wwPDB EM Validation Summary Report

Oct 12, 2024 – 08:47 pm BST

PDB ID	:	8AC3
EMDB ID	:	EMD-15332
Title	:	Complex III2 from Yarrowia lipolytica, apo, int-position
Authors	:	Wieferig, J.P.; Kuhlbrandt, W.
Deposited on	:	2022-07-05
Resolution	:	2.80 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 ⓘ symbol.

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

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

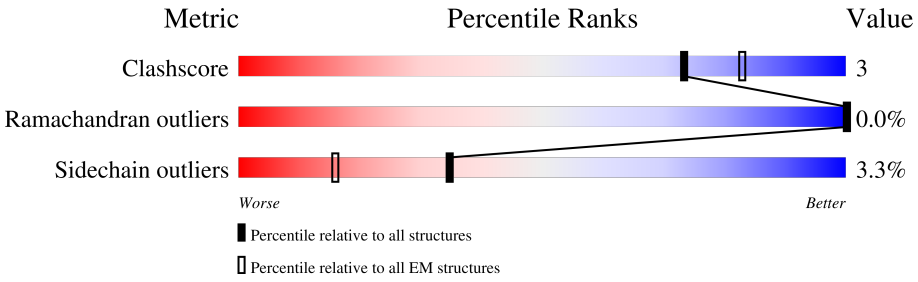
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	93% 6%
1	N	385	92% 7%
2	E	225	24% 73%
2	P	225	62% 19% 17%
3	G	128	88% 9%
3	R	128	91% 5%
4	F	137	47% 48%
4	Q	137	50% 48%

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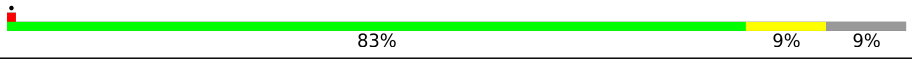
Mol	Chain	Length	Quality of chain
5	A	474	
5	L	474	
6	B	417	
6	M	417	
7	D	330	
7	O	330	
8	H	93	
8	S	93	
9	I	69	
9	T	69	
10	J	82	
10	U	82	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 32540 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
1	C	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		
1	N	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	186	Total	C	N	O	S	0	0
			1445	920	248	268	9		
2	E	61	Total	C	N	O	S	0	0
			465	297	76	89	3		

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

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

- Molecule 4 is a protein called YALI0F24673p.

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

- Molecule 5 is a protein called YALI0A14806p.

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

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

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

- Molecule 7 is a protein called YALI0A17468p.

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

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

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

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

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

- Molecule 10 is a protein called YALI0C12210p.

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

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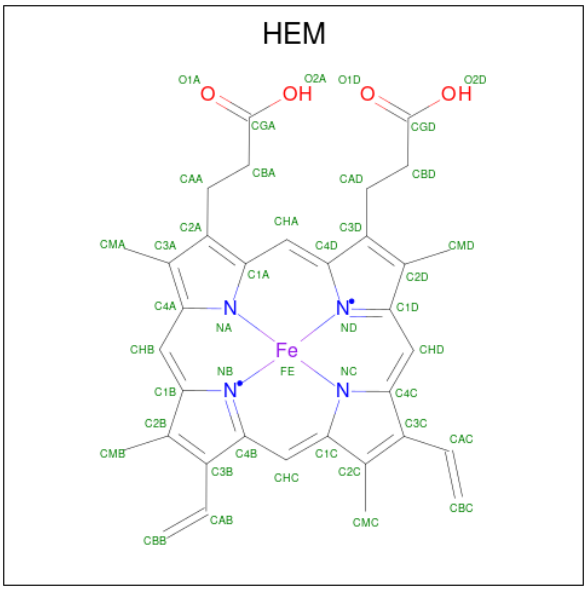
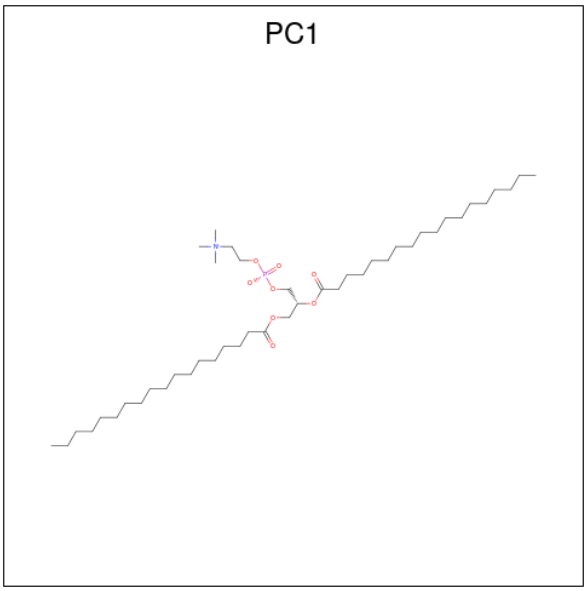
Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	75	Total	C	N	O	0	0
			598	403	99	96		

- 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).



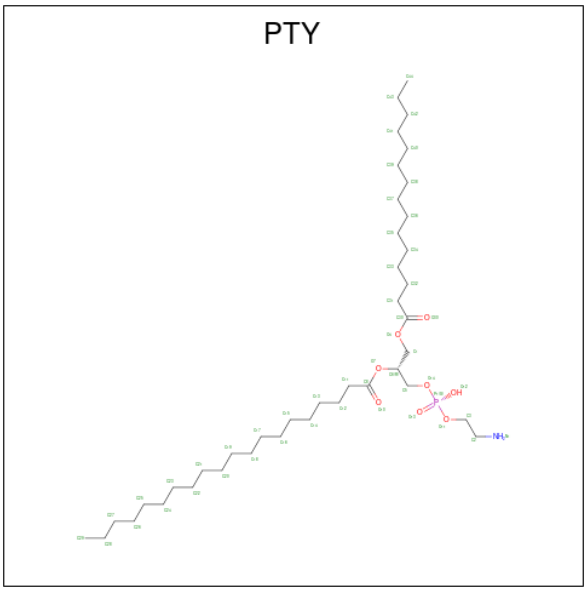
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



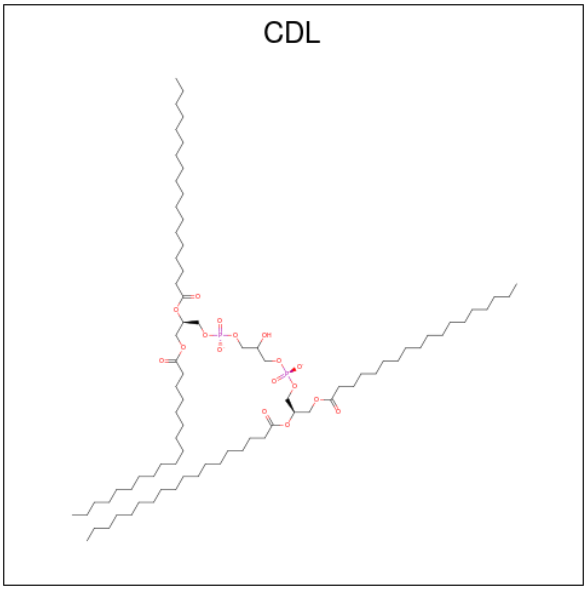
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	T	1	Total	C	N	O	P	0
			32	22	1	8	1	

- 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
			42	25	15	2	
14	A	1	Total	C	O	P	0
			47	30	15	2	
14	D	1	Total	C	O	P	0
			39	20	17	2	
14	H	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			48	29	17	2	
14	L	1	Total	C	O	P	0
			42	25	15	2	

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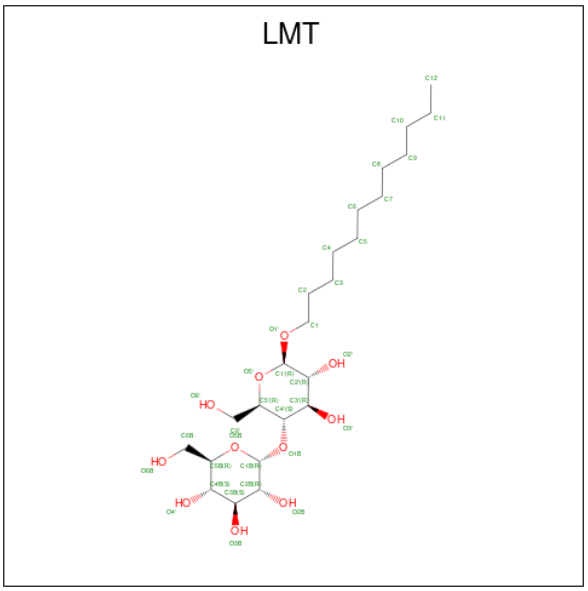
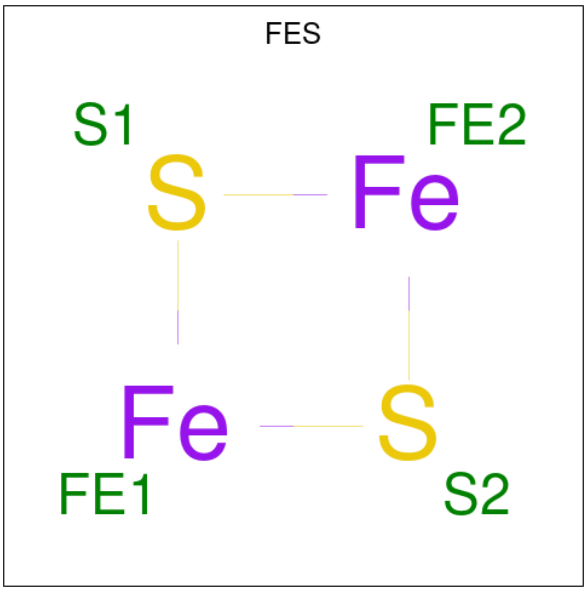
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			47	30	15	2	
14	S	1	Total	C	O	P	0
			39	20	17	2	

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



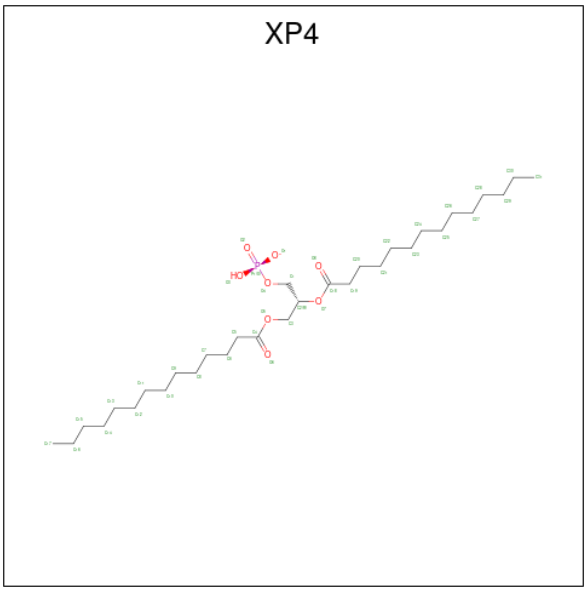
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			35	24	11	
15	J	1	Total	C	O	0
			35	24	11	
15	N	1	Total	C	O	0
			35	24	11	
15	U	1	Total	C	O	0
			35	24	11	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



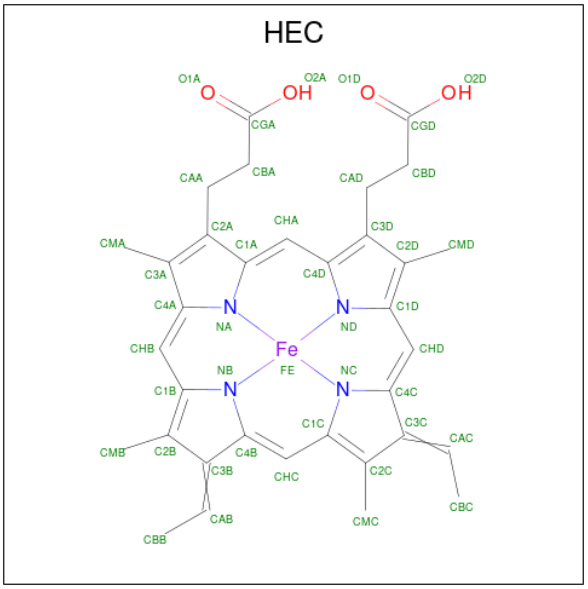
Mol	Chain	Residues	Atoms			AltConf
16	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: $C_{31}H_{60}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			24	15	8	1	
17	U	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

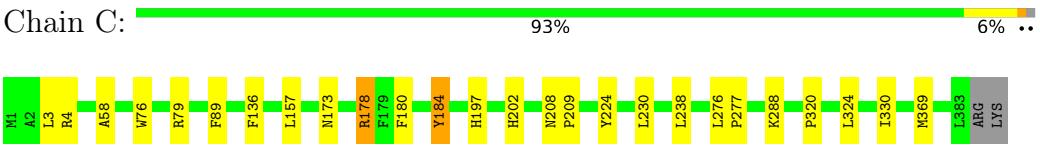


Mol	Chain	Residues	Atoms					AltConf
18	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

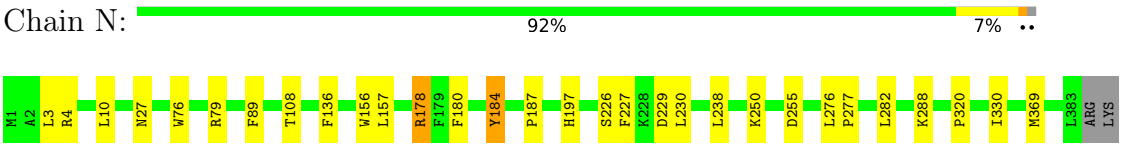
3 Residue-property plots (i)

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.

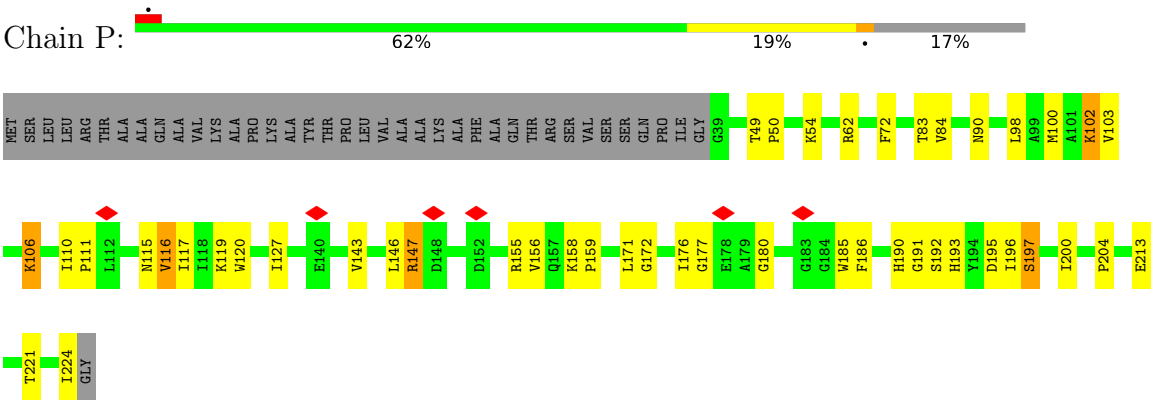
• Molecule 1: Cytochrome b



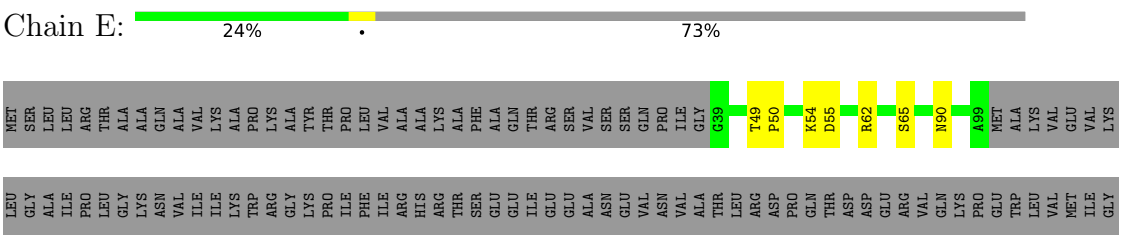
• Molecule 1: Cytochrome b

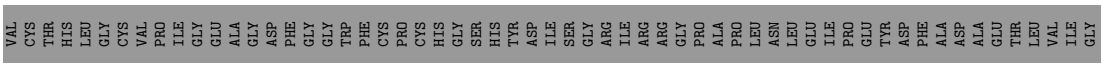


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



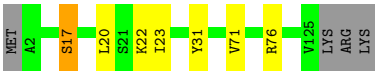


• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain G:

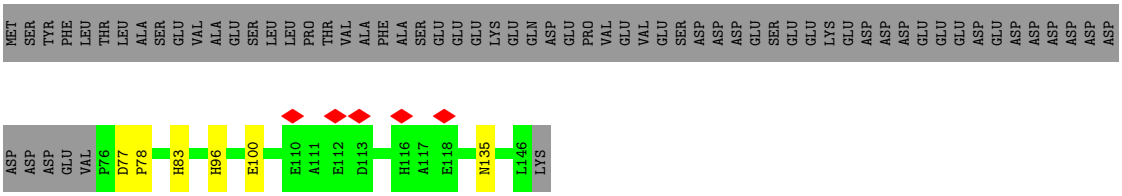
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:



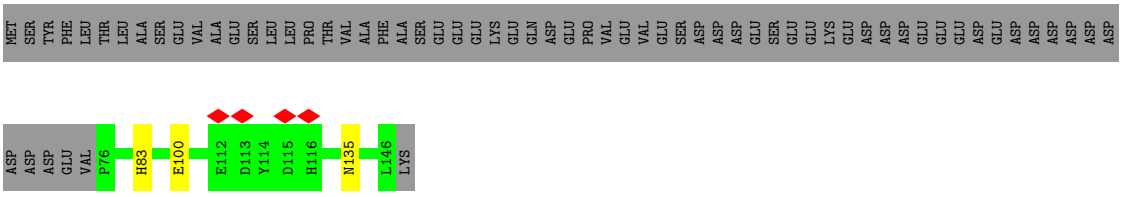
• Molecule 4: YALI0F24673p

Chain F:



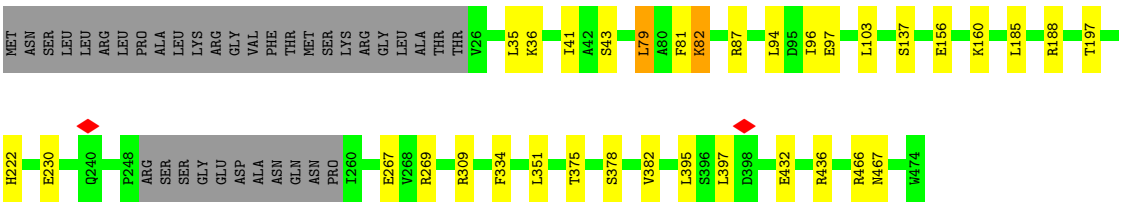
• Molecule 4: YALI0F24673p

Chain Q:



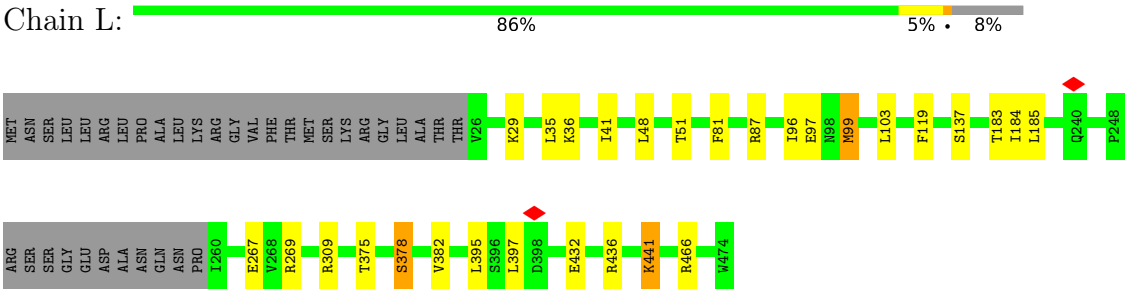
• Molecule 5: YALI0A14806p

Chain A:



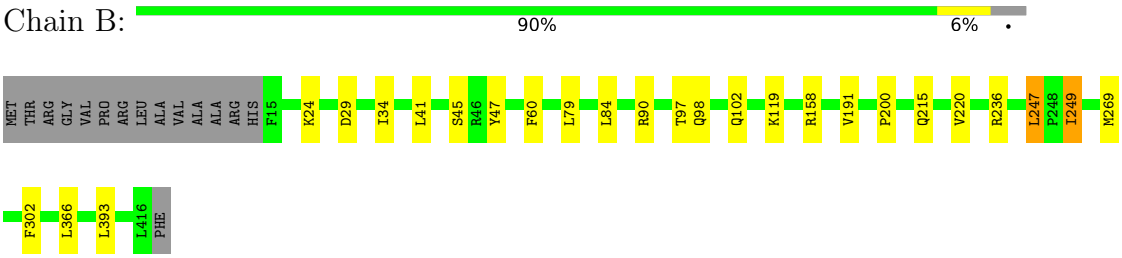
• Molecule 5: YALI0A14806p

Chain L:



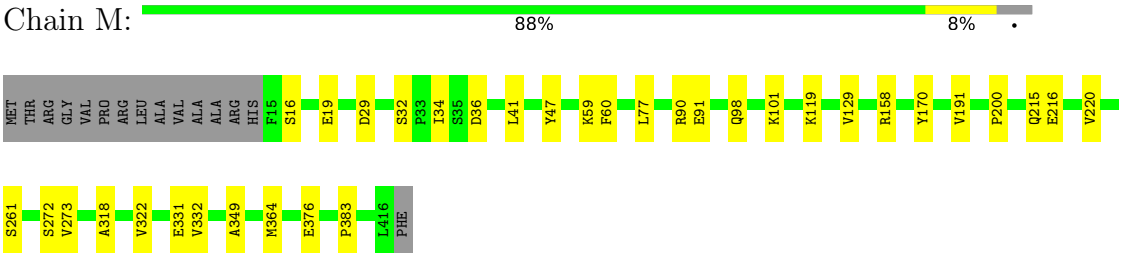
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



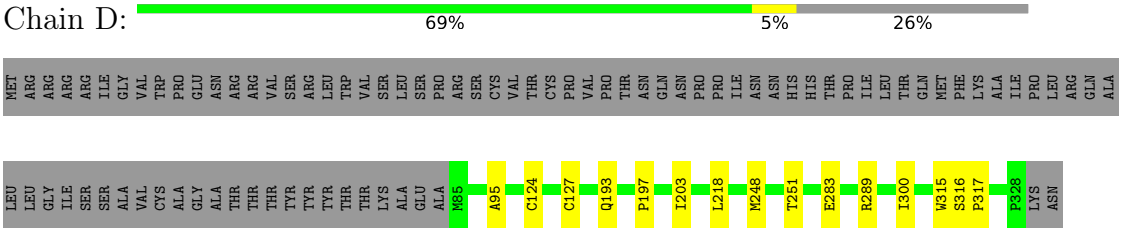
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



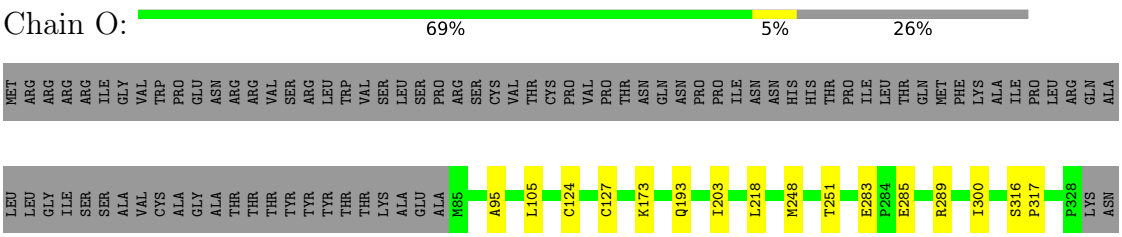
• Molecule 7: YALI0A17468p

Chain D:



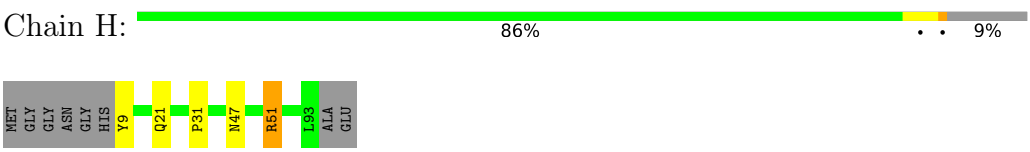
• Molecule 7: YALI0A17468p

Chain O:



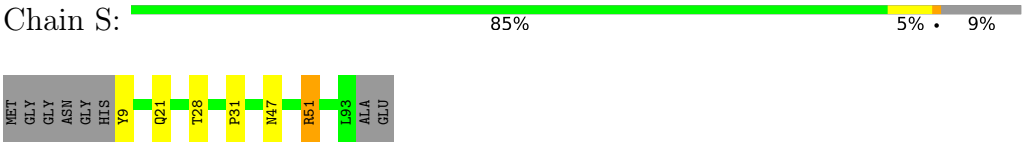
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



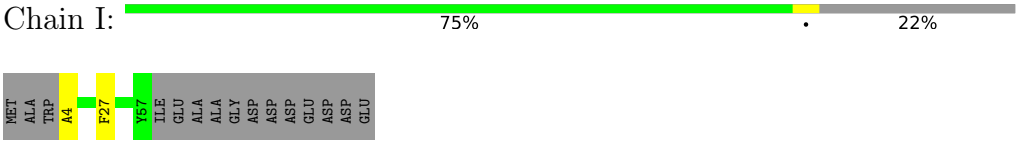
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:



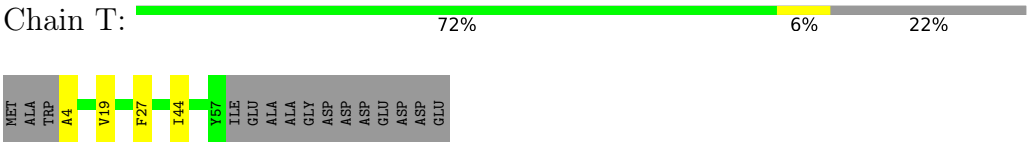
• Molecule 9: Complex III subunit 9

Chain I:



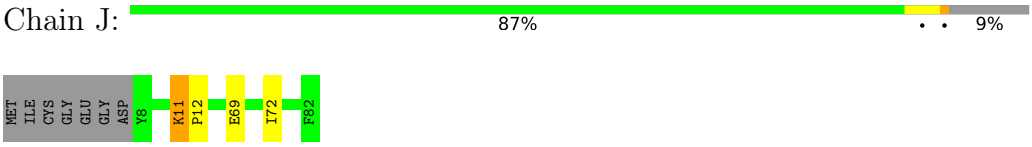
• Molecule 9: Complex III subunit 9

Chain T:



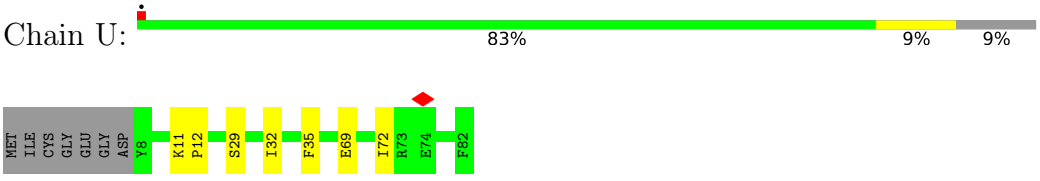
• Molecule 10: YALI0C12210p

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	93285	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	0.061	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XP4, HEM, HEC, CDL, PTY, LMT, 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	0.45	0/3153	0.80	1/4305 (0.0%)
1	N	0.45	0/3153	0.79	1/4305 (0.0%)
2	E	0.45	0/474	0.74	0/637
2	P	0.37	0/1479	0.77	0/2003
3	G	0.41	0/1012	0.74	1/1373 (0.1%)
3	R	0.41	0/1012	0.74	1/1373 (0.1%)
4	F	0.30	0/595	0.67	0/805
4	Q	0.31	0/595	0.68	0/805
5	A	0.38	0/3510	0.77	3/4768 (0.1%)
5	L	0.39	0/3510	0.79	4/4768 (0.1%)
6	B	0.35	0/3069	0.76	3/4178 (0.1%)
6	M	0.35	0/3069	0.76	3/4178 (0.1%)
7	D	0.39	0/1950	0.78	2/2656 (0.1%)
7	O	0.39	0/1950	0.76	1/2656 (0.0%)
8	H	0.40	1/717 (0.1%)	0.72	0/975
8	S	0.41	1/717 (0.1%)	0.71	0/975
9	I	0.48	1/465 (0.2%)	0.68	0/629
9	T	0.49	1/465 (0.2%)	0.69	0/629
10	J	0.37	0/620	0.67	0/846
10	U	0.38	0/620	0.67	0/846
All	All	0.40	4/32135 (0.0%)	0.76	20/43710 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	4	ALA	N-CA	6.48	1.59	1.46
9	I	4	ALA	N-CA	6.39	1.59	1.46
8	S	9	TYR	N-CA	5.15	1.56	1.46
8	H	9	TYR	N-CA	5.00	1.56	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	269	ARG	NE-CZ-NH2	-8.72	115.94	120.30
6	M	90	ARG	CG-CD-NE	-8.10	94.78	111.80
6	B	90	ARG	CG-CD-NE	-7.64	95.75	111.80
5	A	269	ARG	CG-CD-NE	-6.97	97.16	111.80
5	L	309	ARG	CG-CD-NE	-6.94	97.22	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	17	0
1	N	3052	0	3113	19	0
2	E	465	0	459	2	0
2	P	1445	0	1426	26	0
3	G	994	0	1022	4	0
3	R	994	0	1022	5	0
4	F	579	0	511	2	0
4	Q	579	0	511	1	0
5	A	3446	0	3369	22	0
5	L	3446	0	3369	13	0
6	B	3008	0	2991	15	0
6	M	3008	0	2991	15	0
7	D	1893	0	1834	20	0
7	O	1893	0	1834	21	0
8	H	690	0	673	4	0
8	S	690	0	673	5	0
9	I	452	0	435	0	0
9	T	452	0	435	2	0
10	J	598	0	615	2	0
10	U	598	0	615	4	0
11	C	86	0	60	8	0
11	N	86	0	60	7	0
12	C	38	0	50	1	0
12	I	32	0	38	0	0
12	N	38	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	T	32	0	38	2	0
13	C	41	0	58	2	0
13	E	41	0	58	1	0
13	N	41	0	58	8	0
13	P	41	0	58	11	0
14	A	89	0	85	3	0
14	C	48	0	40	1	0
14	D	39	0	22	1	0
14	H	50	0	44	2	0
14	L	89	0	85	0	0
14	N	98	0	84	5	0
14	S	39	0	22	2	0
15	C	35	0	46	1	0
15	J	35	0	46	1	0
15	N	35	0	46	0	0
15	U	35	0	46	0	0
16	P	4	0	0	0	0
17	A	24	0	22	0	0
17	U	24	0	22	1	0
18	D	43	0	32	14	0
18	O	43	0	32	13	0
All	All	32540	0	32213	200	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 200 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)
7:D:124:CYS:SG	18:D:401:HEC:HBB3	1.62	1.38
7:O:124:CYS:SG	18:O:401:HEC:HBB3	1.65	1.34
2:P:84:VAL:CG2	13:P:302:PTY:H441	1.58	1.33
7:O:124:CYS:SG	18:O:401:HEC:CBB	2.33	1.16
7:D:124:CYS:SG	18:D:401:HEC:CBB	2.34	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%)	373 (98%)	8 (2%)	0	100	100
1	N	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
2	E	59/225 (26%)	58 (98%)	1 (2%)	0	100	100
2	P	184/225 (82%)	169 (92%)	14 (8%)	1 (0%)	25	56
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%)	66 (96%)	3 (4%)	0	100	100
4	Q	69/137 (50%)	66 (96%)	3 (4%)	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%)	383 (96%)	17 (4%)	0	100	100
6	M	400/417 (96%)	388 (97%)	12 (3%)	0	100	100
7	D	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
7	O	242/330 (73%)	239 (99%)	3 (1%)	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%)	50 (96%)	2 (4%)	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	3955/4680 (84%)	3852 (97%)	102 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	172	GLY

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%)	322 (97%)	9 (3%)	40 74
1	N	331/333 (99%)	319 (96%)	12 (4%)	30 64
2	E	49/182 (27%)	44 (90%)	5 (10%)	6 19
2	P	154/182 (85%)	135 (88%)	19 (12%)	4 13
3	G	113/117 (97%)	105 (93%)	8 (7%)	12 35
3	R	113/117 (97%)	110 (97%)	3 (3%)	40 74
4	F	61/123 (50%)	58 (95%)	3 (5%)	21 52
4	Q	61/123 (50%)	59 (97%)	2 (3%)	33 67
5	A	377/407 (93%)	366 (97%)	11 (3%)	37 71
5	L	377/407 (93%)	365 (97%)	12 (3%)	34 68
6	B	311/322 (97%)	304 (98%)	7 (2%)	45 78
6	M	311/322 (97%)	298 (96%)	13 (4%)	25 58
7	D	192/268 (72%)	191 (100%)	1 (0%)	86 95
7	O	192/268 (72%)	191 (100%)	1 (0%)	86 95
8	H	67/71 (94%)	66 (98%)	1 (2%)	60 86
8	S	67/71 (94%)	66 (98%)	1 (2%)	60 86
9	I	46/57 (81%)	45 (98%)	1 (2%)	47 79
9	T	46/57 (81%)	45 (98%)	1 (2%)	47 79
10	J	63/68 (93%)	62 (98%)	1 (2%)	58 85
10	U	63/68 (93%)	63 (100%)	0	100 100
All	All	3325/3896 (85%)	3214 (97%)	111 (3%)	35 67

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	193	GLN
9	T	27	PHE
1	N	288	LYS

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Mol	Chain	Res	Type
8	S	51	ARG
6	M	77	LEU

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

Mol	Chain	Res	Type
2	E	90	ASN
6	M	215	GLN
6	M	184	GLN
5	A	74	HIS
1	N	332	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	C	505	-	47,47,99	0.53	0	53,59,111	0.96	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	XP4	A	3003	-	23,23,39	1.46	2 (8%)	27,28,44	2.44	10 (37%)
11	HEM	N	502	1	41,50,50	1.34	4 (9%)	45,82,82	2.46	18 (40%)
14	CDL	N	506	-	47,47,99	0.52	0	53,59,111	0.88	4 (7%)
12	PC1	T	201	-	31,31,53	0.38	0	37,39,61	0.63	0
14	CDL	S	101	-	38,38,99	0.46	0	44,50,111	1.25	5 (11%)
14	CDL	N	504	-	49,49,99	0.36	0	55,61,111	0.64	0
13	PTY	E	401	-	40,40,49	0.48	0	43,45,54	0.52	0
12	PC1	I	201	-	31,31,53	0.39	0	37,39,61	0.67	0
13	PTY	P	302	-	40,40,49	0.50	0	43,45,54	0.66	1 (2%)
11	HEM	N	501	1	41,50,50	1.59	7 (17%)	45,82,82	2.35	13 (28%)
14	CDL	L	3002	-	46,46,99	0.40	0	51,56,111	0.82	3 (5%)
14	CDL	A	3002	-	46,46,99	0.37	0	51,56,111	0.90	3 (5%)
15	LMT	N	507	-	36,36,36	0.56	0	47,47,47	1.20	6 (12%)
15	LMT	J	101	-	36,36,36	0.55	0	47,47,47	1.22	6 (12%)
14	CDL	D	402	-	38,38,99	0.46	0	44,50,111	1.22	4 (9%)
11	HEM	C	502	1	41,50,50	1.37	5 (12%)	45,82,82	2.32	19 (42%)
18	HEC	D	401	7	32,50,50	1.83	8 (25%)	24,82,82	2.91	6 (25%)
14	CDL	A	3001	-	41,41,99	0.57	0	45,51,111	0.77	1 (2%)
15	LMT	U	101	-	36,36,36	0.52	0	47,47,47	1.36	7 (14%)
12	PC1	C	503	-	37,37,53	0.81	1 (2%)	43,45,61	0.98	3 (6%)
12	PC1	N	503	-	37,37,53	0.70	1 (2%)	43,45,61	0.88	2 (4%)
14	CDL	L	3001	-	41,41,99	0.46	0	45,51,111	0.77	1 (2%)
13	PTY	C	504	-	40,40,49	0.37	0	43,45,54	0.55	0
16	FES	P	301	2	0,4,4	-	-	-		
14	CDL	H	701	-	49,49,99	0.36	0	55,61,111	0.67	0
15	LMT	C	506	-	36,36,36	0.52	0	47,47,47	1.25	6 (12%)
17	XP4	U	102	-	23,23,39	1.51	2 (8%)	27,28,44	2.49	7 (25%)
13	PTY	N	505	-	40,40,49	0.38	0	43,45,54	0.73	1 (2%)
11	HEM	C	501	1	41,50,50	1.53	7 (17%)	45,82,82	2.49	17 (37%)
18	HEC	O	401	7	32,50,50	1.83	9 (28%)	24,82,82	2.85	8 (33%)

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	C	505	-	-	29/57/57/110	-
17	XP4	A	3003	-	-	1/24/24/41	-
11	HEM	N	502	1	-	4/12/54/54	-
14	CDL	N	506	-	-	29/57/57/110	-
12	PC1	T	201	-	-	13/35/35/57	-
14	CDL	S	101	-	-	28/48/48/110	-
14	CDL	N	504	-	-	35/59/59/110	-
13	PTY	E	401	-	-	26/44/44/53	-
12	PC1	I	201	-	-	14/35/35/57	-
13	PTY	P	302	-	-	24/44/44/53	-
11	HEM	N	501	1	-	5/12/54/54	-
14	CDL	L	3002	-	-	28/54/54/110	-
14	CDL	A	3002	-	-	30/54/54/110	-
15	LMT	N	507	-	-	12/21/61/61	0/2/2/2
15	LMT	J	101	-	-	12/21/61/61	0/2/2/2
14	CDL	D	402	-	-	29/48/48/110	-
11	HEM	C	502	1	-	4/12/54/54	-
18	HEC	D	401	7	-	2/10/54/54	-
14	CDL	A	3001	-	-	14/48/48/110	-
15	LMT	U	101	-	-	4/21/61/61	0/2/2/2
12	PC1	C	503	-	-	10/41/41/57	-
12	PC1	N	503	-	-	16/41/41/57	-
14	CDL	L	3001	-	-	21/48/48/110	-
13	PTY	C	504	-	-	28/44/44/53	-
16	FES	P	301	2	-	-	0/1/1/1
14	CDL	H	701	-	-	32/59/59/110	-
15	LMT	C	506	-	-	14/21/61/61	0/2/2/2
17	XP4	U	102	-	-	3/24/24/41	-
13	PTY	N	505	-	-	30/44/44/53	-
11	HEM	C	501	1	-	5/12/54/54	-
18	HEC	O	401	7	-	2/10/54/54	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	102	XP4	O7-C18	5.49	1.47	1.35
17	A	3003	XP4	O7-C18	5.06	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	C2B-C3B	4.46	1.45	1.40
11	C	501	HEM	C3C-C2C	-4.42	1.34	1.40
11	N	501	HEM	C3C-C2C	-4.27	1.34	1.40

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	102	XP4	O7-C18-C19	8.44	126.61	111.09
18	O	401	HEC	C1D-C2D-C3D	-7.98	101.44	107.00
18	D	401	HEC	CMB-C2B-C3B	7.84	135.04	125.82
11	N	502	HEM	CHC-C4B-NB	7.73	132.83	124.43
17	A	3003	XP4	O7-C18-C19	7.25	124.42	111.09

There are no chirality outliers.

5 of 504 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-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	C11-O13-P-O11
12	T	201	PC1	O21-C2-C3-O31

There are no ring outliers.

24 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	505	CDL	1	0
11	N	502	HEM	2	0
14	N	506	CDL	2	0
12	T	201	PC1	2	0
14	S	101	CDL	2	0
14	N	504	CDL	3	0
13	E	401	PTY	1	0
13	P	302	PTY	11	0
11	N	501	HEM	5	0
14	A	3002	CDL	2	0
15	J	101	LMT	1	0
14	D	402	CDL	1	0
11	C	502	HEM	2	0
18	D	401	HEC	14	0

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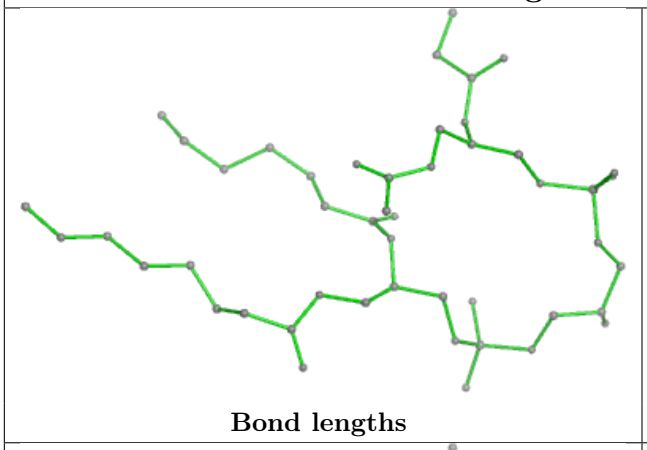
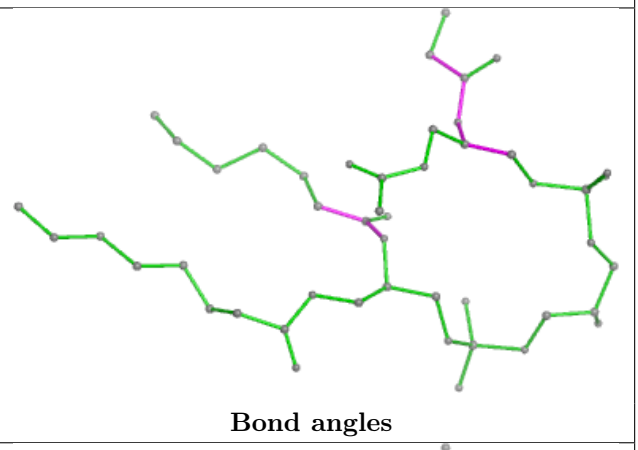
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	3001	CDL	2	0
12	C	503	PC1	1	0
12	N	503	PC1	1	0
13	C	504	PTY	2	0
14	H	701	CDL	2	0
15	C	506	LMT	1	0
17	U	102	XP4	1	0
13	N	505	PTY	8	0
11	C	501	HEM	6	0
18	O	401	HEC	13	0

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.

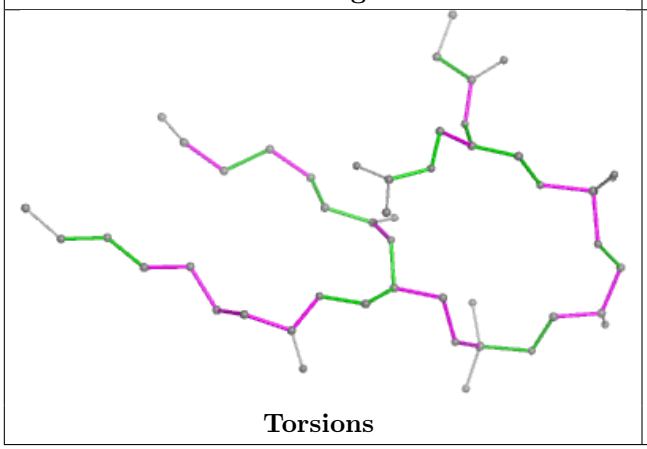
Ligand CDL C 505



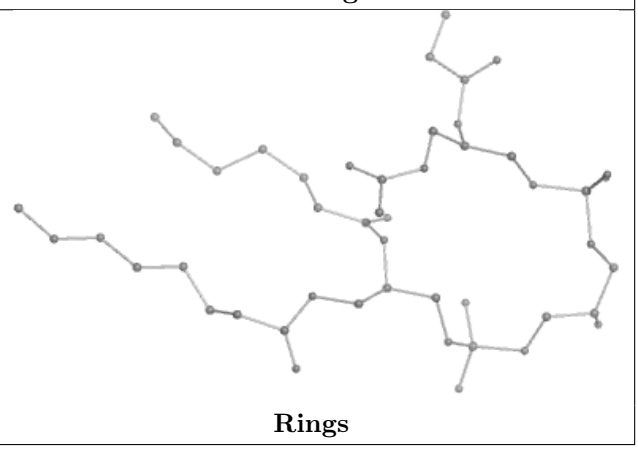
Bond lengths



Bond angles

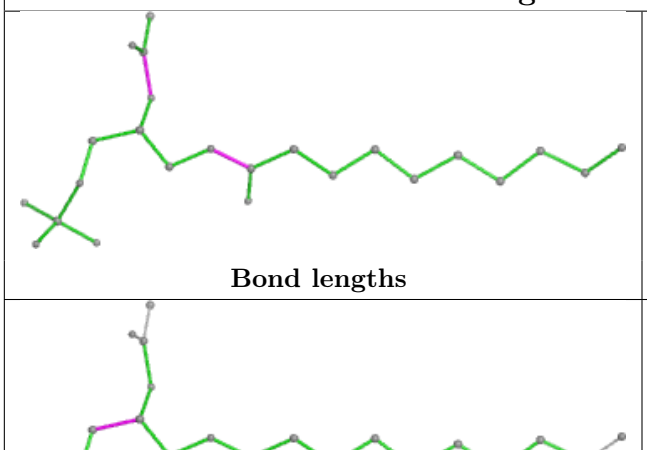


Torsions

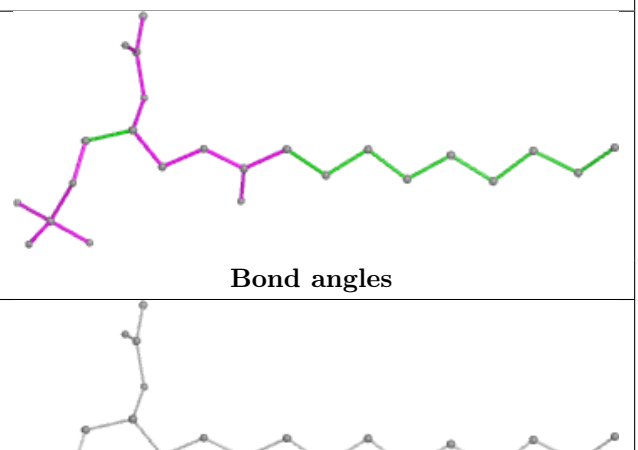


Rings

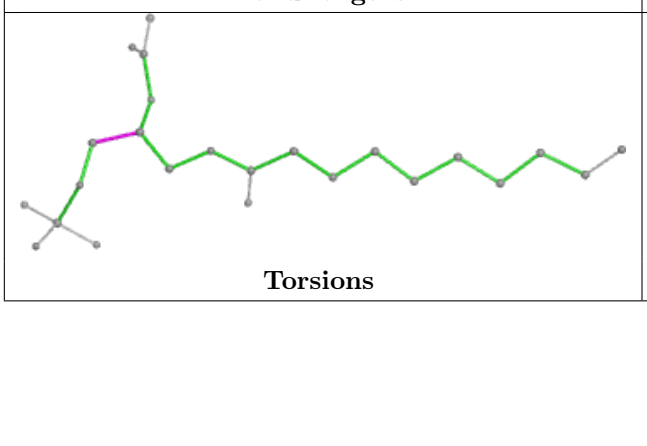
Ligand XP4 A 3003



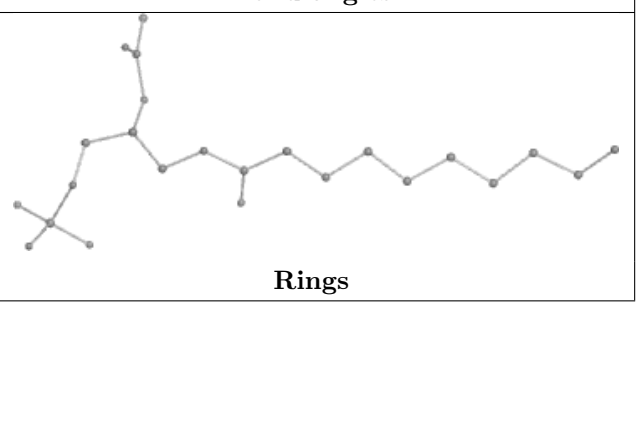
Bond lengths



Bond angles

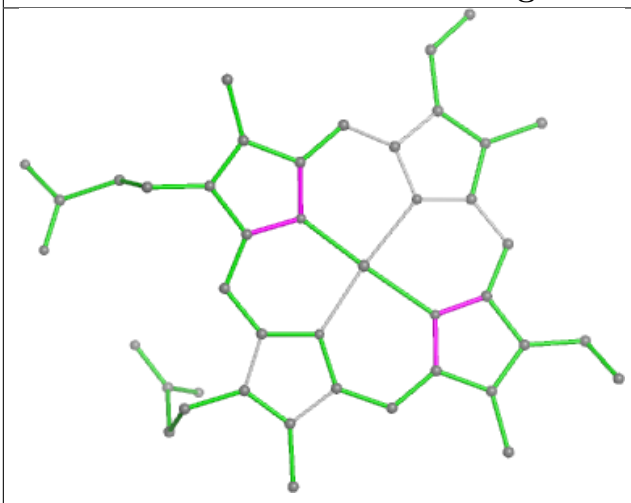


Torsions

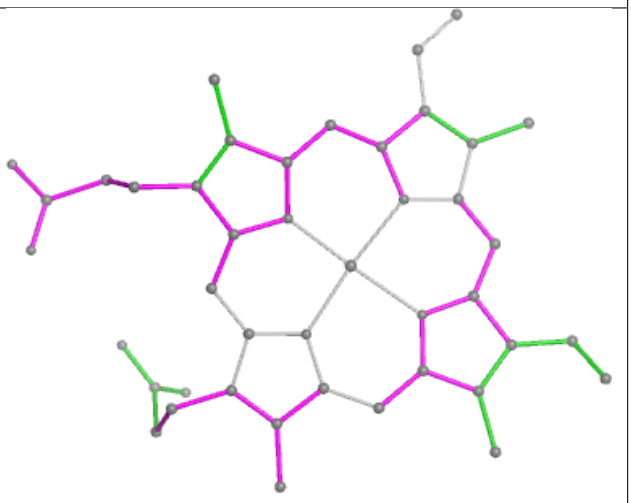


Rings

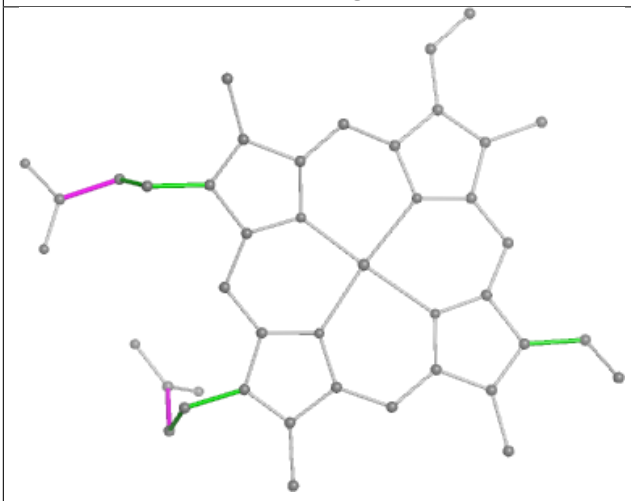
Ligand HEM N 502



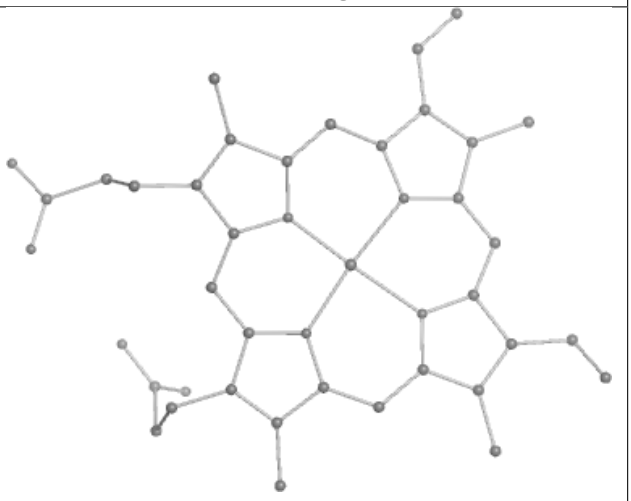
Bond lengths



Bond angles

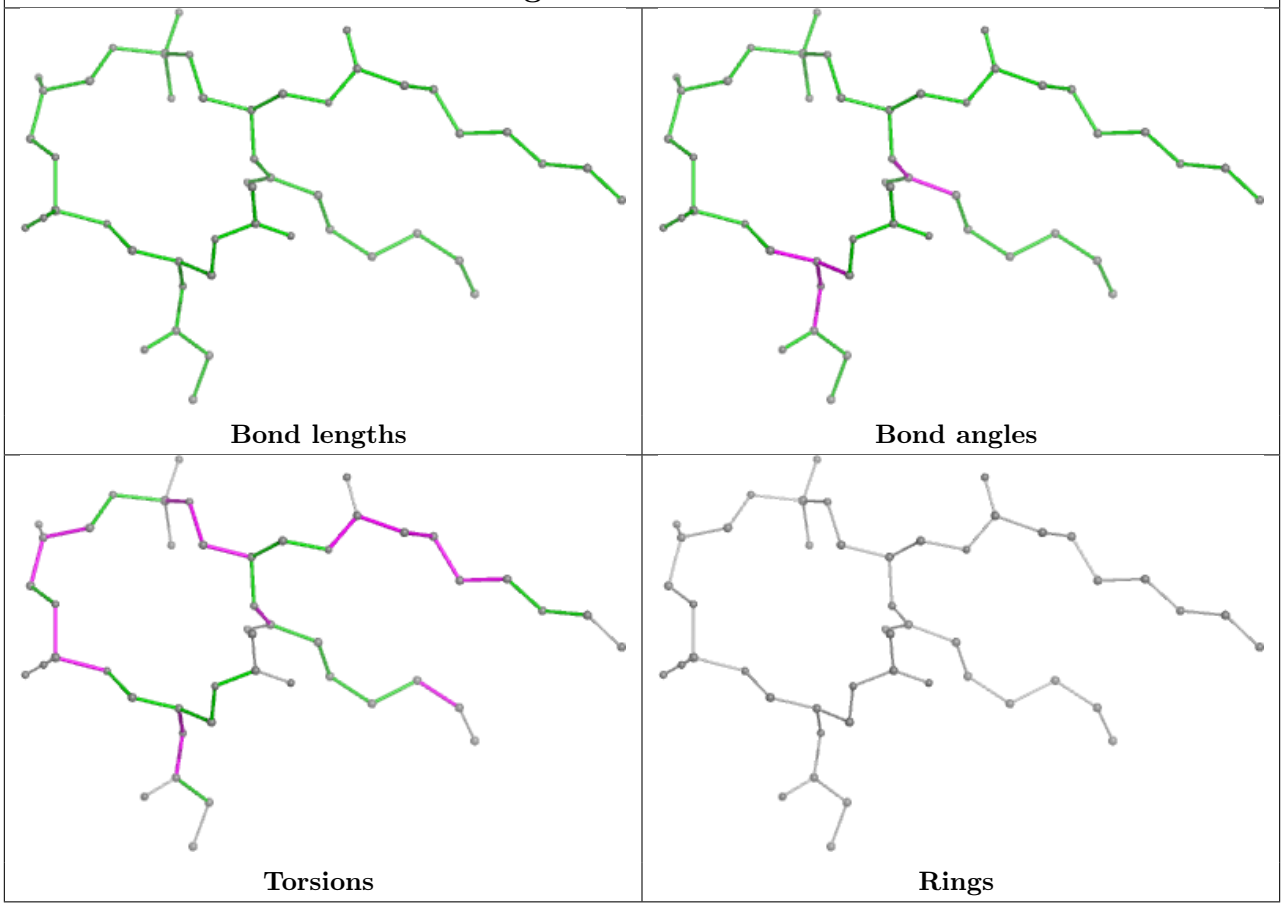


Torsions

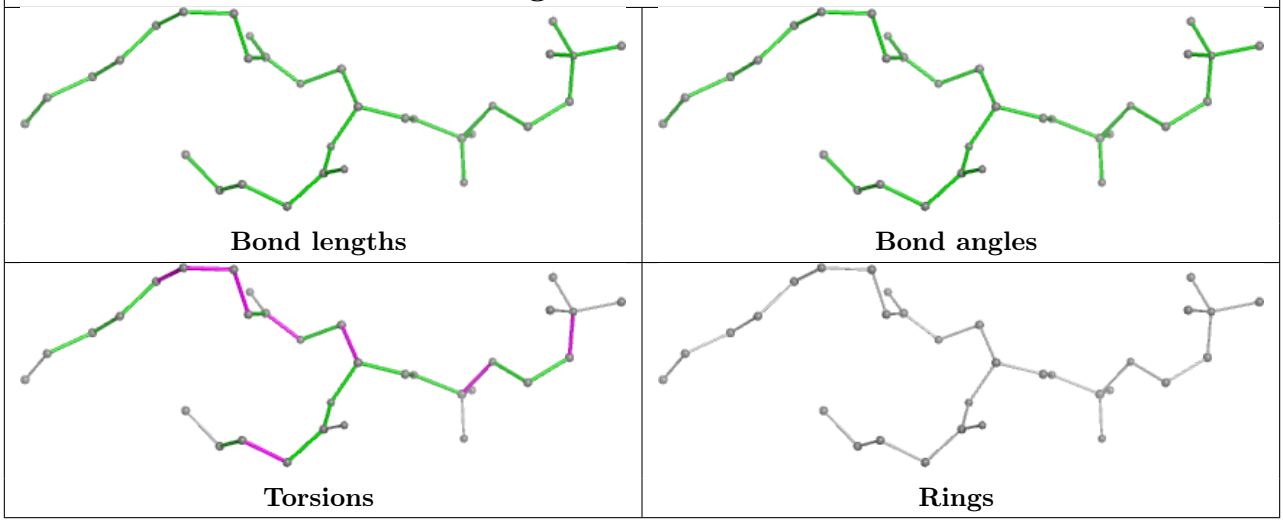


Rings

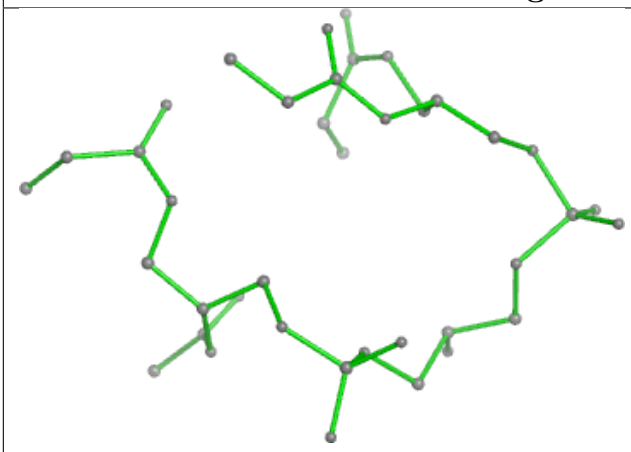
Ligand CDL N 506



Ligand PC1 T 201



Ligand CDL S 101



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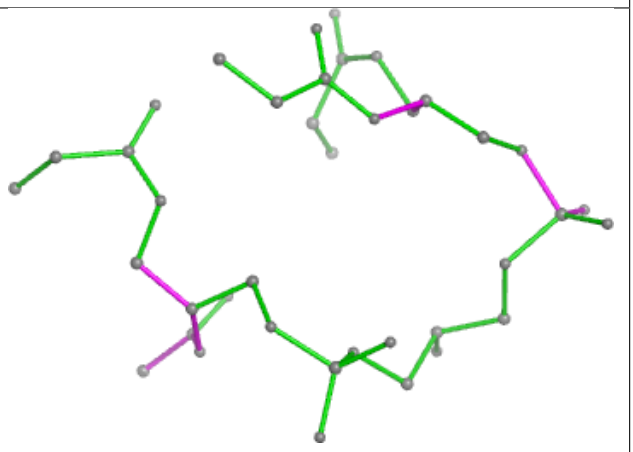
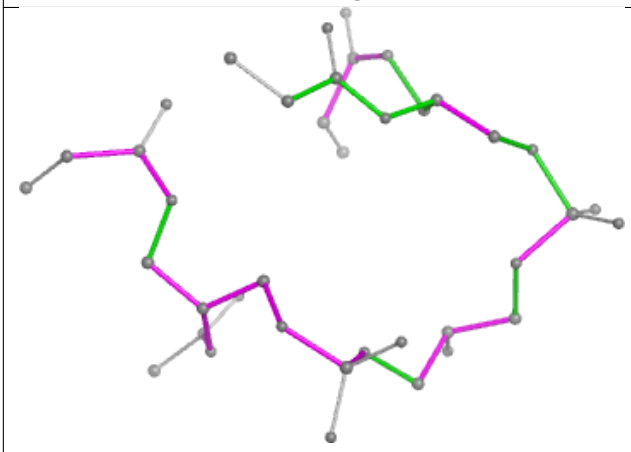
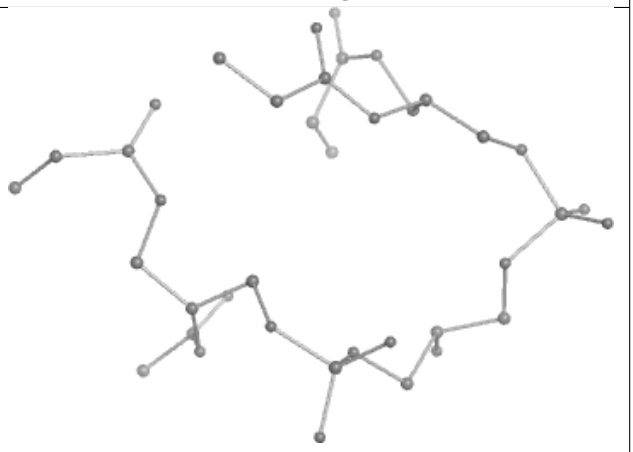


Bond angles

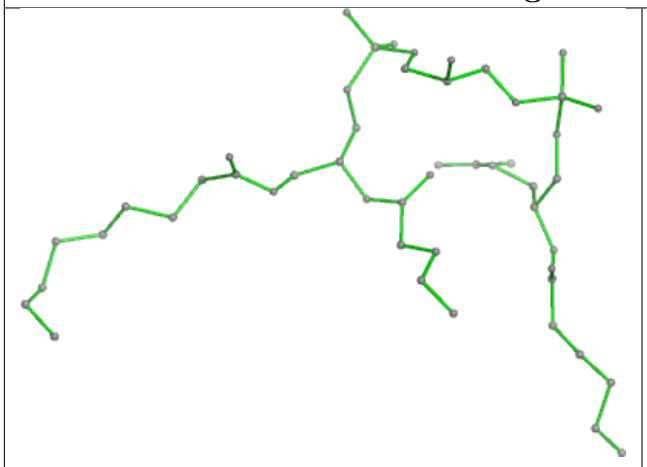


Torsions



Rings

Ligand CDL N 504



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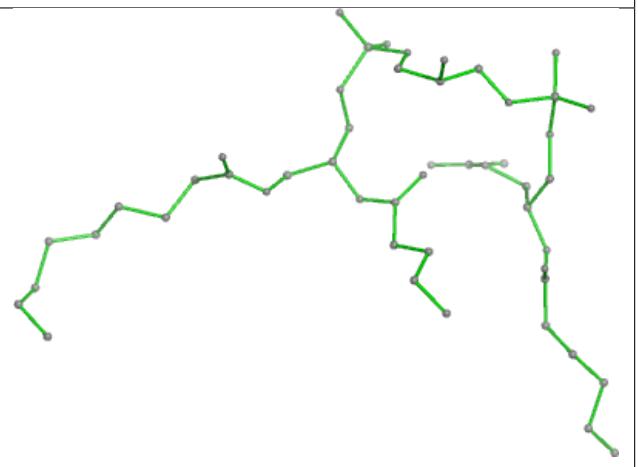

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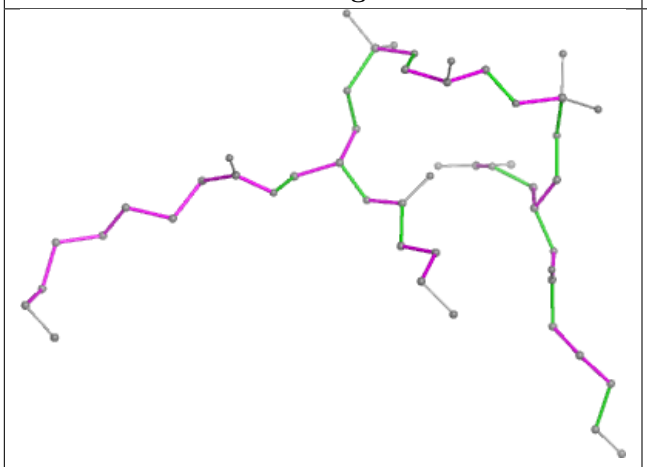

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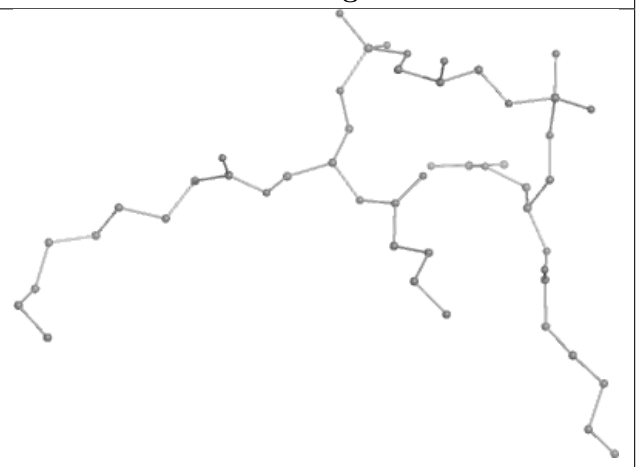
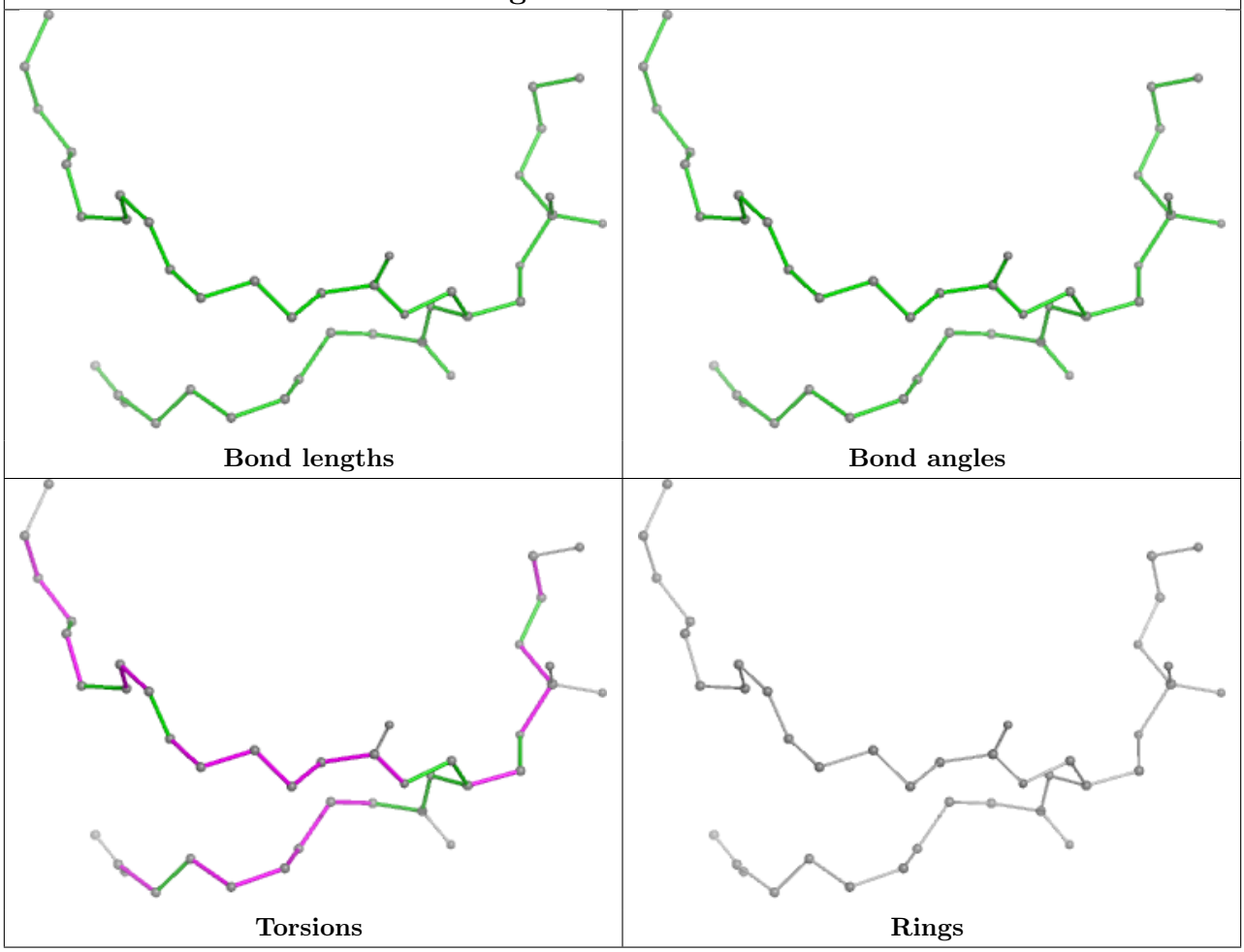
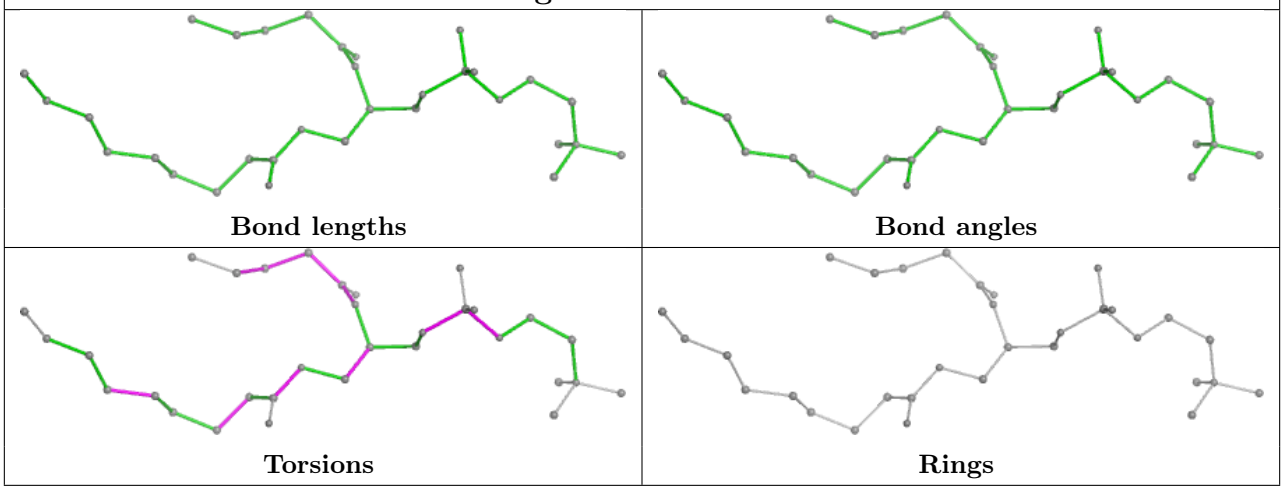


Rings

Ligand PTY E 401



Ligand PC1 I 201



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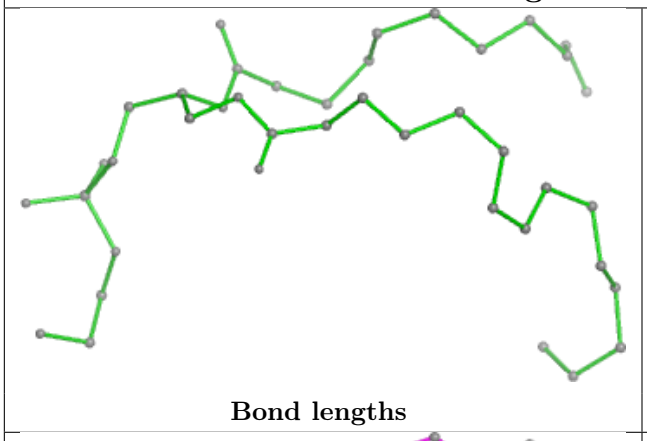

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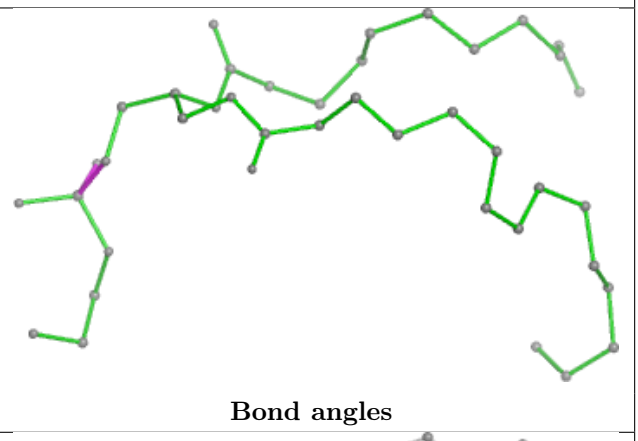
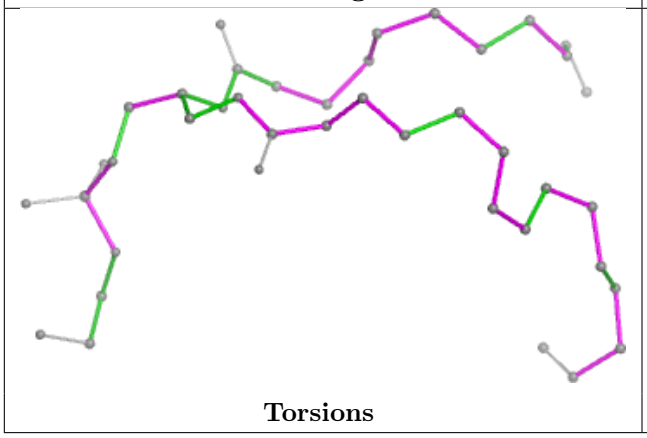


Bond angles



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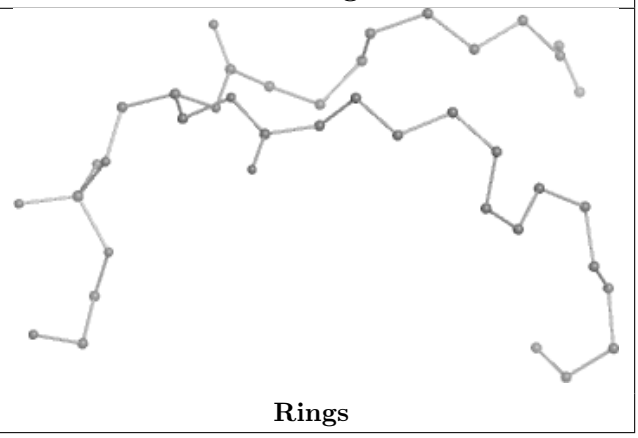
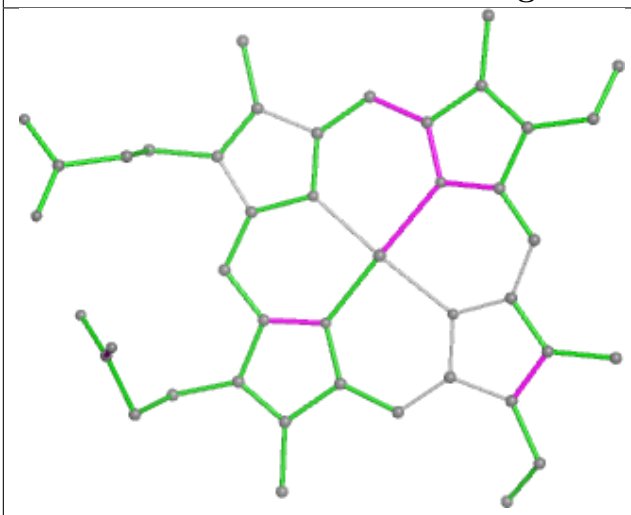


Rings

Ligand HEM N 501



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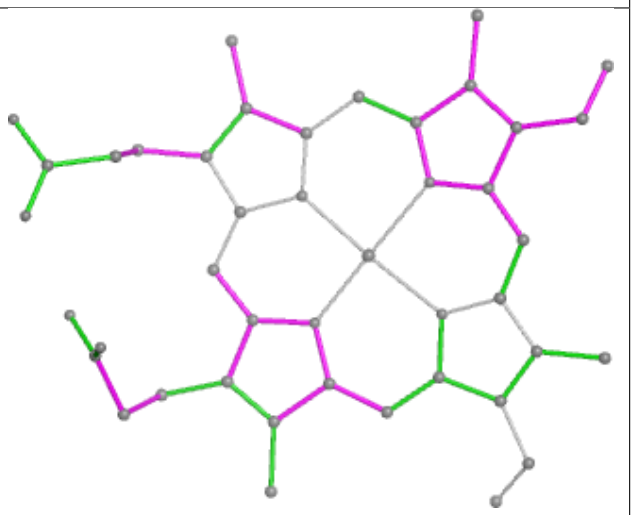
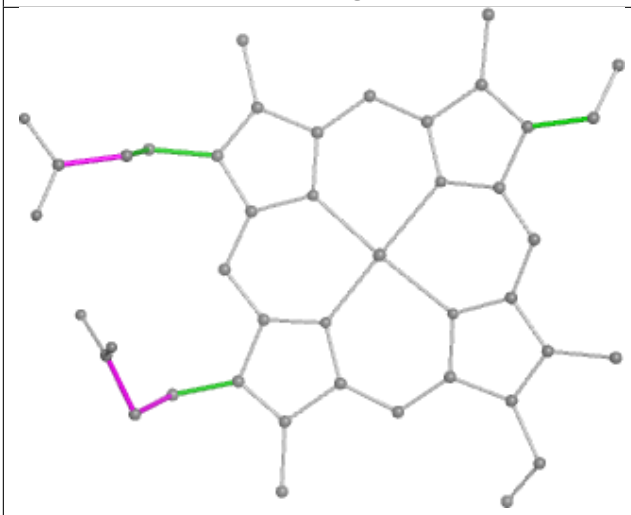
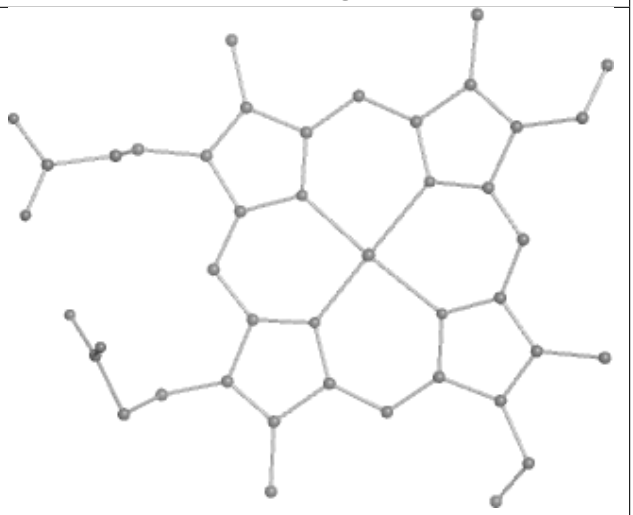


Bond angles

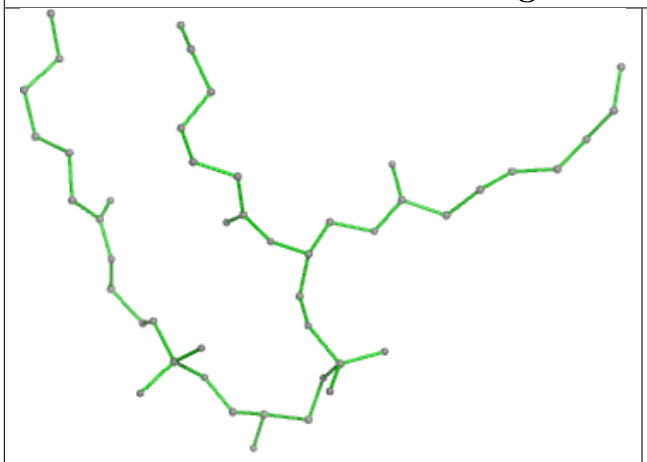


Torsions



Rings

Ligand CDL L 3002



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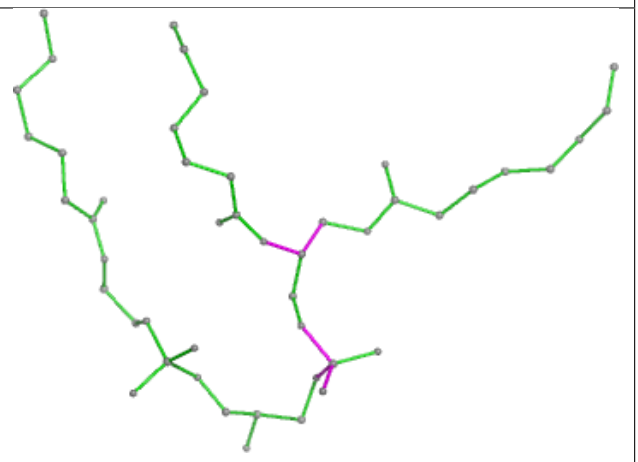

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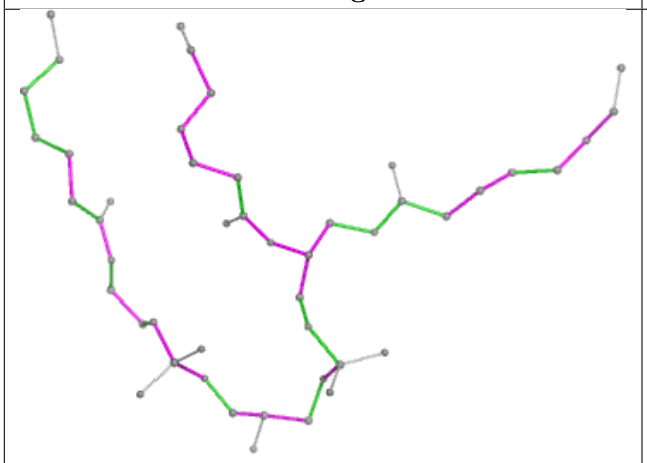
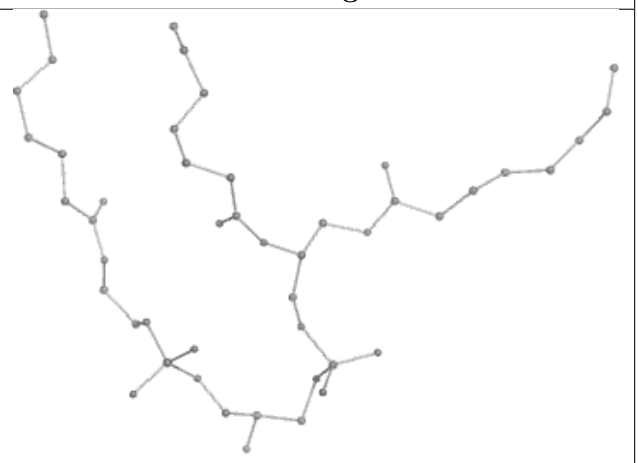
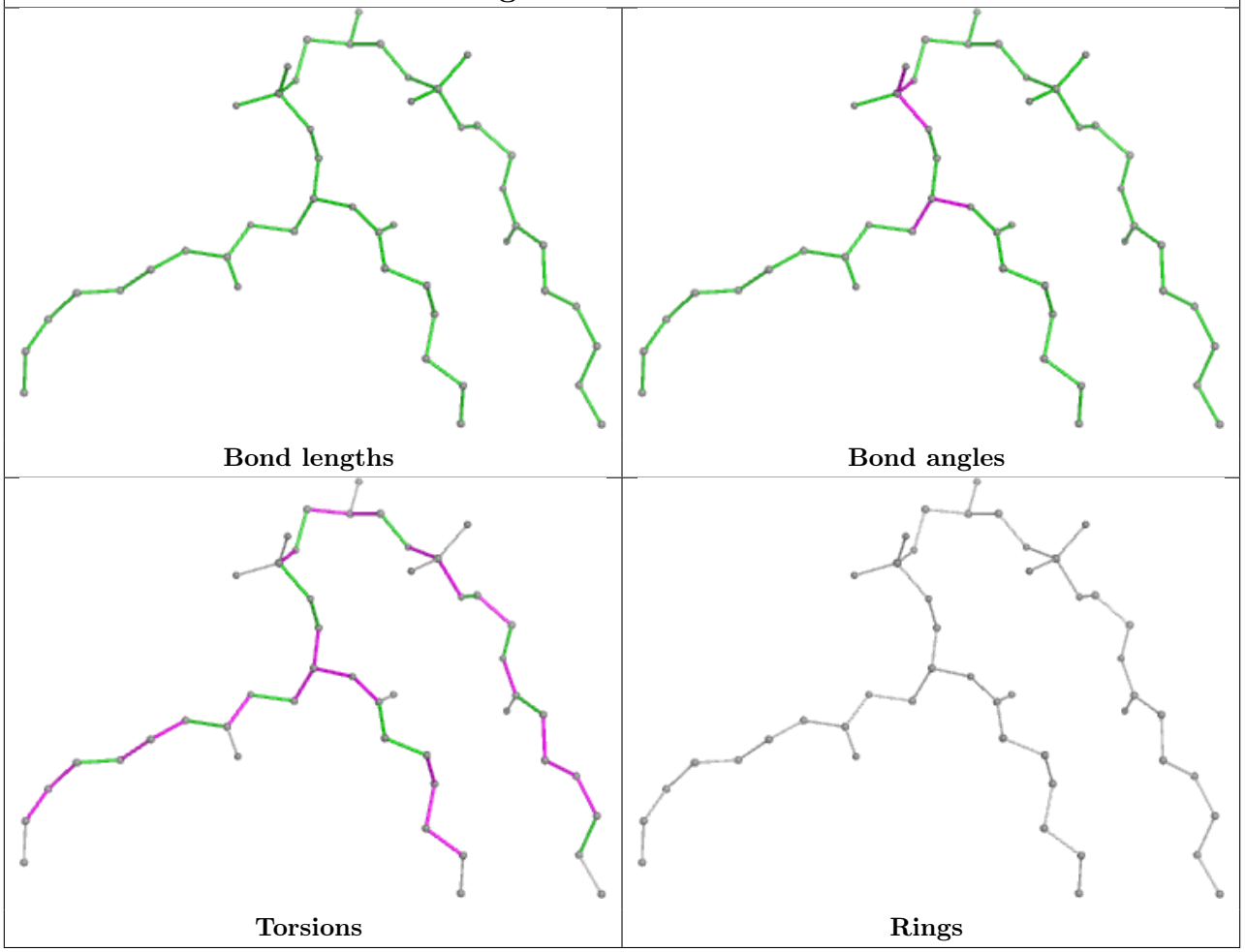


Torsions

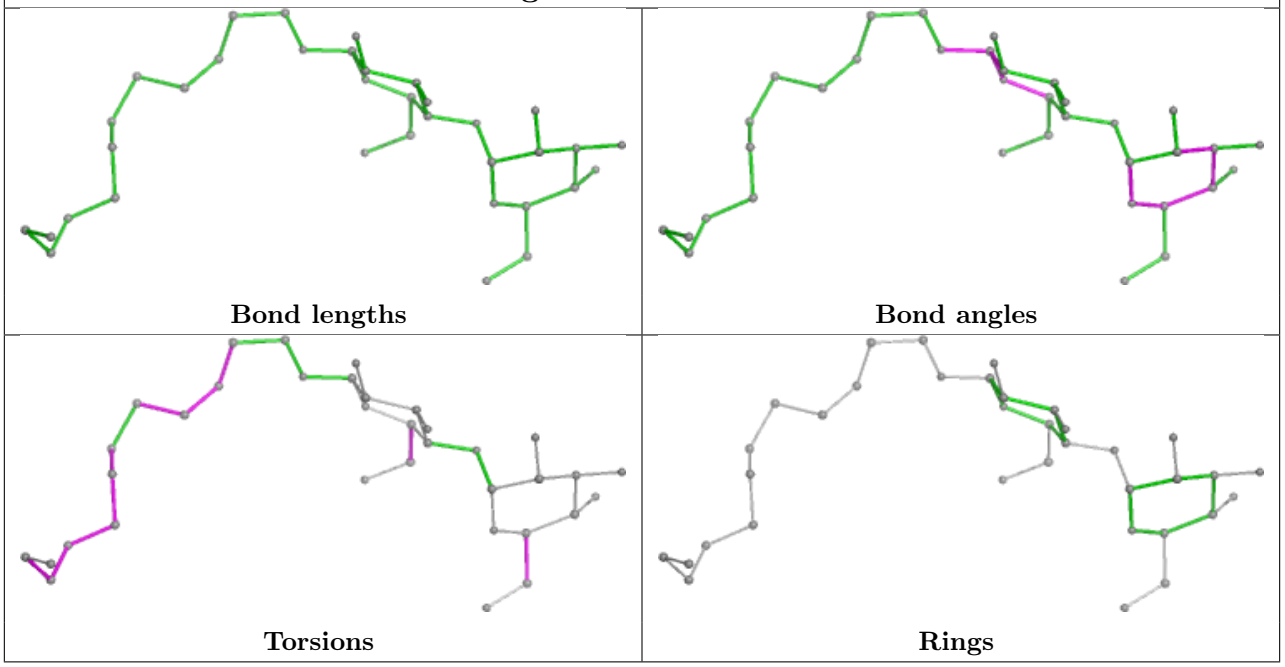


Rings

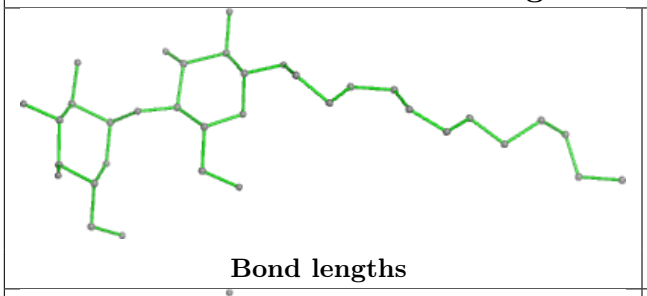
Ligand CDL A 3002



Ligand LMT N 507



Ligand LMT J 101



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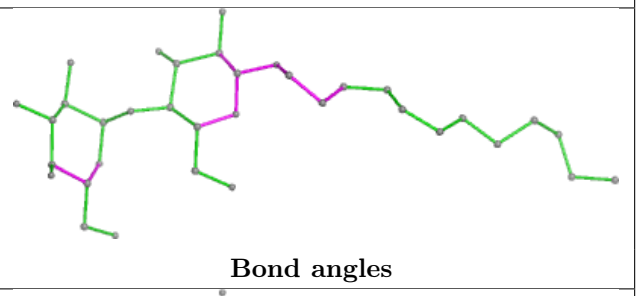
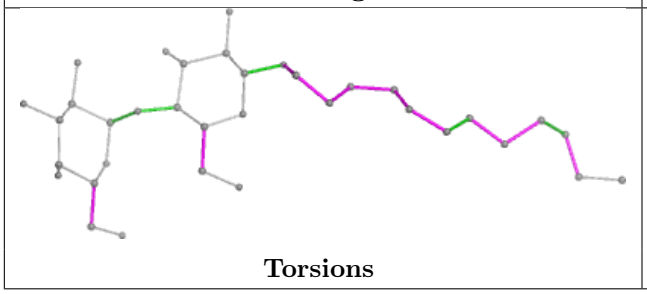


Bond angles



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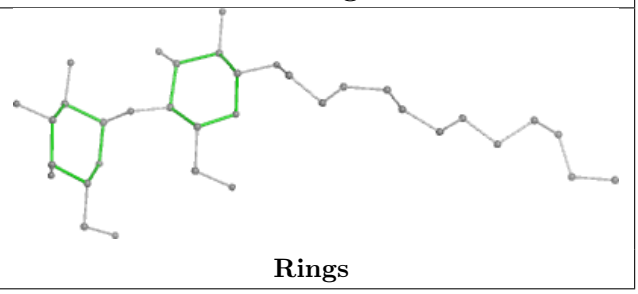
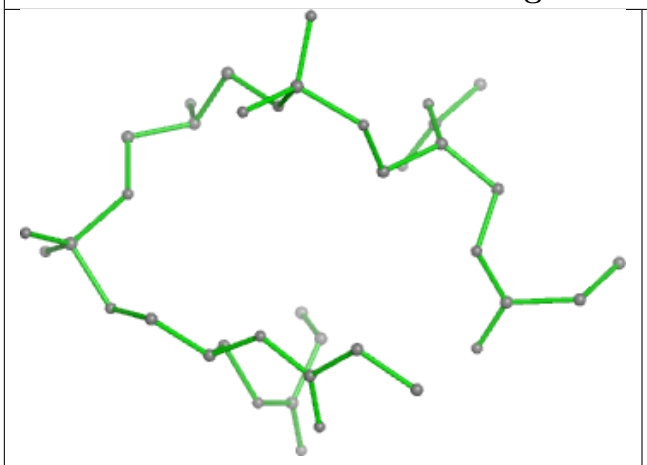


Rings

Ligand CDL D 402



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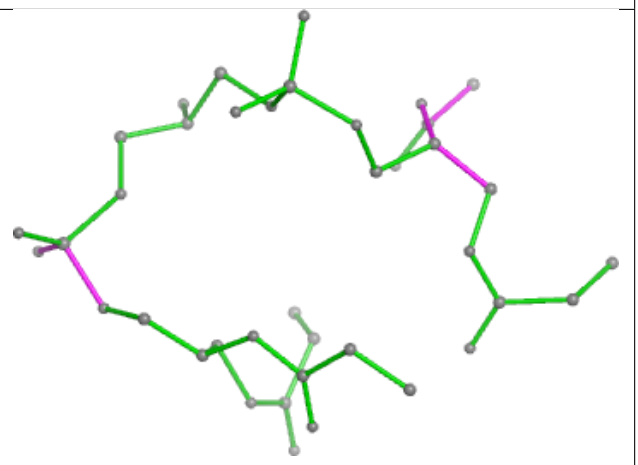
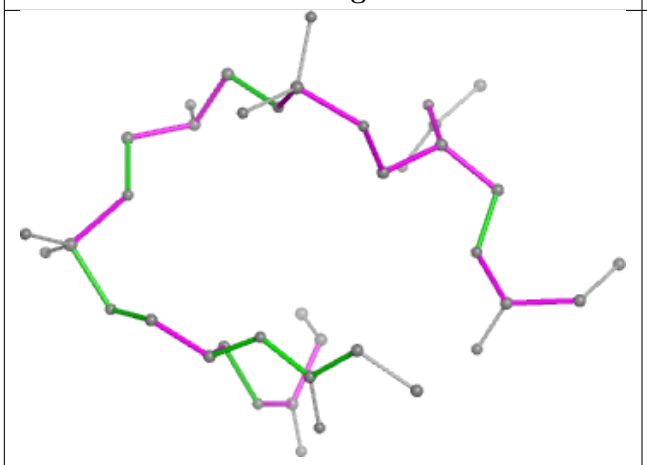


Bond angles



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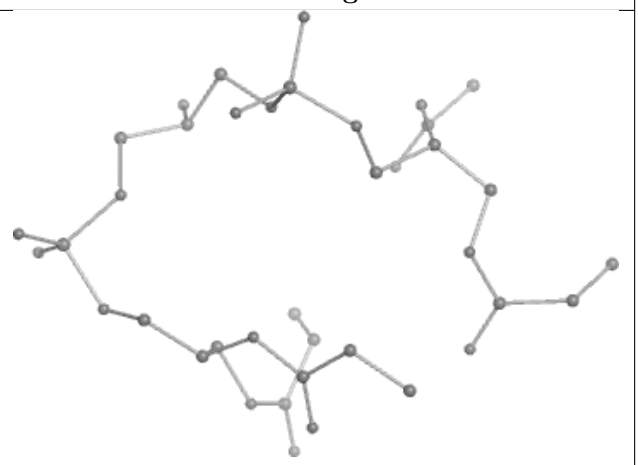
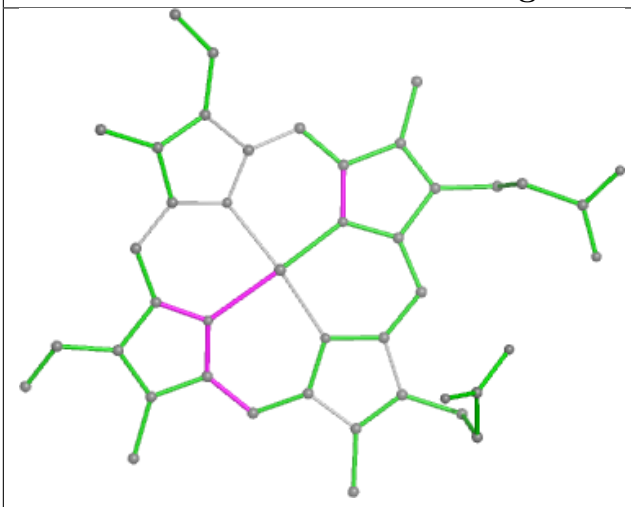


Rings

Ligand HEM C 502



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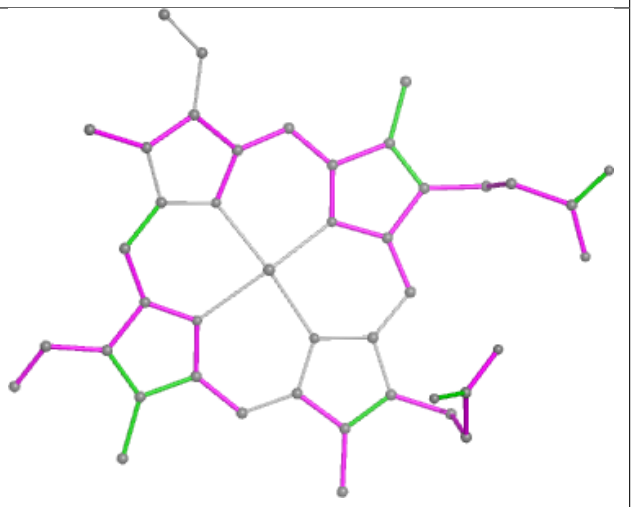

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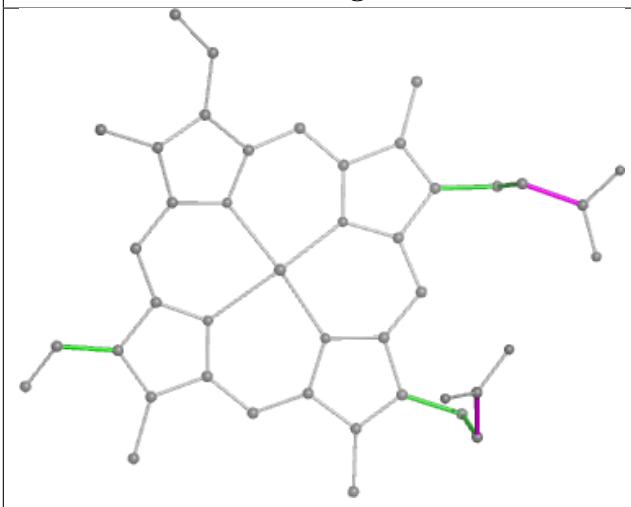

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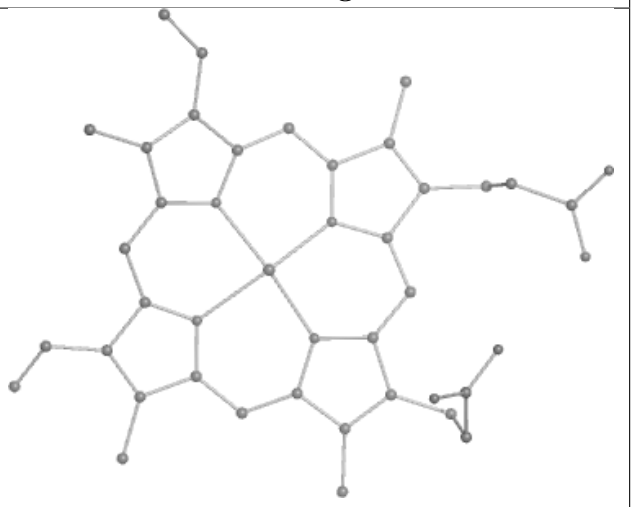
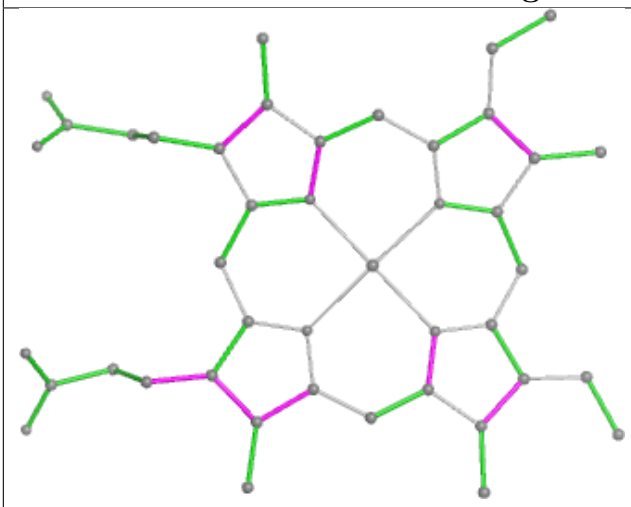


Rings

Ligand HEC D 401



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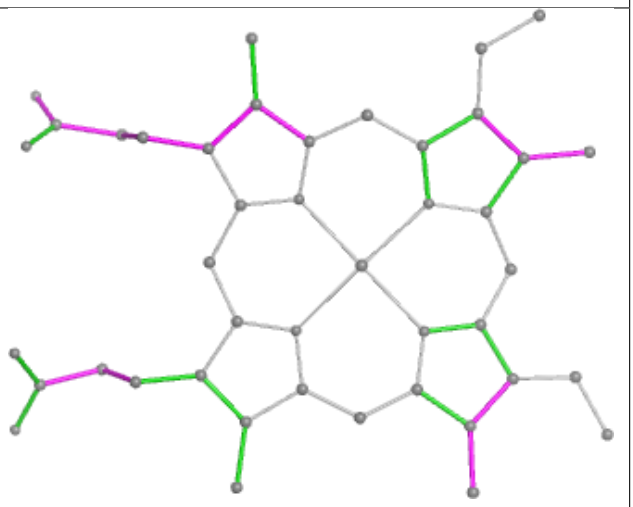
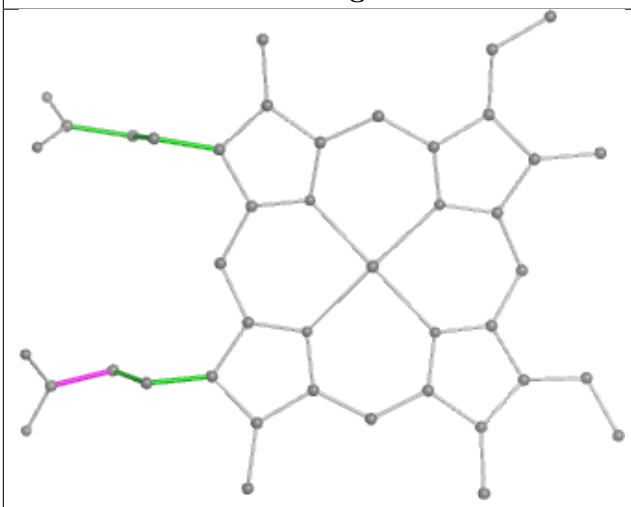
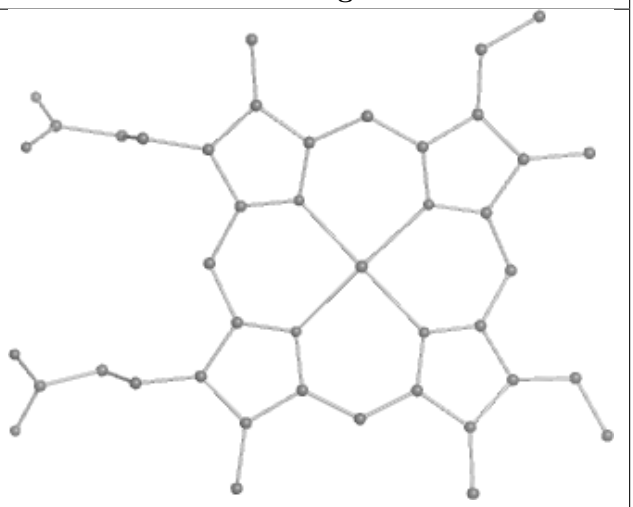


Bond angles

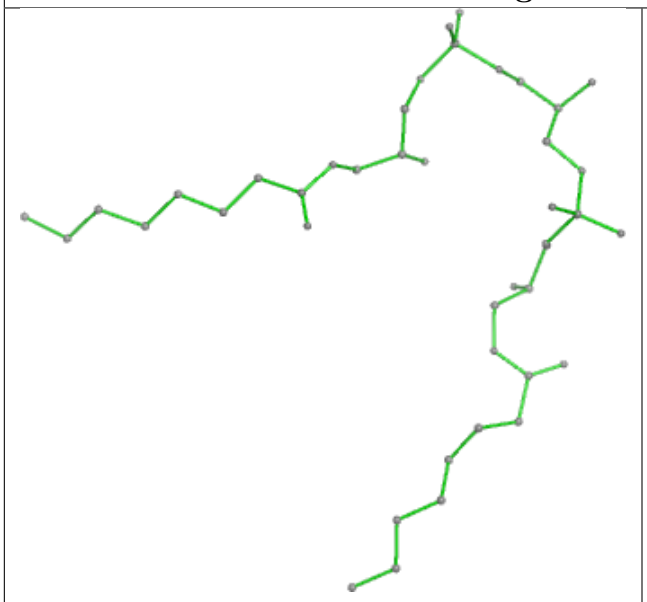


Torsions

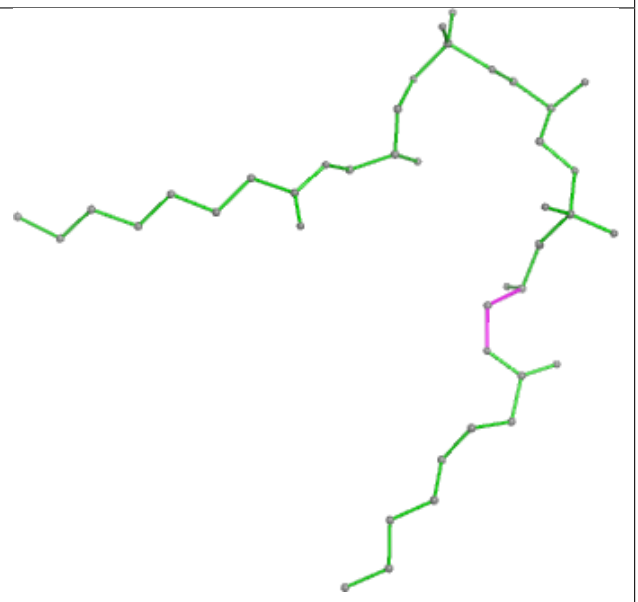


Rings

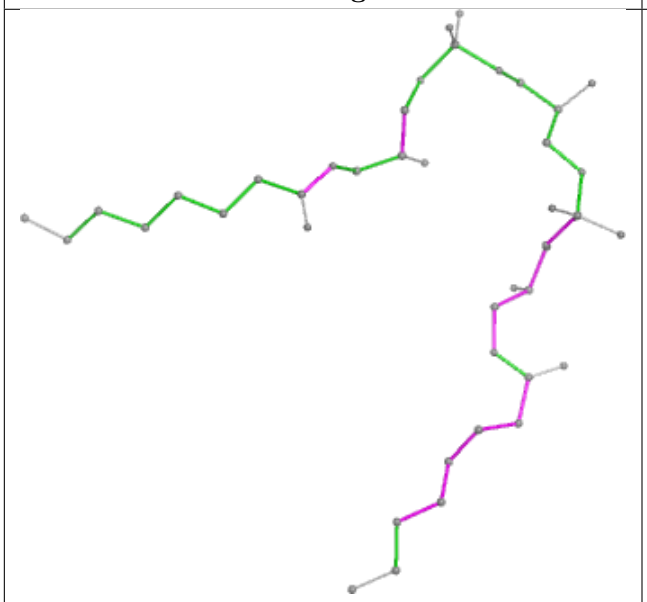
Ligand CDL A 3001



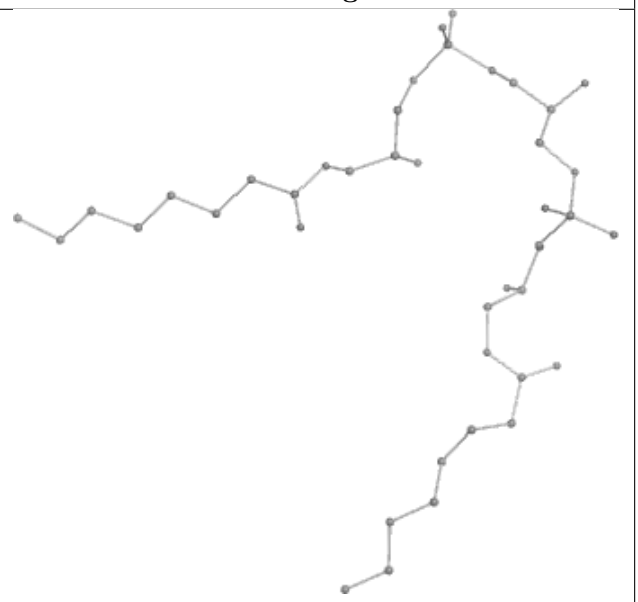
Bond lengths



Bond angles

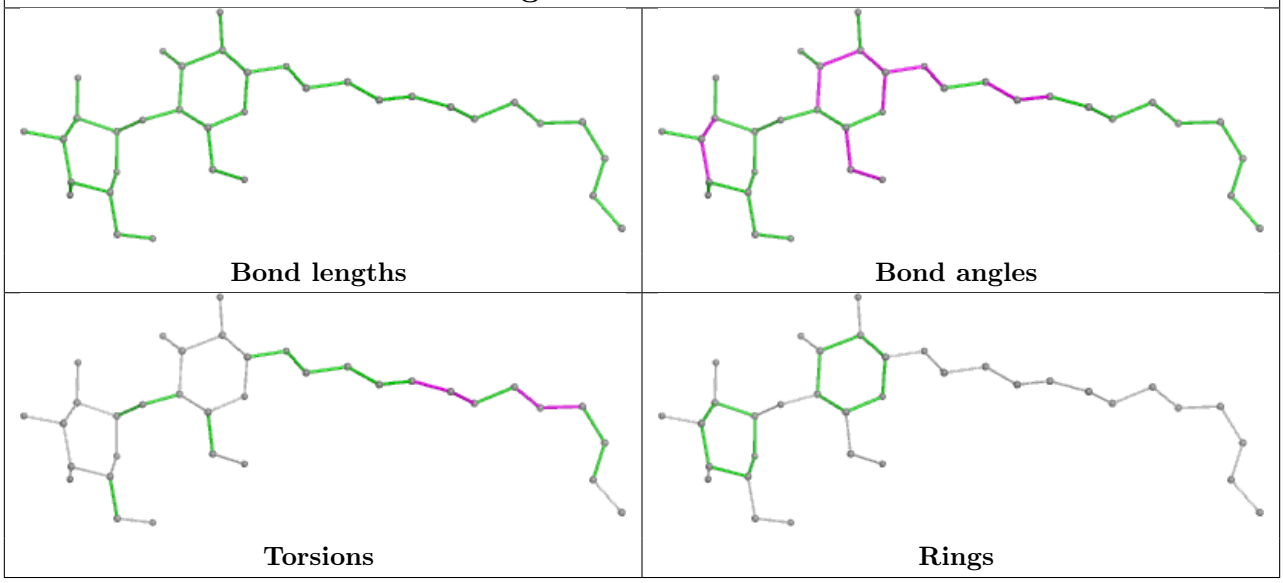


Torsions

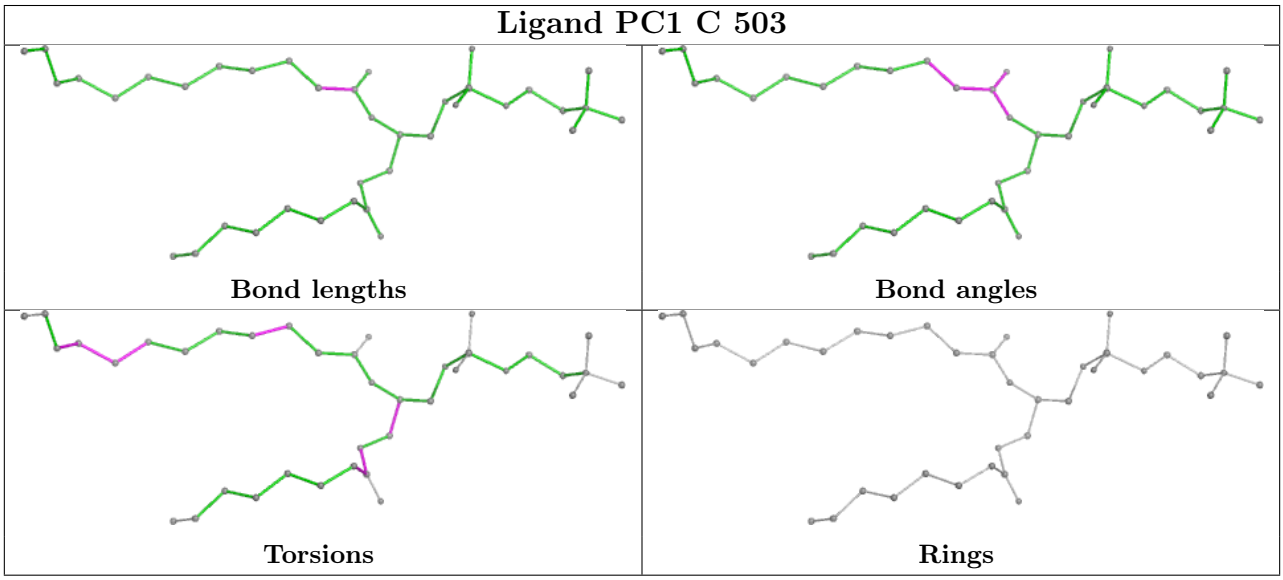


Rings

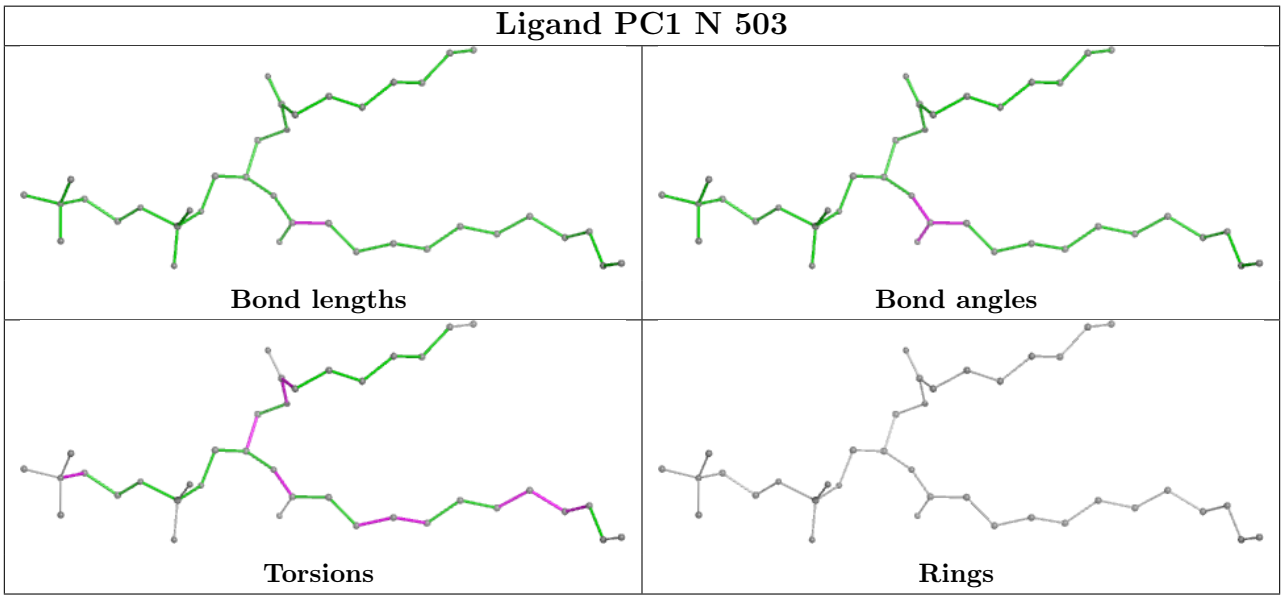
Ligand LMT U 101



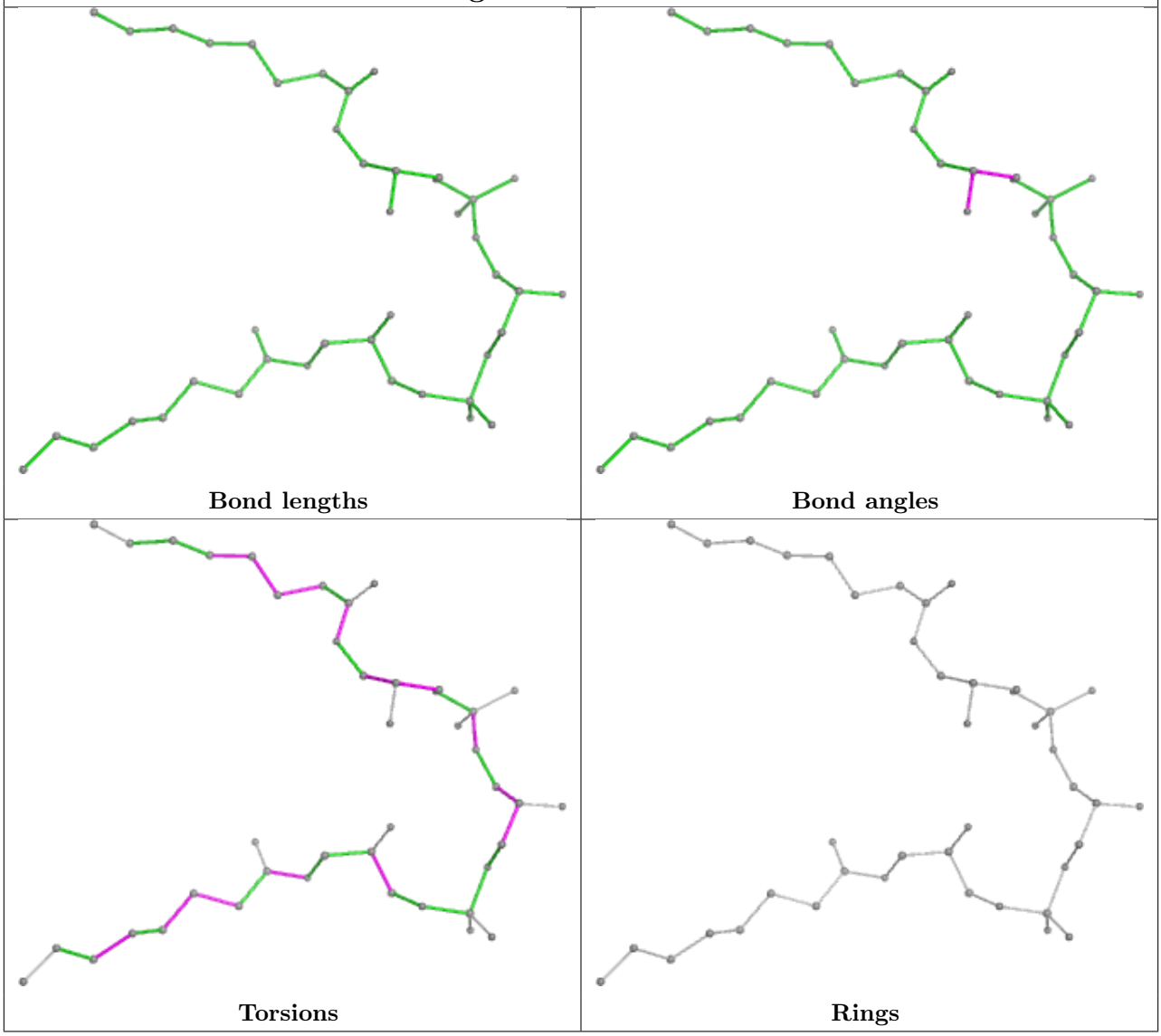
Ligand PC1 C 503



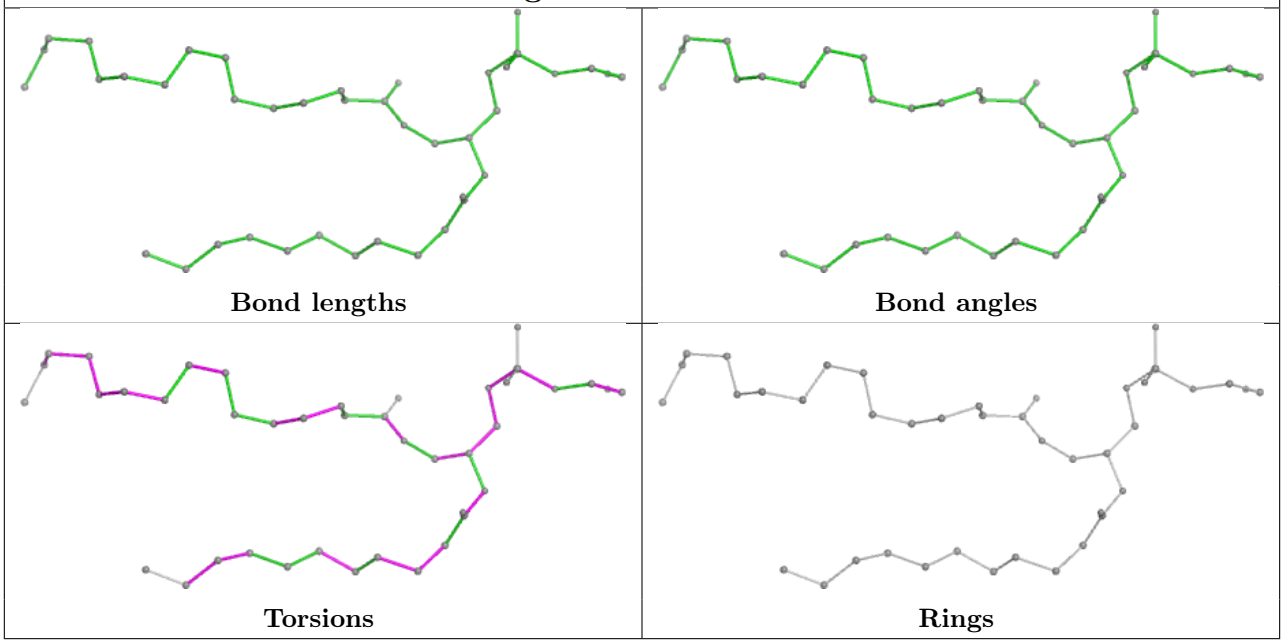
Ligand PC1 N 503



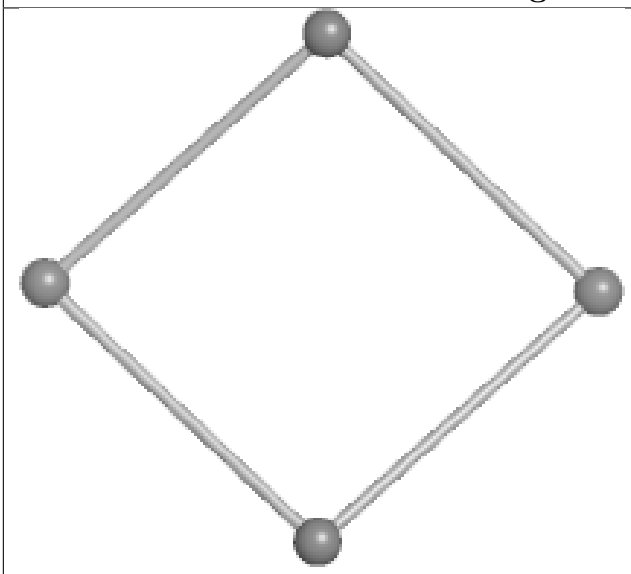
Ligand CDL L 3001



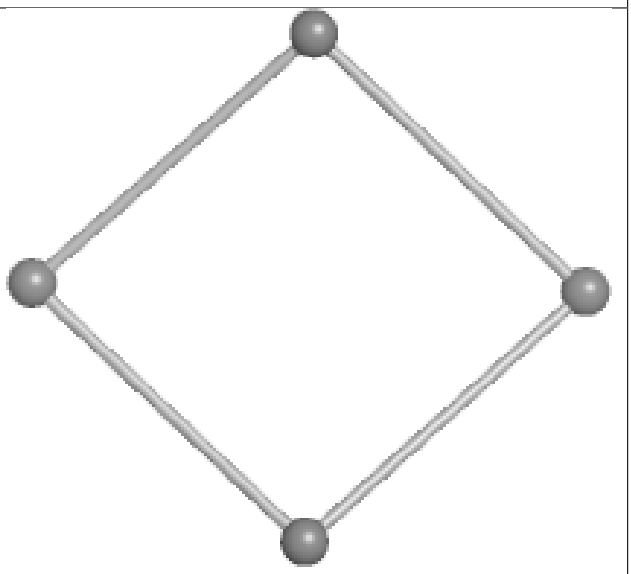
Ligand PTY C 504



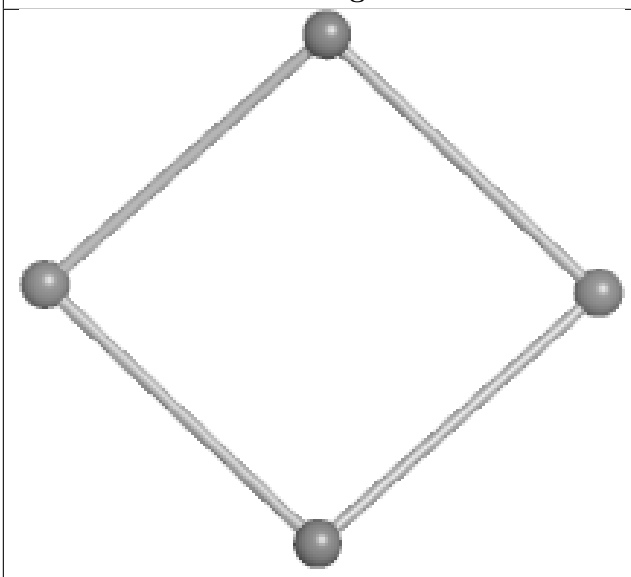
Ligand FES P 301



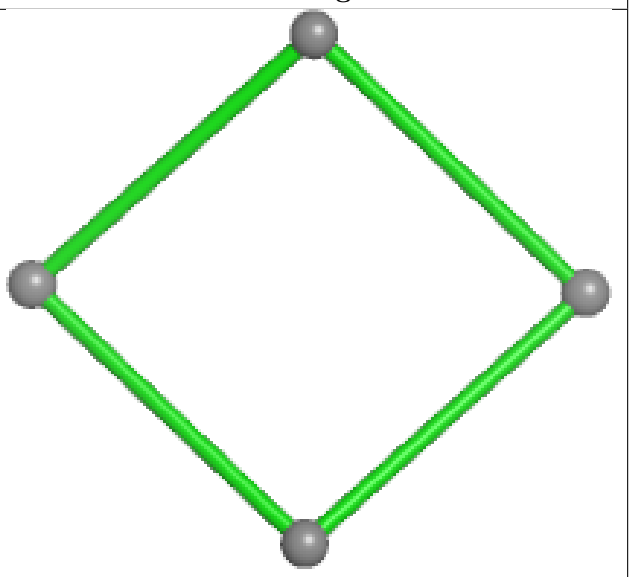
Bond lengths



Bond angles

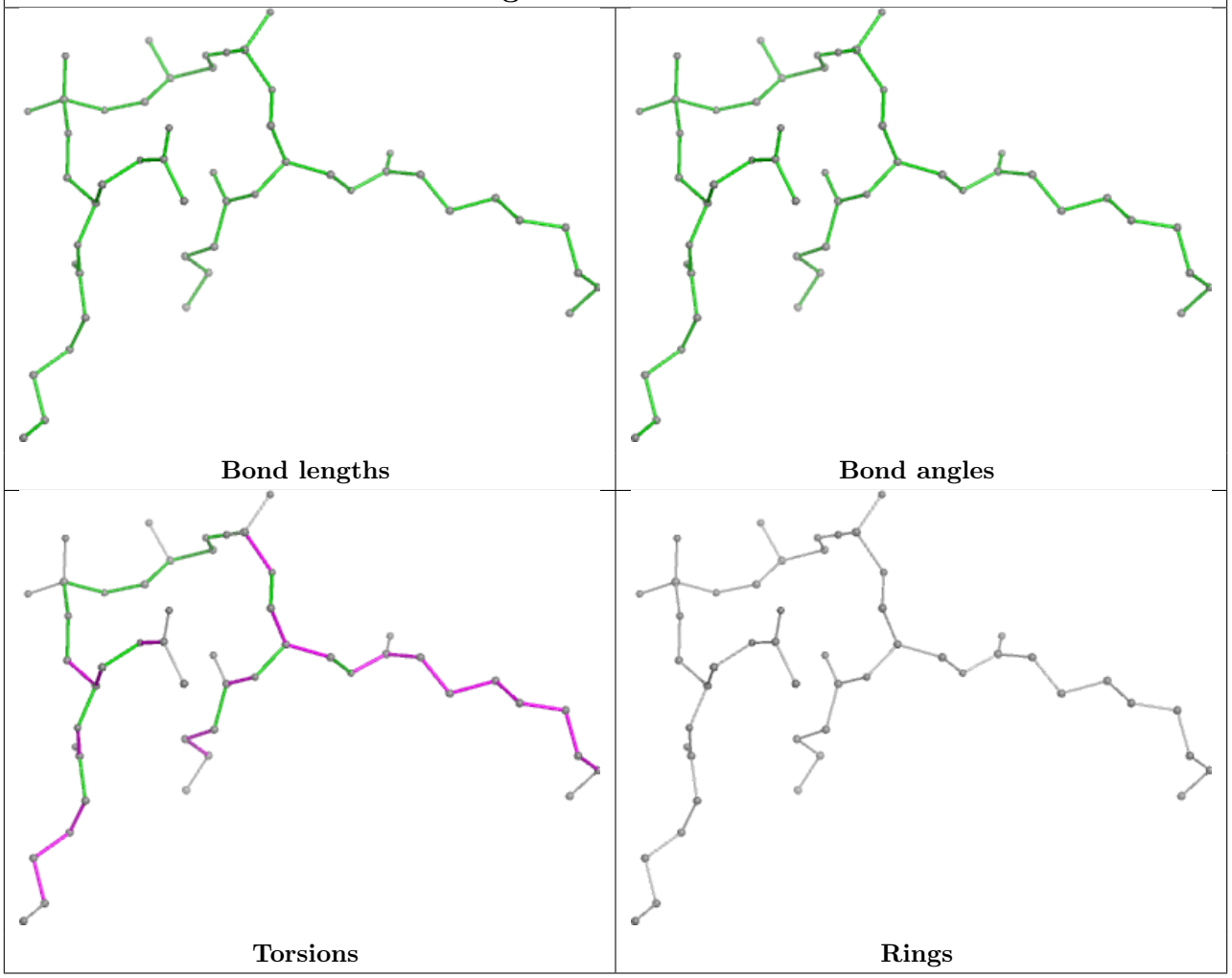


Torsions

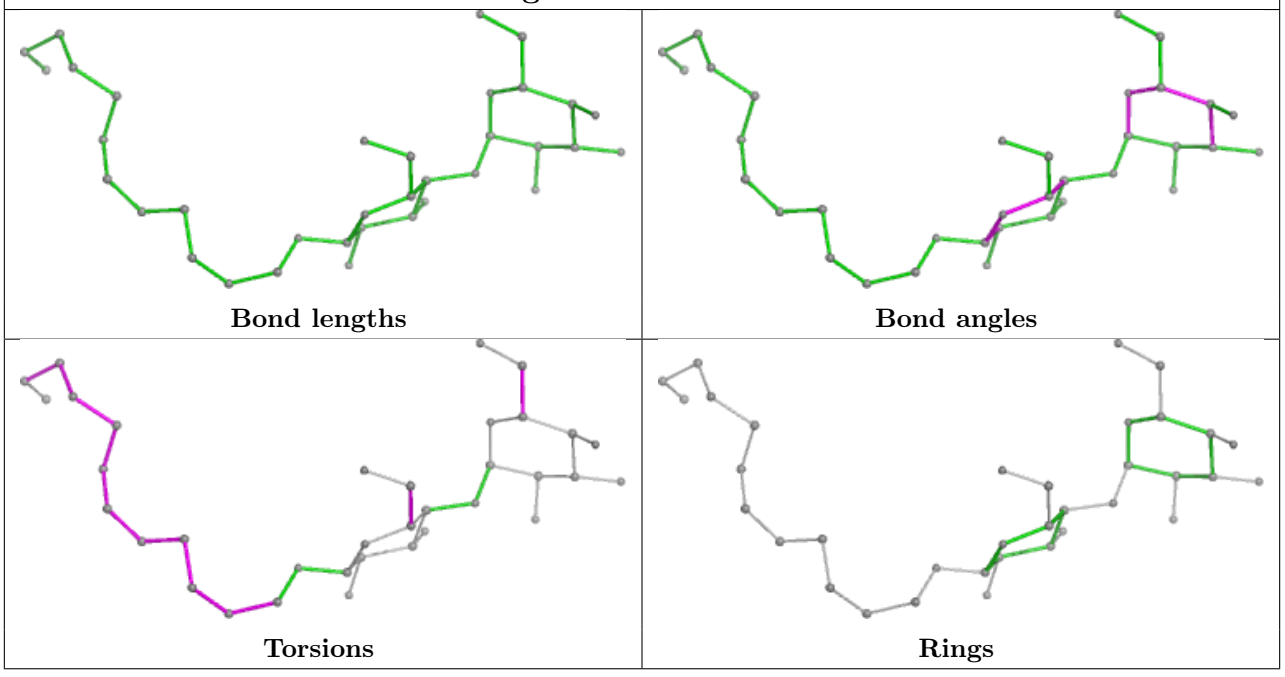


Rings

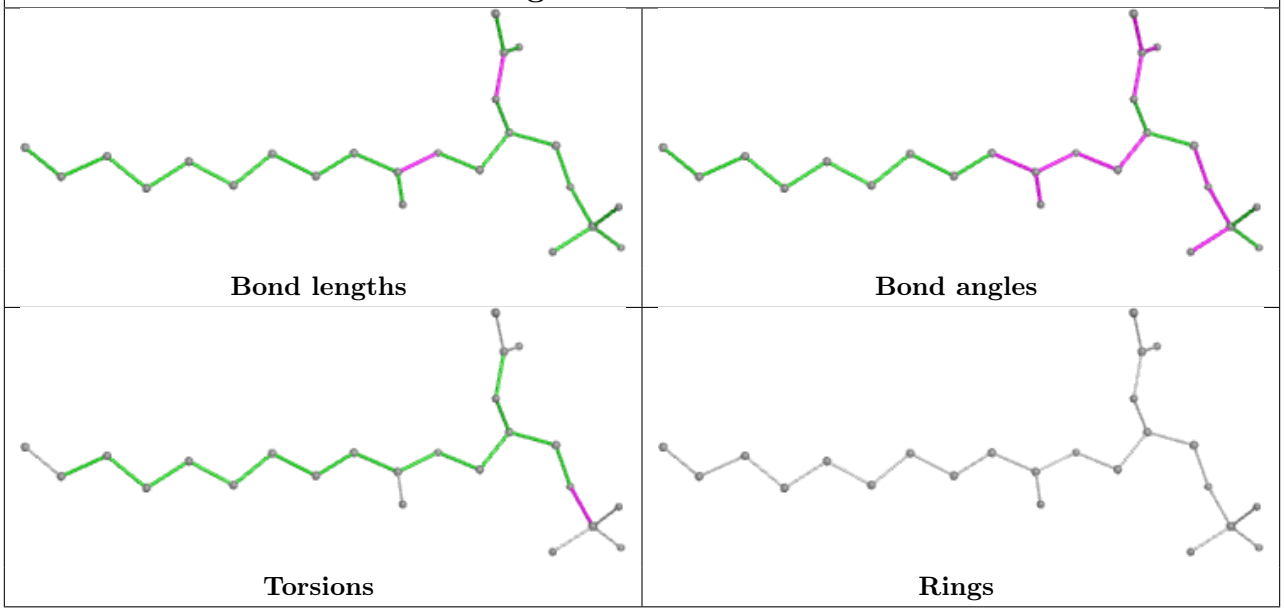
Ligand CDL H 701



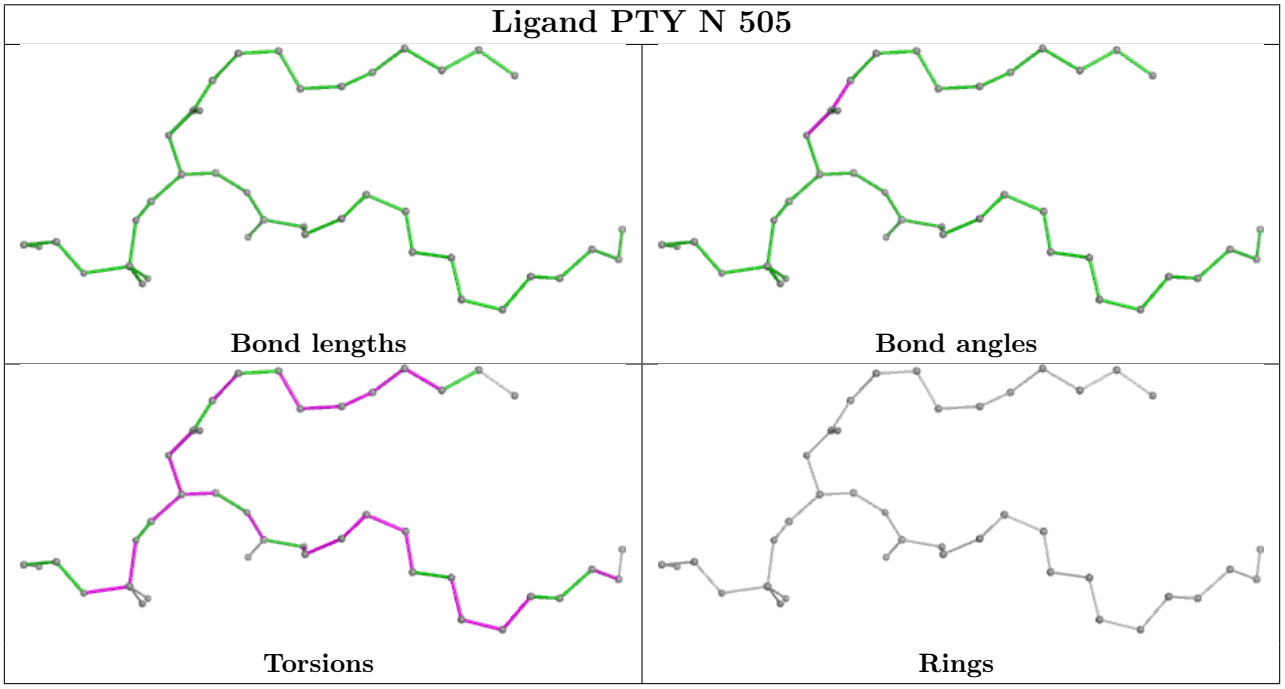
Ligand LMT C 506



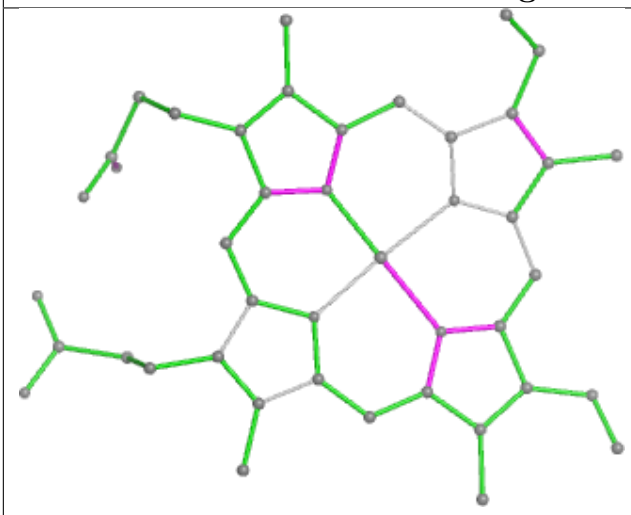
Ligand XP4 U 102



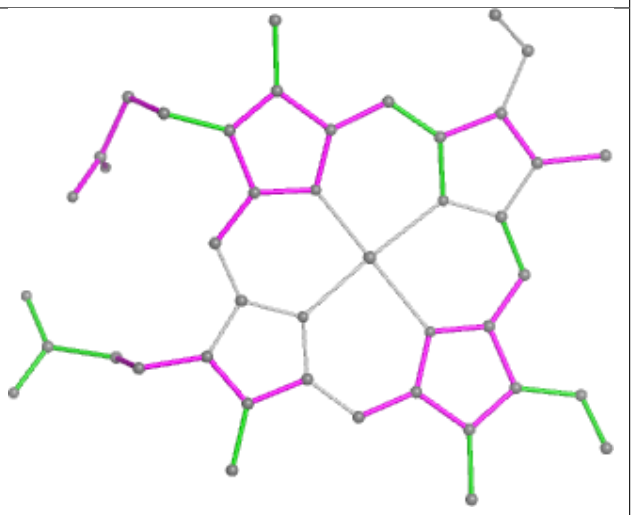
Ligand PTY N 505



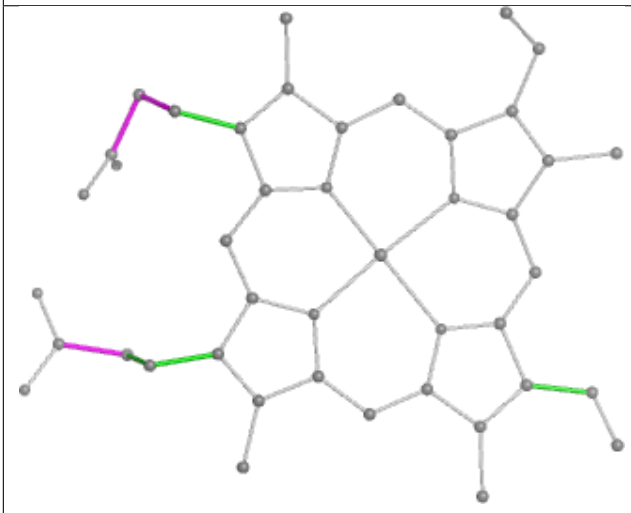
Ligand HEM C 501



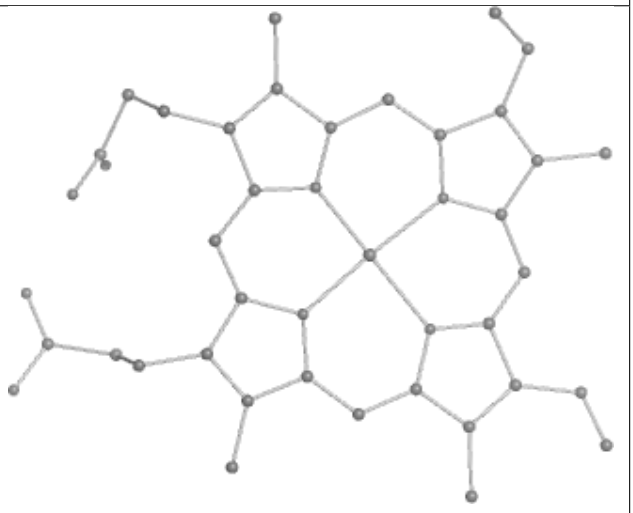
Bond lengths



Bond angles

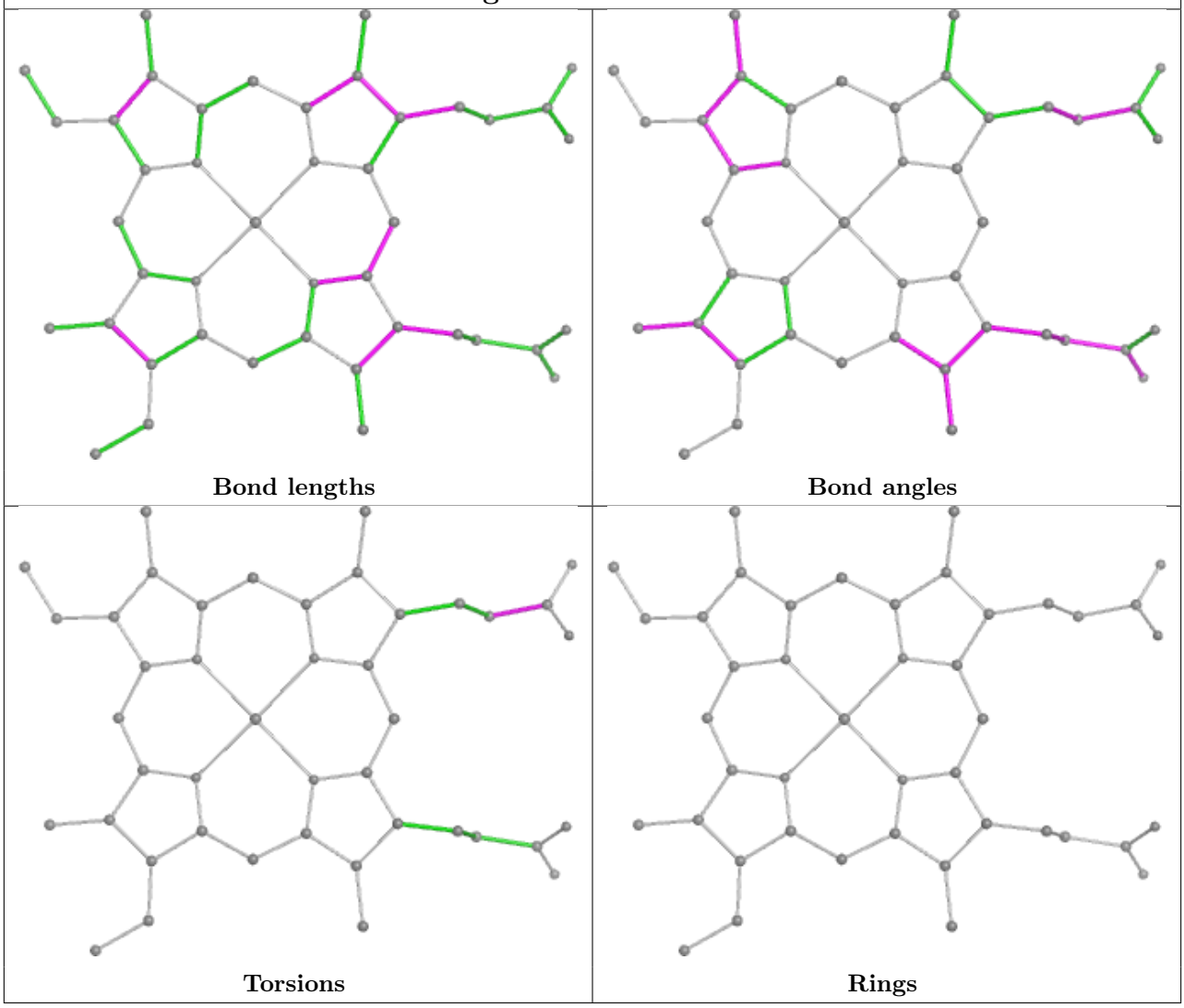


Torsions



Rings

Ligand HEC O 401



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.

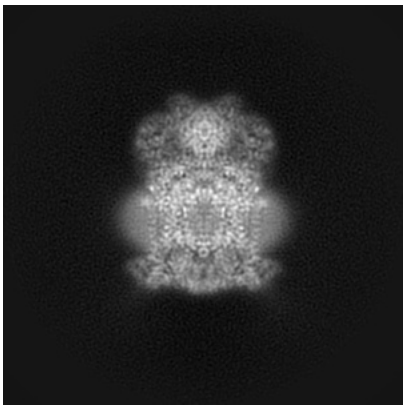
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15332. These allow visual inspection of the internal detail of the map and identification of artifacts.

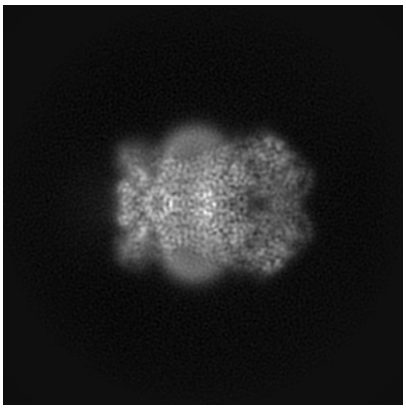
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

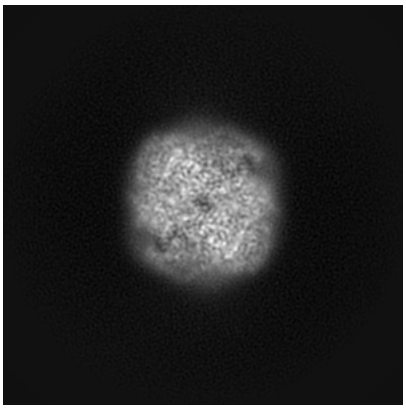
6.1.1 Primary map



X

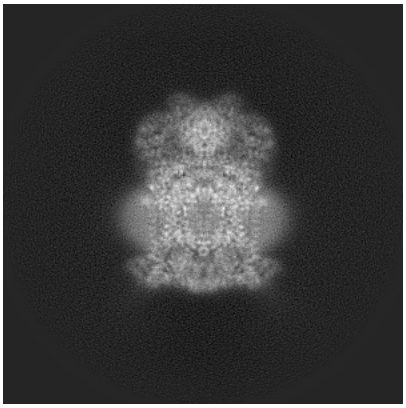


Y

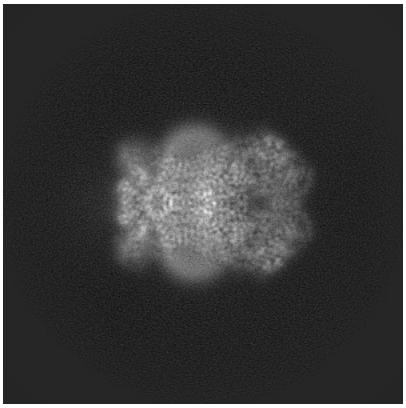


Z

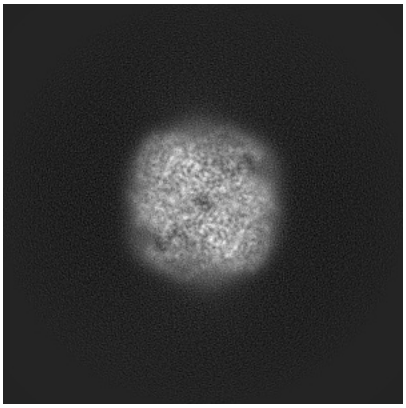
6.1.2 Raw map



X



Y

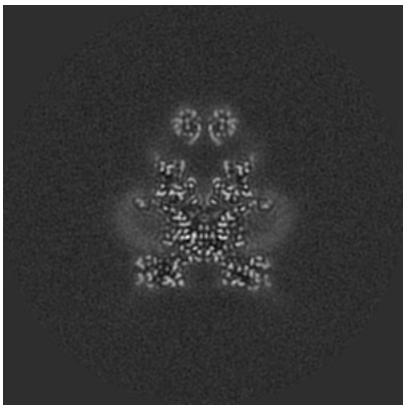


Z

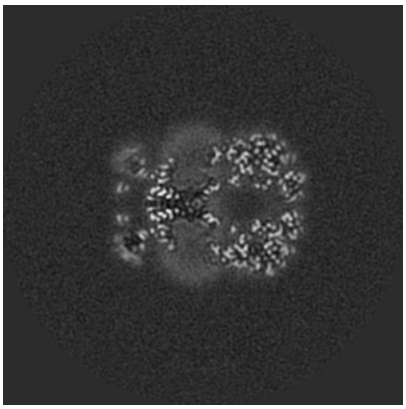
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

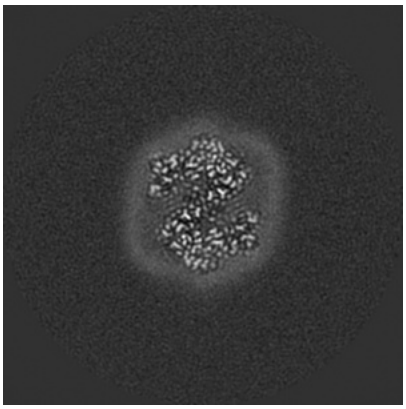
6.2.1 Primary map



X Index: 180

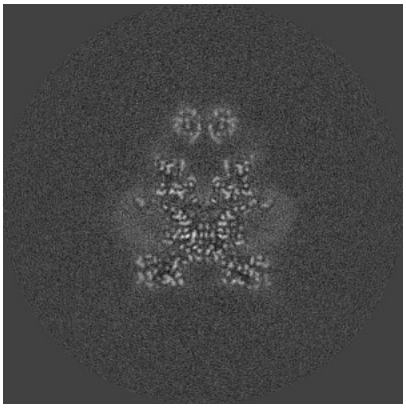


Y Index: 180

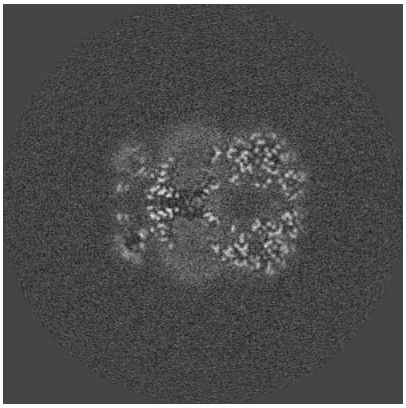


Z Index: 180

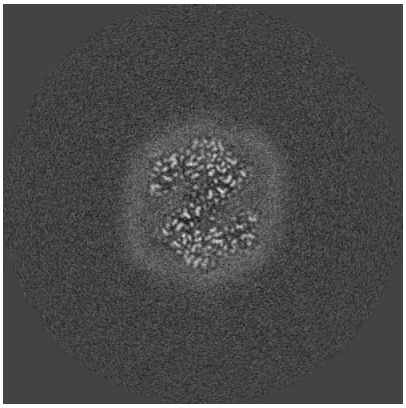
6.2.2 Raw map



X Index: 180



Y Index: 180

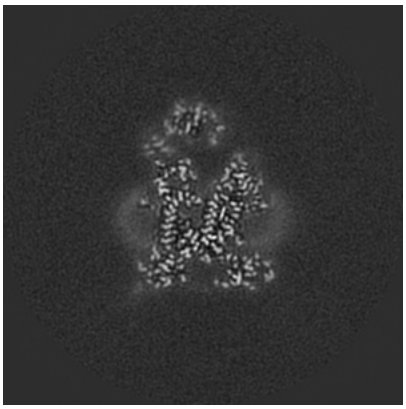


Z Index: 180

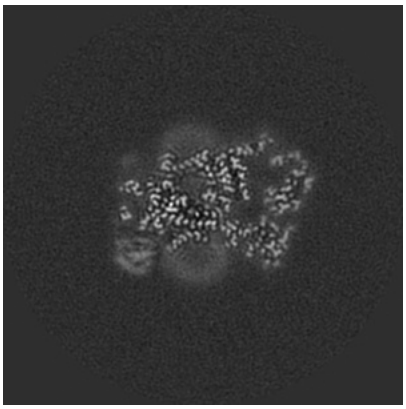
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

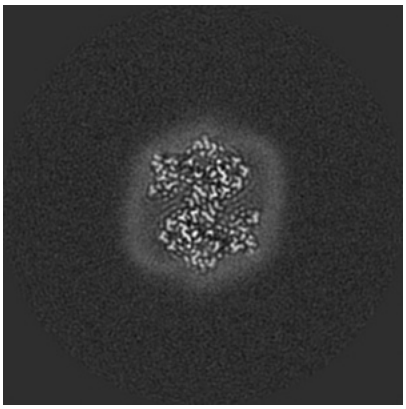
6.3.1 Primary map



X Index: 187

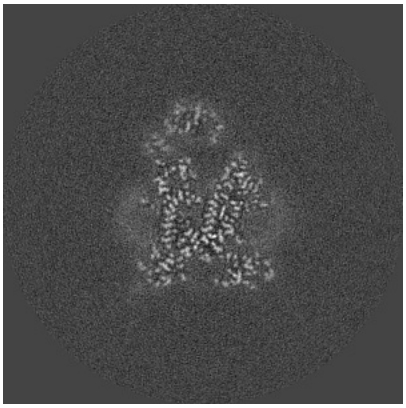


Y Index: 166

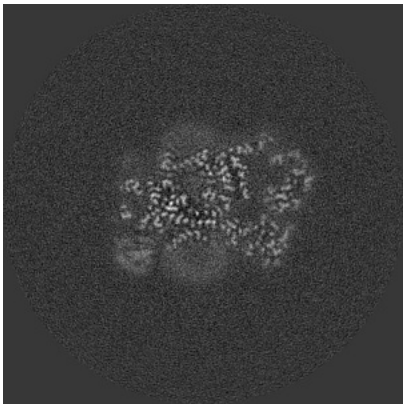


Z Index: 182

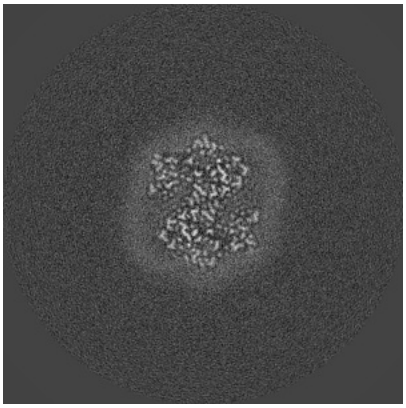
6.3.2 Raw map



X Index: 187



Y Index: 166

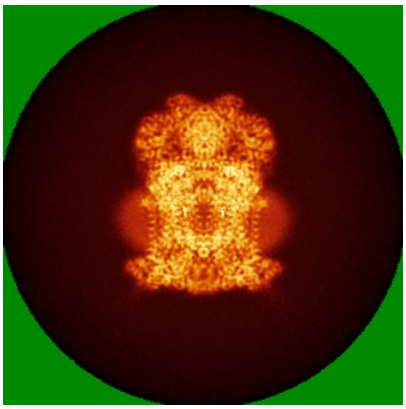


Z Index: 182

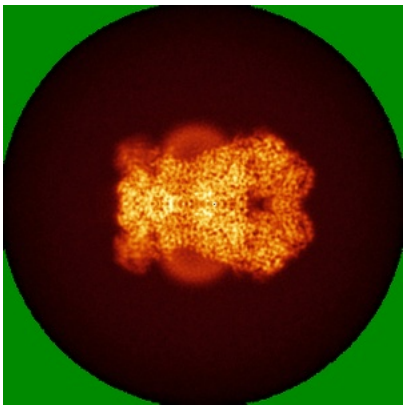
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

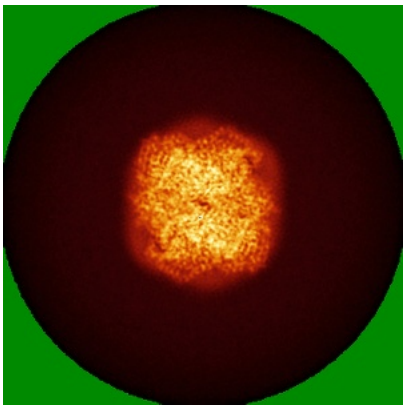
6.4.1 Primary map



X

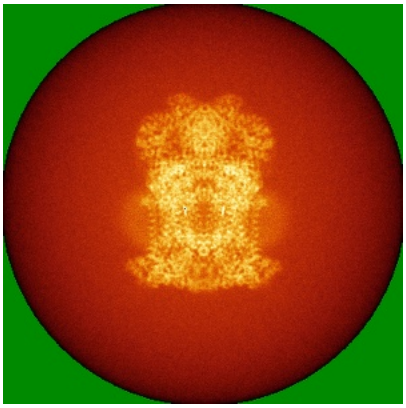


Y

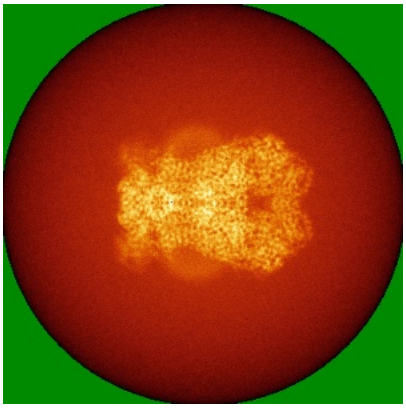


Z

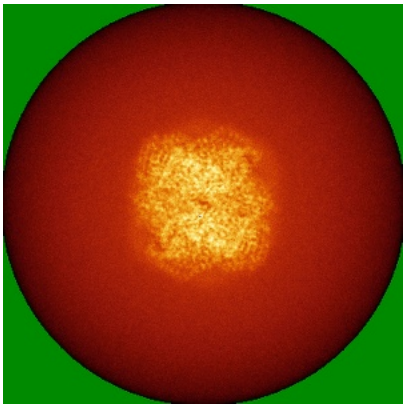
6.4.2 Raw map



X



Y

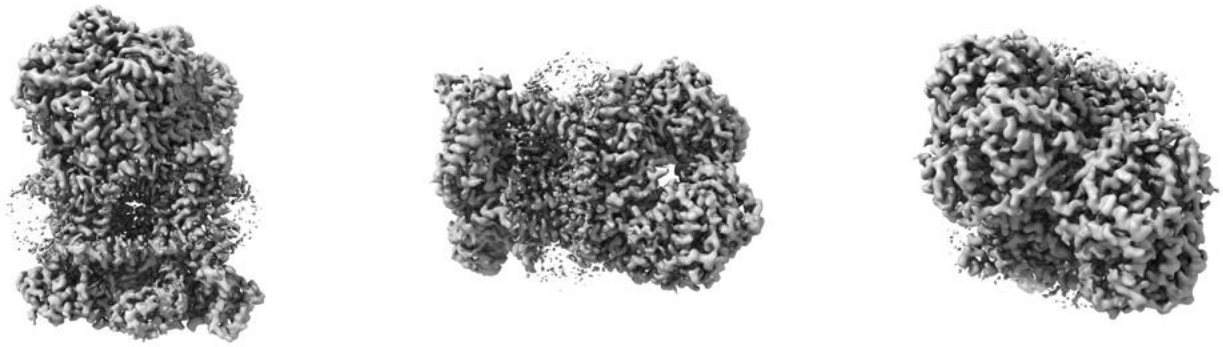


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

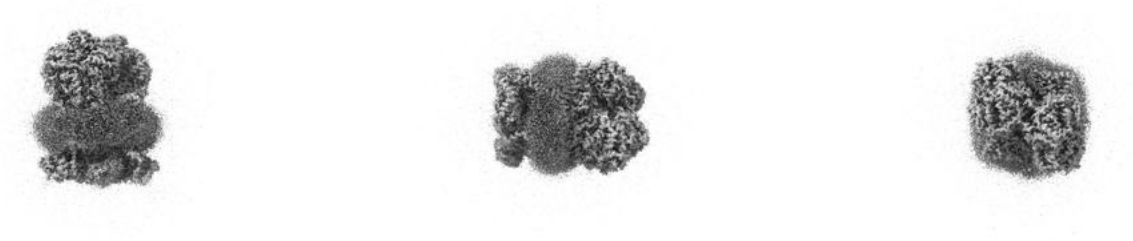
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

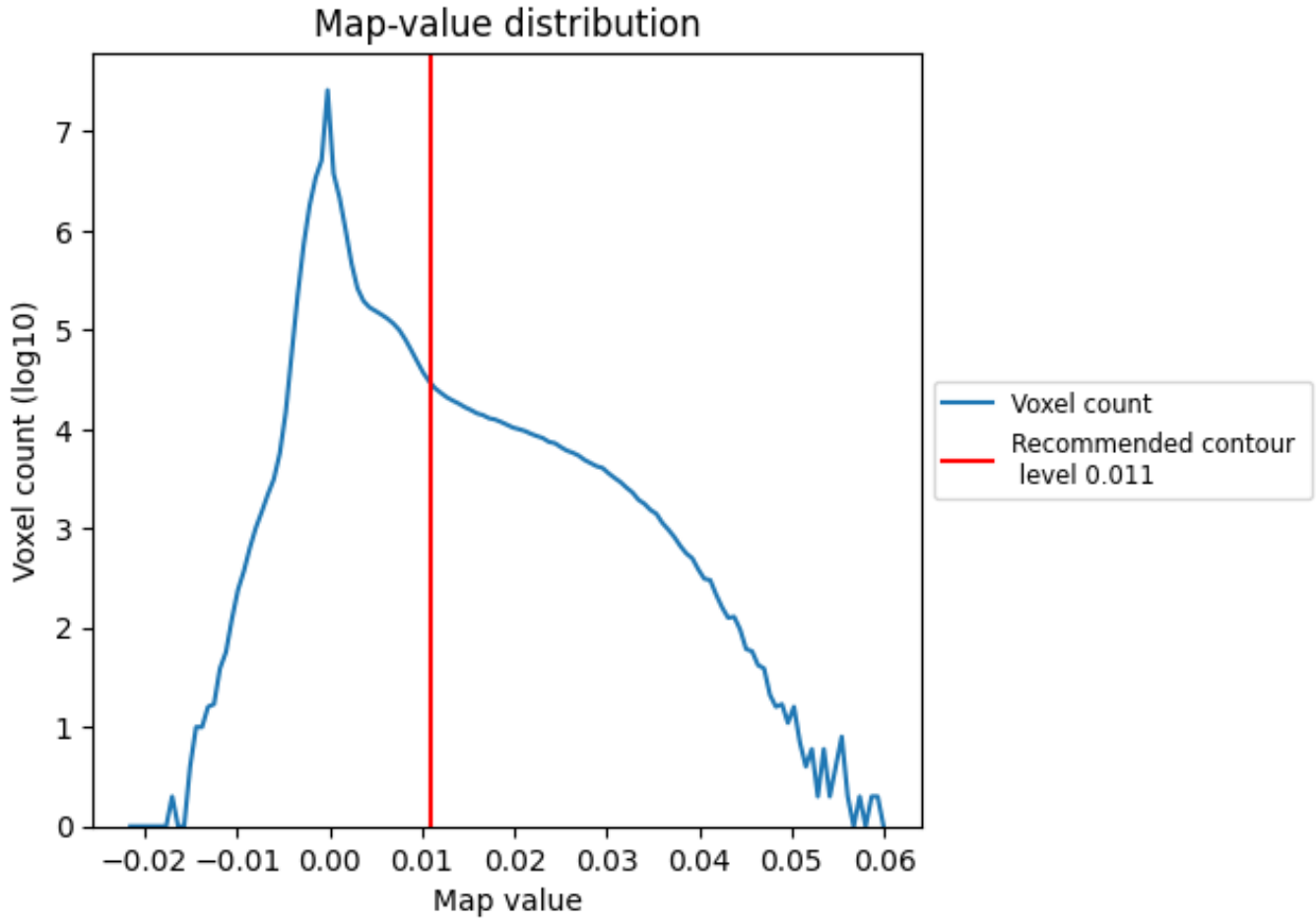
6.6 Mask visualisation (i)

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

7 Map analysis

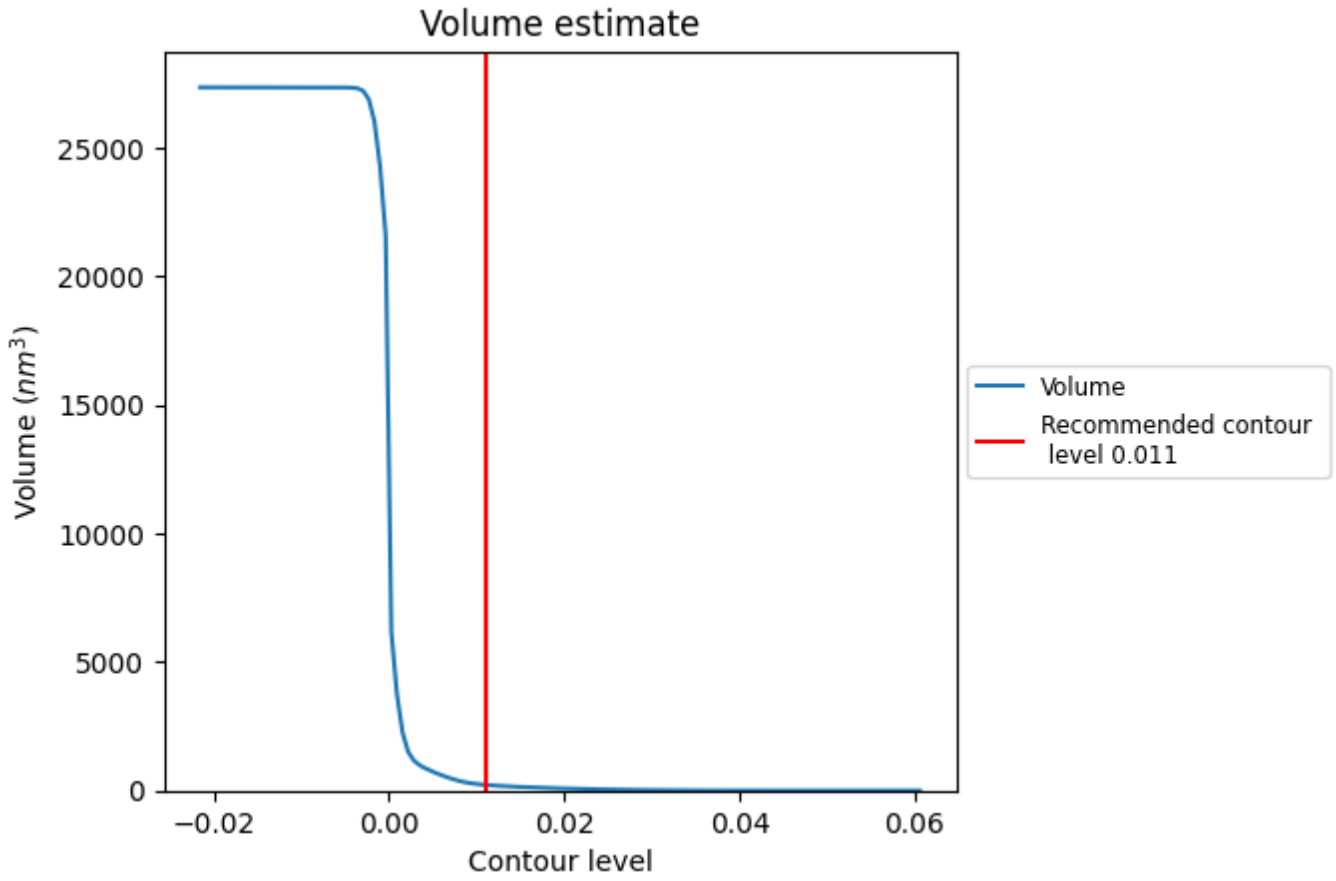
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

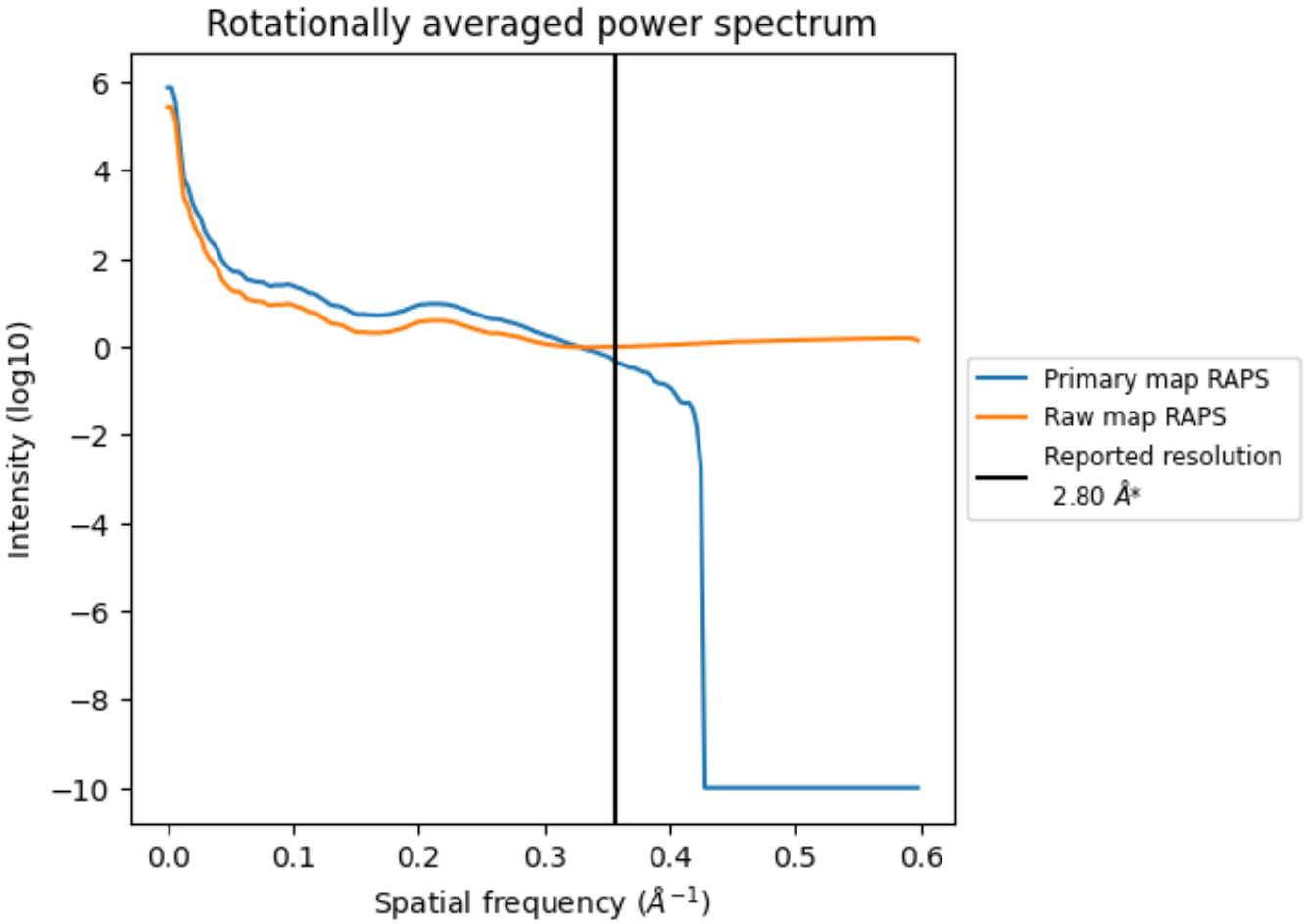
7.2 Volume estimate (i)



The volume at the recommended contour level is 221 nm^3; this corresponds to an approximate mass of 200 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)

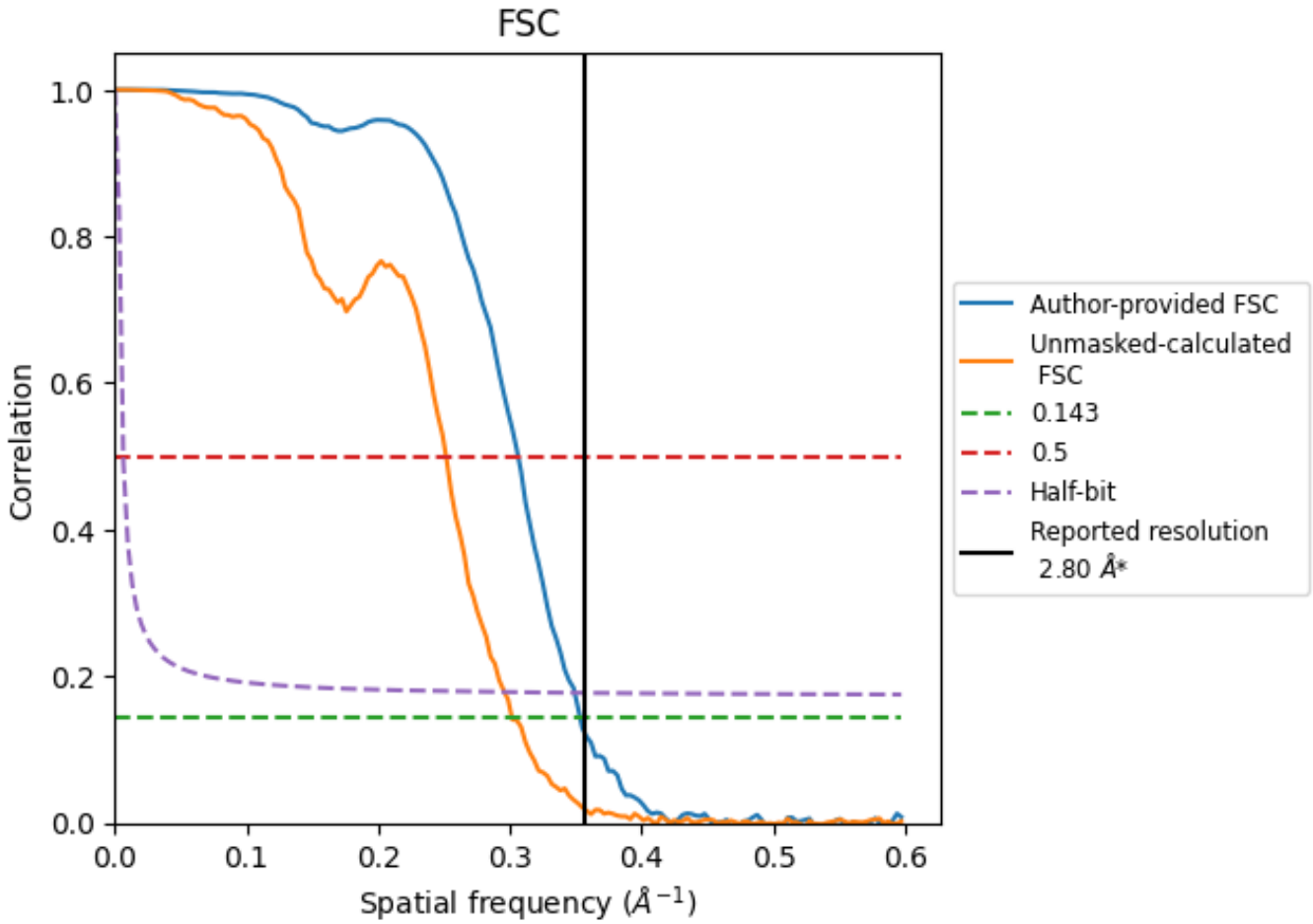


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

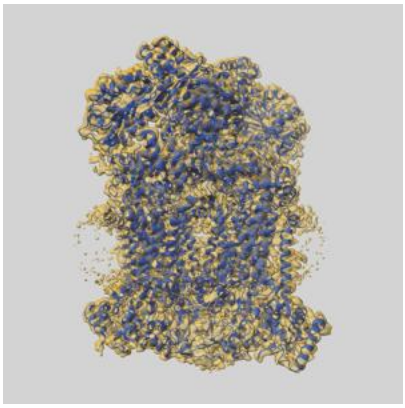
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.26	2.86
Unmasked-calculated*	3.31	3.97	3.38

*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 3.31 differs from the reported value 2.8 by more than 10 %

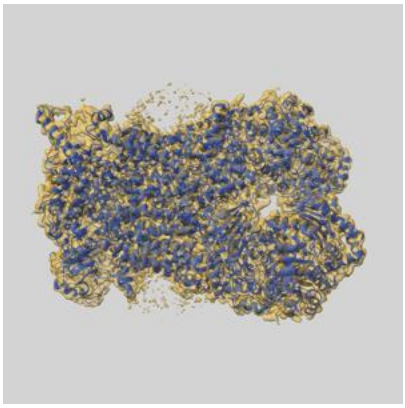
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15332 and PDB model 8AC3. Per-residue inclusion information can be found in section 3 on page 12.

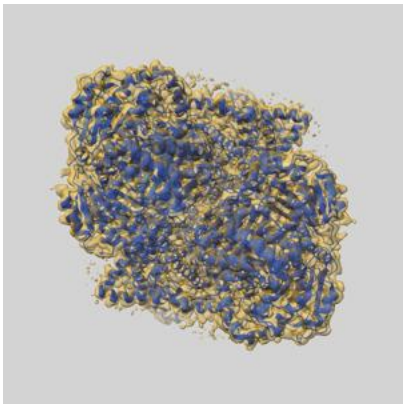
9.1 Map-model overlay



X



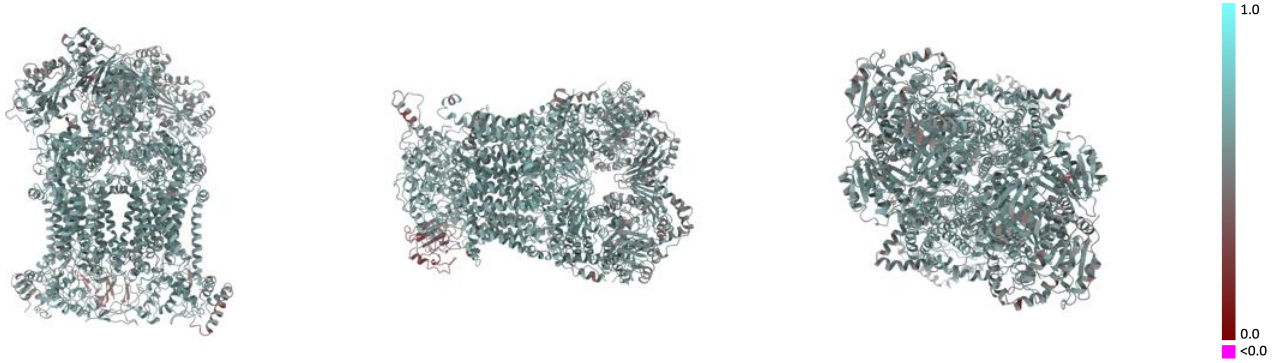
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

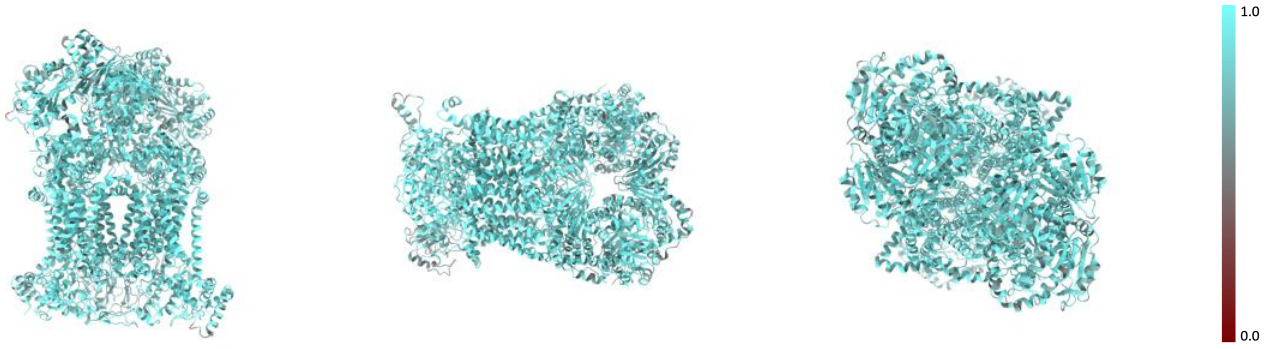
9.2 Q-score mapped to coordinate model (i)



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.

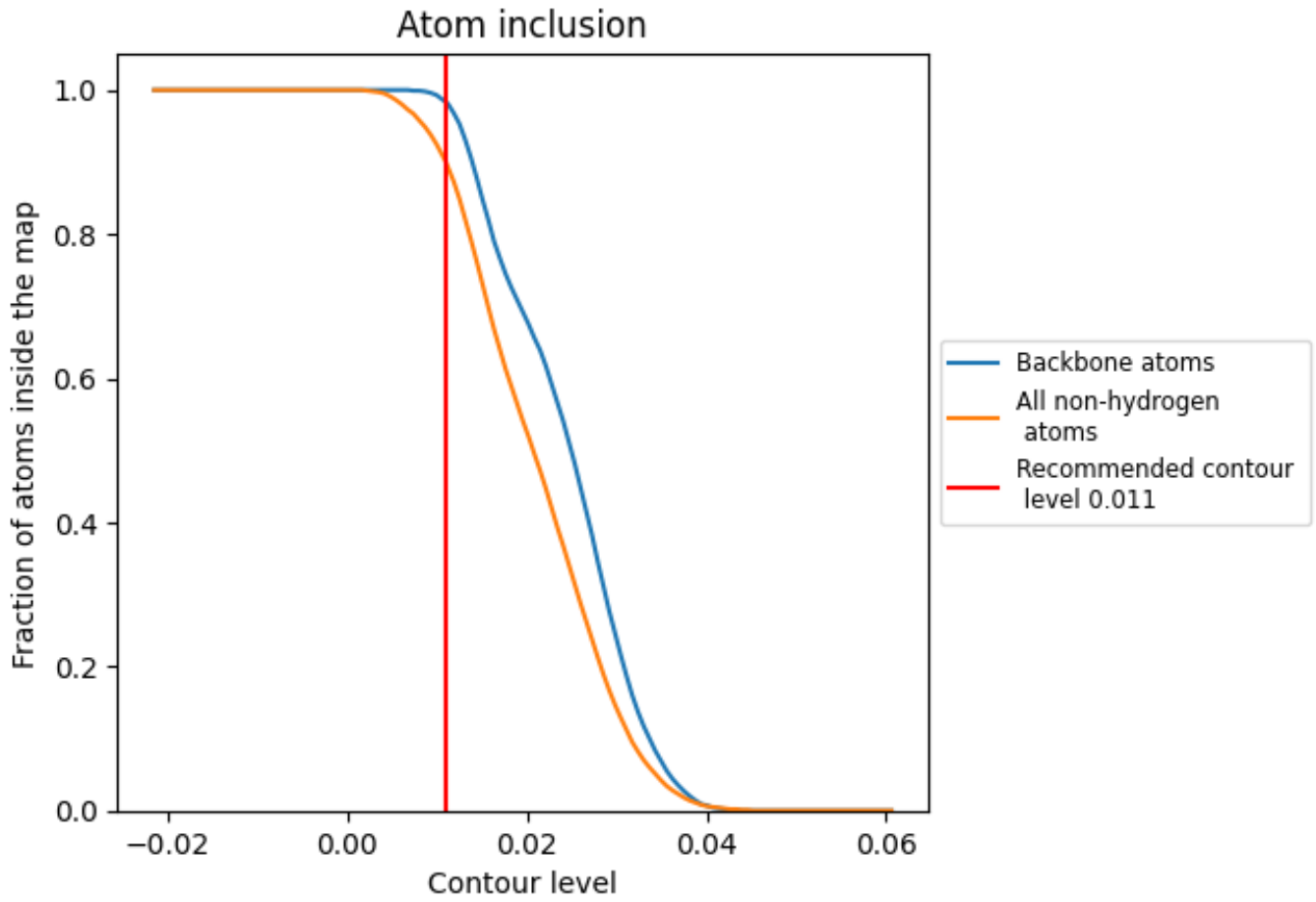
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8990	0.5750
A	0.8840	0.5710
B	0.8750	0.5650
C	0.9490	0.6090
D	0.9320	0.5980
E	0.9260	0.5970
F	0.7730	0.4960
G	0.9050	0.5880
H	0.9410	0.5920
I	0.9410	0.6010
J	0.8590	0.5650
L	0.8840	0.5740
M	0.8750	0.5660
N	0.9480	0.6110
O	0.9360	0.5990
P	0.7940	0.4060
Q	0.7840	0.4990
R	0.8930	0.5870
S	0.9350	0.5950
T	0.9410	0.5950
U	0.8700	0.5790