Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 03:08 am BST

PDB ID	:	8ABB / pdb_00008abb
EMDB ID	:	EMD-15317
Title	:	Complex III2 from Yarrowia lipolytica, ascorbate-reduced, c-position
Authors	:	Wieferig, J.P.; Kuhlbrandt, W.
Deposited on	:	2022-07-04
Resolution	:	3.20 Å(reported)

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

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

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

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

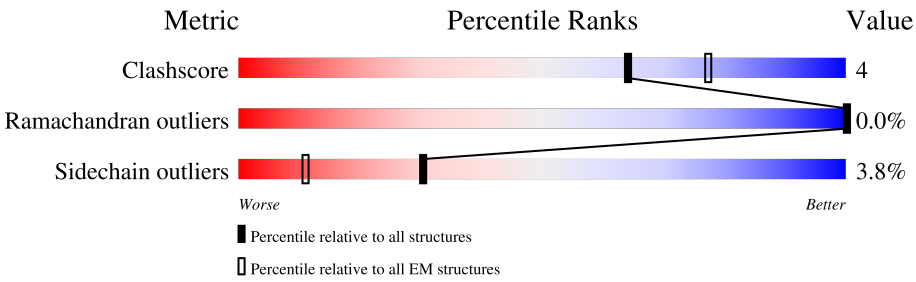
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

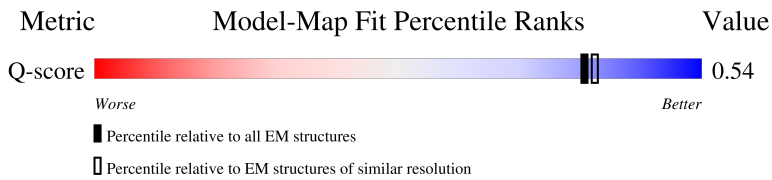
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	91% 8% ••
1	N	385	90% 8% ••
2	E	225	23% • 73%
2	P	225	60% 20% • 17%

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Mol	Chain	Length	Quality of chain
3	G	128	81% 14%
3	R	128	87% 9%
4	F	137	48% 48%
4	Q	137	47% 48%
5	A	474	83% 9% 8%
5	L	474	85% 7% 8%
6	B	417	84% 11%
6	M	417	84% 12%
7	D	330	64% 9% 26%
7	O	330	65% 9% 26%
8	H	93	84% 6% 9%
8	S	93	85% 5% 9%
9	I	69	74% 22%
9	T	69	74% 22%
10	J	82	89% 9%
10	U	82	84% 7% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEC	D	401	X	-	-	-
18	HEC	O	401	X	-	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 32540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

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

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

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

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

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

- Molecule 4 is a protein called YALI0F24673p.

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

- Molecule 5 is a protein called YALI0A14806p.

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

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

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

- Molecule 7 is a protein called YALI0A17468p.

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

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

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

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

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

- Molecule 10 is a protein called YALI0C12210p.

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

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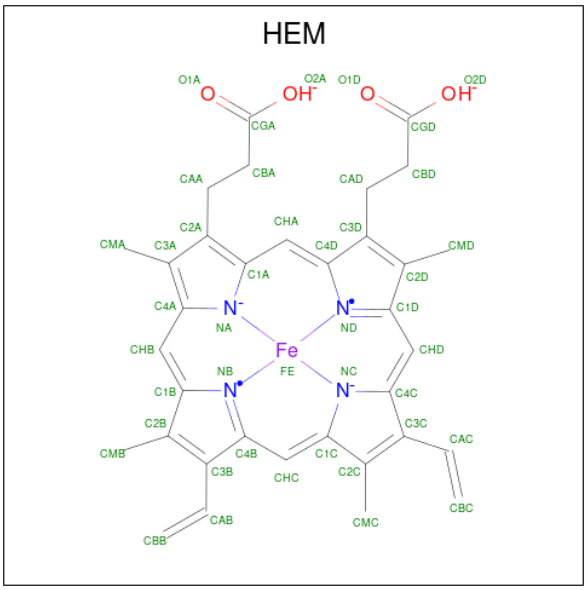
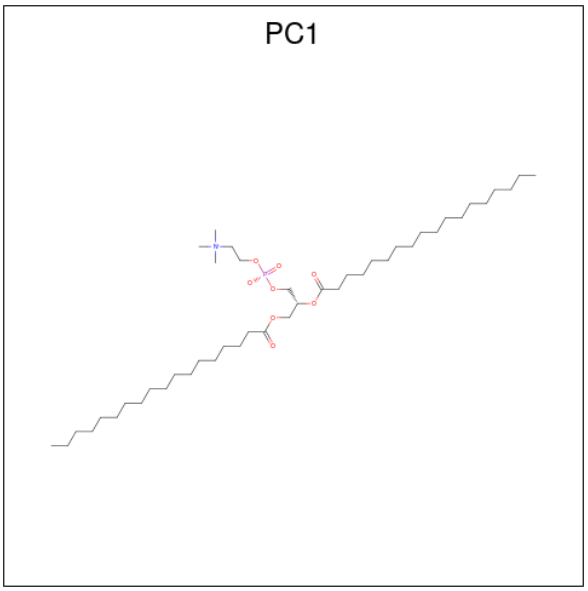
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	75	598	403	99	96	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



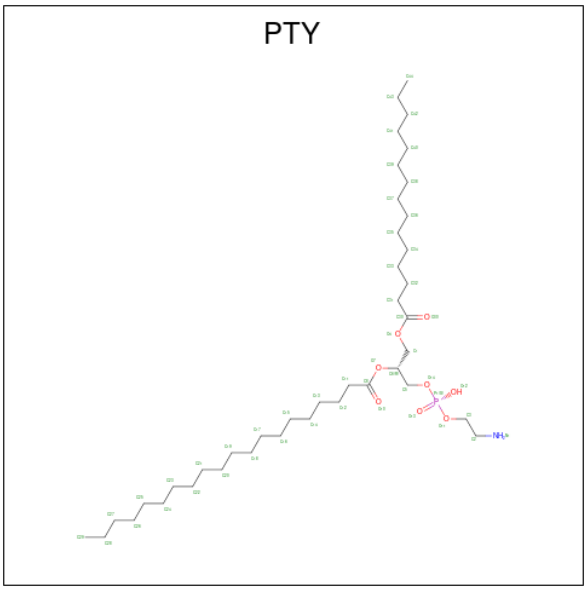
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
11	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
11	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
11	N	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
11	N	1	43	34	1	4	4	0

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



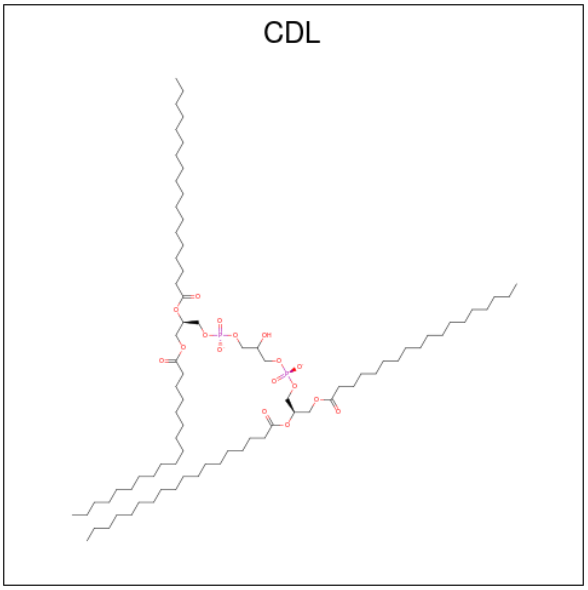
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	I	1	32	22	1	8	1	0
			Total	C	N	O	P	
12	N	1	38	28	1	8	1	0
			Total	C	N	O	P	
12	T	1	32	22	1	8	1	0

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (CCD ID: 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 (CCD ID: 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	

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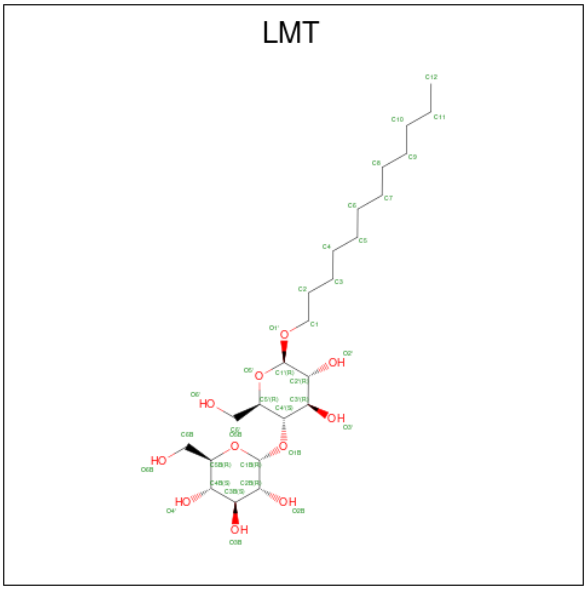
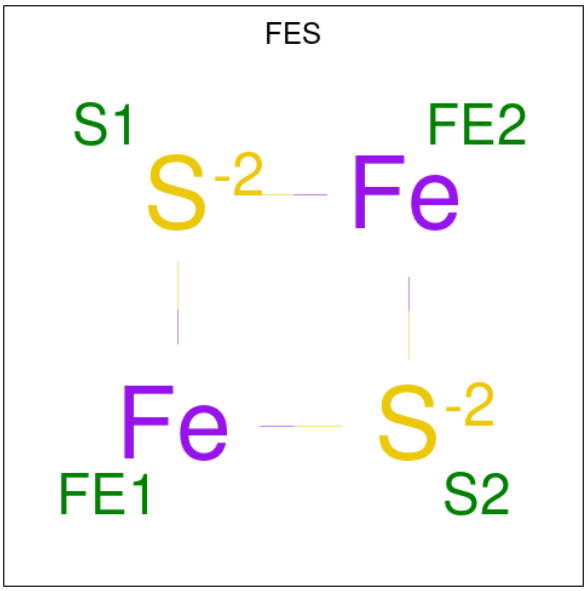
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	L	1	47	30	15	2	0
			Total	C	O	P	
14	S	1	39	20	17	2	0

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



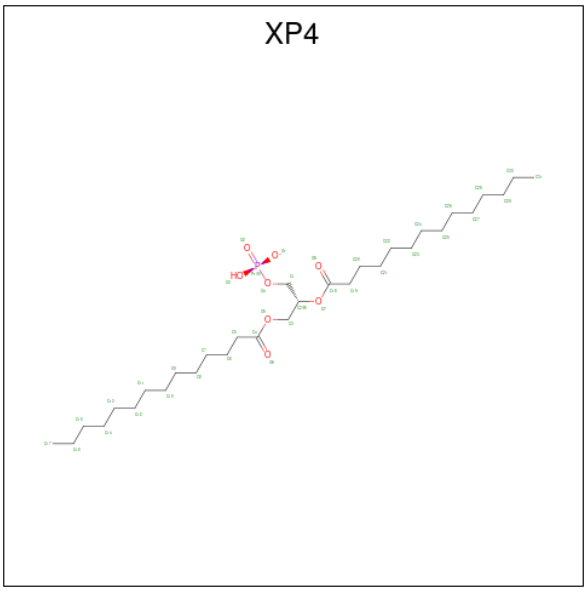
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	C	1	35	24	11	0
			Total	C	O	
15	P	1	35	24	11	0
			Total	C	O	
15	J	1	35	24	11	0
			Total	C	O	
15	N	1	35	24	11	0

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



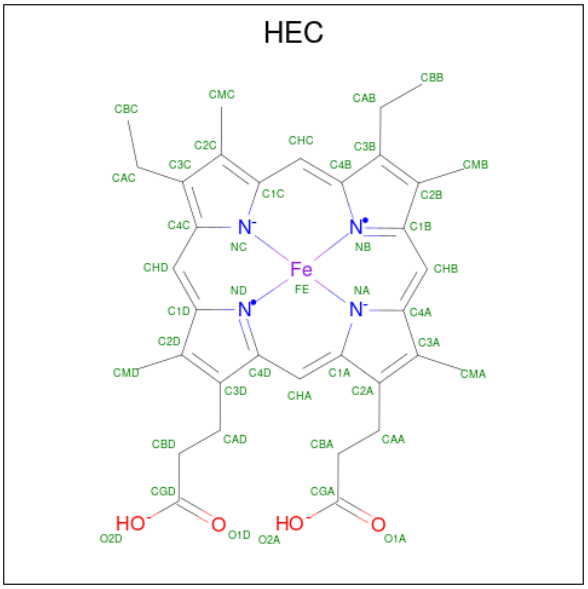
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	P	1	4	2	2	0

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



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

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



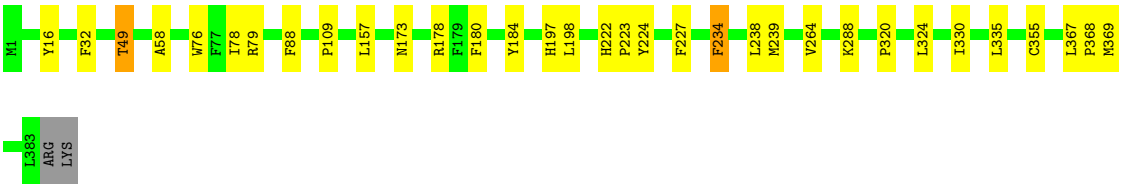
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
18	D	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
18	O	1	43	34	1	4	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome b

Chain C:

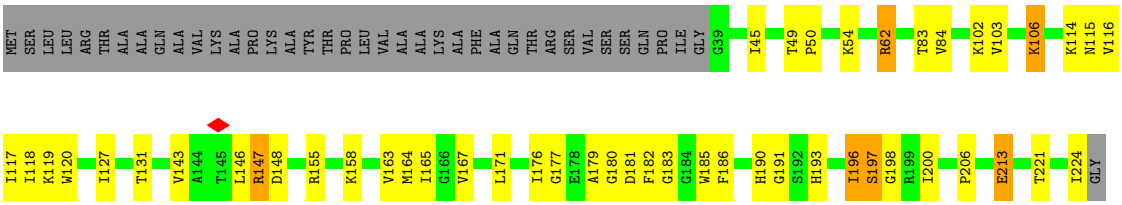


• Molecule 1: Cytochrome b

Chain N:

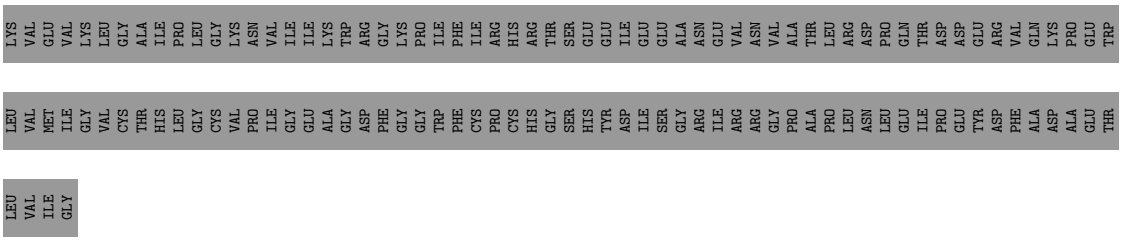
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



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

Chain E:

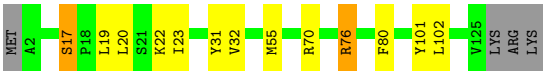


• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain G:

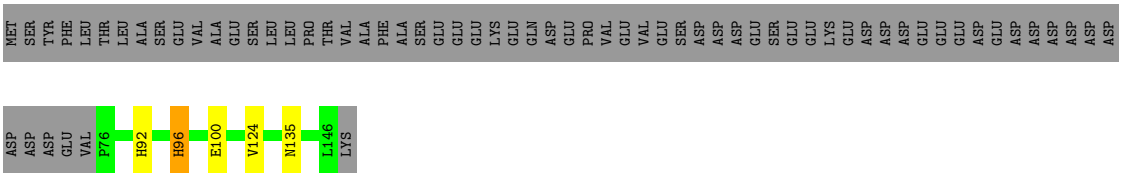
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:



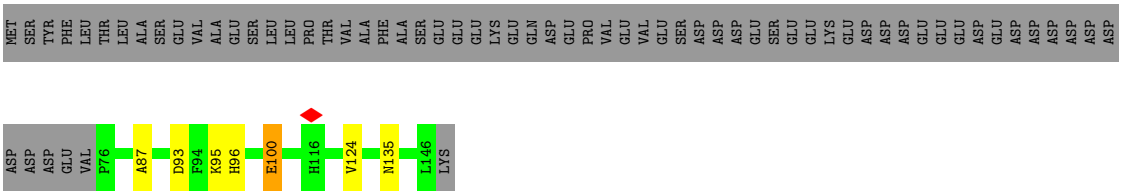
• Molecule 4: YALI0F24673p

Chain F:



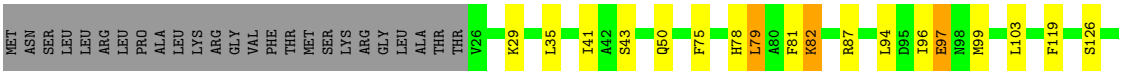
• Molecule 4: YALI0F24673p

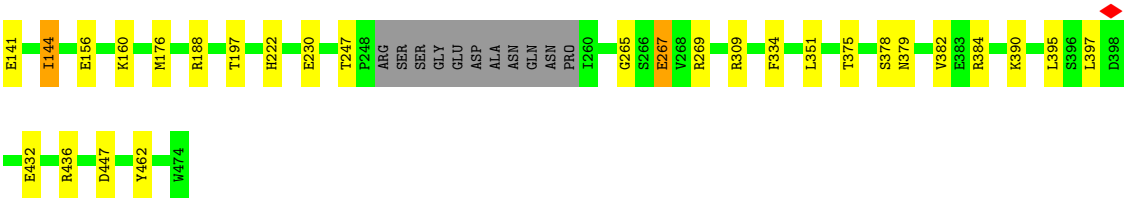
Chain Q:



• Molecule 5: YALI0A14806p

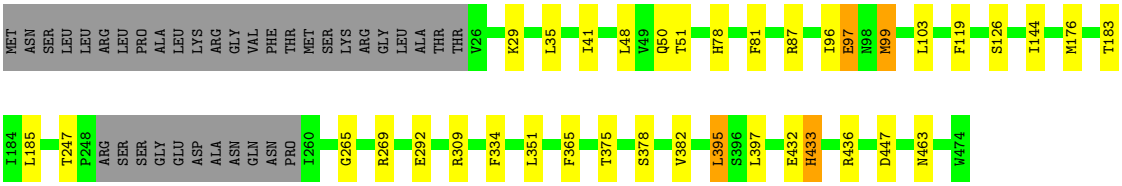
Chain A:





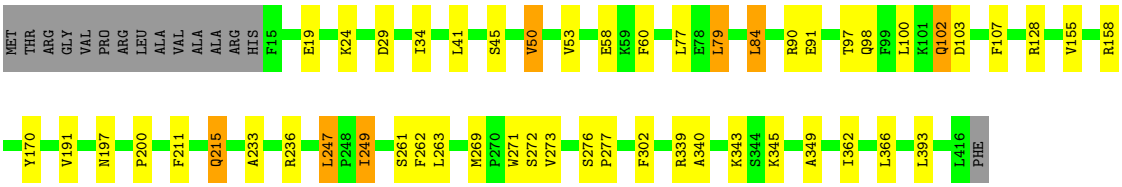
- Molecule 5: YALI0A14806p

Chain L:



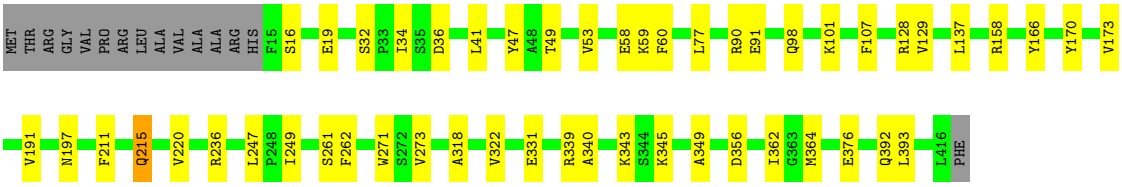
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



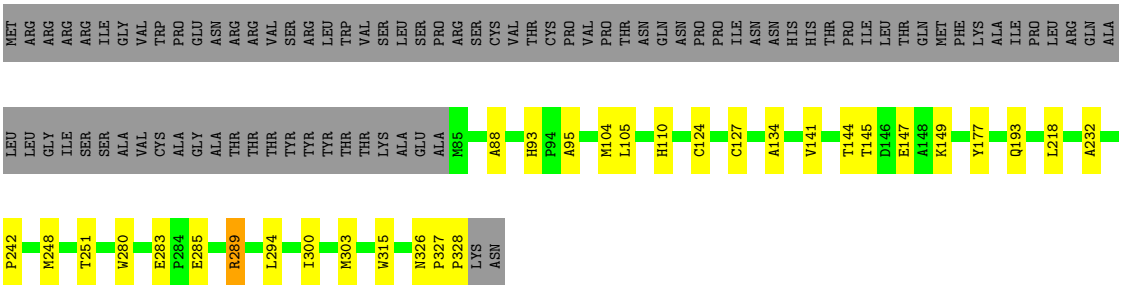
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



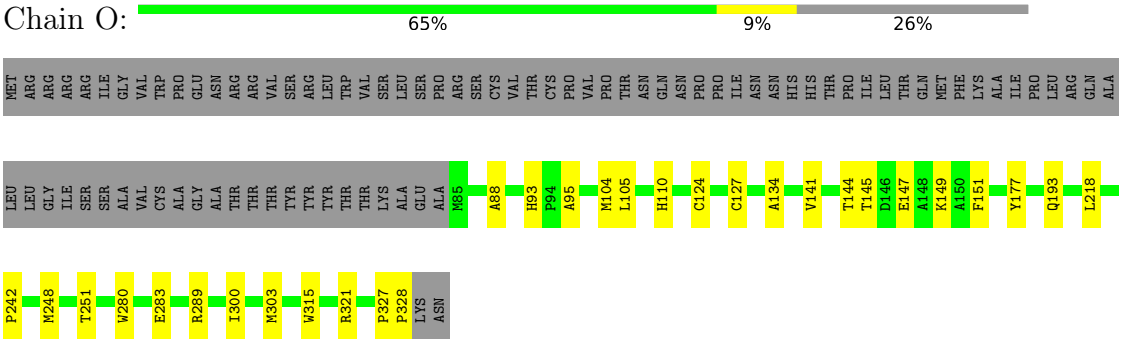
- Molecule 7: YALI0A17468p

Chain D:



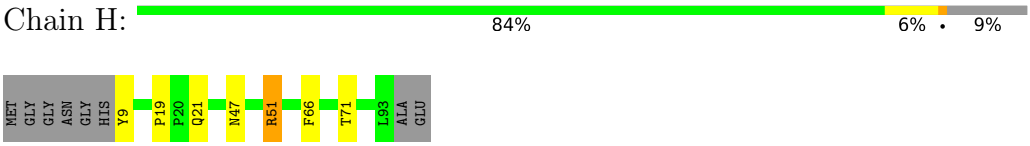
- Molecule 7: YALI0A17468p

Chain O:



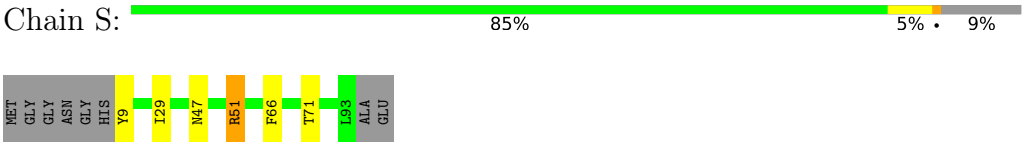
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



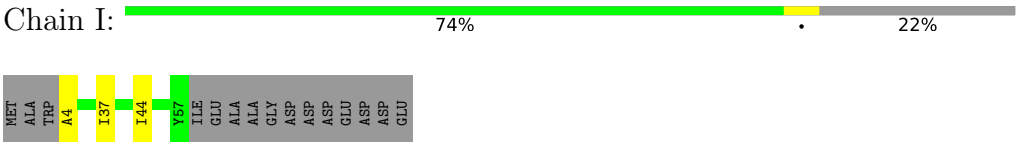
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:



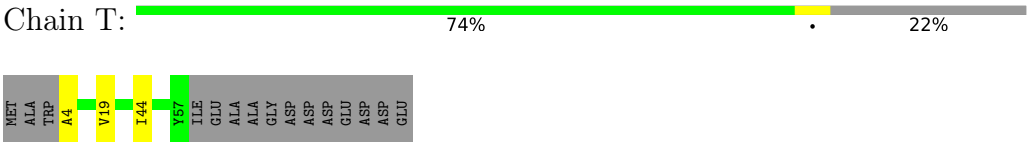
- Molecule 9: Complex III subunit 9

Chain I:



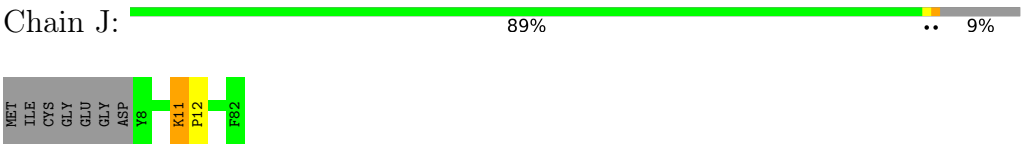
- Molecule 9: Complex III subunit 9

Chain T:



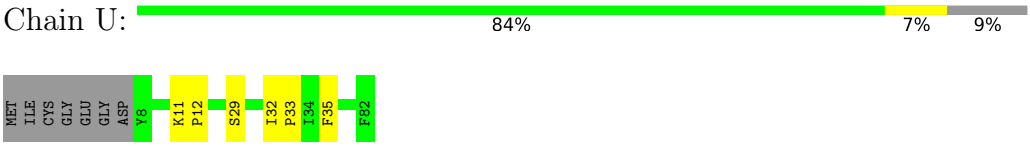
- Molecule 10: YALI0C12210p

Chain J:



- Molecule 10: YALI0C12210p

Chain U:


84%
7%
9%
MET
ILE
CYS
GLY
GLU
GLY
ASP
Y8
K11
P12
S29
I32
P33
I34
F35
F82

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49096	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	-0.020	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: PC1, CDL, HEM, LMT, PTY, HEC, FES, XP4

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	0.67	0/3153	1.15	5/4305 (0.1%)
1	N	0.67	0/3153	1.15	5/4305 (0.1%)
2	E	0.62	0/474	1.12	2/637 (0.3%)
2	P	0.55	0/1479	1.18	5/2003 (0.2%)
3	G	0.59	0/1012	1.09	1/1373 (0.1%)
3	R	0.60	0/1012	1.09	1/1373 (0.1%)
4	F	0.51	0/595	1.11	1/805 (0.1%)
4	Q	0.51	0/595	1.19	3/805 (0.4%)
5	A	0.58	0/3510	1.14	4/4768 (0.1%)
5	L	0.59	0/3510	1.15	4/4768 (0.1%)
6	B	0.56	0/3069	1.13	8/4178 (0.2%)
6	M	0.57	0/3069	1.13	10/4178 (0.2%)
7	D	0.60	0/1950	1.17	6/2656 (0.2%)
7	O	0.60	0/1950	1.16	6/2656 (0.2%)
8	H	0.64	1/717 (0.1%)	1.11	2/975 (0.2%)
8	S	0.65	1/717 (0.1%)	1.11	1/975 (0.1%)
9	I	0.66	1/465 (0.2%)	1.13	0/629
9	T	0.66	1/465 (0.2%)	1.14	0/629
10	J	0.56	0/620	1.10	0/846
10	U	0.56	0/620	1.08	0/846
All	All	0.60	4/32135 (0.0%)	1.14	64/43710 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	9	TYR	N-CA	8.61	1.62	1.46
8	H	9	TYR	N-CA	8.27	1.61	1.46
9	T	4	ALA	N-CA	7.70	1.60	1.46
9	I	4	ALA	N-CA	7.63	1.60	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	283	GLU	CB-CA-C	-9.03	97.06	111.14
6	M	90	ARG	CG-CD-NE	-7.97	94.47	112.00
6	B	90	ARG	CG-CD-NE	-7.96	94.48	112.00
7	D	283	GLU	CB-CA-C	-7.92	98.08	111.15
1	N	49	THR	CA-CB-OG1	-7.86	97.82	109.60
2	P	62	ARG	CB-CG-CD	-7.78	93.40	111.30
1	C	49	THR	CA-CB-OG1	-7.58	98.23	109.60
4	Q	96	HIS	CB-CA-C	-7.42	98.47	110.79
4	Q	93	ASP	CA-CB-CG	7.40	120.00	112.60
2	E	62	ARG	CB-CG-CD	-7.04	95.12	111.30
7	D	283	GLU	CB-CG-CD	-6.96	100.77	112.60
6	B	215	GLN	CB-CA-C	-6.93	97.22	109.62
1	N	16	TYR	CA-C-N	-6.79	114.61	122.14
1	N	16	TYR	C-N-CA	-6.79	114.61	122.14
1	C	16	TYR	CA-C-N	-6.64	114.77	122.14
1	C	16	TYR	C-N-CA	-6.64	114.77	122.14
7	O	93	HIS	CB-CA-C	6.42	118.64	109.08
7	D	93	HIS	CB-CA-C	6.33	118.51	109.08
5	A	379	ASN	CA-CB-CG	-6.24	106.36	112.60
1	C	32	PHE	CA-CB-CG	-6.22	107.58	113.80
5	L	309	ARG	CG-CD-NE	-6.17	98.43	112.00
2	P	182	PHE	N-CA-C	-6.17	103.92	112.30
6	B	197	ASN	CB-CA-C	6.16	120.01	111.63
2	P	148	ASP	CB-CA-C	6.13	117.03	110.65
5	A	309	ARG	CG-CD-NE	-6.07	98.65	112.00
1	N	32	PHE	CA-CB-CG	-6.06	107.74	113.80
6	M	197	ASN	CB-CA-C	6.06	119.87	111.63
6	M	215	GLN	CB-CA-C	-6.05	97.13	109.65
2	P	62	ARG	CB-CA-C	-6.01	100.62	110.85
8	H	71	THR	CA-CB-OG1	-6.01	100.58	109.60
2	E	62	ARG	CB-CA-C	-5.94	100.93	110.79
6	M	49	THR	N-CA-C	-5.93	105.71	113.12
3	G	76	ARG	NE-CZ-NH1	-5.87	115.63	121.50
2	P	181	ASP	N-CA-C	-5.82	105.54	114.16
6	M	392	GLN	CB-CG-CD	-5.81	102.72	112.60
8	S	71	THR	CA-CB-OG1	-5.73	101.00	109.60
6	B	158	ARG	CG-CD-NE	-5.73	99.40	112.00
6	B	211	PHE	CB-CA-C	-5.69	101.97	111.13
6	M	211	PHE	CB-CA-C	-5.62	102.08	111.13
6	M	128	ARG	CG-CD-NE	-5.62	99.63	112.00
4	Q	100	GLU	CB-CA-C	-5.61	101.48	110.79
7	O	321	ARG	CB-CG-CD	-5.61	98.40	111.30
5	L	269	ARG	CG-CD-NE	-5.53	99.83	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	107	PHE	CA-CB-CG	-5.49	108.31	113.80
6	M	158	ARG	CG-CD-NE	-5.49	99.92	112.00
6	B	107	PHE	CA-CB-CG	-5.47	108.33	113.80
5	A	269	ARG	CG-CD-NE	-5.46	100.00	112.00
6	B	128	ARG	CG-CD-NE	-5.45	100.02	112.00
4	F	96	HIS	CB-CA-C	5.34	119.93	110.85
7	O	110	HIS	CA-CB-CG	-5.32	108.48	113.80
7	D	110	HIS	CA-CB-CG	-5.30	108.50	113.80
3	R	76	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	234	PHE	CA-CB-CG	-5.24	108.56	113.80
7	D	289	ARG	CG-CD-NE	-5.22	100.51	112.00
8	H	19	PRO	CB-CA-C	-5.15	104.63	110.92
1	N	234	PHE	CA-CB-CG	-5.15	108.65	113.80
5	A	247	THR	CB-CA-C	5.11	116.70	109.08
7	D	242	PRO	CB-CA-C	-5.05	105.27	111.64
6	M	215	GLN	N-CA-CB	5.04	117.47	110.26
5	L	247	THR	CB-CA-C	5.04	116.59	109.08
7	O	242	PRO	CB-CA-C	-5.04	105.30	111.64
7	O	151	PHE	CB-CA-C	-5.03	102.44	110.79
6	B	91	GLU	CB-CG-CD	5.01	121.12	112.60
5	L	365	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3052	0	3113	23	0
1	N	3052	0	3113	26	0
2	E	465	0	459	6	0
2	P	1445	0	1426	30	0
3	G	994	0	1022	7	0
3	R	994	0	1022	6	0
4	F	579	0	511	2	0
4	Q	579	0	511	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3446	0	3369	28	0
5	L	3446	0	3369	19	0
6	B	3008	0	2991	27	0
6	M	3008	0	2991	21	0
7	D	1893	0	1834	31	0
7	O	1893	0	1834	25	0
8	H	690	0	673	3	0
8	S	690	0	673	3	0
9	I	452	0	435	2	0
9	T	452	0	435	2	0
10	J	598	0	615	1	0
10	U	598	0	615	5	0
11	C	86	0	60	8	0
11	N	86	0	60	8	0
12	C	38	0	50	2	0
12	I	32	0	38	2	0
12	N	38	0	50	3	0
12	T	32	0	38	2	0
13	C	41	0	58	4	0
13	E	41	0	58	2	0
13	N	41	0	58	9	0
13	P	41	0	58	12	0
14	A	89	0	85	3	0
14	C	48	0	40	0	0
14	H	89	0	66	3	0
14	L	89	0	85	1	0
14	N	98	0	84	0	0
14	S	39	0	22	4	0
15	C	35	0	46	0	0
15	J	35	0	46	2	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	2	0
18	D	43	0	32	15	0
18	O	43	0	32	13	0
All	All	32540	0	32213	263	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 (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:84:VAL:CG2	13:P:303:PTY:H441	1.45	1.45
7:O:124:CYS:SG	18:O:401:HEC:HBB3	1.57	1.42
7:D:124:CYS:SG	18:D:401:HEC:HBB3	1.62	1.39
2:P:84:VAL:HG23	13:P:303:PTY:C44	1.65	1.27
7:O:124:CYS:SG	18:O:401:HEC:CBB	2.26	1.23
7:D:124:CYS:SG	18:D:401:HEC:CBB	2.30	1.19
7:O:127:CYS:SG	18:O:401:HEC:CAC	2.38	1.10
7:O:127:CYS:SG	18:O:401:HEC:HBC3	1.92	1.10
7:D:127:CYS:SG	18:D:401:HEC:HBC3	1.93	1.08
7:O:124:CYS:SG	18:O:401:HEC:CAB	2.41	1.08
7:D:124:CYS:SG	18:D:401:HEC:CAB	2.42	1.07
7:D:127:CYS:SG	18:D:401:HEC:CAC	2.42	1.07
7:O:127:CYS:SG	18:O:401:HEC:CBC	2.45	1.04
7:D:127:CYS:SG	18:D:401:HEC:CBC	2.47	1.02
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.41	1.02
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.38	1.01
2:P:84:VAL:HG22	13:P:303:PTY:H441	1.43	1.00
2:P:84:VAL:HG23	13:P:303:PTY:H441	0.94	0.94
2:P:84:VAL:CG2	13:P:303:PTY:C44	2.34	0.93
6:M:91:GLU:HG2	6:M:364:MET:HE1	1.50	0.92
5:A:395:LEU:HD23	6:B:34:ILE:HD12	1.53	0.91
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.10	0.84
1:C:58:ALA:H	1:C:173:ASN:HD22	1.27	0.79
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.69	0.74
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.71	0.72
7:D:124:CYS:SG	18:D:401:HEC:C3B	2.77	0.72
7:O:124:CYS:SG	18:O:401:HEC:C3B	2.78	0.72
7:D:127:CYS:HG	18:D:401:HEC:HBC3	1.52	0.71
2:P:84:VAL:HG23	13:P:303:PTY:C43	2.20	0.71
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.73	0.70
14:H:702:CDL:C72	14:H:702:CDL:HB61	2.23	0.69
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.73	0.69
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	1.92	0.68
14:S:101:CDL:CB6	14:S:101:CDL:C72	2.72	0.67
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.24	0.67
5:A:395:LEU:HD22	6:B:98:GLN:HG2	1.78	0.66
6:B:236:ARG:HD3	6:M:170:TYR:CE1	2.29	0.66
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.26	0.65
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.78	0.65
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.78	0.64
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.43	0.63
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:127:CYS:SG	18:O:401:HEC:C3C	2.87	0.63
14:H:702:CDL:C72	14:H:702:CDL:CB6	2.77	0.63
5:A:395:LEU:CD2	6:B:34:ILE:HD12	2.27	0.62
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.82	0.61
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.82	0.61
5:L:97:GLU:HG3	6:M:343:LYS:HE2	1.83	0.60
6:B:236:ARG:HD3	6:M:170:TYR:CZ	2.37	0.60
9:T:19:VAL:HG22	12:T:201:PC1:H332	1.83	0.60
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.84	0.59
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.84	0.59
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.38	0.59
7:D:127:CYS:SG	18:D:401:HEC:C3C	2.91	0.58
11:C:502:HEM:HBC2	11:C:502:HEM:HMC2	1.85	0.58
2:P:191:GLY:HA3	7:D:232:ALA:HB1	1.85	0.58
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.02	0.58
6:M:318:ALA:O	6:M:322:VAL:HG23	2.04	0.58
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.28	0.58
5:A:395:LEU:HD23	6:B:34:ILE:CD1	2.32	0.57
1:N:234:PHE:CZ	7:O:303:MET:HE2	2.40	0.57
11:N:501:HEM:HBB2	11:N:501:HEM:CMB	2.33	0.57
13:C:504:PTY:H112	13:C:504:PTY:HC12	1.85	0.57
1:C:58:ALA:H	1:C:173:ASN:ND2	2.00	0.56
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.69	0.56
5:A:43:SER:CB	5:A:222:HIS:HD2	2.18	0.56
3:G:55:MET:HE1	3:G:102:LEU:HD21	1.87	0.56
1:N:330:ILE:CD1	12:N:503:PC1:H2A1	2.28	0.56
2:P:155:ARG:NH1	2:P:197:SER:O	2.38	0.56
5:A:378:SER:HA	5:A:432:GLU:OE1	2.06	0.56
1:N:229:ASP:HB2	13:N:505:PTY:H382	1.86	0.56
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.40	0.55
8:H:47:ASN:O	8:H:51:ARG:HG2	2.06	0.55
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.42	0.55
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.42	0.55
1:C:234:PHE:CZ	7:D:303:MET:HE2	2.42	0.54
3:G:71:VAL:HG11	8:H:21:GLN:HG2	1.89	0.54
4:F:124:VAL:HG11	7:D:88:ALA:HB2	1.89	0.54
1:C:264:VAL:HA	2:P:171:LEU:O	2.08	0.54
2:P:84:VAL:CG2	13:P:303:PTY:C43	2.82	0.54
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.88	0.54
2:P:186:PHE:CE1	2:P:191:GLY:HA2	2.43	0.54
6:B:249:ILE:HD11	6:B:302:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:180:GLY:HA2	2:P:186:PHE:HB2	1.90	0.53
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.91	0.53
13:C:504:PTY:H132	2:E:72:PHE:CE2	2.42	0.53
14:S:101:CDL:C72	14:S:101:CDL:HB61	2.38	0.53
14:A:3002:CDL:H132	14:A:3002:CDL:H522	1.91	0.52
2:P:106:LYS:HA	2:P:221:THR:HG22	1.92	0.52
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.91	0.52
1:N:139:MET:HE1	1:N:269:ILE:HA	1.91	0.52
6:M:59:LYS:HB3	6:M:129:VAL:HG13	1.91	0.52
8:S:47:ASN:O	8:S:51:ARG:HG2	2.10	0.52
5:A:97:GLU:HG3	6:B:343:LYS:HE2	1.91	0.51
7:D:145:THR:O	7:D:149:LYS:HG3	2.11	0.51
1:C:238:LEU:HD13	7:D:300:ILE:HG22	1.90	0.51
1:C:330:ILE:CD1	12:C:503:PC1:H2A1	2.27	0.51
11:N:501:HEM:HBB2	11:N:501:HEM:HMB1	1.92	0.51
11:N:501:HEM:HHD	11:N:501:HEM:CBC	2.40	0.50
6:M:262:PHE:HB2	6:M:340:ALA:HB2	1.94	0.50
15:J:101:LMT:H31	2:E:85:GLN:HG3	1.94	0.49
2:E:49:THR:N	2:E:50:PRO:HD2	2.27	0.49
2:P:193:HIS:O	2:P:200:ILE:HD12	2.13	0.49
5:A:96:ILE:HG12	5:A:103:LEU:HD13	1.94	0.49
5:L:119:PHE:HE1	6:M:349:ALA:HB2	1.78	0.49
1:N:227:PHE:HZ	13:N:505:PTY:HC6	1.78	0.49
5:A:119:PHE:HE1	6:B:349:ALA:HB2	1.78	0.49
7:D:105:LEU:HB3	9:I:44:ILE:HD12	1.95	0.49
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.40	0.48
11:C:501:HEM:CMB	11:C:501:HEM:HBB2	2.44	0.48
6:B:262:PHE:HB2	6:B:340:ALA:HB2	1.94	0.48
12:N:503:PC1:O13	12:N:503:PC1:H133	2.14	0.48
17:L:3003:XP4:H8	10:U:35:PHE:HE1	1.78	0.48
6:B:247:LEU:HD13	6:B:393:LEU:HB3	1.93	0.48
5:A:97:GLU:HB3	6:B:339:ARG:HD2	1.96	0.48
7:O:105:LEU:HB3	9:T:44:ILE:HD12	1.96	0.48
4:Q:87:ALA:HB1	4:Q:95:LYS:HD3	1.95	0.47
7:O:248:MET:HB2	18:O:401:HEC:C1D	2.44	0.47
1:N:178:ARG:HE	1:N:178:ARG:HB3	1.49	0.47
2:P:45:ILE:HG21	5:L:176:MET:HE2	1.96	0.47
13:N:505:PTY:H372	13:N:505:PTY:H402	1.58	0.47
13:C:504:PTY:H132	2:E:72:PHE:HE2	1.78	0.47
5:A:81:PHE:HB3	6:B:269:MET:HE3	1.95	0.47
14:S:101:CDL:C72	14:S:101:CDL:HB62	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:249:ILE:HD11	6:M:393:LEU:HD21	1.96	0.47
13:P:303:PTY:H352	13:P:303:PTY:H381	1.63	0.46
5:A:176:MET:HE2	2:E:45:ILE:HG21	1.98	0.46
11:C:502:HEM:HBB2	11:C:502:HEM:CMB	2.45	0.46
2:P:49:THR:N	2:P:50:PRO:HD2	2.30	0.46
2:P:171:LEU:HD12	2:P:190:HIS:CE1	2.50	0.46
1:C:224:TYR:HB3	7:D:315:TRP:CZ2	2.51	0.46
7:D:251:THR:HG21	18:D:401:HEC:HMC1	1.97	0.46
7:O:251:THR:HG21	18:O:401:HEC:HMC1	1.98	0.46
7:D:248:MET:HB2	18:D:401:HEC:C1D	2.45	0.46
14:L:3001:CDL:H1	14:L:3002:CDL:HA4	1.98	0.46
7:O:145:THR:O	7:O:149:LYS:HG3	2.15	0.45
10:U:32:ILE:HB	10:U:33:PRO:HD3	1.98	0.45
2:P:177:GLY:C	2:P:179:ALA:H	2.25	0.45
5:A:82:LYS:HD3	5:A:82:LYS:HA	1.58	0.45
5:A:375:THR:C	5:A:436:ARG:HH12	2.25	0.45
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.98	0.45
3:R:70:ARG:HD2	3:R:101:TYR:OH	2.15	0.45
13:E:401:PTY:H352	13:E:401:PTY:H381	1.29	0.45
1:C:335:LEU:HD23	1:C:355:CYS:SG	2.56	0.45
13:P:303:PTY:H331	13:P:303:PTY:H361	1.63	0.45
1:C:320:PRO:HD2	3:G:31:TYR:CE1	2.52	0.45
5:A:334:PHE:HB3	5:A:351:LEU:HD23	1.98	0.45
10:U:29:SER:HA	10:U:32:ILE:HG12	1.99	0.45
3:G:70:ARG:HD2	3:G:101:TYR:OH	2.17	0.45
18:D:401:HEC:HBA2	18:D:401:HEC:HHA	1.99	0.45
7:O:251:THR:HG21	18:O:401:HEC:CMC	2.47	0.45
7:D:218:LEU:HD11	18:D:401:HEC:HMB3	1.99	0.44
1:N:79:ARG:HD3	1:N:79:ARG:C	2.42	0.44
3:G:76:ARG:HD3	3:G:80:PHE:CE2	2.53	0.44
5:L:96:ILE:HG12	5:L:103:LEU:HD13	1.99	0.44
1:C:79:ARG:HD3	1:C:79:ARG:C	2.42	0.44
7:D:134:ALA:HA	7:D:177:TYR:HA	2.00	0.44
1:N:335:LEU:HD22	8:S:66:PHE:HD1	1.83	0.44
13:E:401:PTY:H132	13:E:401:PTY:H161	1.64	0.44
4:Q:124:VAL:HG11	7:O:88:ALA:HB2	1.98	0.44
7:O:134:ALA:HA	7:O:177:TYR:HA	2.00	0.44
1:N:367:LEU:HB3	1:N:368:PRO:HD3	2.00	0.44
5:L:395:LEU:HD12	6:M:34:ILE:HG22	1.99	0.44
15:J:101:LMT:H71	15:J:101:LMT:H41	1.82	0.44
5:L:81:PHE:HE1	5:L:103:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:104:MET:HE2	7:O:104:MET:HB3	1.79	0.44
7:D:218:LEU:HD11	18:D:401:HEC:CMB	2.48	0.44
1:N:238:LEU:HD13	7:O:300:ILE:HG22	2.00	0.44
13:N:505:PTY:H331	13:N:505:PTY:H362	1.41	0.44
7:O:327:PRO:HA	7:O:328:PRO:HD3	1.84	0.44
1:C:335:LEU:HD22	8:H:66:PHE:HD1	1.82	0.44
5:L:375:THR:C	5:L:436:ARG:HH12	2.25	0.44
1:C:76:TRP:CG	7:D:285:GLU:HG3	2.53	0.43
7:D:251:THR:HG21	18:D:401:HEC:CMC	2.48	0.43
1:N:49:THR:HG21	1:N:78:ILE:HD13	2.00	0.43
5:A:99:MET:SD	5:A:126:SER:HB3	2.58	0.43
6:B:263:LEU:HA	6:B:277:PRO:HG2	1.99	0.43
7:D:144:THR:OG1	7:D:147:GLU:HG3	2.18	0.43
5:L:265:GLY:HA3	5:L:447:ASP:HB3	2.00	0.43
1:C:227:PHE:CZ	13:C:504:PTY:H322	2.53	0.43
2:P:147:ARG:HE	2:P:147:ARG:HB2	1.20	0.43
5:A:334:PHE:CB	5:A:351:LEU:HD23	2.48	0.43
17:L:3003:XP4:H8	10:U:35:PHE:CE1	2.52	0.43
12:I:201:PC1:H322	12:I:201:PC1:H351	1.62	0.43
1:N:335:LEU:HD23	1:N:355:CYS:SG	2.58	0.43
13:N:505:PTY:H341	13:N:505:PTY:H151	2.01	0.43
5:L:97:GLU:HB3	6:M:339:ARG:HD3	1.99	0.43
5:L:334:PHE:HB3	5:L:351:LEU:HD23	2.01	0.43
5:A:75:PHE:HD1	5:A:79:LEU:HD22	1.84	0.43
1:C:49:THR:HG21	1:C:78:ILE:HD13	2.00	0.43
1:C:264:VAL:HG22	2:P:171:LEU:O	2.19	0.43
3:R:55:MET:HE1	3:R:102:LEU:HD21	2.00	0.43
7:O:144:THR:OG1	7:O:147:GLU:HG3	2.18	0.43
1:N:227:PHE:CZ	13:N:505:PTY:H322	2.54	0.43
2:P:83:THR:HA	13:P:303:PTY:H121	2.01	0.43
14:S:101:CDL:H311	14:S:101:CDL:HA62	1.60	0.43
14:H:702:CDL:HA62	14:H:702:CDL:H311	1.56	0.42
1:N:222:HIS:CG	1:N:223:PRO:HA	2.54	0.42
6:M:247:LEU:HD13	6:M:393:LEU:HB3	2.01	0.42
1:C:222:HIS:CG	1:C:223:PRO:HA	2.54	0.42
6:B:102:GLN:H	6:B:102:GLN:HG3	1.55	0.42
1:N:320:PRO:HD2	3:R:31:TYR:CE1	2.53	0.42
3:R:76:ARG:HD3	3:R:80:PHE:CE2	2.55	0.42
5:L:432:GLU:HG3	5:L:433:HIS:N	2.34	0.42
11:C:501:HEM:HBB2	11:C:501:HEM:HMB1	2.01	0.42
2:P:196:ILE:H	2:P:196:ILE:HG12	1.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:267:GLU:OE1	5:A:462:TYR:HB2	2.19	0.42
6:B:170:TYR:CE2	6:M:236:ARG:HG2	2.55	0.42
6:M:53:VAL:HG12	6:M:173:VAL:HG13	2.02	0.42
5:L:334:PHE:CB	5:L:351:LEU:HD23	2.50	0.42
6:M:137:LEU:HD13	6:M:166:TYR:HB2	2.01	0.42
1:C:88:PHE:CD1	1:C:239:MET:HE3	2.55	0.42
1:C:367:LEU:HB3	1:C:368:PRO:HD3	2.00	0.42
10:J:11:LYS:HD2	10:J:12:PRO:HD2	2.02	0.42
2:P:103:VAL:HG22	2:P:120:TRP:CD1	2.55	0.42
2:P:147:ARG:HD2	2:P:206:PRO:HA	2.02	0.42
5:A:265:GLY:HA3	5:A:447:ASP:HB3	2.02	0.42
1:N:88:PHE:CD1	1:N:239:MET:HE3	2.55	0.42
1:N:226:SER:HB3	13:N:505:PTY:H321	2.02	0.42
18:O:401:HEC:HBA2	18:O:401:HEC:HHA	2.01	0.42
2:P:103:VAL:HG23	2:P:224:ILE:HD12	2.01	0.42
7:D:141:VAL:HG11	7:D:280:TRP:CE2	2.55	0.42
6:B:50:VAL:HG22	6:B:53:VAL:HB	2.00	0.42
7:D:326:ASN:OD1	2:E:40:LYS:HA	2.19	0.42
5:A:160:LYS:HD2	5:A:160:LYS:HA	1.87	0.41
6:B:269:MET:HE2	6:B:272:SER:OG	2.19	0.41
1:N:224:TYR:OH	5:L:463:ASN:HB2	2.20	0.41
1:C:320:PRO:HD2	3:G:31:TYR:CZ	2.55	0.41
9:I:37:ILE:HD13	9:I:37:ILE:HA	1.93	0.41
1:N:43:GLN:OE1	1:N:43:GLN:HA	2.20	0.41
6:M:47:TYR:HB3	6:M:220:VAL:CG1	2.51	0.41
6:B:100:LEU:HB2	6:B:103:ASP:OD2	2.19	0.41
7:D:104:MET:HE2	7:D:104:MET:HB3	1.84	0.41
1:N:224:TYR:HB3	7:O:315:TRP:CZ2	2.55	0.41
2:P:165:ILE:HG22	2:P:167:VAL:HG22	2.03	0.41
5:A:35:LEU:HG	5:A:41:ILE:HD11	2.03	0.41
5:L:99:MET:SD	5:L:126:SER:HB3	2.61	0.41
11:C:502:HEM:HBB2	11:C:502:HEM:HMB1	2.03	0.41
2:P:164:MET:SD	2:P:198:GLY:HA3	2.60	0.41
13:P:303:PTY:H141	13:P:303:PTY:H311	2.02	0.41
5:A:144:ILE:H	5:A:144:ILE:HG12	1.76	0.41
1:N:324:LEU:HD23	1:N:324:LEU:HA	1.88	0.41
5:L:176:MET:HE1	8:S:29:ILE:HG22	2.02	0.41
2:P:127:ILE:HG12	2:P:163:VAL:HG22	2.03	0.41
6:B:29:ASP:HB2	6:B:200:PRO:HD3	2.03	0.41
12:I:201:PC1:H143	12:I:201:PC1:H112	1.77	0.41
5:L:395:LEU:HD12	6:M:34:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:141:VAL:HG11	7:O:280:TRP:CE2	2.56	0.41
5:A:384:ARG:HG2	6:B:79:LEU:HD11	2.03	0.41
6:B:155:VAL:HG21	6:B:233:ALA:HB2	2.03	0.41
11:N:502:HEM:HBC2	11:N:502:HEM:CMC	2.51	0.41
13:N:505:PTY:H342	13:N:505:PTY:H311	1.40	0.41
13:P:303:PTY:H132	13:P:303:PTY:H161	1.84	0.40
13:N:505:PTY:H111	12:T:201:PC1:O31	2.21	0.40
2:P:213:GLU:H	2:P:213:GLU:HG3	1.52	0.40
1:N:320:PRO:HD2	3:R:31:TYR:CZ	2.57	0.40
7:O:218:LEU:HD11	18:O:401:HEC:CMB	2.51	0.40
7:D:105:LEU:HD21	7:D:294:LEU:HD13	2.04	0.40
7:D:327:PRO:HA	7:D:328:PRO:HD3	1.84	0.40
5:L:35:LEU:HG	5:L:41:ILE:HD11	2.03	0.40
5:L:78:HIS:HA	6:M:271:TRP:CD1	2.56	0.40
2:P:177:GLY:HA2	2:P:185:TRP:CD1	2.56	0.40
5:A:78:HIS:HA	6:B:271:TRP:CD1	2.56	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%)	375 (98%)	6 (2%)	0	100	100
1	N	381/385 (99%)	374 (98%)	7 (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%)	24	59
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	14 (4%)	0	100	100
6	M	400/417 (96%)	389 (97%)	11 (3%)	0	100	100
7	D	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
7	O	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
9	I	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
9	T	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
10	J	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
10	U	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
All	All	3955/4680 (84%)	3861 (98%)	93 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	183	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	331/333 (99%)	323 (98%)	8 (2%)	43	70
1	N	331/333 (99%)	323 (98%)	8 (2%)	43	70
2	E	49/182 (27%)	45 (92%)	4 (8%)	10	39
2	P	154/182 (85%)	135 (88%)	19 (12%)	4	22
3	G	113/117 (97%)	102 (90%)	11 (10%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	113/117 (97%)	108 (96%)	5 (4%)	25	59
4	F	61/123 (50%)	58 (95%)	3 (5%)	22	55
4	Q	61/123 (50%)	60 (98%)	1 (2%)	55	75
5	A	377/407 (93%)	363 (96%)	14 (4%)	30	63
5	L	377/407 (93%)	362 (96%)	15 (4%)	28	61
6	B	311/322 (97%)	294 (94%)	17 (6%)	19	52
6	M	311/322 (97%)	296 (95%)	15 (5%)	23	56
7	D	192/268 (72%)	191 (100%)	1 (0%)	81	85
7	O	192/268 (72%)	191 (100%)	1 (0%)	81	85
8	H	67/71 (94%)	66 (98%)	1 (2%)	57	76
8	S	67/71 (94%)	66 (98%)	1 (2%)	57	76
9	I	46/57 (81%)	46 (100%)	0	100	100
9	T	46/57 (81%)	46 (100%)	0	100	100
10	J	63/68 (93%)	62 (98%)	1 (2%)	55	75
10	U	63/68 (93%)	63 (100%)	0	100	100
All	All	3325/3896 (85%)	3200 (96%)	125 (4%)	30	62

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	109	PRO
1	C	157	LEU
1	C	178	ARG
1	C	197	HIS
1	C	198	LEU
1	C	288	LYS
1	C	324	LEU
1	C	369	MET
2	P	54	LYS
2	P	62	ARG
2	P	102	LYS
2	P	106	LYS
2	P	114	LYS
2	P	115	ASN
2	P	116	VAL
2	P	117	ILE
2	P	118	ILE

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Mol	Chain	Res	Type
2	P	119	LYS
2	P	131	THR
2	P	143	VAL
2	P	146	LEU
2	P	147	ARG
2	P	158	LYS
2	P	176	ILE
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	19	LEU
3	G	22	LYS
3	G	23	ILE
3	G	32	VAL
3	G	40	LEU
3	G	50	GLU
3	G	112	GLU
3	G	123	GLU
4	F	92	HIS
4	F	96	HIS
4	F	100	GLU
5	A	29	LYS
5	A	50	GLN
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	141	GLU
5	A	144	ILE
5	A	197	THR
5	A	230	GLU
5	A	267	GLU
5	A	390	LYS
5	A	397	LEU
6	B	19	GLU
6	B	45	SER
6	B	50	VAL
6	B	58	GLU

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Mol	Chain	Res	Type
6	B	60	PHE
6	B	77	LEU
6	B	79	LEU
6	B	84	LEU
6	B	102	GLN
6	B	215	GLN
6	B	247	LEU
6	B	249	ILE
6	B	261	SER
6	B	273	VAL
6	B	276	SER
6	B	345	LYS
6	B	362	ILE
7	D	193	GLN
8	H	51	ARG
10	J	11	LYS
1	N	109	PRO
1	N	178	ARG
1	N	197	HIS
1	N	198	LEU
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
3	R	17	SER
3	R	19	LEU
3	R	22	LYS
3	R	23	ILE
3	R	32	VAL
4	Q	100	GLU
5	L	29	LYS
5	L	48	LEU
5	L	50	GLN
5	L	51	THR
5	L	87	ARG
5	L	97	GLU
5	L	99	MET
5	L	144	ILE

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Mol	Chain	Res	Type
5	L	183	THR
5	L	185	LEU
5	L	292	GLU
5	L	378	SER
5	L	395	LEU
5	L	397	LEU
5	L	433	HIS
6	M	16	SER
6	M	19	GLU
6	M	32	SER
6	M	58	GLU
6	M	60	PHE
6	M	77	LEU
6	M	101	LYS
6	M	215	GLN
6	M	261	SER
6	M	273	VAL
6	M	331	GLU
6	M	345	LYS
6	M	356	ASP
6	M	362	ILE
6	M	376	GLU
7	O	193	GLN
8	S	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	ASN
1	C	177	GLN
1	C	202	HIS
1	C	332	ASN
2	P	90	ASN
2	P	129	HIS
2	P	157	GLN
2	P	193	HIS
3	G	54	ASN
3	G	84	HIS
4	F	92	HIS
4	F	97	HIS
4	F	109	GLN
5	A	159	ASN

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Mol	Chain	Res	Type
5	A	222	HIS
5	A	316	HIS
5	A	410	GLN
6	B	87	HIS
6	B	122	GLN
6	B	184	GLN
6	B	319	HIS
6	B	408	HIS
7	D	193	GLN
7	D	269	GLN
9	I	49	GLN
10	J	70	HIS
1	N	177	GLN
1	N	202	HIS
1	N	332	ASN
2	E	85	GLN
2	E	90	ASN
3	R	84	HIS
4	Q	97	HIS
4	Q	109	GLN
5	L	316	HIS
5	L	410	GLN
6	M	28	GLN
6	M	63	GLN
6	M	87	HIS
6	M	122	GLN
6	M	184	GLN
6	M	196	ASN
6	M	408	HIS
7	O	118	GLN
7	O	193	GLN
7	O	269	GLN
9	T	49	GLN
10	U	70	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PC1	I	201	-	31,31,53	0.36	0	37,39,61	0.62	0
14	CDL	L	3001	-	41,41,99	0.46	0	45,51,111	0.70	1 (2%)
14	CDL	N	506	-	47,47,99	0.53	0	53,59,111	1.00	4 (7%)
12	PC1	T	201	-	31,31,53	0.37	0	37,39,61	0.60	0
11	HEM	N	502	1	50,50,50	1.61	9 (18%)	66,82,82	2.48	24 (36%)
14	CDL	H	701	-	49,49,99	0.38	0	55,61,111	0.78	0
18	HEC	O	401	7	50,50,50	2.56	24 (48%)	68,82,82	2.90	35 (51%)
17	XP4	L	3003	-	23,23,39	1.47	2 (8%)	27,28,44	2.27	8 (29%)
14	CDL	C	505	-	47,47,99	0.48	0	53,59,111	0.95	3 (5%)
13	PTY	C	504	-	40,40,49	0.38	0	43,45,54	0.62	0
12	PC1	C	503	-	37,37,53	0.73	1 (2%)	43,45,61	1.14	5 (11%)
13	PTY	E	401	-	40,40,49	0.50	0	43,45,54	0.58	0
14	CDL	A	3001	-	41,41,99	0.54	0	45,51,111	0.72	1 (2%)
14	CDL	H	702	-	38,38,99	0.49	0	44,50,111	1.29	5 (11%)
18	HEC	D	401	7	50,50,50	2.54	24 (48%)	68,82,82	2.86	34 (50%)
13	PTY	N	505	-	40,40,49	0.37	0	43,45,54	0.71	1 (2%)
15	LMT	C	506	-	36,36,36	0.57	0	47,47,47	1.42	7 (14%)
14	CDL	L	3002	-	46,46,99	0.41	0	51,56,111	0.87	3 (5%)
15	LMT	P	302	-	36,36,36	0.50	0	47,47,47	1.08	6 (12%)
11	HEM	C	501	1	50,50,50	1.62	8 (16%)	66,82,82	2.22	22 (33%)
14	CDL	S	101	-	38,38,99	0.47	0	44,50,111	1.23	6 (13%)
11	HEM	C	502	1	50,50,50	1.47	8 (16%)	66,82,82	2.52	22 (33%)
16	FES	P	301	2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CDL	N	504	-	49,49,99	0.36	0	55,61,111	0.76	0
15	LMT	N	507	-	36,36,36	0.56	0	47,47,47	1.21	5 (10%)
14	CDL	A	3002	-	46,46,99	0.36	0	51,56,111	0.89	3 (5%)
12	PC1	N	503	-	37,37,53	0.71	1 (2%)	43,45,61	0.94	2 (4%)
15	LMT	J	101	-	36,36,36	0.55	0	47,47,47	1.19	4 (8%)
17	XP4	A	3003	-	23,23,39	1.52	2 (8%)	27,28,44	2.54	9 (33%)
13	PTY	P	303	-	40,40,49	0.50	0	43,45,54	0.67	1 (2%)
11	HEM	N	501	1	50,50,50	1.58	9 (18%)	66,82,82	2.23	29 (43%)

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	I	201	-	-	15/35/35/57	-
14	CDL	L	3001	-	-	22/48/48/110	-
14	CDL	N	506	-	-	31/57/57/110	-
12	PC1	T	201	-	-	13/35/35/57	-
11	HEM	N	502	1	-	4/14/54/54	-
14	CDL	H	701	-	-	34/59/59/110	-
18	HEC	O	401	7	1/1/3/7	10/14/54/54	-
17	XP4	L	3003	-	-	3/24/24/41	-
14	CDL	C	505	-	-	31/57/57/110	-
13	PTY	C	504	-	-	30/44/44/53	-
12	PC1	C	503	-	-	15/41/41/57	-
13	PTY	E	401	-	-	29/44/44/53	-
14	CDL	A	3001	-	-	16/48/48/110	-
14	CDL	H	702	-	-	28/48/48/110	-
18	HEC	D	401	7	1/1/3/7	8/14/54/54	-
13	PTY	N	505	-	-	28/44/44/53	-
15	LMT	C	506	-	-	15/21/61/61	0/2/2/2
14	CDL	L	3002	-	-	22/54/54/110	-
15	LMT	P	302	-	-	6/21/61/61	0/2/2/2
11	HEM	C	501	1	-	5/14/54/54	-
14	CDL	S	101	-	-	25/48/48/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	C	502	1	-	4/14/54/54	-
16	FES	P	301	2	-	-	0/1/1/1
14	CDL	N	504	-	-	40/59/59/110	-
15	LMT	N	507	-	-	12/21/61/61	0/2/2/2
14	CDL	A	3002	-	-	28/54/54/110	-
12	PC1	N	503	-	-	12/41/41/57	-
15	LMT	J	101	-	-	11/21/61/61	0/2/2/2
17	XP4	A	3003	-	-	1/24/24/41	-
13	PTY	P	303	-	-	26/44/44/53	-
11	HEM	N	501	1	-	5/14/54/54	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	401	HEC	C4B-NB	-6.31	1.29	1.40
18	D	401	HEC	C4B-NB	-5.81	1.30	1.40
17	A	3003	XP4	O7-C18	5.28	1.47	1.35
17	L	3003	XP4	O7-C18	5.18	1.46	1.35
18	O	401	HEC	C1D-ND	-4.69	1.32	1.40
18	O	401	HEC	C4C-NC	-4.39	1.31	1.39
11	C	502	HEM	FE-NB	4.37	2.08	1.94
18	D	401	HEC	C4A-NA	-4.35	1.31	1.39
11	N	502	HEM	FE-NB	4.35	2.08	1.94
18	D	401	HEC	C4C-NC	-4.15	1.31	1.39
11	N	501	HEM	FE-NB	4.13	2.07	1.94
17	A	3003	XP4	O5-C4	4.12	1.45	1.33
18	D	401	HEC	CHA-C1A	4.02	1.46	1.38
18	D	401	HEC	FE-ND	3.94	2.07	1.94
18	O	401	HEC	C4A-NA	-3.94	1.32	1.39
11	C	501	HEM	FE-NB	3.89	2.06	1.94
18	O	401	HEC	FE-ND	3.82	2.06	1.94
18	O	401	HEC	CHA-C1A	3.80	1.45	1.38
11	N	502	HEM	C1B-NB	-3.79	1.33	1.40
11	C	501	HEM	C4D-ND	-3.79	1.33	1.40
18	O	401	HEC	C3B-C2B	3.71	1.44	1.36
18	D	401	HEC	C1A-NA	-3.71	1.32	1.39
11	N	501	HEM	C1B-NB	-3.70	1.33	1.40
18	O	401	HEC	C1C-NC	-3.68	1.32	1.39
17	L	3003	XP4	O5-C4	3.68	1.44	1.33
11	C	501	HEM	C1B-NB	-3.68	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	401	HEC	C1B-NB	-3.66	1.31	1.38
18	D	401	HEC	C3B-C2B	3.60	1.44	1.36
11	N	501	HEM	C4B-NB	-3.60	1.31	1.38
18	D	401	HEC	C1D-ND	-3.59	1.34	1.40
18	D	401	HEC	C3D-C2D	3.58	1.44	1.36
18	O	401	HEC	CHA-C4D	3.54	1.47	1.39
18	D	401	HEC	CHB-C4A	3.48	1.45	1.38
11	N	501	HEM	FE-NC	3.47	2.06	1.95
18	D	401	HEC	C1B-NB	-3.46	1.31	1.38
11	N	502	HEM	C3C-C4C	-3.39	1.40	1.46
18	D	401	HEC	C1C-NC	-3.39	1.33	1.39
18	D	401	HEC	CHC-C4B	3.39	1.45	1.38
11	C	501	HEM	C4B-NB	-3.36	1.31	1.38
11	C	501	HEM	FE-NC	3.31	2.06	1.95
18	D	401	HEC	CHA-C4D	3.29	1.46	1.39
18	O	401	HEC	CHB-C4A	3.27	1.44	1.38
11	C	502	HEM	C1B-NB	-3.26	1.34	1.40
11	N	502	HEM	C4D-ND	-3.22	1.34	1.40
18	O	401	HEC	C3D-C2D	3.22	1.43	1.36
11	N	502	HEM	C4B-NB	-3.21	1.32	1.38
18	O	401	HEC	FE-NA	3.20	2.06	1.95
18	O	401	HEC	C1A-NA	-3.18	1.33	1.39
18	D	401	HEC	C2A-C3A	3.18	1.43	1.36
11	N	502	HEM	C1C-C2C	-3.14	1.39	1.45
18	D	401	HEC	CAB-C3B	-3.13	1.43	1.51
18	O	401	HEC	C2A-C3A	3.13	1.43	1.36
18	D	401	HEC	FE-NC	3.12	2.05	1.95
11	C	502	HEM	C3C-C4C	-3.10	1.40	1.46
11	C	501	HEM	C1C-NC	-3.09	1.33	1.39
18	D	401	HEC	CHD-C1D	3.08	1.44	1.38
18	O	401	HEC	C4D-ND	-3.07	1.32	1.38
18	O	401	HEC	FE-NC	3.06	2.05	1.95
18	O	401	HEC	CAB-C3B	-3.04	1.43	1.51
18	D	401	HEC	FE-NB	2.94	2.03	1.94
11	C	502	HEM	C1C-C2C	-2.93	1.39	1.45
11	C	502	HEM	FE-NC	2.83	2.04	1.95
18	O	401	HEC	CHD-C1D	2.82	1.44	1.38
11	N	501	HEM	C4D-ND	-2.82	1.35	1.40
18	D	401	HEC	C4D-ND	-2.79	1.33	1.38
18	O	401	HEC	FE-NB	2.77	2.03	1.94
18	D	401	HEC	FE-NA	2.74	2.04	1.95
11	N	501	HEM	C1C-NC	-2.73	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	401	HEC	CHC-C4B	2.70	1.44	1.38
11	C	502	HEM	C4D-ND	-2.68	1.35	1.40
18	D	401	HEC	CHD-C4C	2.61	1.45	1.39
11	N	502	HEM	FE-NC	2.57	2.03	1.95
11	N	502	HEM	FE-ND	-2.57	1.86	1.94
18	O	401	HEC	CHD-C4C	2.55	1.45	1.39
11	C	502	HEM	C4B-NB	-2.55	1.33	1.38
11	N	502	HEM	C4C-NC	-2.42	1.35	1.39
11	C	501	HEM	FE-ND	-2.40	1.87	1.94
11	C	502	HEM	FE-ND	-2.35	1.87	1.94
11	N	501	HEM	FE-ND	-2.31	1.87	1.94
12	C	503	PC1	C22-C21	2.29	1.57	1.50
18	O	401	HEC	C3C-C2C	2.22	1.44	1.38
11	N	501	HEM	O2D-CGD	-2.19	1.23	1.30
18	D	401	HEC	C3C-C2C	2.14	1.44	1.38
18	D	401	HEC	CHC-C1C	2.13	1.44	1.39
18	O	401	HEC	C4B-C3B	-2.10	1.41	1.45
11	N	501	HEM	C1D-C2D	2.06	1.48	1.44
11	C	501	HEM	C4A-NA	-2.03	1.35	1.39
12	N	503	PC1	C22-C21	2.02	1.56	1.50

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	502	HEM	CHD-C4C-NC	8.70	133.85	124.44
11	N	502	HEM	CHD-C4C-NC	8.60	133.74	124.44
18	O	401	HEC	C1B-C2B-C3B	-8.58	97.94	106.96
18	D	401	HEC	C1B-C2B-C3B	-8.50	98.02	106.96
17	A	3003	XP4	O7-C18-C19	8.06	125.91	111.09
11	C	502	HEM	CHC-C4B-NB	7.04	132.07	124.42
11	N	502	HEM	CHC-C4B-NB	6.86	131.88	124.42
18	O	401	HEC	CAA-CBA-CGA	-6.81	98.95	113.60
17	L	3003	XP4	O7-C18-C19	6.68	123.39	111.09
18	D	401	HEC	CAA-CBA-CGA	-6.36	99.91	113.60
18	D	401	HEC	C2B-C1B-NB	6.35	117.49	109.88
18	O	401	HEC	C1C-C2C-C3C	-6.32	99.44	106.83
11	C	501	HEM	CHC-C4B-NB	6.15	131.09	124.42
18	D	401	HEC	C1C-C2C-C3C	-6.12	99.67	106.83
11	N	501	HEM	CHC-C4B-NB	6.10	131.04	124.42
18	O	401	HEC	C2B-C1B-NB	5.99	117.06	109.88
18	O	401	HEC	CAA-C2A-C1A	5.93	136.07	124.89
18	D	401	HEC	CAA-C2A-C1A	5.88	135.97	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	502	HEM	C4C-NC-C1C	5.81	111.04	105.35
11	N	501	HEM	CHD-C1D-ND	5.50	130.39	124.42
11	C	502	HEM	CHD-C1D-ND	5.46	130.35	124.42
11	C	502	HEM	C4C-NC-C1C	5.43	110.67	105.35
18	D	401	HEC	C2D-C1D-ND	5.13	115.92	109.84
18	O	401	HEC	C2D-C1D-ND	5.06	115.84	109.84
11	C	502	HEM	C4C-CHD-C1D	-4.99	115.30	126.06
17	A	3003	XP4	O7-C18-O8	-4.81	113.42	122.96
11	C	501	HEM	CHD-C1D-ND	4.75	129.58	124.42
11	N	502	HEM	CHD-C1D-ND	4.72	129.55	124.42
18	D	401	HEC	C1D-C2D-C3D	-4.70	102.02	106.96
11	C	502	HEM	CHD-C1D-C2D	-4.61	117.78	124.98
11	C	502	HEM	C1B-NB-C4B	4.54	109.76	105.07
17	L	3003	XP4	O7-C18-O8	-4.43	114.15	122.96
11	C	502	HEM	CHA-C4D-ND	4.43	129.83	124.37
11	C	501	HEM	CAC-C3C-C4C	4.40	135.52	124.90
11	N	502	HEM	C4C-CHD-C1D	-4.29	116.79	126.06
11	C	501	HEM	CAD-CBD-CGD	-4.22	104.52	113.60
18	D	401	HEC	C3D-C4D-ND	4.22	114.44	110.36
18	O	401	HEC	C1D-C2D-C3D	-4.20	102.55	106.96
18	O	401	HEC	CAD-C3D-C4D	4.15	131.91	124.66
18	O	401	HEC	C2C-C1C-NC	4.12	116.35	110.08
11	N	502	HEM	C4C-C3C-C2C	4.12	110.13	106.75
17	L	3003	XP4	P1-O4-C1	4.10	129.59	118.30
11	C	501	HEM	C1B-NB-C4B	4.09	109.29	105.07
11	C	501	HEM	CBA-CAA-C2A	-4.03	101.43	112.63
11	N	502	HEM	CHD-C1D-C2D	-4.00	118.73	124.98
18	D	401	HEC	CMD-C2D-C1D	3.98	131.10	125.04
14	H	702	CDL	CB4-OB6-CB5	3.94	125.23	117.90
18	D	401	HEC	C2A-C1A-NA	3.92	114.14	110.32
11	N	501	HEM	CMC-C2C-C1C	3.91	131.60	124.71
14	S	101	CDL	CB4-OB6-CB5	3.88	125.13	117.90
11	C	501	HEM	CHD-C1D-C2D	-3.83	118.99	124.98
18	O	401	HEC	CMD-C2D-C1D	3.80	130.83	125.04
17	A	3003	XP4	P1-O4-C1	3.78	128.71	118.30
18	O	401	HEC	CBC-CAC-C3C	3.77	122.84	112.43
15	J	101	LMT	C1-O1'-C1'	-3.76	107.60	113.84
11	N	501	HEM	C1B-NB-C4B	3.76	108.95	105.07
11	N	501	HEM	CHD-C1D-C2D	-3.75	119.11	124.98
18	D	401	HEC	C2C-C1C-NC	3.75	115.79	110.08
18	O	401	HEC	CHB-C1B-C2B	-3.74	119.14	124.98
18	O	401	HEC	C2A-C1A-NA	3.73	113.96	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	503	PC1	O22-C21-C22	3.69	138.11	123.73
18	O	401	HEC	CAA-C2A-C3A	-3.67	121.04	127.88
15	C	506	LMT	O5'-C1'-C2'	3.67	118.11	110.35
18	D	401	HEC	CAB-C3B-C4B	-3.67	120.05	124.81
11	N	502	HEM	CBD-CAD-C3D	-3.66	102.45	112.63
15	C	506	LMT	C1'-O5'-C5'	3.65	120.86	113.69
17	A	3003	XP4	O1-P1-O4	3.57	116.24	106.73
11	C	501	HEM	C3B-C2B-C1B	-3.56	103.85	106.49
11	N	501	HEM	CBC-CAC-C3C	-3.53	110.08	127.62
18	D	401	HEC	C1A-C2A-C3A	-3.52	102.54	107.13
11	C	502	HEM	CBD-CAD-C3D	-3.51	102.88	112.63
18	O	401	HEC	CAB-C3B-C4B	-3.49	120.28	124.81
18	D	401	HEC	CAA-C2A-C3A	-3.49	121.38	127.88
11	N	501	HEM	CBA-CAA-C2A	-3.47	102.99	112.63
17	A	3003	XP4	O4-P1-O2	-3.44	96.81	106.47
18	O	401	HEC	CHC-C4B-C3B	-3.43	118.89	125.33
18	D	401	HEC	CMC-C2C-C1C	3.41	130.56	125.37
11	N	501	HEM	CAC-C3C-C4C	3.36	133.02	124.90
11	N	501	HEM	C3B-C2B-C1B	-3.32	104.02	106.49
18	D	401	HEC	CHB-C1B-C2B	-3.30	119.82	124.98
11	N	502	HEM	C1B-NB-C4B	3.30	108.48	105.07
18	O	401	HEC	C1A-C2A-C3A	-3.30	102.83	107.13
11	N	502	HEM	C1C-CHC-C4B	-3.28	118.98	126.06
11	N	501	HEM	CAD-CBD-CGD	-3.28	106.55	113.60
11	C	502	HEM	CHA-C4D-C3D	-3.27	119.18	125.33
14	H	702	CDL	OA5-PA1-OA3	-3.26	96.33	109.07
11	N	502	HEM	CHA-C4D-ND	3.25	128.39	124.37
18	O	401	HEC	C3D-C4D-ND	3.25	113.50	110.36
11	C	501	HEM	CBC-CAC-C3C	-3.24	111.52	127.62
11	N	502	HEM	O2A-CGA-O1A	-3.23	115.25	123.30
11	C	502	HEM	O2A-CGA-O1A	-3.23	115.26	123.30
15	J	101	LMT	C1'-O5'-C5'	-3.21	107.39	113.69
17	L	3003	XP4	O5-C4-O6	-3.20	115.53	123.59
11	N	501	HEM	C4A-NA-C1A	3.19	108.47	105.35
11	C	502	HEM	C1A-CHA-C4D	-3.19	118.77	126.34
12	C	503	PC1	O21-C21-C22	-3.18	104.65	111.50
15	C	506	LMT	O5B-C5B-C4B	3.18	115.46	109.69
11	C	502	HEM	C1C-CHC-C4B	-3.17	119.22	126.06
15	C	506	LMT	C1B-O5B-C5B	3.16	119.89	113.69
15	N	507	LMT	O5B-C5B-C4B	3.14	115.40	109.69
11	C	501	HEM	C4A-NA-C1A	3.14	108.43	105.35
18	O	401	HEC	CMC-C2C-C1C	3.08	130.06	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	O	401	HEC	C3B-C4B-NB	3.07	113.58	110.17
14	N	506	CDL	OB6-CB4-CB3	3.05	119.43	108.40
18	D	401	HEC	CAB-C3B-C2B	3.04	132.73	127.53
11	N	501	HEM	CHA-C4D-ND	3.03	128.12	124.37
18	D	401	HEC	C3B-C4B-NB	3.02	113.53	110.17
11	C	501	HEM	CAC-C3C-C2C	-3.01	118.68	128.60
17	A	3003	XP4	O5-C4-C5	2.99	121.30	111.91
11	N	501	HEM	C2A-C1A-NA	-2.99	106.81	110.15
11	C	501	HEM	CMC-C2C-C1C	2.98	129.97	124.71
11	C	501	HEM	CHA-C1A-NA	2.96	129.29	123.85
18	D	401	HEC	CBD-CAD-C3D	-2.96	104.41	112.63
11	N	501	HEM	CHA-C1A-NA	2.93	129.24	123.85
18	O	401	HEC	CMA-C3A-C4A	2.92	129.86	124.71
11	N	501	HEM	C1A-CHA-C4D	-2.92	119.42	126.34
17	A	3003	XP4	O5-C4-O6	-2.91	116.24	123.59
18	D	401	HEC	C3C-C4C-NC	2.91	113.39	110.15
18	O	401	HEC	C3C-C4C-NC	2.90	113.39	110.15
14	C	505	CDL	OB6-CB4-CB3	2.89	118.86	108.40
18	O	401	HEC	CAB-C3B-C2B	2.88	132.46	127.53
11	C	501	HEM	CHA-C4D-C3D	-2.88	119.93	125.33
11	C	502	HEM	CHD-C4C-C3C	-2.86	120.37	125.26
14	L	3001	CDL	OB6-CB4-CB3	-2.86	99.53	109.56
11	N	502	HEM	C3B-C2B-C1B	-2.86	104.37	106.49
11	C	501	HEM	C1A-CHA-C4D	-2.84	119.59	126.34
17	L	3003	XP4	O4-P1-O2	-2.84	98.50	106.47
11	N	502	HEM	CHC-C4B-C3B	-2.83	119.03	125.13
14	S	101	CDL	OB6-CB5-C51	2.83	116.30	111.09
15	N	507	LMT	C1B-O5B-C5B	2.81	119.20	113.69
15	C	506	LMT	C1-O1'-C1'	-2.80	109.20	113.84
18	D	401	HEC	CHC-C4B-C3B	-2.80	120.08	125.33
11	C	502	HEM	C4C-C3C-C2C	2.79	109.05	106.75
11	N	501	HEM	CHD-C4C-NC	2.79	127.45	124.44
11	N	501	HEM	CAC-C3C-C2C	-2.78	119.43	128.60
11	C	501	HEM	CHA-C4D-ND	2.77	127.79	124.37
15	P	302	LMT	O1'-C1'-C2'	2.76	112.62	108.30
18	D	401	HEC	CBB-CAB-C3B	2.76	120.03	112.43
18	O	401	HEC	CBD-CAD-C3D	-2.75	104.97	112.63
11	C	502	HEM	O2D-CGD-CBD	2.75	122.86	114.03
18	D	401	HEC	CBC-CAC-C3C	2.74	119.98	112.43
14	S	101	CDL	OA5-PA1-OA3	-2.73	98.39	109.07
14	H	702	CDL	OB6-CB4-CB6	2.72	118.24	108.40
11	N	502	HEM	C1A-CHA-C4D	-2.71	119.90	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	501	HEM	C4C-CHD-C1D	-2.70	120.23	126.06
12	C	503	PC1	O21-C21-O22	-2.70	117.18	123.70
14	A	3002	CDL	OA2-PA1-OA3	2.67	119.50	109.07
18	D	401	HEC	CMB-C2B-C3B	2.67	133.37	126.12
14	L	3002	CDL	OA5-PA1-OA3	-2.66	98.66	109.07
17	L	3003	XP4	O1-P1-O4	2.65	113.79	106.73
14	N	506	CDL	CB4-OB6-CB5	2.64	124.28	117.79
18	D	401	HEC	C3A-C4A-NA	2.64	114.55	109.69
14	S	101	CDL	OB6-CB4-CB6	2.63	117.91	108.40
14	H	702	CDL	OB6-CB5-C51	2.62	115.90	111.09
15	N	507	LMT	O1'-C1'-C2'	-2.60	104.25	108.30
18	O	401	HEC	CMB-C2B-C1B	2.58	128.97	125.04
14	L	3002	CDL	OA2-PA1-OA3	2.58	119.14	109.07
18	O	401	HEC	CMB-C2B-C3B	2.56	133.08	126.12
18	O	401	HEC	CHC-C4B-NB	2.55	127.52	124.37
12	N	503	PC1	O22-C21-C22	2.52	133.57	123.73
11	N	502	HEM	CHD-C4C-C3C	-2.52	120.95	125.26
18	O	401	HEC	CBB-CAB-C3B	2.51	119.36	112.43
11	N	501	HEM	CMC-C2C-C3C	-2.48	122.22	128.30
11	C	501	HEM	C2A-C1A-NA	-2.48	107.37	110.15
17	L	3003	XP4	O5-C4-C5	2.48	119.68	111.91
15	N	507	LMT	C3B-C4B-C5B	2.47	114.65	110.24
11	N	502	HEM	CMB-C2B-C1B	2.47	128.80	125.04
14	A	3002	CDL	OA5-PA1-OA3	-2.44	99.52	109.07
18	O	401	HEC	CAC-C3C-C2C	2.43	130.75	126.86
18	D	401	HEC	CAD-C3D-C4D	2.43	128.90	124.66
17	A	3003	XP4	O5-C3-C2	-2.42	101.39	108.43
11	C	502	HEM	CHB-C1B-NB	2.42	127.36	124.37
11	N	502	HEM	CHC-C1C-NC	2.42	127.05	124.44
12	C	503	PC1	C23-C22-C21	2.41	122.39	113.62
11	C	501	HEM	CMC-C2C-C3C	-2.40	122.41	128.30
14	A	3001	CDL	OB8-CB6-CB4	2.40	117.36	105.77
11	N	501	HEM	CHA-C4D-C3D	-2.39	120.85	125.33
18	D	401	HEC	C4A-C3A-C2A	-2.38	103.46	106.94
11	C	502	HEM	CHC-C4B-C3B	-2.38	120.01	125.13
18	O	401	HEC	C4D-C3D-C2D	-2.37	103.44	106.90
14	C	505	CDL	CB4-OB6-CB5	2.37	123.62	117.79
11	N	502	HEM	CHA-C4D-C3D	-2.37	120.89	125.33
11	N	501	HEM	O2D-CGD-O1D	-2.36	117.42	123.30
18	D	401	HEC	CMB-C2B-C1B	2.34	128.61	125.04
11	N	502	HEM	CHB-C1B-NB	2.34	127.26	124.37
18	O	401	HEC	CHC-C1C-C2C	-2.34	120.63	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	502	HEM	CAD-C3D-C4D	2.32	128.71	124.66
18	D	401	HEC	CHB-C4A-C3A	-2.32	120.62	125.48
17	A	3003	XP4	O7-C2-C3	-2.32	100.01	108.40
11	N	501	HEM	O2A-CGA-O1A	-2.31	117.53	123.30
11	C	502	HEM	CHA-C1A-NA	2.31	128.09	123.85
15	P	302	LMT	C4-C3-C2	-2.30	102.77	114.42
18	D	401	HEC	CHD-C4C-C3C	-2.29	120.35	125.36
15	P	302	LMT	O5B-C5B-C4B	2.27	113.82	109.69
18	O	401	HEC	CMC-C2C-C3C	2.26	130.50	125.61
11	N	501	HEM	CAA-C2A-C1A	2.26	129.34	124.89
11	N	502	HEM	O2D-CGD-CBD	2.26	121.29	114.03
14	H	702	CDL	OB6-CB4-CB3	2.24	116.52	108.40
11	N	502	HEM	C4A-NA-C1A	2.24	107.54	105.35
17	L	3003	XP4	O5-C3-C2	-2.22	101.97	108.43
11	N	502	HEM	CHA-C1A-NA	2.21	127.92	123.85
15	P	302	LMT	C4B-C3B-C2B	2.21	114.67	110.82
18	O	401	HEC	CHD-C1D-C2D	-2.20	120.62	126.73
15	C	506	LMT	O2'-C2'-C1'	-2.19	104.72	110.05
11	N	501	HEM	CBB-CAB-C3B	-2.17	116.80	127.62
18	D	401	HEC	CHC-C1C-C2C	-2.17	121.10	127.24
11	N	501	HEM	C4C-NC-C1C	2.16	107.47	105.35
14	C	505	CDL	OA6-CA5-C11	2.16	116.16	111.50
11	C	502	HEM	O1D-CGD-CBD	-2.16	116.14	123.08
11	N	501	HEM	CMB-C2B-C1B	2.16	128.33	125.04
11	N	501	HEM	CHC-C4B-C3B	-2.16	120.49	125.13
15	J	101	LMT	O2'-C2'-C1'	2.15	115.27	110.05
18	D	401	HEC	C4D-C3D-C2D	-2.14	103.77	106.90
12	N	503	PC1	C23-C22-C21	2.12	121.33	113.62
11	C	501	HEM	C4C-NC-C1C	2.11	107.41	105.35
11	C	501	HEM	CAA-C2A-C1A	2.11	129.04	124.89
15	P	302	LMT	C2'-C3'-C4'	2.11	114.49	109.68
18	D	401	HEC	CAD-CBD-CGD	-2.10	109.09	113.60
14	L	3002	CDL	OA6-CA4-CA6	2.09	115.98	108.40
14	N	506	CDL	OB6-CB5-OB7	-2.09	118.65	123.70
15	J	101	LMT	O5B-C5B-C4B	2.09	113.49	109.69
15	P	302	LMT	C1'-O5'-C5'	-2.08	109.60	113.69
15	C	506	LMT	O5'-C5'-C4'	2.08	114.14	109.75
13	N	505	PTY	O7-C8-C11	2.07	115.97	111.50
18	O	401	HEC	C3A-C4A-NA	2.07	113.51	109.69
15	N	507	LMT	C4B-C3B-C2B	2.07	114.43	110.82
12	C	503	PC1	O12-P-O14	2.06	122.42	112.24
14	S	101	CDL	OA4-PA1-OA3	2.05	122.39	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	303	PTY	O12-P1-O14	-2.05	98.24	107.75
14	A	3002	CDL	OA6-CA4-CA6	2.03	115.75	108.40
14	S	101	CDL	OB6-CB4-CB3	2.02	115.72	108.40
11	C	502	HEM	CAD-C3D-C4D	2.02	128.19	124.66
11	C	501	HEM	CHD-C4C-NC	2.02	126.62	124.44
18	D	401	HEC	CMA-C3A-C4A	2.01	128.26	124.71
11	N	501	HEM	CHB-C4A-NA	2.01	127.55	123.85
11	C	501	HEM	C4C-CHD-C1D	-2.01	121.71	126.06
11	N	501	HEM	O2A-CGA-CBA	2.01	120.48	114.03
11	C	502	HEM	CBB-CAB-C3B	-2.00	117.65	127.62
18	O	401	HEC	CHD-C4C-C3C	-2.00	120.98	125.36
14	N	506	CDL	OB6-CB5-C51	2.00	116.38	110.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	D	401	HEC	NA
18	O	401	HEC	NA

All (529) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	I	201	PC1	C11-O13-P-O14
12	I	201	PC1	C11-O13-P-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	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	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	CB2-C1-CA2-OA2
14	C	505	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
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-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	CA2-OA2-PA1-OA5
14	A	3002	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	CA2-OA2-PA1-OA4
14	H	702	CDL	CA2-OA2-PA1-OA5
14	H	702	CDL	OA9-CA7-OA8-CA6
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
14	N	504	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	CB2-C1-CA2-OA2
14	N	506	CDL	CA2-C1-CB2-OB2
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-OB2
14	N	506	CDL	CB3-OB5-PB2-OB4
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	S	101	CDL	CA2-OA2-PA1-OA4
14	S	101	CDL	CA2-OA2-PA1-OA5
14	S	101	CDL	C31-CA7-OA8-CA6
14	S	101	CDL	CB3-OB5-PB2-OB4
14	S	101	CDL	C51-CB5-OB6-CB4
15	P	302	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
15	J	101	LMT	C2-C1-O1'-C1'
14	H	702	CDL	OB9-CB7-OB8-CB6
14	S	101	CDL	OA9-CA7-OA8-CA6
14	S	101	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	CB4-CB6-OB8-CB7
14	H	702	CDL	C71-CB7-OB8-CB6
18	D	401	HEC	C4B-C3B-CAB-CBB
18	O	401	HEC	C4B-C3B-CAB-CBB
12	T	201	PC1	O32-C31-O31-C3
14	H	701	CDL	OB9-CB7-OB8-CB6
14	N	504	CDL	OB9-CB7-OB8-CB6
18	D	401	HEC	C4C-C3C-CAC-CBC
18	O	401	HEC	C4C-C3C-CAC-CBC
14	H	702	CDL	OB7-CB5-OB6-CB4
18	D	401	HEC	C2B-C3B-CAB-CBB
18	O	401	HEC	C2B-C3B-CAB-CBB
14	S	101	CDL	OB7-CB5-OB6-CB4
18	D	401	HEC	C2C-C3C-CAC-CBC
18	O	401	HEC	C2C-C3C-CAC-CBC
13	C	504	PTY	O10-C8-O7-C6
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	C71-CB7-OB8-CB6
14	S	101	CDL	C71-CB7-OB8-CB6
14	N	504	CDL	C51-CB5-OB6-CB4
14	H	701	CDL	OA9-CA7-OA8-CA6
14	L	3001	CDL	C31-CA7-OA8-CA6
14	A	3001	CDL	OA9-CA7-OA8-CA6
14	L	3001	CDL	OA9-CA7-OA8-CA6
14	L	3001	CDL	OB9-CB7-OB8-CB6
14	H	701	CDL	C31-CA7-OA8-CA6
14	A	3002	CDL	O1-C1-CB2-OB2
14	H	702	CDL	O1-C1-CA2-OA2
14	N	504	CDL	O1-C1-CA2-OA2
14	N	506	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
14	L	3002	CDL	O1-C1-CB2-OB2
13	P	303	PTY	C37-C38-C39-C40
14	A	3001	CDL	OB6-CB4-CB6-OB8
12	I	201	PC1	C32-C33-C34-C35
13	N	505	PTY	C31-C32-C33-C34
13	C	504	PTY	C31-C32-C33-C34
13	E	401	PTY	C13-C14-C15-C16
15	J	101	LMT	C2-C3-C4-C5
13	C	504	PTY	C35-C36-C37-C38
13	P	303	PTY	C35-C36-C37-C38
13	N	505	PTY	C33-C34-C35-C36
13	E	401	PTY	C35-C36-C37-C38
14	A	3001	CDL	C31-CA7-OA8-CA6
13	N	505	PTY	C37-C38-C39-C40
13	E	401	PTY	C40-C41-C42-C43
15	J	101	LMT	O5B-C5B-C6B-O6B
15	N	507	LMT	O5B-C5B-C6B-O6B
15	J	101	LMT	C4-C5-C6-C7
15	C	506	LMT	O5B-C5B-C6B-O6B
15	C	506	LMT	O5'-C5'-C6'-O6'
14	A	3002	CDL	C11-CA5-OA6-CA4
15	N	507	LMT	O5'-C5'-C6'-O6'
14	H	702	CDL	CB2-C1-CA2-OA2
14	H	702	CDL	CA2-C1-CB2-OB2
14	N	504	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	S	101	CDL	CB2-C1-CA2-OA2
14	S	101	CDL	CA2-C1-CB2-OB2
12	C	503	PC1	C32-C31-O31-C3
13	P	303	PTY	C31-C30-O4-C1
15	C	506	LMT	C4'-C5'-C6'-O6'
15	N	507	LMT	C4'-C5'-C6'-O6'
13	P	303	PTY	C33-C34-C35-C36
13	C	504	PTY	C16-C17-C18-C19
14	H	702	CDL	O1-C1-CB2-OB2
14	S	101	CDL	O1-C1-CA2-OA2
14	L	3002	CDL	CA7-C31-C32-C33
14	L	3002	CDL	C11-CA5-OA6-CA4
13	E	401	PTY	C30-C31-C32-C33
14	A	3001	CDL	CB7-C71-C72-C73
14	A	3002	CDL	CA7-C31-C32-C33
14	N	504	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	CB7-C71-C72-C73
13	P	303	PTY	C30-C31-C32-C33
13	N	505	PTY	C8-C11-C12-C13
14	C	505	CDL	CA7-C31-C32-C33
14	H	701	CDL	CA5-C11-C12-C13
14	H	701	CDL	CB7-C71-C72-C73
14	N	506	CDL	CA7-C31-C32-C33
12	I	201	PC1	C21-C22-C23-C24
12	T	201	PC1	C21-C22-C23-C24
12	T	201	PC1	C31-C32-C33-C34
12	C	503	PC1	O32-C31-O31-C3
13	P	303	PTY	O30-C30-O4-C1
14	N	504	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	L	3002	CDL	O1-C1-CA2-OA2
14	S	101	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	OA7-CA5-OA6-CA4
14	L	3002	CDL	OA7-CA5-OA6-CA4
12	N	503	PC1	C32-C31-O31-C3
13	E	401	PTY	C8-C11-C12-C13
14	L	3001	CDL	OB6-CB4-CB6-OB8
12	T	201	PC1	C11-O13-P-O11
13	C	504	PTY	C5-O14-P1-O11
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
14	A	3002	CDL	CB3-OB5-PB2-OB2
14	N	504	CDL	CA2-OA2-PA1-OA5
14	N	506	CDL	CB2-OB2-PB2-OB5
14	S	101	CDL	CB3-OB5-PB2-OB2
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	N	504	CDL	CB2-C1-CA2-OA2
14	L	3001	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-CA6
12	I	201	PC1	C31-C32-C33-C34
14	A	3002	CDL	C52-C53-C54-C55
14	H	701	CDL	C73-C74-C75-C76
15	P	302	LMT	C4-C5-C6-C7
15	N	507	LMT	C7-C8-C9-C10
13	P	303	PTY	C16-C17-C18-C19
13	N	505	PTY	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
13	E	401	PTY	C16-C17-C18-C19
14	N	504	CDL	C74-C75-C76-C77
12	N	503	PC1	O32-C31-O31-C3
13	E	401	PTY	O14-C5-C6-O7
13	P	303	PTY	C31-C32-C33-C34
14	A	3001	CDL	C71-C72-C73-C74
13	P	303	PTY	C13-C14-C15-C16
14	H	701	CDL	C71-C72-C73-C74
14	L	3001	CDL	CB7-C71-C72-C73
13	P	303	PTY	C40-C41-C42-C43
13	N	505	PTY	C16-C17-C18-C19
13	E	401	PTY	C38-C39-C40-C41
15	C	506	LMT	C4-C5-C6-C7
13	P	303	PTY	C34-C35-C36-C37
15	C	506	LMT	C5-C6-C7-C8
14	N	506	CDL	OB7-CB5-OB6-CB4
14	N	504	CDL	C71-C72-C73-C74
13	C	504	PTY	C8-C11-C12-C13
14	H	701	CDL	CB5-C51-C52-C53
13	E	401	PTY	C11-C12-C13-C14
13	E	401	PTY	C14-C15-C16-C17
14	H	701	CDL	C74-C75-C76-C77
13	C	504	PTY	C38-C39-C40-C41
14	A	3001	CDL	C73-C74-C75-C76
14	L	3001	CDL	C71-C72-C73-C74
14	L	3002	CDL	C12-C13-C14-C15
15	C	506	LMT	C6-C7-C8-C9
14	N	504	CDL	C73-C74-C75-C76
14	L	3001	CDL	C72-C73-C74-C75
14	L	3002	CDL	C11-C12-C13-C14
12	I	201	PC1	C32-C31-O31-C3
13	E	401	PTY	C31-C30-O4-C1
15	C	506	LMT	C3-C4-C5-C6
13	E	401	PTY	C31-C32-C33-C34
13	E	401	PTY	C12-C13-C14-C15
14	H	701	CDL	C51-CB5-OB6-CB4
14	N	506	CDL	C51-CB5-OB6-CB4
14	L	3002	CDL	CA5-C11-C12-C13
14	C	505	CDL	CA2-C1-CB2-OB2
14	C	505	CDL	OB7-CB5-OB6-CB4
15	N	507	LMT	C1-C2-C3-C4
12	C	503	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	C31-CA7-OA8-CA6
12	I	201	PC1	O32-C31-O31-C3
12	T	201	PC1	C33-C34-C35-C36
13	C	504	PTY	C37-C38-C39-C40
15	C	506	LMT	C11-C10-C9-C8
12	N	503	PC1	C28-C29-C2A-C2B
12	C	503	PC1	C27-C28-C29-C2A
13	E	401	PTY	C33-C34-C35-C36
12	N	503	PC1	C27-C28-C29-C2A
14	H	701	CDL	OB7-CB5-OB6-CB4
14	A	3002	CDL	C33-C34-C35-C36
13	P	303	PTY	C41-C42-C43-C44
13	N	505	PTY	C30-C31-C32-C33
13	P	303	PTY	C14-C15-C16-C17
14	C	505	CDL	C51-CB5-OB6-CB4
15	J	101	LMT	C4B-C5B-C6B-O6B
13	E	401	PTY	O30-C30-O4-C1
14	N	506	CDL	O1-C1-CB2-OB2
15	N	507	LMT	C4B-C5B-C6B-O6B
15	N	507	LMT	C2-C3-C4-C5
12	C	503	PC1	O21-C2-C3-O31
12	N	503	PC1	O21-C2-C3-O31
12	C	503	PC1	C26-C27-C28-C29
15	C	506	LMT	C1-C2-C3-C4
12	N	503	PC1	C33-C34-C35-C36
18	D	401	HEC	C1A-C2A-CAA-CBA
18	O	401	HEC	C1A-C2A-CAA-CBA
15	J	101	LMT	C7-C8-C9-C10
12	N	503	PC1	C26-C27-C28-C29
13	C	504	PTY	C39-C40-C41-C42
13	N	505	PTY	C14-C15-C16-C17
15	J	101	LMT	C1-C2-C3-C4
14	C	505	CDL	CA3-OA5-PA1-OA2
14	H	701	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	CA3-OA5-PA1-OA2
13	P	303	PTY	C11-C12-C13-C14
13	N	505	PTY	C34-C35-C36-C37
14	L	3002	CDL	OB5-CB3-CB4-OB6
13	N	505	PTY	O14-C5-C6-C1
13	P	303	PTY	C8-C11-C12-C13
13	N	505	PTY	C36-C37-C38-C39
15	N	507	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	H	701	CDL	C11-C12-C13-C14
14	L	3002	CDL	CB2-C1-CA2-OA2
13	C	504	PTY	C40-C41-C42-C43
15	J	101	LMT	C6-C7-C8-C9
13	N	505	PTY	O4-C1-C6-C5
14	N	504	CDL	CB3-CB4-CB6-OB8
12	I	201	PC1	C33-C34-C35-C36
13	N	505	PTY	C12-C13-C14-C15
14	C	505	CDL	C13-C14-C15-C16
14	N	504	CDL	OA9-CA7-OA8-CA6
12	I	201	PC1	C34-C35-C36-C37
15	N	507	LMT	C9-C10-C11-C12
13	P	303	PTY	C38-C39-C40-C41
13	N	505	PTY	C41-C42-C43-C44
15	J	101	LMT	C9-C10-C11-C12
14	L	3002	CDL	C34-C35-C36-C37
15	J	101	LMT	O1'-C1-C2-C3
13	C	504	PTY	C41-C42-C43-C44
13	E	401	PTY	C41-C42-C43-C44
15	J	101	LMT	C3-C4-C5-C6
13	N	505	PTY	C17-C18-C19-C20
15	P	302	LMT	C3-C4-C5-C6
14	N	504	CDL	C75-C76-C77-C78
14	H	701	CDL	C75-C76-C77-C78
13	C	504	PTY	C14-C15-C16-C17
14	A	3002	CDL	C12-C13-C14-C15
14	A	3002	CDL	C34-C35-C36-C37
14	N	504	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	O1-C1-CA2-OA2
15	C	506	LMT	C4B-C5B-C6B-O6B
15	N	507	LMT	C3-C4-C5-C6
13	C	504	PTY	C13-C14-C15-C16
14	C	505	CDL	C11-C12-C13-C14
14	H	701	CDL	OA7-CA5-OA6-CA4
18	D	401	HEC	C3A-C2A-CAA-CBA
18	O	401	HEC	C3A-C2A-CAA-CBA
14	A	3002	CDL	C51-CB5-OB6-CB4
14	N	506	CDL	C13-C14-C15-C16
15	C	506	LMT	C7-C8-C9-C10
15	C	506	LMT	C9-C10-C11-C12
14	H	701	CDL	C11-CA5-OA6-CA4
14	L	3001	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
14	N	506	CDL	C11-C12-C13-C14
13	E	401	PTY	C32-C33-C34-C35
14	N	504	CDL	OB5-CB3-CB4-CB6
14	S	101	CDL	OB5-CB3-CB4-CB6
13	C	504	PTY	C30-C31-C32-C33
14	C	505	CDL	CA5-C11-C12-C13
14	L	3001	CDL	C73-C74-C75-C76
12	I	201	PC1	C22-C23-C24-C25
11	C	501	HEM	C3D-CAD-CBD-CGD
15	P	302	LMT	C7-C8-C9-C10
14	H	701	CDL	CB3-CB4-CB6-OB8
14	N	504	CDL	CA3-CA4-CA6-OA8
13	N	505	PTY	C38-C39-C40-C41
14	A	3001	CDL	CB3-OB5-PB2-OB2
13	C	504	PTY	C17-C18-C19-C20
13	E	401	PTY	C36-C37-C38-C39
13	N	505	PTY	O4-C1-C6-O7
14	H	702	CDL	OB6-CB4-CB6-OB8
14	N	504	CDL	OA6-CA4-CA6-OA8
14	S	101	CDL	OB6-CB4-CB6-OB8
12	N	503	PC1	C22-C23-C24-C25
14	L	3001	CDL	CB2-C1-CA2-OA2
13	C	504	PTY	C32-C33-C34-C35
15	N	507	LMT	C6-C7-C8-C9
12	C	503	PC1	C22-C23-C24-C25
13	E	401	PTY	O14-C5-C6-C1
14	A	3002	CDL	OA5-CA3-CA4-CA6
14	H	701	CDL	OA5-CA3-CA4-CA6
14	H	701	CDL	OB5-CB3-CB4-CB6
14	H	702	CDL	OA5-CA3-CA4-CA6
14	N	504	CDL	OA5-CA3-CA4-CA6
14	L	3002	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	OA5-CA3-CA4-CA6
14	C	505	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	CA6-CA4-OA6-CA5
14	H	702	CDL	CB6-CB4-OB6-CB5
14	L	3002	CDL	CA6-CA4-OA6-CA5
13	C	504	PTY	O4-C1-C6-C5
14	H	701	CDL	CA3-CA4-CA6-OA8
14	N	506	CDL	CA4-CA3-OA5-PA1
14	S	101	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
13	N	505	PTY	O14-C5-C6-O7
14	H	701	CDL	OA5-CA3-CA4-OA6
14	N	504	CDL	OB5-CB3-CB4-OB6
14	N	506	CDL	OA5-CA3-CA4-OA6
15	N	507	LMT	C11-C10-C9-C8
17	L	3003	XP4	C5-C6-C7-C8
14	A	3002	CDL	O1-C1-CA2-OA2
14	C	505	CDL	OB6-CB4-CB6-OB8
14	H	701	CDL	OA6-CA4-CA6-OA8
14	N	504	CDL	OB6-CB4-CB6-OB8
14	N	504	CDL	C51-C52-C53-C54
15	P	302	LMT	O1'-C1-C2-C3
13	C	504	PTY	C3-O11-P1-O14
14	N	504	CDL	CB3-OB5-PB2-OB2
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	C	505	CDL	CA4-CA3-OA5-PA1
13	C	504	PTY	C5-O14-P1-O12
13	C	504	PTY	C5-O14-P1-O13
13	P	303	PTY	C5-O14-P1-O13
13	N	505	PTY	C5-O14-P1-O12
14	C	505	CDL	CA3-OA5-PA1-OA4
14	C	505	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	CB3-OB5-PB2-OB4
14	H	701	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB3-OB5-PB2-OB3
14	N	504	CDL	CA2-OA2-PA1-OA3
14	N	504	CDL	CB3-OB5-PB2-OB4
14	N	506	CDL	CA3-OA5-PA1-OA4
14	S	101	CDL	CB3-OB5-PB2-OB3
13	C	504	PTY	O14-C5-C6-C1
14	H	702	CDL	OB5-CB3-CB4-CB6
14	C	505	CDL	C32-C33-C34-C35
13	C	504	PTY	O14-C5-C6-O7
13	P	303	PTY	O14-C5-C6-O7
14	C	505	CDL	OA5-CA3-CA4-OA6
14	H	701	CDL	OB5-CB3-CB4-OB6
14	H	702	CDL	OA5-CA3-CA4-OA6
14	S	101	CDL	OA5-CA3-CA4-OA6
14	N	506	CDL	CA5-C11-C12-C13
12	T	201	PC1	C1-C2-C3-O31
13	C	504	PTY	O4-C1-C6-O7
14	H	701	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
14	N	506	CDL	C32-C33-C34-C35
14	L	3002	CDL	C33-C34-C35-C36
14	A	3001	CDL	C32-C33-C34-C35
14	H	701	CDL	C72-C73-C74-C75
14	S	101	CDL	CB6-CB4-OB6-CB5
15	C	506	LMT	O1'-C1-C2-C3
13	C	504	PTY	C6-C5-O14-P1
14	L	3002	CDL	C51-CB5-OB6-CB4
14	H	702	CDL	OB5-CB3-CB4-OB6
14	S	101	CDL	OB5-CB3-CB4-OB6
11	N	501	HEM	C3D-CAD-CBD-CGD
15	P	302	LMT	C6-C7-C8-C9
15	C	506	LMT	C2'-C1'-O1'-C1
13	P	303	PTY	C3-O11-P1-O14
13	E	401	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	S	101	CDL	CB2-OB2-PB2-OB5
12	C	503	PC1	C1-C2-C3-O31
12	N	503	PC1	C1-C2-C3-O31
14	H	702	CDL	CB3-CB4-CB6-OB8
12	T	201	PC1	C11-C12-N-C14
12	N	503	PC1	O22-C21-O21-C2
14	N	506	CDL	C31-C32-C33-C34
13	C	504	PTY	C31-C30-O4-C1
14	H	702	CDL	CB4-CB3-OB5-PB2
14	S	101	CDL	CB4-CB3-OB5-PB2
14	A	3002	CDL	CB2-C1-CA2-OA2
11	C	502	HEM	CAD-CBD-CGD-O2D
13	C	504	PTY	O30-C30-O4-C1
11	N	502	HEM	CAD-CBD-CGD-O2D
17	A	3003	XP4	O4-C1-C2-O7
11	C	502	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAA-CBA-CGA-O1A
14	N	504	CDL	C72-C73-C74-C75
11	C	501	HEM	CAA-CBA-CGA-O1A
14	H	702	CDL	CA3-CA4-CA6-OA8
11	C	502	HEM	CAA-CBA-CGA-O2A
14	L	3002	CDL	OB7-CB5-OB6-CB4
14	H	701	CDL	O1-C1-CB2-OB2
14	A	3002	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
11	N	502	HEM	CAA-CBA-CGA-O1A
14	N	504	CDL	CA3-CA4-OA6-CA5
14	N	504	CDL	CA6-CA4-OA6-CA5
12	C	503	PC1	C11-C12-N-C15
14	L	3002	CDL	C31-C32-C33-C34
11	C	502	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAA-CBA-CGA-O2A
11	N	502	HEM	CAD-CBD-CGD-O1D
14	N	504	CDL	C11-C12-C13-C14
14	H	701	CDL	C51-C52-C53-C54
11	C	501	HEM	CAA-CBA-CGA-O2A
11	N	501	HEM	CAA-CBA-CGA-O2A
14	C	505	CDL	C31-C32-C33-C34
13	P	303	PTY	C12-C13-C14-C15
14	N	504	CDL	CB5-C51-C52-C53
14	N	504	CDL	OA7-CA5-OA6-CA4
14	A	3002	CDL	CA5-C11-C12-C13
14	A	3002	CDL	C11-C12-C13-C14
14	A	3001	CDL	OB5-CB3-CB4-CB6
14	H	701	CDL	CA2-C1-CB2-OB2
13	N	505	PTY	O30-C30-O4-C1
15	C	506	LMT	C2-C3-C4-C5
18	O	401	HEC	CAA-CBA-CGA-O1A
13	E	401	PTY	C39-C40-C41-C42
18	O	401	HEC	CAA-CBA-CGA-O2A
18	D	401	HEC	CAA-CBA-CGA-O2A
14	N	506	CDL	OA5-CA3-CA4-CA6
14	N	506	CDL	OB6-CB4-CB6-OB8
18	D	401	HEC	CAA-CBA-CGA-O1A
14	H	701	CDL	C72-C71-CB7-OB8
14	N	504	CDL	CB2-OB2-PB2-OB5
12	C	503	PC1	C11-C12-N-C13
12	C	503	PC1	C11-C12-N-C14
14	H	702	CDL	C32-C31-CA7-OA9
14	C	505	CDL	C32-C31-CA7-OA8
14	N	506	CDL	C32-C31-CA7-OA8
11	N	501	HEM	CAD-CBD-CGD-O2D
13	P	303	PTY	O4-C30-C31-C32
14	N	504	CDL	C72-C71-CB7-OB8
12	I	201	PC1	O21-C21-C22-C23
12	N	503	PC1	O31-C31-C32-C33
13	P	303	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	OA5-CA3-CA4-CA6
12	I	201	PC1	O21-C2-C3-O31
14	A	3002	CDL	OA6-CA4-CA6-OA8
13	N	505	PTY	C31-C30-O4-C1
11	C	501	HEM	CAD-CBD-CGD-O2D
18	O	401	HEC	CAD-CBD-CGD-O1D
12	C	503	PC1	O31-C31-C32-C33
14	A	3001	CDL	C72-C71-CB7-OB8
14	A	3001	CDL	C33-C34-C35-C36
12	I	201	PC1	C22-C21-O21-C2
11	N	501	HEM	CAD-CBD-CGD-O1D
13	C	504	PTY	C36-C37-C38-C39
14	A	3001	CDL	C72-C73-C74-C75
12	C	503	PC1	C21-C22-C23-C24
13	P	303	PTY	O30-C30-C31-C32
14	H	701	CDL	C72-C71-CB7-OB9
14	N	504	CDL	C72-C71-CB7-OB9
11	C	501	HEM	CAD-CBD-CGD-O1D
12	T	201	PC1	C11-C12-N-C15
13	P	303	PTY	C3-O11-P1-O12
14	C	505	CDL	CA2-OA2-PA1-OA3
14	A	3002	CDL	CB2-OB2-PB2-OB3
14	H	702	CDL	CB2-OB2-PB2-OB3
14	N	506	CDL	CA2-OA2-PA1-OA3
14	N	506	CDL	CB3-OB5-PB2-OB3
14	S	101	CDL	CB2-OB2-PB2-OB3
12	I	201	PC1	O22-C21-C22-C23
12	N	503	PC1	O32-C31-C32-C33
14	C	505	CDL	C32-C31-CA7-OA9
14	N	506	CDL	C32-C31-CA7-OA9
12	C	503	PC1	O22-C21-O21-C2
13	E	401	PTY	C34-C35-C36-C37
12	T	201	PC1	C12-C11-O13-P
13	E	401	PTY	C2-C3-O11-P1
14	C	505	CDL	CB6-CB4-OB6-CB5
14	H	701	CDL	CA3-CA4-OA6-CA5
14	N	506	CDL	CB6-CB4-OB6-CB5
13	E	401	PTY	O4-C30-C31-C32
18	O	401	HEC	CAD-CBD-CGD-O2D
12	T	201	PC1	C11-C12-N-C13
12	C	503	PC1	O32-C31-C32-C33
14	L	3001	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
17	L	3003	XP4	C2-C1-O4-P1
17	L	3003	XP4	O4-C1-C2-O7
14	L	3001	CDL	C72-C71-CB7-OB8
14	H	702	CDL	C32-C31-CA7-OA8
13	E	401	PTY	O30-C30-C31-C32

There are no ring outliers.

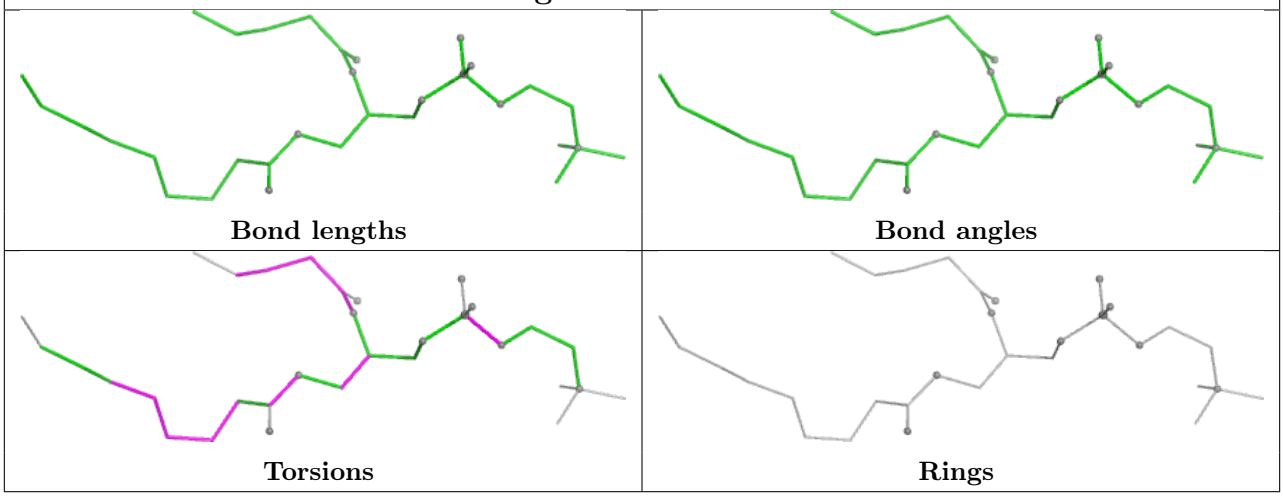
22 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	201	PC1	2	0
14	L	3001	CDL	1	0
12	T	201	PC1	2	0
11	N	502	HEM	2	0
18	O	401	HEC	13	0
17	L	3003	XP4	2	0
13	C	504	PTY	4	0
12	C	503	PC1	2	0
13	E	401	PTY	2	0
14	A	3001	CDL	2	0
14	H	702	CDL	3	0
18	D	401	HEC	15	0
13	N	505	PTY	9	0
14	L	3002	CDL	1	0
11	C	501	HEM	5	0
14	S	101	CDL	4	0
11	C	502	HEM	3	0
14	A	3002	CDL	2	0
12	N	503	PC1	3	0
15	J	101	LMT	2	0
13	P	303	PTY	12	0
11	N	501	HEM	6	0

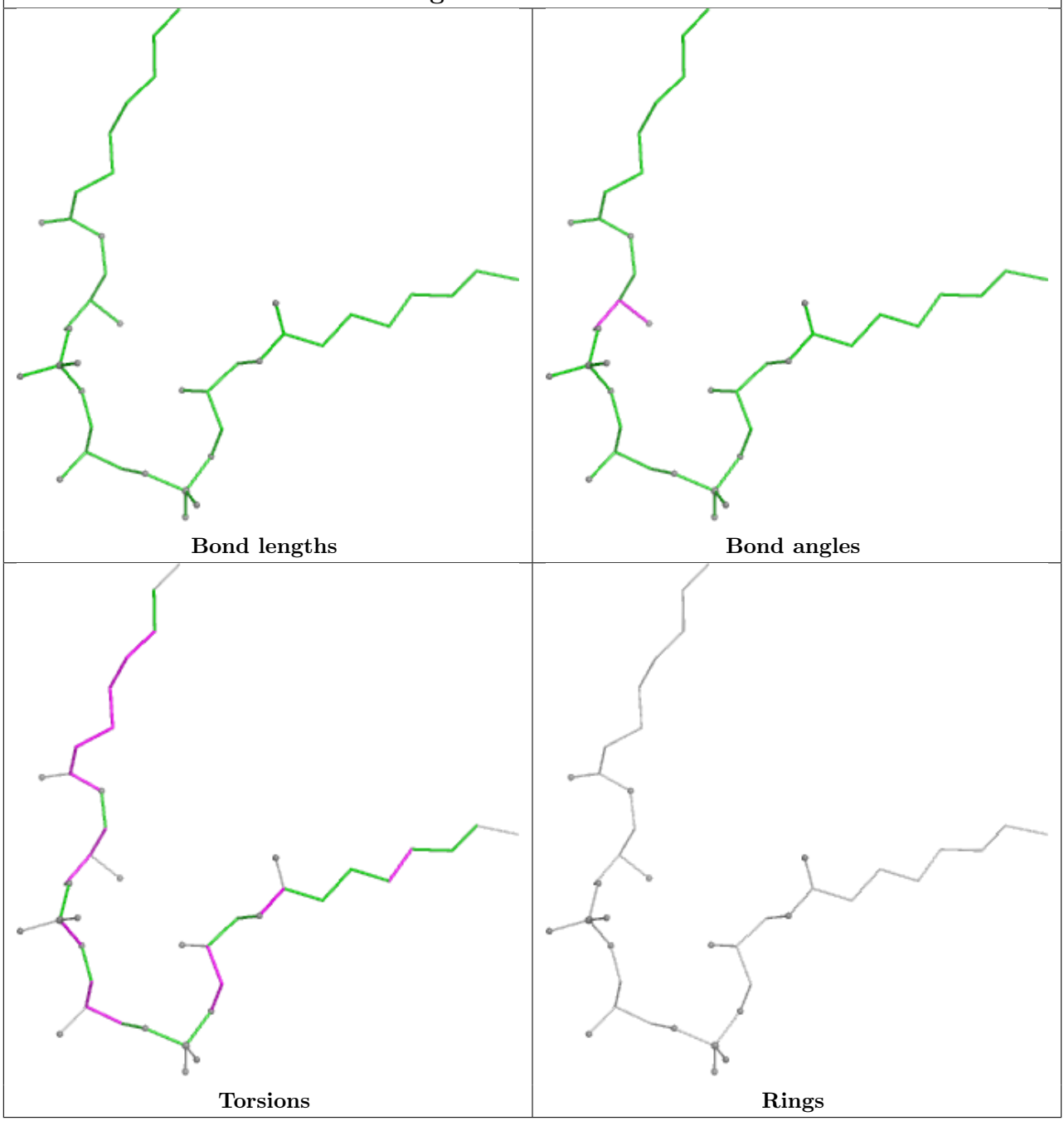
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 I 201



Ligand CDL L 3001



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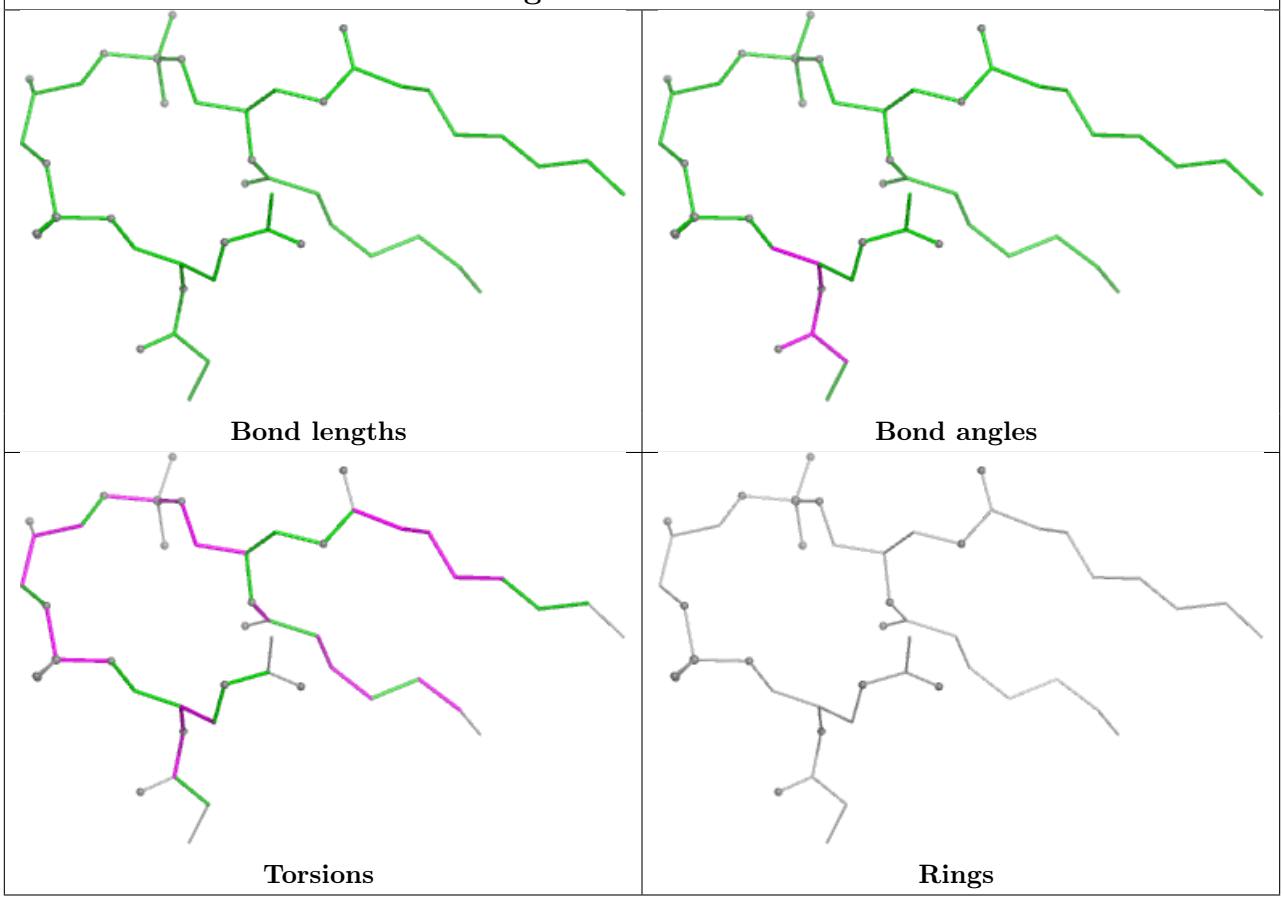
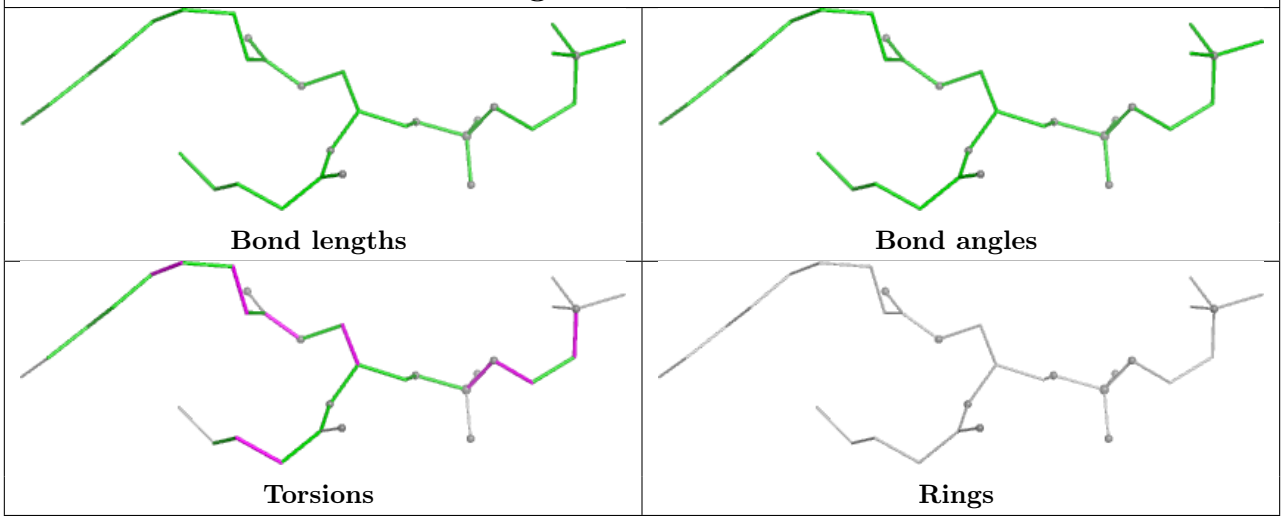
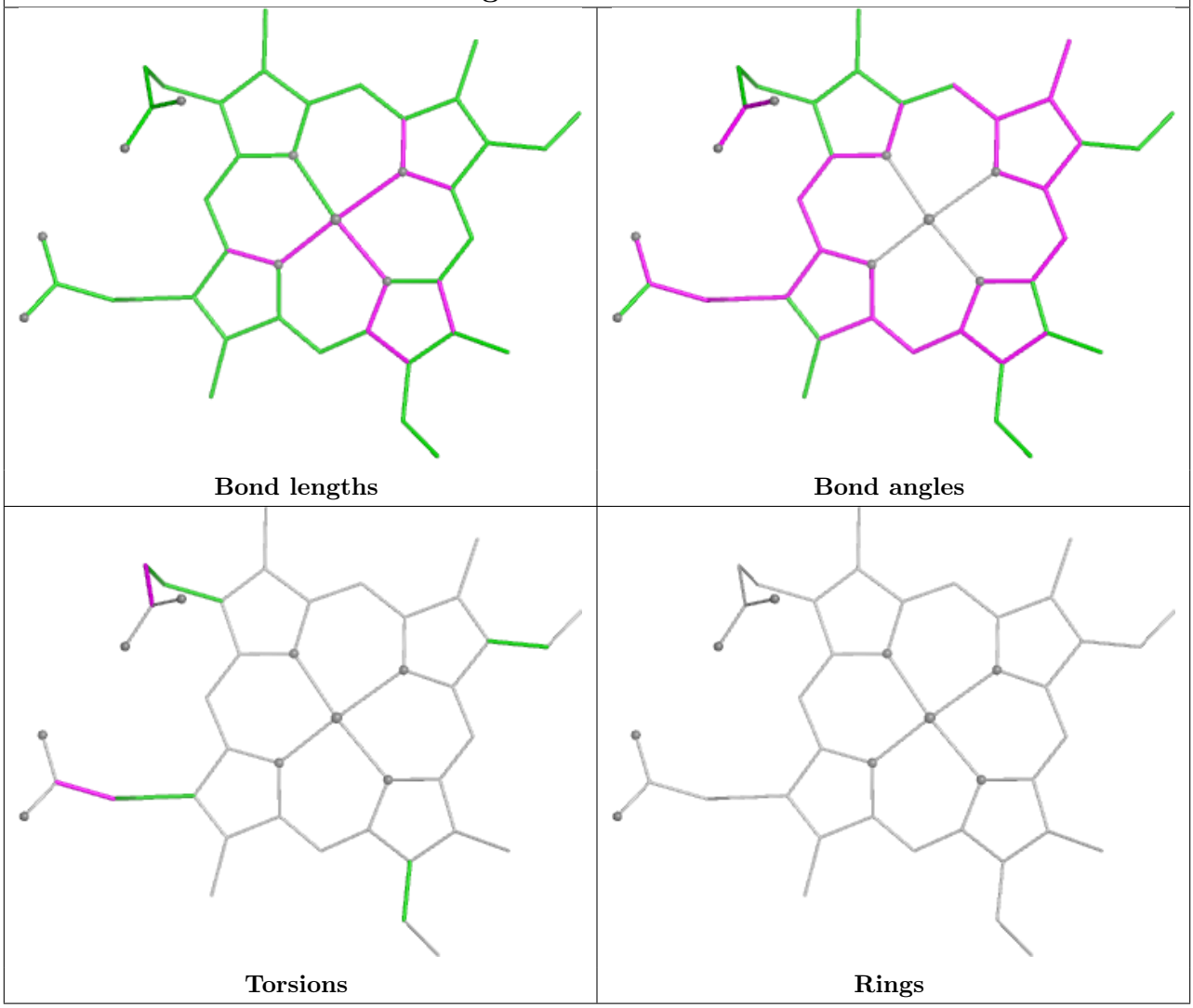


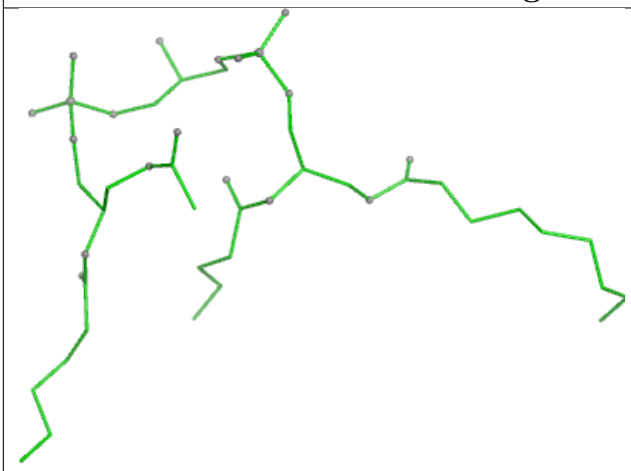
Ligand PC1 T 201



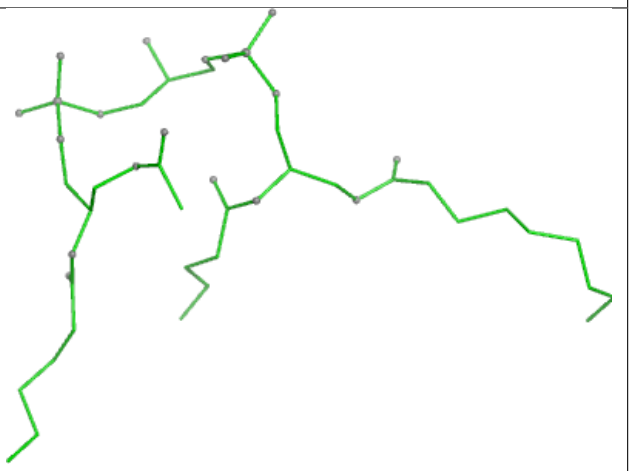
Ligand HEM N 502



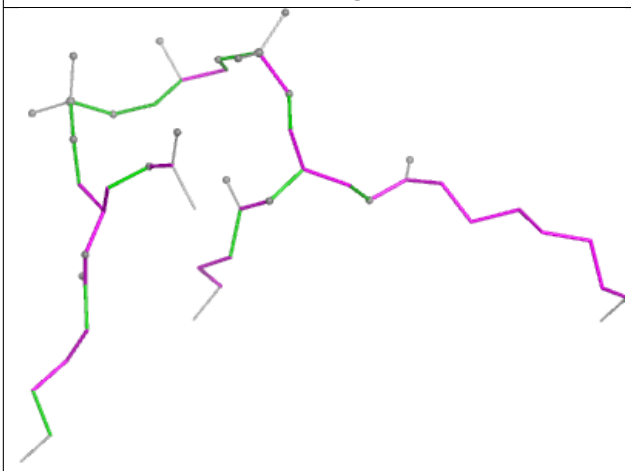
Ligand CDL H 701



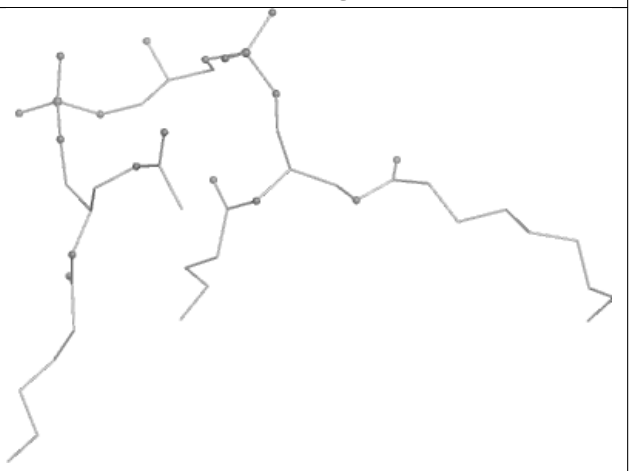
Bond lengths



Bond angles

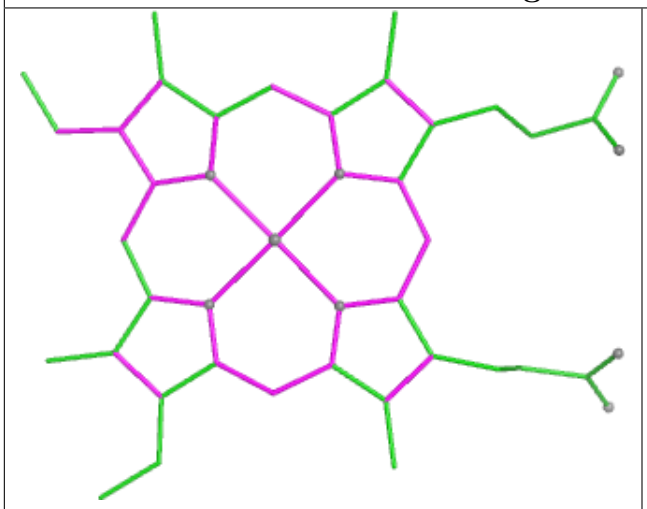


Torsions

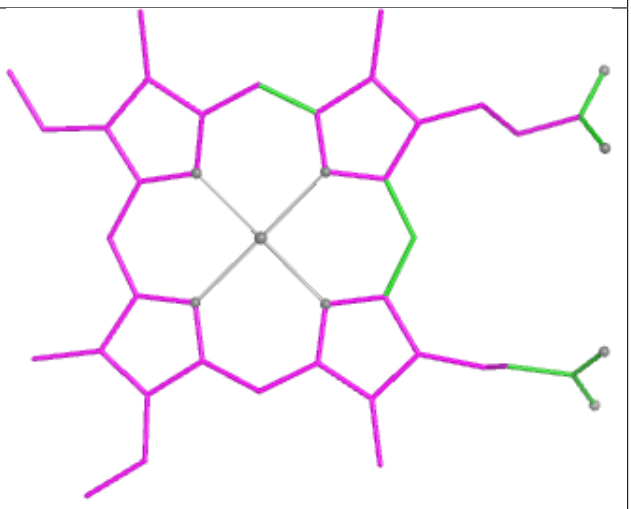


Rings

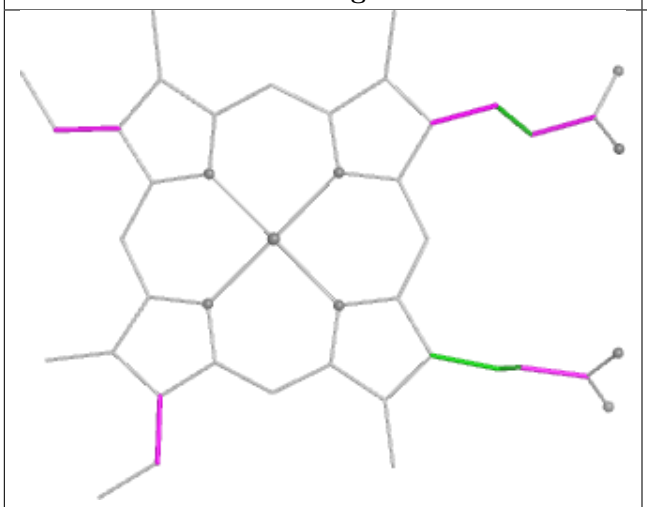
Ligand HEC O 401



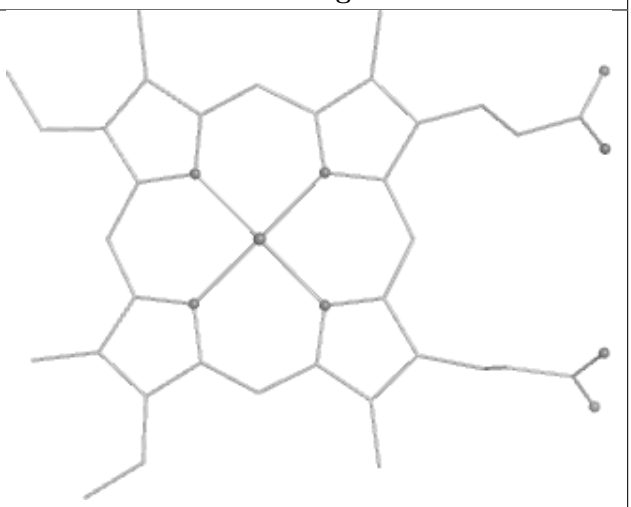
Bond lengths



Bond angles

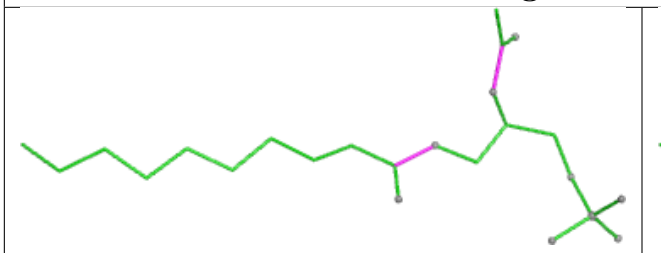


Torsions



Rings

Ligand XP4 L 3003



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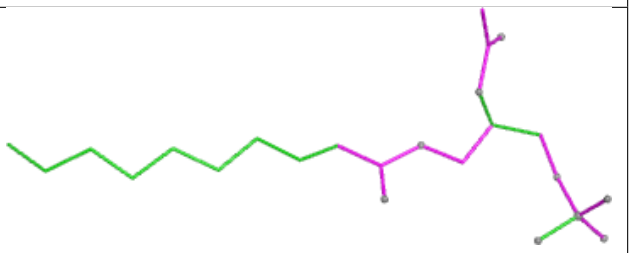
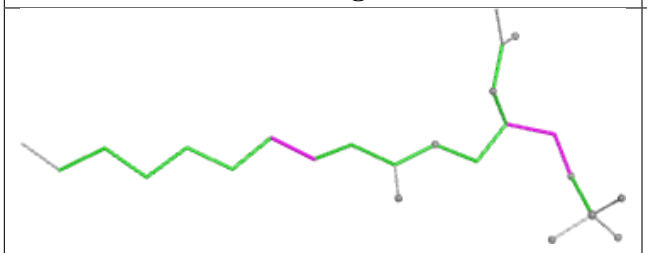


Bond angles



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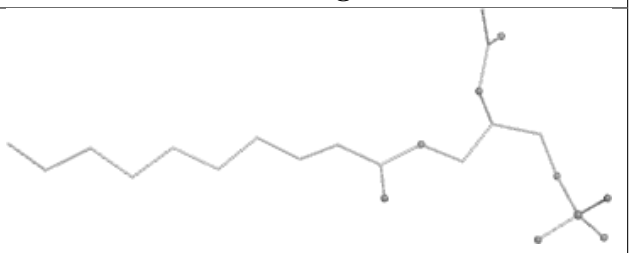
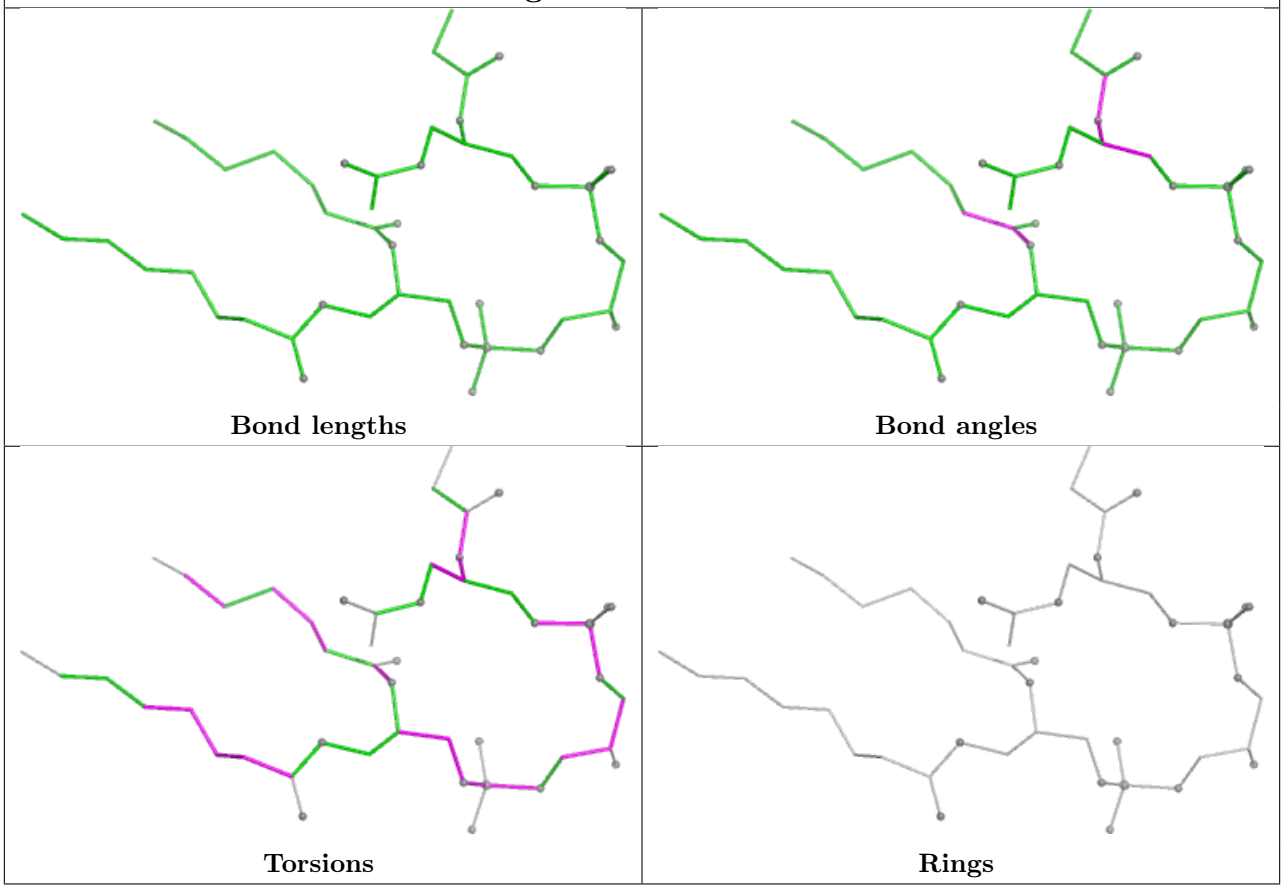
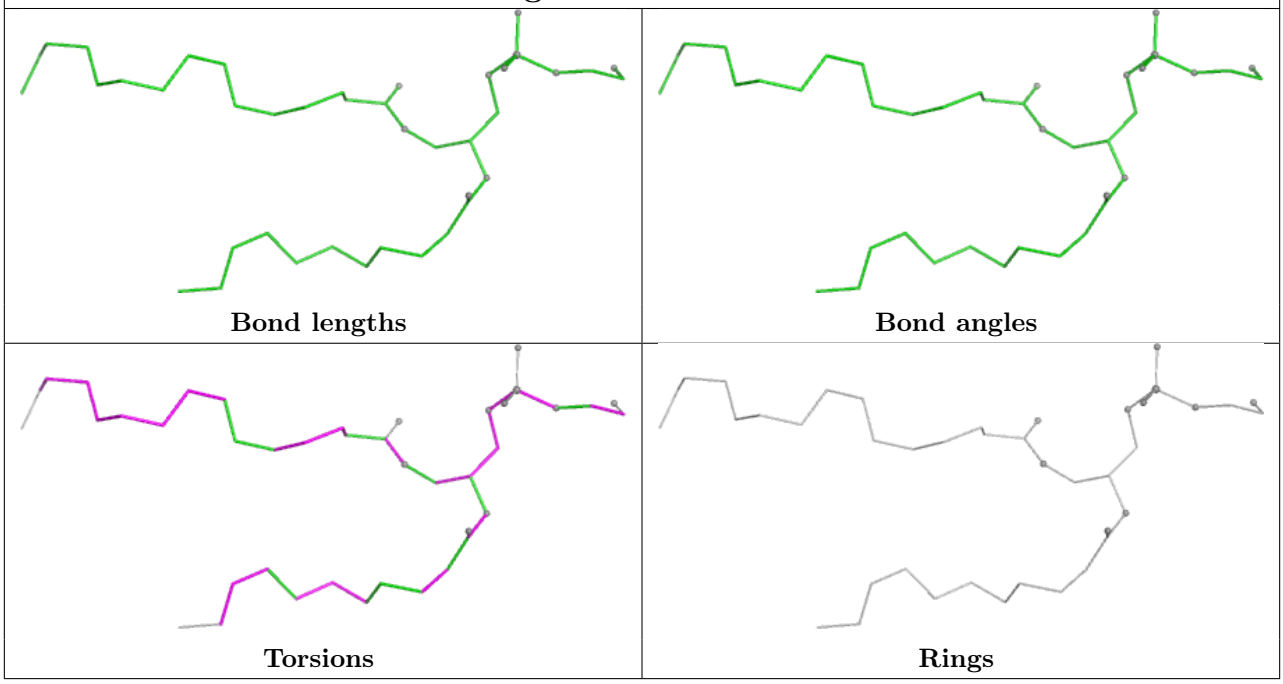


Rings

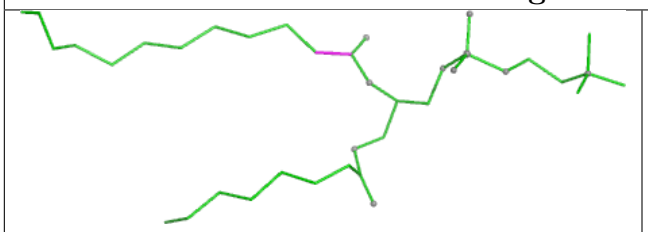
Ligand CDL C 505



Ligand PTY C 504



Ligand PC1 C 503



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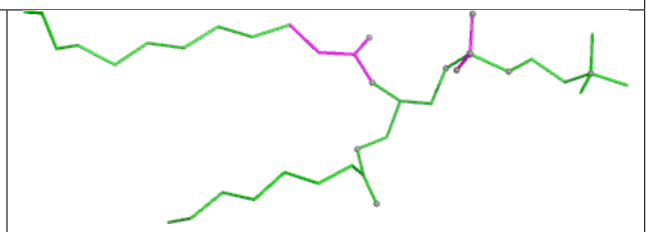
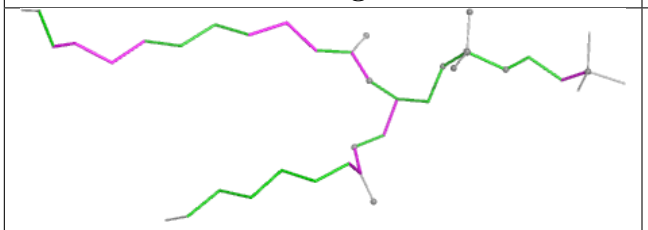


Bond angles



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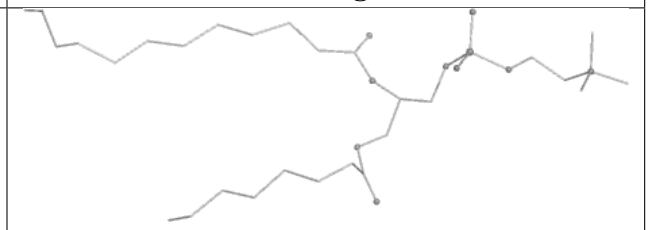
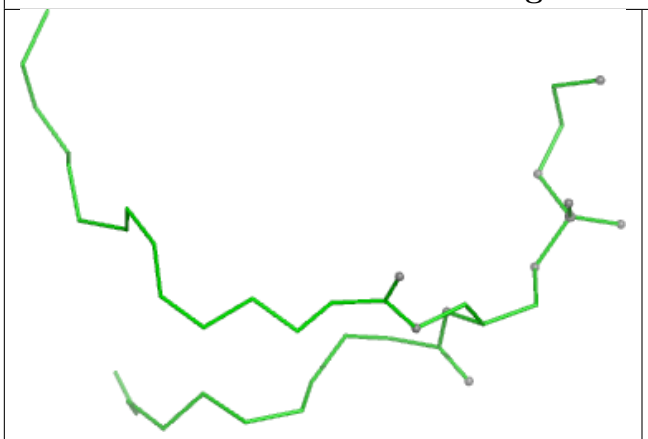


Rings

Ligand PTY E 401



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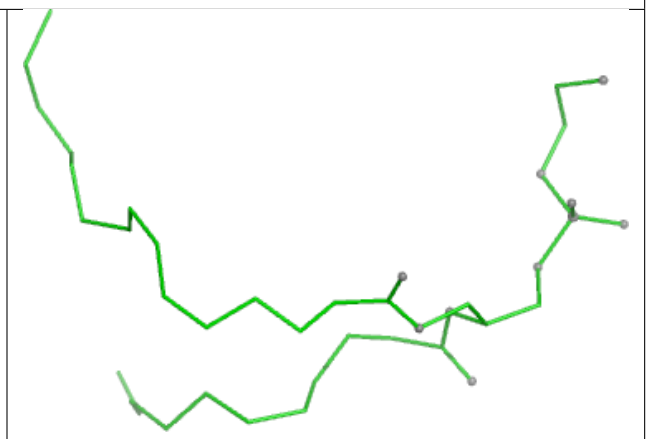

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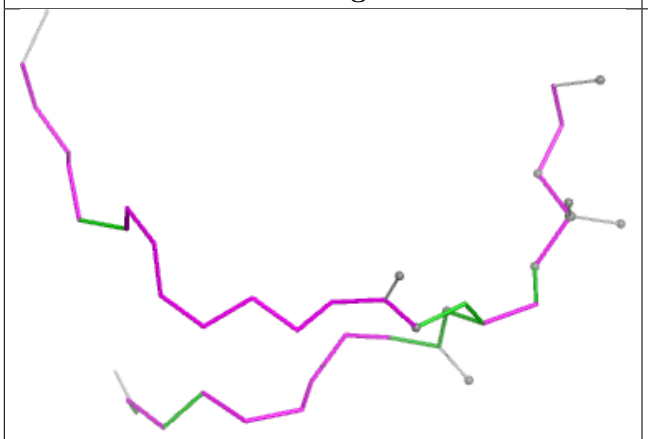

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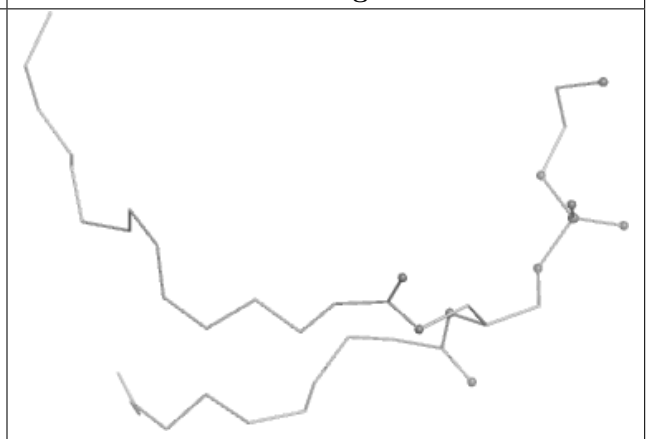
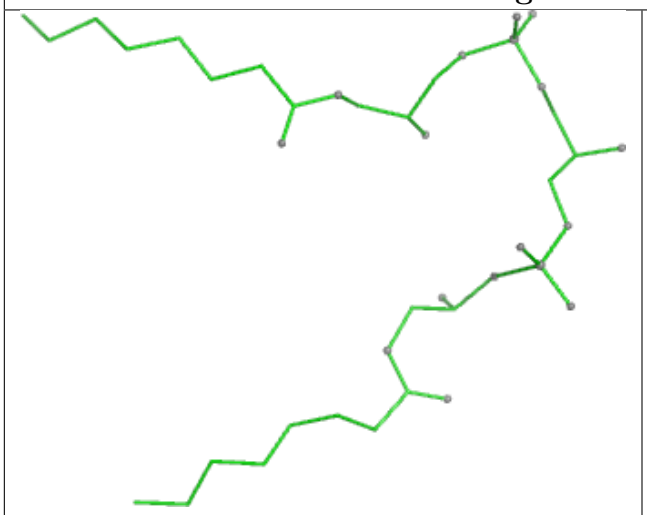


Rings

Ligand CDL A 3001



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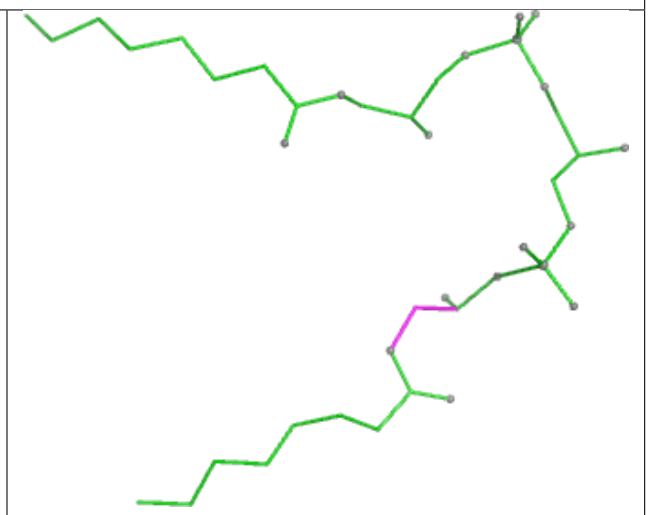
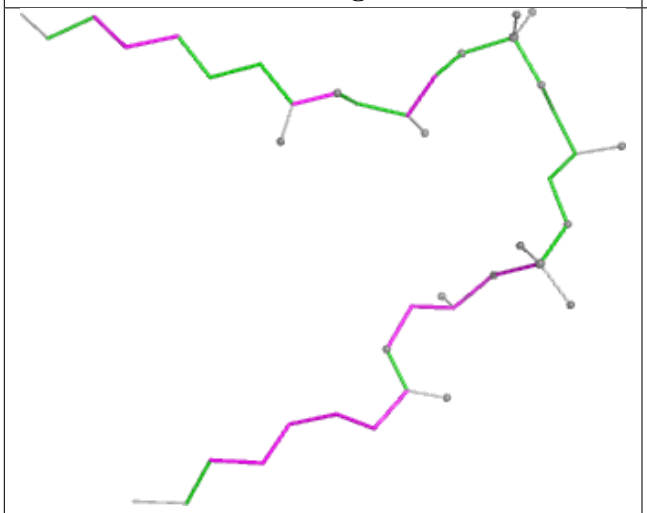
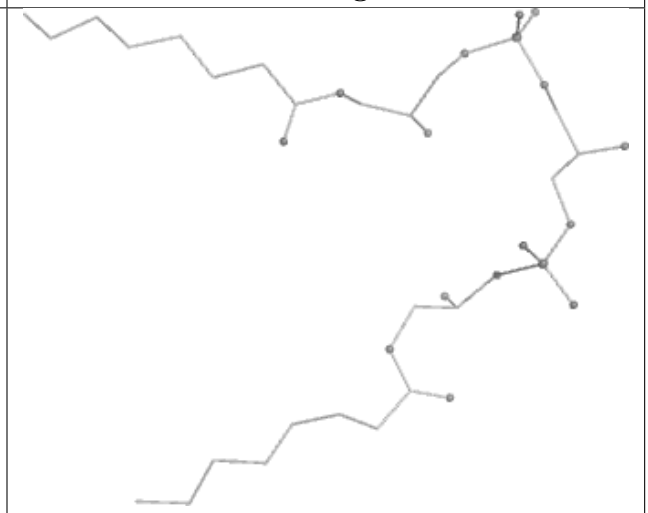


Bond angles

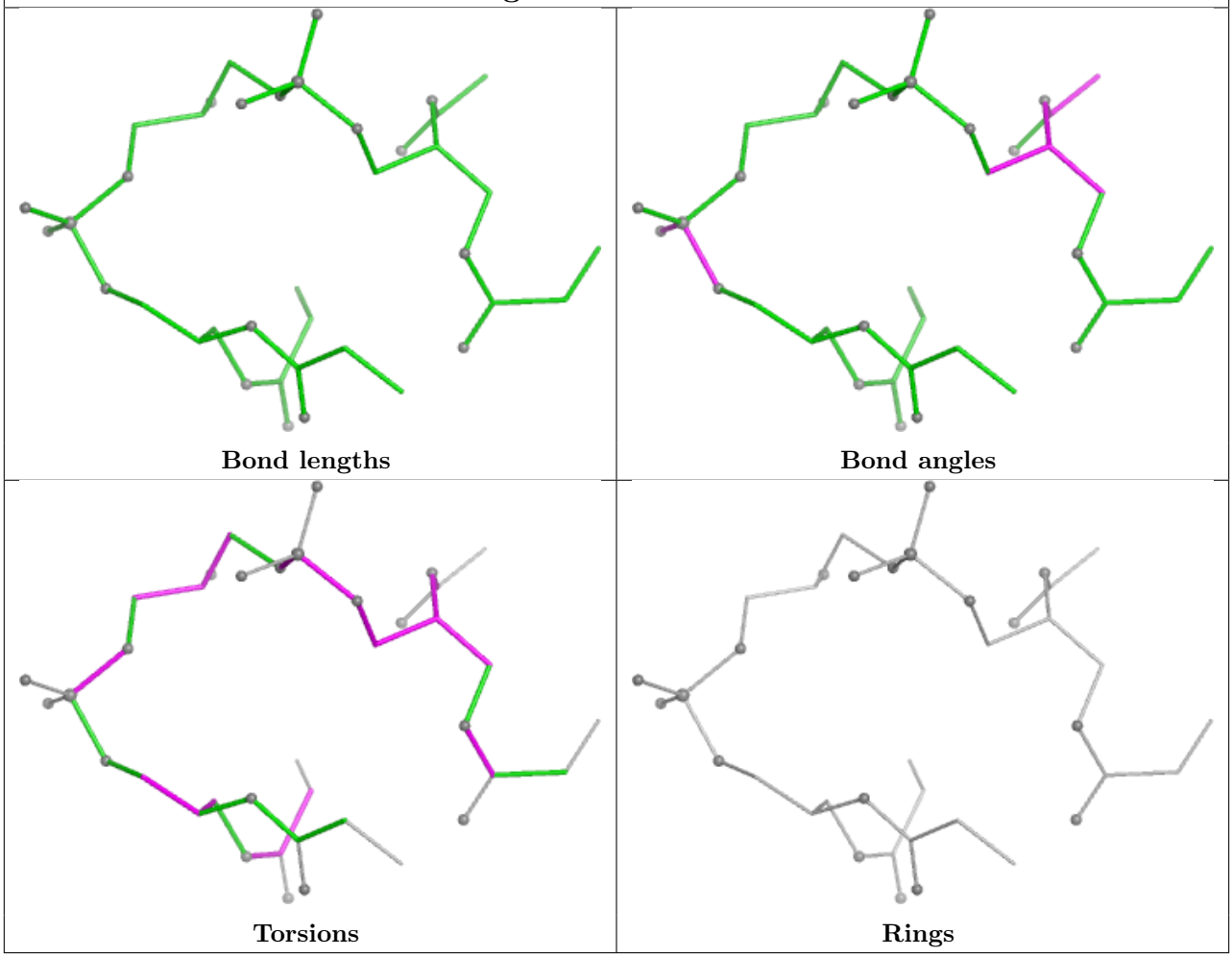


Torsions

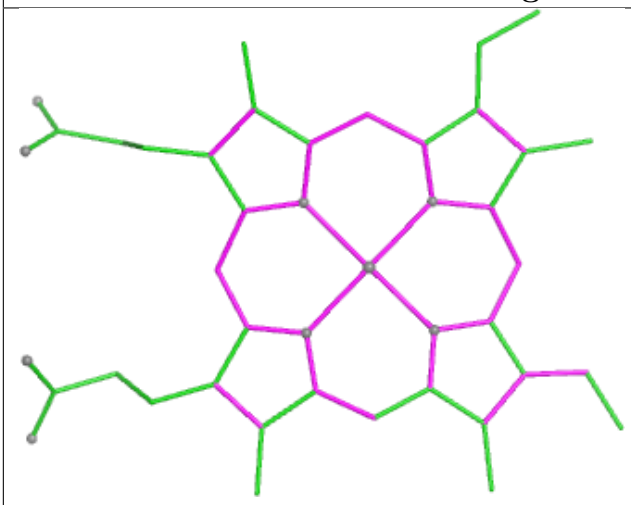


Rings

Ligand CDL H 702



Ligand HEC D 401



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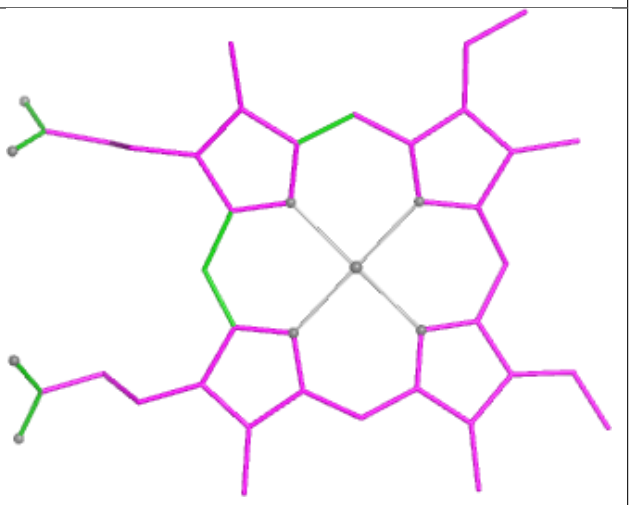
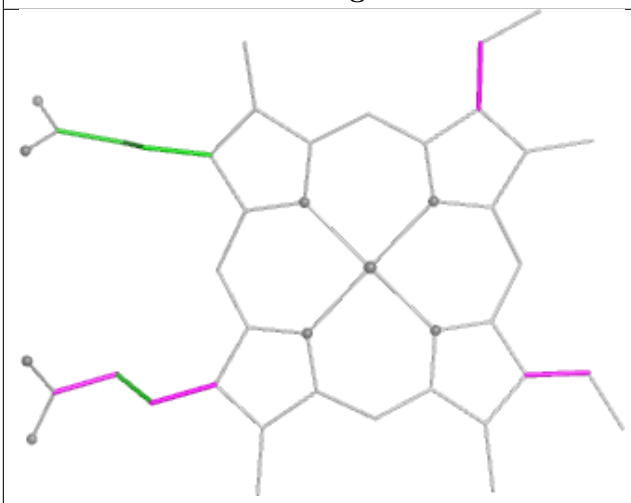
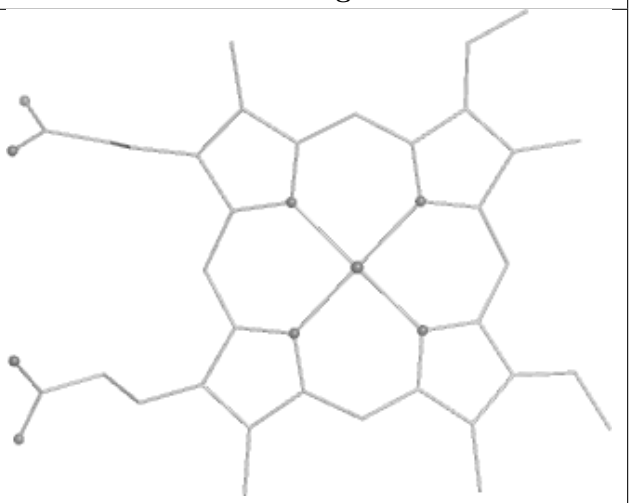


Bond angles

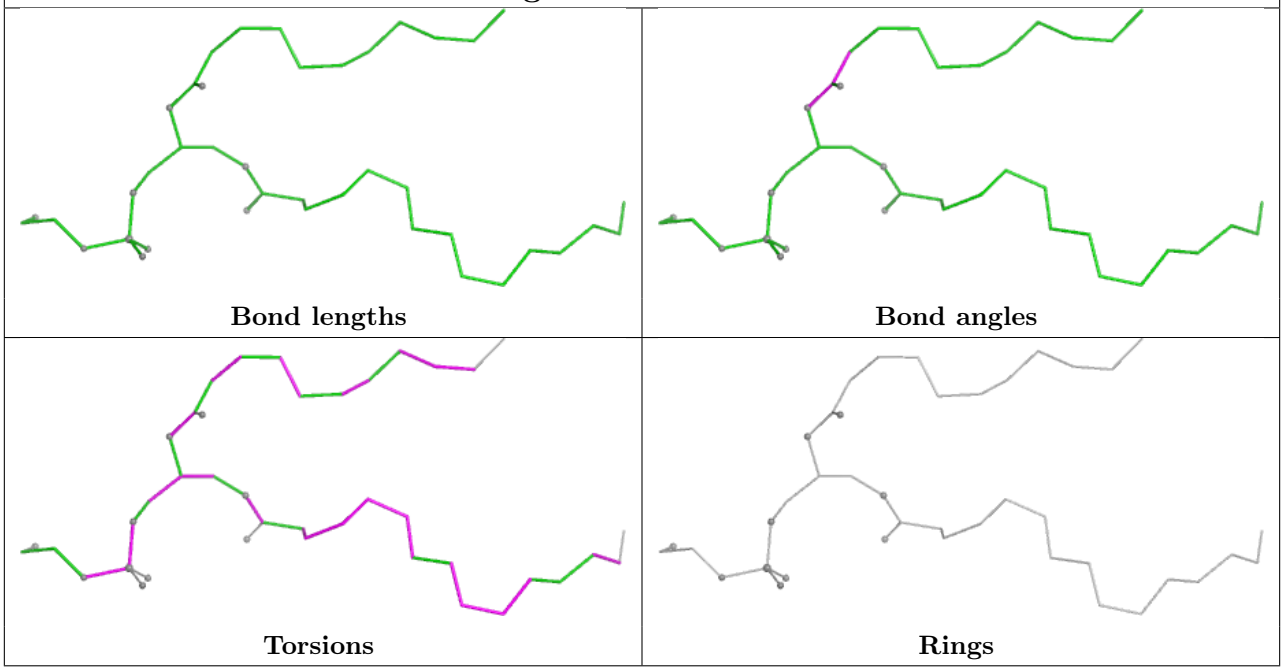


Torsions

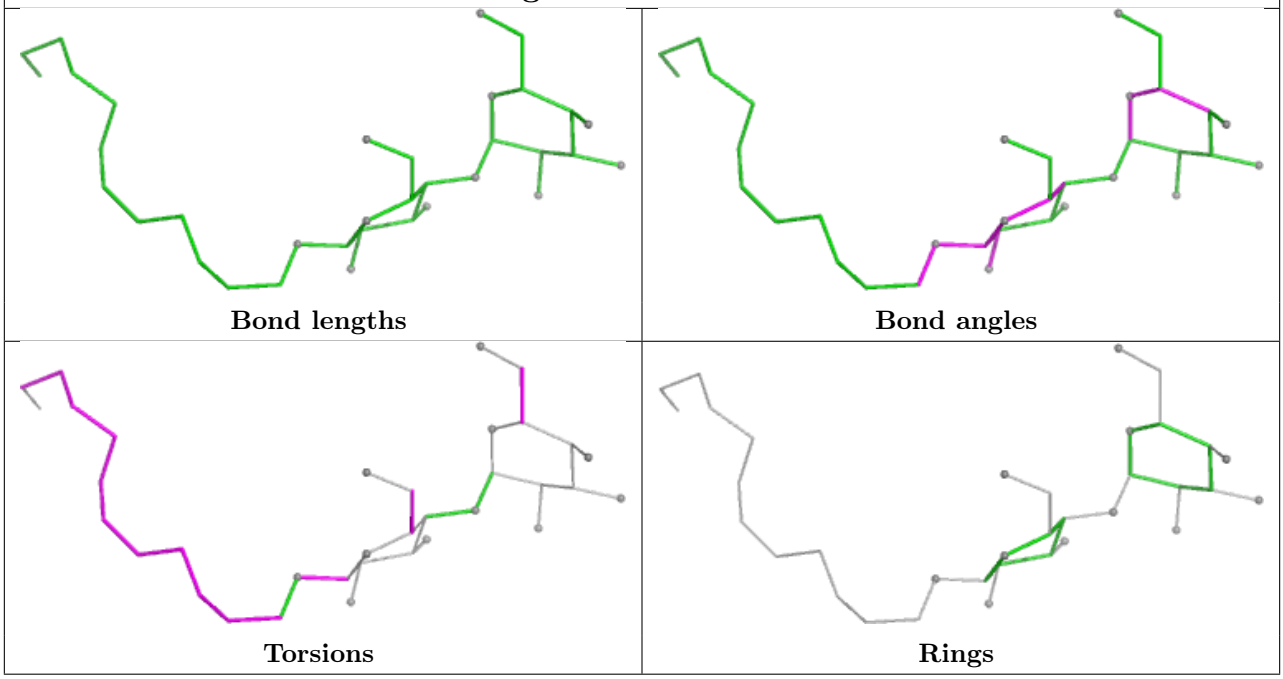


Rings

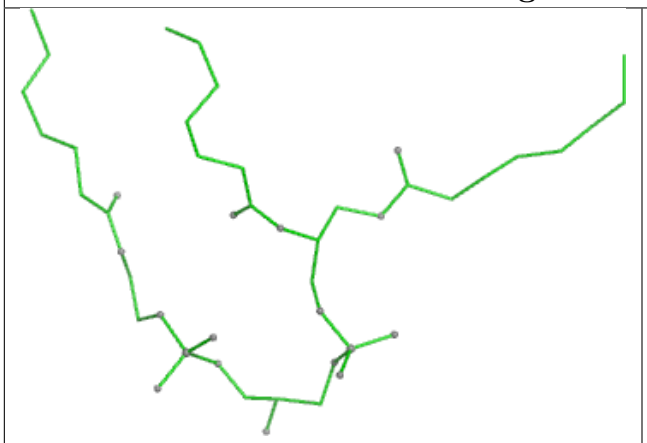
Ligand PTY N 505



Ligand LMT C 506

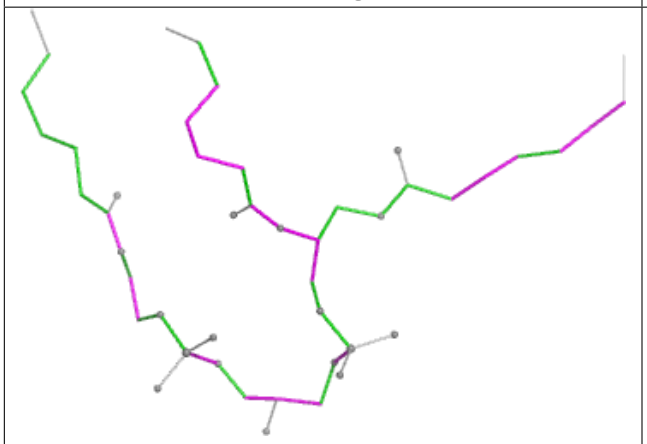


Ligand CDL L 3002

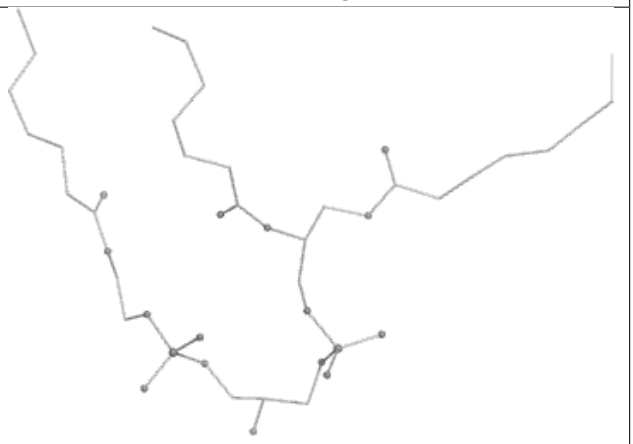


Bond lengths

Bond angles

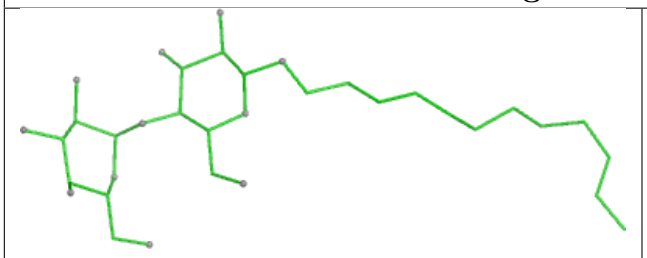


Torsions

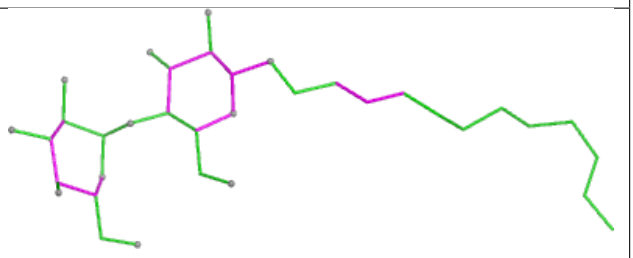


Rings

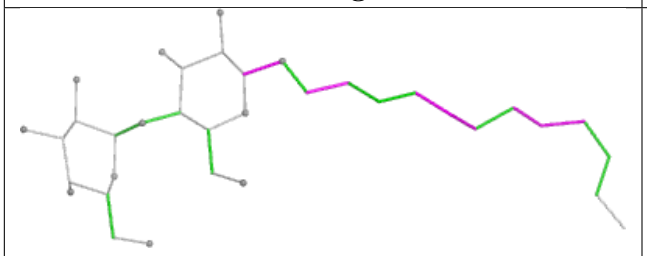
Ligand LMT P 302



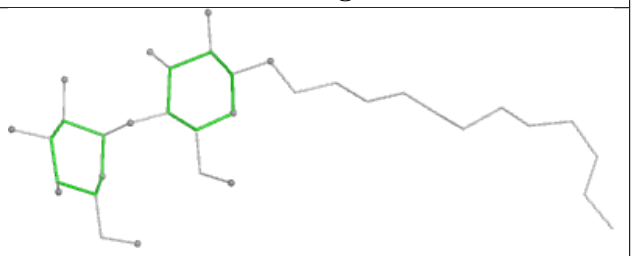
Bond lengths



Bond angles

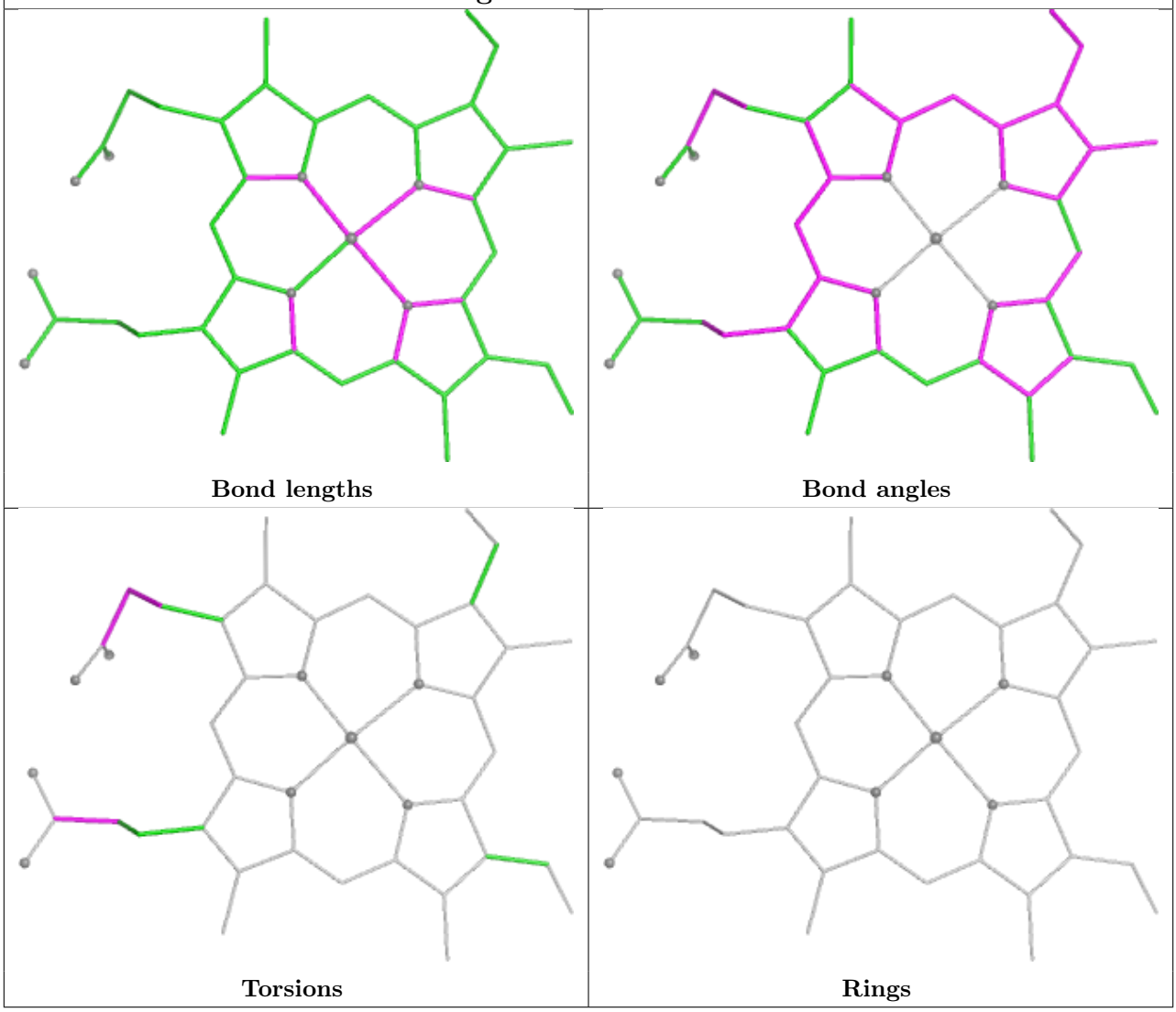


Torsions

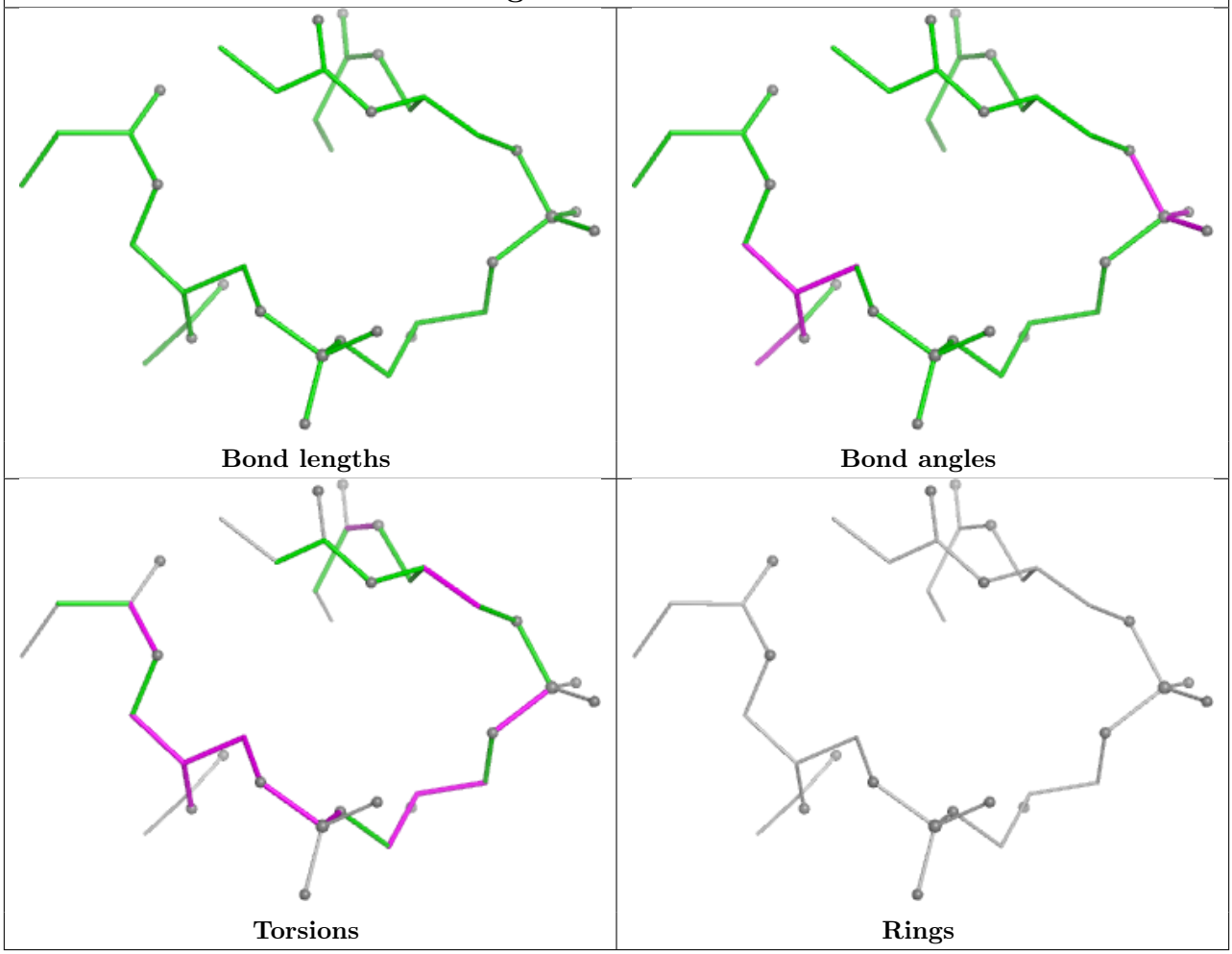


Rings

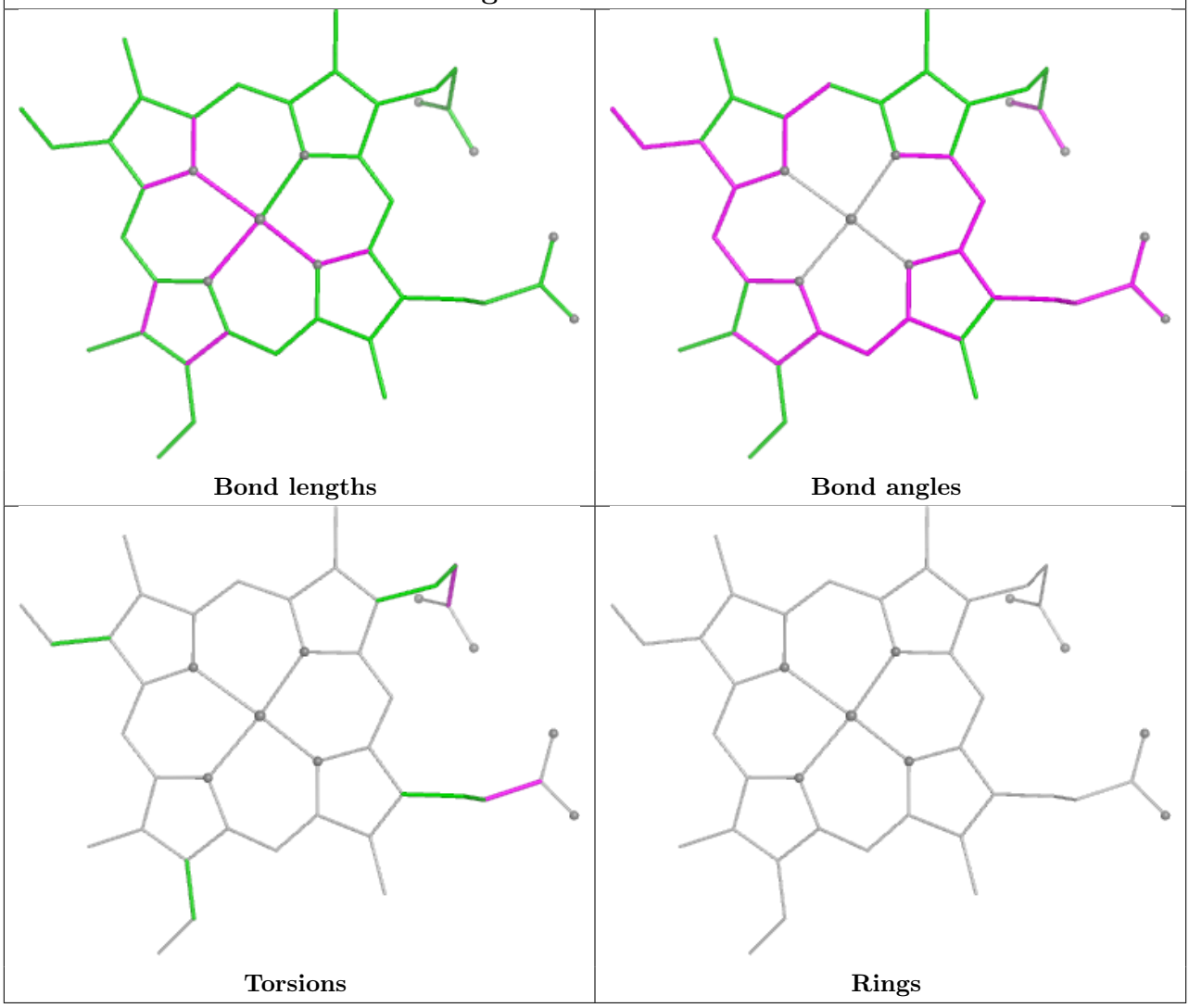
Ligand HEM C 501



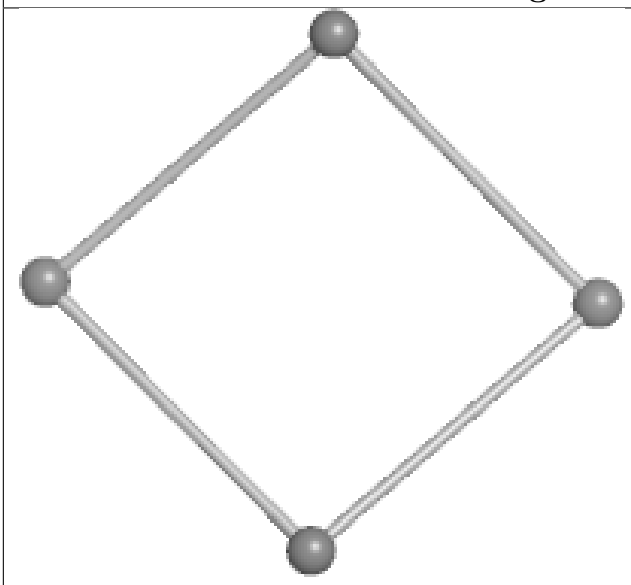
Ligand CDL S 101



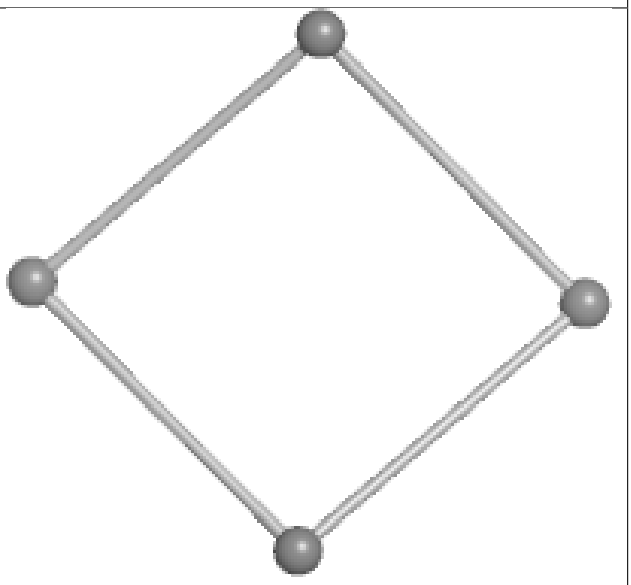
Ligand HEM C 502



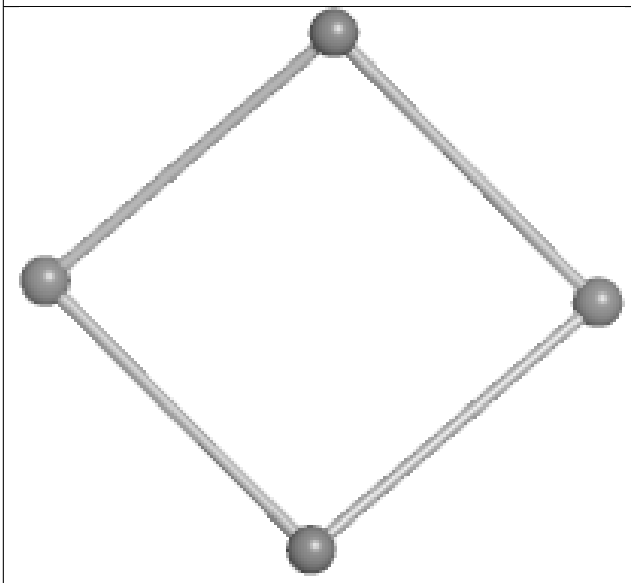
Ligand FES P 301



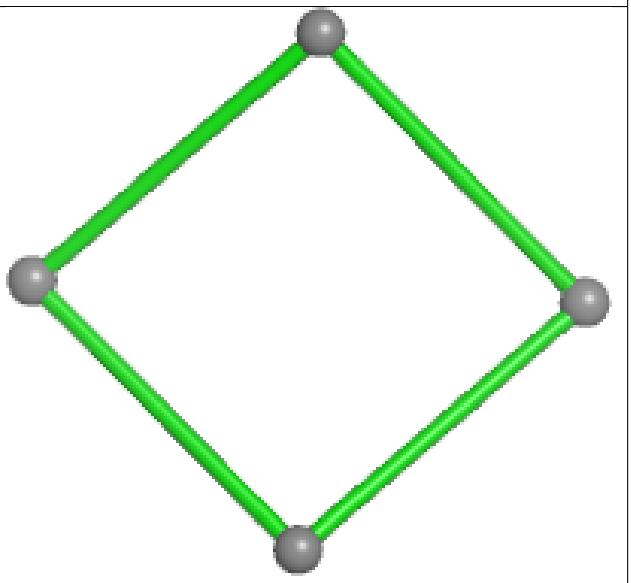
Bond lengths



Bond angles

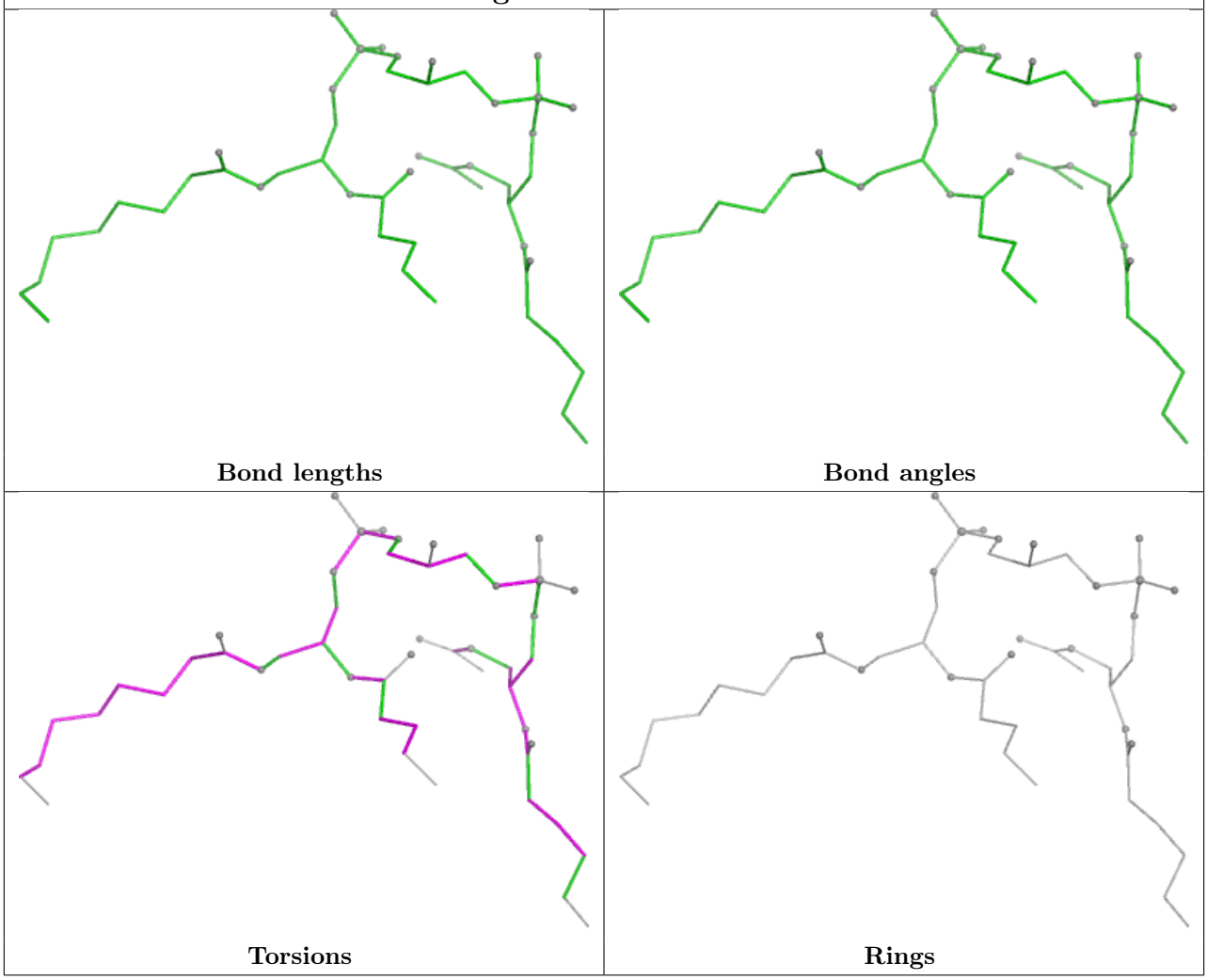


Torsions

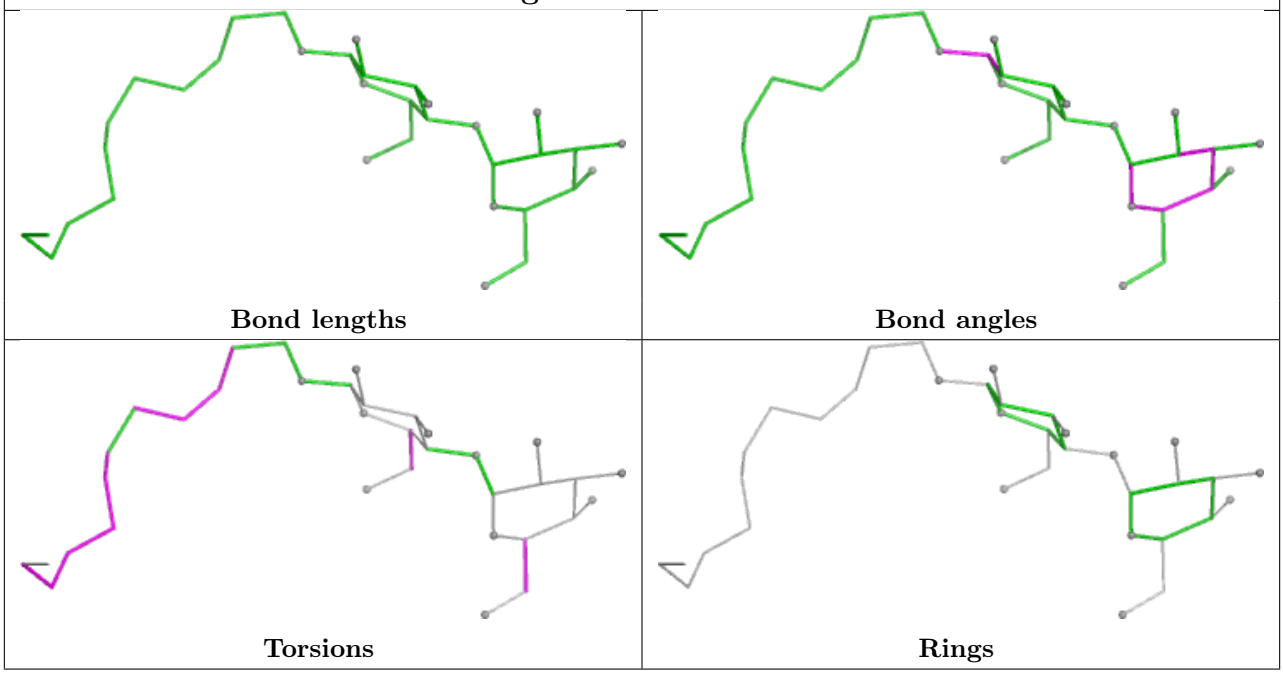


Rings

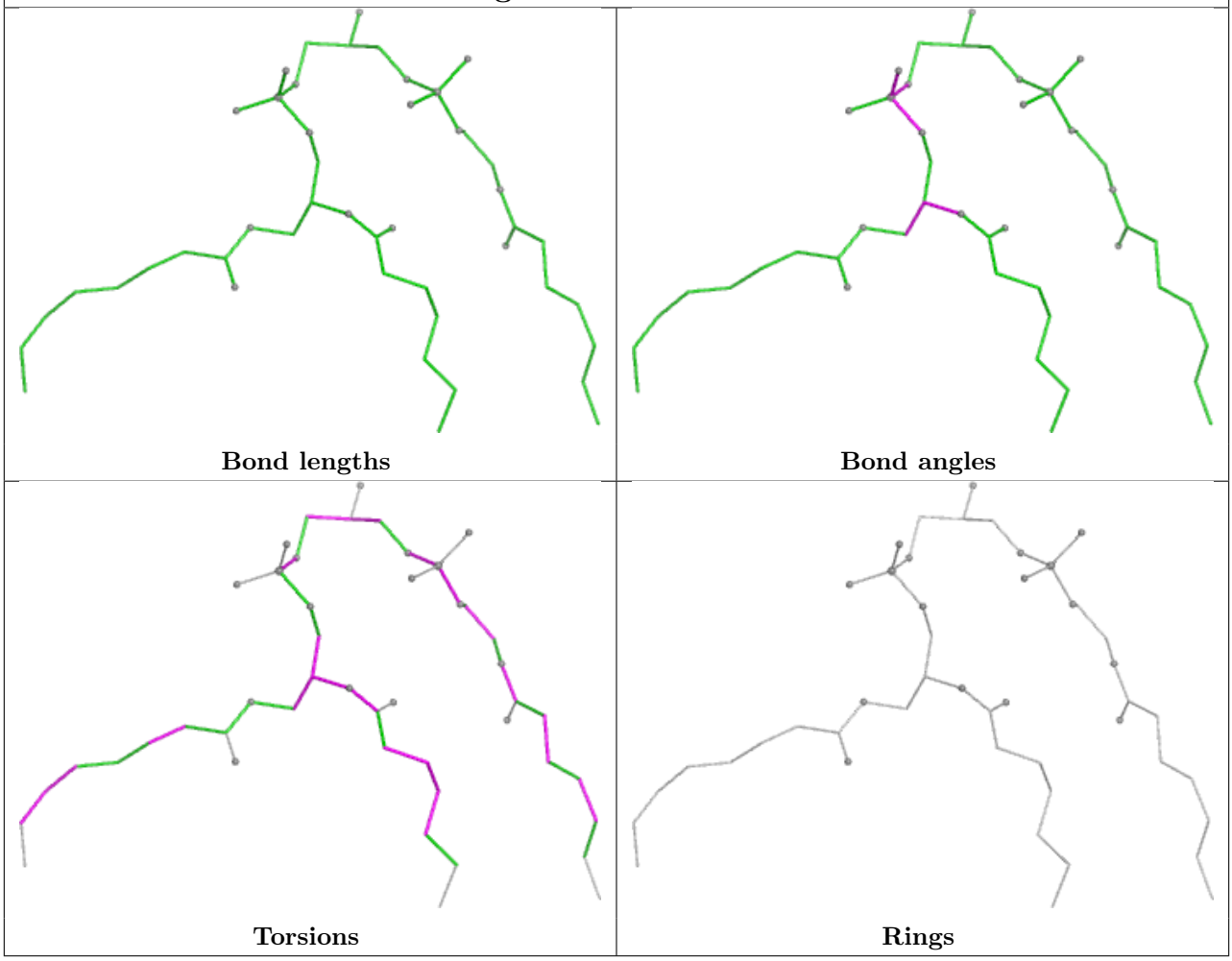
Ligand CDL N 504



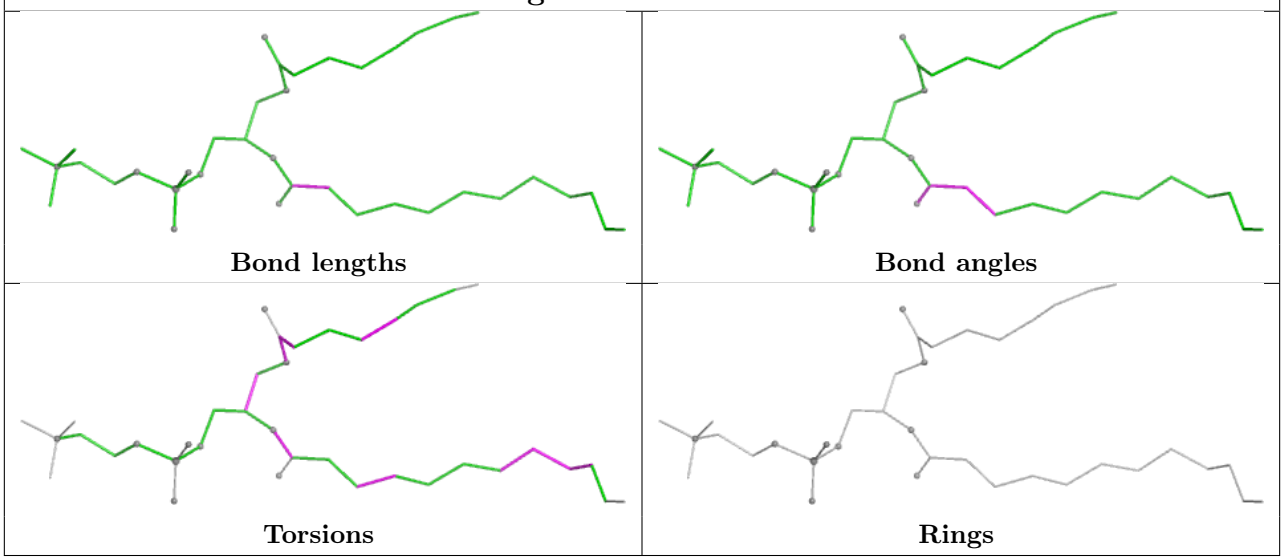
Ligand LMT N 507



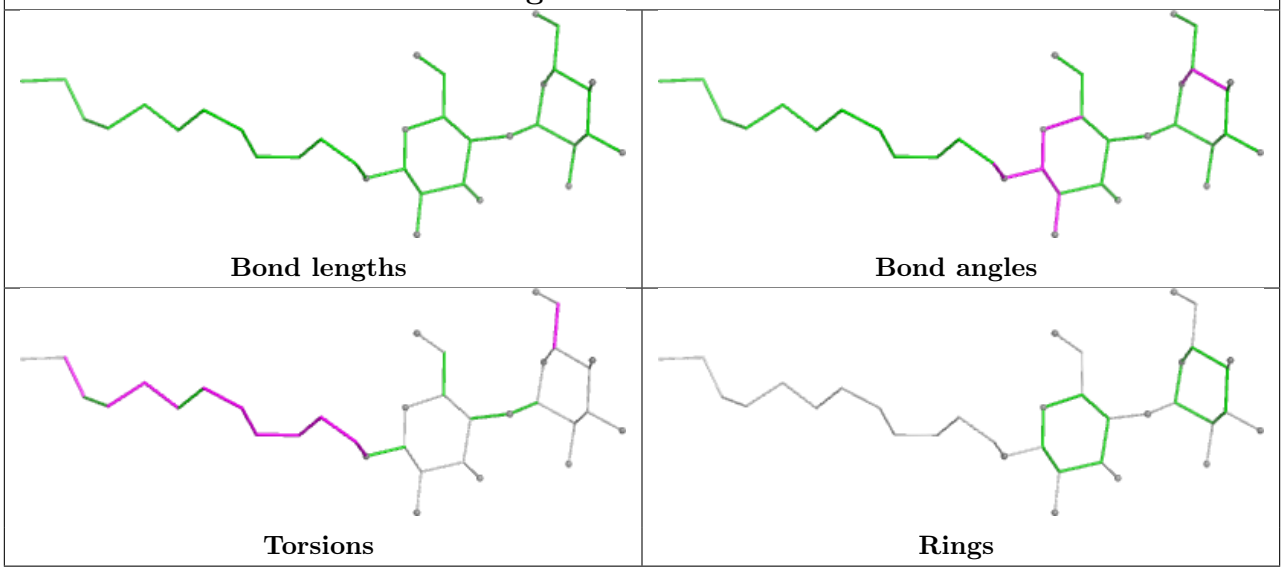
Ligand CDL A 3002



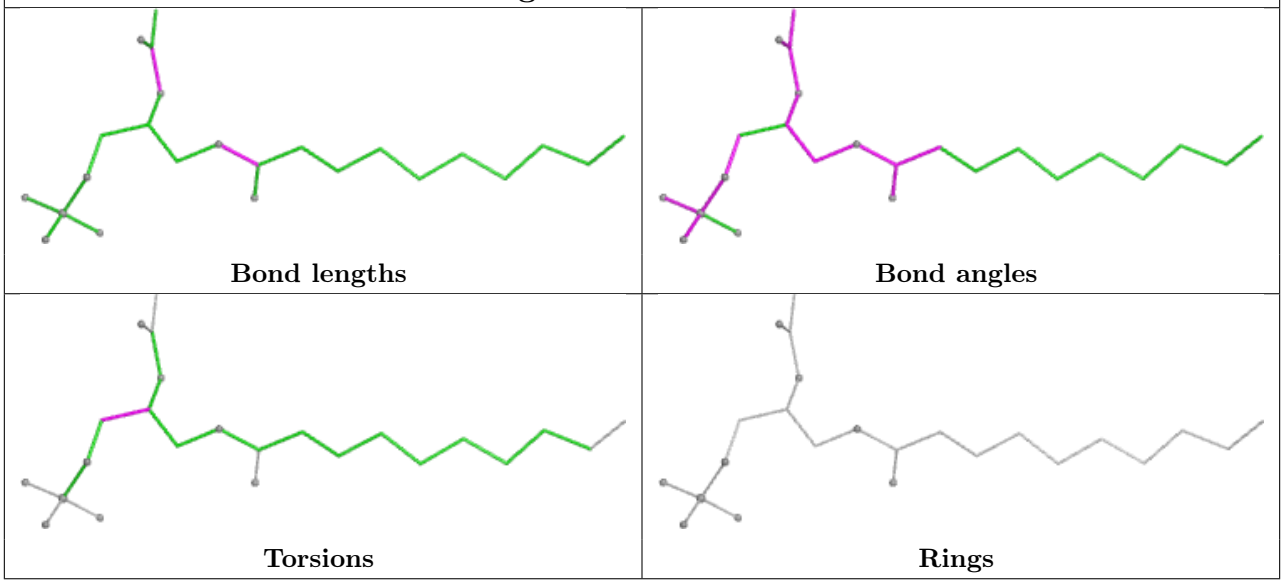
Ligand PC1 N 503



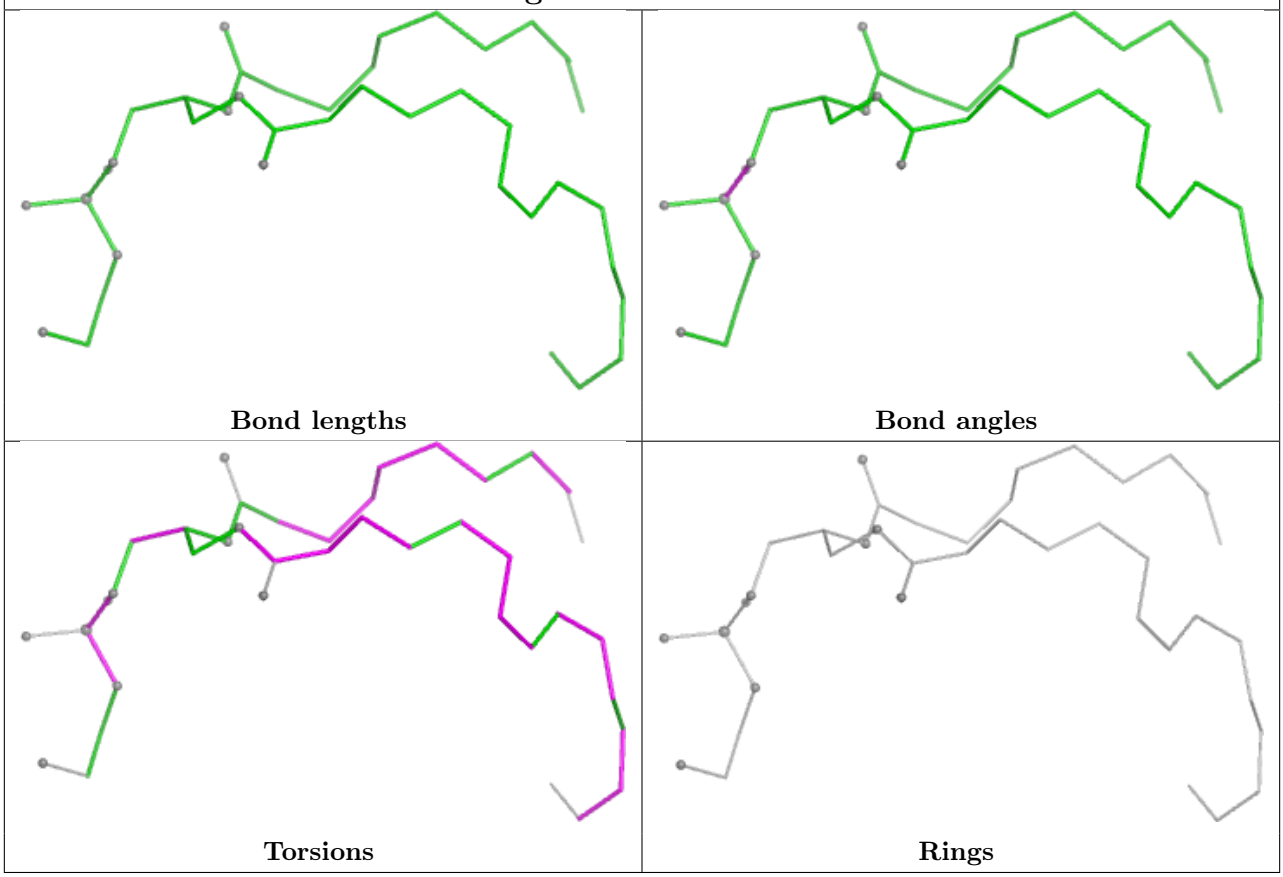
Ligand LMT J 101

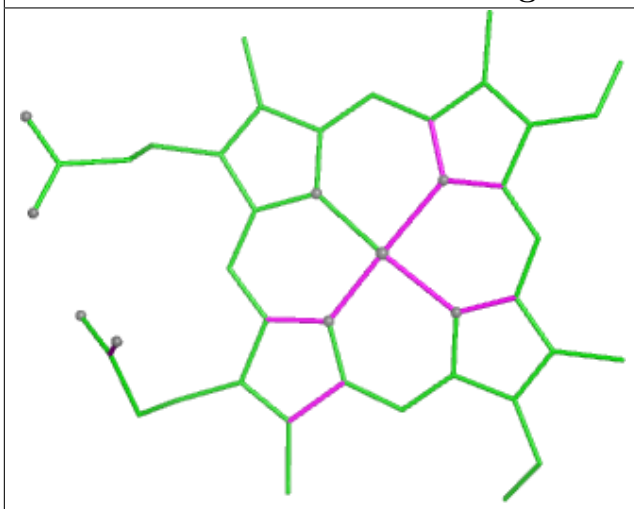
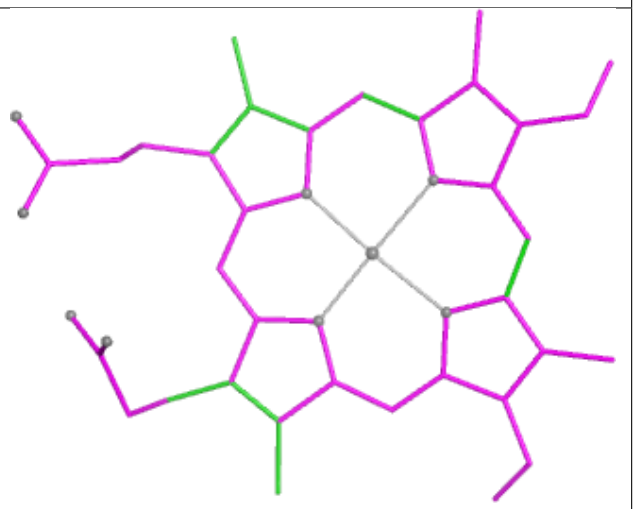
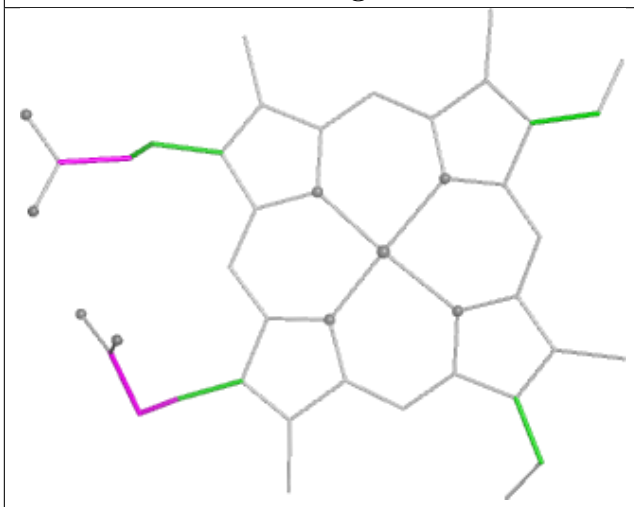
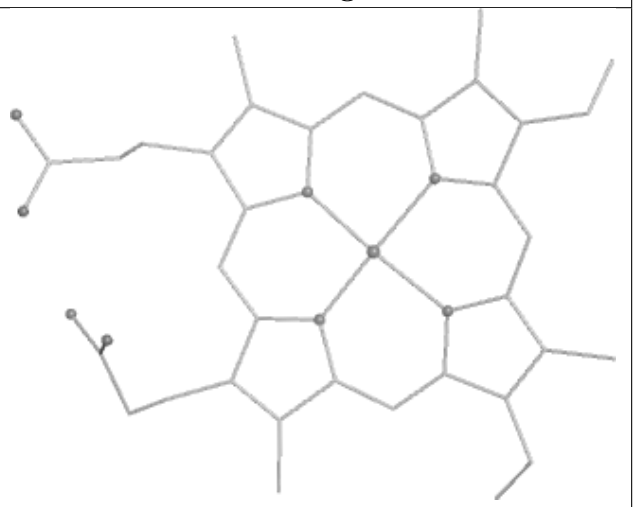


Ligand XP4 A 3003



Ligand PTY P 303



Ligand HEM N 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

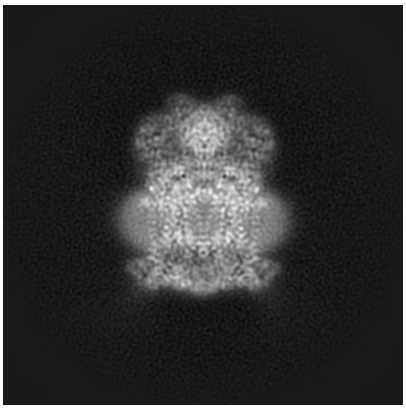
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15317. These allow visual inspection of the internal detail of the map and identification of artifacts.

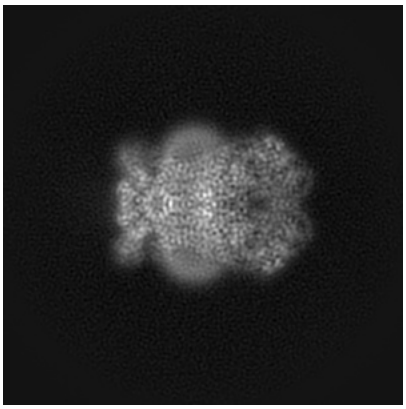
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

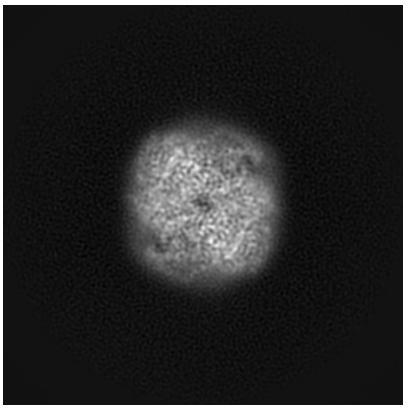
6.1.1 Primary map



X

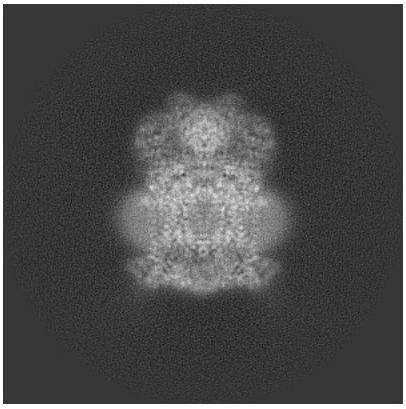


Y

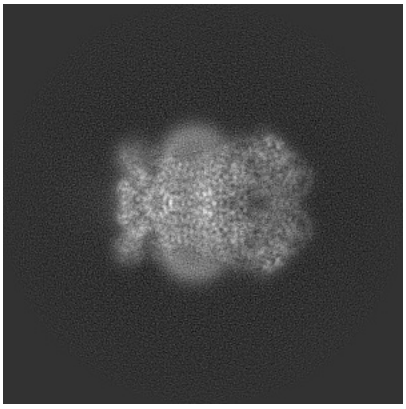


Z

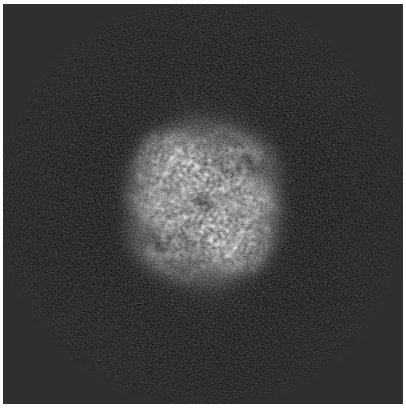
6.1.2 Raw map



X



Y

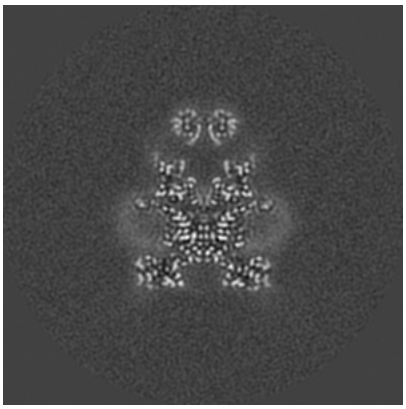


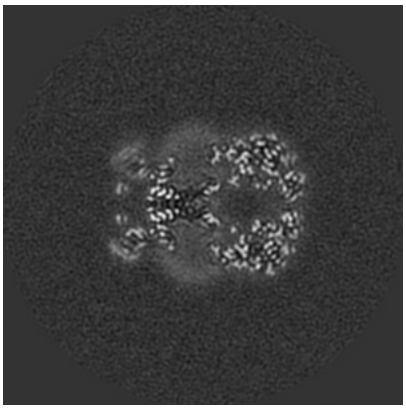
Z

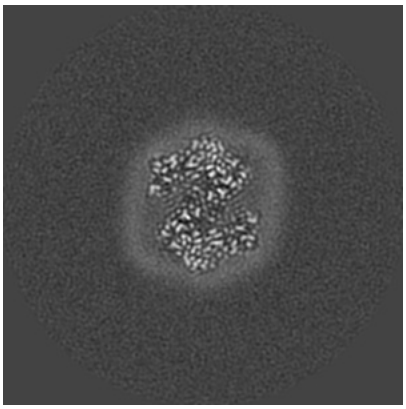
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

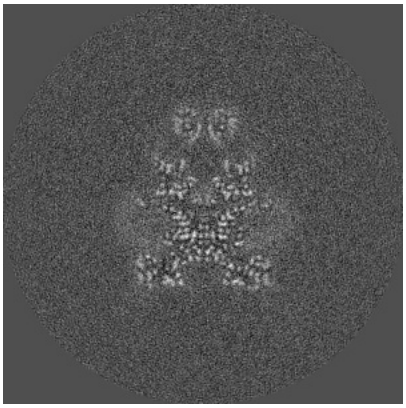
6.2.1 Primary map

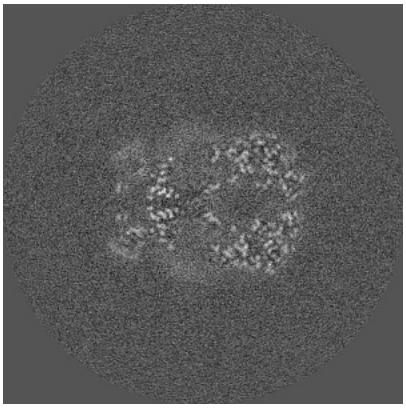

X Index: 180

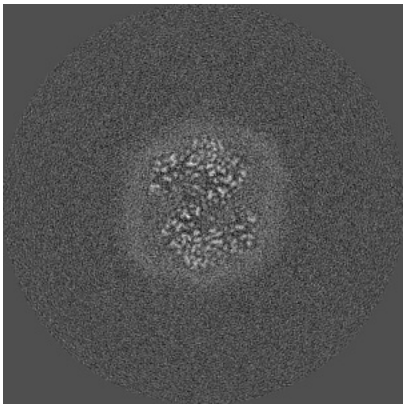

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

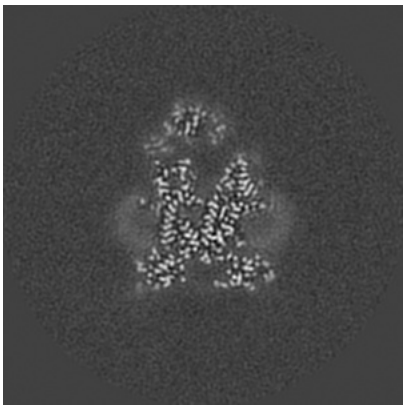

Y Index: 180

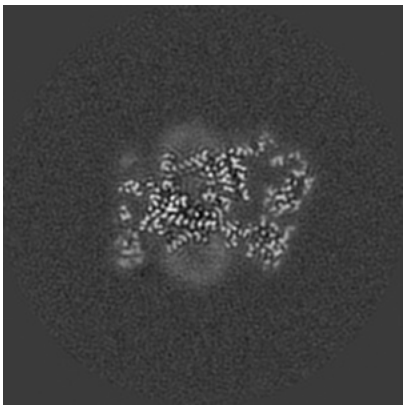

Z Index: 180

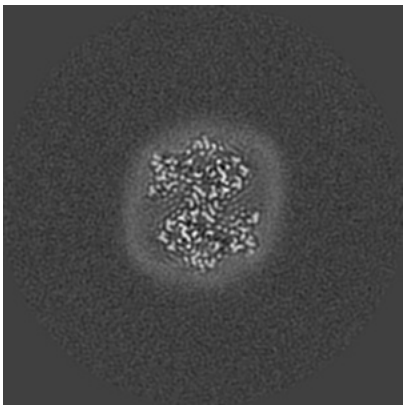
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

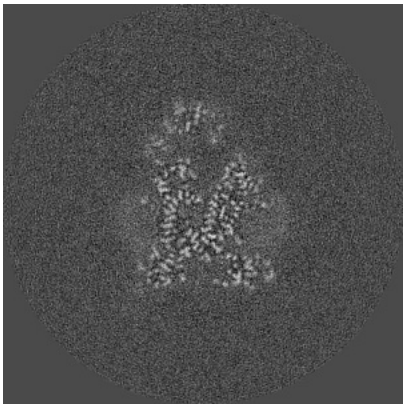
6.3.1 Primary map

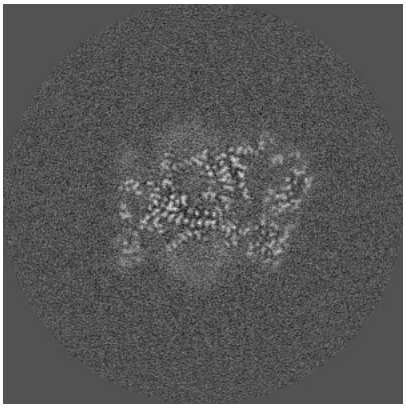

X Index: 186

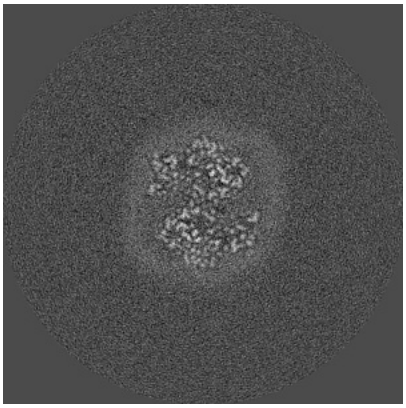

Y Index: 166


Z Index: 182

6.3.2 Raw map


X Index: 187

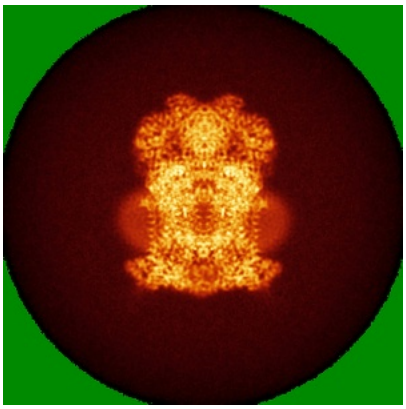

Y Index: 166

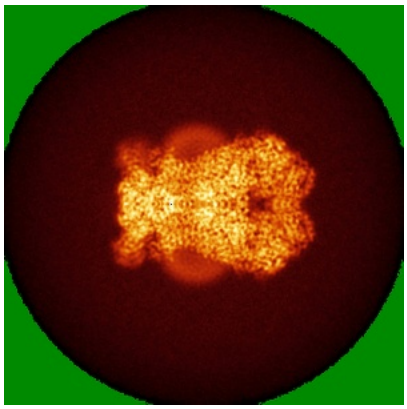

Z Index: 181

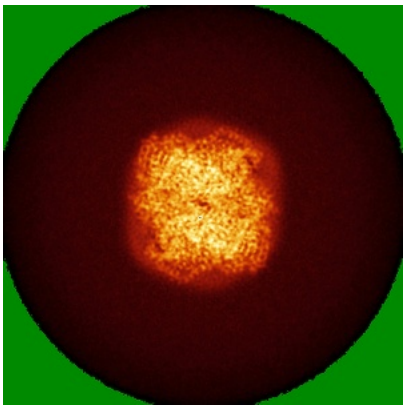
The images above show the largest variance slices of the map in three orthogonal directions.

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

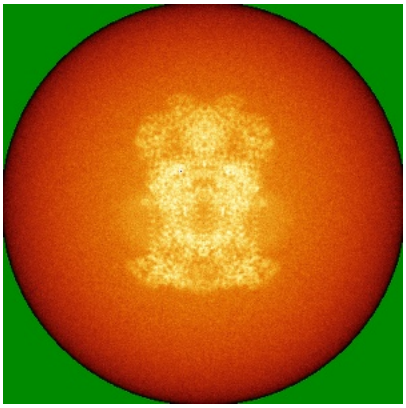
6.4.1 Primary map

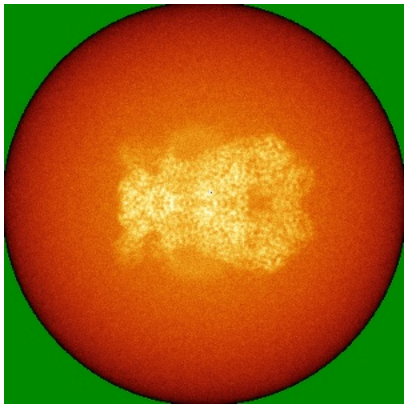

X

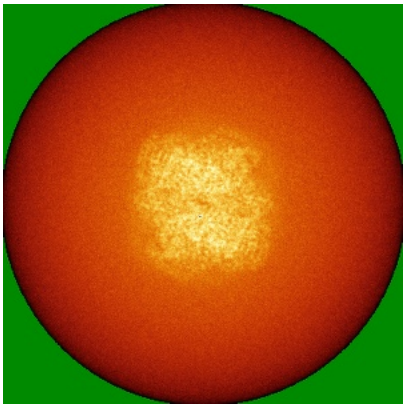

Y


Z

6.4.2 Raw map


X

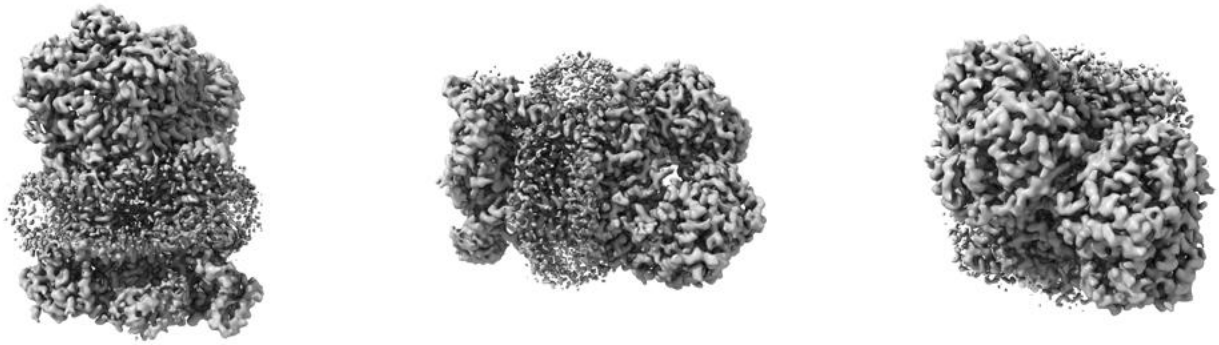

Y


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)

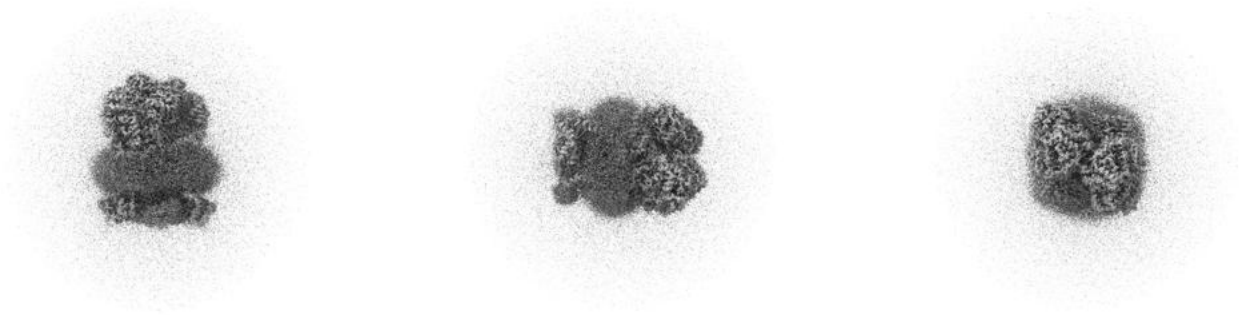
6.5.1 Primary map



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.

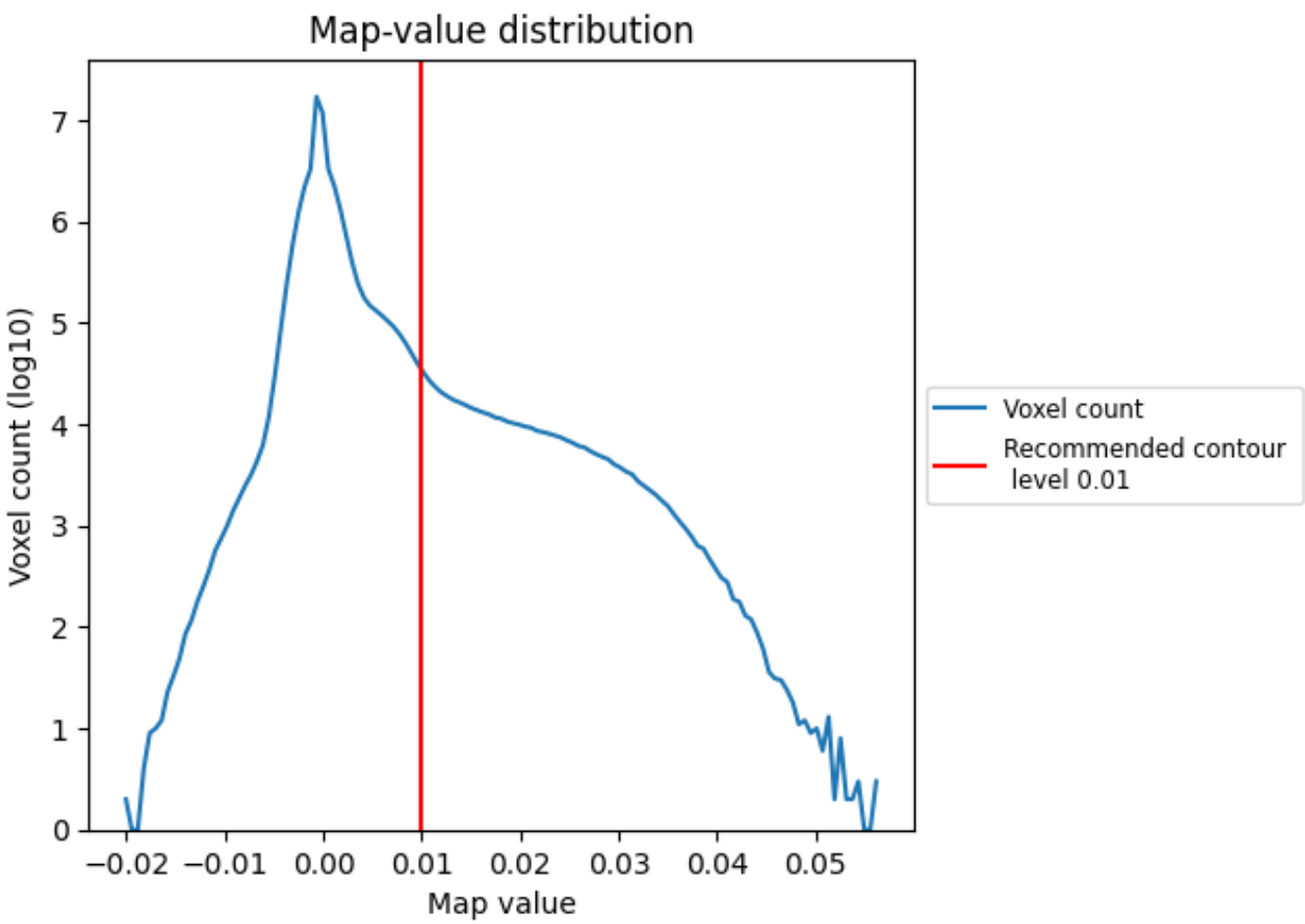
6.6 Mask visualisation (i)

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

7 Map analysis (i)

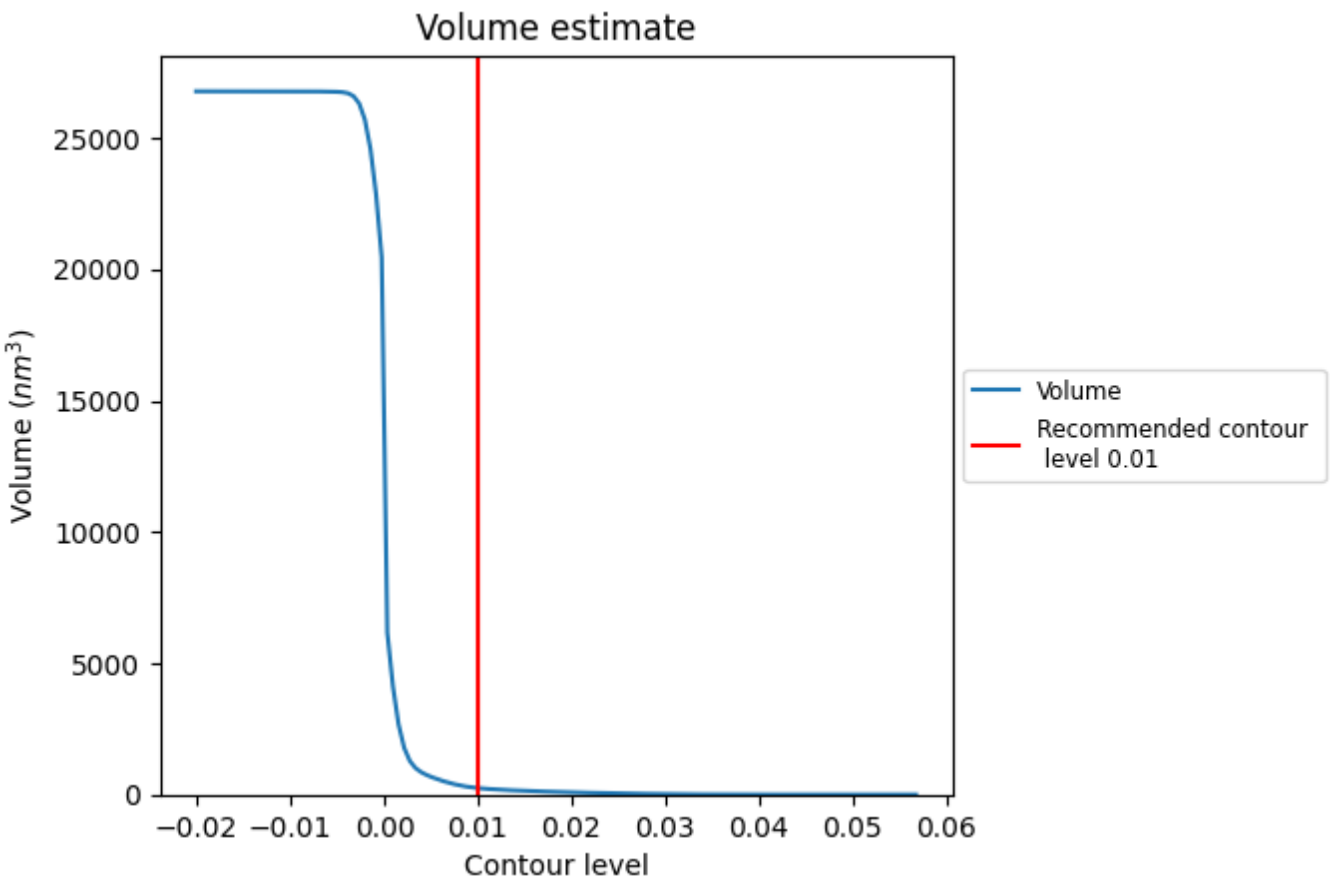
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

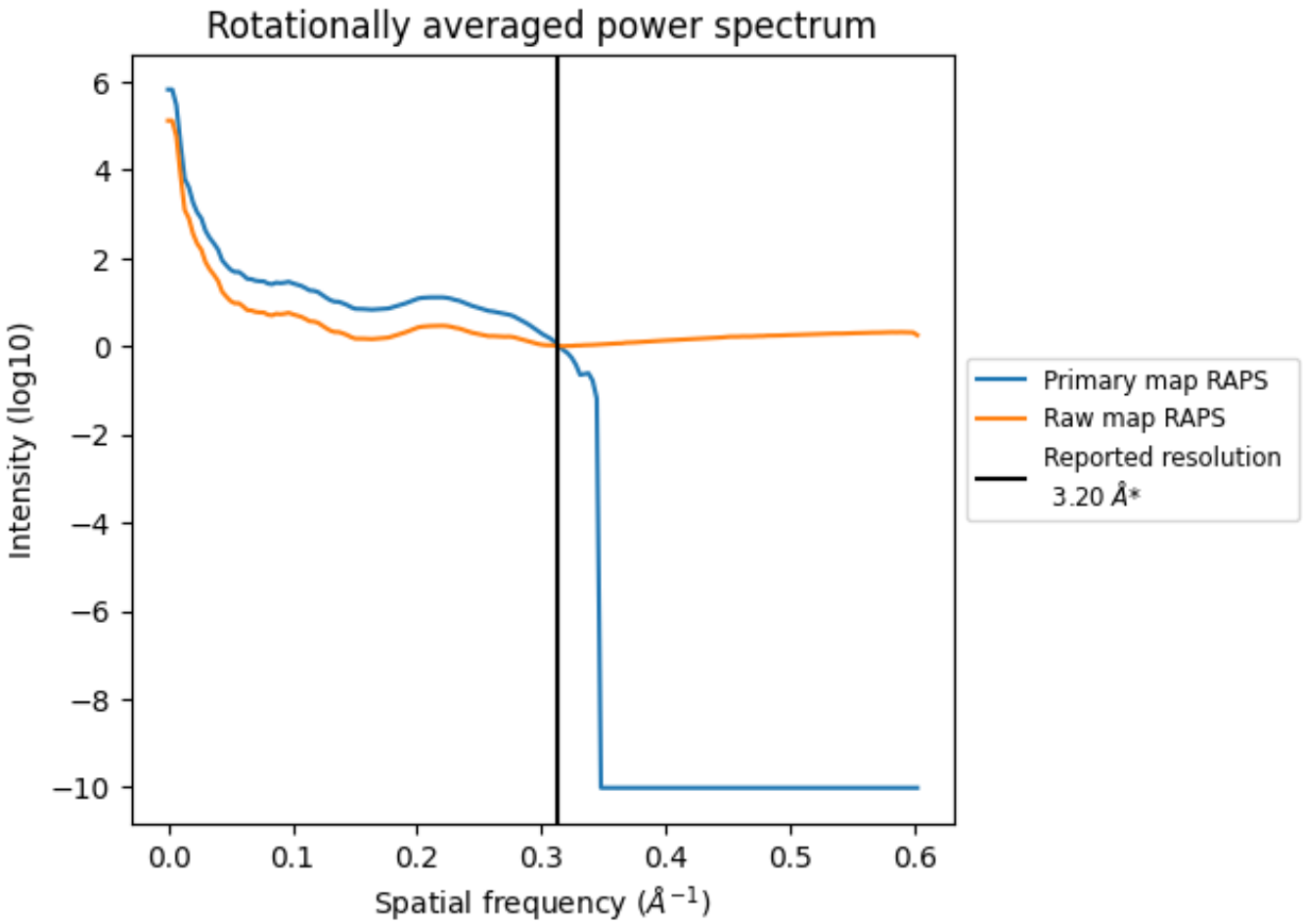
7.2 Volume estimate (i)



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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)

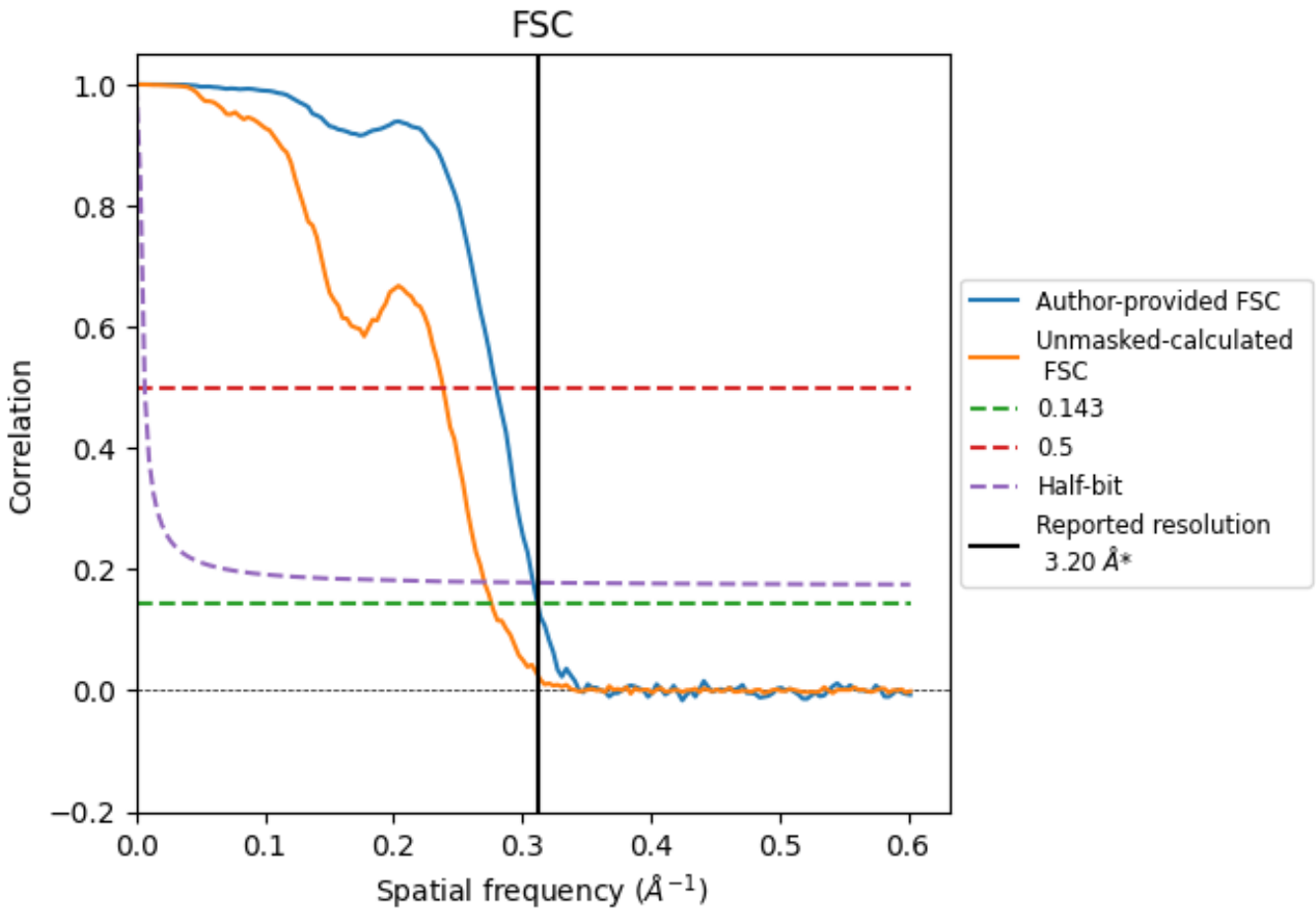


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

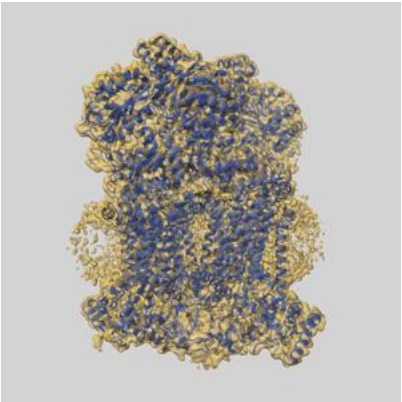
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.57	3.24
Unmasked-calculated*	3.62	4.19	3.70

*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 3.62 differs from the reported value 3.2 by more than 10 %

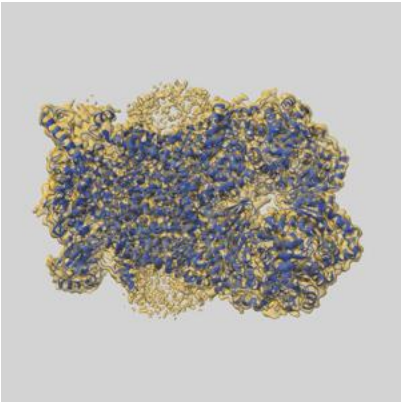
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15317 and PDB model 8ABB. Per-residue inclusion information can be found in section 3 on page 12.

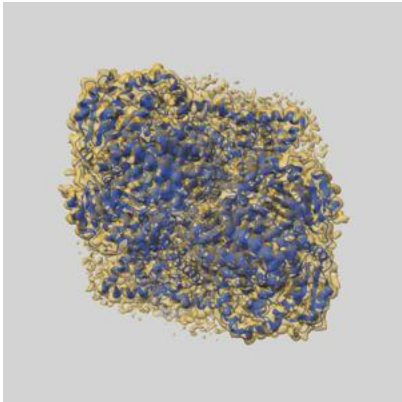
9.1 Map-model overlay (i)



X



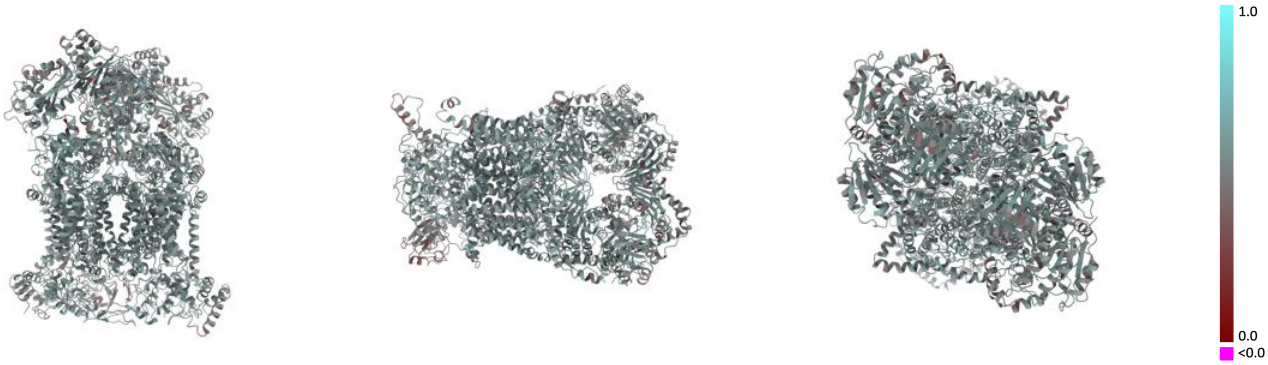
Y



Z

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

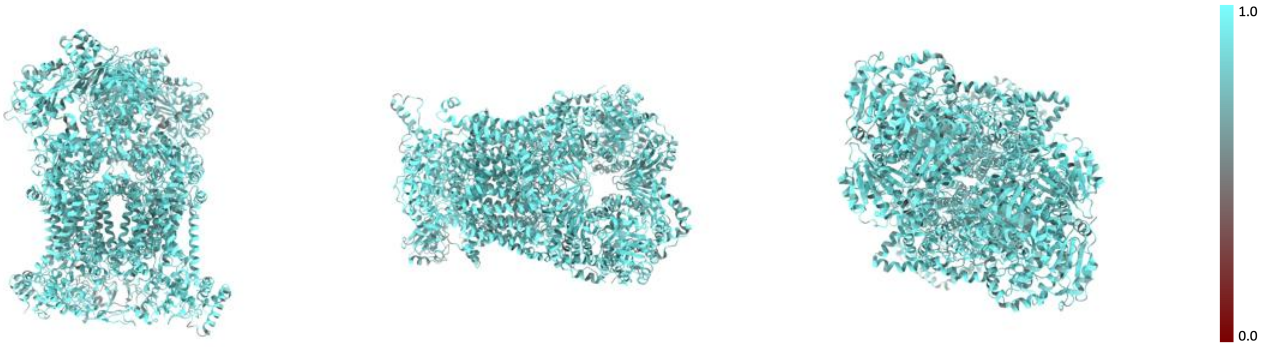
9.2 Q-score mapped to coordinate model (i)



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.

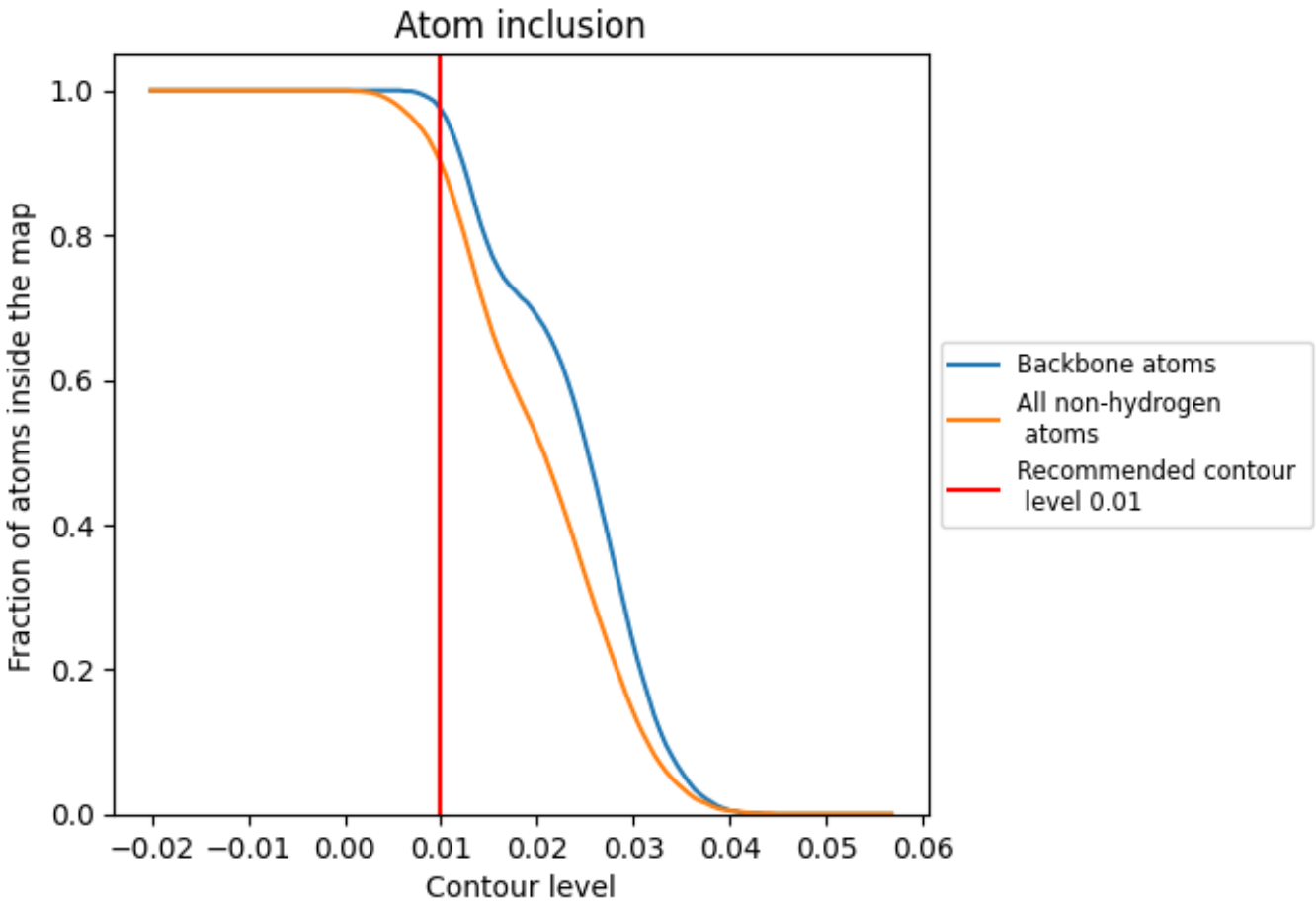
9.3 Atom inclusion mapped to coordinate model (i)



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, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.5400
A	0.8930	0.5380
B	0.8890	0.5290
C	0.9370	0.5680
D	0.9220	0.5570
E	0.9060	0.5580
F	0.8190	0.4720
G	0.8990	0.5420
H	0.9410	0.5580
I	0.9280	0.5530
J	0.8570	0.5310
L	0.8900	0.5380
M	0.8870	0.5280
N	0.9340	0.5660
O	0.9190	0.5580
P	0.8230	0.4610
Q	0.8150	0.4790
R	0.8990	0.5380
S	0.9270	0.5570
T	0.9220	0.5440
U	0.8710	0.5370