Full wwPDB EM Validation Report

Sep 28, 2024 – 06:06 pm BST

PDB ID	:	8AB9
EMDB ID	:	EMD-15315
Title	:	Complex III2 from Yarrowia lipolytica, ascorbate-reduced, b-position
Authors	:	Wieferig, J.P.; Kuhlbrandt, W.
Deposited on	:	2022-07-04
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

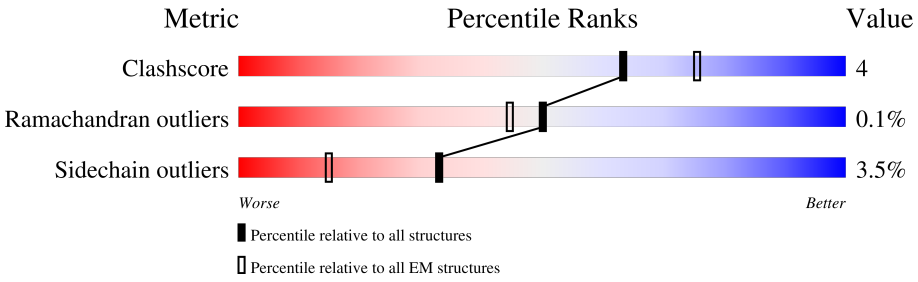
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	90% 9%
1	N	385	91% 8%
2	E	225	22% 73%
2	P	225	12% 57% 22% 17%
3	G	128	86% 9%
3	R	128	89% 6%
4	F	137	49% 48%
4	Q	137	47% 5% 48%

Continued on next page...

Continued from previous page...

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

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.

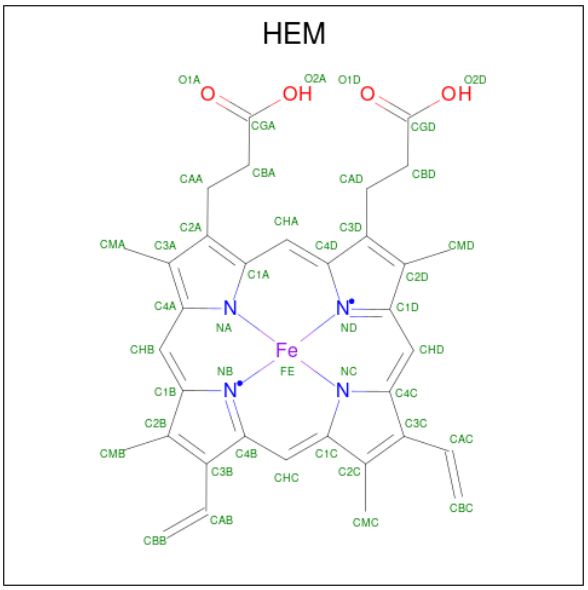
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	75	Total	C	N	O	0	0
			598	403	99	96		

Continued on next page...

Continued from previous page...

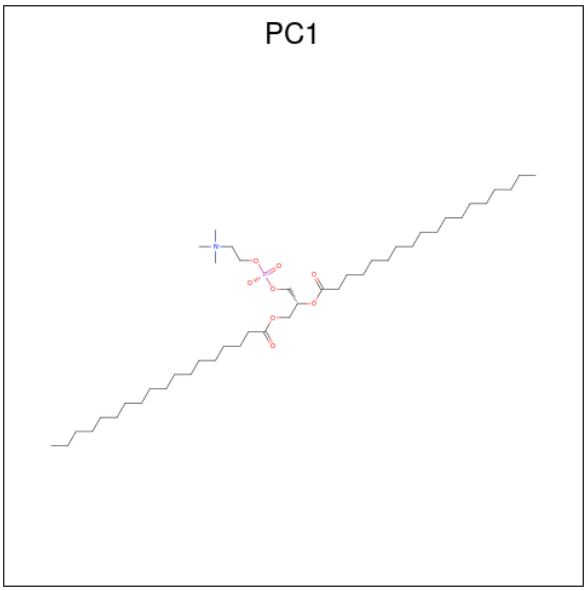
Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	75	Total	C	N	O	0	0
			598	403	99	96		

- 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).



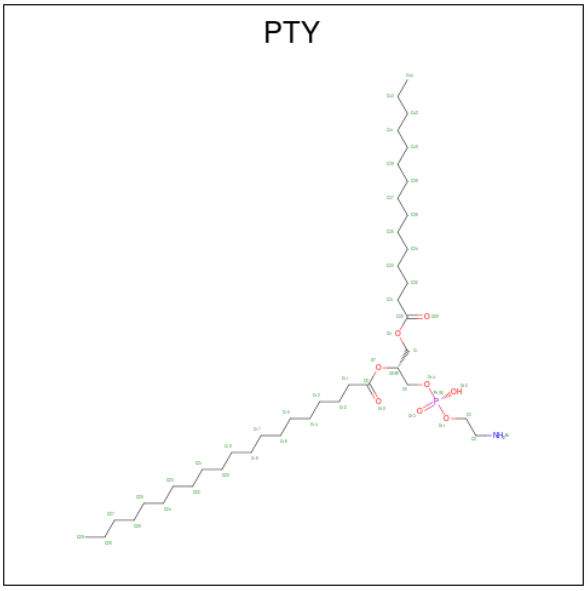
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



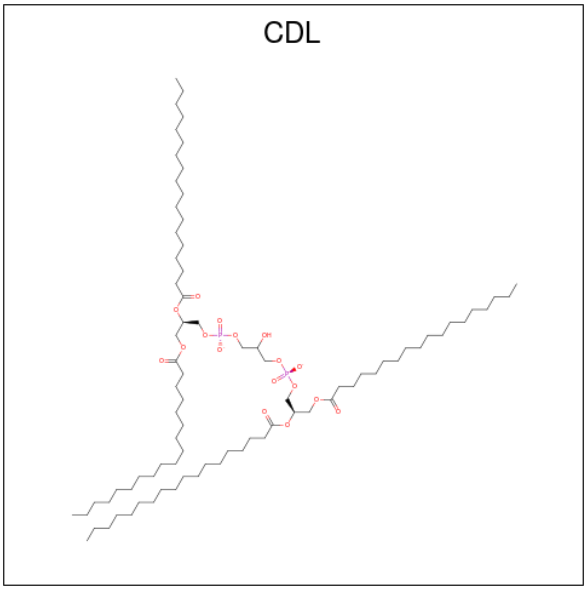
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	T	1	Total	C	N	O	P	0
			32	22	1	8	1	

- 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: $C_{81}H_{156}O_{17}P_2$).



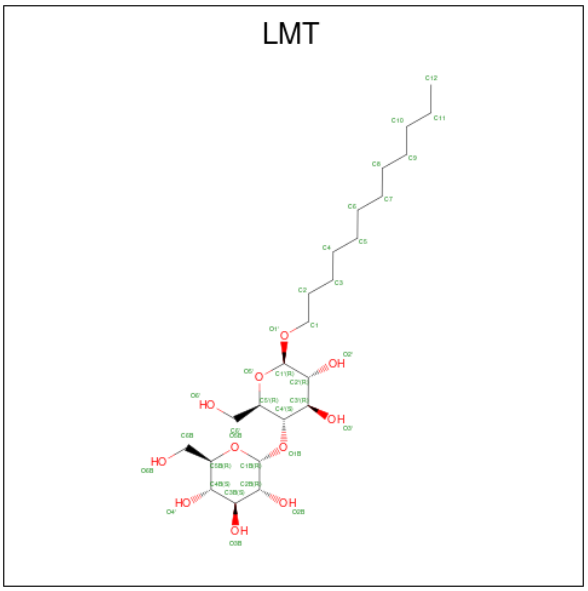
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	A	1	Total	C	O	P	0
			42	25	15	2	
14	A	1	Total	C	O	P	0
			47	30	15	2	
14	H	1	Total	C	O	P	0
			50	31	17	2	
14	H	1	Total	C	O	P	0
			39	20	17	2	
14	N	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			48	29	17	2	
14	L	1	Total	C	O	P	0
			42	25	15	2	

Continued on next page...

Continued from previous page...

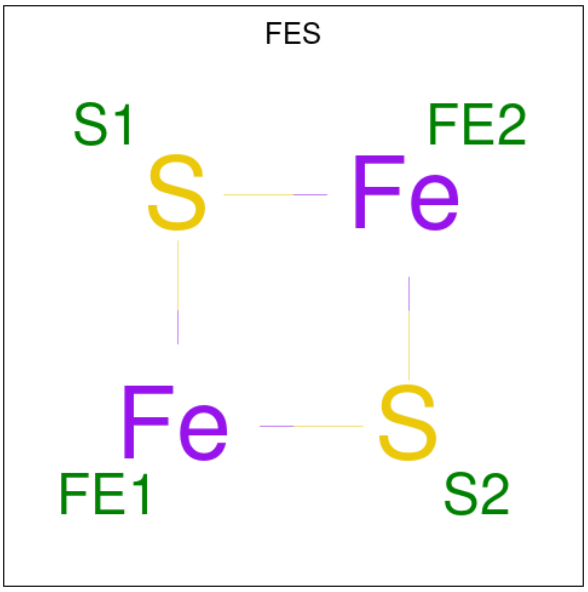
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			47	30	15	2	
14	O	1	Total	C	O	P	0
			39	20	17	2	

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



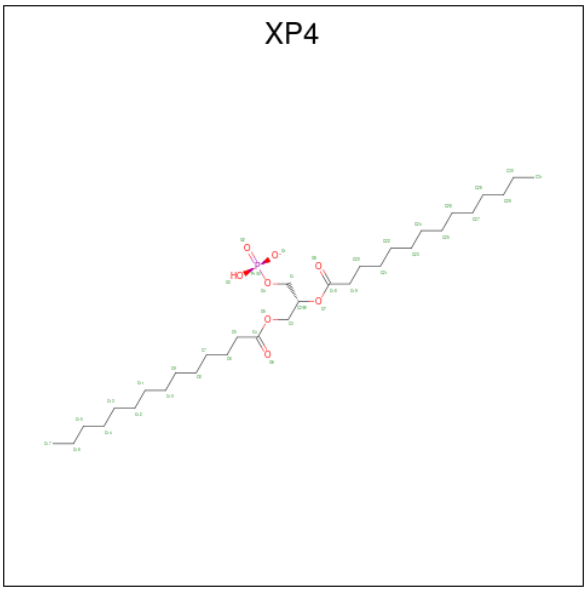
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			35	24	11	
15	P	1	Total	C	O	0
			35	24	11	
15	J	1	Total	C	O	0
			35	24	11	
15	N	1	Total	C	O	0
			35	24	11	

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



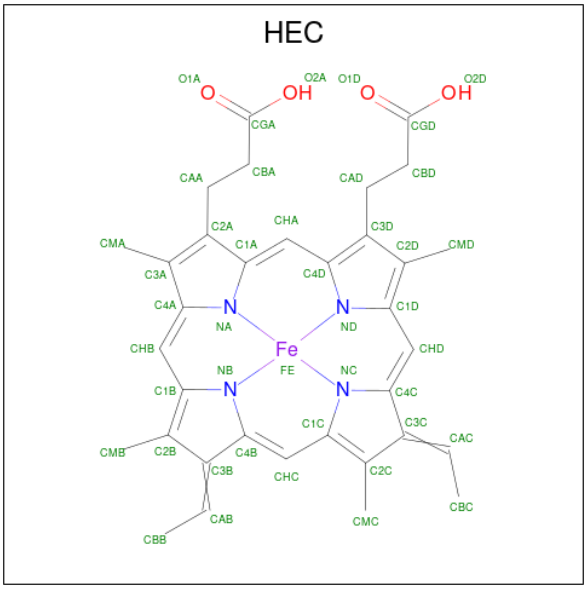
Mol	Chain	Residues	Atoms			AltConf
16	P	1	Total	Fe	S	0
			4	2	2	

- 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	L	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).

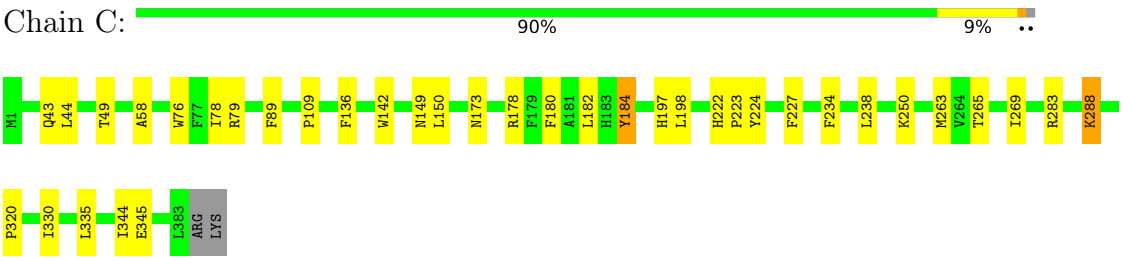


Mol	Chain	Residues	Atoms					AltConf
18	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

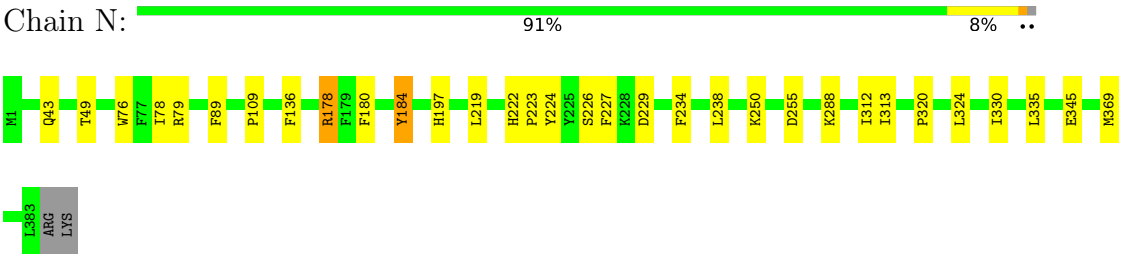
3 Residue-property plots (i)

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.

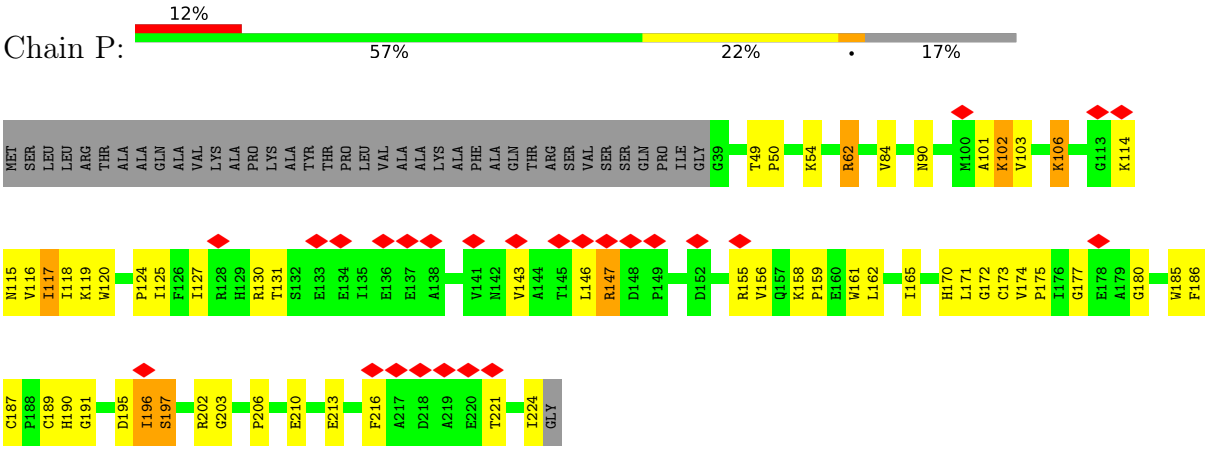
• Molecule 1: Cytochrome b



• Molecule 1: Cytochrome b

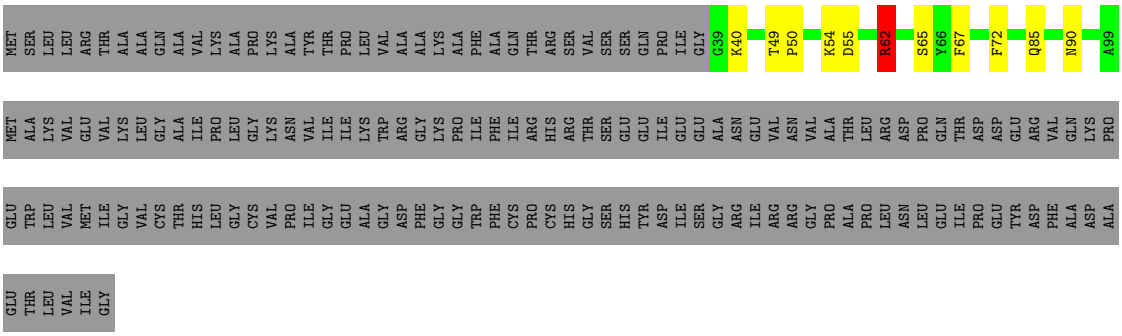


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

Chain E:



• Molecule 3: Cytochrome b-c1 complex subunit 7

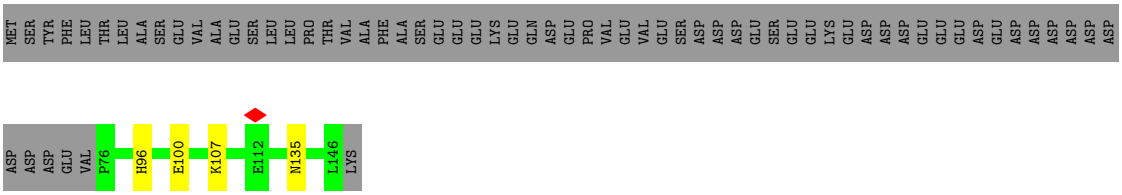
Chain G:

• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:

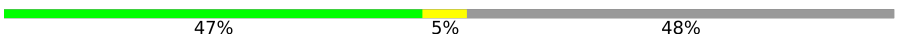
• Molecule 4: YALI0F24673p

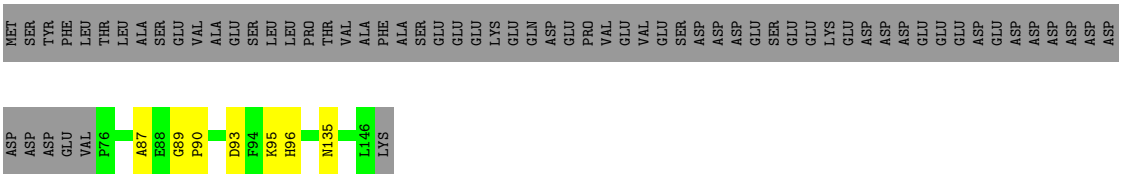
Chain F:



• Molecule 4: YALI0F24673p

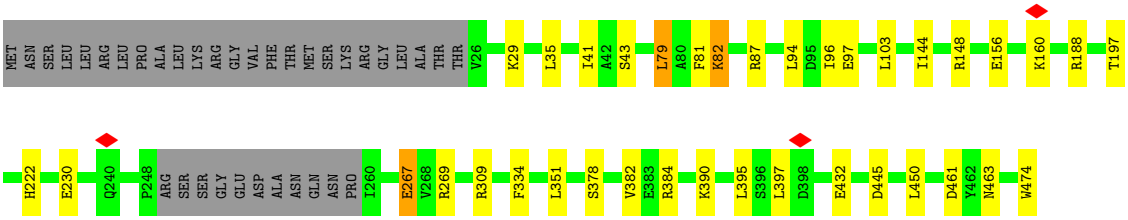
Chain Q:





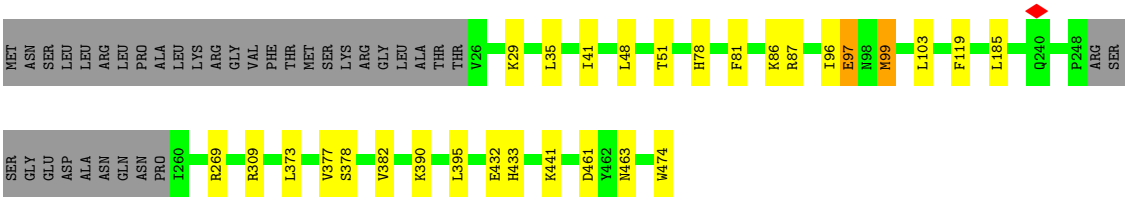
• Molecule 5: YALI0A14806p

Chain A:



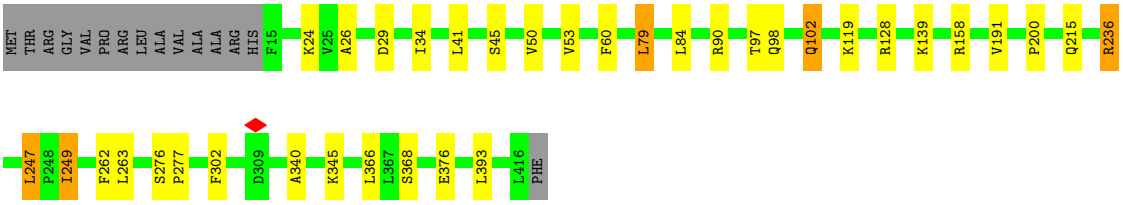
• Molecule 5: YALI0A14806p

Chain L:



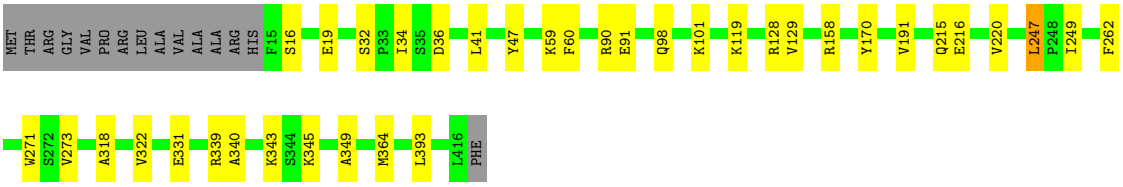
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



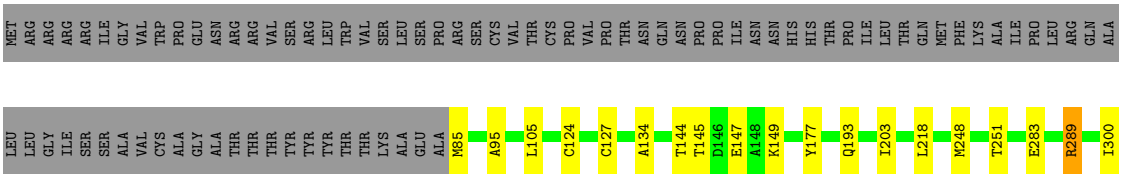
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

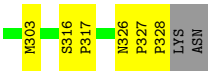
Chain M:



• Molecule 7: YALI0A17468p

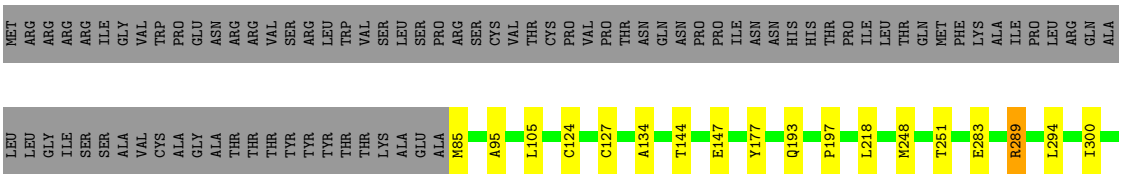
Chain D:





• Molecule 7: YALI0A17468p

Chain O:



• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:

• Molecule 8: Cytochrome b-c1 complex subunit 8

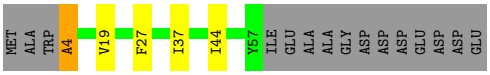
Chain S:

• Molecule 9: Complex III subunit 9

Chain I:

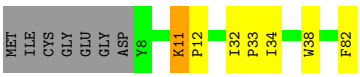
• Molecule 9: Complex III subunit 9

Chain T:



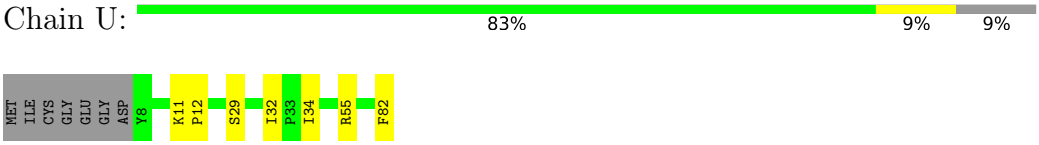
• Molecule 10: YALI0C12210p

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	33680	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	0.057	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	299.16, 299.16, 299.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	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: FES, XP4, PC1, PTY, LMT, CDL, HEC, HEM

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	0.47	0/3153	0.81	1/4305 (0.0%)
1	N	0.46	0/3153	0.79	0/4305
2	E	0.45	0/474	0.77	2/637 (0.3%)
2	P	0.38	0/1479	0.80	1/2003 (0.0%)
3	G	0.40	0/1012	0.75	1/1373 (0.1%)
3	R	0.41	0/1012	0.75	1/1373 (0.1%)
4	F	0.32	0/595	0.69	0/805
4	Q	0.33	0/595	0.74	1/805 (0.1%)
5	A	0.41	0/3510	0.80	2/4768 (0.0%)
5	L	0.41	0/3510	0.81	2/4768 (0.0%)
6	B	0.37	0/3069	0.79	5/4178 (0.1%)
6	M	0.38	0/3069	0.79	4/4178 (0.1%)
7	D	0.40	0/1950	0.82	3/2656 (0.1%)
7	O	0.41	0/1950	0.81	2/2656 (0.1%)
8	H	0.50	1/717 (0.1%)	0.77	0/975
8	S	0.48	1/717 (0.1%)	0.76	0/975
9	I	0.52	1/465 (0.2%)	0.74	0/629
9	T	0.53	1/465 (0.2%)	0.75	0/629
10	J	0.39	0/620	0.71	0/846
10	U	0.39	0/620	0.72	0/846
All	All	0.42	4/32135 (0.0%)	0.79	25/43710 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
9	T	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	9	TYR	N-CA	8.68	1.63	1.46
8	S	9	TYR	N-CA	7.85	1.62	1.46
9	T	4	ALA	N-CA	7.70	1.61	1.46
9	I	4	ALA	N-CA	7.26	1.60	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	215	GLN	CB-CA-C	-7.98	94.44	110.40
6	B	215	GLN	CB-CA-C	-7.89	94.62	110.40
6	M	90	ARG	CG-CD-NE	-7.69	95.66	111.80
6	B	90	ARG	CG-CD-NE	-7.49	96.07	111.80
6	M	158	ARG	CG-CD-NE	-6.21	98.76	111.80
5	L	309	ARG	CG-CD-NE	-6.11	98.97	111.80
7	O	283	GLU	CB-CA-C	-6.06	98.28	110.40
5	A	269	ARG	CG-CD-NE	-6.02	99.15	111.80
7	O	289	ARG	CG-CD-NE	-5.99	99.23	111.80
5	A	309	ARG	CG-CD-NE	-5.90	99.41	111.80
5	L	269	ARG	NE-CZ-NH2	-5.84	117.38	120.30
6	B	158	ARG	CG-CD-NE	-5.76	99.70	111.80
4	Q	96	HIS	CB-CA-C	-5.66	99.09	110.40
3	R	76	ARG	NE-CZ-NH1	-5.54	117.53	120.30
7	D	289	ARG	CG-CD-NE	-5.51	100.23	111.80
7	D	283	GLU	CB-CA-C	-5.45	99.51	110.40
2	E	62	ARG	CB-CA-C	-5.29	99.81	110.40
6	B	128	ARG	CG-CD-NE	-5.27	100.73	111.80
7	D	283	GLU	CB-CG-CD	-5.24	100.04	114.20
1	C	283	ARG	CG-CD-NE	5.22	122.75	111.80
2	E	62	ARG	CB-CG-CD	-5.22	98.03	111.60
3	G	76	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	P	62	ARG	CB-CA-C	-5.09	100.23	110.40
6	B	236	ARG	CG-CD-NE	5.03	122.36	111.80
6	M	128	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	4	ALA	Peptide
9	T	4	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3052	0	3113	50	0
1	N	3052	0	3113	21	0
2	E	465	0	459	7	0
2	P	1445	0	1426	65	0
3	G	994	0	1022	4	0
3	R	994	0	1022	6	0
4	F	579	0	511	1	0
4	Q	579	0	511	3	0
5	A	3446	0	3369	23	0
5	L	3446	0	3369	16	0
6	B	3008	0	2991	21	0
6	M	3008	0	2991	23	0
7	D	1893	0	1834	25	0
7	O	1893	0	1834	23	0
8	H	690	0	673	3	0
8	S	690	0	673	5	0
9	I	452	0	435	2	0
9	T	452	0	435	3	0
10	J	598	0	615	4	0
10	U	598	0	615	3	0
11	C	86	0	60	8	0
11	N	86	0	60	6	0
12	C	38	0	50	2	0
12	I	32	0	38	1	0
12	N	38	0	50	3	0
12	T	32	0	38	1	0
13	C	41	0	58	4	0
13	E	41	0	58	2	0
13	N	41	0	58	5	0
13	P	41	0	58	8	0
14	A	89	0	85	2	0
14	C	48	0	40	0	0
14	H	89	0	66	2	0
14	L	89	0	85	0	0
14	N	98	0	84	1	0
14	O	39	0	22	1	0
15	C	35	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	35	0	46	1	0
15	N	35	0	46	0	0
15	P	35	0	46	0	0
16	P	4	0	0	0	0
17	A	24	0	22	0	0
17	L	24	0	22	0	0
18	D	43	0	32	13	0
18	O	43	0	32	13	0
All	All	32540	0	32213	261	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 4.

All (261) 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	1.67	1.34
7:O:124:CYS:SG	18:O:401:HEC:HBB3	1.66	1.33
2:P:84:VAL:CG2	13:P:303:PTY:H441	1.65	1.25
1:C:288:LYS:NZ	2:P:171:LEU:HD23	1.55	1.19
7:O:127:CYS:SG	18:O:401:HEC:CAC	2.30	1.19
7:D:124:CYS:SG	18:D:401:HEC:CBB	2.39	1.10
7:O:127:CYS:SG	18:O:401:HEC:HBC3	1.93	1.09
7:O:124:CYS:SG	18:O:401:HEC:CBB	2.39	1.09
7:D:127:CYS:SG	18:D:401:HEC:CAC	2.41	1.08
7:O:127:CYS:SG	18:O:401:HEC:CBC	2.42	1.08
2:P:84:VAL:HG23	13:P:303:PTY:H441	1.16	1.06
1:C:288:LYS:NZ	2:P:171:LEU:CD2	2.20	1.05
1:C:150:LEU:HD23	2:P:171:LEU:HD21	1.34	1.04
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.43	1.01
7:D:127:CYS:SG	18:D:401:HEC:HBC3	2.00	1.00
2:P:84:VAL:HG23	13:P:303:PTY:C44	1.92	1.00
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.44	0.99
7:D:127:CYS:SG	18:D:401:HEC:CBC	2.52	0.97
7:O:124:CYS:SG	18:O:401:HEC:CAB	2.54	0.95
1:C:288:LYS:HZ2	2:P:171:LEU:CD2	1.81	0.94
7:D:124:CYS:SG	18:D:401:HEC:CAB	2.56	0.94
1:C:150:LEU:HD23	2:P:171:LEU:CD2	1.97	0.94
5:A:395:LEU:HD23	6:B:34:ILE:HD12	1.56	0.88
2:P:84:VAL:HG22	13:P:303:PTY:H441	1.55	0.86
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:ND2	2:P:171:LEU:O	2.13	0.82
1:C:288:LYS:HZ1	2:P:171:LEU:HD23	1.42	0.81
1:C:288:LYS:HZ1	2:P:171:LEU:CD2	1.91	0.81
1:C:269:ILE:HD12	2:P:189:CYS:SG	2.21	0.80
1:C:265:THR:OG1	2:P:174:VAL:HG22	1.82	0.79
1:C:58:ALA:H	1:C:173:ASN:HD22	1.28	0.78
6:B:236:ARG:HD3	6:M:170:TYR:CE1	2.20	0.77
2:P:124:PRO:HG2	2:P:174:VAL:HG11	1.67	0.75
1:C:142:TRP:HB3	1:C:269:ILE:HD13	1.71	0.72
1:C:288:LYS:HZ2	2:P:171:LEU:HD23	1.37	0.72
1:C:150:LEU:CD2	2:P:171:LEU:HD21	2.18	0.72
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.71	0.72
5:A:395:LEU:HD22	6:B:98:GLN:HG2	1.73	0.70
1:C:344:ILE:CD1	2:P:190:HIS:HA	2.23	0.69
7:O:218:LEU:HD11	18:O:401:HEC:HMB2	1.76	0.68
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.76	0.68
2:P:202:ARG:HH12	8:H:93:LEU:HB3	1.59	0.68
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.76	0.68
7:O:127:CYS:SG	18:O:401:HEC:C3C	2.81	0.67
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.24	0.67
2:P:84:VAL:CG2	13:P:303:PTY:C44	2.56	0.67
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.77	0.67
7:O:124:CYS:SG	18:O:401:HEC:C3B	2.84	0.67
2:P:180:GLY:HA2	2:P:186:PHE:HB2	1.78	0.66
7:D:218:LEU:HD11	18:D:401:HEC:HMB2	1.78	0.66
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.76	0.66
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.26	0.66
1:C:288:LYS:NZ	2:P:171:LEU:HD21	2.11	0.65
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.79	0.65
2:P:186:PHE:CE1	2:P:191:GLY:HA2	2.32	0.64
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.78	0.64
1:C:142:TRP:HH2	2:P:174:VAL:HG13	1.60	0.64
7:D:251:THR:HG21	18:D:401:HEC:HMC2	1.77	0.64
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	1.96	0.64
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.80	0.64
7:O:251:THR:HG21	18:O:401:HEC:HMC2	1.79	0.64
1:C:238:LEU:HD13	7:D:300:ILE:HG22	1.79	0.63
1:C:344:ILE:HD12	2:P:190:HIS:C	2.19	0.62
1:C:149:ASN:HB2	2:P:171:LEU:O	1.99	0.62
8:S:47:ASN:O	8:S:51:ARG:HG2	2.00	0.62
7:D:124:CYS:SG	18:D:401:HEC:C3B	2.88	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:501:HEM:CMB	11:C:501:HEM:HBB2	2.31	0.61
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.30	0.60
1:C:150:LEU:HD21	2:P:171:LEU:HD11	1.82	0.60
7:D:127:CYS:SG	18:D:401:HEC:C3C	2.89	0.60
6:M:91:GLU:HG2	6:M:364:MET:HE1	1.84	0.60
1:N:238:LEU:HD13	7:O:300:ILE:HG22	1.83	0.59
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.83	0.59
2:P:171:LEU:HD12	2:P:190:HIS:CE1	2.38	0.59
8:H:47:ASN:O	8:H:51:ARG:HG2	2.02	0.59
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.85	0.58
3:R:71:VAL:HG11	8:S:21:GLN:HG2	1.86	0.58
2:P:130:ARG:HD2	2:P:162:LEU:HB2	1.84	0.58
7:D:203:ILE:HG12	18:D:401:HEC:HMA3	1.86	0.58
1:C:344:ILE:HD12	2:P:190:HIS:HA	1.84	0.58
1:C:149:ASN:CB	2:P:171:LEU:O	2.52	0.57
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.86	0.57
11:C:501:HEM:HBB2	11:C:501:HEM:HMB1	1.86	0.57
1:C:58:ALA:H	1:C:173:ASN:ND2	2.00	0.57
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.52	0.57
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.33	0.57
5:A:378:SER:HA	5:A:432:GLU:OE1	2.05	0.56
6:M:91:GLU:HG2	6:M:364:MET:CE	2.35	0.56
1:C:149:ASN:ND2	2:P:172:GLY:HA3	2.21	0.56
1:N:335:LEU:HD22	8:S:66:PHE:HD1	1.71	0.56
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.41	0.55
6:M:249:ILE:CD1	6:M:393:LEU:HD21	2.37	0.55
2:P:155:ARG:NH1	2:P:197:SER:O	2.39	0.55
11:N:501:HEM:HBB2	11:N:501:HEM:CMB	2.37	0.55
13:C:504:PTY:H132	2:E:72:PHE:CE2	2.42	0.54
1:N:330:ILE:CD1	12:N:503:PC1:H2A1	2.30	0.54
1:C:263:MET:CE	2:P:119:LYS:HB3	2.38	0.54
1:C:288:LYS:HZ2	2:P:171:LEU:HD21	1.65	0.54
7:D:127:CYS:HG	18:D:401:HEC:HBC3	1.70	0.53
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.90	0.53
6:M:318:ALA:O	6:M:322:VAL:HG23	2.09	0.53
2:P:177:GLY:HA2	2:P:185:TRP:CD1	2.45	0.52
2:P:84:VAL:HG23	13:P:303:PTY:C43	2.39	0.52
5:A:43:SER:CB	5:A:222:HIS:HD2	2.22	0.52
5:L:81:PHE:HE1	5:L:103:LEU:HD23	1.75	0.52
1:C:335:LEU:HD22	8:H:66:PHE:HD1	1.73	0.52
9:T:19:VAL:HG22	12:T:201:PC1:H332	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.91	0.52
11:C:502:HEM:HBC2	11:C:502:HEM:HMC2	1.92	0.51
13:C:504:PTY:H132	2:E:72:PHE:CD2	2.45	0.51
1:C:344:ILE:HD12	2:P:190:HIS:CA	2.40	0.51
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.45	0.51
6:B:236:ARG:HD3	6:M:170:TYR:CZ	2.45	0.51
11:N:501:HEM:HBB2	11:N:501:HEM:HMB1	1.92	0.51
1:C:344:ILE:HD11	2:P:190:HIS:HA	1.93	0.51
5:A:96:ILE:HG12	5:A:103:LEU:HD13	1.92	0.51
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.10	0.51
6:M:59:LYS:HB3	6:M:129:VAL:HG13	1.91	0.51
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.76	0.50
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.93	0.50
6:B:26:ALA:HB2	6:B:366:LEU:HD11	1.94	0.50
14:H:701:CDL:OB3	14:H:702:CDL:O1	2.29	0.50
1:N:345:GLU:OE2	7:O:85:MET:N	2.45	0.50
7:O:197:PRO:HG3	18:O:401:HEC:HMD3	1.94	0.50
6:B:236:ARG:HD3	6:M:170:TYR:CD1	2.46	0.49
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.47	0.49
6:B:50:VAL:HG22	6:B:53:VAL:HB	1.93	0.49
1:C:142:TRP:HZ3	2:P:173:CYS:HA	1.78	0.49
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.48	0.49
4:Q:87:ALA:HB1	4:Q:95:LYS:HD3	1.95	0.49
5:A:81:PHE:HE1	5:A:103:LEU:HD23	1.78	0.48
2:P:103:VAL:HG23	2:P:224:ILE:HD12	1.96	0.48
12:N:503:PC1:O13	12:N:503:PC1:H133	2.14	0.48
1:C:150:LEU:HD23	2:P:171:LEU:HD22	1.91	0.48
2:P:120:TRP:CE3	2:P:125:ILE:HD11	2.49	0.48
1:C:320:PRO:HD2	3:G:31:TYR:CZ	2.49	0.48
5:A:35:LEU:HG	5:A:41:ILE:HD11	1.96	0.48
1:N:229:ASP:HB2	13:N:505:PTY:H382	1.95	0.48
2:E:49:THR:N	2:E:50:PRO:HD2	2.29	0.47
10:U:29:SER:HA	10:U:32:ILE:HG12	1.97	0.47
6:B:249:ILE:HD11	6:B:302:PHE:HB2	1.96	0.47
2:P:116:VAL:HG23	2:P:127:ILE:O	2.15	0.47
6:B:247:LEU:HD13	6:B:393:LEU:HB3	1.95	0.47
5:L:96:ILE:HG12	5:L:103:LEU:HD13	1.95	0.47
6:M:249:ILE:HD11	6:M:393:LEU:HD21	1.96	0.47
5:A:395:LEU:CD2	6:B:34:ILE:HD12	2.35	0.47
5:L:395:LEU:HD12	6:M:34:ILE:HG22	1.97	0.47
7:O:144:THR:OG1	7:O:147:GLU:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:117:ILE:HG22	2:P:124:PRO:HB3	1.96	0.47
7:D:144:THR:OG1	7:D:147:GLU:HG3	2.15	0.47
2:P:165:ILE:HD12	2:P:210:GLU:HB2	1.97	0.46
5:A:384:ARG:HG2	6:B:79:LEU:HD11	1.96	0.46
15:J:101:LMT:H31	2:E:85:GLN:HG3	1.95	0.46
1:N:227:PHE:HZ	13:N:505:PTY:HC6	1.81	0.46
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.96	0.46
5:L:395:LEU:HD12	6:M:34:ILE:CG2	2.46	0.46
1:C:234:PHE:CZ	7:D:303:MET:HE2	2.50	0.46
2:P:147:ARG:HE	2:P:147:ARG:HB2	1.06	0.46
2:P:156:VAL:HG21	2:P:159:PRO:HA	1.98	0.46
12:I:201:PC1:H351	12:I:201:PC1:H322	1.72	0.46
1:C:227:PHE:CZ	13:C:504:PTY:H322	2.51	0.45
7:D:326:ASN:OD1	2:E:40:LYS:HA	2.16	0.45
1:C:150:LEU:HD21	2:P:171:LEU:CD1	2.46	0.45
5:A:334:PHE:HB3	5:A:351:LEU:HD23	1.98	0.45
11:C:501:HEM:HHD	11:C:501:HEM:CBC	2.46	0.45
1:C:222:HIS:CG	1:C:223:PRO:HA	2.52	0.45
2:P:175:PRO:HB2	2:P:185:TRP:HB3	1.99	0.45
1:N:320:PRO:HD2	3:R:31:TYR:CZ	2.52	0.45
13:P:303:PTY:H331	13:P:303:PTY:H361	1.68	0.45
7:D:327:PRO:HA	7:D:328:PRO:HD3	1.82	0.45
1:N:43:GLN:OE1	1:N:43:GLN:HA	2.17	0.45
12:C:503:PC1:O13	12:C:503:PC1:H133	2.17	0.45
5:L:35:LEU:HG	5:L:41:ILE:HD11	1.98	0.45
1:C:345:GLU:OE2	7:D:85:MET:N	2.50	0.45
5:A:445:ASP:HB3	2:E:62:ARG:HH21	1.82	0.45
6:M:247:LEU:HD13	6:M:393:LEU:HB3	1.99	0.45
7:D:145:THR:O	7:D:149:LYS:HG3	2.18	0.44
1:N:222:HIS:CG	1:N:223:PRO:HA	2.52	0.44
14:N:504:CDL:HA21	8:S:51:ARG:HH21	1.82	0.44
7:O:105:LEU:HB3	9:T:44:ILE:HD12	2.00	0.44
13:C:504:PTY:H112	13:C:504:PTY:HC12	2.00	0.44
1:N:49:THR:HG21	1:N:78:ILE:HD13	1.99	0.44
1:C:49:THR:HG21	1:C:78:ILE:HD13	2.00	0.44
2:P:196:ILE:H	2:P:196:ILE:HG12	1.56	0.44
7:D:134:ALA:HA	7:D:177:TYR:HA	2.00	0.44
2:P:147:ARG:NH1	2:P:203:GLY:O	2.51	0.43
5:L:78:HIS:HA	6:M:271:TRP:CD1	2.52	0.43
5:A:160:LYS:HD2	5:A:160:LYS:HA	1.85	0.43
5:L:96:ILE:O	5:L:99:MET:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:432:GLU:HG3	5:L:433:HIS:N	2.33	0.43
5:L:474:TRP:CD1	10:U:34:ILE:HG13	2.53	0.43
1:C:43:GLN:HA	1:C:43:GLN:OE1	2.17	0.43
1:C:44:LEU:HD23	11:C:501:HEM:HMC2	2.00	0.43
5:A:82:LYS:HD3	5:A:82:LYS:HA	1.57	0.43
9:I:16:SER:HB3	10:J:38:TRP:CE2	2.54	0.43
2:E:49:THR:N	2:E:50:PRO:CD	2.82	0.43
1:C:224:TYR:OH	5:A:463:ASN:HB2	2.18	0.43
6:B:262:PHE:HB2	6:B:340:ALA:HB2	2.01	0.43
10:J:11:LYS:HD2	10:J:12:PRO:HD2	2.01	0.43
1:N:320:PRO:HD2	3:R:31:TYR:CE1	2.53	0.43
18:O:401:HEC:CBC	18:O:401:HEC:HMC1	2.49	0.43
6:B:236:ARG:CD	6:M:170:TYR:CZ	3.02	0.43
1:N:226:SER:HB3	13:N:505:PTY:H321	2.01	0.43
7:O:248:MET:HB2	18:O:401:HEC:C1D	2.49	0.43
2:P:174:VAL:HA	2:P:175:PRO:HD3	1.87	0.42
7:D:248:MET:HB2	18:D:401:HEC:C1D	2.48	0.42
6:M:262:PHE:HB2	6:M:340:ALA:HB2	2.01	0.42
7:O:134:ALA:HA	7:O:177:TYR:HA	2.01	0.42
7:O:327:PRO:HA	7:O:328:PRO:HD3	1.79	0.42
2:P:49:THR:N	2:P:50:PRO:CD	2.83	0.42
5:A:267:GLU:HA	5:A:450:LEU:O	2.18	0.42
5:L:395:LEU:HA	6:M:34:ILE:HG21	2.01	0.42
13:E:401:PTY:H161	13:E:401:PTY:H132	1.74	0.42
5:L:119:PHE:HE1	6:M:349:ALA:HB2	1.85	0.42
2:P:102:LYS:HB2	2:P:102:LYS:HE3	1.62	0.42
2:P:173:CYS:HB2	2:P:187:CYS:SG	2.59	0.42
5:A:79:LEU:HD12	5:A:79:LEU:HA	1.83	0.42
2:P:106:LYS:HA	2:P:221:THR:HG22	2.01	0.41
1:N:224:TYR:OH	5:L:463:ASN:HB2	2.20	0.41
1:C:142:TRP:CZ3	2:P:173:CYS:HA	2.54	0.41
13:P:303:PTY:H352	13:P:303:PTY:H381	1.85	0.41
10:J:32:ILE:HB	10:J:33:PRO:HD3	2.01	0.41
1:N:234:PHE:CZ	7:O:303:MET:HE2	2.54	0.41
1:N:312:ILE:HG13	1:N:313:ILE:HG13	2.01	0.41
13:N:505:PTY:H341	13:N:505:PTY:H151	2.02	0.41
13:N:505:PTY:H402	13:N:505:PTY:H372	1.59	0.41
13:E:401:PTY:H141	13:E:401:PTY:H311	2.01	0.41
5:L:373:LEU:HD23	5:L:377:VAL:HG11	2.01	0.41
2:P:161:TRP:HB2	2:P:216:PHE:HZ	1.86	0.41
2:P:180:GLY:CA	2:P:186:PHE:HB2	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:26:ALA:CB	6:B:366:LEU:HD11	2.50	0.41
6:B:102:GLN:H	6:B:102:GLN:HG3	1.55	0.41
5:L:97:GLU:HG3	6:M:343:LYS:HE2	2.01	0.41
5:A:474:TRP:CD1	10:J:34:ILE:HG13	2.56	0.41
1:N:178:ARG:HE	1:N:178:ARG:HB3	1.43	0.41
3:R:84:HIS:O	8:S:50:ARG:NH2	2.53	0.41
1:C:288:LYS:HG2	2:P:170:HIS:CD2	2.56	0.41
2:P:189:CYS:HB3	2:P:190:HIS:CE1	2.56	0.41
7:D:105:LEU:HB3	9:I:44:ILE:HD12	2.03	0.41
14:H:702:CDL:H311	14:H:702:CDL:HA62	1.61	0.41
2:P:118:ILE:HD13	2:P:127:ILE:HD12	2.02	0.41
3:G:76:ARG:HD3	3:G:80:PHE:CE2	2.55	0.41
3:R:76:ARG:HD3	3:R:80:PHE:CE2	2.56	0.41
6:M:47:TYR:HB3	6:M:220:VAL:CG1	2.51	0.41
1:C:150:LEU:CD2	2:P:171:LEU:CD2	2.83	0.40
2:P:147:ARG:HD2	2:P:206:PRO:HA	2.04	0.40
5:A:334:PHE:CB	5:A:351:LEU:HD23	2.51	0.40
14:O:402:CDL:HA62	14:O:402:CDL:H311	1.68	0.40
3:G:27:LEU:HD23	3:G:27:LEU:HA	1.94	0.40
7:D:316:SER:OG	7:D:317:PRO:HD3	2.21	0.40
1:N:219:LEU:HD23	1:N:219:LEU:HA	1.91	0.40
6:B:29:ASP:HB2	6:B:200:PRO:HD3	2.04	0.40
6:B:263:LEU:HA	6:B:277:PRO:HG2	2.03	0.40
4:Q:89:GLY:HA3	4:Q:90:PRO:HD3	1.91	0.40
5:L:97:GLU:HB3	6:M:339:ARG:HD3	2.04	0.40
5:A:148:ARG:HH11	5:A:148:ARG:HD3	1.69	0.40
7:O:316:SER:OG	7:O:317:PRO:HD3	2.20	0.40
9:T:37:ILE:HD13	9:T:37:ILE:HA	1.95	0.40
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.94	0.40
5:A:144:ILE:H	5:A:144:ILE:HG12	1.73	0.40
7:O:105:LEU:HD21	7:O:294:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	381/385 (99%)	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%)	170 (92%)	13 (7%)	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%)	386 (96%)	13 (3%)	1 (0%)	37	66
6	M	400/417 (96%)	387 (97%)	13 (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%)	50 (96%)	2 (4%)	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%)	3854 (97%)	99 (2%)	2 (0%)	50	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	101	ALA
6	B	368	SER

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%)	36	62
1	N	331/333 (99%)	319 (96%)	12 (4%)	30	57
2	E	49/182 (27%)	43 (88%)	6 (12%)	4	16
2	P	154/182 (85%)	137 (89%)	17 (11%)	5	20
3	G	113/117 (97%)	104 (92%)	9 (8%)	10	32
3	R	113/117 (97%)	109 (96%)	4 (4%)	31	58
4	F	61/123 (50%)	58 (95%)	3 (5%)	21	49
4	Q	61/123 (50%)	60 (98%)	1 (2%)	58	76
5	A	377/407 (93%)	365 (97%)	12 (3%)	34	61
5	L	377/407 (93%)	365 (97%)	12 (3%)	34	61
6	B	311/322 (97%)	300 (96%)	11 (4%)	31	58
6	M	311/322 (97%)	300 (96%)	11 (4%)	31	58
7	D	192/268 (72%)	191 (100%)	1 (0%)	86	91
7	O	192/268 (72%)	191 (100%)	1 (0%)	86	91
8	H	67/71 (94%)	66 (98%)	1 (2%)	60	77
8	S	67/71 (94%)	66 (98%)	1 (2%)	60	77
9	I	46/57 (81%)	46 (100%)	0	100	100
9	T	46/57 (81%)	45 (98%)	1 (2%)	47	69
10	J	63/68 (93%)	61 (97%)	2 (3%)	34	61
10	U	63/68 (93%)	61 (97%)	2 (3%)	34	61
All	All	3325/3896 (85%)	3208 (96%)	117 (4%)	33	58

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ARG
1	C	89	PHE
1	C	109	PRO
1	C	136	PHE
1	C	178	ARG
1	C	184	TYR
1	C	197	HIS
1	C	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	250	LYS
1	C	288	LYS
2	P	54	LYS
2	P	62	ARG
2	P	90	ASN
2	P	102	LYS
2	P	106	LYS
2	P	114	LYS
2	P	115	ASN
2	P	117	ILE
2	P	131	THR
2	P	143	VAL
2	P	146	LEU
2	P	147	ARG
2	P	158	LYS
2	P	195	ASP
2	P	196	ILE
2	P	197	SER
2	P	213	GLU
3	G	3	SER
3	G	6	SER
3	G	17	SER
3	G	22	LYS
3	G	23	ILE
3	G	40	LEU
3	G	50	GLU
3	G	112	GLU
3	G	123	GLU
4	F	96	HIS
4	F	100	GLU
4	F	107	LYS
5	A	29	LYS
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	197	THR
5	A	230	GLU
5	A	267	GLU
5	A	390	LYS
5	A	397	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	461	ASP
6	B	45	SER
6	B	60	PHE
6	B	79	LEU
6	B	102	GLN
6	B	119	LYS
6	B	139	LYS
6	B	247	LEU
6	B	249	ILE
6	B	276	SER
6	B	345	LYS
6	B	376	GLU
7	D	193	GLN
8	H	51	ARG
10	J	11	LYS
10	J	82	PHE
1	N	79	ARG
1	N	89	PHE
1	N	109	PRO
1	N	136	PHE
1	N	178	ARG
1	N	184	TYR
1	N	197	HIS
1	N	250	LYS
1	N	255	ASP
1	N	288	LYS
1	N	324	LEU
1	N	369	MET
2	E	54	LYS
2	E	55	ASP
2	E	62	ARG
2	E	65	SER
2	E	67	PHE
2	E	90	ASN
3	R	17	SER
3	R	22	LYS
3	R	23	ILE
3	R	94	LYS
4	Q	93	ASP
5	L	29	LYS
5	L	48	LEU
5	L	51	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	86	LYS
5	L	87	ARG
5	L	97	GLU
5	L	99	MET
5	L	185	LEU
5	L	378	SER
5	L	390	LYS
5	L	441	LYS
5	L	461	ASP
6	M	16	SER
6	M	19	GLU
6	M	32	SER
6	M	60	PHE
6	M	101	LYS
6	M	119	LYS
6	M	216	GLU
6	M	247	LEU
6	M	273	VAL
6	M	331	GLU
6	M	345	LYS
7	O	193	GLN
8	S	51	ARG
9	T	27	PHE
10	U	55	ARG
10	U	82	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	C	173	ASN
1	C	202	HIS
1	C	332	ASN
2	P	90	ASN
3	G	54	ASN
3	G	84	HIS
5	A	222	HIS
6	B	215	GLN
10	J	70	HIS
1	N	14	ASN
1	N	202	HIS
1	N	332	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	85	GLN
2	E	90	ASN
3	R	84	HIS
6	M	87	HIS
6	M	92	HIS
6	M	184	GLN
6	M	215	GLN
10	U	70	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
12	PC1	T	201	-	31,31,53	0.38	0	37,39,61	0.61	0
13	PTY	P	303	-	40,40,49	0.46	0	43,45,54	0.76	1 (2%)
14	CDL	H	701	-	49,49,99	0.39	0	55,61,111	0.75	0
15	LMT	J	101	-	36,36,36	0.51	0	47,47,47	1.06	2 (4%)
14	CDL	A	3002	-	46,46,99	0.39	0	51,56,111	0.92	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CDL	O	402	-	38,38,99	0.54	0	44,50,111	1.28	5 (11%)
14	CDL	A	3001	-	41,41,99	0.74	2 (4%)	45,51,111	0.74	1 (2%)
14	CDL	L	3001	-	41,41,99	0.66	1 (2%)	45,51,111	0.78	1 (2%)
11	HEM	C	502	1	41,50,50	1.54	5 (12%)	45,82,82	2.53	21 (46%)
13	PTY	N	505	-	40,40,49	0.39	0	43,45,54	0.64	0
15	LMT	C	506	-	36,36,36	0.60	0	47,47,47	1.35	7 (14%)
14	CDL	H	702	-	38,38,99	0.53	0	44,50,111	1.21	6 (13%)
14	CDL	N	506	-	47,47,99	0.50	0	53,59,111	0.91	2 (3%)
12	PC1	C	503	-	37,37,53	0.82	1 (2%)	43,45,61	1.04	4 (9%)
18	HEC	O	401	7	32,50,50	1.69	10 (31%)	24,82,82	2.89	7 (29%)
16	FES	P	301	2	0,4,4	-	-	-		
14	CDL	L	3002	-	46,46,99	0.39	0	51,56,111	0.86	3 (5%)
12	PC1	I	201	-	31,31,53	0.42	0	37,39,61	0.74	1 (2%)
14	CDL	C	505	-	47,47,99	0.51	0	53,59,111	0.92	3 (5%)
15	LMT	P	302	-	36,36,36	0.61	0	47,47,47	1.16	6 (12%)
13	PTY	C	504	-	40,40,49	0.36	0	43,45,54	0.52	0
18	HEC	D	401	7	32,50,50	1.68	8 (25%)	24,82,82	2.80	7 (29%)
14	CDL	N	504	-	49,49,99	0.37	0	55,61,111	0.75	2 (3%)
13	PTY	E	401	-	40,40,49	0.55	0	43,45,54	0.63	0
12	PC1	N	503	-	37,37,53	0.65	0	43,45,61	0.90	1 (2%)
11	HEM	C	501	1	41,50,50	1.55	10 (24%)	45,82,82	2.37	15 (33%)
17	XP4	L	3003	-	23,23,39	1.60	2 (8%)	27,28,44	2.39	10 (37%)
11	HEM	N	501	1	41,50,50	1.50	7 (17%)	45,82,82	2.30	14 (31%)
11	HEM	N	502	1	41,50,50	1.43	7 (17%)	45,82,82	2.33	18 (40%)
15	LMT	N	507	-	36,36,36	0.59	0	47,47,47	1.28	6 (12%)
17	XP4	A	3003	-	23,23,39	1.63	2 (8%)	27,28,44	2.35	6 (22%)

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
12	PC1	T	201	-	-	13/35/35/57	-
13	PTY	P	303	-	-	25/44/44/53	-
14	CDL	H	701	-	-	34/59/59/110	-
15	LMT	J	101	-	-	11/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	A	3002	-	-	26/54/54/110	-
14	CDL	O	402	-	-	28/48/48/110	-
14	CDL	A	3001	-	-	16/48/48/110	-
14	CDL	L	3001	-	-	20/48/48/110	-
11	HEM	C	502	1	-	4/12/54/54	-
13	PTY	N	505	-	-	27/44/44/53	-
15	LMT	C	506	-	-	14/21/61/61	0/2/2/2
14	CDL	H	702	-	-	28/48/48/110	-
14	CDL	N	506	-	-	29/57/57/110	-
12	PC1	C	503	-	-	14/41/41/57	-
18	HEC	O	401	7	-	5/10/54/54	-
16	FES	P	301	2	-	-	0/1/1/1
14	CDL	L	3002	-	-	28/54/54/110	-
12	PC1	I	201	-	-	17/35/35/57	-
14	CDL	C	505	-	-	30/57/57/110	-
15	LMT	P	302	-	-	8/21/61/61	0/2/2/2
13	PTY	C	504	-	-	30/44/44/53	-
18	HEC	D	401	7	-	4/10/54/54	-
14	CDL	N	504	-	-	36/59/59/110	-
13	PTY	E	401	-	-	27/44/44/53	-
12	PC1	N	503	-	-	11/41/41/57	-
11	HEM	C	501	1	-	5/12/54/54	-
17	XP4	L	3003	-	-	2/24/24/41	-
11	HEM	N	501	1	-	5/12/54/54	-
11	HEM	N	502	1	-	4/12/54/54	-
15	LMT	N	507	-	-	12/21/61/61	0/2/2/2
17	XP4	A	3003	-	-	2/24/24/41	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	3003	XP4	O7-C18	5.63	1.47	1.35
17	A	3003	XP4	O7-C18	5.61	1.47	1.35
11	C	502	HEM	C1B-NB	-5.00	1.31	1.40
17	A	3003	XP4	O5-C4	4.25	1.45	1.33
11	N	501	HEM	C4B-NB	-4.15	1.30	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	3003	XP4	O5-C4	4.13	1.45	1.33
18	D	401	HEC	C3C-C2C	4.08	1.45	1.40
11	N	502	HEM	C1B-NB	-3.94	1.33	1.40
11	C	501	HEM	C4B-NB	-3.91	1.30	1.38
18	O	401	HEC	C3C-C2C	3.84	1.44	1.40
18	O	401	HEC	C2B-C3B	3.71	1.44	1.40
11	C	501	HEM	C1B-NB	-3.63	1.34	1.40
18	D	401	HEC	C2B-C3B	3.62	1.44	1.40
11	N	501	HEM	C1B-NB	-3.61	1.34	1.40
11	N	502	HEM	C4B-NB	-3.54	1.31	1.38
11	N	501	HEM	C3C-C2C	-3.45	1.35	1.40
11	C	502	HEM	C4B-NB	-3.39	1.31	1.38
11	C	502	HEM	C4D-ND	-3.25	1.34	1.40
11	C	501	HEM	C3C-C2C	-2.95	1.36	1.40
14	L	3001	CDL	C31-CA7	2.66	1.58	1.50
11	C	501	HEM	C4D-ND	-2.63	1.35	1.40
11	N	501	HEM	C4D-ND	-2.60	1.35	1.40
18	D	401	HEC	C1B-NB	-2.48	1.31	1.36
18	D	401	HEC	C3D-C2D	2.47	1.45	1.37
18	O	401	HEC	C2A-C3A	2.47	1.45	1.37
14	A	3001	CDL	C31-CA7	2.44	1.57	1.50
18	D	401	HEC	CAA-C2A	-2.41	1.48	1.52
12	C	503	PC1	C22-C21	2.36	1.57	1.50
11	N	502	HEM	C4D-C3D	2.35	1.49	1.45
11	C	502	HEM	FE-NB	2.34	2.08	1.96
18	O	401	HEC	C1B-NB	-2.33	1.31	1.36
18	O	401	HEC	C3D-C2D	2.33	1.44	1.37
11	C	501	HEM	FE-NB	2.32	2.08	1.96
18	D	401	HEC	C1D-ND	-2.32	1.31	1.36
11	C	502	HEM	FE-ND	-2.31	1.85	1.96
11	C	501	HEM	C1D-C2D	2.26	1.48	1.44
11	N	501	HEM	CHB-C1B	2.26	1.40	1.35
18	O	401	HEC	C4D-CHA	2.24	1.47	1.41
11	C	501	HEM	C4D-C3D	2.24	1.48	1.45
18	O	401	HEC	C1D-ND	-2.23	1.31	1.36
11	C	501	HEM	CHC-C4B	-2.23	1.34	1.41
14	A	3001	CDL	C32-C31	2.21	1.60	1.52
11	N	502	HEM	C4D-ND	-2.21	1.36	1.40
18	D	401	HEC	C2A-C3A	2.19	1.44	1.37
18	O	401	HEC	C2A-C1A	2.18	1.47	1.42
11	C	501	HEM	FE-ND	-2.17	1.86	1.96
11	C	501	HEM	O2D-CGD	-2.14	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	C4D-ND	-2.12	1.31	1.36
18	O	401	HEC	CAA-C2A	-2.12	1.48	1.52
11	N	501	HEM	O2D-CGD	-2.09	1.23	1.30
11	N	501	HEM	C1D-C2D	2.05	1.48	1.44
11	N	502	HEM	FE-NB	2.04	2.07	1.96
18	O	401	HEC	CAD-C3D	-2.03	1.49	1.52
11	N	502	HEM	CHB-C1B	2.03	1.40	1.35
11	N	502	HEM	FE-ND	-2.01	1.87	1.96

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	3003	XP4	O7-C18-C19	8.19	126.16	111.09
17	L	3003	XP4	O7-C18-C19	7.84	125.52	111.09
18	O	401	HEC	CMB-C2B-C3B	7.71	134.89	125.82
18	D	401	HEC	C1D-C2D-C3D	-7.11	102.05	107.00
11	C	501	HEM	CBA-CAA-C2A	-7.00	100.68	112.62
18	D	401	HEC	CMB-C2B-C3B	6.85	133.87	125.82
18	O	401	HEC	C1D-C2D-C3D	-6.39	102.55	107.00
11	C	502	HEM	CHC-C4B-NB	6.38	131.37	124.43
11	N	502	HEM	CHC-C4B-NB	6.01	130.96	124.43
11	N	501	HEM	CBA-CAA-C2A	-6.00	102.39	112.62
11	C	501	HEM	CHC-C4B-NB	5.86	130.80	124.43
11	N	501	HEM	CHC-C4B-NB	5.79	130.72	124.43
11	C	502	HEM	CHD-C1D-ND	5.33	130.22	124.43
17	L	3003	XP4	O7-C18-O8	-5.08	112.86	122.96
17	A	3003	XP4	O7-C18-O8	-4.97	113.08	122.96
11	C	502	HEM	CHD-C1D-C2D	-4.91	117.30	124.98
18	O	401	HEC	CMC-C2C-C3C	4.89	131.57	125.82
11	N	502	HEM	CHD-C1D-ND	4.88	129.73	124.43
18	D	401	HEC	CAA-CBA-CGA	-4.84	100.18	113.76
18	O	401	HEC	CAA-CBA-CGA	-4.77	100.40	113.76
11	C	502	HEM	C4C-CHD-C1D	-4.76	116.28	122.56
11	N	502	HEM	C4C-CHD-C1D	-4.64	116.44	122.56
11	C	501	HEM	CHD-C1D-ND	4.39	129.20	124.43
18	D	401	HEC	CMC-C2C-C3C	4.37	130.96	125.82
11	N	502	HEM	CHD-C1D-C2D	-4.37	118.16	124.98
11	N	501	HEM	CHD-C1D-ND	4.34	129.15	124.43
11	N	501	HEM	C1B-NB-C4B	4.24	109.45	105.07
18	O	401	HEC	CBD-CAD-C3D	-4.21	105.44	112.62
11	C	502	HEM	C2C-C3C-C4C	4.09	109.75	106.90
11	C	501	HEM	CMA-C3A-C4A	-4.08	122.20	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	501	HEM	C3B-C2B-C1B	-4.04	103.49	106.49
11	N	501	HEM	CHA-C4D-ND	4.03	129.36	124.38
11	N	502	HEM	CBD-CAD-C3D	-3.77	102.15	112.63
11	C	501	HEM	C4A-C3A-C2A	3.76	109.61	107.00
14	O	402	CDL	CB4-OB6-CB5	3.71	124.80	117.90
17	L	3003	XP4	P1-O4-C1	3.69	128.45	118.30
11	N	501	HEM	CAD-CBD-CGD	-3.62	105.80	113.60
11	C	502	HEM	CHA-C4D-ND	3.60	128.83	124.38
18	D	401	HEC	CBD-CAD-C3D	-3.59	106.50	112.62
11	C	502	HEM	CHC-C4B-C3B	-3.58	119.09	124.57
18	O	401	HEC	CMA-C3A-C2A	3.54	131.61	124.94
15	N	507	LMT	O5B-C5B-C4B	3.52	116.09	109.69
11	C	501	HEM	C1B-NB-C4B	3.50	108.69	105.07
11	N	502	HEM	CHA-C4D-ND	3.49	128.69	124.38
11	C	501	HEM	CHA-C4D-ND	3.47	128.67	124.38
14	H	702	CDL	CB4-OB6-CB5	3.47	124.36	117.90
15	P	302	LMT	O1'-C1'-C2'	3.45	113.69	108.30
11	C	502	HEM	CBD-CAD-C3D	-3.41	103.16	112.63
11	N	502	HEM	CHC-C4B-C3B	-3.38	119.39	124.57
11	C	501	HEM	CAD-CBD-CGD	-3.38	106.33	113.60
11	N	502	HEM	C1B-NB-C4B	3.38	108.56	105.07
17	A	3003	XP4	P1-O4-C1	3.33	127.48	118.30
11	C	501	HEM	CHC-C4B-C3B	-3.31	119.50	124.57
14	O	402	CDL	OB6-CB5-C51	3.30	117.16	111.09
11	N	501	HEM	CHD-C1D-C2D	-3.24	119.92	124.98
11	N	502	HEM	CMB-C2B-C1B	3.23	129.96	125.04
11	N	502	HEM	C2C-C3C-C4C	3.21	109.14	106.90
14	N	506	CDL	OB6-CB4-CB3	3.21	120.01	108.40
11	C	501	HEM	CHD-C1D-C2D	-3.18	120.01	124.98
11	N	501	HEM	CHA-C4D-C3D	-3.17	119.39	125.33
15	N	507	LMT	C1B-O5B-C5B	3.16	119.90	113.69
15	C	506	LMT	O5B-C5B-C4B	3.12	115.36	109.69
15	P	302	LMT	C1'-O5'-C5'	-3.12	107.57	113.69
17	A	3003	XP4	O4-P1-O2	-3.05	97.91	106.47
11	N	502	HEM	CAD-C3D-C4D	3.04	129.97	124.66
15	C	506	LMT	C1B-O5B-C5B	3.00	119.58	113.69
15	C	506	LMT	C4B-C3B-C2B	2.98	116.03	110.82
11	C	502	HEM	C3B-C2B-C1B	-2.96	104.29	106.49
15	N	507	LMT	O1'-C1'-C2'	-2.92	103.75	108.30
12	C	503	PC1	O22-C21-C22	2.91	135.09	123.73
15	C	506	LMT	C3B-C4B-C5B	2.91	115.43	110.24
11	C	502	HEM	CMB-C2B-C1B	2.88	129.42	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	702	CDL	OB6-CB5-C51	2.87	116.38	111.09
18	D	401	HEC	O1D-CGD-CBD	-2.83	113.99	123.08
11	C	502	HEM	O2A-CGA-O1A	-2.81	116.28	123.30
11	C	501	HEM	CHA-C4D-C3D	-2.80	120.06	125.33
11	C	501	HEM	O2D-CGD-O1D	-2.78	116.37	123.30
11	C	502	HEM	O1D-CGD-CBD	-2.77	114.18	123.08
17	L	3003	XP4	O5-C4-C5	2.76	120.58	111.91
15	N	507	LMT	C3B-C4B-C5B	2.72	115.09	110.24
14	N	504	CDL	OB6-CB5-C51	-2.71	105.67	111.50
11	C	502	HEM	C3C-C4C-NC	-2.70	105.84	110.94
14	H	702	CDL	OA5-PA1-OA3	-2.70	98.52	109.07
11	C	502	HEM	CHA-C4D-C3D	-2.69	120.28	125.33
15	C	506	LMT	O5'-C1'-C2'	2.68	116.01	110.35
11	C	501	HEM	CMB-C2B-C1B	2.67	129.11	125.04
17	L	3003	XP4	O5-C4-O6	-2.67	116.84	123.59
11	C	502	HEM	CAD-C3D-C4D	2.62	129.24	124.66
15	C	506	LMT	C1'-O5'-C5'	2.61	118.82	113.69
18	D	401	HEC	O2D-CGD-CBD	2.59	122.34	114.03
11	N	502	HEM	CHA-C4D-C3D	-2.55	120.53	125.33
14	L	3001	CDL	OB6-CB4-CB3	-2.55	100.62	109.56
14	A	3002	CDL	OA6-CA5-C11	-2.55	106.01	111.50
11	C	502	HEM	C1B-NB-C4B	2.54	107.70	105.07
15	J	101	LMT	C1-O1'-C1'	-2.54	109.63	113.84
14	O	402	CDL	OA5-PA1-OA3	-2.54	99.15	109.07
15	P	302	LMT	O5B-C5B-C4B	2.53	114.30	109.69
17	A	3003	XP4	O5-C4-O6	-2.53	117.21	123.59
11	C	502	HEM	O2D-CGD-CBD	2.52	122.13	114.03
14	C	505	CDL	CB4-OB6-CB5	2.51	123.96	117.79
14	L	3002	CDL	OA2-PA1-OA3	2.49	118.78	109.07
14	C	505	CDL	OB6-CB4-CB3	2.46	117.33	108.40
11	C	502	HEM	CMC-C2C-C3C	2.46	129.28	124.68
13	P	303	PTY	O12-P1-O14	-2.45	96.39	107.75
14	L	3002	CDL	OA6-CA4-CA6	2.45	117.25	108.40
15	C	506	LMT	C1-O1'-C1'	-2.44	109.79	113.84
11	N	502	HEM	C3C-C4C-NC	-2.44	106.34	110.94
12	N	503	PC1	O22-C21-C22	2.44	133.23	123.73
17	L	3003	XP4	O3-P1-O4	-2.43	100.25	106.73
12	C	503	PC1	O21-C21-C22	-2.43	106.26	111.50
14	L	3002	CDL	OA5-PA1-OA3	-2.42	99.60	109.07
11	N	501	HEM	CHB-C1B-NB	2.41	127.36	124.38
11	N	501	HEM	O2D-CGD-O1D	-2.39	117.34	123.30
17	L	3003	XP4	O4-P1-O2	-2.39	99.78	106.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	3002	CDL	OA2-PA1-OA3	2.38	118.38	109.07
11	N	502	HEM	CHB-C1B-NB	2.38	127.32	124.38
15	J	101	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
14	A	3001	CDL	OB8-CB6-CB4	2.34	117.06	105.77
14	N	506	CDL	CB4-OB6-CB5	2.33	123.53	117.79
11	N	501	HEM	C4A-C3A-C2A	2.32	108.61	107.00
14	A	3002	CDL	OA5-PA1-OA3	-2.32	100.02	109.07
14	O	402	CDL	OB6-CB4-CB6	2.30	116.74	108.40
17	A	3003	XP4	O5-C4-C5	2.30	119.13	111.91
11	N	502	HEM	O2A-CGA-O1A	-2.29	117.59	123.30
14	O	402	CDL	OB6-CB4-CB3	2.27	116.61	108.40
15	N	507	LMT	C4B-C3B-C2B	2.25	114.76	110.82
11	C	501	HEM	C3B-C2B-C1B	-2.24	104.83	106.49
17	L	3003	XP4	O7-C2-C3	-2.22	100.35	108.40
11	N	502	HEM	C3B-C2B-C1B	-2.21	104.85	106.49
15	N	507	LMT	C1-O1'-C1'	-2.18	110.22	113.84
17	L	3003	XP4	O3-P1-O1	2.18	115.96	107.64
14	H	702	CDL	OB6-CB4-CB3	2.18	116.28	108.40
11	N	502	HEM	CBA-CAA-C2A	-2.16	108.93	112.62
17	L	3003	XP4	O1-P1-O4	2.16	112.48	106.73
11	N	501	HEM	O2A-CGA-CBA	2.14	120.91	114.03
12	C	503	PC1	O12-P-O14	2.14	122.83	112.24
11	N	501	HEM	CHC-C4B-C3B	-2.13	121.30	124.57
18	O	401	HEC	CAA-C2A-C3A	-2.13	121.13	127.25
11	C	502	HEM	C4B-CHC-C1C	-2.12	119.77	122.56
14	H	702	CDL	OB6-CB4-CB6	2.11	116.04	108.40
11	C	502	HEM	C2D-C1D-ND	2.10	112.40	109.88
12	C	503	PC1	O21-C21-O22	-2.10	118.62	123.70
15	P	302	LMT	C4B-C3B-C2B	2.10	114.49	110.82
14	H	702	CDL	OA6-CA5-C11	2.10	116.65	110.80
15	P	302	LMT	C1-O1'-C1'	-2.08	110.39	113.84
15	P	302	LMT	C2'-C3'-C4'	2.06	114.39	109.68
11	C	501	HEM	CAD-C3D-C4D	2.06	128.26	124.66
14	N	504	CDL	OB7-CB5-C51	2.06	131.77	123.73
11	C	502	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
14	C	505	CDL	OB6-CB4-CB6	2.05	115.84	108.40
11	N	502	HEM	O2D-CGD-CBD	2.05	120.61	114.03
12	I	201	PC1	O12-P-O14	2.02	122.24	112.24

There are no chirality outliers.

All (515) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	I	201	PC1	C11-O13-P-O14
12	I	201	PC1	C11-O13-P-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	C11-O13-P-O14
12	T	201	PC1	C11-O13-P-O11
12	T	201	PC1	O21-C2-C3-O31
13	C	504	PTY	N1-C2-C3-O11
13	C	504	PTY	C11-C8-O7-C6
13	C	504	PTY	C3-O11-P1-O13
13	P	303	PTY	C5-O14-P1-O11
13	P	303	PTY	C5-O14-P1-O12
13	P	303	PTY	C5-O14-P1-O13
13	N	505	PTY	C11-C8-O7-C6
13	N	505	PTY	C3-O11-P1-O12
13	N	505	PTY	C3-O11-P1-O13
13	N	505	PTY	C5-O14-P1-O13
13	E	401	PTY	N1-C2-C3-O11
13	E	401	PTY	C3-O11-P1-O13
13	E	401	PTY	C5-O14-P1-O12
14	C	505	CDL	O1-C1-CA2-OA2
14	C	505	CDL	CA2-C1-CB2-OB2
14	C	505	CDL	CA3-OA5-PA1-OA3
14	C	505	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	CB2-OB2-PB2-OB3
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB3-OB5-PB2-OB2
14	C	505	CDL	CB3-OB5-PB2-OB3
14	C	505	CDL	CB3-OB5-PB2-OB4
14	A	3001	CDL	OA5-CA3-CA4-OA6
14	A	3001	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	CA2-OA2-PA1-OA3
14	A	3002	CDL	CA2-OA2-PA1-OA4
14	A	3002	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	CA2-C1-CB2-OB2
14	H	702	CDL	CA2-OA2-PA1-OA4
14	H	702	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	C51-CB5-OB6-CB4
14	N	504	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	504	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	CB2-C1-CA2-OA2
14	N	506	CDL	CA3-OA5-PA1-OA3
14	N	506	CDL	C11-CA5-OA6-CA4
14	N	506	CDL	CB2-OB2-PB2-OB3
14	N	506	CDL	CB2-OB2-PB2-OB4
14	N	506	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	CB3-OB5-PB2-OB4
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	L	3001	CDL	CB3-CB4-CB6-OB8
14	L	3002	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	CA2-OA2-PA1-OA3
14	L	3002	CDL	CA2-OA2-PA1-OA4
14	L	3002	CDL	CA2-OA2-PA1-OA5
14	L	3002	CDL	CB2-OB2-PB2-OB3
14	L	3002	CDL	CB3-OB5-PB2-OB3
14	L	3002	CDL	OB5-CB3-CB4-OB6
14	O	402	CDL	CA2-C1-CB2-OB2
14	O	402	CDL	CA2-OA2-PA1-OA4
14	O	402	CDL	CA2-OA2-PA1-OA5
14	O	402	CDL	CB3-OB5-PB2-OB4
14	O	402	CDL	C51-CB5-OB6-CB4
15	P	302	LMT	O5'-C1'-O1'-C1
15	J	101	LMT	C2-C1-O1'-C1'
14	H	702	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	OB9-CB7-OB8-CB6
14	O	402	CDL	OA9-CA7-OA8-CA6
14	O	402	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	CB4-CB6-OB8-CB7
14	H	702	CDL	C71-CB7-OB8-CB6
14	O	402	CDL	C31-CA7-OA8-CA6
14	O	402	CDL	C71-CB7-OB8-CB6
12	T	201	PC1	O32-C31-O31-C3
14	A	3001	CDL	OA9-CA7-OA8-CA6
14	H	701	CDL	OB9-CB7-OB8-CB6
14	N	504	CDL	OB9-CB7-OB8-CB6
14	H	702	CDL	OB7-CB5-OB6-CB4
14	O	402	CDL	OB7-CB5-OB6-CB4
14	H	701	CDL	OA9-CA7-OA8-CA6
14	H	701	CDL	C31-CA7-OA8-CA6
13	C	504	PTY	O10-C8-O7-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	N	505	PTY	O10-C8-O7-C6
14	C	505	CDL	OA7-CA5-OA6-CA4
14	N	504	CDL	OB7-CB5-OB6-CB4
14	N	506	CDL	OA7-CA5-OA6-CA4
12	T	201	PC1	C32-C31-O31-C3
14	H	701	CDL	C71-CB7-OB8-CB6
14	N	504	CDL	C71-CB7-OB8-CB6
14	L	3001	CDL	C31-CA7-OA8-CA6
14	L	3001	CDL	C71-CB7-OB8-CB6
14	N	504	CDL	C51-CB5-OB6-CB4
14	L	3001	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	C31-CA7-OA8-CA6
13	P	303	PTY	C37-C38-C39-C40
14	L	3001	CDL	OA9-CA7-OA8-CA6
14	A	3002	CDL	O1-C1-CB2-OB2
14	N	504	CDL	O1-C1-CA2-OA2
14	N	506	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	OB5-CB3-CB4-OB6
14	L	3002	CDL	O1-C1-CB2-OB2
14	O	402	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	C51-CB5-OB6-CB4
13	E	401	PTY	C35-C36-C37-C38
14	A	3002	CDL	C11-CA5-OA6-CA4
14	L	3002	CDL	C11-CA5-OA6-CA4
13	N	505	PTY	C31-C32-C33-C34
13	C	504	PTY	C35-C36-C37-C38
13	N	505	PTY	C33-C34-C35-C36
14	A	3002	CDL	OB7-CB5-OB6-CB4
12	I	201	PC1	C32-C33-C34-C35
13	C	504	PTY	C31-C32-C33-C34
13	E	401	PTY	C13-C14-C15-C16
15	J	101	LMT	C2-C3-C4-C5
15	J	101	LMT	C4-C5-C6-C7
15	C	506	LMT	O5'-C5'-C6'-O6'
13	P	303	PTY	C35-C36-C37-C38
13	N	505	PTY	C37-C38-C39-C40
15	C	506	LMT	O5B-C5B-C6B-O6B
15	N	507	LMT	O5B-C5B-C6B-O6B
14	C	505	CDL	CB2-C1-CA2-OA2
14	H	702	CDL	CB2-C1-CA2-OA2
14	N	504	CDL	CB2-C1-CA2-OA2
14	N	504	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA7-CA5-OA6-CA4
12	C	503	PC1	C32-C31-O31-C3
13	P	303	PTY	C31-C30-O4-C1
15	N	507	LMT	C4'-C5'-C6'-O6'
13	P	303	PTY	C33-C34-C35-C36
14	L	3002	CDL	CA7-C31-C32-C33
15	N	507	LMT	O5'-C5'-C6'-O6'
14	H	702	CDL	O1-C1-CA2-OA2
13	N	505	PTY	C8-C11-C12-C13
14	A	3002	CDL	OA7-CA5-OA6-CA4
15	C	506	LMT	C4'-C5'-C6'-O6'
15	J	101	LMT	O5B-C5B-C6B-O6B
12	I	201	PC1	C32-C31-O31-C3
14	A	3002	CDL	CA7-C31-C32-C33
12	I	201	PC1	C21-C22-C23-C24
12	T	201	PC1	C21-C22-C23-C24
13	E	401	PTY	C30-C31-C32-C33
14	C	505	CDL	CA7-C31-C32-C33
14	A	3001	CDL	CB7-C71-C72-C73
14	H	701	CDL	CB7-C71-C72-C73
14	N	504	CDL	CA5-C11-C12-C13
14	N	504	CDL	CB7-C71-C72-C73
12	T	201	PC1	C31-C32-C33-C34
14	H	701	CDL	CA5-C11-C12-C13
14	N	506	CDL	CA7-C31-C32-C33
13	P	303	PTY	O30-C30-O4-C1
14	N	504	CDL	OA9-CA7-OA8-CA6
13	E	401	PTY	C40-C41-C42-C43
14	H	702	CDL	O1-C1-CB2-OB2
14	N	504	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	O	402	CDL	O1-C1-CA2-OA2
12	N	503	PC1	C32-C31-O31-C3
14	N	504	CDL	C31-CA7-OA8-CA6
12	C	503	PC1	O32-C31-O31-C3
12	I	201	PC1	O32-C31-O31-C3
14	L	3001	CDL	OB6-CB4-CB6-OB8
13	N	505	PTY	C3-O11-P1-O14
13	N	505	PTY	C5-O14-P1-O11
13	E	401	PTY	C5-O14-P1-O11
14	C	505	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	3002	CDL	CA2-OA2-PA1-OA5
14	H	701	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CA2-OA2-PA1-OA5
14	N	504	CDL	CA2-OA2-PA1-OA5
14	N	506	CDL	CB2-OB2-PB2-OB5
14	N	506	CDL	CB3-OB5-PB2-OB2
14	O	402	CDL	CB3-OB5-PB2-OB2
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	L	3001	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-CA6
12	N	503	PC1	O32-C31-O31-C3
14	A	3001	CDL	C71-C72-C73-C74
15	C	506	LMT	C5-C6-C7-C8
13	P	303	PTY	C16-C17-C18-C19
13	P	303	PTY	C34-C35-C36-C37
13	E	401	PTY	C16-C17-C18-C19
13	E	401	PTY	C32-C33-C34-C35
14	H	701	CDL	C73-C74-C75-C76
14	N	504	CDL	C74-C75-C76-C77
14	L	3002	CDL	C12-C13-C14-C15
14	C	505	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	O1-C1-CA2-OA2
12	I	201	PC1	C34-C35-C36-C37
15	N	507	LMT	C7-C8-C9-C10
13	E	401	PTY	C38-C39-C40-C41
15	P	302	LMT	C4-C5-C6-C7
13	E	401	PTY	C8-C11-C12-C13
14	L	3001	CDL	CB7-C71-C72-C73
13	N	505	PTY	C32-C33-C34-C35
13	E	401	PTY	C14-C15-C16-C17
14	A	3002	CDL	C12-C13-C14-C15
14	H	701	CDL	C11-C12-C13-C14
14	H	701	CDL	C74-C75-C76-C77
14	N	504	CDL	C71-C72-C73-C74
14	H	701	CDL	C71-C72-C73-C74
13	C	504	PTY	C38-C39-C40-C41
12	I	201	PC1	C33-C34-C35-C36
13	P	303	PTY	C40-C41-C42-C43
14	N	504	CDL	C73-C74-C75-C76
13	N	505	PTY	C16-C17-C18-C19
13	C	504	PTY	C8-C11-C12-C13
13	P	303	PTY	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	E	401	PTY	C12-C13-C14-C15
15	J	101	LMT	O1'-C1-C2-C3
15	C	506	LMT	C4-C5-C6-C7
15	C	506	LMT	C6-C7-C8-C9
14	H	701	CDL	CB3-CB4-CB6-OB8
14	C	505	CDL	C51-CB5-OB6-CB4
12	T	201	PC1	C33-C34-C35-C36
13	P	303	PTY	C14-C15-C16-C17
13	E	401	PTY	C11-C12-C13-C14
15	C	506	LMT	C3-C4-C5-C6
14	O	402	CDL	CB2-C1-CA2-OA2
12	C	503	PC1	C28-C29-C2A-C2B
14	C	505	CDL	OB7-CB5-OB6-CB4
14	H	701	CDL	OA7-CA5-OA6-CA4
15	N	507	LMT	C1-C2-C3-C4
13	E	401	PTY	C31-C32-C33-C34
13	E	401	PTY	C31-C30-O4-C1
14	N	506	CDL	C11-C12-C13-C14
15	C	506	LMT	C1-C2-C3-C4
13	C	504	PTY	C13-C14-C15-C16
13	C	504	PTY	C37-C38-C39-C40
13	C	504	PTY	C39-C40-C41-C42
13	P	303	PTY	C41-C42-C43-C44
14	A	3001	CDL	C73-C74-C75-C76
14	H	701	CDL	CB5-C51-C52-C53
13	P	303	PTY	C38-C39-C40-C41
15	J	101	LMT	C6-C7-C8-C9
14	A	3002	CDL	C33-C34-C35-C36
12	N	503	PC1	C26-C27-C28-C29
14	L	3001	CDL	C71-C72-C73-C74
14	H	701	CDL	C11-CA5-OA6-CA4
14	H	701	CDL	C51-CB5-OB6-CB4
14	N	506	CDL	C51-CB5-OB6-CB4
13	E	401	PTY	O14-C5-C6-O7
15	N	507	LMT	C5-C6-C7-C8
15	P	302	LMT	C6-C7-C8-C9
14	L	3002	CDL	O1-C1-CA2-OA2
14	H	701	CDL	OB7-CB5-OB6-CB4
14	N	506	CDL	OB7-CB5-OB6-CB4
12	C	503	PC1	O21-C2-C3-O31
12	N	503	PC1	O21-C2-C3-O31
12	C	503	PC1	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	L	3002	CDL	C33-C34-C35-C36
15	N	507	LMT	C2-C3-C4-C5
12	I	201	PC1	C31-C32-C33-C34
17	L	3003	XP4	C5-C6-C7-C8
13	C	504	PTY	C5-O14-P1-O11
14	N	506	CDL	CA3-OA5-PA1-OA2
15	C	506	LMT	C4B-C5B-C6B-O6B
14	A	3002	CDL	OA5-CA3-CA4-CA6
12	C	503	PC1	C27-C28-C29-C2A
12	N	503	PC1	C28-C29-C2A-C2B
13	E	401	PTY	O30-C30-O4-C1
13	N	505	PTY	C36-C37-C38-C39
13	C	504	PTY	O4-C1-C6-C5
13	P	303	PTY	C11-C12-C13-C14
13	N	505	PTY	O4-C1-C6-C5
14	L	3002	CDL	C13-C14-C15-C16
13	N	505	PTY	C14-C15-C16-C17
14	H	701	CDL	C75-C76-C77-C78
15	J	101	LMT	C9-C10-C11-C12
14	N	504	CDL	CB5-C51-C52-C53
12	N	503	PC1	C27-C28-C29-C2A
13	N	505	PTY	C41-C42-C43-C44
14	N	506	CDL	C13-C14-C15-C16
14	A	3001	CDL	OB6-CB4-CB6-OB8
13	C	504	PTY	C41-C42-C43-C44
13	C	504	PTY	C17-C18-C19-C20
14	N	504	CDL	C75-C76-C77-C78
15	N	507	LMT	C3-C4-C5-C6
12	C	503	PC1	C22-C23-C24-C25
13	C	504	PTY	C40-C41-C42-C43
15	J	101	LMT	C7-C8-C9-C10
13	P	303	PTY	C31-C32-C33-C34
13	N	505	PTY	C34-C35-C36-C37
13	E	401	PTY	C41-C42-C43-C44
15	N	507	LMT	C9-C10-C11-C12
14	L	3002	CDL	CA6-CA4-OA6-CA5
14	L	3002	CDL	C34-C35-C36-C37
13	C	504	PTY	O14-C5-C6-O7
14	C	505	CDL	OA5-CA3-CA4-OA6
14	N	504	CDL	OA5-CA3-CA4-OA6
14	N	506	CDL	OA5-CA3-CA4-OA6
14	L	3002	CDL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	506	CDL	OB6-CB4-CB6-OB8
14	C	505	CDL	C13-C14-C15-C16
14	L	3001	CDL	CB2-C1-CA2-OA2
12	N	503	PC1	C22-C23-C24-C25
14	L	3002	CDL	C51-CB5-OB6-CB4
14	A	3002	CDL	C13-C14-C15-C16
14	L	3001	CDL	C34-C35-C36-C37
13	N	505	PTY	O14-C5-C6-C1
13	E	401	PTY	O14-C5-C6-C1
14	H	702	CDL	OB5-CB3-CB4-CB6
14	N	504	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA5-CA3-CA4-CA6
14	O	402	CDL	OB5-CB3-CB4-CB6
13	N	505	PTY	C30-C31-C32-C33
14	A	3002	CDL	C34-C35-C36-C37
14	N	506	CDL	CA5-C11-C12-C13
14	H	701	CDL	C12-C13-C14-C15
14	N	504	CDL	C11-C12-C13-C14
13	P	303	PTY	C8-C11-C12-C13
12	T	201	PC1	C1-C2-C3-O31
14	N	504	CDL	CA3-CA4-CA6-OA8
14	N	504	CDL	CB3-CB4-CB6-OB8
15	P	302	LMT	O1'-C1-C2-C3
14	A	3001	CDL	C33-C34-C35-C36
13	P	303	PTY	C13-C14-C15-C16
14	A	3001	CDL	CB3-OB5-PB2-OB2
14	L	3002	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	C32-C33-C34-C35
15	C	506	LMT	C9-C10-C11-C12
15	C	506	LMT	C11-C10-C9-C8
13	N	505	PTY	O4-C1-C6-O7
14	N	504	CDL	OA6-CA4-CA6-OA8
14	O	402	CDL	OB6-CB4-CB6-OB8
15	N	507	LMT	C4B-C5B-C6B-O6B
13	N	505	PTY	C38-C39-C40-C41
14	A	3002	CDL	CB2-C1-CA2-OA2
14	L	3002	CDL	CB2-C1-CA2-OA2
13	N	505	PTY	C12-C13-C14-C15
11	N	501	HEM	C3D-CAD-CBD-CGD
13	C	504	PTY	C30-C31-C32-C33
15	C	506	LMT	C7-C8-C9-C10
14	H	701	CDL	OA5-CA3-CA4-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	701	CDL	OB5-CB3-CB4-CB6
14	L	3001	CDL	O1-C1-CA2-OA2
14	A	3002	CDL	CA6-CA4-OA6-CA5
14	C	505	CDL	CA4-CA3-OA5-PA1
14	H	701	CDL	CA3-CA4-CA6-OA8
14	H	702	CDL	CB3-CB4-CB6-OB8
13	P	303	PTY	O14-C5-C6-O7
13	N	505	PTY	O14-C5-C6-O7
14	H	701	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OB5-CB3-CB4-OB6
14	N	504	CDL	OB5-CB3-CB4-OB6
14	O	402	CDL	OA5-CA3-CA4-OA6
14	A	3001	CDL	OB5-CB3-CB4-CB6
13	C	504	PTY	C32-C33-C34-C35
14	H	701	CDL	OA6-CA4-CA6-OA8
14	H	701	CDL	OB6-CB4-CB6-OB8
14	H	702	CDL	OB6-CB4-CB6-OB8
14	N	504	CDL	OB6-CB4-CB6-OB8
14	L	3002	CDL	OB7-CB5-OB6-CB4
15	C	506	LMT	O1'-C1-C2-C3
13	E	401	PTY	C3-O11-P1-O14
14	C	505	CDL	CA3-OA5-PA1-OA2
13	C	504	PTY	C6-C5-O14-P1
13	N	505	PTY	C5-O14-P1-O12
14	C	505	CDL	CA3-OA5-PA1-OA4
14	H	701	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB3-OB5-PB2-OB3
14	N	504	CDL	CA2-OA2-PA1-OA3
14	N	506	CDL	CA3-OA5-PA1-OA4
14	O	402	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	OA5-CA3-CA4-CA6
14	N	504	CDL	OA5-CA3-CA4-CA6
14	O	402	CDL	OA5-CA3-CA4-CA6
12	I	201	PC1	C22-C21-O21-C2
14	L	3002	CDL	C11-C12-C13-C14
14	H	701	CDL	OB5-CB3-CB4-OB6
14	L	3002	CDL	CA5-C11-C12-C13
12	C	503	PC1	C1-C2-C3-O31
14	O	402	CDL	CB3-CB4-CB6-OB8
18	O	401	HEC	C3A-C2A-CAA-CBA
13	C	504	PTY	O4-C1-C6-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	C	505	CDL	OB6-CB4-CB6-OB8
14	L	3002	CDL	OA6-CA4-CA6-OA8
14	N	506	CDL	CA4-CA3-OA5-PA1
13	E	401	PTY	C39-C40-C41-C42
14	C	505	CDL	CA5-C11-C12-C13
14	N	504	CDL	C72-C73-C74-C75
14	H	702	CDL	CB6-CB4-OB6-CB5
14	O	402	CDL	CB6-CB4-OB6-CB5
13	C	504	PTY	O14-C5-C6-C1
14	C	505	CDL	OA5-CA3-CA4-CA6
13	E	401	PTY	C36-C37-C38-C39
12	C	503	PC1	O22-C21-O21-C2
14	A	3002	CDL	CA5-C11-C12-C13
14	O	402	CDL	OB5-CB3-CB4-OB6
13	C	504	PTY	C3-O11-P1-O14
13	P	303	PTY	C3-O11-P1-O14
14	A	3002	CDL	CB2-OB2-PB2-OB5
14	H	702	CDL	CB2-OB2-PB2-OB5
14	L	3002	CDL	CB2-OB2-PB2-OB5
14	O	402	CDL	CB2-OB2-PB2-OB5
14	A	3002	CDL	C51-C52-C53-C54
13	N	505	PTY	C31-C30-O4-C1
15	P	302	LMT	C7-C8-C9-C10
13	N	505	PTY	O30-C30-O4-C1
14	A	3001	CDL	C72-C73-C74-C75
14	H	702	CDL	CB4-CB3-OB5-PB2
13	C	504	PTY	C15-C16-C17-C18
13	C	504	PTY	C31-C30-O4-C1
14	C	505	CDL	C11-C12-C13-C14
14	C	505	CDL	C32-C33-C34-C35
13	C	504	PTY	C12-C13-C14-C15
11	N	502	HEM	CAA-CBA-CGA-O1A
15	P	302	LMT	C2'-C1'-O1'-C1
14	O	402	CDL	C32-C31-CA7-OA9
11	N	502	HEM	CAD-CBD-CGD-O1D
11	C	501	HEM	CAA-CBA-CGA-O2A
14	H	702	CDL	CA3-CA4-CA6-OA8
11	C	502	HEM	CAA-CBA-CGA-O2A
11	N	502	HEM	CAA-CBA-CGA-O2A
11	N	502	HEM	CAD-CBD-CGD-O2D
18	O	401	HEC	CAA-CBA-CGA-O1A
15	J	101	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	506	CDL	C71-CB7-OB8-CB6
11	C	502	HEM	CAD-CBD-CGD-O2D
13	C	504	PTY	C36-C37-C38-C39
18	D	401	HEC	CAA-CBA-CGA-O1A
14	C	505	CDL	CB6-CB4-OB6-CB5
11	C	501	HEM	CAA-CBA-CGA-O1A
11	N	501	HEM	CAA-CBA-CGA-O2A
14	O	402	CDL	CB4-CB3-OB5-PB2
11	C	502	HEM	CAA-CBA-CGA-O1A
14	N	504	CDL	OA7-CA5-OA6-CA4
13	P	303	PTY	O14-C5-C6-C1
12	C	503	PC1	C33-C34-C35-C36
11	C	502	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAA-CBA-CGA-O1A
13	C	504	PTY	O30-C30-O4-C1
12	I	201	PC1	O22-C21-O21-C2
15	C	506	LMT	C2'-C1'-O1'-C1
12	I	201	PC1	O21-C2-C3-O31
14	N	506	CDL	CA2-C1-CB2-OB2
13	P	303	PTY	C12-C13-C14-C15
14	L	3001	CDL	C72-C73-C74-C75
18	D	401	HEC	CAA-CBA-CGA-O2A
18	O	401	HEC	CAA-CBA-CGA-O2A
12	N	503	PC1	O22-C21-O21-C2
15	N	507	LMT	C6-C7-C8-C9
11	C	501	HEM	C3D-CAD-CBD-CGD
15	N	507	LMT	C11-C10-C9-C8
14	A	3002	CDL	C52-C53-C54-C55
12	T	201	PC1	C11-C12-N-C14
14	N	506	CDL	OA5-CA3-CA4-CA6
14	C	505	CDL	C31-C32-C33-C34
14	O	402	CDL	C32-C31-CA7-OA8
15	J	101	LMT	C1-C2-C3-C4
14	A	3002	CDL	OA6-CA4-CA6-OA8
14	H	701	CDL	C51-C52-C53-C54
14	N	504	CDL	CB2-OB2-PB2-OB5
14	H	702	CDL	C32-C31-CA7-OA9
14	A	3001	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	C72-C71-CB7-OB8
14	N	506	CDL	C32-C31-CA7-OA8
11	N	501	HEM	CAD-CBD-CGD-O2D
15	J	101	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	501	HEM	CAD-CBD-CGD-O2D
14	A	3001	CDL	C72-C71-CB7-OB8
12	N	503	PC1	C1-C2-C3-O31
13	P	303	PTY	O4-C30-C31-C32
14	N	504	CDL	C72-C71-CB7-OB8
18	D	401	HEC	CAD-CBD-CGD-O1D
12	I	201	PC1	C36-C37-C38-C39
17	A	3003	XP4	C5-C6-C7-C8
11	N	501	HEM	CAD-CBD-CGD-O1D
18	D	401	HEC	CAD-CBD-CGD-O2D
14	H	701	CDL	O1-C1-CB2-OB2
14	N	504	CDL	C51-C52-C53-C54
12	I	201	PC1	O21-C21-C22-C23
12	N	503	PC1	O31-C31-C32-C33
14	C	505	CDL	C32-C31-CA7-OA8
12	C	503	PC1	C22-C21-O21-C2
12	C	503	PC1	O31-C31-C32-C33
14	L	3002	CDL	C52-C53-C54-C55
14	O	402	CDL	C72-C71-CB7-OB8
14	C	505	CDL	C32-C31-CA7-OA9
13	C	504	PTY	C14-C15-C16-C17
18	O	401	HEC	CAD-CBD-CGD-O1D
13	E	401	PTY	C37-C38-C39-C40
14	H	701	CDL	CA2-C1-CB2-OB2
12	I	201	PC1	C22-C23-C24-C25
14	H	701	CDL	C72-C71-CB7-OB9
14	O	402	CDL	C72-C71-CB7-OB9
14	A	3002	CDL	C31-CA7-OA8-CA6
14	N	504	CDL	C72-C71-CB7-OB9
14	H	701	CDL	C72-C73-C74-C75
14	N	506	CDL	C32-C31-CA7-OA9
12	T	201	PC1	C1-O11-P-O14
13	C	504	PTY	C5-O14-P1-O13
12	C	503	PC1	C23-C24-C25-C26
13	P	303	PTY	O30-C30-C31-C32
11	C	501	HEM	CAD-CBD-CGD-O1D
18	O	401	HEC	CAD-CBD-CGD-O2D
14	A	3002	CDL	OA9-CA7-OA8-CA6
12	C	503	PC1	O32-C31-C32-C33
12	I	201	PC1	O22-C21-C22-C23
12	N	503	PC1	O32-C31-C32-C33
13	E	401	PTY	O4-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	506	CDL	OB9-CB7-OB8-CB6
14	L	3001	CDL	C32-C33-C34-C35
17	A	3003	XP4	O4-C1-C2-O7
17	L	3003	XP4	O4-C1-C2-O7
15	P	302	LMT	C3-C4-C5-C6
14	H	702	CDL	C32-C31-CA7-OA8
14	H	702	CDL	C72-C71-CB7-OB8
15	P	302	LMT	C2-C1-O1'-C1'
12	T	201	PC1	C11-C12-N-C15
13	E	401	PTY	O30-C30-C31-C32

There are no ring outliers.

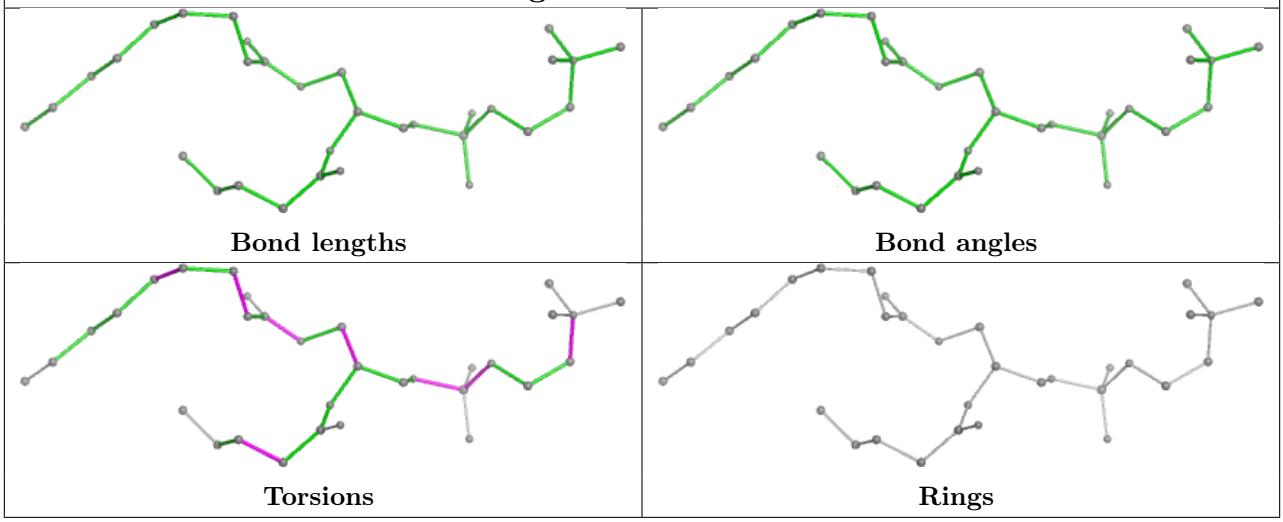
21 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	201	PC1	1	0
13	P	303	PTY	8	0
14	H	701	CDL	1	0
15	J	101	LMT	1	0
14	A	3002	CDL	1	0
14	O	402	CDL	1	0
14	A	3001	CDL	2	0
11	C	502	HEM	1	0
13	N	505	PTY	5	0
14	H	702	CDL	2	0
12	C	503	PC1	2	0
18	O	401	HEC	13	0
12	I	201	PC1	1	0
13	C	504	PTY	4	0
18	D	401	HEC	13	0
14	N	504	CDL	1	0
13	E	401	PTY	2	0
12	N	503	PC1	3	0
11	C	501	HEM	7	0
11	N	501	HEM	5	0
11	N	502	HEM	1	0

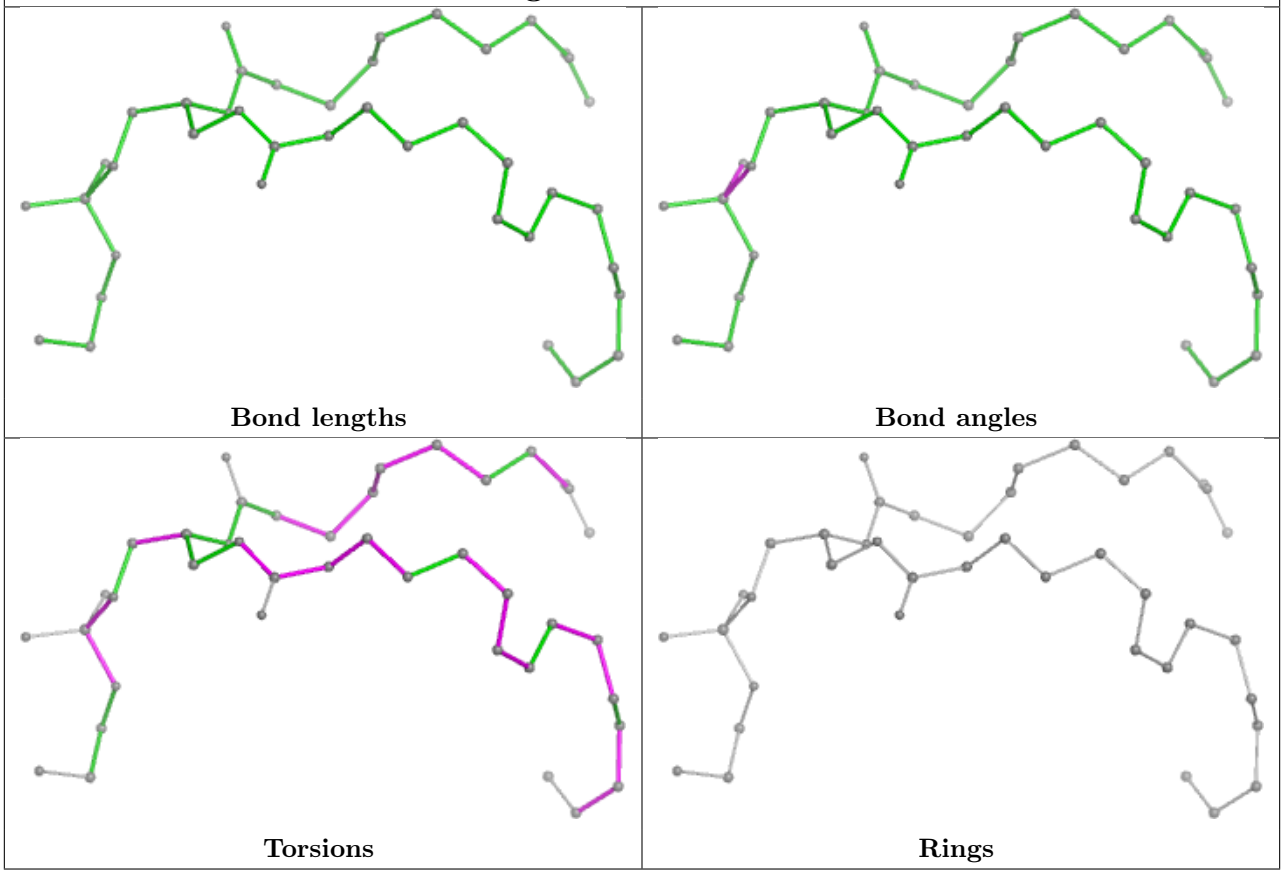
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

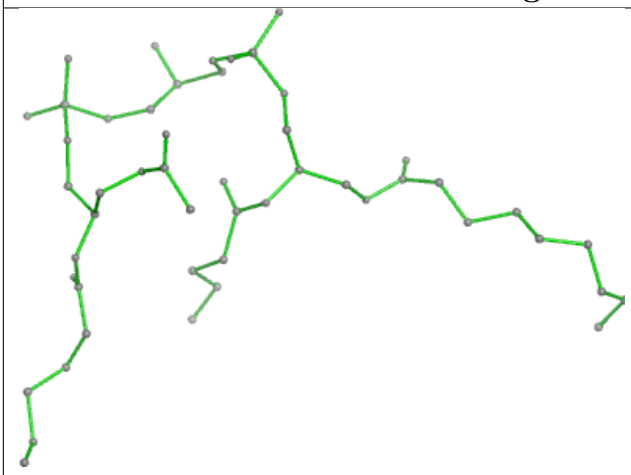
Ligand PC1 T 201



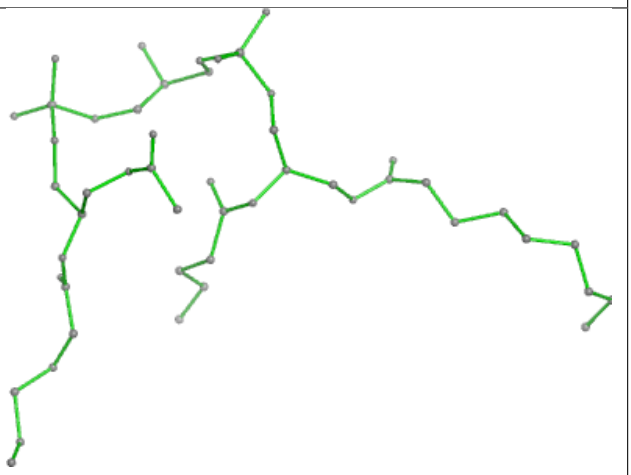
Ligand PTY P 303



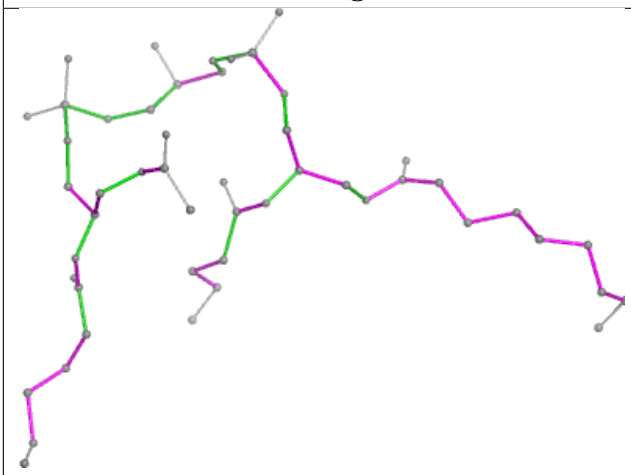
Ligand CDL H 701



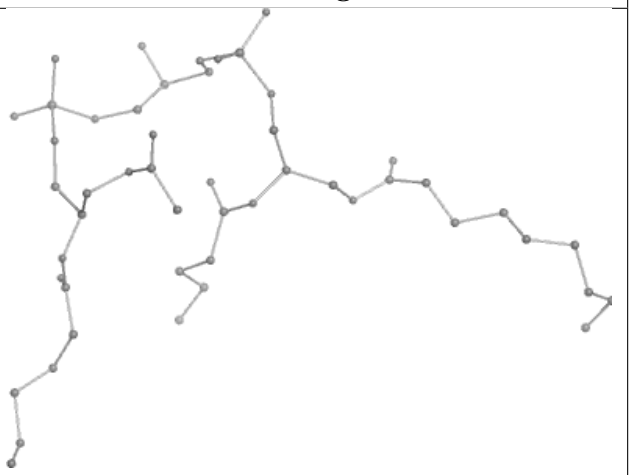
Bond lengths



Bond angles

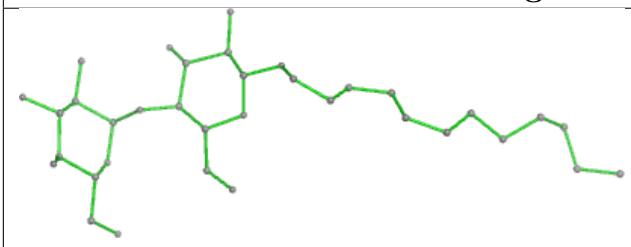


Torsions

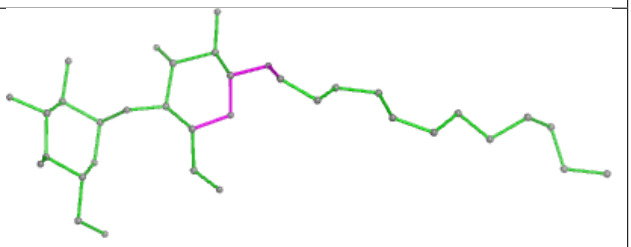


Rings

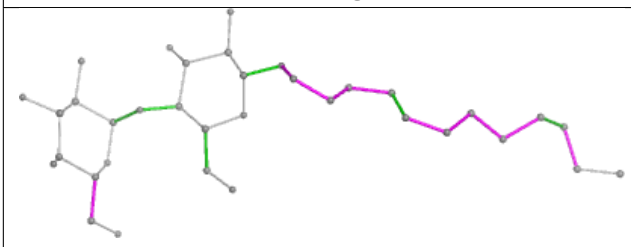
Ligand LMT J 101



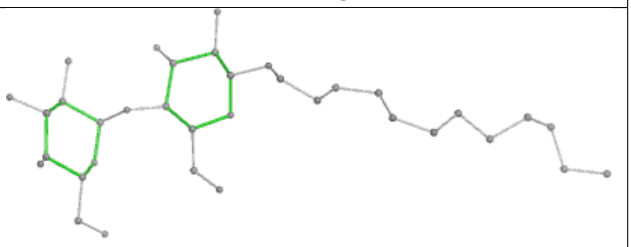
Bond lengths



Bond angles

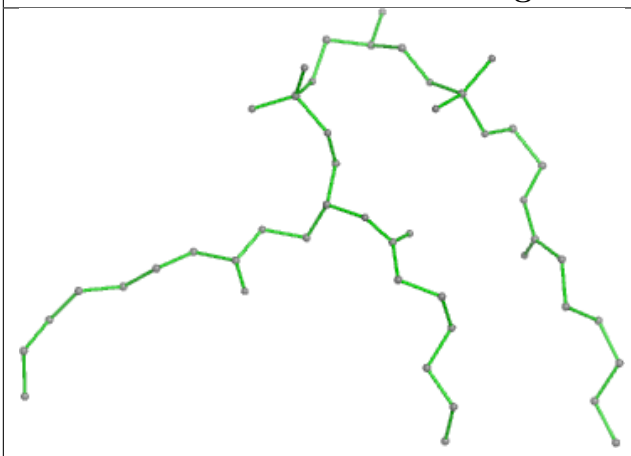


Torsions

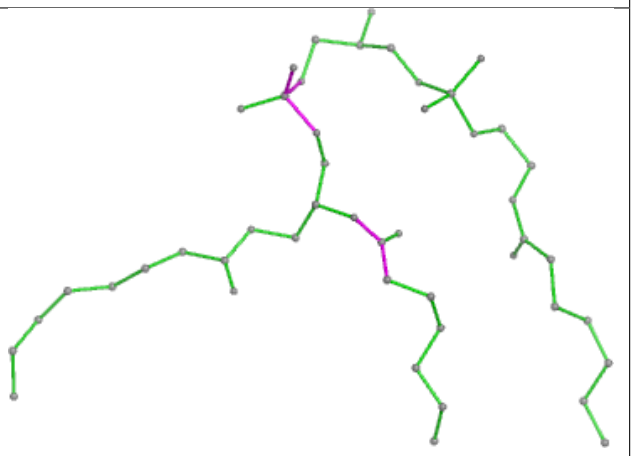


Rings

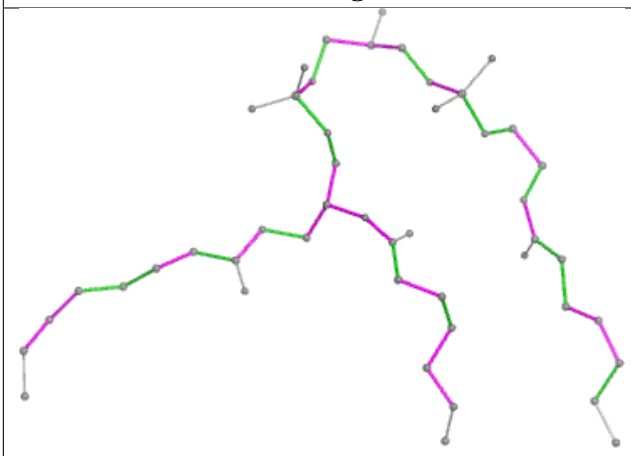
Ligand CDL A 3002



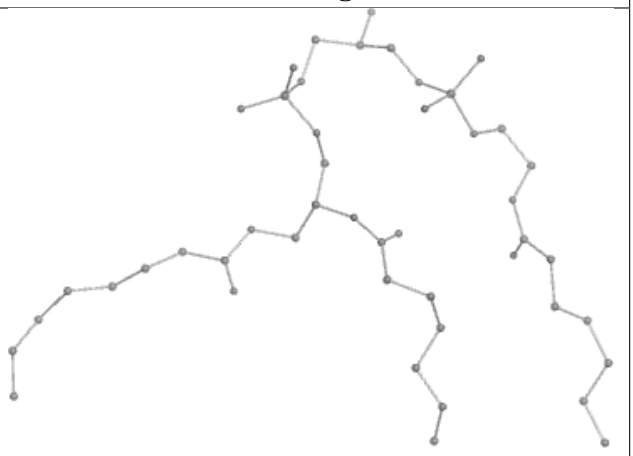
Bond lengths



Bond angles

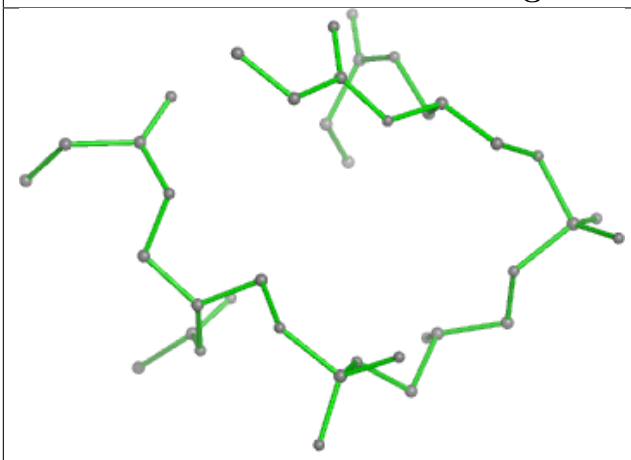


Torsions

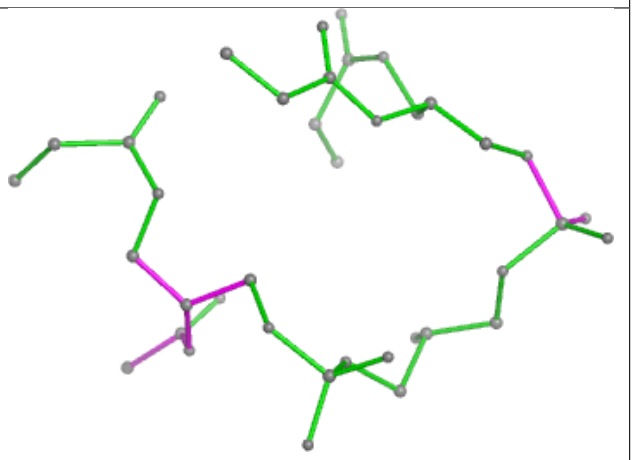


Rings

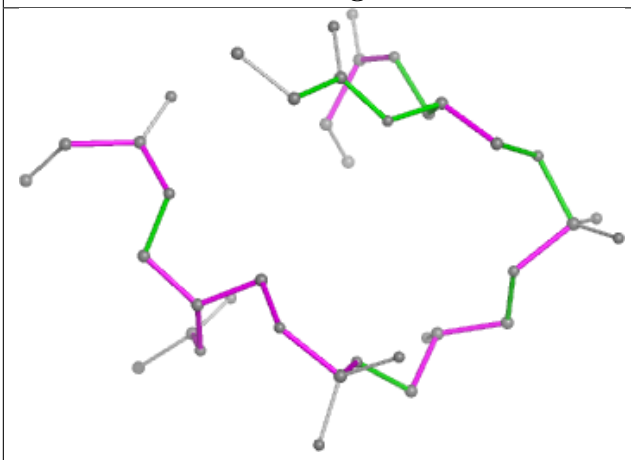
Ligand CDL O 402



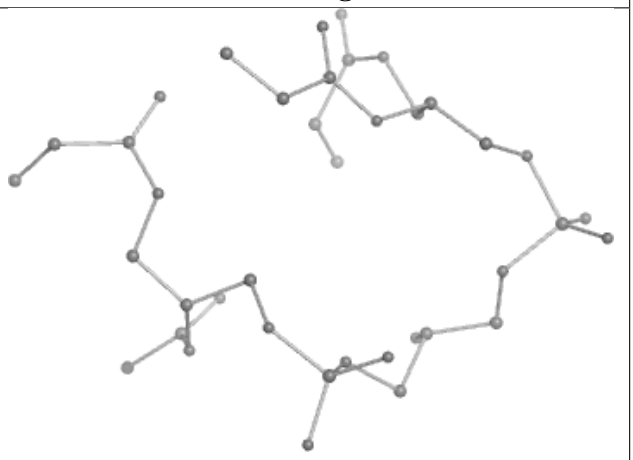
Bond lengths



Bond angles

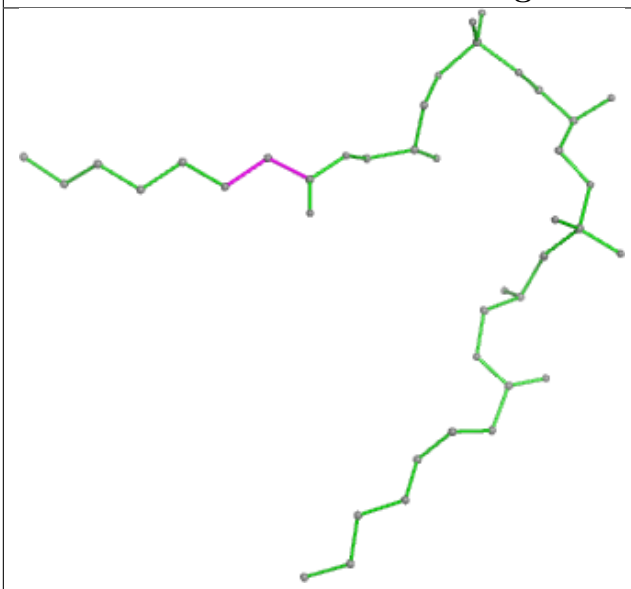


Torsions

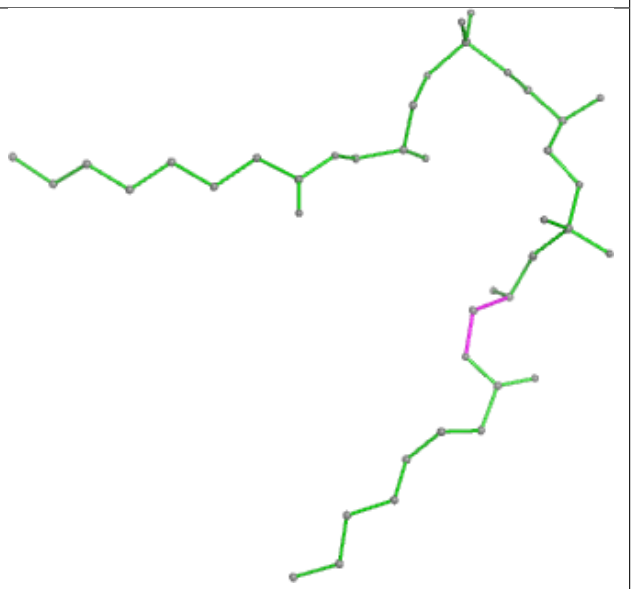


Rings

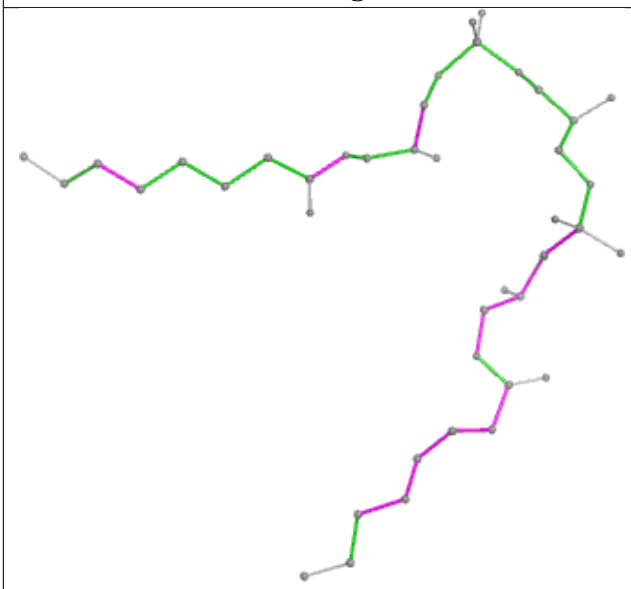
Ligand CDL A 3001



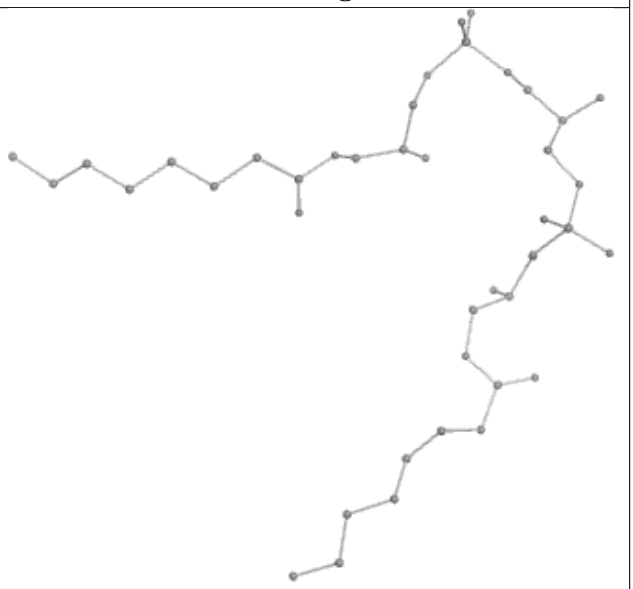
Bond lengths



Bond angles

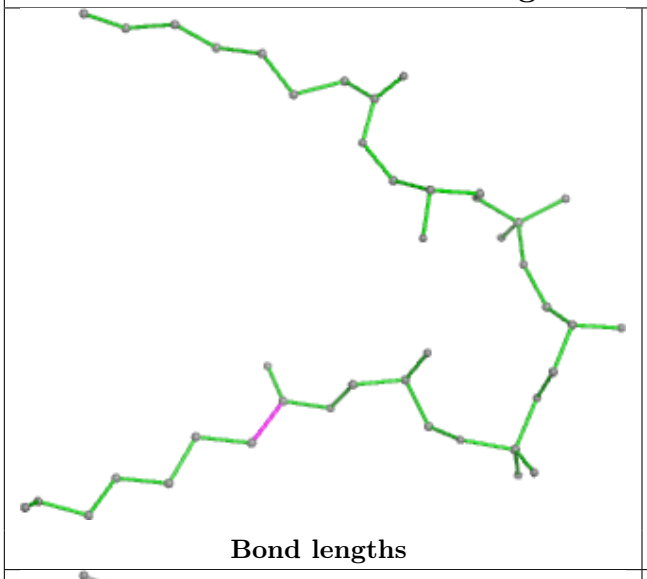


Torsions

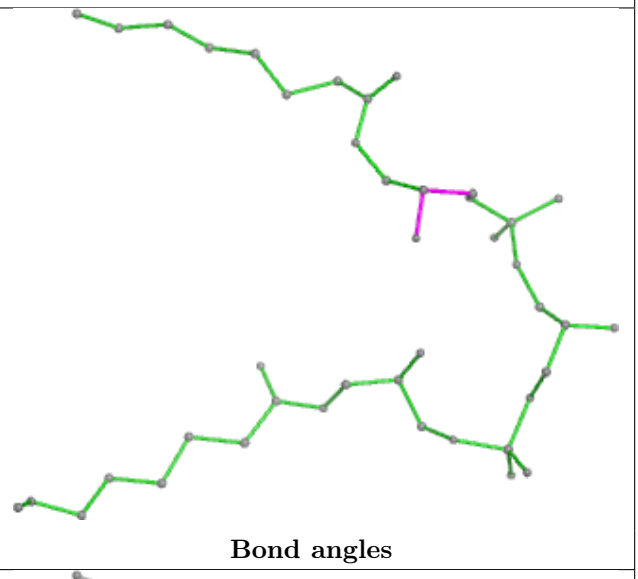


Rings

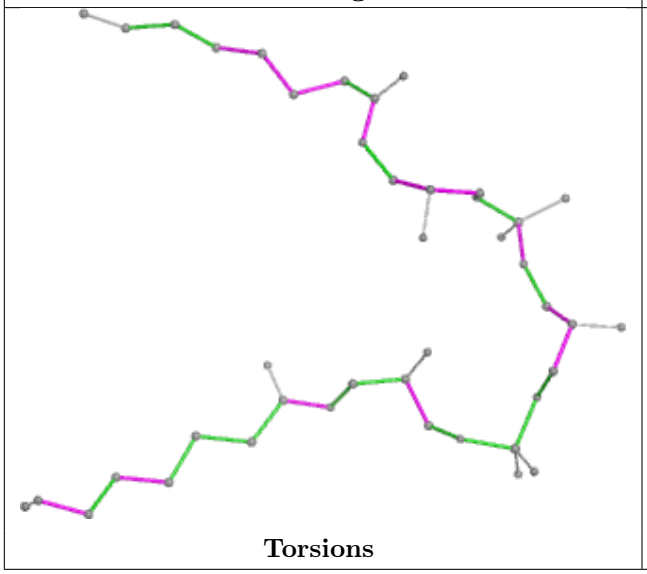
Ligand CDL L 3001



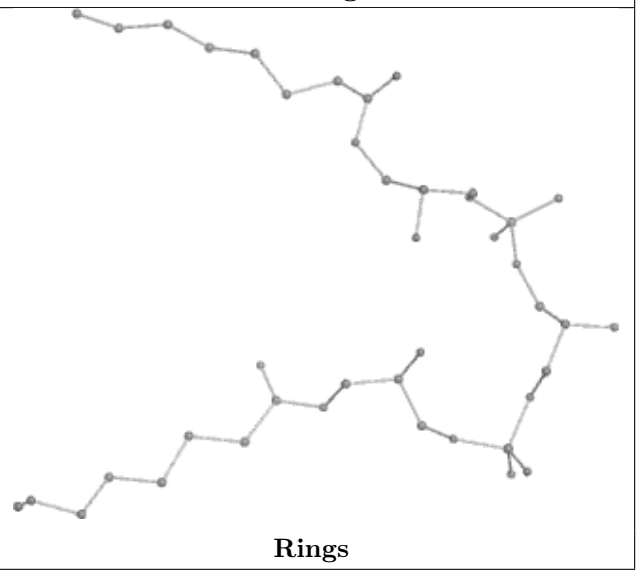
Bond lengths



Bond angles

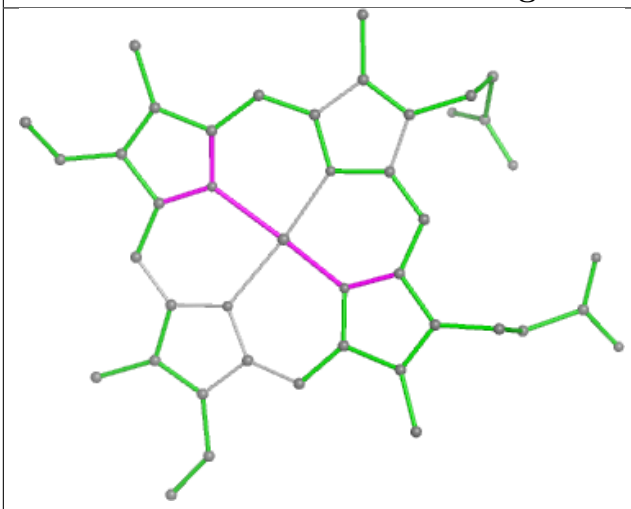


Torsions

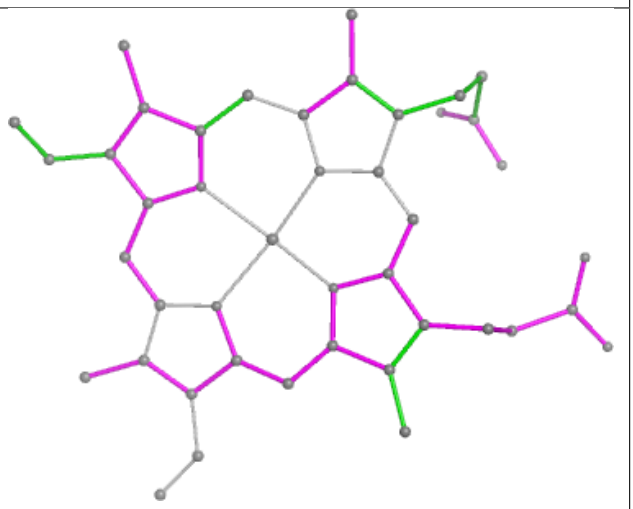


Rings

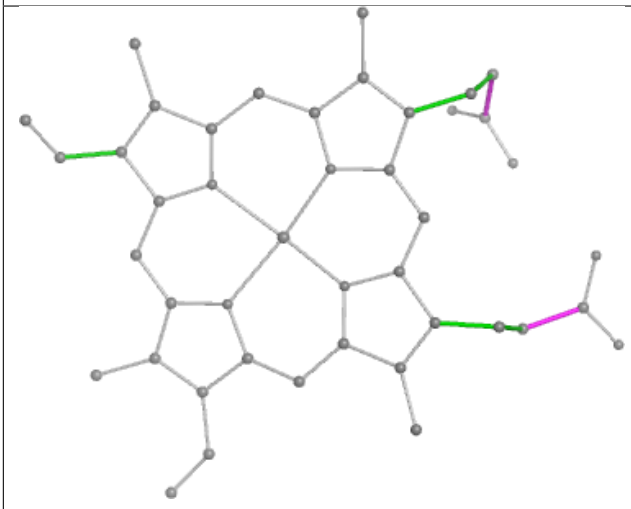
Ligand HEM C 502



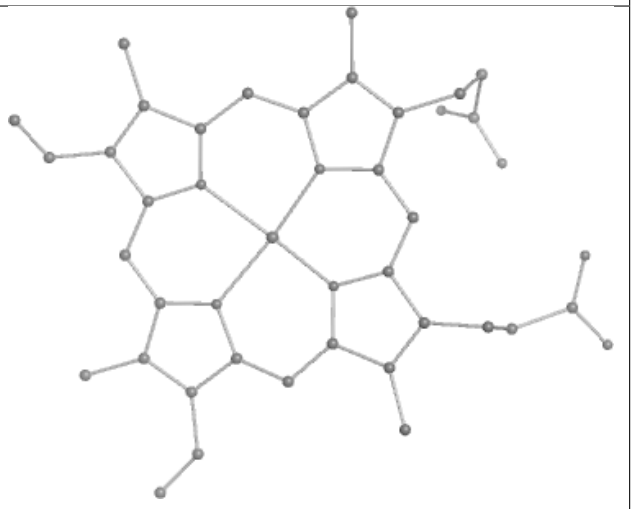
Bond lengths



Bond angles

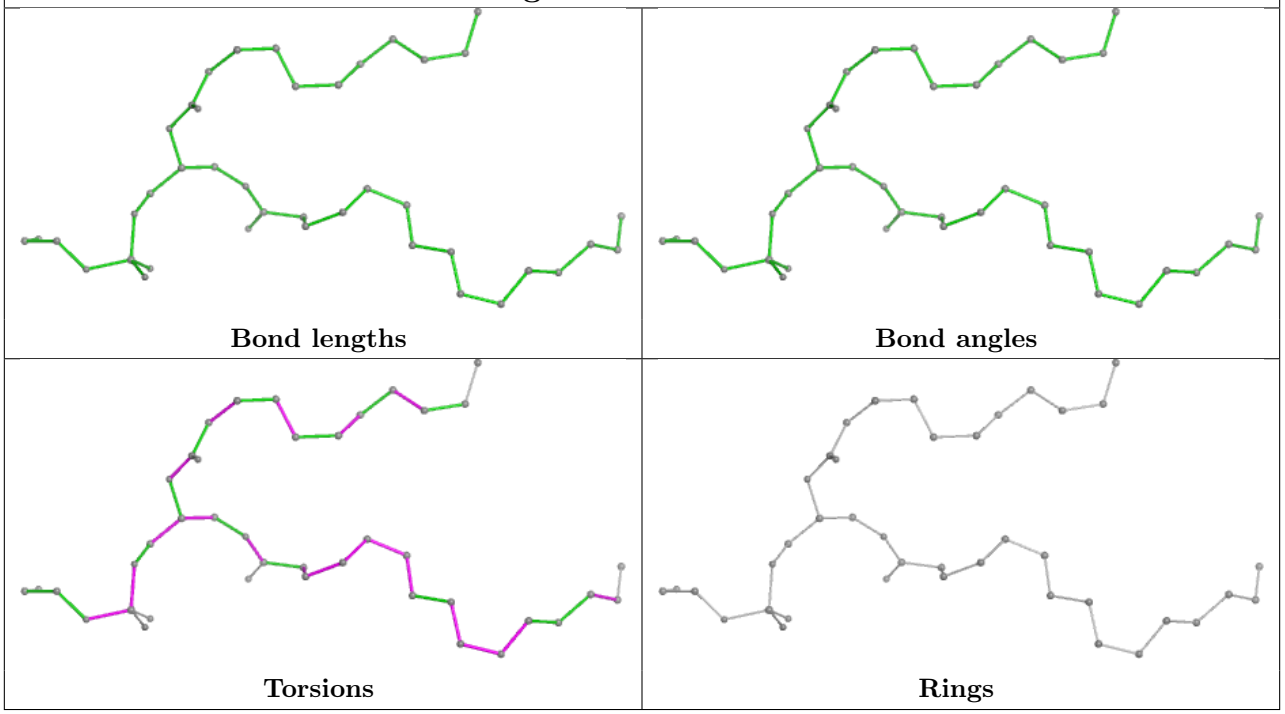


Torsions

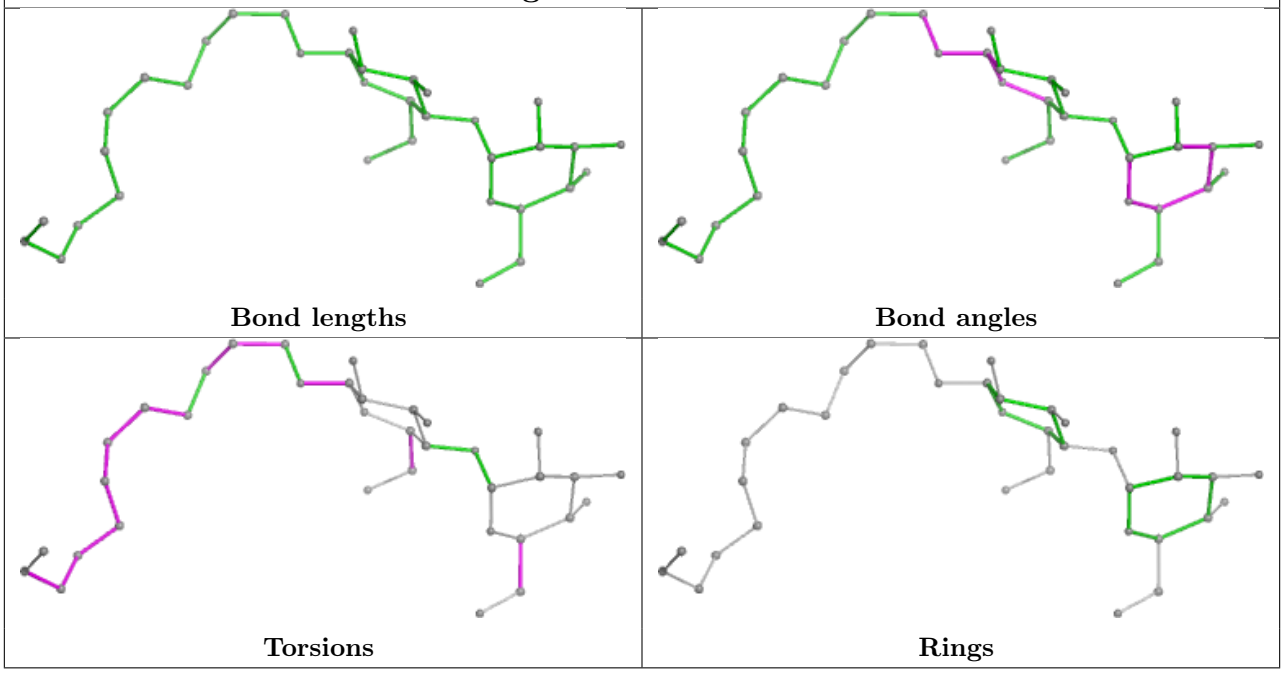


Rings

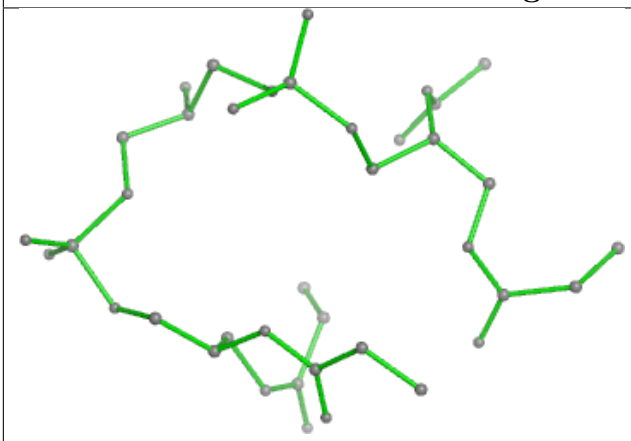
Ligand PTY N 505



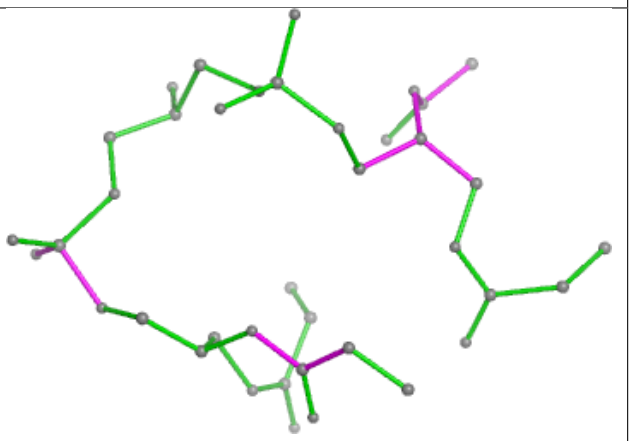
Ligand LMT C 506



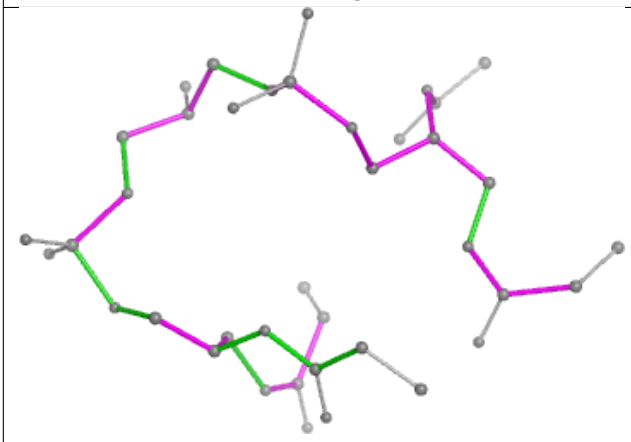
Ligand CDL H 702



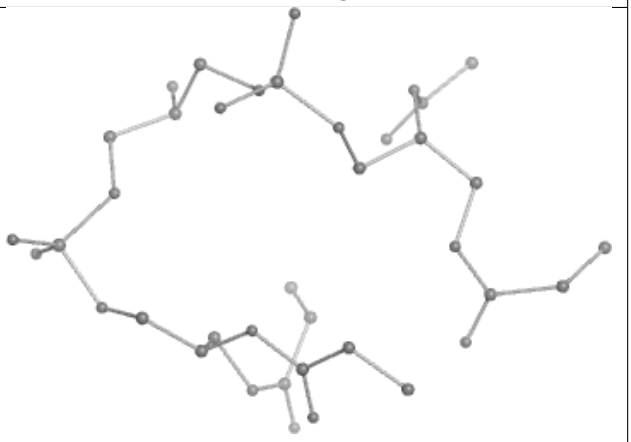
Bond lengths



Bond angles

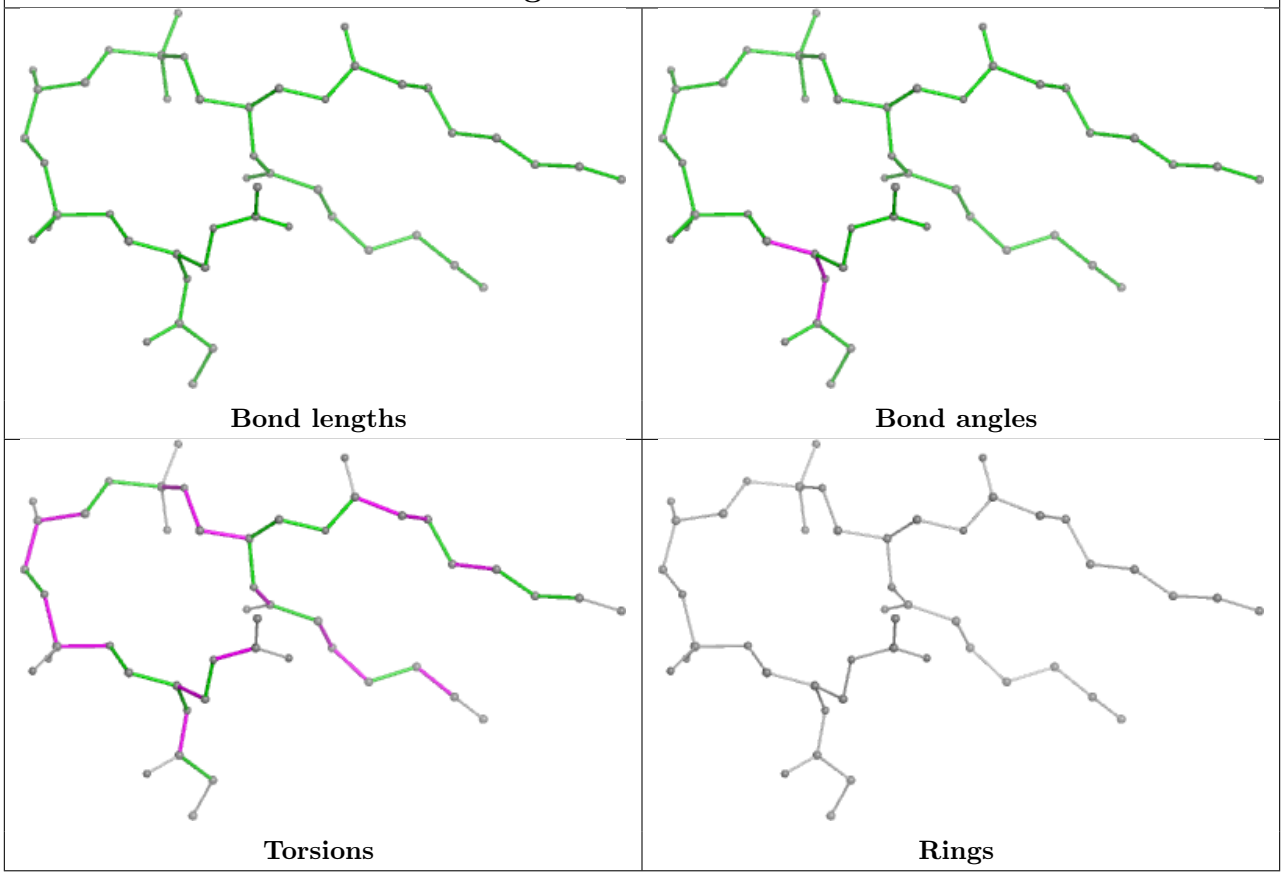


Torsions

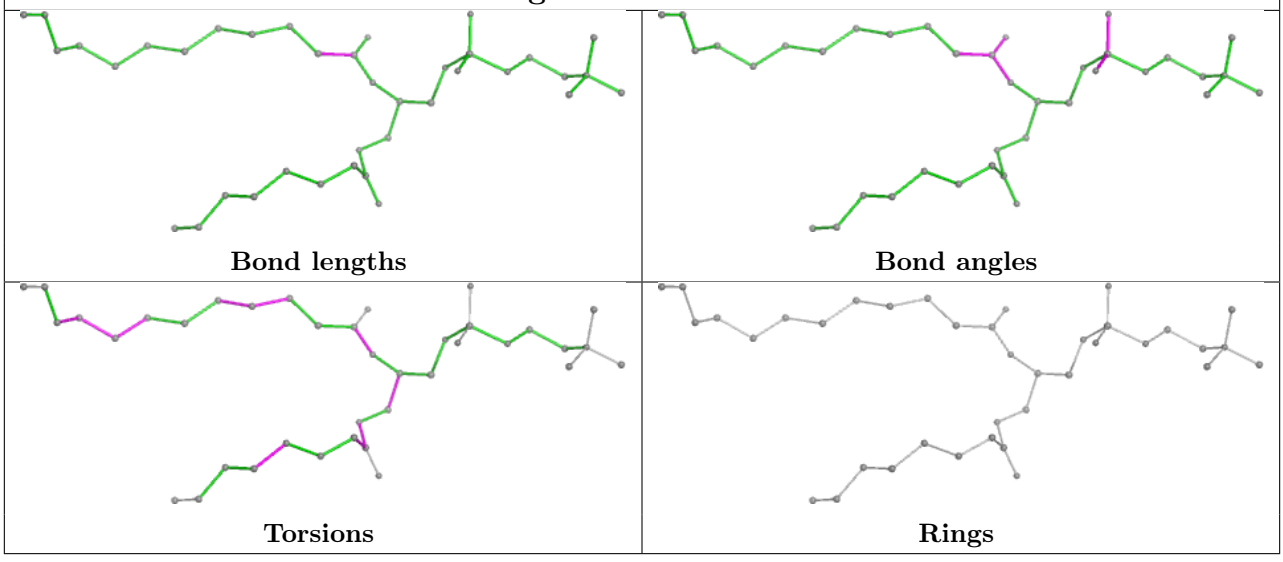


Rings

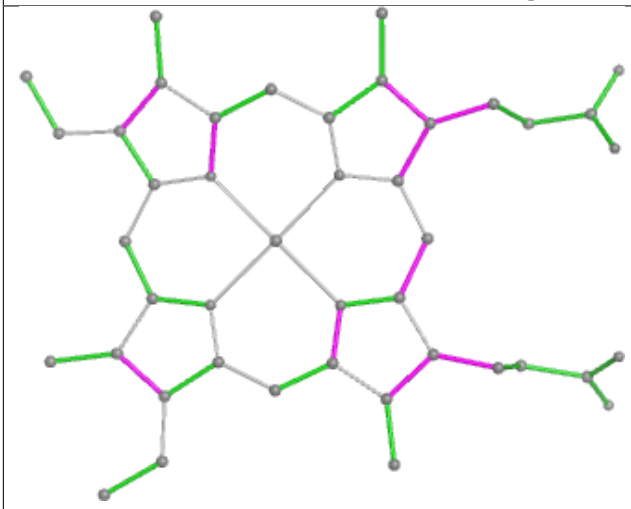
Ligand CDL N 506



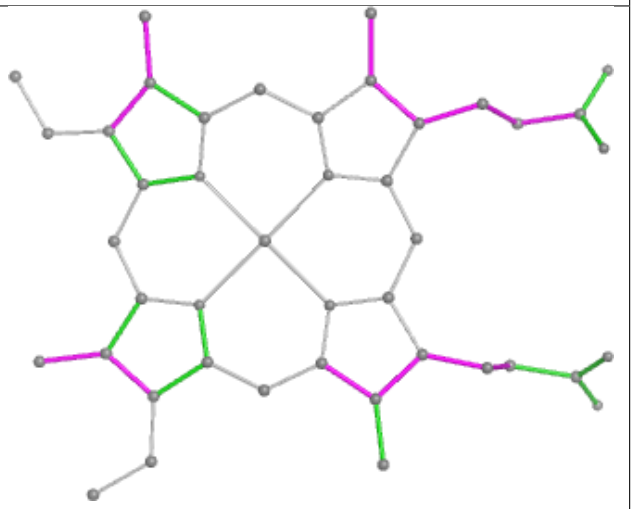
Ligand PC1 C 503



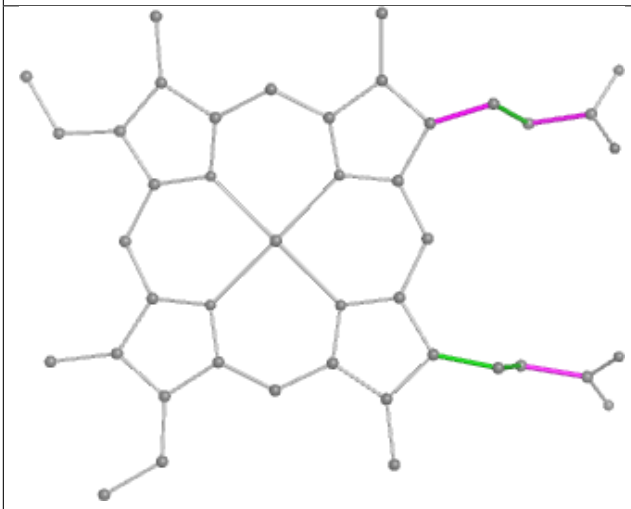
Ligand HEC O 401



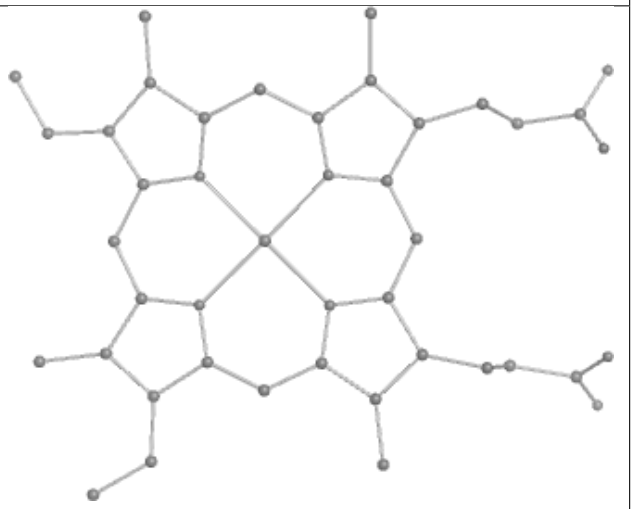
Bond lengths



Bond angles

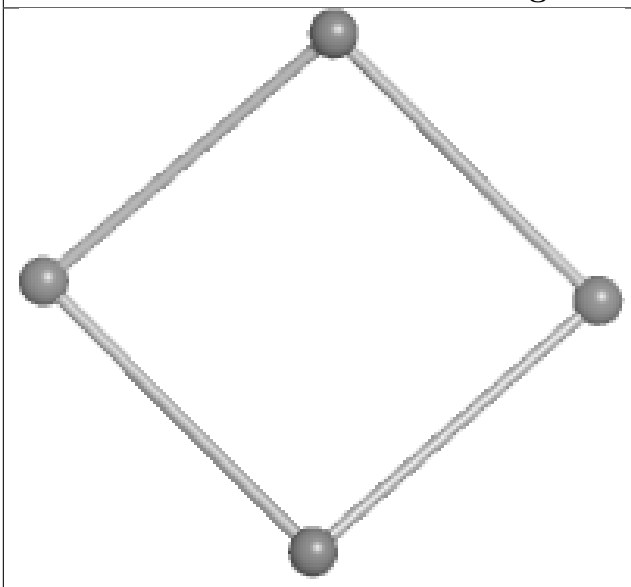


Torsions

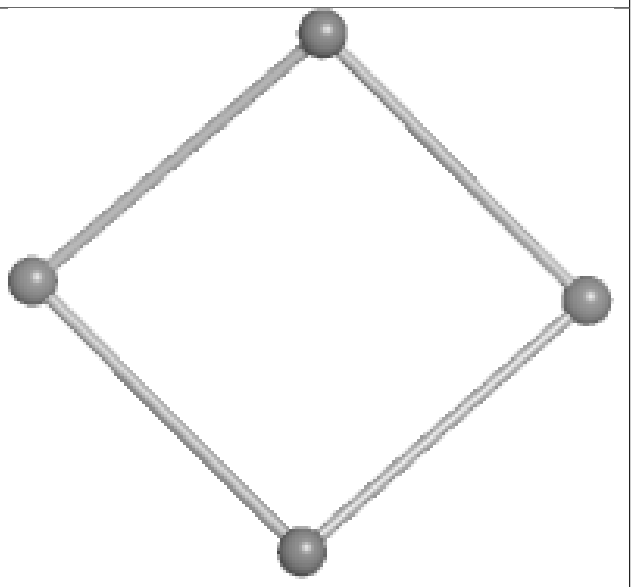


Rings

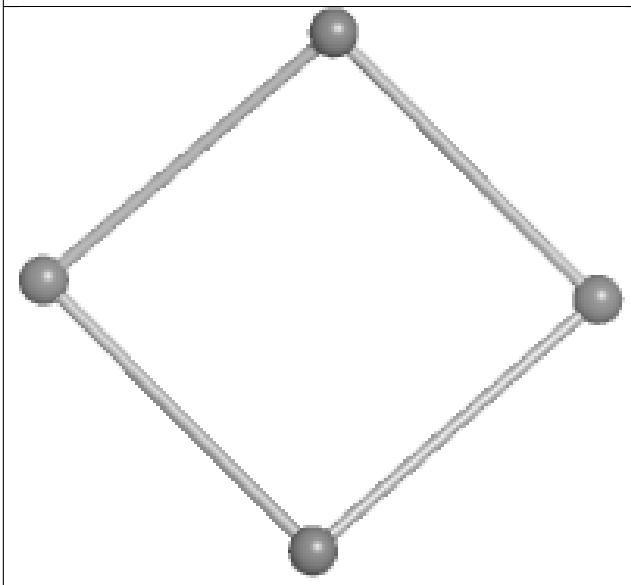
Ligand FES P 301



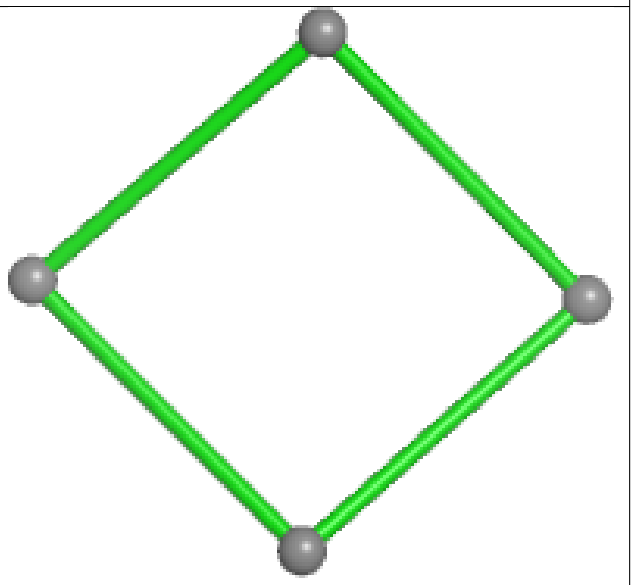
Bond lengths



Bond angles

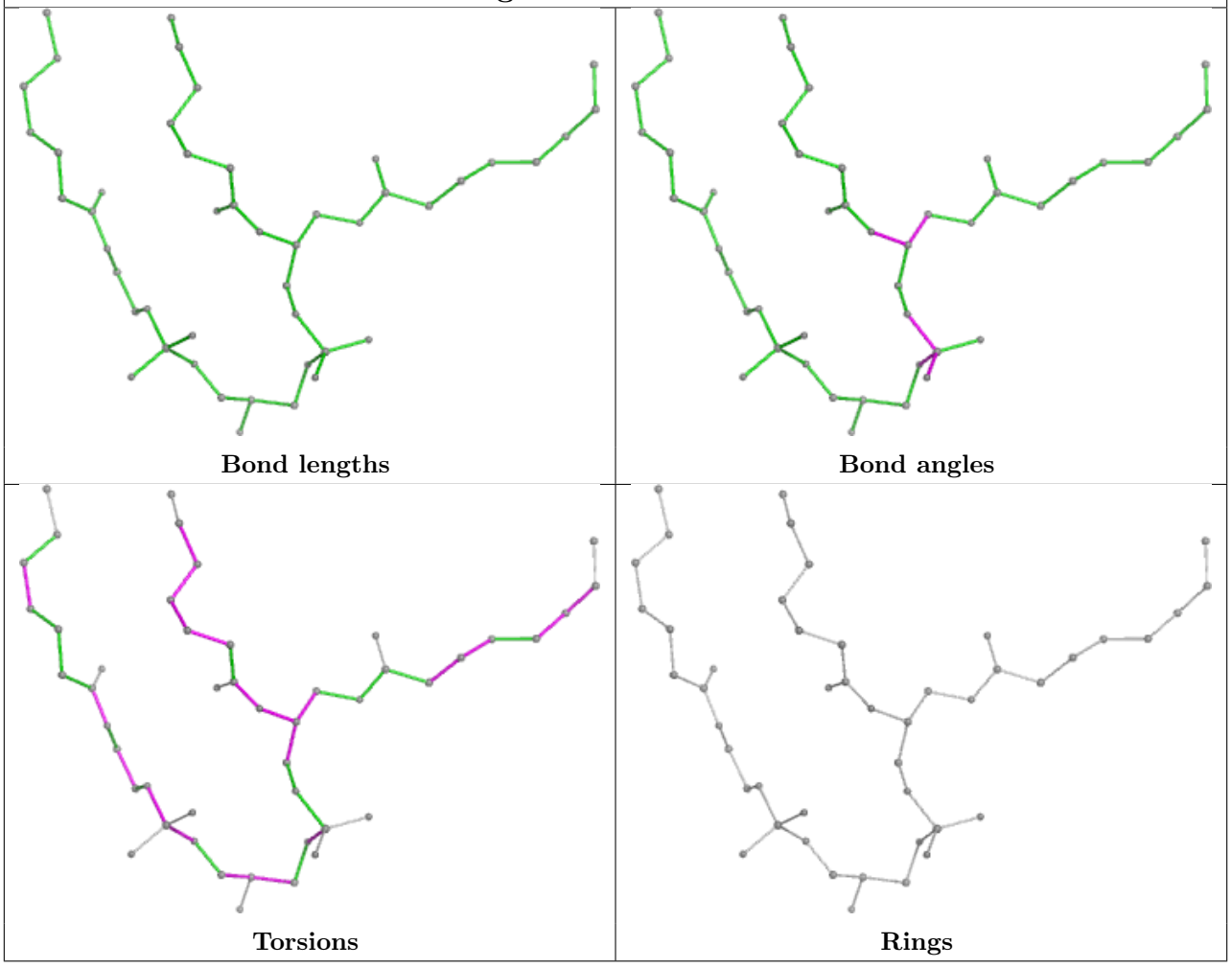


Torsions

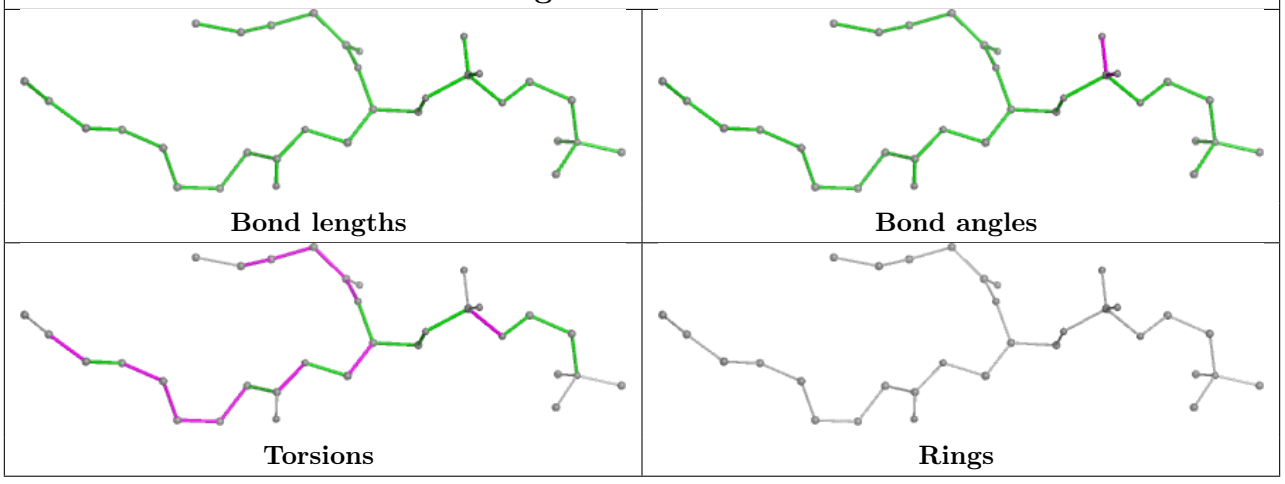


Rings

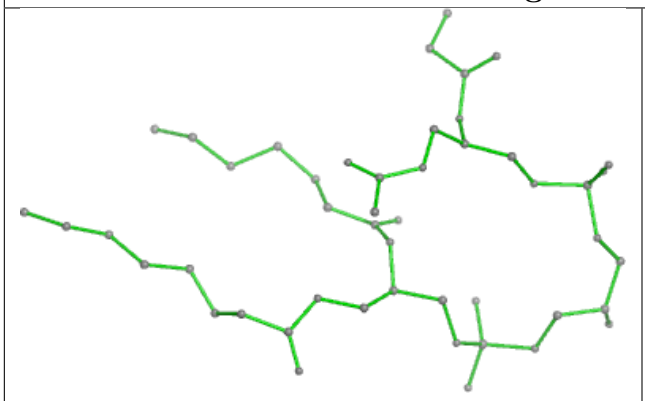
Ligand CDL L 3002



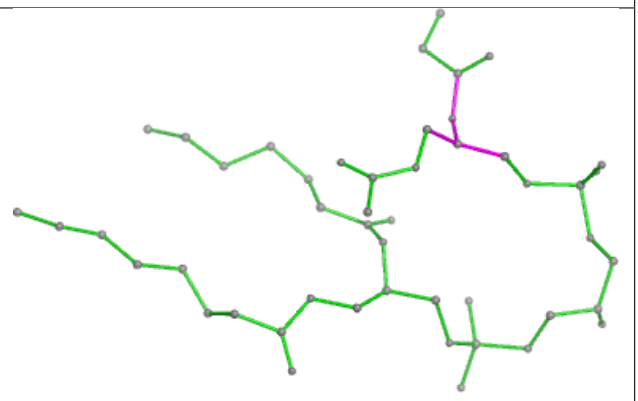
Ligand PC1 I 201



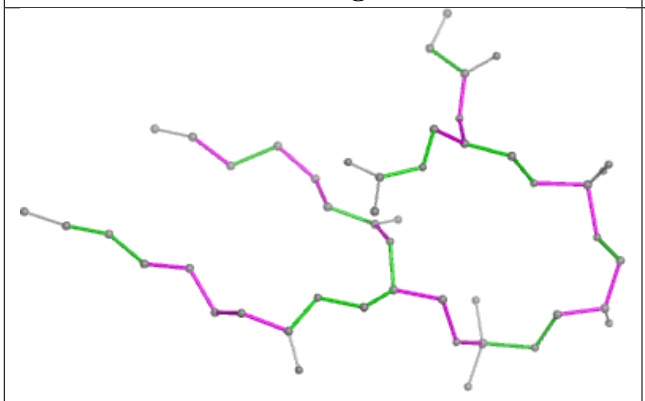
Ligand CDL C 505



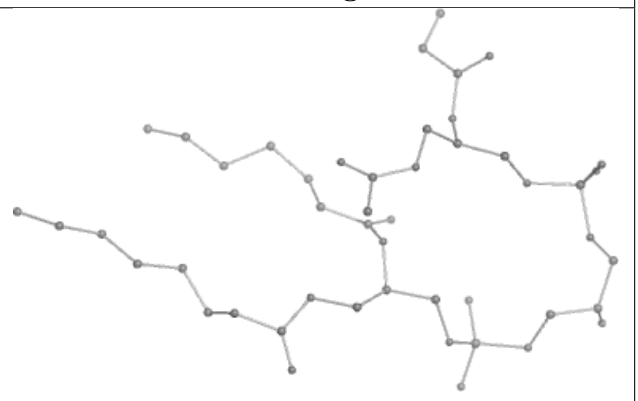
Bond lengths



Bond angles

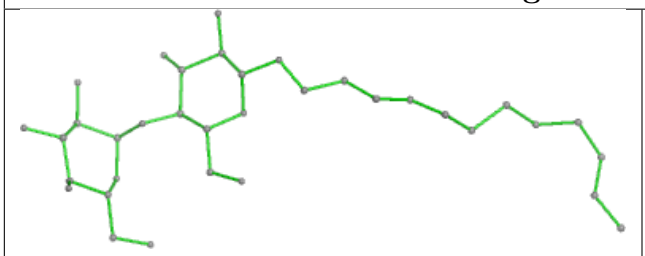


Torsions

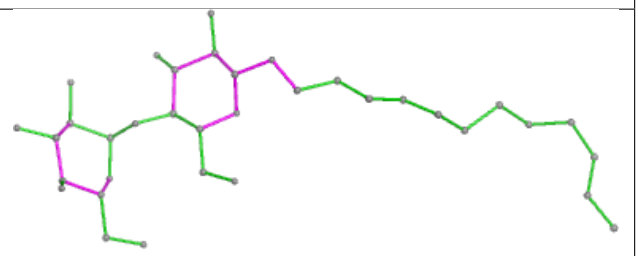


Rings

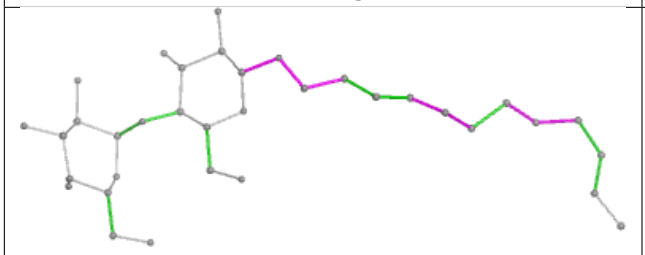
Ligand LMT P 302



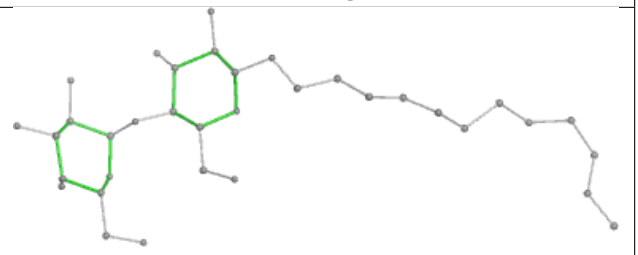
Bond lengths



Bond angles

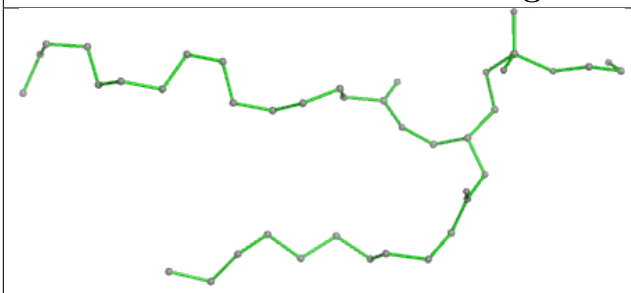


Torsions

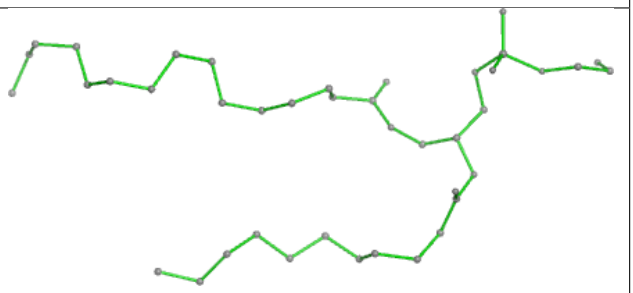


Rings

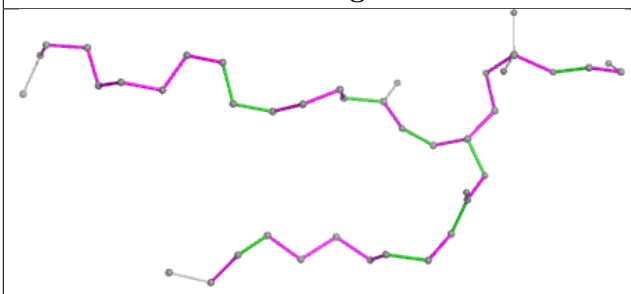
Ligand PTY C 504



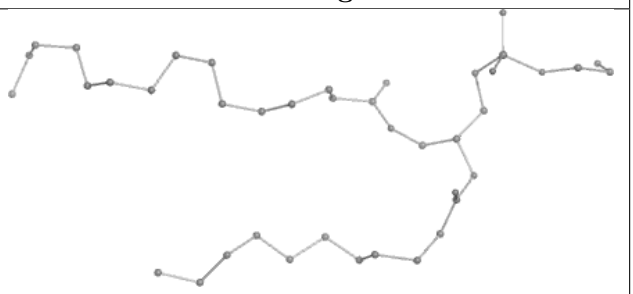
Bond lengths



Bond angles

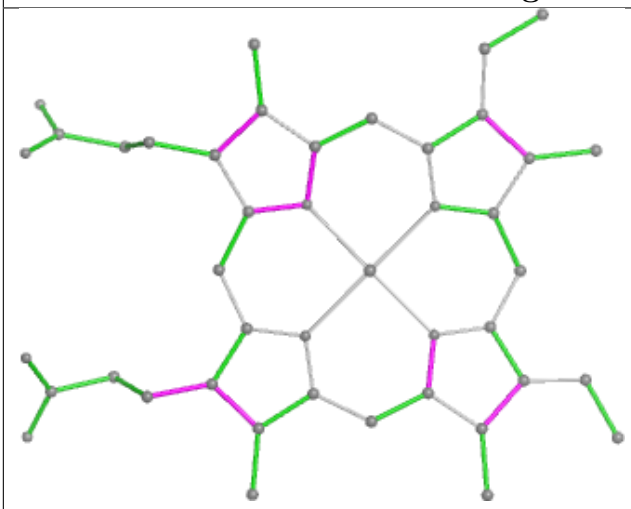


Torsions

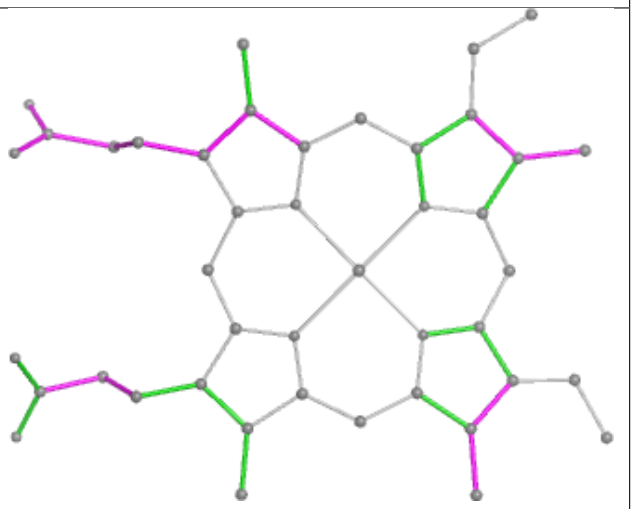


Rings

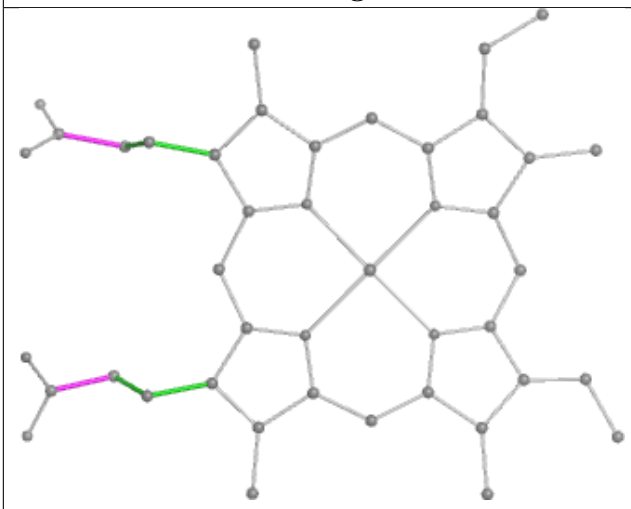
Ligand HEC D 401



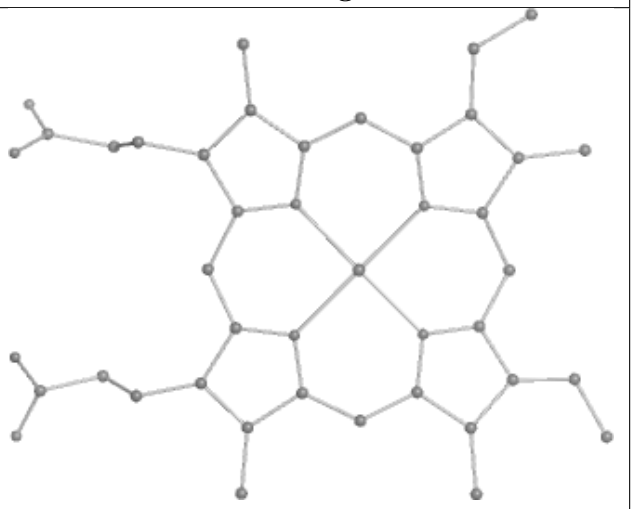
Bond lengths



Bond angles

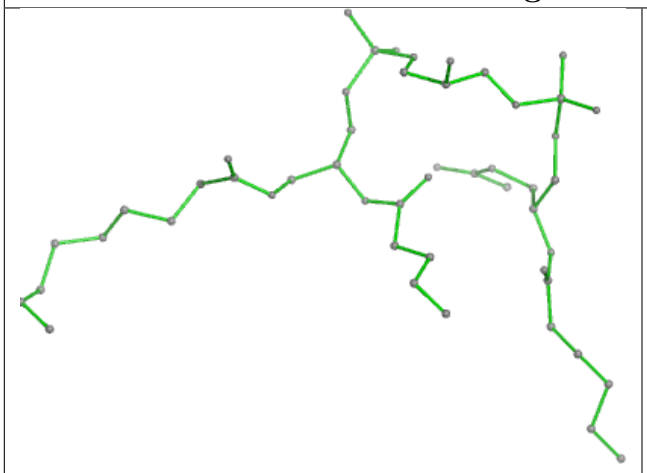


Torsions

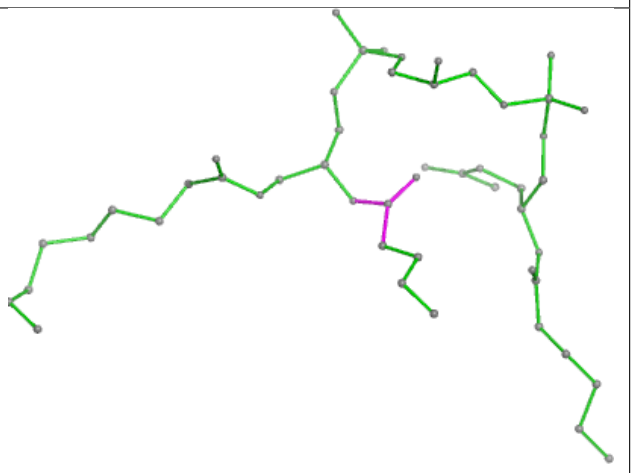


Rings

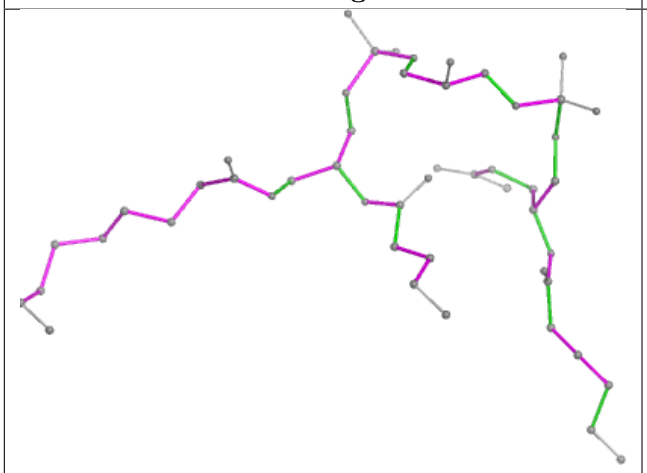
Ligand CDL N 504



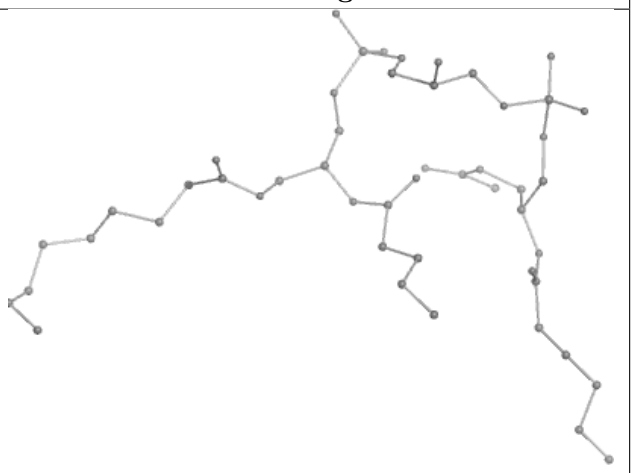
Bond lengths



Bond angles

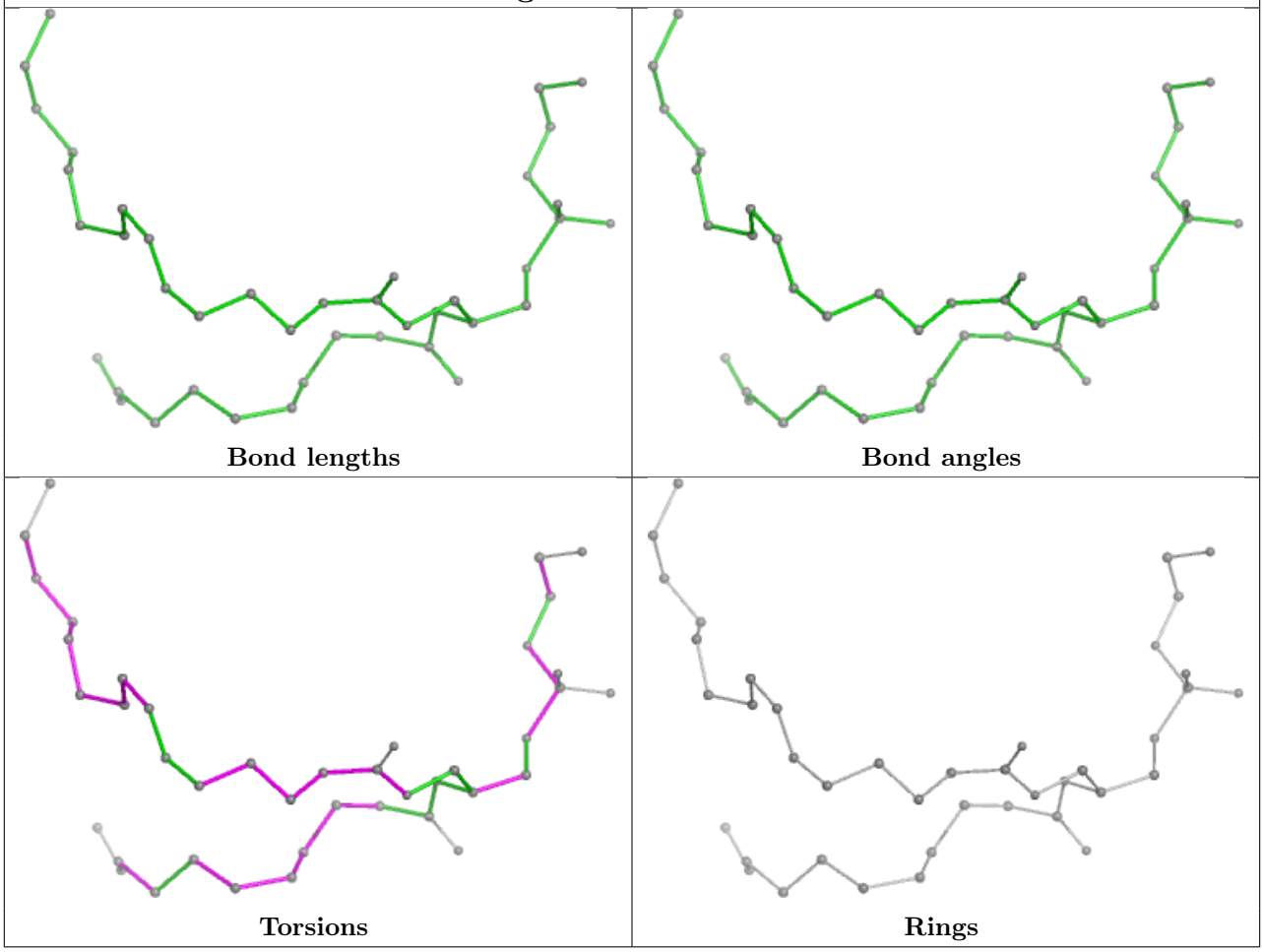


Torsions

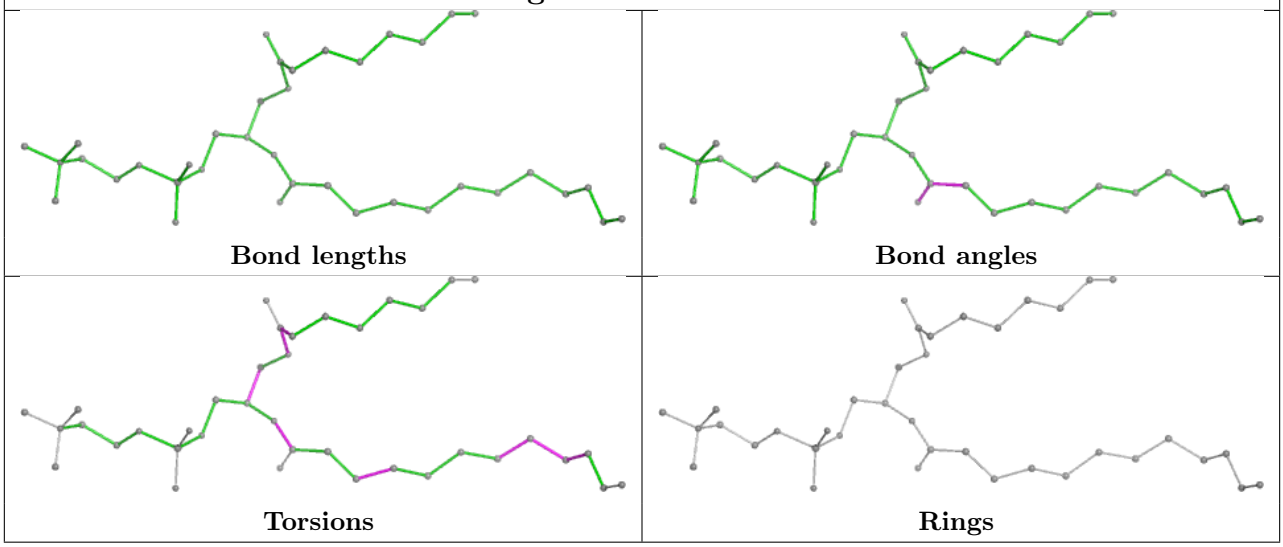


Rings

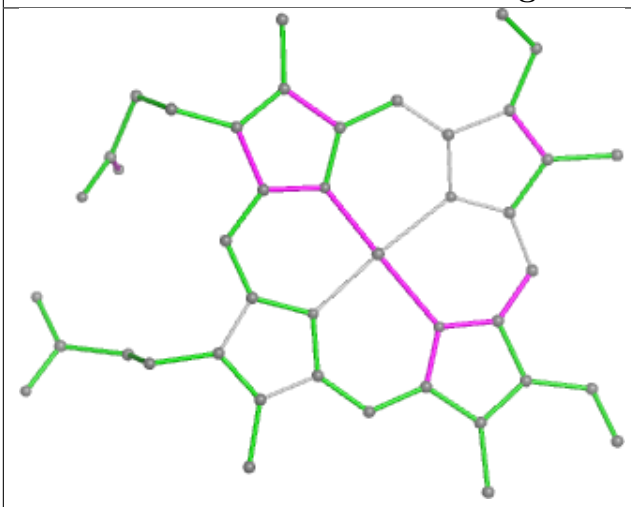
Ligand PTY E 401



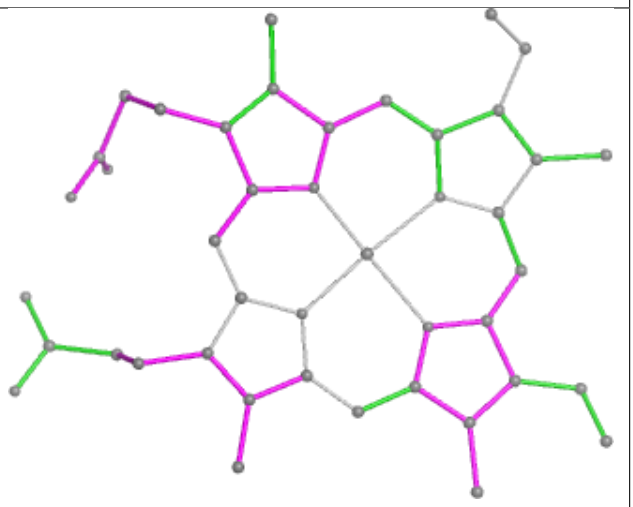
Ligand PC1 N 503



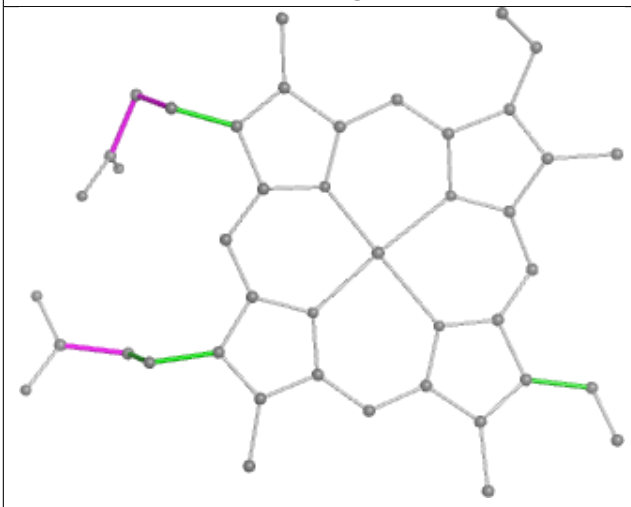
Ligand HEM C 501



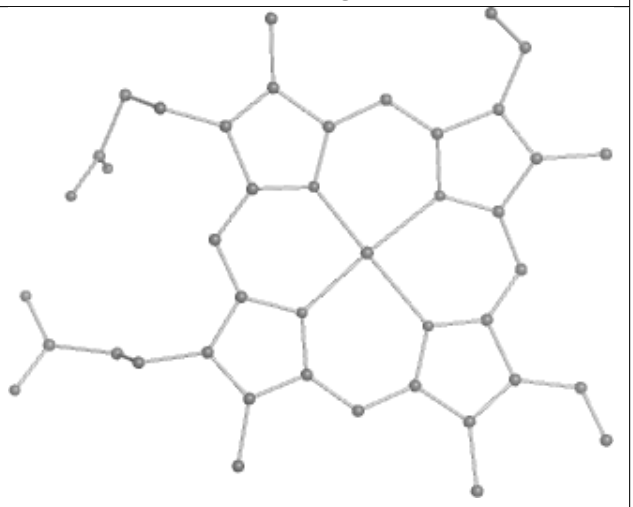
Bond lengths



Bond angles

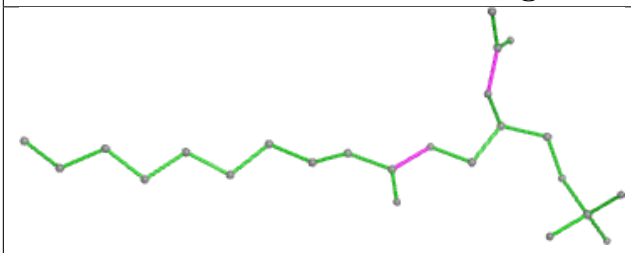


Torsions

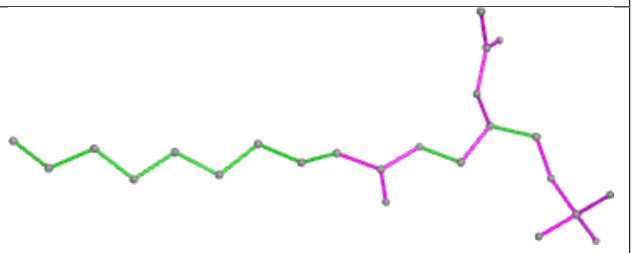


Rings

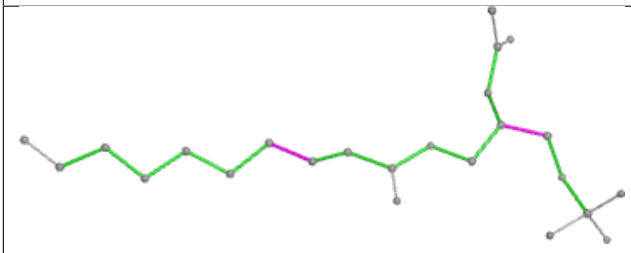
Ligand XP4 L 3003



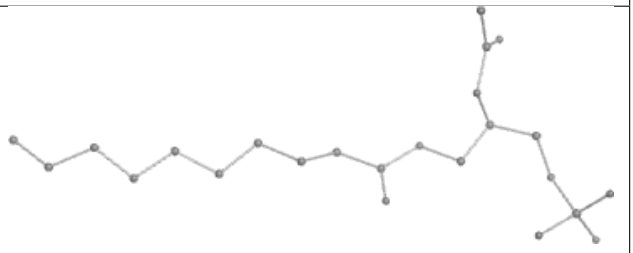
Bond lengths



Bond angles

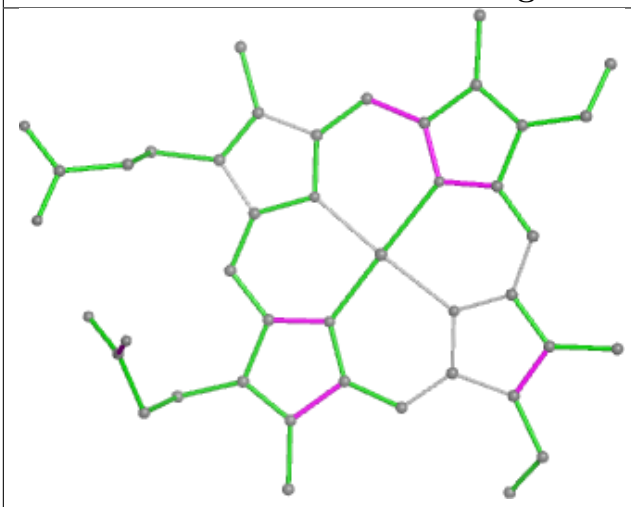


Torsions

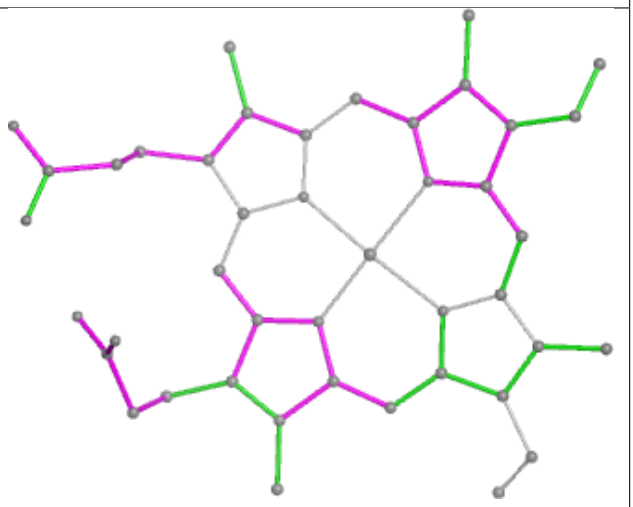


Rings

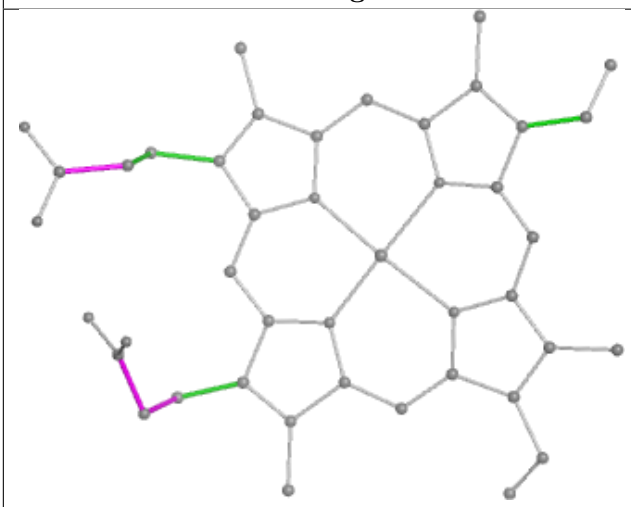
Ligand HEM N 501



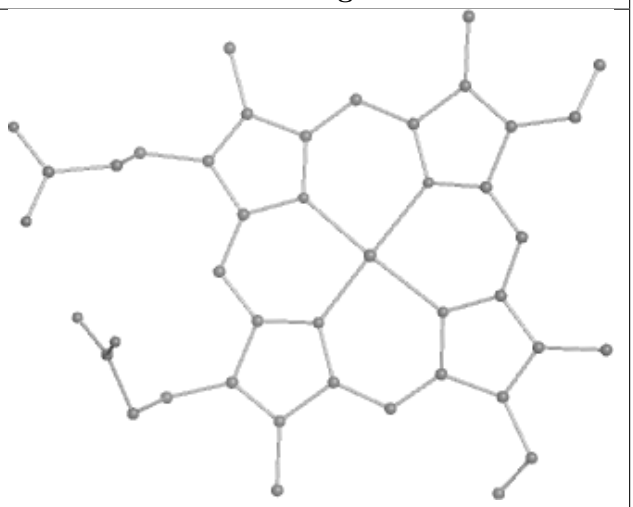
Bond lengths



Bond angles

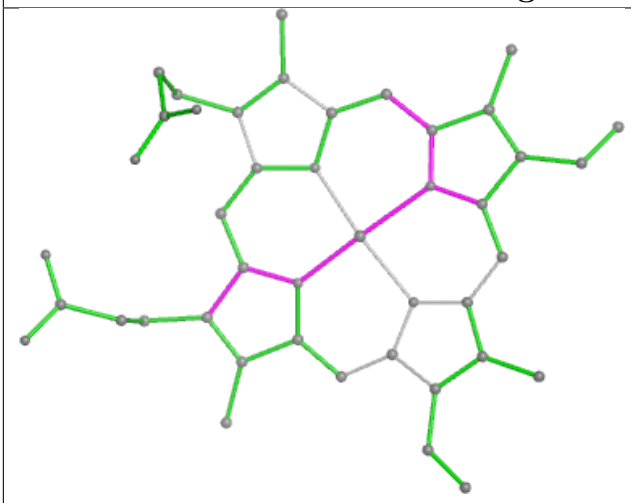


Torsions

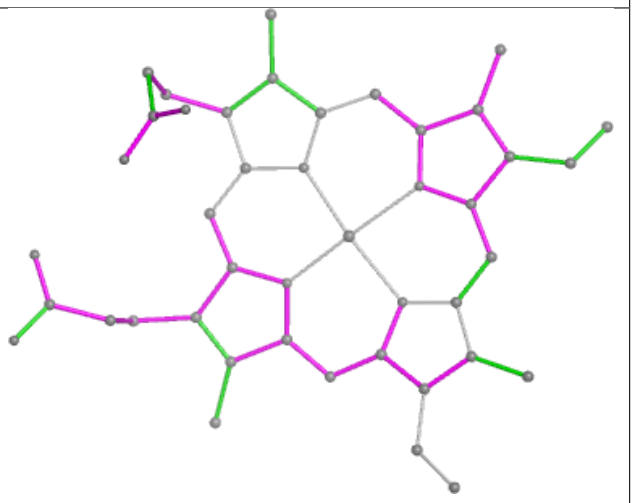


Rings

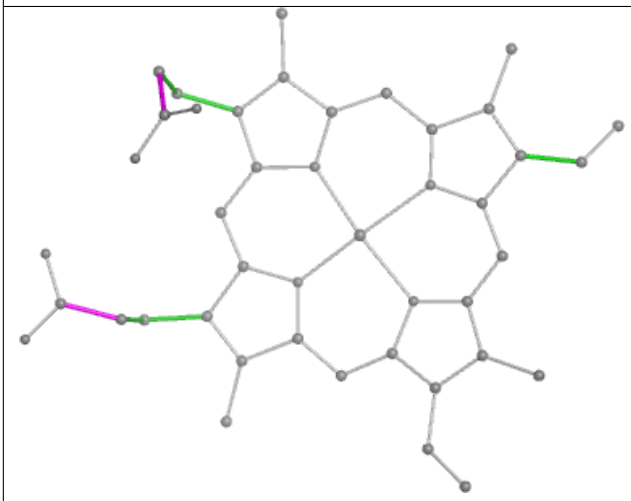
Ligand HEM N 502



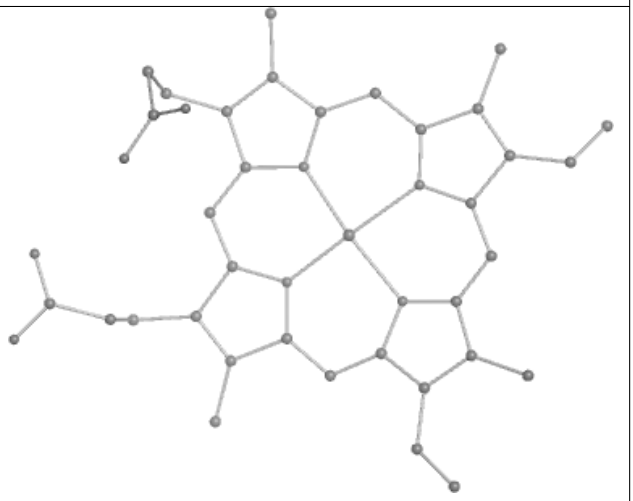
Bond lengths



Bond angles

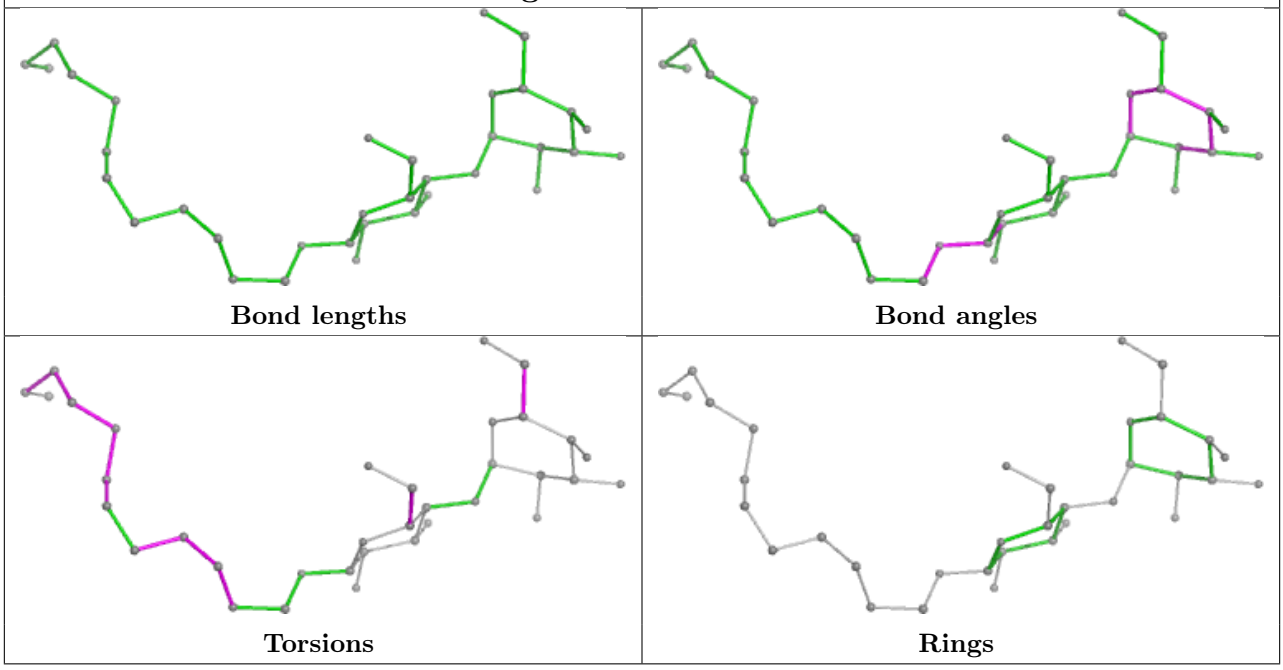


Torsions

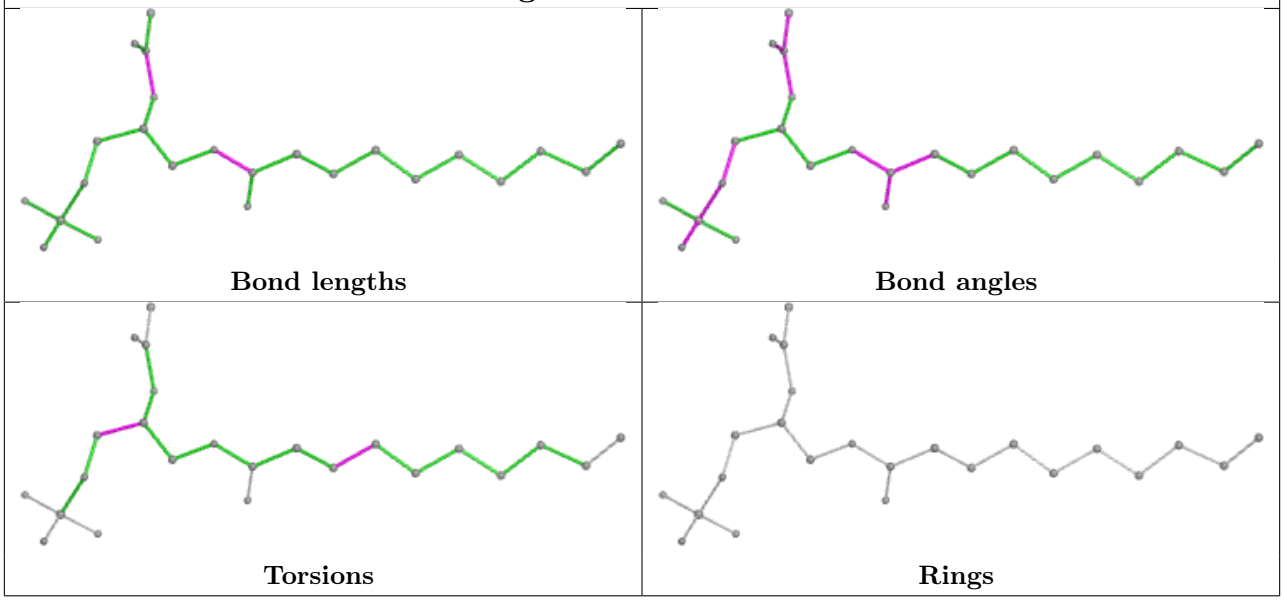


Rings

Ligand LMT N 507



Ligand XP4 A 3003



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.

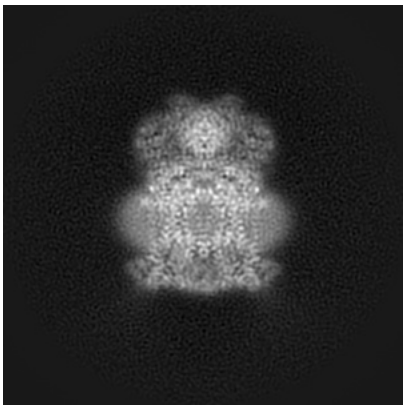
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15315. These allow visual inspection of the internal detail of the map and identification of artifacts.

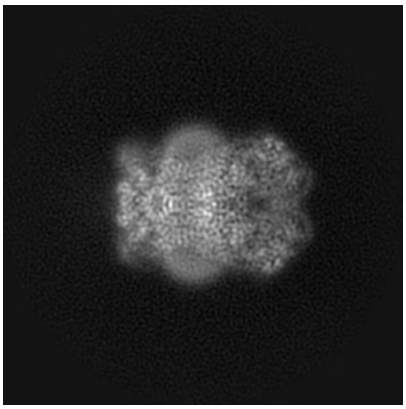
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

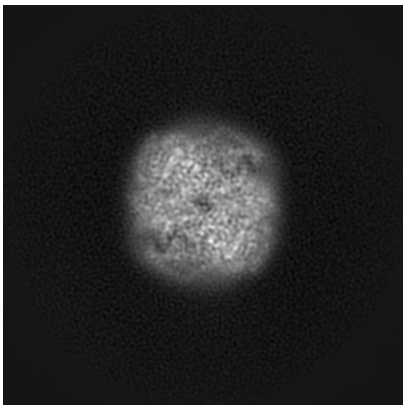
6.1.1 Primary map



X

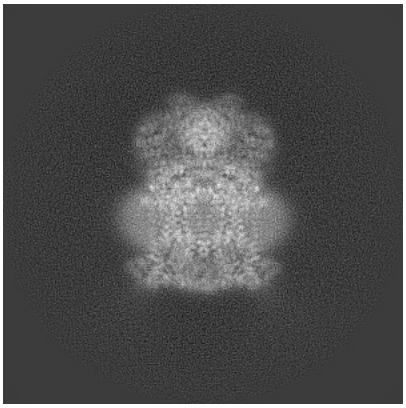


Y

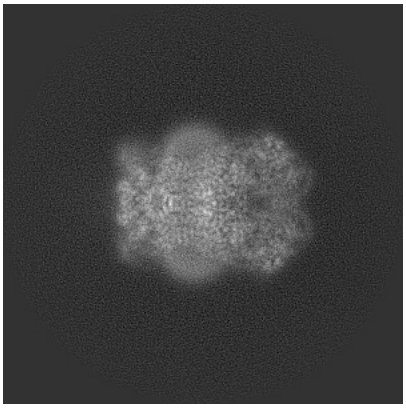


Z

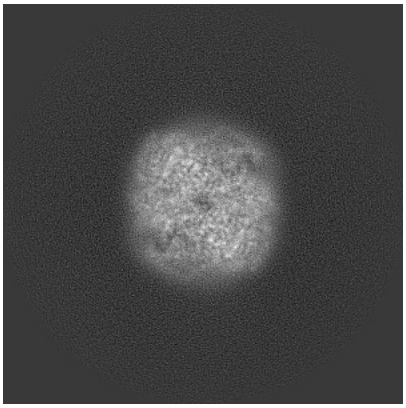
6.1.2 Raw map



X



Y

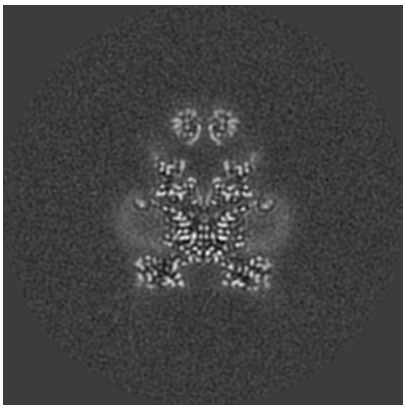


Z

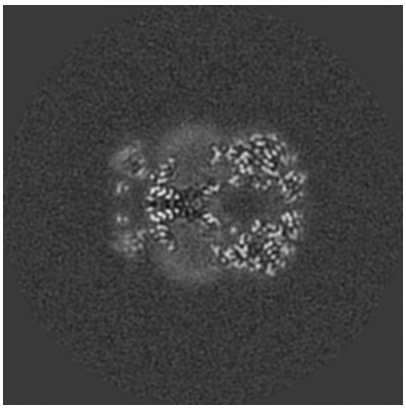
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

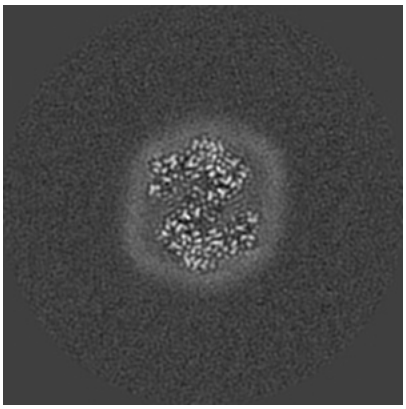
6.2.1 Primary map



X Index: 180

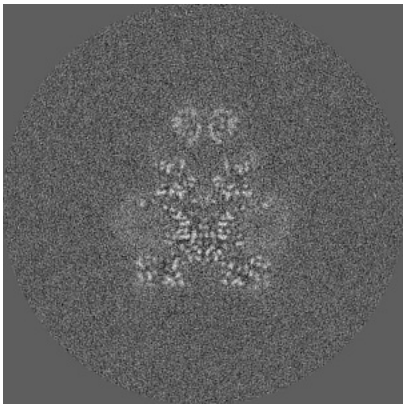


Y Index: 180

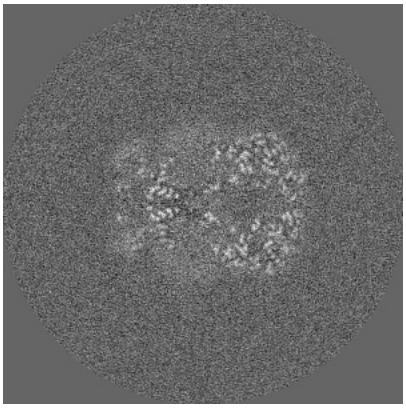


Z Index: 180

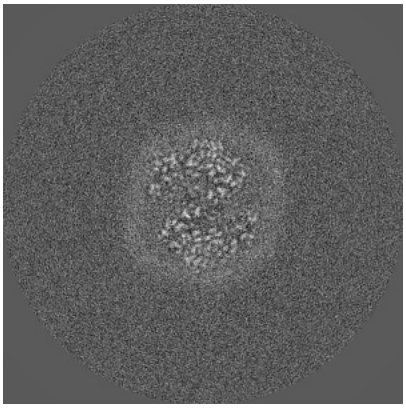
6.2.2 Raw map



X Index: 180



Y Index: 180

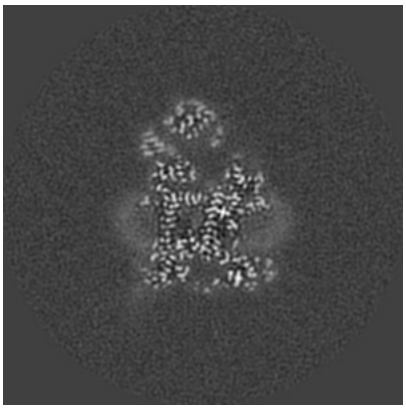


Z Index: 180

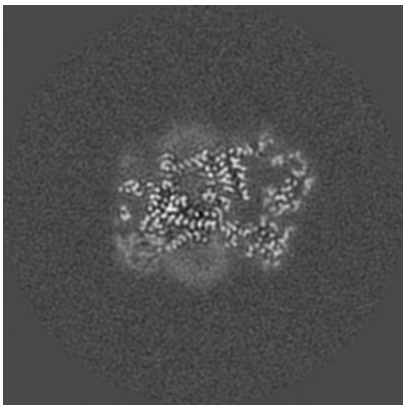
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

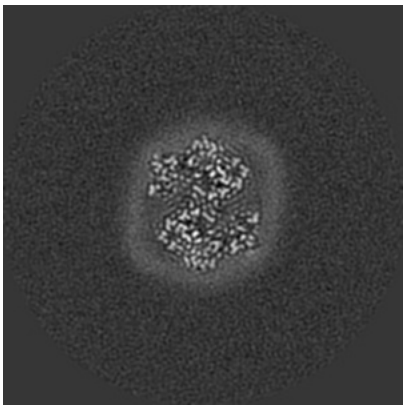
6.3.1 Primary map



X Index: 189

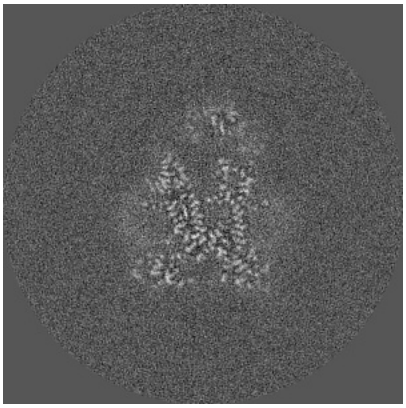


Y Index: 166

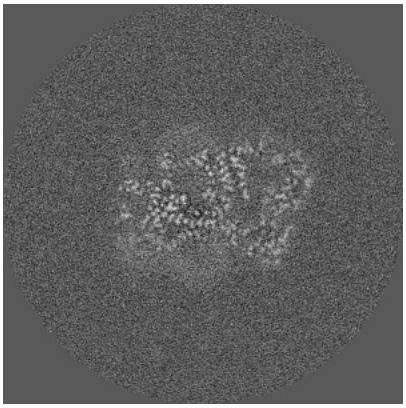


Z Index: 181

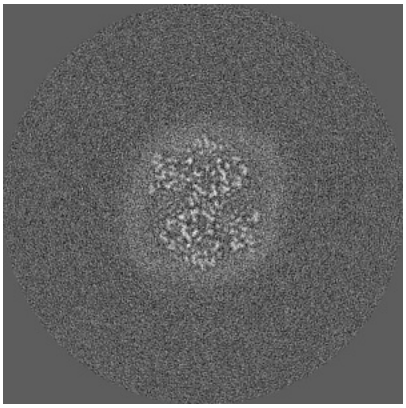
6.3.2 Raw map



X Index: 174



Y Index: 166

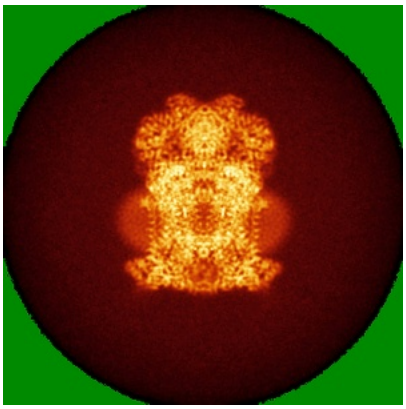


Z Index: 182

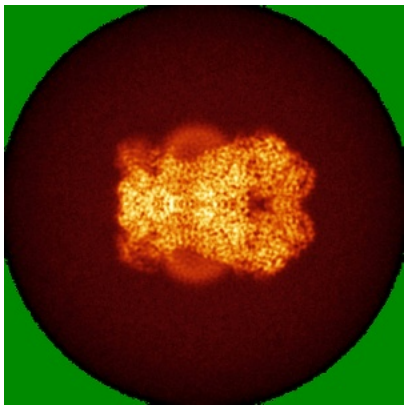
The images above show the largest variance slices of the map in three orthogonal directions.

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

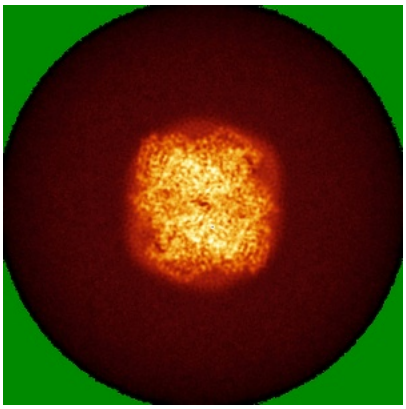
6.4.1 Primary map



X

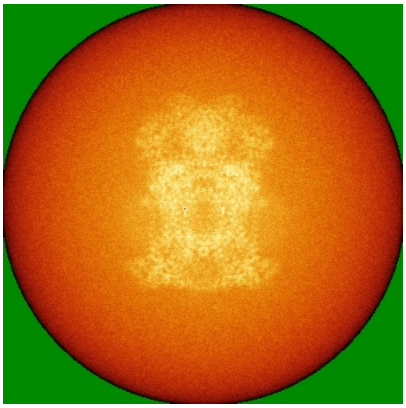


Y

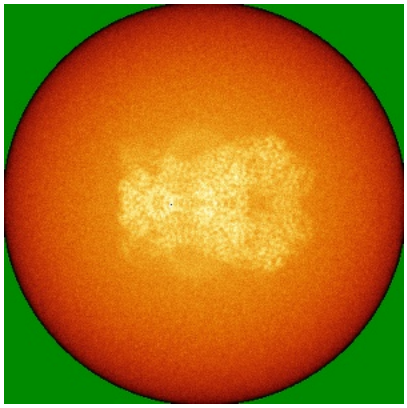


Z

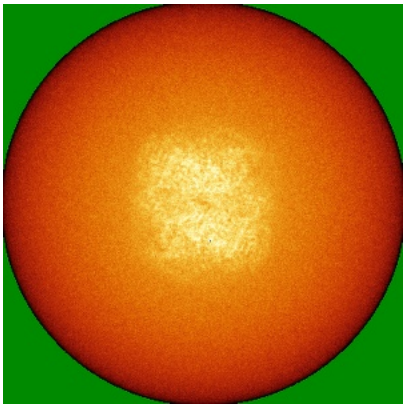
6.4.2 Raw map



X



Y

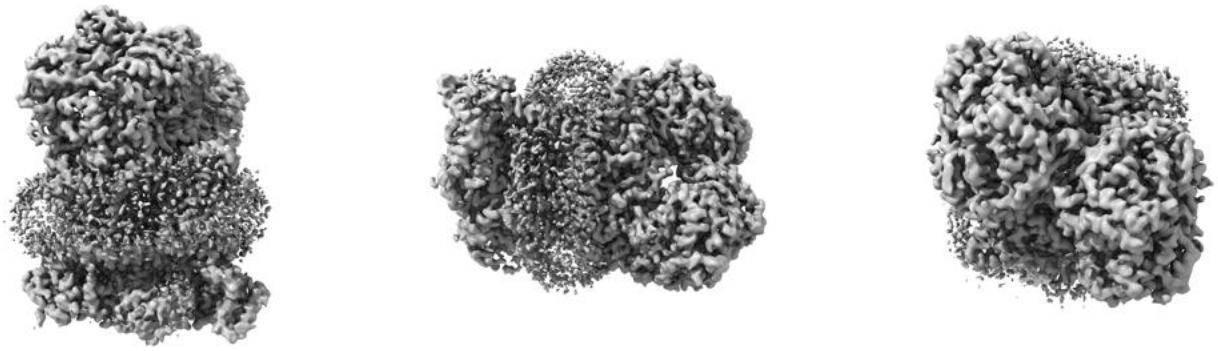


Z

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)

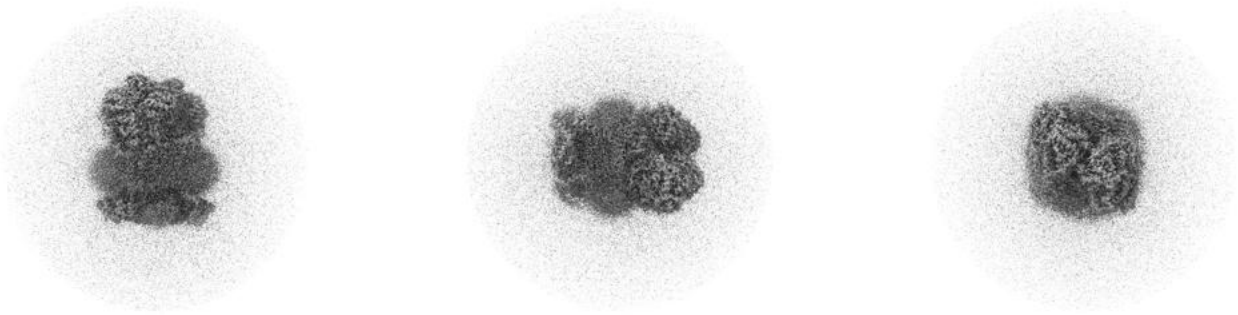
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

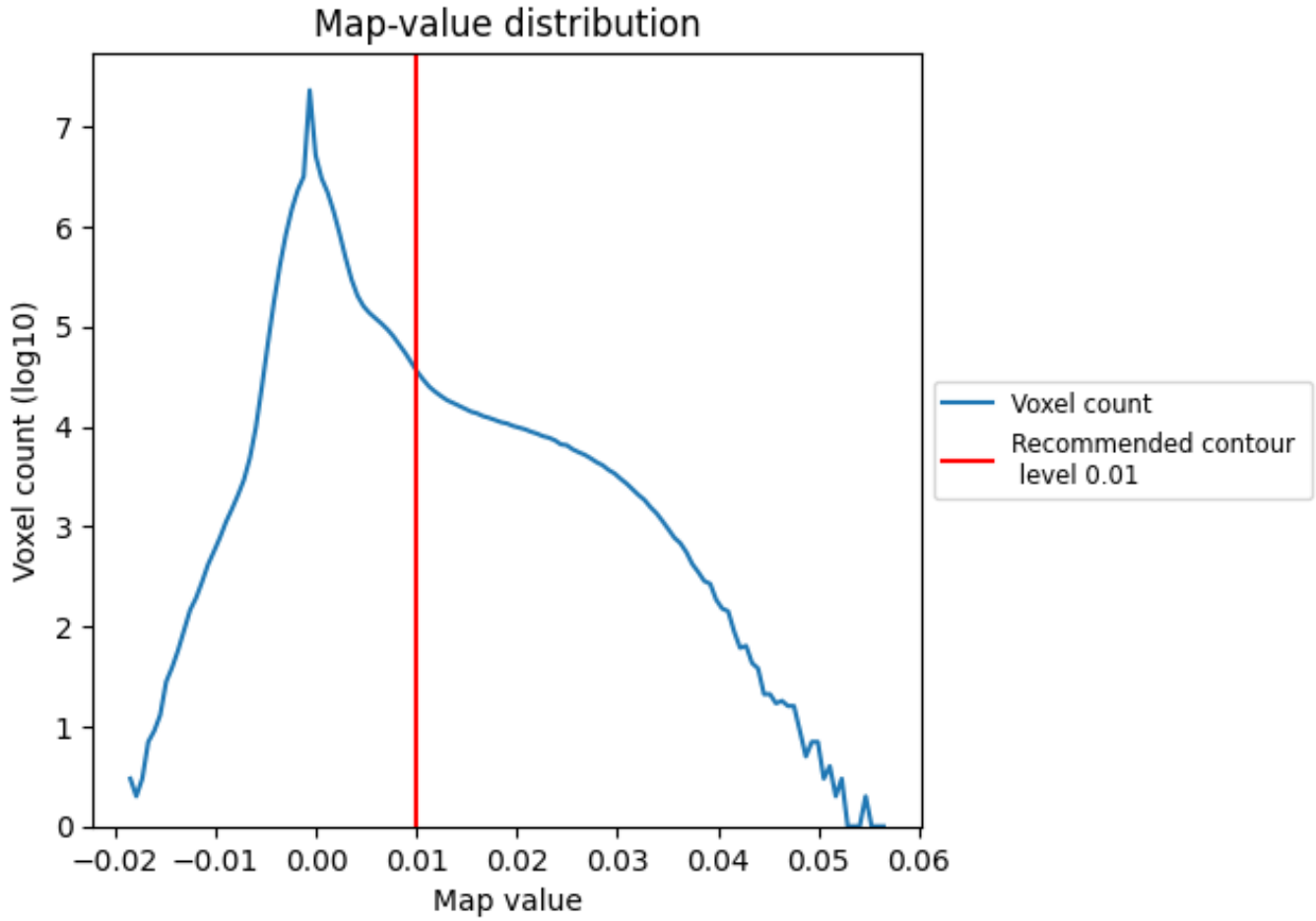
6.6 Mask visualisation (i)

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

7 Map analysis

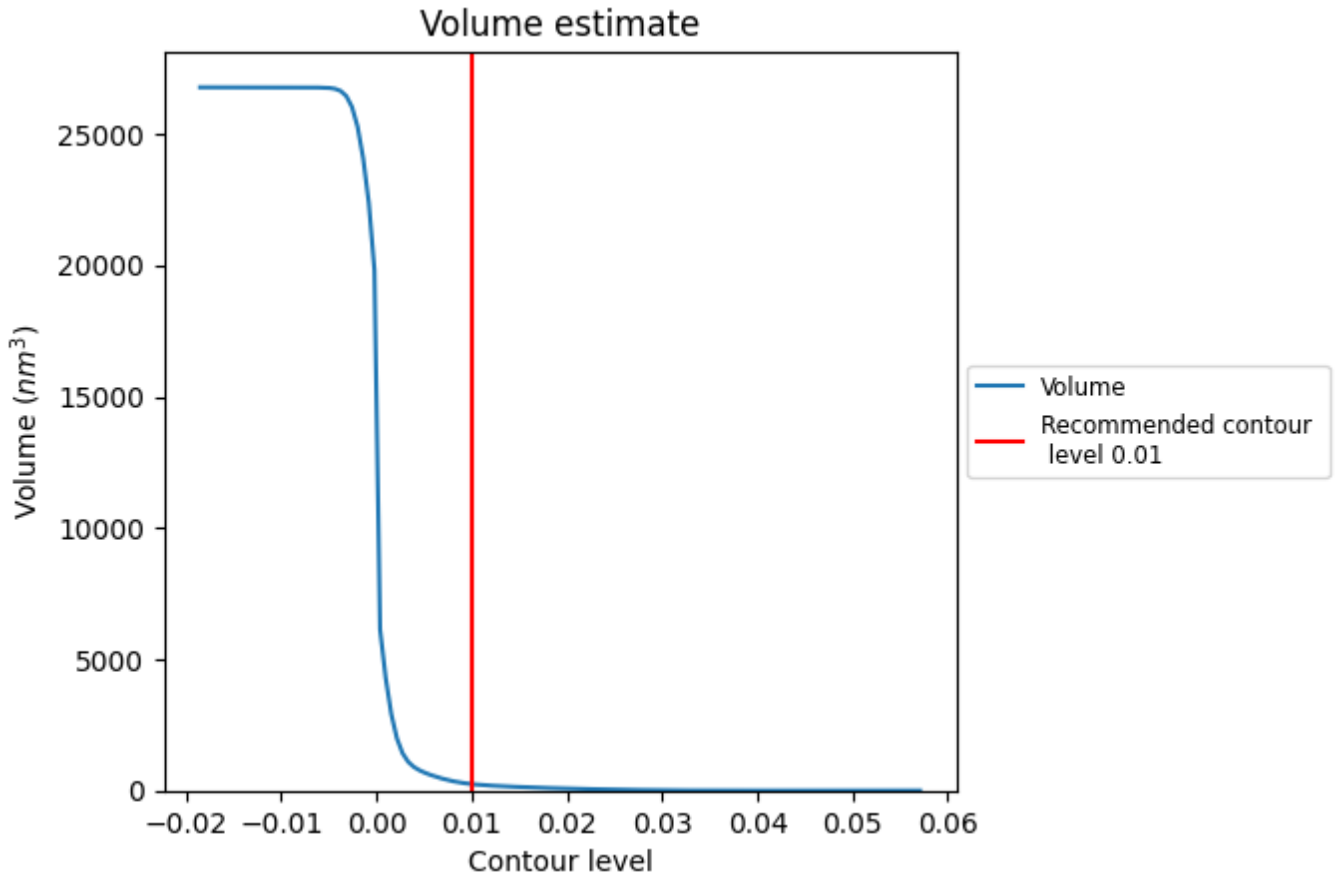
This section contains the results of statistical analysis of the map.

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.

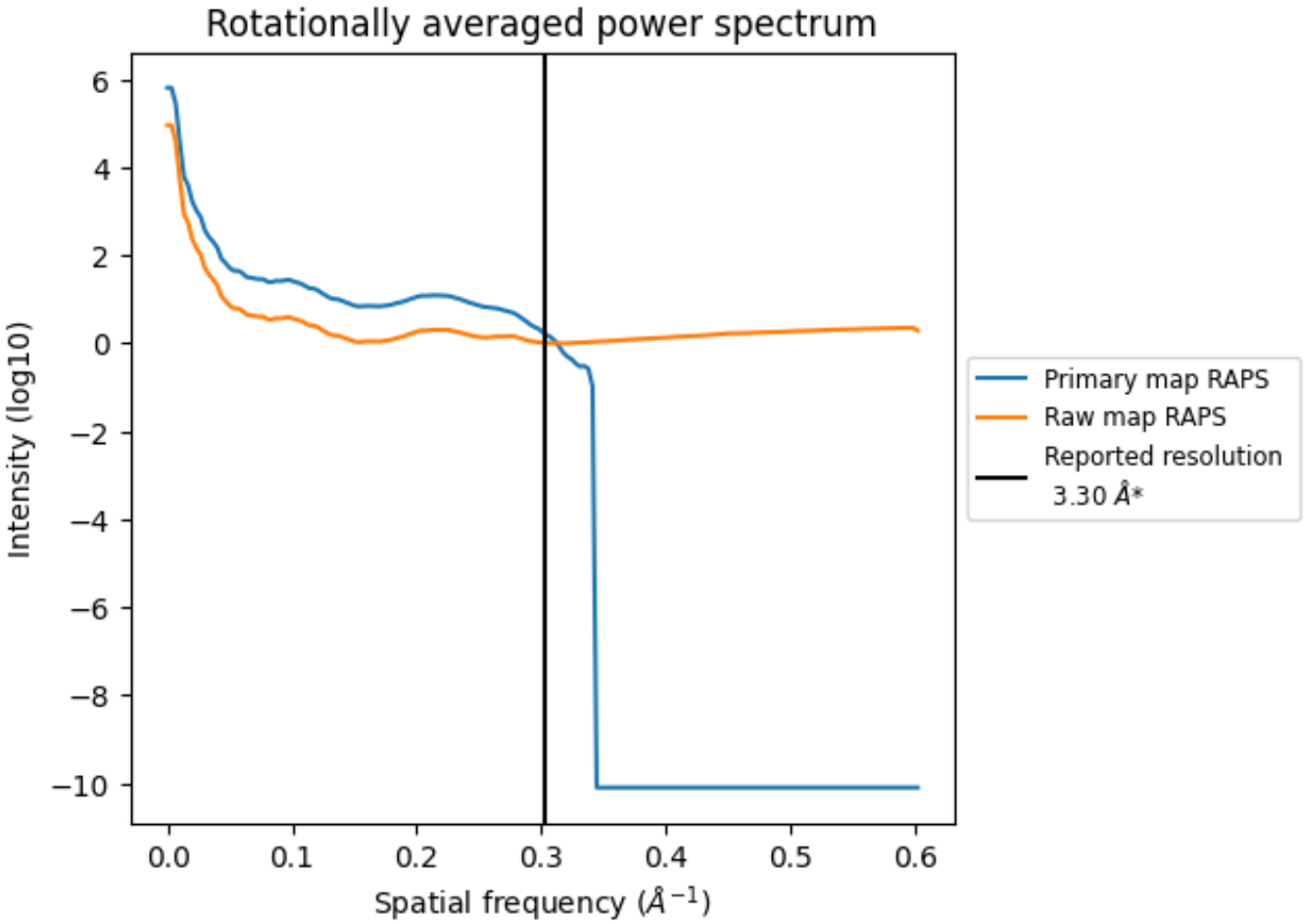
7.2 Volume estimate



The volume at the recommended contour level is 248 nm^3; this corresponds to an approximate mass of 224 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)

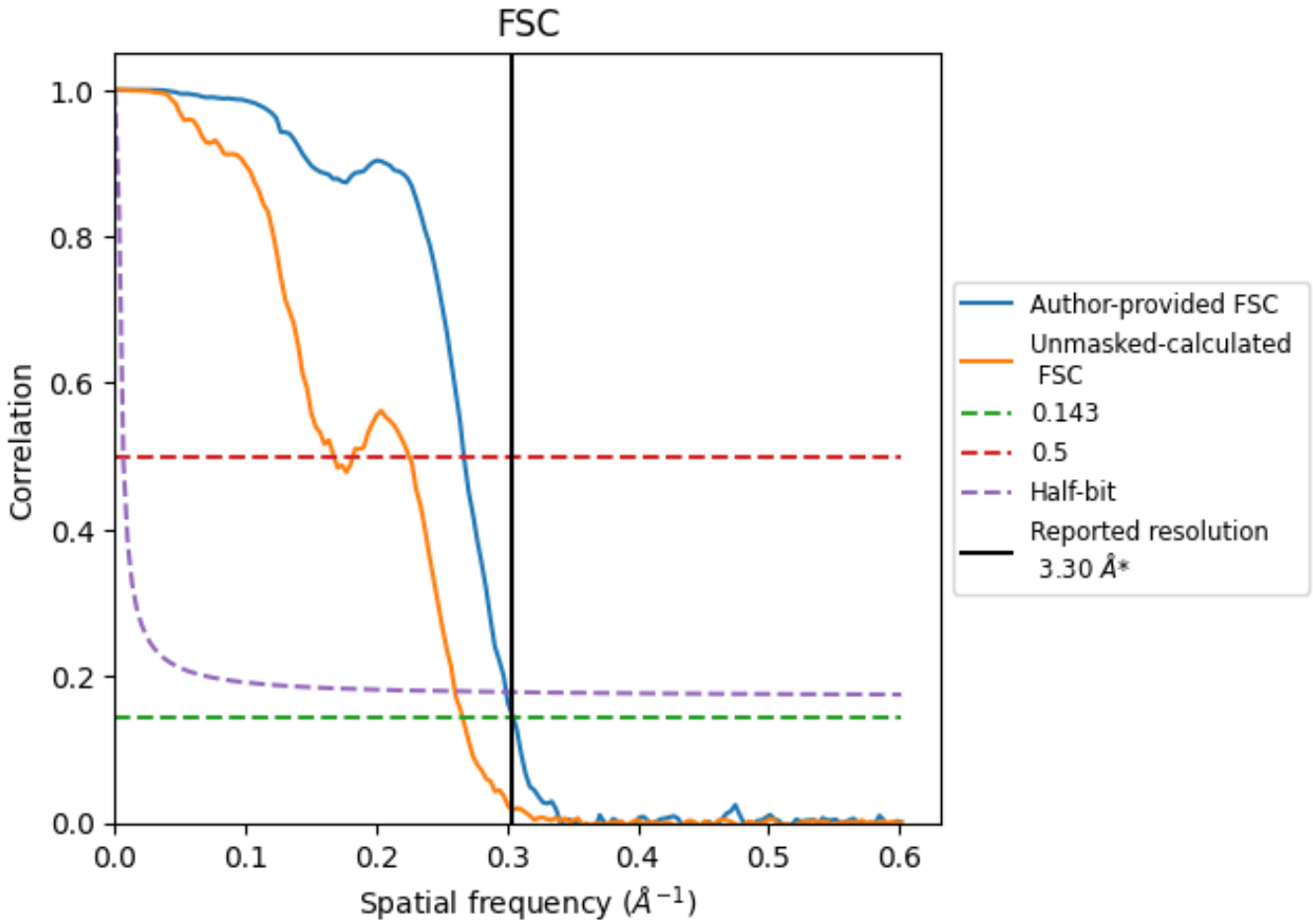


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

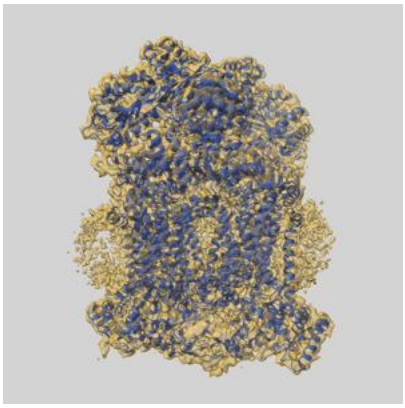
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.74	3.34
Unmasked-calculated*	3.76	5.97	3.84

*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 3.76 differs from the reported value 3.3 by more than 10 %

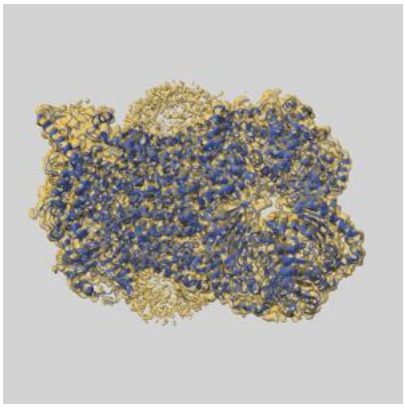
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15315 and PDB model 8AB9. Per-residue inclusion information can be found in section 3 on page 12.

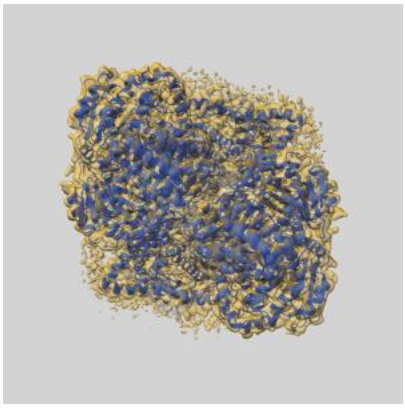
9.1 Map-model overlay



X



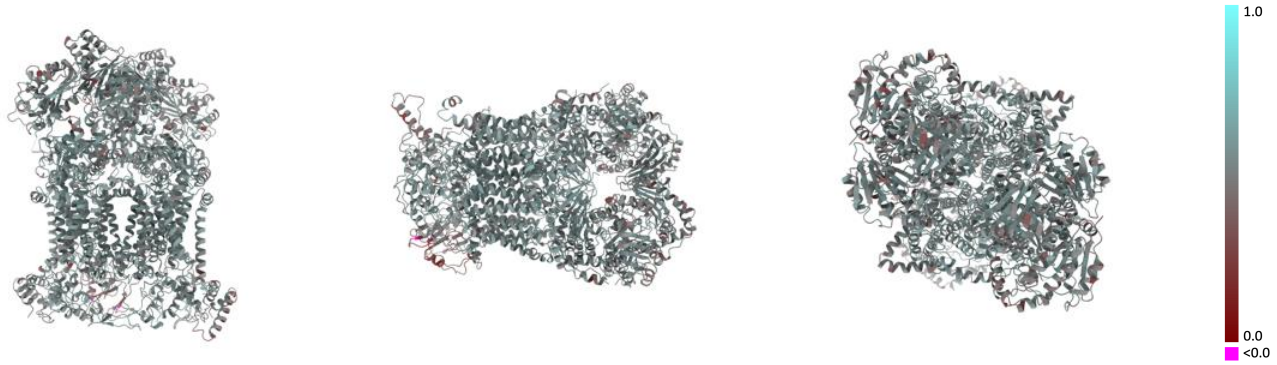
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

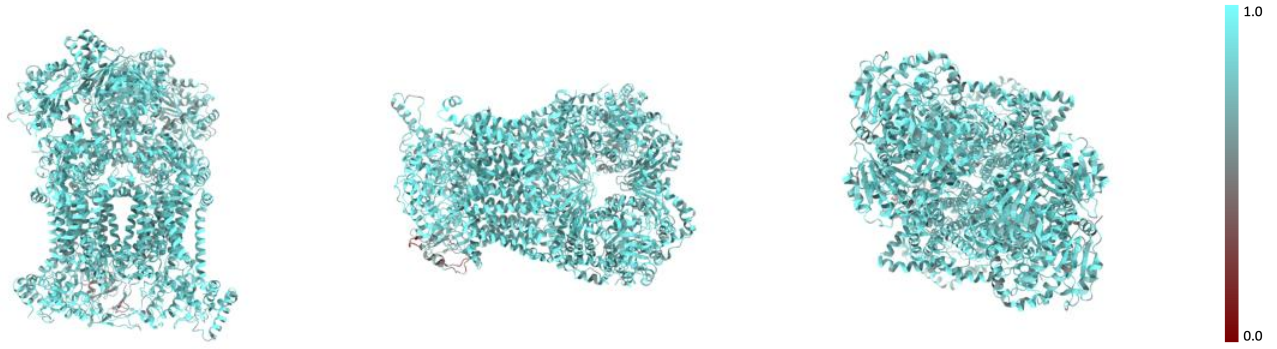
9.2 Q-score mapped to coordinate model (i)



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.

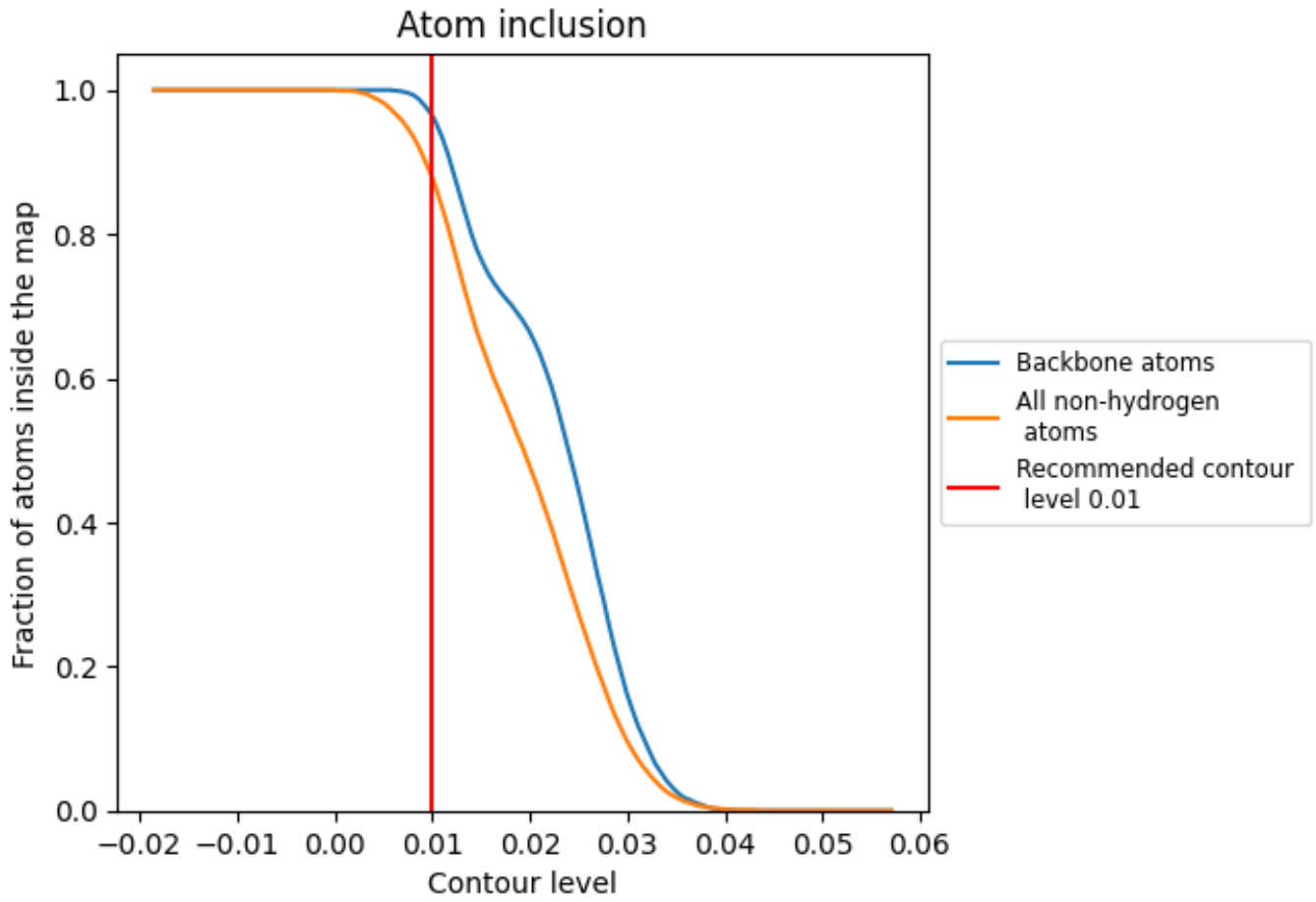
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.5240
A	0.8750	0.5230
B	0.8700	0.5190
C	0.9160	0.5530
D	0.9080	0.5450
E	0.9040	0.5480
F	0.8110	0.4540
G	0.8770	0.5260
H	0.9240	0.5440
I	0.9030	0.5380
J	0.8340	0.5120
L	0.8760	0.5220
M	0.8660	0.5140
N	0.9170	0.5550
O	0.9100	0.5420
P	0.7050	0.3940
Q	0.8080	0.4640
R	0.8820	0.5330
S	0.9300	0.5470
T	0.8990	0.5330
U	0.8470	0.5200