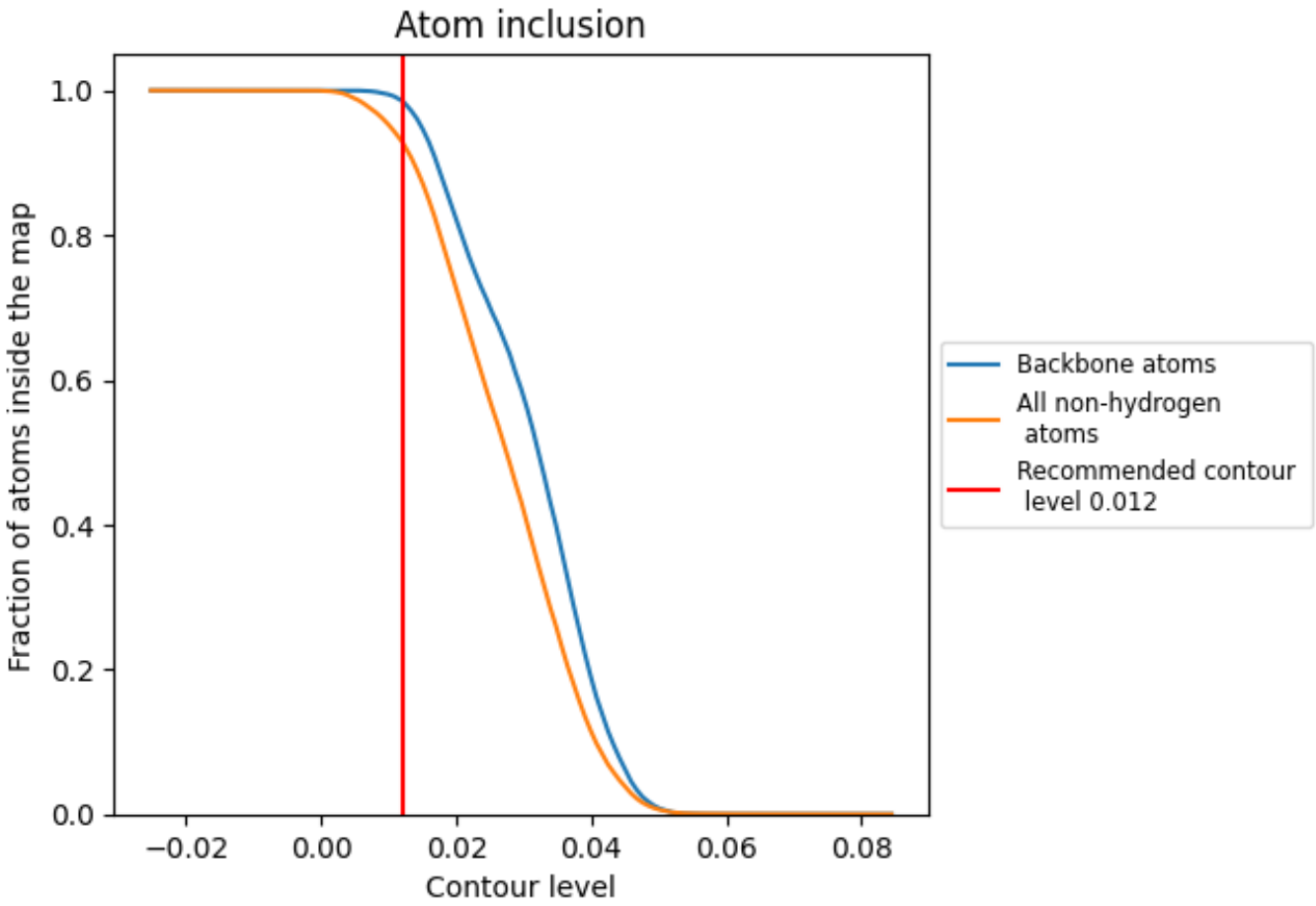
9.3 Atom inclusion mapped to coordinate model (i)



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