



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 07:44 AM UTC

PDB ID : 8YIN / pdb_00008yin
EMDB ID : EMD-39323
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex in YF23694-bound state
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-02-29
Resolution : 2.74 Å(reported)
Based on initial model : 6YMX

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

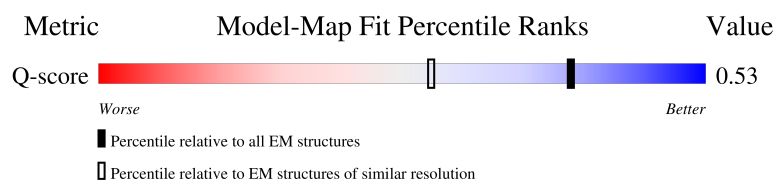
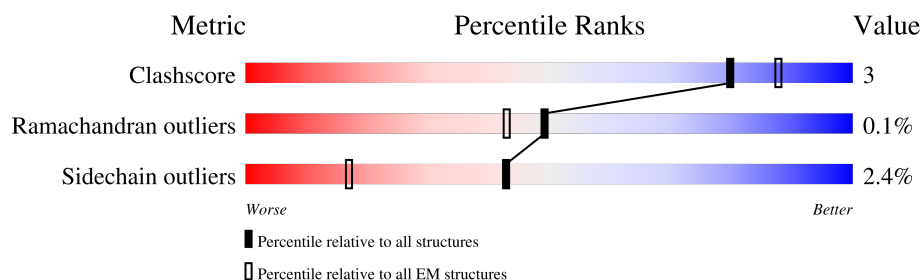
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

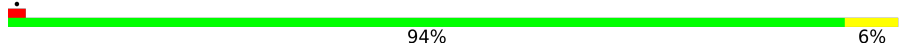
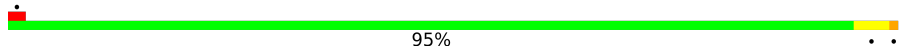
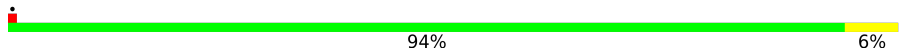
The reported resolution of this entry is 2.74 Å.

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.



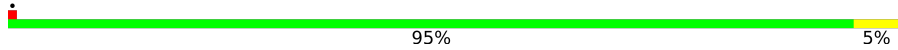
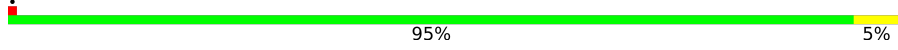
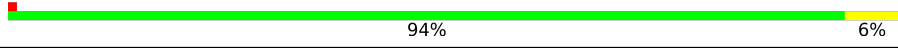
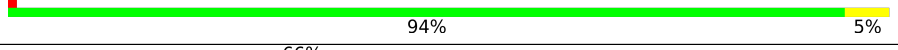
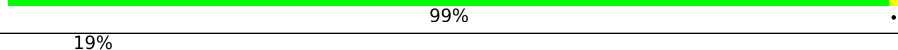
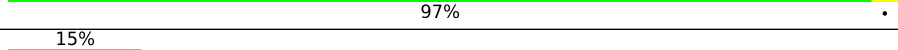
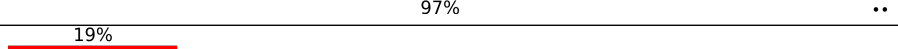
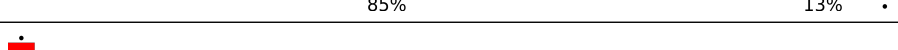
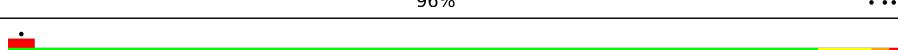
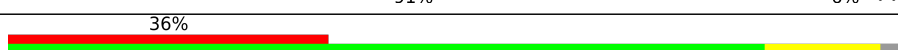
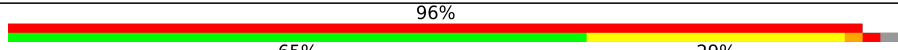
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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 $\leq 5\%$. 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	A	431	
1	L	431	
2	C	385	
2	N	385	

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Mol	Chain	Length	Quality of chain
3	B	352	
3	M	352	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	H	93	
6	S	93	
7	F	75	
7	Q	75	
8	G	126	
8	R	126	
9	I	55	
9	T	55	
10	U	52	
10	V	52	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 32364 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 COR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
1	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
2	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
3	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
4	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
6	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 7 is a protein called QCR6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
7	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
8	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	54	Total	C	N	O	0	0
			442	295	74	73		
9	T	54	Total	C	N	O	0	0
			443	295	74	74		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

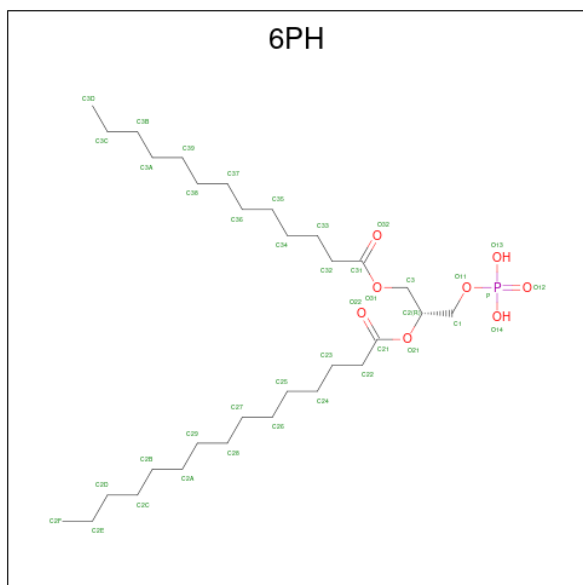
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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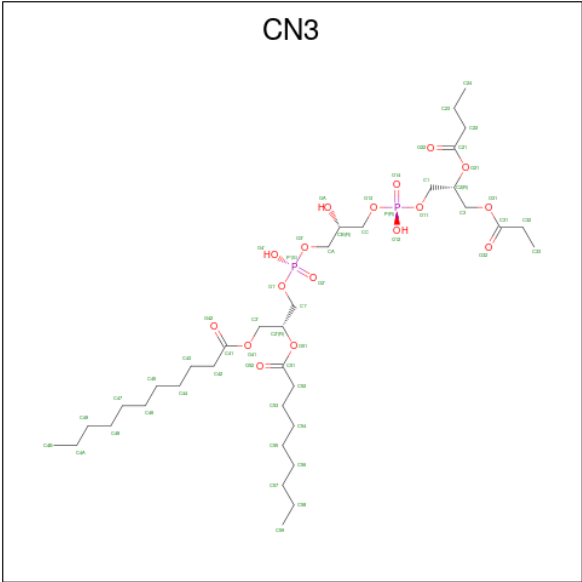
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: $C_{31}H_{61}O_8P$).



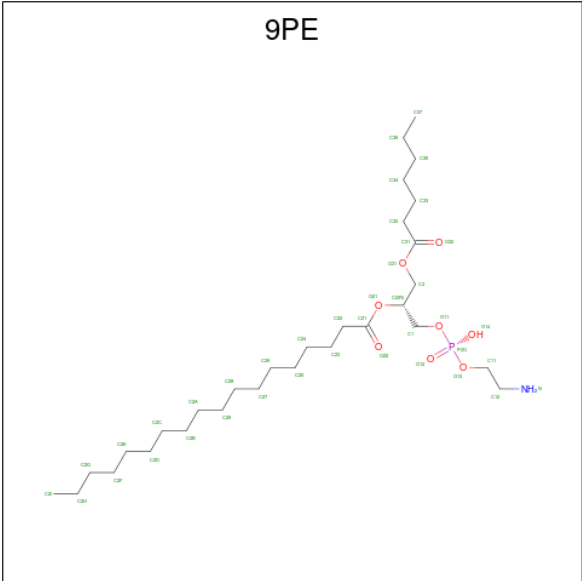
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			40	31	8	1	
11	E	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 12 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			55	36	17	2	
12	N	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 13 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



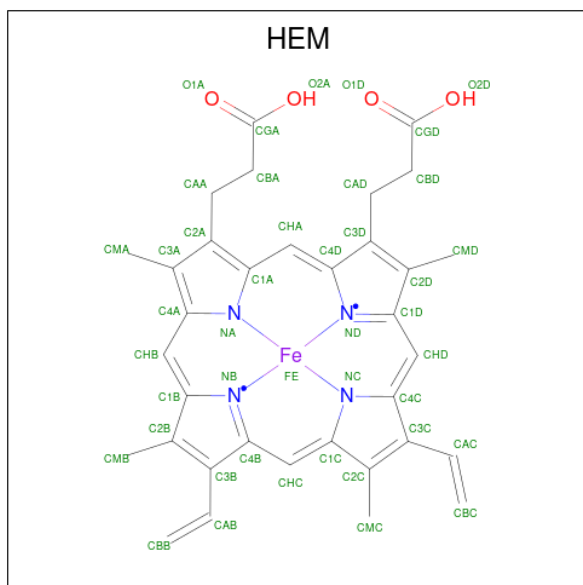
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

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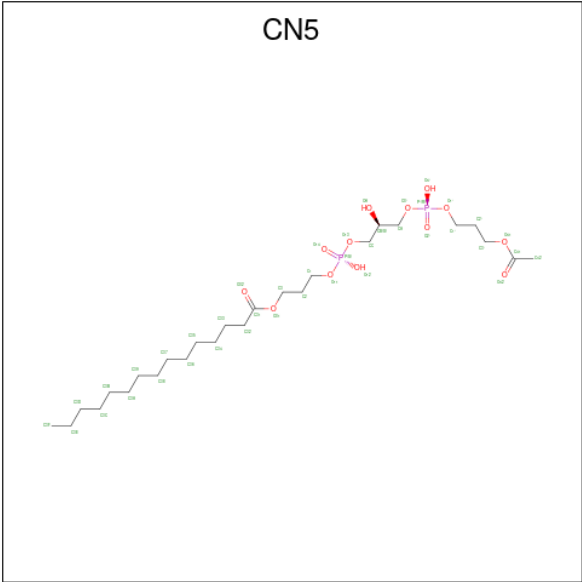
Mol	Chain	Residues	Atoms					AltConf
13	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



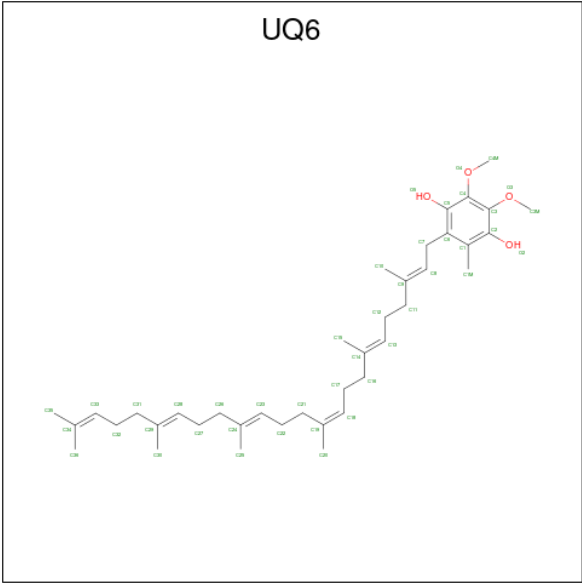
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



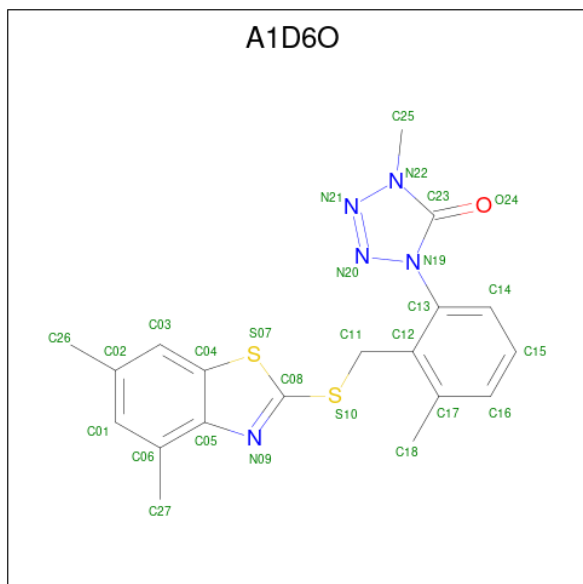
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: C₃₉H₆₀O₄).



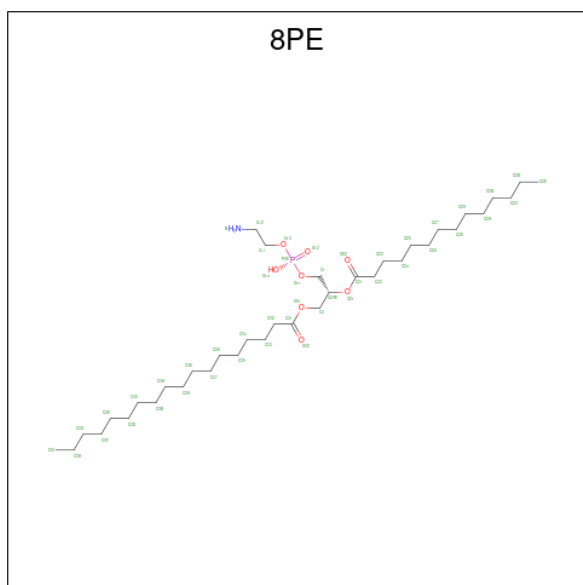
Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total	C	O		0
			43	39	4		
16	N	1	Total	C	O		0
			43	39	4		

- Molecule 17 is 1-[2-[(4,6-dimethyl-1,3-benzothiazol-2-yl)sulfanylmethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (CCD ID: A1D6O) (formula: $C_{19}H_{19}N_5OS_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	C	1	Total	C	N	O	S	0
			27	19	5	1	2	
17	N	1	Total	C	N	O	S	0
			27	19	5	1	2	

- Molecule 18 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).

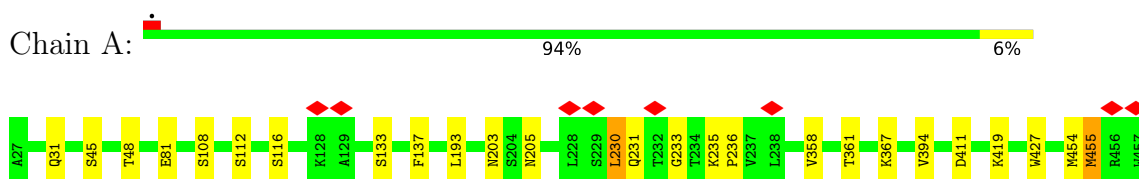


Mol	Chain	Residues	Atoms					AltConf
18	H	1	Total 47	C 37	N 1	O 8	P 1	0
18	S	1	Total 47	C 37	N 1	O 8	P 1	0

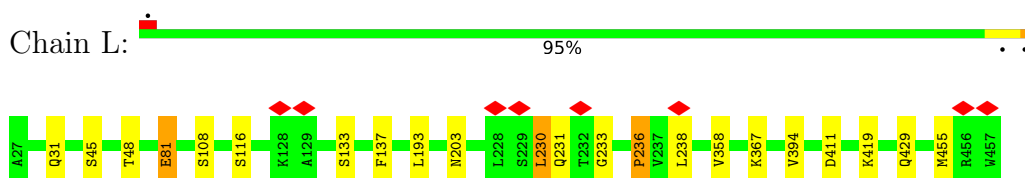
3 Residue-property plots [i](#)

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.

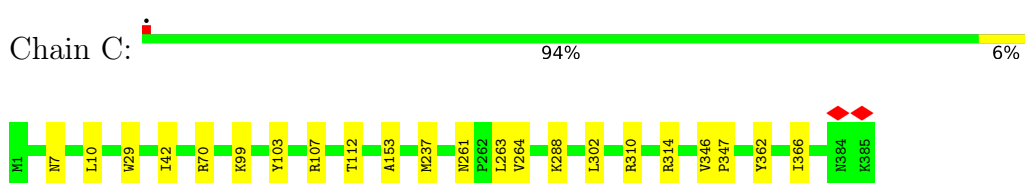
- Molecule 1: COR1 isoform 1



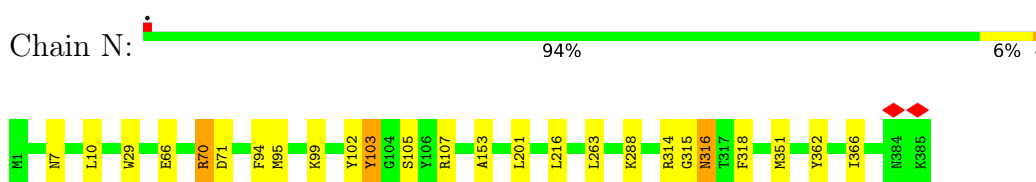
- Molecule 1: COR1 isoform 1



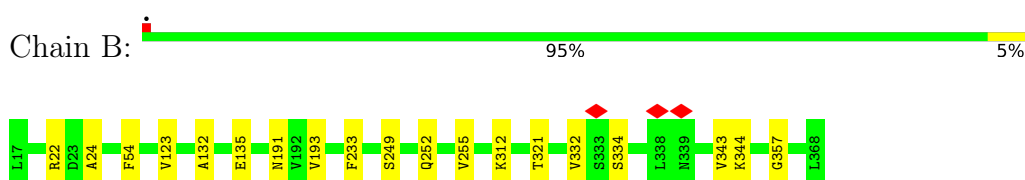
- Molecule 2: Cytochrome b



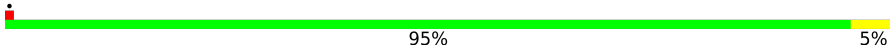
- Molecule 2: Cytochrome b



- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

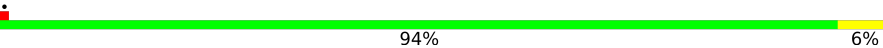


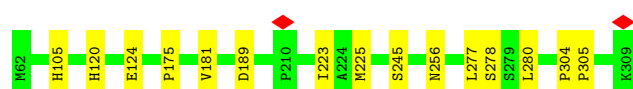
- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  95% 5%

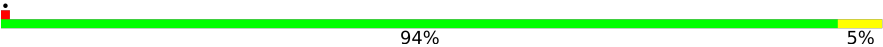


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  94% 6%



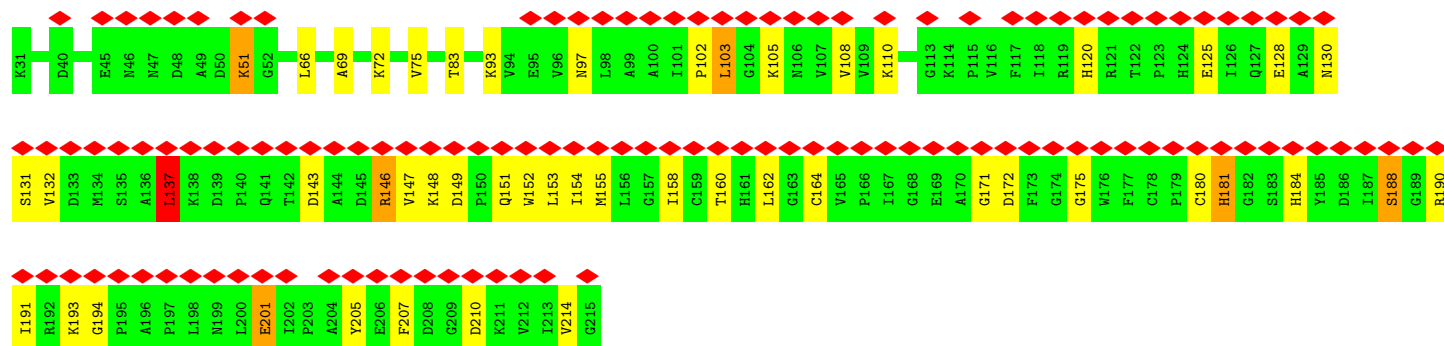
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:  94% 5%



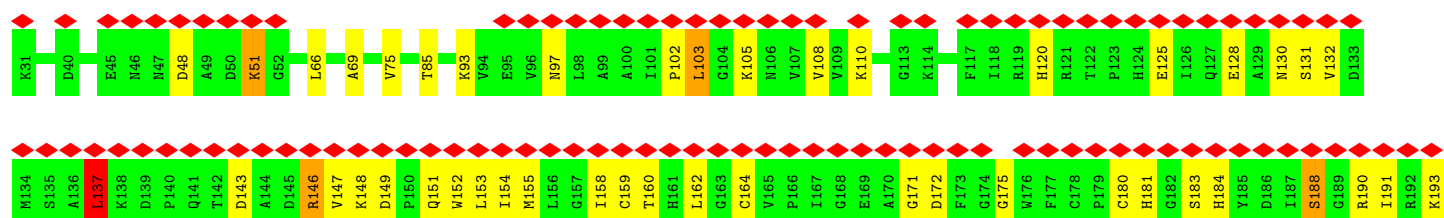
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:  66% 73% 23%



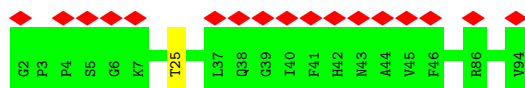
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:  66% 71% 25%

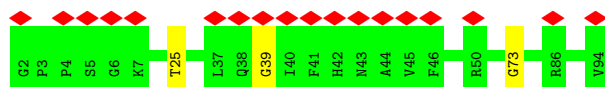




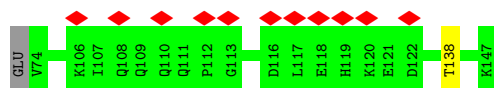
- Molecule 6: Cytochrome b-c1 complex subunit 8



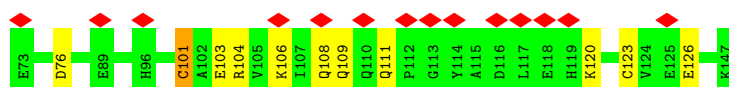
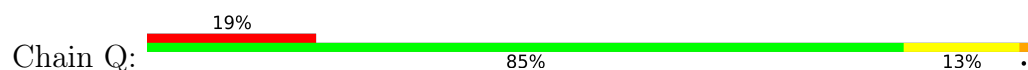
- Molecule 6: Cytochrome b-c1 complex subunit 8



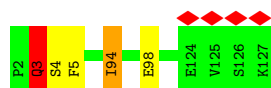
- Molecule 7: QCR6 isoform 1



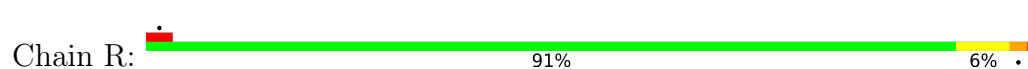
- Molecule 7: QCR6 isoform 1



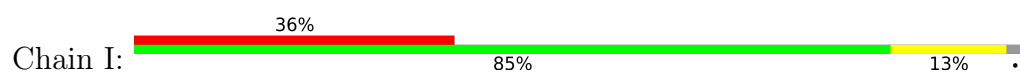
- Molecule 8: Cytochrome b-c1 complex subunit 7



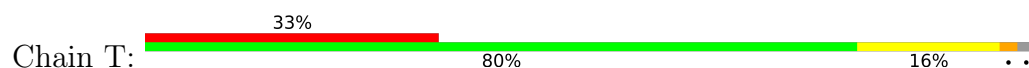
- Molecule 8: Cytochrome b-c1 complex subunit 7



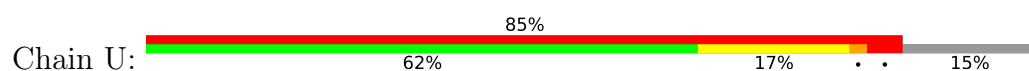
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



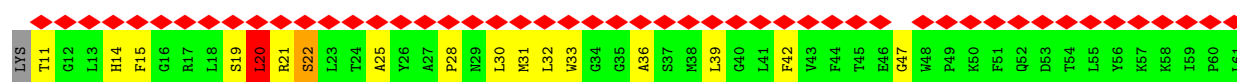
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.48	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.682	Depositor
Minimum map value	-2.774	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8PE, 6PH, CN5, UQ6, CN3, 9PE, A1D6O, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	1/3405 (0.0%)	0.54	0/4615
1	L	0.38	3/3405 (0.1%)	0.55	0/4615
2	C	0.31	0/3192	0.55	1/4354 (0.0%)
2	N	0.33	0/3192	0.56	2/4354 (0.0%)
3	B	0.26	0/2781	0.48	0/3764
3	M	0.26	0/2781	0.48	0/3764
4	D	0.28	0/2022	0.52	0/2751
4	O	0.29	0/2022	0.49	0/2751
5	E	0.37	0/1444	0.83	4/1957 (0.2%)
5	P	0.38	1/1444 (0.1%)	0.82	4/1957 (0.2%)
6	H	0.22	0/804	0.52	0/1088
6	S	0.22	0/804	0.52	0/1088
7	F	0.25	0/638	0.54	0/858
7	Q	0.29	0/647	0.69	1/870 (0.1%)
8	G	0.66	2/1040 (0.2%)	0.83	4/1408 (0.3%)
8	R	0.55	1/1040 (0.1%)	0.93	5/1408 (0.4%)
9	I	0.24	0/455	0.56	0/614
9	T	0.23	0/456	0.64	1/615 (0.2%)
10	U	0.63	0/358	1.49	8/483 (1.7%)
10	V	1.16	3/419 (0.7%)	1.19	8/567 (1.4%)
All	All	0.36	11/32349 (0.0%)	0.62	38/43881 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	C	0	1
5	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	P	0	1
10	U	0	1
10	V	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	3	GLN	C-N	16.89	1.57	1.33
10	V	19	SER	C-N	16.61	1.59	1.33
8	R	5	PHE	C-N	13.94	1.52	1.33
10	V	20	LEU	C-N	12.11	1.51	1.33
1	L	236	PRO	C-N	8.96	1.45	1.33
1	L	233	GLY	C-N	8.62	1.44	1.33
8	G	5	PHE	C-N	-8.45	1.23	1.33
10	V	22	SER	C-N	7.83	1.44	1.33
5	P	159	CYS	C-N	-6.86	1.24	1.33
1	L	238	LEU	C-N	-6.06	1.26	1.33
1	A	233	GLY	C-N	5.42	1.40	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	5	PHE	O-C-N	16.75	146.19	122.41
8	R	5	PHE	CA-C-N	-15.23	98.66	120.29
8	R	5	PHE	C-N-CA	-15.23	98.66	120.29
10	U	31	MET	N-CA-C	-13.25	94.50	114.64
8	G	5	PHE	O-C-N	13.16	138.46	122.27
10	U	40	GLY	O-C-N	10.79	136.72	122.70
8	G	5	PHE	CA-C-N	-10.71	106.52	120.44
8	G	5	PHE	C-N-CA	-10.71	106.52	120.44
8	G	3	GLN	O-C-N	10.61	136.80	122.26
10	U	40	GLY	CA-C-N	-9.06	105.28	121.14
10	U	40	GLY	C-N-CA	-9.06	105.28	121.14
5	E	201	GLU	CA-CB-CG	8.68	131.46	114.10
5	P	201	GLU	CA-CB-CG	8.67	131.45	114.10
10	U	33	TRP	N-CA-C	-7.87	103.82	113.50
10	V	19	SER	CA-C-N	6.89	137.64	121.52
10	V	19	SER	C-N-CA	6.89	137.64	121.52
5	P	201	GLU	CB-CG-CD	6.86	124.27	112.60
5	E	201	GLU	CB-CG-CD	6.85	124.25	112.60
10	V	22	SER	O-C-N	-6.82	112.92	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	21	ARG	CA-C-N	6.71	133.59	122.66
10	V	21	ARG	C-N-CA	6.71	133.59	122.66
10	V	19	SER	O-C-N	-6.57	115.31	123.33
7	Q	101	CYS	N-CA-C	-6.37	105.67	113.50
8	R	5	PHE	CA-CB-CG	6.25	120.05	113.80
2	N	103	TYR	N-CA-C	-6.18	105.59	113.01
9	T	18	VAL	N-CA-C	-6.10	106.86	112.96
5	P	160	THR	CA-C-N	6.06	129.91	120.82
5	P	160	THR	C-N-CA	6.06	129.91	120.82
5	E	160	THR	CA-C-N	6.04	129.88	120.82
5	E	160	THR	C-N-CA	6.04	129.88	120.82
10	U	35	GLY	N-CA-C	-5.89	106.06	115.66
8	R	6	THR	N-CA-C	-5.86	104.97	111.36
2	N	103	TYR	CB-CA-C	5.84	122.09	110.17
10	V	47	GLY	CA-C-N	5.83	130.86	123.34
10	V	47	GLY	C-N-CA	5.83	130.86	123.34
10	U	30	LEU	CA-C-N	5.63	131.71	121.41
10	U	30	LEU	C-N-CA	5.63	131.71	121.41
2	C	103	TYR	N-CA-C	-5.62	106.50	113.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	70	ARG	Sidechain
5	E	137	LEU	Peptide
1	L	455	MET	Peptide
5	P	137	LEU	Peptide
10	U	39	LEU	Mainchain
10	V	20	LEU	Mainchain

5.2 Too-close contacts ⓘ

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	A	3344	0	3323	14	0
1	L	3344	0	3323	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3090	0	3129	13	0
2	N	3090	0	3129	18	0
3	B	2735	0	2774	10	0
3	M	2735	0	2774	11	0
4	D	1961	0	1890	7	0
4	O	1961	0	1890	8	0
5	E	1411	0	1390	23	0
5	P	1411	0	1390	25	0
6	H	773	0	736	0	0
6	S	773	0	736	2	0
7	F	624	0	583	0	0
7	Q	633	0	589	7	0
8	G	1019	0	1034	2	0
8	R	1019	0	1034	7	0
9	I	442	0	440	6	0
9	T	443	0	440	8	0
10	U	347	0	345	8	0
10	V	406	0	414	11	0
11	A	40	0	59	0	0
11	E	40	0	59	4	0
12	C	55	0	66	0	0
12	N	55	0	66	1	0
13	C	40	0	59	1	0
13	N	40	0	59	3	0
14	C	86	0	60	1	0
14	D	43	0	30	0	0
14	N	86	0	60	0	0
14	O	43	0	30	0	0
15	C	41	0	50	0	0
16	C	43	0	60	1	0
16	N	43	0	60	2	0
17	C	27	0	0	0	0
17	N	27	0	0	0	0
18	H	47	0	73	1	0
18	S	47	0	73	3	0
All	All	32364	0	32227	173	0

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

All (173) 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)
10:V:22:SER:HA	10:V:25:ALA:HB3	1.49	0.95
3:B:252:GLN:HG3	3:B:343:VAL:HG22	1.55	0.88
10:U:38:MET:HA	10:U:41:LEU:HD23	1.58	0.84
10:V:14:HIS:CE1	10:V:20:LEU:HD22	2.13	0.84
9:T:23:ALA:HB2	10:U:39:LEU:HD13	1.67	0.77
2:N:66:GLU:O	2:N:70:ARG:HG3	1.87	0.73
8:R:4:SER:O	8:R:8:ILE:HG13	1.89	0.71
10:V:14:HIS:NE2	10:V:20:LEU:HD22	2.07	0.69
9:T:15:ALA:HB1	10:U:32:LEU:C	2.16	0.69
9:T:10:PHE:HB2	9:T:16:VAL:HG11	1.75	0.68
4:O:121:THR:OG1	4:O:124:GLU:HG2	1.93	0.68
1:A:108:SER:HG	1:A:116:SER:HG	1.41	0.68
1:L:108:SER:HG	1:L:116:SER:HG	1.41	0.66
3:M:252:GLN:HG2	3:M:343:VAL:HG22	1.77	0.65
10:V:15:PHE:HA	10:V:20:LEU:HB2	1.78	0.64
3:B:249:SER:HA	3:B:252:GLN:OE1	1.98	0.63
7:Q:101:CYS:O	7:Q:123:CYS:SG	2.57	0.63
5:E:146:ARG:HD3	5:E:147:VAL:HG23	1.82	0.61
7:Q:103:GLU:HG3	7:Q:104:ARG:HG3	1.81	0.61
5:P:146:ARG:HD3	5:P:147:VAL:HG23	1.82	0.61
5:E:102:PRO:HB2	5:E:105:LYS:HD3	1.82	0.61
1:L:45:SER:HB2	3:M:22:ARG:HH22	1.67	0.60
4:D:280:LEU:HD13	5:E:66:LEU:HB2	1.83	0.60
10:V:30:LEU:HA	10:V:33:TRP:HB2	1.83	0.59
5:P:102:PRO:HB2	5:P:105:LYS:HD3	1.82	0.59
9:T:18:VAL:HG21	10:U:33:TRP:CZ2	2.38	0.59
5:P:130:ASN:HD22	5:P:143:ASP:HB3	1.67	0.58
14:C:403:HEM:HBC2	14:C:403:HEM:HHD	1.84	0.58
5:E:110:LYS:HD2	2:N:263:LEU:HD11	1.84	0.57
5:E:164:CYS:CB	5:E:180:CYS:HB2	2.35	0.57
5:P:164:CYS:CB	5:P:180:CYS:HB2	2.35	0.57
1:L:358:VAL:HG12	1:L:419:LYS:HE3	1.87	0.56
1:A:358:VAL:HG12	1:A:419:LYS:HE3	1.87	0.56
3:M:54:PHE:HD1	3:M:123:VAL:HG21	1.70	0.56
5:P:103:LEU:HA	5:P:120:HIS:HB3	1.88	0.56
9:I:8:LYS:HG3	9:I:12:LYS:HD2	1.86	0.56
1:L:203:ASN:HD22	1:L:230:LEU:HB3	1.70	0.56
1:A:203:ASN:HD22	1:A:230:LEU:HB3	1.70	0.56
2:C:42:ILE:HG12	11:E:301:6PH:H2D	1.87	0.55
7:Q:108:GLN:HA	7:Q:111:GLN:HG3	1.87	0.55
5:E:137:LEU:HD23	5:E:190:ARG:HG3	1.88	0.55
5:P:137:LEU:HD23	5:P:190:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:54:PHE:HD1	3:B:123:VAL:HG21	1.70	0.55
4:O:289:LYS:HZ3	6:S:39:GLY:H	1.53	0.55
5:E:103:LEU:HA	5:E:120:HIS:HB3	1.88	0.55
3:M:255:VAL:HG22	3:M:321:THR:HG21	1.89	0.55
5:E:205:TYR:HB3	5:E:214:VAL:HA	1.89	0.55
1:A:45:SER:HB2	3:B:22:ARG:HH22	1.69	0.54
3:B:255:VAL:HG22	3:B:321:THR:HG21	1.89	0.54
10:U:26:TYR:O	10:U:30:LEU:HB2	2.07	0.54
4:D:105:HIS:HE1	4:D:175:PRO:HD2	1.73	0.54
4:O:105:HIS:HE1	4:O:175:PRO:HD2	1.73	0.54
9:I:29:GLN:HG3	9:I:30:THR:HG23	1.89	0.54
5:P:205:TYR:HB3	5:P:214:VAL:HA	1.89	0.54
5:E:164:CYS:HG	5:E:180:CYS:CB	2.17	0.53
5:E:130:ASN:HD22	5:E:143:ASP:HB3	1.72	0.53
2:C:362:TYR:HA	2:C:366:ILE:HB	1.91	0.52
4:O:243:THR:HB	7:Q:76:ASP:HB3	1.90	0.52
1:A:454:MET:O	1:A:455:MET:HB2	2.10	0.51
9:T:14:ASN:HA	9:T:17:PHE:HB3	1.92	0.51
2:N:7:ASN:HB3	2:N:10:LEU:HB2	1.92	0.51
2:C:107:ARG:HD3	2:C:314:ARG:HG3	1.93	0.51
4:O:223:ILE:HG12	4:O:225:MET:H	1.76	0.51
2:N:362:TYR:HA	2:N:366:ILE:HB	1.91	0.51
7:Q:106:LYS:HA	7:Q:109:GLN:HG2	1.93	0.50
2:C:7:ASN:HB3	2:C:10:LEU:HB2	1.92	0.50
5:P:164:CYS:HB3	5:P:181:HIS:NE2	2.27	0.50
9:T:18:VAL:HG21	10:U:33:TRP:CH2	2.46	0.50
5:P:164:CYS:SG	5:P:180:CYS:CB	2.99	0.50
7:Q:101:CYS:SG	7:Q:126:GLU:OE1	2.69	0.50
5:E:164:CYS:SG	5:E:180:CYS:CB	2.99	0.50
4:D:223:ILE:HG12	4:D:225:MET:H	1.76	0.50
5:E:191:ILE:HD12	5:E:194:GLY:H	1.77	0.50
10:V:39:LEU:HD13	10:V:42:PHE:HD1	1.77	0.50
8:R:94:ILE:HG23	8:R:98:GLU:HG3	1.93	0.49
4:O:280:LEU:HD13	5:P:66:LEU:HB2	1.94	0.49
5:E:164:CYS:HB3	5:E:181:HIS:NE2	2.27	0.49
2:N:107:ARG:HD3	2:N:314:ARG:HG3	1.93	0.49
2:N:94:PHE:HB3	18:S:101:8PE:H3AA	1.94	0.49
5:P:191:ILE:HD12	5:P:194:GLY:H	1.77	0.49
2:N:351:MET:HE1	6:S:73:GLY:HA3	1.95	0.48
8:G:94:ILE:HG23	8:G:98:GLU:HG3	1.93	0.48
2:C:153:ALA:HB2	2:C:288:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:153:ALA:HB2	2:N:288:LYS:HG3	1.96	0.48
1:L:367:LYS:HD3	1:L:411:ASP:HA	1.96	0.47
5:E:51:LYS:HA	5:E:51:LYS:HD3	1.74	0.47
1:A:367:LYS:HD3	1:A:411:ASP:HA	1.96	0.47
5:E:69:ALA:HB2	9:I:25:ALA:HB1	1.97	0.47
5:E:188:SER:HB2	5:E:190:ARG:HD3	1.97	0.47
5:P:69:ALA:HB2	9:T:25:ALA:HB1	1.96	0.47
5:P:51:LYS:HA	5:P:51:LYS:HD3	1.74	0.46
5:P:188:SER:HB2	5:P:190:ARG:HD3	1.97	0.46
4:D:120:HIS:HB3	4:D:124:GLU:HB3	1.97	0.46
2:C:112:THR:HG23	13:N:404:9PE:H3A	1.97	0.46
2:N:7:ASN:HD21	13:N:404:9PE:H23A	1.80	0.46
1:A:137:PHE:HE1	1:A:193:LEU:HD22	1.81	0.46
5:E:149:ASP:HA	5:E:207:PHE:HZ	1.80	0.46
1:L:137:PHE:HE1	1:L:193:LEU:HD22	1.81	0.46
5:P:149:ASP:HA	5:P:207:PHE:HZ	1.80	0.46
10:V:14:HIS:CD2	10:V:20:LEU:HD13	2.50	0.46
3:M:233:PHE:HB3	3:M:357:GLY:HA2	1.99	0.45
4:D:277:LEU:HD11	11:E:301:6PH:H36	1.97	0.45
3:B:233:PHE:HB3	3:B:357:GLY:HA2	1.99	0.45
8:R:3:GLN:O	8:R:4:SER:HB3	2.17	0.45
2:C:310:ARG:O	8:G:3:GLN:HB2	2.15	0.45
1:A:230:LEU:HD23	1:A:231:GLN:H	1.82	0.45
1:L:230:LEU:HD23	1:L:231:GLN:H	1.82	0.45
2:N:71:ASP:HB3	5:P:85:THR:HG22	1.98	0.44
5:P:164:CYS:SG	5:P:180:CYS:HB2	2.58	0.44
1:A:427:TRP:HE1	9:I:12:LYS:HG3	1.82	0.44
3:B:24:ALA:HB3	3:B:191:ASN:OD1	2.17	0.44
5:E:164:CYS:SG	5:E:180:CYS:HB2	2.57	0.44
9:I:16:VAL:HG23	10:V:32:LEU:HD21	1.99	0.44
4:O:304:PRO:HA	4:O:305:PRO:HD3	1.91	0.44
3:M:24:ALA:HB3	3:M:191:ASN:OD1	2.17	0.44
2:N:216:LEU:HD13	8:R:75:ILE:HG21	1.99	0.44
11:E:301:6PH:H26	11:E:301:6PH:H29	1.77	0.44
2:N:95:MET:HG2	18:S:101:8PE:H37A	1.99	0.44
12:N:401:CN3:H67	12:N:401:CN3:H23	2.00	0.44
5:P:48:ASP:CG	5:P:51:LYS:HB2	2.43	0.43
3:M:132:ALA:HA	3:M:135:GLU:HG2	2.00	0.43
9:T:12:LYS:HG2	9:T:13:ARG:HE	1.83	0.43
3:M:312:LYS:HD3	3:M:312:LYS:HA	1.76	0.43
5:P:151:GLN:HG3	5:P:152:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:120:LYS:HB3	7:Q:120:LYS:HE2	1.78	0.43
2:N:103:TYR:O	2:N:315:GLY:HA2	2.18	0.43
13:N:404:9PE:H2G	13:N:404:9PE:H2D	1.73	0.43
4:O:247:MET:HE3	4:O:247:MET:HB2	1.83	0.43
2:C:263:LEU:HD11	5:P:110:LYS:HD2	2.00	0.43
3:B:132:ALA:HA	3:B:135:GLU:HG2	2.00	0.43
5:E:191:ILE:HD12	5:E:194:GLY:N	2.34	0.42
3:M:332:VAL:HG22	3:M:334:SER:H	1.84	0.42
1:A:112:SER:O	1:A:112:SER:OG	2.32	0.42
9:I:13:ARG:HB2	9:I:16:VAL:HB	2.00	0.42
10:U:33:TRP:O	10:U:36:ALA:HB3	2.20	0.42
5:E:151:GLN:HG3	5:E:152:TRP:CD1	2.54	0.42
10:V:33:TRP:HA	10:V:36:ALA:HB3	2.02	0.42
2:C:237:MET:HG2	11:E:301:6PH:H29A	2.01	0.42
2:N:201:LEU:HD21	16:N:403:UQ6:H3M3	2.01	0.42
16:C:406:UQ6:H1M1	16:C:406:UQ6:H71	1.78	0.42
1:A:205:ASN:HD21	1:A:235:LYS:HD3	1.85	0.42
3:B:312:LYS:HD3	3:B:312:LYS:HA	1.76	0.42
10:V:28:PRO:HA	10:V:31:MET:HG3	2.01	0.42
3:B:332:VAL:HG22	3:B:334:SER:H	1.84	0.41
1:L:81:GLU:H	1:L:81:GLU:HG2	1.55	0.41
5:P:172:ASP:H	5:P:184:HIS:CE1	2.38	0.41
1:A:31:GLN:HE21	1:A:394:VAL:HG13	1.86	0.41
5:E:172:ASP:H	5:E:184:HIS:CE1	2.38	0.41
2:N:99:LYS:HA	18:S:101:8PE:H32A	2.02	0.41
1:L:31:GLN:HE21	1:L:394:VAL:HG13	1.86	0.41
10:U:34:GLY:C	10:U:36:ALA:H	2.27	0.41
2:C:346:VAL:HA	2:C:347:PRO:HA	1.91	0.41
5:P:191:ILE:H	5:P:191:ILE:HG12	1.71	0.41
16:N:403:UQ6:H222	16:N:403:UQ6:H201	1.71	0.41
2:N:318:PHE:HB3	8:R:36:ALA:HB1	2.03	0.41
5:P:191:ILE:HD12	5:P:194:GLY:N	2.34	0.41
1:A:454:MET:HE3	1:A:454:MET:HB2	1.93	0.41
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.91	0.41
1:A:361:THR:HG21	8:R:123:ILE:HG23	2.01	0.41
4:D:181:VAL:HG21	4:D:256:ASN:HA	2.03	0.41
2:N:29:TRP:HB3	2:N:99:LYS:HG3	2.02	0.41
5:P:171:GLY:HA3	5:P:175:GLY:HA3	2.02	0.41
13:C:402:9PE:H29A	13:C:402:9PE:H2C	1.95	0.41
5:E:171:GLY:HA3	5:E:175:GLY:HA3	2.02	0.41
3:M:252:GLN:CG	3:M:343:VAL:HG22	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:TRP:HB3	2:C:99:LYS:HG3	2.02	0.40
5:P:183:SER:HB3	5:P:195:PRO:HD2	2.03	0.40
5:E:164:CYS:HB3	5:E:181:HIS:CE1	2.56	0.40
3:M:53:ARG:HD3	3:M:53:ARG:HA	1.95	0.40
2:C:261:ASN:HD22	2:C:264:VAL:HG12	1.86	0.40
2:C:302:LEU:HD11	18:H:101:8PE:H3IB	2.04	0.40
2:N:102:TYR:HA	2:N:316:ASN:ND2	2.37	0.40
8:R:119:GLU:HB3	10:V:11:THR:HG22	2.04	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	A	429/431 (100%)	390 (91%)	38 (9%)	1 (0%)	43	62
1	L	429/431 (100%)	390 (91%)	38 (9%)	1 (0%)	43	62
2	C	383/385 (100%)	362 (94%)	21 (6%)	0	100	100
2	N	383/385 (100%)	362 (94%)	21 (6%)	0	100	100
3	B	350/352 (99%)	327 (93%)	23 (7%)	0	100	100
3	M	350/352 (99%)	327 (93%)	23 (7%)	0	100	100
4	D	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
4	O	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
5	E	183/185 (99%)	162 (88%)	21 (12%)	0	100	100
5	P	183/185 (99%)	162 (88%)	21 (12%)	0	100	100
6	H	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
6	S	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
7	F	72/75 (96%)	69 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Q	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
8	G	124/126 (98%)	119 (96%)	4 (3%)	1 (1%)	16	29
8	R	124/126 (98%)	119 (96%)	4 (3%)	1 (1%)	16	29
9	I	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
9	T	52/55 (94%)	47 (90%)	5 (10%)	0	100	100
10	U	42/52 (81%)	33 (79%)	9 (21%)	0	100	100
10	V	49/52 (94%)	34 (69%)	15 (31%)	0	100	100
All	All	3952/4004 (99%)	3657 (92%)	291 (7%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	G	4	SER
1	L	236	PRO
1	A	236	PRO
8	R	4	SER

5.3.2 Protein sidechains ⓘ

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	A	370/370 (100%)	365 (99%)	5 (1%)	59	74
1	L	370/370 (100%)	365 (99%)	5 (1%)	59	74
2	C	338/338 (100%)	338 (100%)	0	100	100
2	N	338/338 (100%)	335 (99%)	3 (1%)	70	82
3	B	301/301 (100%)	299 (99%)	2 (1%)	76	85
3	M	301/301 (100%)	299 (99%)	2 (1%)	76	85
4	D	206/206 (100%)	203 (98%)	3 (2%)	57	73
4	O	206/206 (100%)	203 (98%)	3 (2%)	57	73
5	E	151/151 (100%)	126 (83%)	25 (17%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	151/151 (100%)	129 (85%)	22 (15%)	3	4
6	H	77/77 (100%)	76 (99%)	1 (1%)	61	75
6	S	77/77 (100%)	76 (99%)	1 (1%)	61	75
7	F	67/68 (98%)	66 (98%)	1 (2%)	57	73
7	Q	68/68 (100%)	68 (100%)	0	100	100
8	G	110/110 (100%)	108 (98%)	2 (2%)	51	69
8	R	110/110 (100%)	106 (96%)	4 (4%)	31	53
9	I	44/45 (98%)	44 (100%)	0	100	100
9	T	45/45 (100%)	45 (100%)	0	100	100
10	U	35/43 (81%)	33 (94%)	2 (6%)	18	34
10	V	42/43 (98%)	41 (98%)	1 (2%)	43	63
All	All	3407/3418 (100%)	3325 (98%)	82 (2%)	43	63

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	81	GLU
1	A	133	SER
1	A	230	LEU
1	A	455	MET
3	B	193	VAL
3	B	344	LYS
4	D	189	ASP
4	D	245	SER
4	D	278	SER
5	E	51	LYS
5	E	72	LYS
5	E	75	VAL
5	E	83	THR
5	E	93	LYS
5	E	97	ASN
5	E	103	LEU
5	E	108	VAL
5	E	125	GLU
5	E	128	GLU
5	E	131	SER
5	E	132	VAL

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Mol	Chain	Res	Type
5	E	137	LEU
5	E	146	ARG
5	E	148	LYS
5	E	153	LEU
5	E	154	ILE
5	E	155	MET
5	E	158	ILE
5	E	162	LEU
5	E	181	HIS
5	E	188	SER
5	E	193	LYS
5	E	201	GLU
5	E	210	ASP
6	H	25	THR
2	N	70	ARG
2	N	105	SER
2	N	316	ASN
7	F	138	THR
8	G	3	GLN
8	G	94	ILE
1	L	48	THR
1	L	81	GLU
1	L	133	SER
1	L	230	LEU
1	L	429	GLN
3	M	193	VAL
3	M	344	LYS
4	O	245	SER
4	O	278	SER
4	O	289	LYS
6	S	25	THR
5	P	51	LYS
5	P	75	VAL
5	P	93	LYS
5	P	97	ASN
5	P	103	LEU
5	P	108	VAL
5	P	125	GLU
5	P	128	GLU
5	P	131	SER
5	P	132	VAL
5	P	137	LEU

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Mol	Chain	Res	Type
5	P	146	ARG
5	P	148	LYS
5	P	153	LEU
5	P	154	ILE
5	P	155	MET
5	P	158	ILE
5	P	162	LEU
5	P	188	SER
5	P	193	LYS
5	P	201	GLU
5	P	210	ASP
8	R	3	GLN
8	R	4	SER
8	R	6	THR
8	R	94	ILE
10	U	30	LEU
10	U	33	TRP
10	V	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	102	GLN
1	A	156	HIS
1	A	187	ASN
1	A	199	ASN
1	A	203	ASN
1	A	205	ASN
1	A	227	ASN
1	A	283	GLN
1	A	298	GLN
1	A	317	HIS
1	A	352	ASN
1	A	385	ASN
1	A	388	ASN
2	C	57	ASN
2	C	67	HIS
2	C	215	ASN
2	C	261	ASN
2	C	332	ASN
3	B	36	HIS

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Mol	Chain	Res	Type
3	B	52	ASN
3	B	58	ASN
4	D	127	ASN
5	E	97	ASN
5	E	120	HIS
5	E	184	HIS
6	H	55	GLN
2	N	7	ASN
2	N	57	ASN
2	N	67	HIS
2	N	74	ASN
2	N	215	ASN
2	N	261	ASN
2	N	316	ASN
2	N	332	ASN
7	F	111	GLN
8	G	30	ASN
8	G	79	HIS
8	G	85	HIS
9	I	44	ASN
1	L	42	HIS
1	L	102	GLN
1	L	156	HIS
1	L	187	ASN
1	L	199	ASN
1	L	203	ASN
1	L	205	ASN
1	L	227	ASN
1	L	283	GLN
1	L	298	GLN
1	L	314	ASN
1	L	316	ASN
1	L	317	HIS
1	L	352	ASN
1	L	385	ASN
1	L	388	ASN
3	M	36	HIS
3	M	52	ASN
3	M	58	ASN
4	O	127	ASN
5	P	46	ASN
5	P	97	ASN

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Mol	Chain	Res	Type
5	P	120	HIS
5	P	184	HIS
8	R	30	ASN
9	T	44	ASN
10	U	29	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
13	9PE	N	404	-	39,39,39	0.99	4 (10%)	42,44,44	1.07	2 (4%)
14	HEM	D	401	4	50,50,50	1.44	7 (14%)	67,82,82	1.13	4 (5%)
11	6PH	E	301	-	39,39,39	0.94	4 (10%)	42,44,44	1.22	2 (4%)
13	9PE	C	402	-	39,39,39	0.97	4 (10%)	42,44,44	1.08	2 (4%)
18	8PE	S	101	-	46,46,46	0.90	4 (8%)	49,51,51	1.33	2 (4%)
14	HEM	C	403	2	50,50,50	1.57	9 (18%)	67,82,82	1.57	12 (17%)
14	HEM	N	405	2	50,50,50	1.55	8 (16%)	67,82,82	1.52	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEM	C	404	2	50,50,50	1.36	6 (12%)	67,82,82	1.20	6 (8%)
14	HEM	N	402	2	50,50,50	1.32	5 (10%)	67,82,82	1.10	5 (7%)
14	HEM	O	401	4	50,50,50	1.44	7 (14%)	67,82,82	1.13	4 (5%)
15	CN5	C	405	-	40,40,40	0.33	0	44,48,48	0.43	0
17	A1D6O	C	407	-	30,30,30	2.01	7 (23%)	40,44,44	4.49	17 (42%)
12	CN3	C	401	-	54,54,54	1.18	8 (14%)	60,66,66	1.23	5 (8%)
12	CN3	N	401	-	54,54,54	1.18	8 (14%)	60,66,66	1.21	4 (6%)
18	8PE	H	101	-	46,46,46	0.91	4 (8%)	49,51,51	1.12	2 (4%)
17	A1D6O	N	406	-	30,30,30	2.01	7 (23%)	40,44,44	4.48	17 (42%)
16	UQ6	C	406	-	43,43,43	1.62	11 (25%)	54,55,55	1.58	13 (24%)
11	6PH	A	501	-	39,39,39	0.95	4 (10%)	42,44,44	1.17	2 (4%)
16	UQ6	N	403	-	43,43,43	1.69	10 (23%)	54,55,55	1.54	11 (20%)

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
13	9PE	N	404	-	-	21/43/43/43	-
14	HEM	D	401	4	-	2/14/54/54	-
11	6PH	E	301	-	-	22/41/41/41	-
13	9PE	C	402	-	-	15/43/43/43	-
18	8PE	S	101	-	-	31/50/50/50	-
14	HEM	C	403	2	-	7/14/54/54	-
14	HEM	N	405	2	-	6/14/54/54	-
14	HEM	C	404	2	-	4/14/54/54	-
14	HEM	N	402	2	-	2/14/54/54	-
14	HEM	O	401	4	-	0/14/54/54	-
15	CN5	C	405	-	-	23/44/44/44	-
17	A1D6O	C	407	-	-	2/9/9/9	0/4/4/4
12	CN3	C	401	-	-	30/65/65/65	-
12	CN3	N	401	-	-	26/65/65/65	-
18	8PE	H	101	-	-	18/50/50/50	-
17	A1D6O	N	406	-	-	2/9/9/9	0/4/4/4
16	UQ6	C	406	-	-	11/39/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	6PH	A	501	-	-	21/41/41/41	-
16	UQ6	N	403	-	-	10/39/39/39	0/1/1/1

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	407	A1D6O	C08-S07	-5.39	1.68	1.75
17	N	406	A1D6O	C08-S07	-5.28	1.68	1.75
16	N	403	UQ6	C7-C6	5.19	1.57	1.51
17	C	407	A1D6O	C08-S10	5.13	1.83	1.74
17	N	406	A1D6O	C08-S10	5.12	1.83	1.74
16	C	406	UQ6	C7-C6	4.72	1.56	1.51
14	N	405	HEM	FE-NB	4.68	2.09	1.94
14	C	403	HEM	FE-NB	4.53	2.08	1.94
14	O	401	HEM	FE-NB	4.20	2.07	1.94
14	D	401	HEM	FE-NB	4.17	2.07	1.94
14	N	405	HEM	FE-ND	4.03	2.07	1.94
14	C	403	HEM	FE-NC	3.73	2.07	1.95
16	N	403	UQ6	C16-C14	3.65	1.58	1.51
14	C	403	HEM	FE-ND	3.64	2.06	1.94
17	N	406	A1D6O	O24-C23	-3.53	1.16	1.22
17	C	407	A1D6O	O24-C23	-3.48	1.16	1.22
17	N	406	A1D6O	C23-N19	-3.47	1.33	1.38
16	C	406	UQ6	C16-C14	3.44	1.58	1.51
14	N	402	HEM	FE-ND	3.43	2.05	1.94
14	C	404	HEM	FE-ND	3.42	2.05	1.94
17	C	407	A1D6O	C23-N19	-3.40	1.34	1.38
14	D	401	HEM	FE-NA	3.29	2.06	1.95
14	O	401	HEM	FE-NA	3.29	2.06	1.95
14	C	404	HEM	CAB-C3B	3.17	1.55	1.47
14	D	401	HEM	CAB-C3B	3.16	1.55	1.47
14	O	401	HEM	CAB-C3B	3.15	1.55	1.47
14	C	404	HEM	FE-NA	3.14	2.05	1.95
14	D	401	HEM	CAC-C3C	3.12	1.55	1.47
14	O	401	HEM	CAC-C3C	3.12	1.55	1.47
14	N	402	HEM	CAB-C3B	3.11	1.55	1.47
14	N	405	HEM	CAB-C3B	3.07	1.55	1.47
14	N	405	HEM	FE-NC	3.06	2.05	1.95
14	N	402	HEM	CAC-C3C	3.05	1.55	1.47
14	C	404	HEM	CAC-C3C	3.02	1.55	1.47
14	D	401	HEM	FE-ND	2.98	2.04	1.94
14	O	401	HEM	FE-ND	2.98	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	403	HEM	CAB-C3B	2.97	1.55	1.47
14	N	402	HEM	FE-NA	2.85	2.04	1.95
16	N	403	UQ6	C11-C9	2.85	1.57	1.51
16	N	403	UQ6	C12-C13	2.83	1.59	1.50
14	C	403	HEM	FE-NA	2.79	2.04	1.95
12	N	401	CN3	O51-C2'	-2.78	1.40	1.46
18	H	101	8PE	O21-C2	-2.77	1.40	1.46
11	A	501	6PH	O21-C2	-2.75	1.40	1.46
14	N	405	HEM	CAC-C3C	2.72	1.54	1.47
12	N	401	CN3	O21-C2	-2.71	1.40	1.46
16	C	406	UQ6	C12-C13	2.70	1.58	1.50
14	N	405	HEM	FE-NA	2.69	2.04	1.95
11	E	301	6PH	O21-C2	-2.67	1.40	1.46
12	C	401	CN3	O21-C2	-2.66	1.40	1.46
14	C	403	HEM	CAC-C3C	2.66	1.54	1.47
12	C	401	CN3	O51-C2'	-2.63	1.40	1.46
13	N	404	9PE	O21-C2	-2.60	1.40	1.46
11	A	501	6PH	O31-C31	2.60	1.40	1.33
16	N	403	UQ6	O3-C3	2.53	1.43	1.38
13	C	402	9PE	O21-C2	-2.51	1.40	1.46
17	C	407	A1D6O	C13-C12	-2.49	1.37	1.40
17	N	406	A1D6O	C13-C12	-2.46	1.37	1.40
18	S	101	8PE	O21-C21	2.43	1.41	1.34
16	C	406	UQ6	O3-C3	2.42	1.42	1.38
12	C	401	CN3	O31-C31	2.41	1.40	1.33
12	N	401	CN3	O41-C3'	-2.39	1.39	1.45
18	H	101	8PE	O31-C31	2.38	1.40	1.33
16	C	406	UQ6	C11-C9	2.38	1.56	1.51
18	S	101	8PE	O31-C3	-2.37	1.39	1.45
12	N	401	CN3	O31-C3	-2.37	1.39	1.45
16	N	403	UQ6	C17-C18	2.36	1.57	1.50
16	C	406	UQ6	C21-C19	2.35	1.56	1.51
16	N	403	UQ6	C7-C8	2.34	1.55	1.50
13	N	404	9PE	O31-C3	-2.34	1.39	1.45
12	C	401	CN3	O41-C3'	-2.33	1.40	1.45
12	N	401	CN3	O41-C41	2.33	1.40	1.33
11	E	301	6PH	O31-C31	2.33	1.40	1.33
14	D	401	HEM	C2A-C3A	-2.32	1.32	1.38
12	N	401	CN3	O31-C31	2.32	1.40	1.33
14	C	403	HEM	C3C-C2C	-2.31	1.32	1.37
13	N	404	9PE	O31-C31	2.30	1.40	1.33
14	C	403	HEM	C2A-C3A	-2.30	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	101	8PE	O21-C2	-2.30	1.41	1.46
14	O	401	HEM	C2A-C3A	-2.29	1.32	1.38
14	N	405	HEM	C2A-C3A	-2.28	1.32	1.38
14	C	404	HEM	C2A-C3A	-2.27	1.33	1.38
13	C	402	9PE	O31-C31	2.27	1.40	1.33
18	H	101	8PE	O31-C3	-2.26	1.40	1.45
12	C	401	CN3	O41-C41	2.25	1.39	1.33
13	N	404	9PE	O21-C21	2.24	1.40	1.34
13	C	402	9PE	O31-C3	-2.24	1.40	1.45
12	C	401	CN3	O21-C21	2.23	1.40	1.34
12	C	401	CN3	O31-C3	-2.22	1.40	1.45
12	C	401	CN3	O51-C51	2.22	1.40	1.34
12	N	401	CN3	O21-C21	2.21	1.40	1.34
18	S	101	8PE	O31-C31	2.20	1.39	1.33
16	N	403	UQ6	C31-C29	2.19	1.55	1.51
16	N	403	UQ6	C21-C19	2.19	1.55	1.51
16	C	406	UQ6	C7-C8	2.19	1.55	1.50
18	H	101	8PE	O21-C21	2.18	1.40	1.34
13	C	402	9PE	O21-C21	2.18	1.40	1.34
11	A	501	6PH	O21-C21	2.16	1.40	1.34
14	D	401	HEM	FE-NC	2.16	2.02	1.95
16	N	403	UQ6	C26-C24	2.15	1.55	1.51
12	N	401	CN3	O51-C51	2.14	1.40	1.34
17	N	406	A1D6O	C04-S07	-2.13	1.70	1.74
16	C	406	UQ6	C17-C18	2.13	1.56	1.50
11	E	301	6PH	O31-C3	-2.13	1.40	1.45
14	O	401	HEM	FE-NC	2.13	2.02	1.95
16	C	406	UQ6	C22-C23	2.13	1.56	1.50
17	C	407	A1D6O	C04-S07	-2.11	1.70	1.74
16	C	406	UQ6	C31-C29	2.09	1.55	1.51
14	C	403	HEM	CMB-C2B	2.09	1.55	1.50
16	C	406	UQ6	C26-C24	2.08	1.55	1.51
14	C	404	HEM	CMB-C2B	2.08	1.55	1.50
11	E	301	6PH	O21-C21	2.07	1.40	1.34
11	A	501	6PH	O31-C3	-2.06	1.40	1.45
14	N	402	HEM	CMB-C2B	2.06	1.55	1.50
17	C	407	A1D6O	N19-N20	-2.05	1.34	1.36
14	N	405	HEM	CMB-C2B	2.04	1.55	1.50
17	N	406	A1D6O	N19-N20	-2.01	1.34	1.36

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	407	A1D6O	N19-C23-N22	16.33	108.92	101.46
17	N	406	A1D6O	N19-C23-N22	16.32	108.92	101.46
17	C	407	A1D6O	C04-S07-C08	12.00	98.75	88.77
17	N	406	A1D6O	C04-S07-C08	11.99	98.74	88.77
17	N	406	A1D6O	S07-C08-N09	-10.17	104.24	116.34
17	C	407	A1D6O	S07-C08-N09	-10.13	104.30	116.34
17	C	407	A1D6O	C11-S10-C08	8.66	117.35	102.46
17	N	406	A1D6O	C11-S10-C08	8.58	117.20	102.46
17	N	406	A1D6O	C05-C04-S07	-5.61	105.50	109.71
17	C	407	A1D6O	C05-C04-S07	-5.59	105.52	109.71
18	S	101	8PE	O21-C21-C22	5.16	122.64	111.48
14	N	405	HEM	CAD-C3D-C4D	5.10	133.59	124.70
14	C	403	HEM	CAD-C3D-C4D	4.99	133.39	124.70
12	C	401	CN3	O51-C51-C52	4.62	121.47	111.48
17	C	407	A1D6O	C23-N19-N20	-4.58	107.49	110.53
17	C	407	A1D6O	C13-N19-N20	4.56	127.95	120.14
17	N	406	A1D6O	C13-N19-N20	4.51	127.86	120.14
17	N	406	A1D6O	C23-N19-N20	-4.47	107.57	110.53
14	N	405	HEM	CAD-C3D-C2D	-4.46	119.52	127.87
11	E	301	6PH	O21-C21-C22	4.42	121.04	111.48
16	C	406	UQ6	C7-C8-C9	-4.35	121.18	127.42
17	N	406	A1D6O	C05-N09-C08	4.35	118.42	110.14
17	C	407	A1D6O	C05-N09-C08	4.32	118.36	110.14
17	C	407	A1D6O	C06-C01-C02	-4.24	118.09	122.13
14	C	403	HEM	CAD-C3D-C2D	-4.19	120.03	127.87
17	N	406	A1D6O	C06-C01-C02	-4.17	118.16	122.13
13	C	402	9PE	O21-C21-C22	4.09	120.33	111.48
17	C	407	A1D6O	C11-C12-C17	4.07	123.61	119.60
17	N	406	A1D6O	C11-C12-C17	4.07	123.61	119.60
12	N	401	CN3	O21-C21-C22	3.92	119.97	111.48
11	A	501	6PH	O21-C21-C22	3.88	119.88	111.48
16	C	406	UQ6	C20-C19-C21	3.82	121.86	115.23
12	N	401	CN3	O51-C51-C52	3.74	119.56	111.48
18	H	101	8PE	O21-C21-C22	3.69	119.47	111.48
16	N	403	UQ6	C15-C14-C16	3.67	121.61	115.23
12	C	401	CN3	O21-C21-C22	3.66	119.40	111.48
17	C	407	A1D6O	C01-C06-C05	3.61	122.20	118.45
13	N	404	9PE	O21-C21-C22	3.60	119.27	111.48
17	N	406	A1D6O	C01-C06-C05	3.54	122.14	118.45
17	C	407	A1D6O	C25-N22-N21	3.54	126.89	121.08
17	N	406	A1D6O	C25-N22-N21	3.51	126.85	121.08
17	C	407	A1D6O	C03-C04-S07	3.48	134.76	126.07
16	N	403	UQ6	C10-C9-C11	3.48	121.27	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	406	A1D6O	C03-C04-S07	3.47	134.73	126.07
16	C	406	UQ6	C12-C13-C14	-3.32	120.03	127.62
12	N	401	CN3	O31-C31-C32	3.30	121.16	111.15
12	C	401	CN3	O31-C31-C32	3.29	121.14	111.15
14	D	401	HEM	CMB-C2B-C1B	-3.17	120.08	125.03
14	O	401	HEM	CMB-C2B-C1B	-3.13	120.14	125.03
16	N	403	UQ6	C1M-C1-C2	-3.03	115.47	120.52
11	E	301	6PH	O31-C31-C32	3.03	121.07	111.83
16	N	403	UQ6	C10-C9-C8	-3.03	115.85	123.63
18	S	101	8PE	O31-C31-C32	2.99	120.94	111.83
16	C	406	UQ6	C27-C28-C29	-2.89	121.02	127.62
16	N	403	UQ6	C27-C28-C29	-2.88	121.02	127.62
14	N	402	HEM	CMB-C2B-C1B	-2.83	120.62	125.03
16	N	403	UQ6	C22-C23-C24	-2.82	121.18	127.62
18	H	101	8PE	O31-C31-C32	2.80	120.37	111.83
14	N	405	HEM	C4D-ND-C1D	2.78	108.50	105.21
14	C	404	HEM	CMB-C2B-C1B	-2.76	120.73	125.03
14	O	401	HEM	CAA-CBA-CGA	-2.75	106.36	113.67
14	D	401	HEM	CAA-CBA-CGA	-2.72	106.46	113.67
14	N	405	HEM	CHA-C4D-C3D	2.72	130.24	125.23
16	N	403	UQ6	C20-C19-C21	2.70	119.92	115.23
14	C	403	HEM	CHA-C4D-C3D	2.70	130.21	125.23
12	C	401	CN3	O41-C41-C42	2.67	119.98	111.83
17	C	407	A1D6O	C04-C05-N09	-2.63	113.07	115.40
12	N	401	CN3	O41-C41-C42	2.63	119.84	111.83
13	N	404	9PE	O31-C31-C32	2.60	119.77	111.83
14	C	404	HEM	CAA-C2A-C1A	2.60	130.02	124.94
17	N	406	A1D6O	C04-C05-N09	-2.59	113.10	115.40
17	C	407	A1D6O	S07-C08-S10	2.59	125.39	118.20
17	N	406	A1D6O	S07-C08-S10	2.58	125.38	118.20
14	C	403	HEM	CAC-C3C-C4C	2.58	130.97	124.82
11	A	501	6PH	O31-C31-C32	2.56	119.64	111.83
14	D	401	HEM	C3B-C2B-C1B	2.51	108.30	106.41
14	O	401	HEM	C3B-C2B-C1B	2.50	108.29	106.41
14	N	405	HEM	C1D-C2D-C3D	2.47	109.58	106.98
16	C	406	UQ6	C25-C24-C26	2.46	119.50	115.23
16	C	406	UQ6	C20-C19-C18	-2.45	117.32	123.63
16	N	403	UQ6	C30-C29-C31	2.45	119.48	115.23
16	N	403	UQ6	C25-C24-C26	2.43	119.45	115.23
14	N	405	HEM	CBD-CAD-C3D	2.43	119.24	112.53
16	C	406	UQ6	C6-C7-C8	2.40	116.16	112.06
14	N	405	HEM	C3D-C4D-ND	-2.39	107.55	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	406	UQ6	C30-C29-C31	2.37	119.34	115.23
14	N	405	HEM	C2A-C1A-NA	-2.34	107.56	110.15
14	C	403	HEM	CHD-C1D-ND	2.32	126.92	124.42
14	C	403	HEM	C4D-ND-C1D	2.30	107.93	105.21
14	C	403	HEM	CAC-C3C-C2C	-2.30	120.97	128.43
14	C	403	HEM	C1D-C2D-C3D	2.28	109.38	106.98
13	C	402	9PE	O31-C31-C32	2.28	118.78	111.83
16	C	406	UQ6	C10-C9-C11	2.26	119.16	115.23
14	N	402	HEM	CMC-C2C-C1C	-2.26	120.74	124.73
14	C	404	HEM	CMC-C2C-C1C	-2.25	120.76	124.73
16	C	406	UQ6	C15-C14-C16	2.24	119.12	115.23
16	C	406	UQ6	C17-C18-C19	-2.23	122.51	127.62
17	C	407	A1D6O	C11-C12-C13	-2.23	118.01	123.64
14	C	403	HEM	CBD-CAD-C3D	2.23	118.70	112.53
14	C	403	HEM	C2A-C1A-NA	-2.22	107.68	110.15
14	C	403	HEM	CHA-C4D-ND	-2.21	121.64	124.37
14	C	403	HEM	CHD-C4C-C3C	2.20	128.92	125.21
17	N	406	A1D6O	C11-C12-C13	-2.20	118.10	123.64
16	N	403	UQ6	C17-C18-C19	-2.16	122.69	127.62
16	N	403	UQ6	C1M-C1-C6	2.16	123.54	120.43
16	C	406	UQ6	C2-C1-C6	2.15	121.19	118.59
16	C	406	UQ6	C22-C23-C24	-2.14	122.72	127.62
14	C	404	HEM	CAC-C3C-C4C	-2.14	119.71	124.82
14	N	402	HEM	C4D-ND-C1D	2.14	107.74	105.21
14	N	405	HEM	CMB-C2B-C1B	-2.14	121.70	125.03
14	N	405	HEM	CHD-C1D-ND	2.11	126.69	124.42
14	O	401	HEM	CAC-C3C-C4C	-2.11	119.78	124.82
14	D	401	HEM	CAC-C3C-C4C	-2.10	119.81	124.82
14	N	405	HEM	C2D-C1D-ND	-2.08	107.49	109.90
14	N	402	HEM	CAC-C3C-C4C	-2.07	119.88	124.82
12	C	401	CN3	O51-C51-O52	-2.05	118.90	123.70
14	C	404	HEM	CHA-C4D-ND	2.05	126.90	124.37
14	N	402	HEM	C3D-C4D-ND	-2.04	107.94	110.17
17	N	406	A1D6O	C03-C02-C01	2.04	120.38	118.11
17	C	407	A1D6O	C03-C02-C01	2.02	120.36	118.11
14	C	404	HEM	CAD-CBD-CGD	-2.02	108.31	113.67

There are no chirality outliers.

All (253) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	6PH	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
11	A	501	6PH	C1-O11-P-O13
11	A	501	6PH	C1-O11-P-O14
11	A	501	6PH	C22-C21-O21-C2
11	E	301	6PH	C1-O11-P-O12
11	E	301	6PH	C1-O11-P-O13
11	E	301	6PH	C1-O11-P-O14
11	E	301	6PH	O22-C21-O21-C2
11	E	301	6PH	C22-C21-O21-C2
12	C	401	CN3	CC-O13-P-O11
12	C	401	CN3	CA-O3'-P'-O1'
12	C	401	CN3	CA-O3'-P'-O2'
12	C	401	CN3	CA-O3'-P'-O4'
12	C	401	CN3	O52-C51-O51-C2'
12	C	401	CN3	C52-C51-O51-C2'
12	N	401	CN3	CC-O13-P-O11
12	N	401	CN3	CC-O13-P-O12
12	N	401	CN3	CA-O3'-P'-O1'
12	N	401	CN3	CA-O3'-P'-O2'
13	C	402	9PE	C1-O11-P-O12
13	C	402	9PE	C1-O11-P-O13
13	N	404	9PE	C1-O11-P-O12
13	N	404	9PE	O13-C11-C12-N
14	C	403	HEM	C2D-C3D-CAD-CBD
14	C	404	HEM	C1A-C2A-CAA-CBA
14	N	405	HEM	C2D-C3D-CAD-CBD
14	N	405	HEM	C4D-C3D-CAD-CBD
15	C	405	CN5	CC-O13-P-O11
15	C	405	CN5	CC-O13-P-O12
15	C	405	CN5	CC-O13-P-O14
15	C	405	CN5	CB-CC-O13-P
16	C	406	UQ6	C1-C6-C7-C8
18	H	101	8PE	O13-C11-C12-N
18	S	101	8PE	C1-O11-P-O12
18	S	101	8PE	C11-O13-P-O11
18	S	101	8PE	C11-O13-P-O12
18	S	101	8PE	C11-O13-P-O14
18	S	101	8PE	O13-C11-C12-N
18	S	101	8PE	C22-C21-O21-C2
12	C	401	CN3	O32-C31-O31-C3
12	N	401	CN3	O32-C31-O31-C3
18	H	101	8PE	O32-C31-O31-C3
12	C	401	CN3	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
12	N	401	CN3	C32-C31-O31-C3
18	H	101	8PE	C32-C31-O31-C3
11	A	501	6PH	O22-C21-O21-C2
18	S	101	8PE	O22-C21-O21-C2
16	C	406	UQ6	C20-C19-C21-C22
16	C	406	UQ6	C18-C19-C21-C22
15	C	405	CN5	O42-C41-O41-C3'
14	C	403	HEM	C4D-C3D-CAD-CBD
15	C	405	CN5	C42-C41-O41-C3'
18	S	101	8PE	C32-C31-O31-C3
16	N	403	UQ6	C18-C19-C21-C22
16	C	406	UQ6	C9-C11-C12-C13
16	C	406	UQ6	C24-C26-C27-C28
16	N	403	UQ6	C14-C16-C17-C18
16	N	403	UQ6	C24-C26-C27-C28
16	N	403	UQ6	C29-C31-C32-C33
18	S	101	8PE	O32-C31-O31-C3
12	C	401	CN3	CA-CB-CC-O13
12	N	401	CN3	CA-CB-CC-O13
12	C	401	CN3	C42-C41-O41-C3'
12	N	401	CN3	C42-C41-O41-C3'
13	N	404	9PE	C32-C31-O31-C3
16	N	403	UQ6	C20-C19-C21-C22
12	C	401	CN3	OA-CB-CC-O13
12	N	401	CN3	OA-CB-CC-O13
13	C	402	9PE	C21-C22-C23-C24
18	H	101	8PE	C31-C32-C33-C34
12	N	401	CN3	O42-C41-O41-C3'
12	N	401	CN3	C22-C21-O21-C2
11	E	301	6PH	O21-C2-C3-O31
16	C	406	UQ6	C14-C16-C17-C18
16	C	406	UQ6	C29-C31-C32-C33
15	C	405	CN5	C31-C32-C33-C34
12	C	401	CN3	O42-C41-O41-C3'
12	C	401	CN3	C41-C42-C43-C44
13	N	404	9PE	O32-C31-O31-C3
12	N	401	CN3	O22-C21-O21-C2
15	C	405	CN5	C38-C39-C3A-C3B
15	C	405	CN5	O11-C1-C2-C3
18	S	101	8PE	C1-C2-O21-C21
15	C	405	CN5	C1-C2-C3-O31
11	A	501	6PH	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	H	101	8PE	C37-C38-C39-C3A
15	C	405	CN5	C32-C31-O31-C3
18	H	101	8PE	C3C-C3D-C3E-C3F
18	S	101	8PE	C34-C35-C36-C37
18	S	101	8PE	C24-C25-C26-C27
12	N	401	CN3	C41-C42-C43-C44
13	C	402	9PE	C2D-C2E-C2F-C2G
12	N	401	CN3	C21-C22-C23-C24
11	E	301	6PH	C21-C22-C23-C24
13	N	404	9PE	C2C-C2D-C2E-C2F
12	N	401	CN3	C52-C53-C54-C55
12	C	401	CN3	C1'-C2'-C3'-O41
11	E	301	6PH	C2A-C2B-C2C-C2D
13	N	404	9PE	C2A-C2B-C2C-C2D
18	H	101	8PE	C38-C39-C3A-C3B
18	H	101	8PE	C26-C27-C28-C29
18	S	101	8PE	C21-C22-C23-C24
18	S	101	8PE	C2A-C2B-C2C-C2D
11	A	501	6PH	C32-C33-C34-C35
15	C	405	CN5	O32-C31-O31-C3
11	E	301	6PH	C35-C36-C37-C38
15	C	405	CN5	C39-C3A-C3B-C3C
18	S	101	8PE	C37-C38-C39-C3A
12	C	401	CN3	C52-C53-C54-C55
18	S	101	8PE	C35-C36-C37-C38
12	C	401	CN3	C53-C54-C55-C56
18	S	101	8PE	C36-C37-C38-C39
15	C	405	CN5	C3B-C3C-C3D-C3E
15	C	405	CN5	C36-C37-C38-C39
11	E	301	6PH	C25-C26-C27-C28
11	A	501	6PH	O21-C2-C3-O31
11	A	501	6PH	C38-C39-C3A-C3B
13	N	404	9PE	C32-C33-C34-C35
18	S	101	8PE	C3D-C3E-C3F-C3G
15	C	405	CN5	CA-CB-CC-O13
12	C	401	CN3	C46-C47-C48-C49
18	H	101	8PE	C21-C22-C23-C24
18	H	101	8PE	C36-C37-C38-C39
14	C	404	HEM	C3A-C2A-CAA-CBA
11	A	501	6PH	C24-C25-C26-C27
13	N	404	9PE	C28-C29-C2A-C2B
11	A	501	6PH	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
11	E	301	6PH	C23-C24-C25-C26
11	E	301	6PH	C32-C31-O31-C3
11	A	501	6PH	C1-C2-C3-O31
18	S	101	8PE	C1-C2-C3-O31
13	N	404	9PE	C2E-C2F-C2G-C2H
11	A	501	6PH	C23-C24-C25-C26
13	N	404	9PE	C33-C34-C35-C36
12	N	401	CN3	C53-C54-C55-C56
18	S	101	8PE	C22-C23-C24-C25
13	N	404	9PE	O21-C2-C3-O31
13	N	404	9PE	C29-C2A-C2B-C2C
12	C	401	CN3	C55-C56-C57-C58
16	C	406	UQ6	C19-C21-C22-C23
11	E	301	6PH	C32-C33-C34-C35
13	N	404	9PE	C2F-C2G-C2H-C2I
11	A	501	6PH	C26-C27-C28-C29
18	S	101	8PE	C3E-C3F-C3G-C3H
12	N	401	CN3	C2-C1-O11-P
11	E	301	6PH	C29-C2A-C2B-C2C
12	N	401	CN3	O1'-C1'-C2'-C3'
18	H	101	8PE	O11-C1-C2-C3
13	C	402	9PE	C2F-C2G-C2H-C2I
11	E	301	6PH	O32-C31-O31-C3
13	C	402	9PE	C25-C26-C27-C28
11	A	501	6PH	C39-C3A-C3B-C3C
17	C	407	A1D6O	S10-C11-C12-C13
17	N	406	A1D6O	S10-C11-C12-C13
13	C	402	9PE	C2C-C2D-C2E-C2F
11	E	301	6PH	C1-C2-C3-O31
18	S	101	8PE	C23-C24-C25-C26
11	E	301	6PH	O11-C1-C2-O21
13	N	404	9PE	C2D-C2E-C2F-C2G
13	N	404	9PE	C34-C35-C36-C37
18	H	101	8PE	C3D-C3E-C3F-C3G
12	N	401	CN3	C51-C52-C53-C54
18	H	101	8PE	C39-C3A-C3B-C3C
15	C	405	CN5	O3'-CA-CB-OA
18	S	101	8PE	C2B-C2C-C2D-C2E
11	A	501	6PH	C2-C1-O11-P
14	N	405	HEM	C2C-C3C-CAC-CBC
12	C	401	CN3	C42-C43-C44-C45
15	C	405	CN5	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
12	N	401	CN3	C44-C45-C46-C47
18	S	101	8PE	C31-C32-C33-C34
12	C	401	CN3	C1-C2-C3-O31
14	C	403	HEM	C4C-C3C-CAC-CBC
12	C	401	CN3	C56-C57-C58-C59
12	C	401	CN3	O51-C2'-C3'-O41
18	S	101	8PE	O21-C2-C3-O31
13	C	402	9PE	C32-C33-C34-C35
15	C	405	CN5	C37-C38-C39-C3A
15	C	405	CN5	C32-C33-C34-C35
11	E	301	6PH	C22-C23-C24-C25
13	C	402	9PE	C2B-C2C-C2D-C2E
11	E	301	6PH	O11-C1-C2-C3
18	H	101	8PE	C25-C26-C27-C28
15	C	405	CN5	OA-CB-CC-O13
18	S	101	8PE	C27-C28-C29-C2A
12	N	401	CN3	O1'-C1'-C2'-O51
18	H	101	8PE	O11-C1-C2-O21
17	C	407	A1D6O	S10-C11-C12-C17
12	C	401	CN3	O21-C2-C3-O31
16	C	406	UQ6	C12-C11-C9-C10
16	N	403	UQ6	C15-C14-C16-C17
17	N	406	A1D6O	S10-C11-C12-C17
11	A	501	6PH	C25-C26-C27-C28
15	C	405	CN5	C34-C35-C36-C37
13	C	402	9PE	C32-C31-O31-C3
13	C	402	9PE	C24-C25-C26-C27
12	C	401	CN3	C1'-O1'-P'-O2'
12	C	401	CN3	C1'-O1'-P'-O3'
12	C	401	CN3	C1'-O1'-P'-O4'
12	N	401	CN3	CA-O3'-P'-O4'
13	C	402	9PE	C1-O11-P-O14
13	N	404	9PE	C1-O11-P-O13
13	N	404	9PE	C1-O11-P-O14
18	H	101	8PE	C1-O11-P-O12
12	N	401	CN3	C52-C51-O51-C2'
18	S	101	8PE	C3F-C3G-C3H-C3I
12	N	401	CN3	O52-C51-O51-C2'
13	C	402	9PE	C2E-C2F-C2G-C2H
13	C	402	9PE	O32-C31-O31-C3
11	A	501	6PH	C33-C34-C35-C36
12	C	401	CN3	C44-C45-C46-C47

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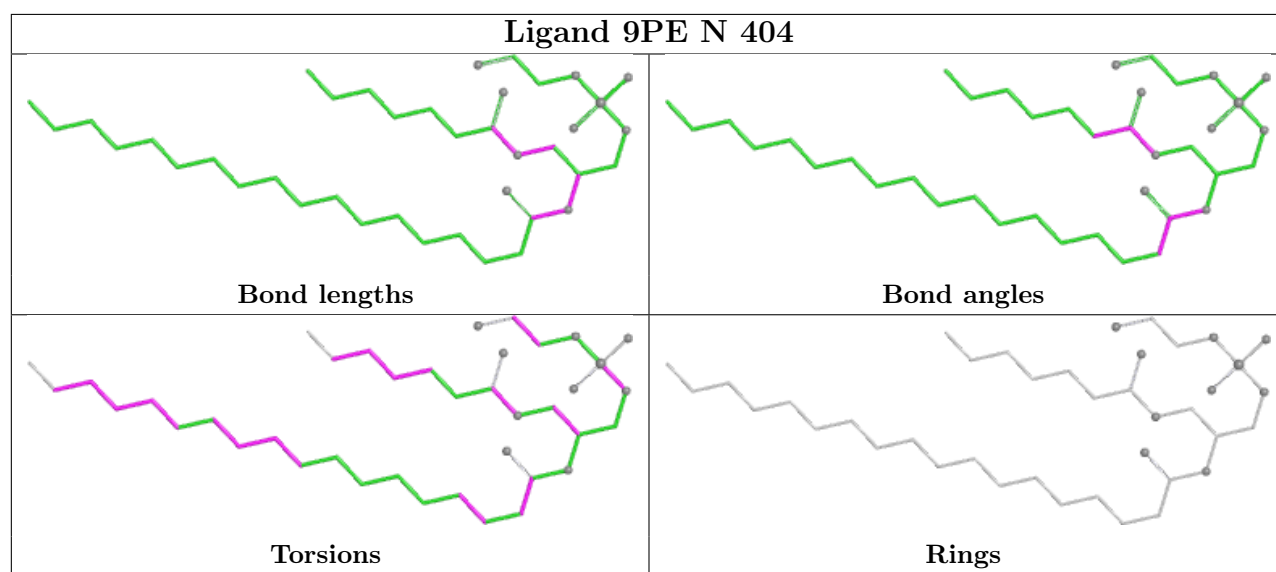
Mol	Chain	Res	Type	Atoms
13	N	404	9PE	C1-C2-C3-O31
16	N	403	UQ6	C9-C11-C12-C13
15	C	405	CN5	C1'-C2'-C3'-O41
12	C	401	CN3	O1'-C1'-C2'-O51
14	N	405	HEM	C4C-C3C-CAC-CBC
12	N	401	CN3	O3'-CA-CB-OA
18	S	101	8PE	C39-C3A-C3B-C3C
16	N	403	UQ6	C19-C21-C22-C23
12	N	401	CN3	C47-C48-C49-C4A
14	N	405	HEM	CAA-CBA-CGA-O1A
14	N	405	HEM	CAA-CBA-CGA-O2A
11	A	501	6PH	C29-C2A-C2B-C2C
11	E	301	6PH	C36-C37-C38-C39
16	C	406	UQ6	C12-C11-C9-C8
16	N	403	UQ6	C13-C14-C16-C17
18	H	101	8PE	C3F-C3G-C3H-C3I
11	E	301	6PH	C26-C27-C28-C29
11	A	501	6PH	C2B-C2C-C2D-C2E
13	N	404	9PE	C22-C23-C24-C25
14	C	403	HEM	CAA-CBA-CGA-O2A
16	C	406	UQ6	C5-C6-C7-C8
14	C	403	HEM	CAA-CBA-CGA-O1A
14	C	404	HEM	CAA-CBA-CGA-O1A
12	C	401	CN3	O1'-C1'-C2'-C3'
12	C	401	CN3	C45-C46-C47-C48
14	C	403	HEM	CAD-CBD-CGD-O1D
14	N	402	HEM	CAA-CBA-CGA-O1A
11	E	301	6PH	C3A-C3B-C3C-C3D
16	N	403	UQ6	C25-C24-C26-C27
13	N	404	9PE	O21-C21-C22-C23
14	D	401	HEM	CAA-CBA-CGA-O1A
14	D	401	HEM	CAA-CBA-CGA-O2A
14	N	402	HEM	CAA-CBA-CGA-O2A
14	C	404	HEM	CAA-CBA-CGA-O2A
18	S	101	8PE	O21-C21-C22-C23
18	H	101	8PE	O21-C21-C22-C23
13	C	402	9PE	C27-C28-C29-C2A
14	C	403	HEM	CAD-CBD-CGD-O2D
13	N	404	9PE	O22-C21-C22-C23
11	A	501	6PH	C28-C29-C2A-C2B
18	S	101	8PE	O22-C21-C22-C23
18	S	101	8PE	C28-C29-C2A-C2B

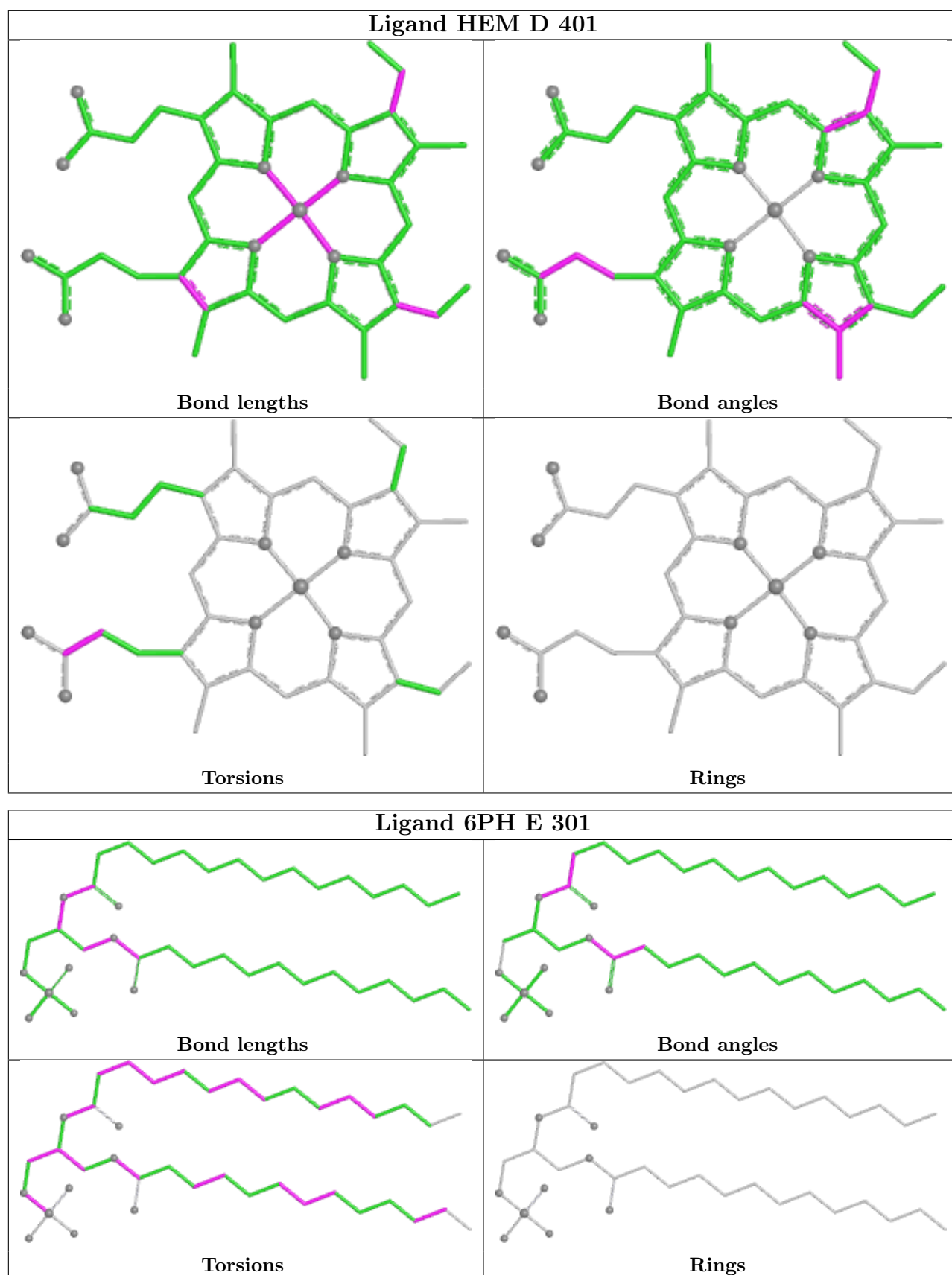
There are no ring outliers.

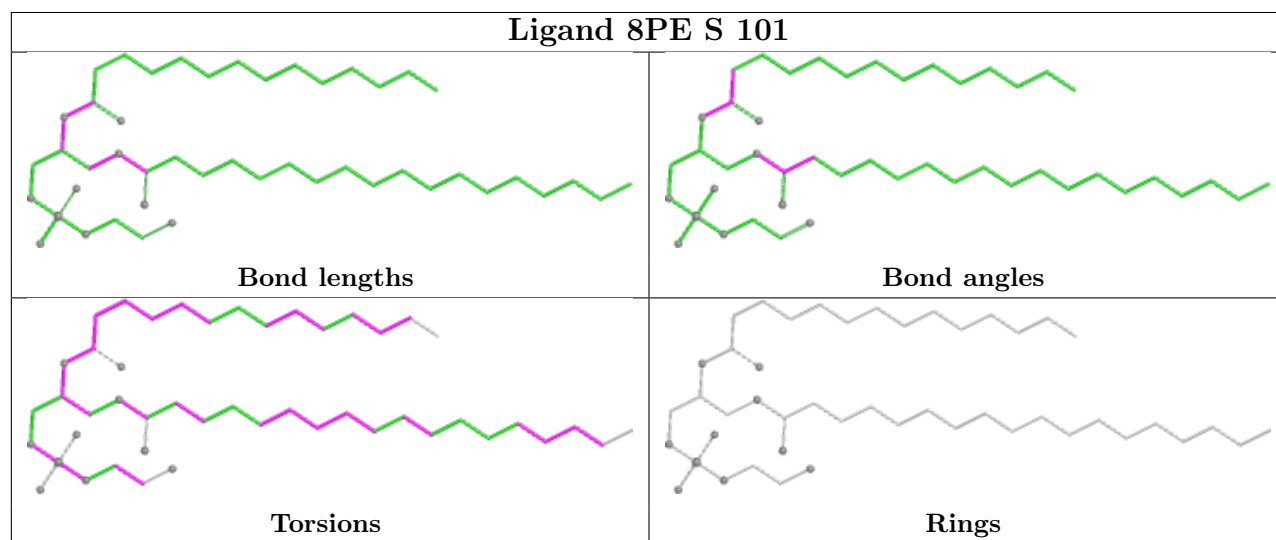
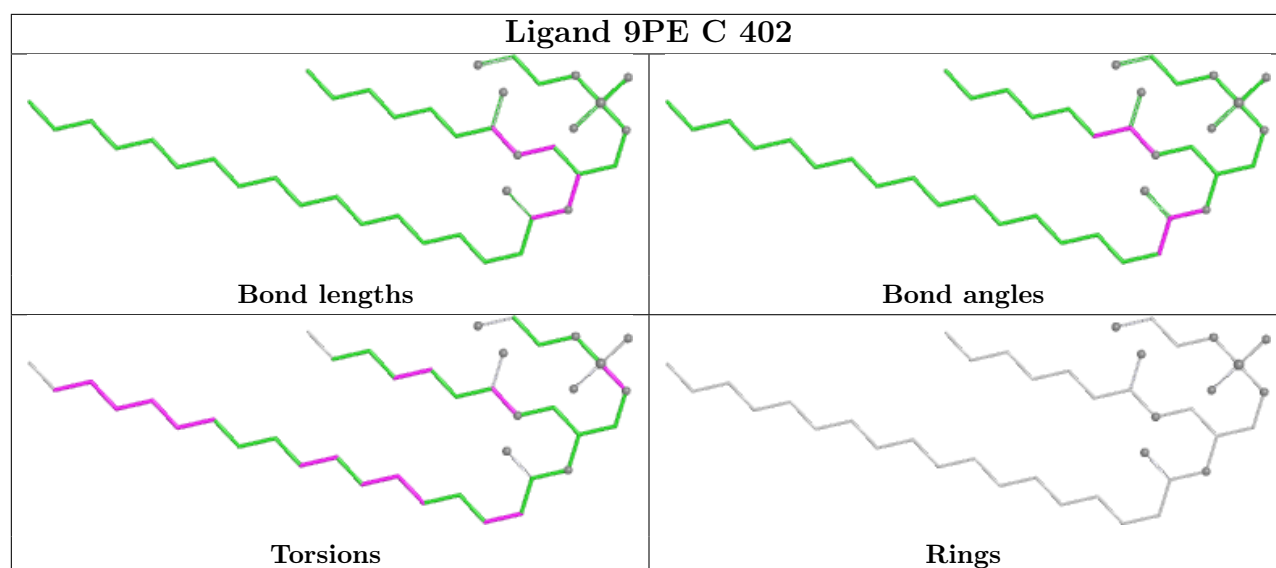
9 monomers are involved in 17 short contacts:

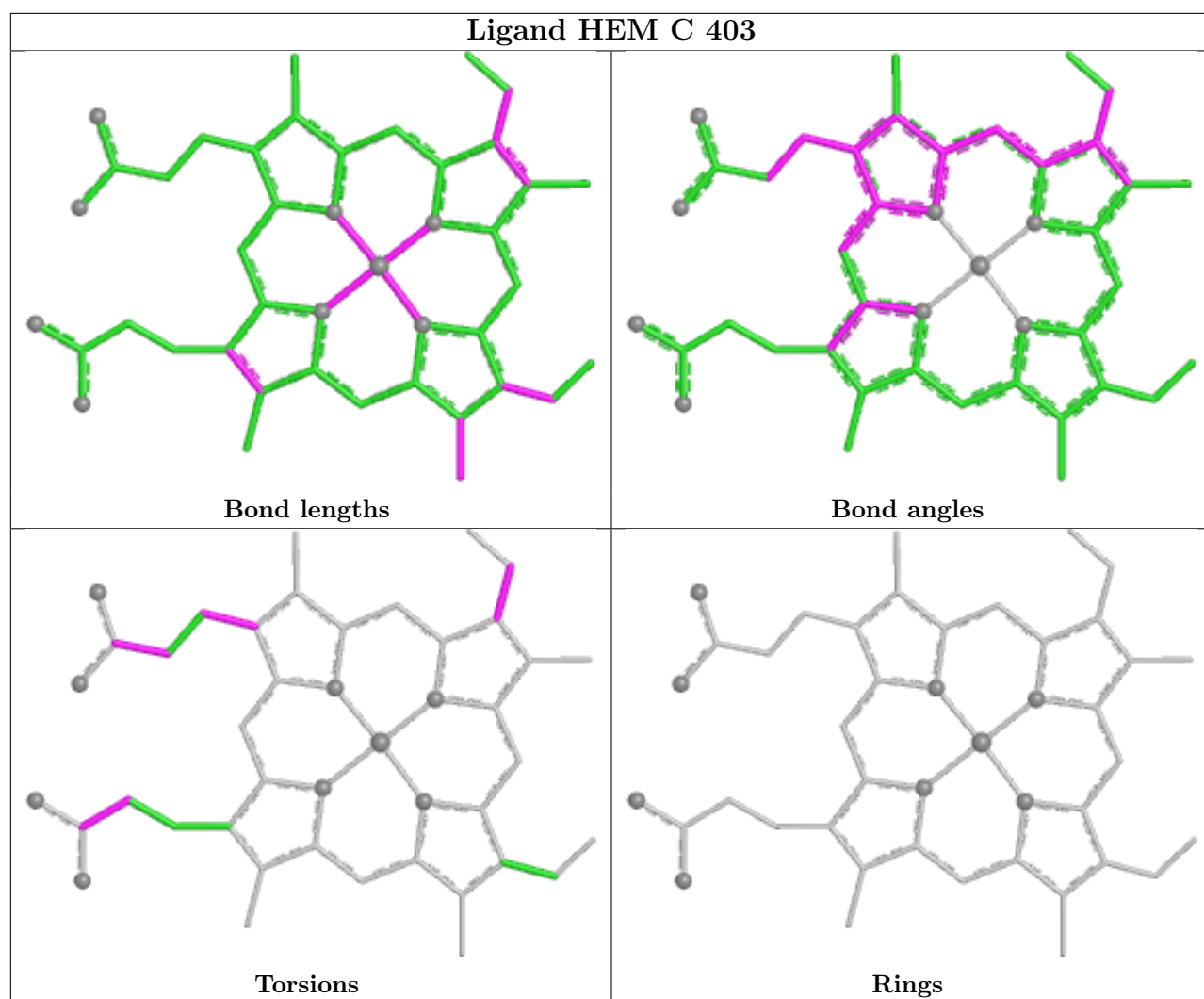
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	404	9PE	3	0
11	E	301	6PH	4	0
13	C	402	9PE	1	0
18	S	101	8PE	3	0
14	C	403	HEM	1	0
12	N	401	CN3	1	0
18	H	101	8PE	1	0
16	C	406	UQ6	1	0
16	N	403	UQ6	2	0

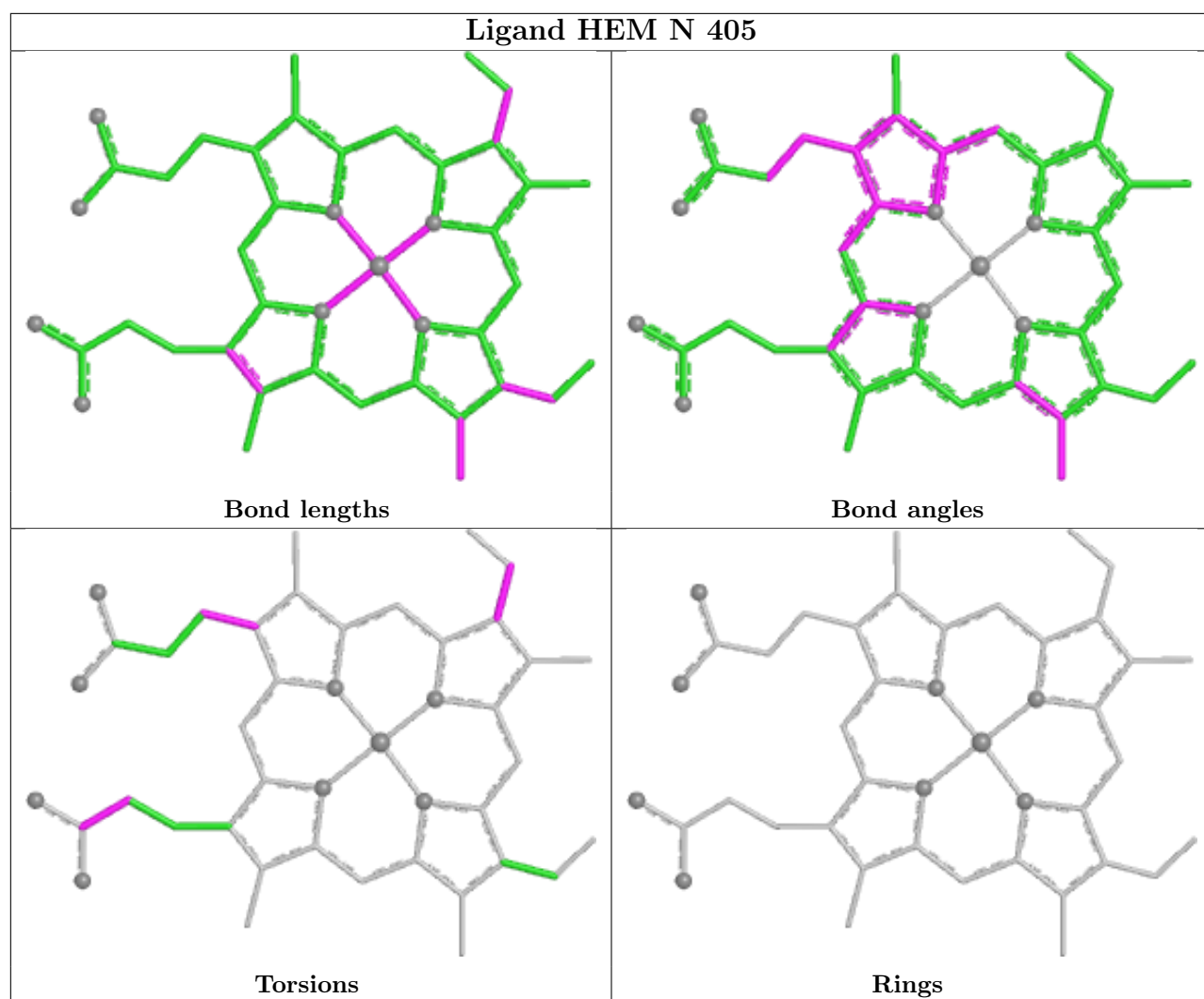
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

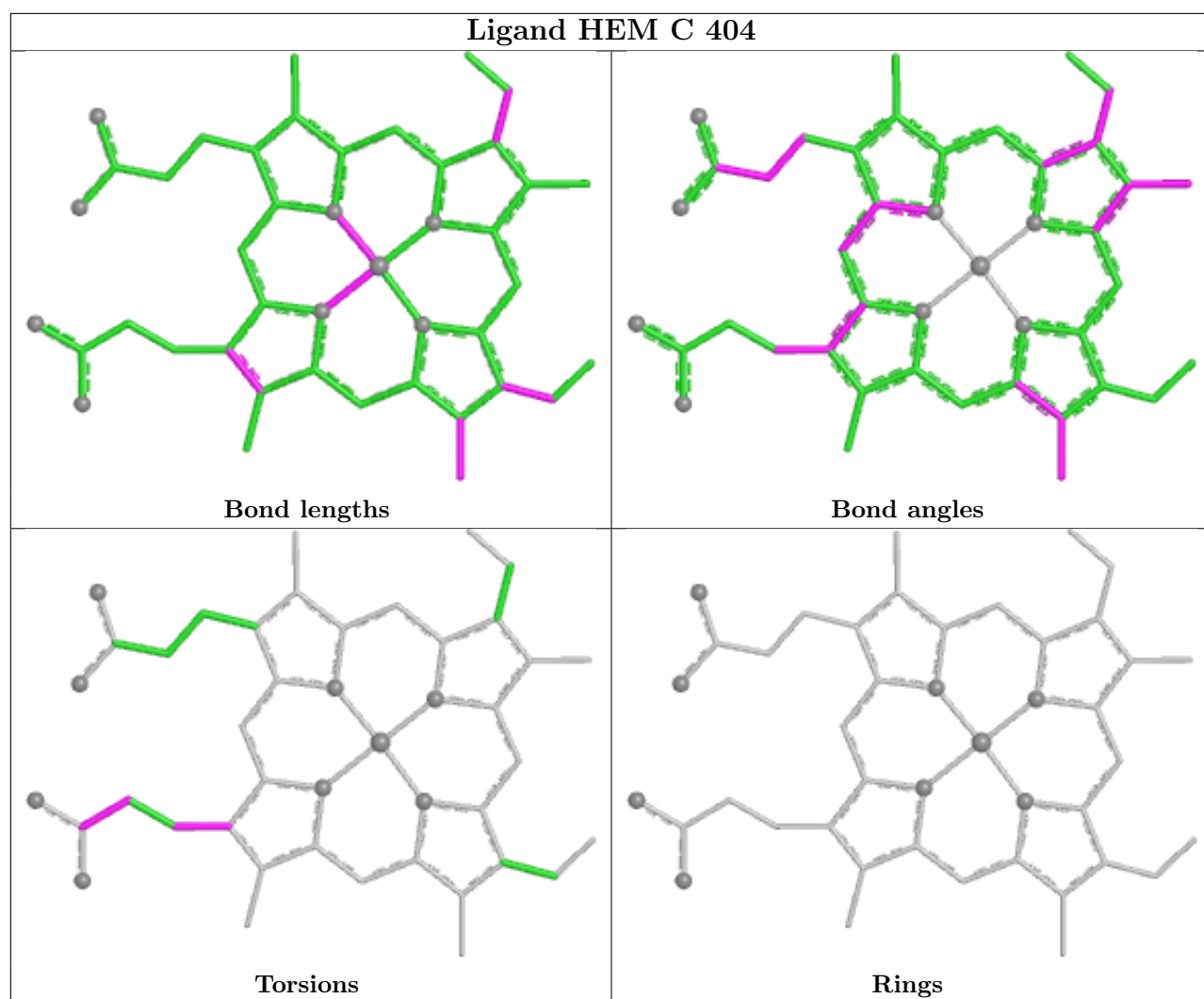


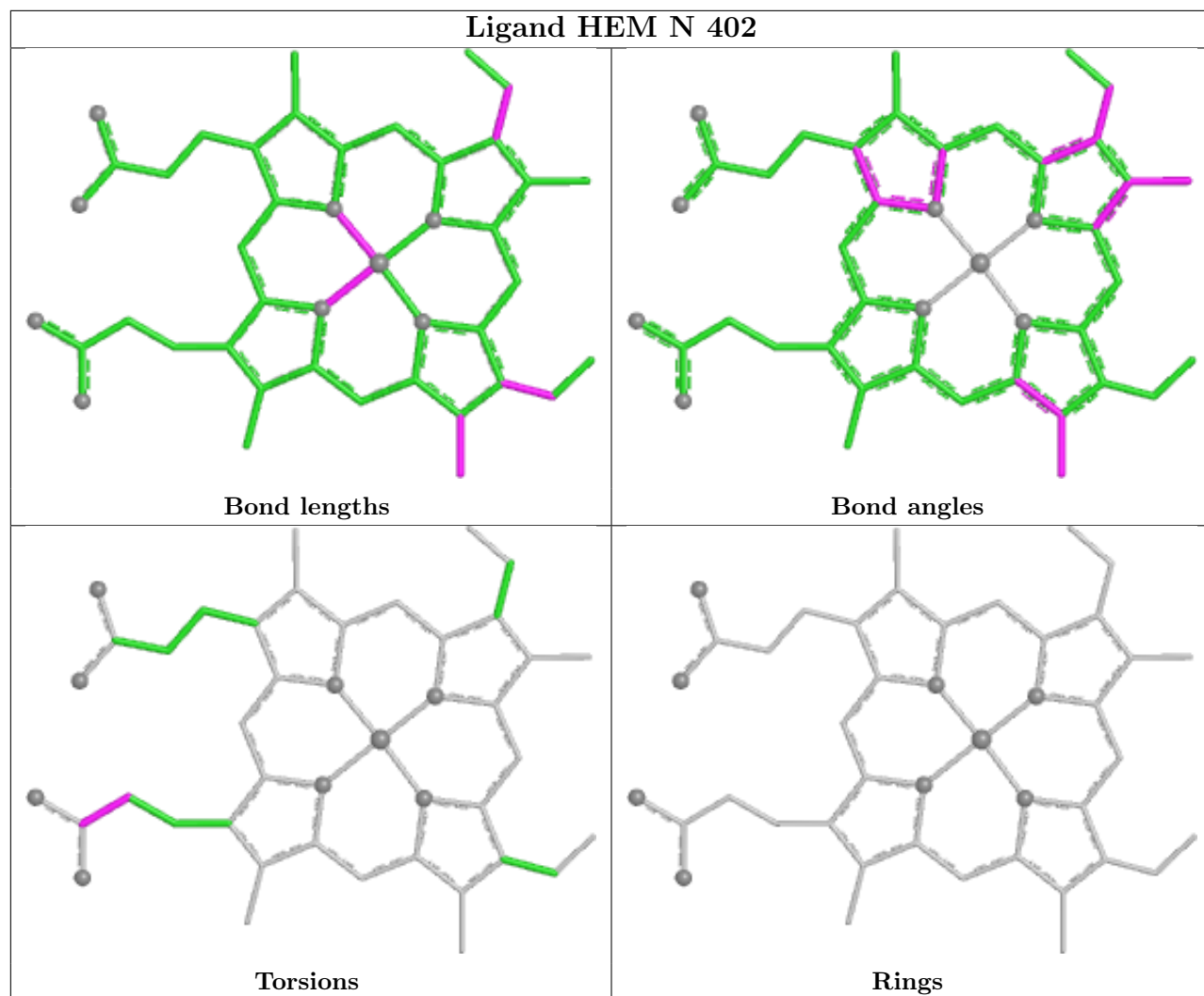


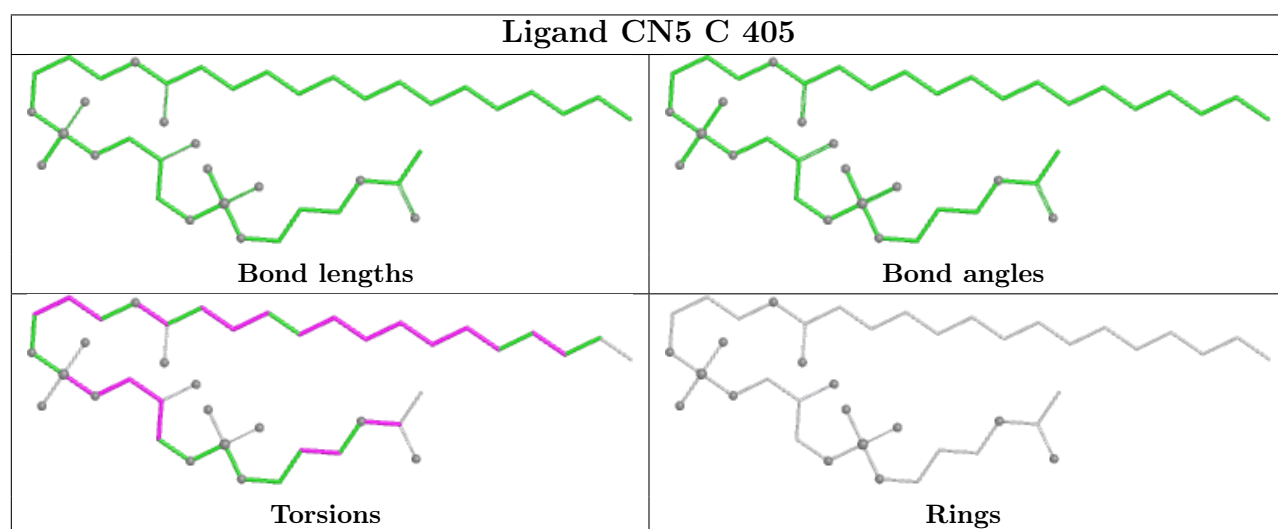
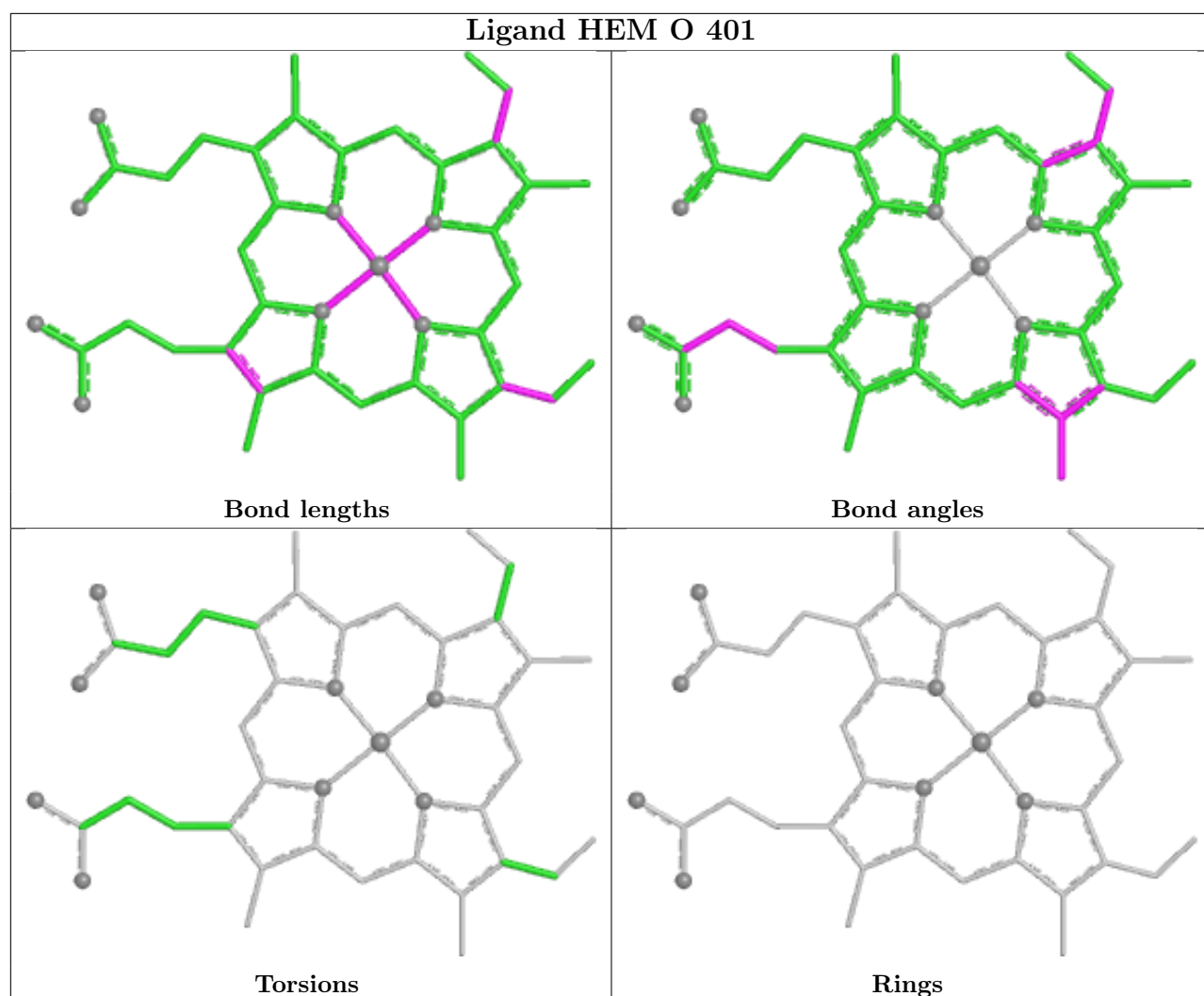




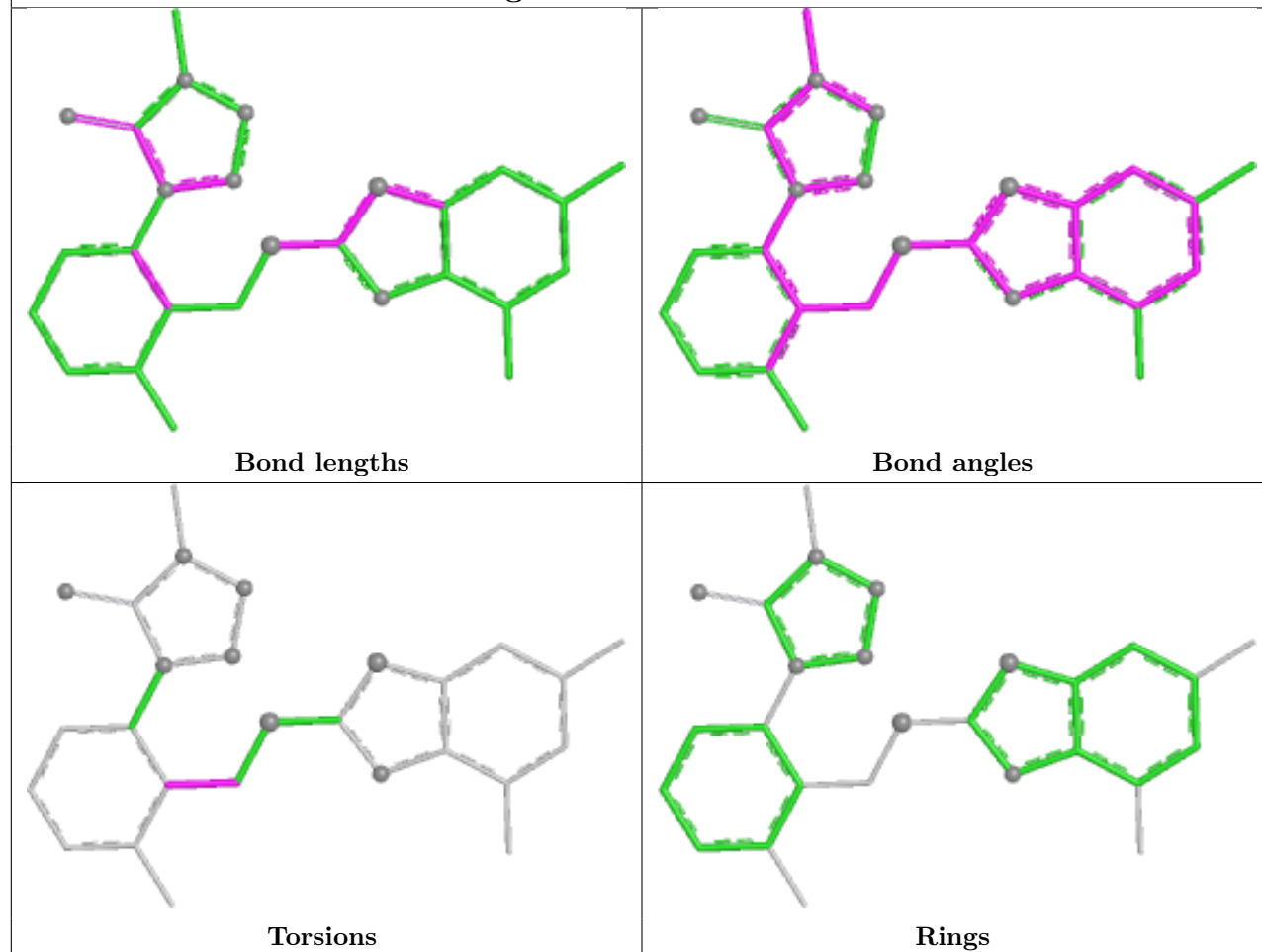




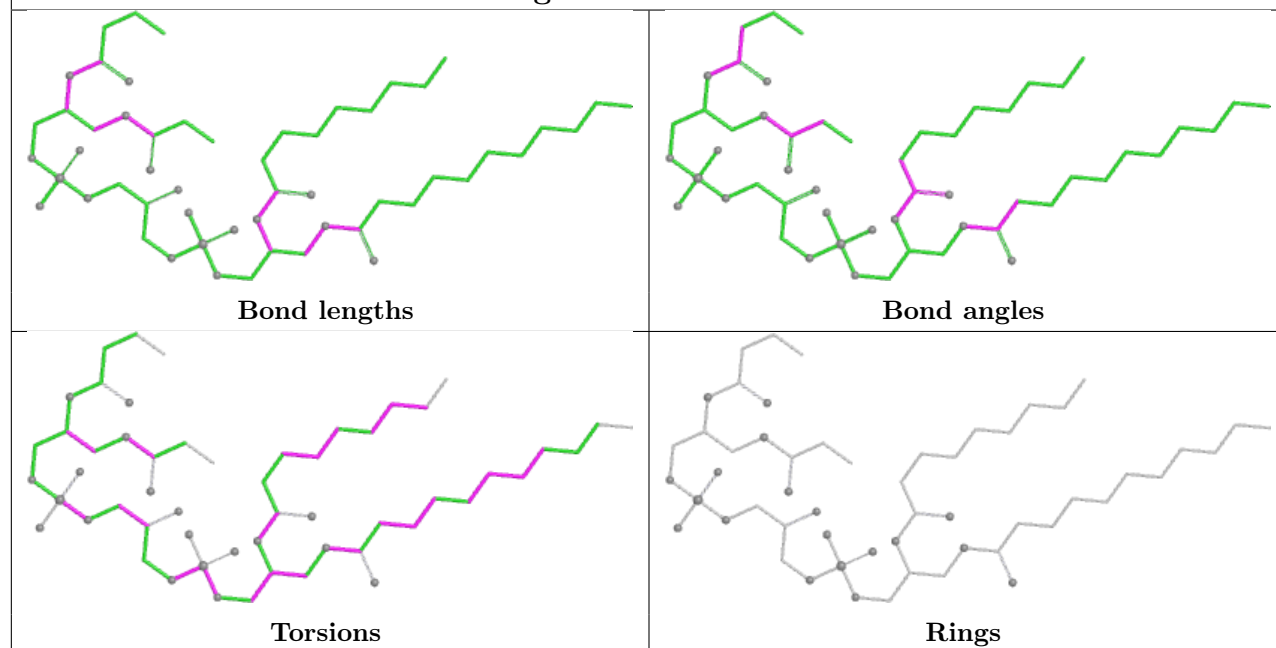


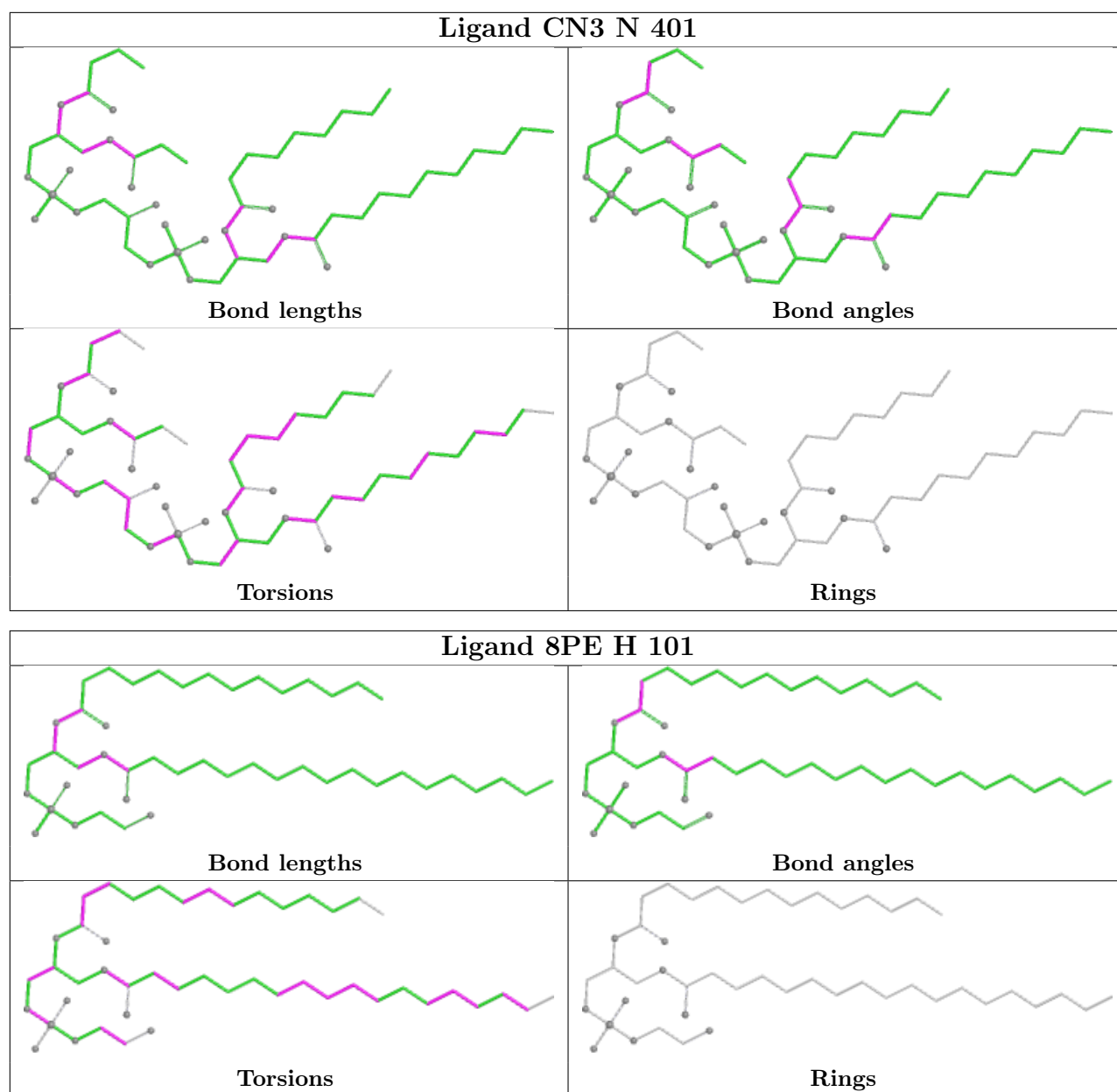


Ligand A1D6O C 407

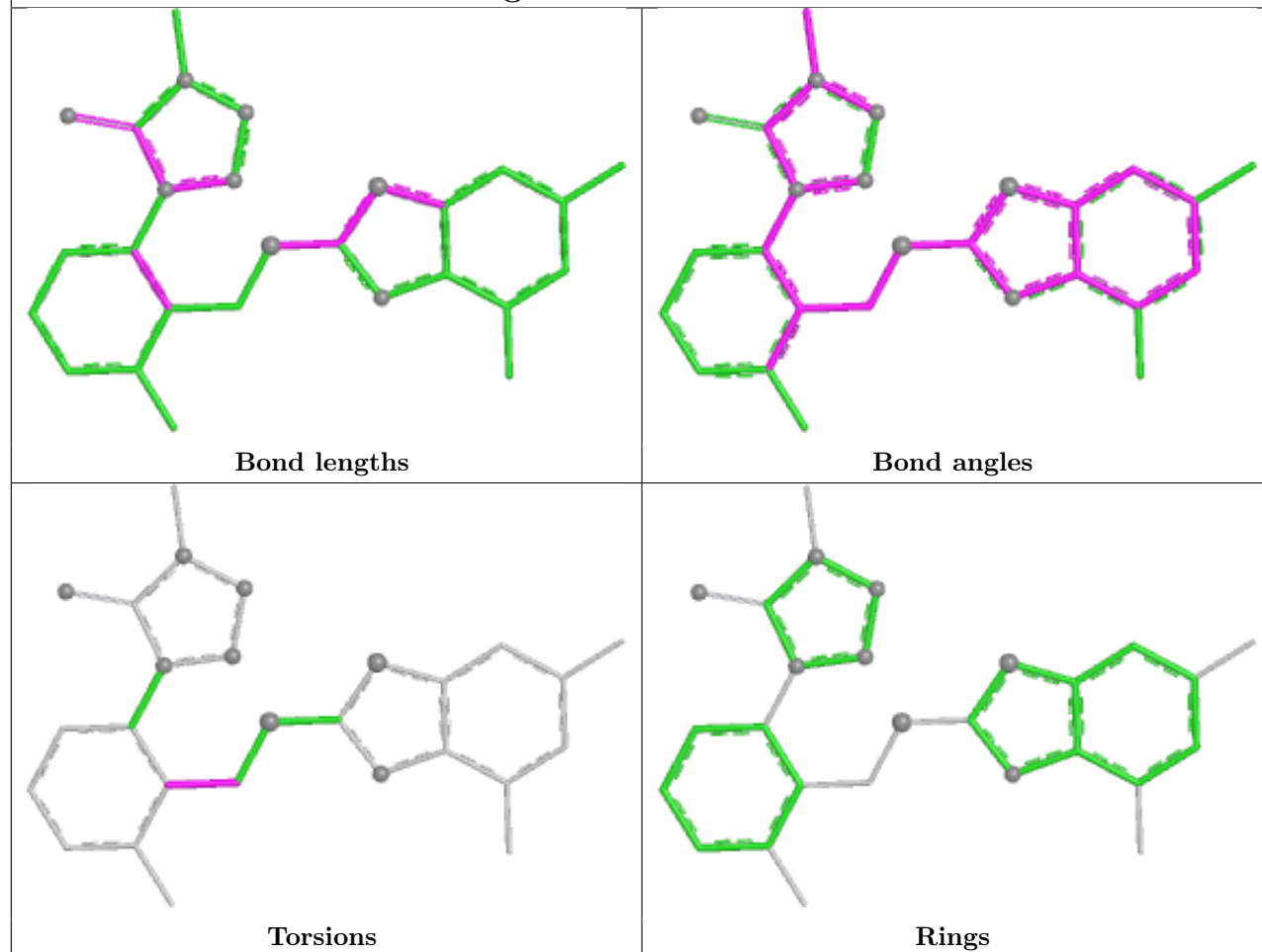


Ligand CN3 C 401

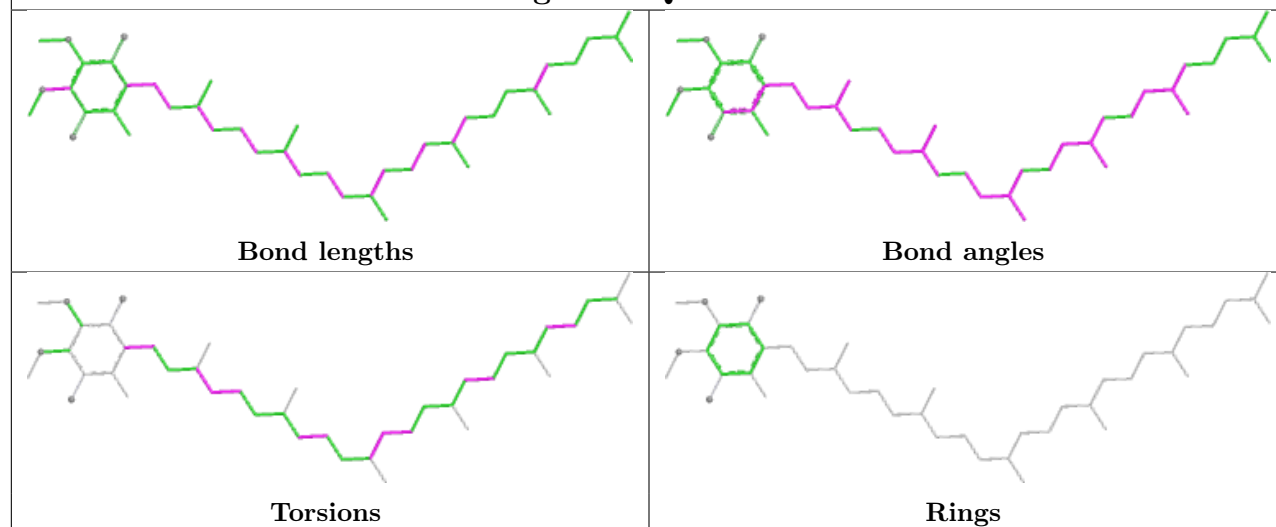


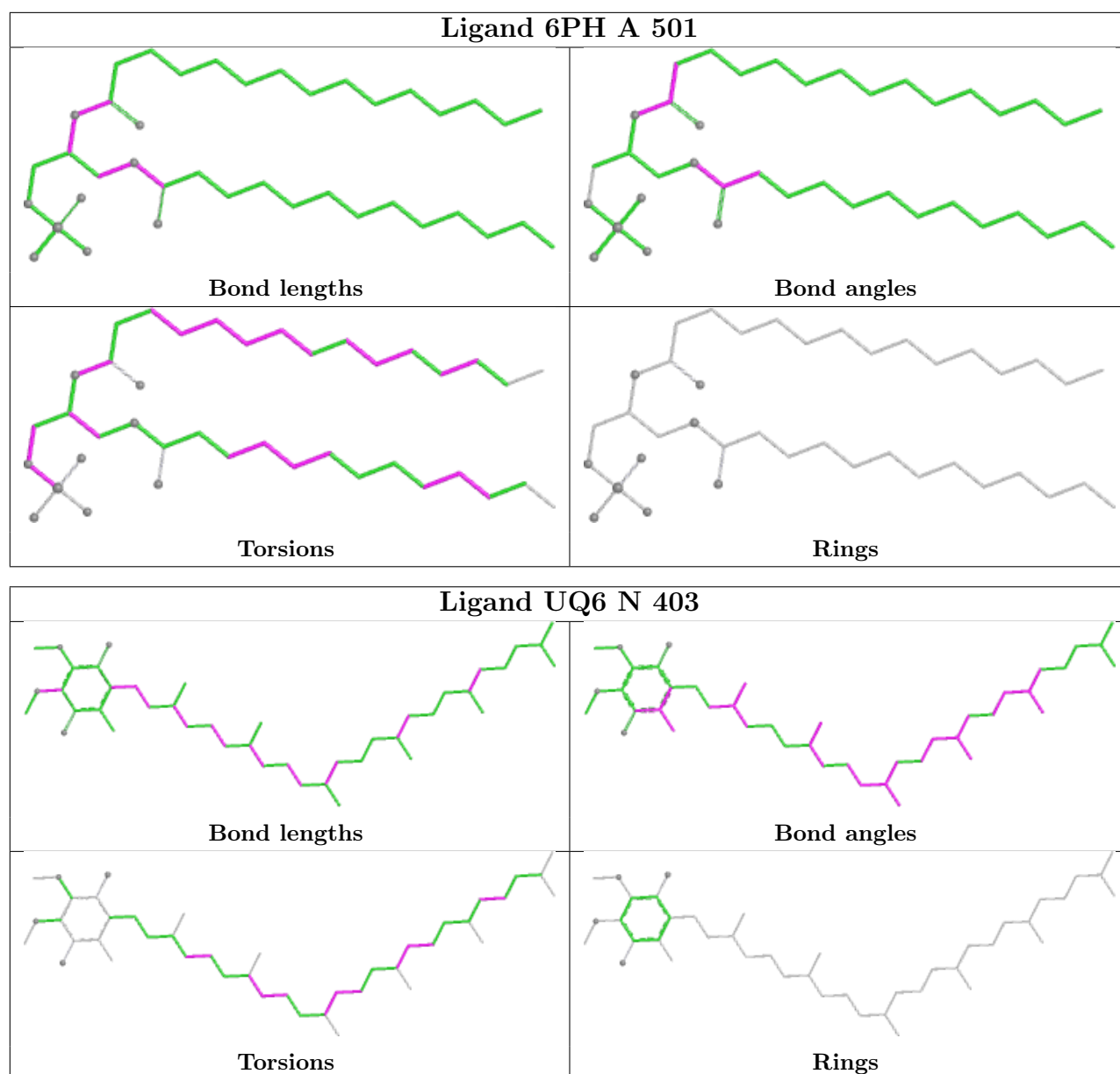


Ligand A1D6O N 406



Ligand UQ6 C 406





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.

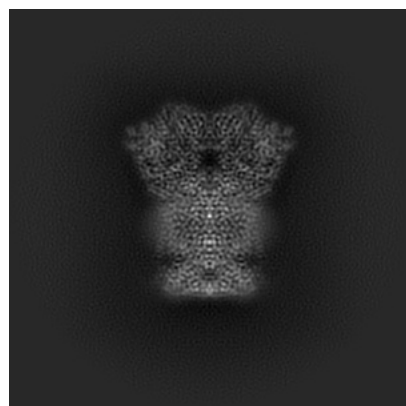
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39323. These allow visual inspection of the internal detail of the map and identification of artifacts.

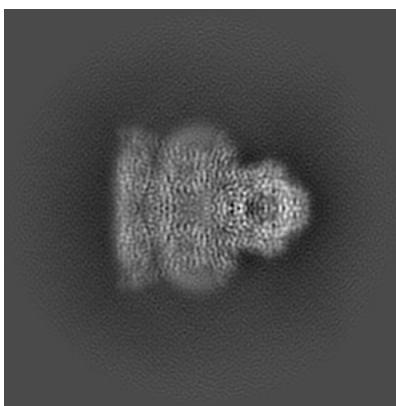
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

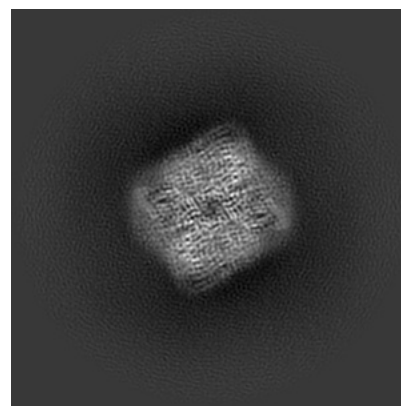
6.1.1 Primary map



X

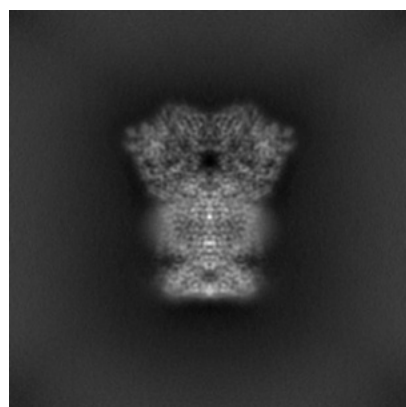


Y

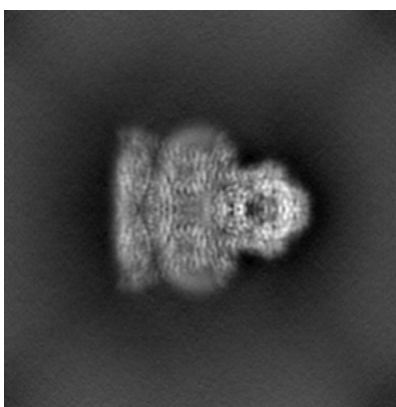


Z

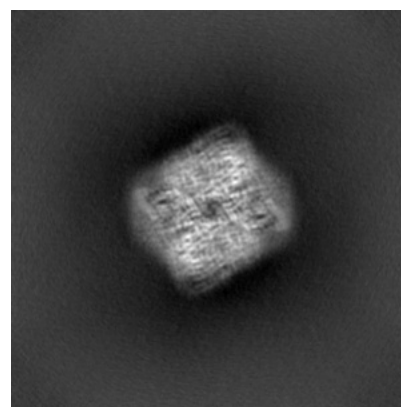
6.1.2 Raw map



X



Y

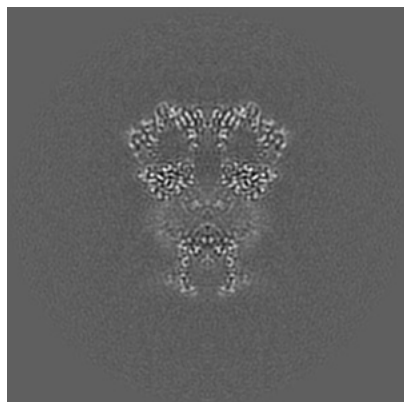


Z

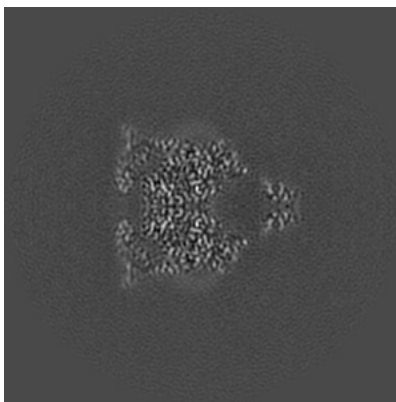
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

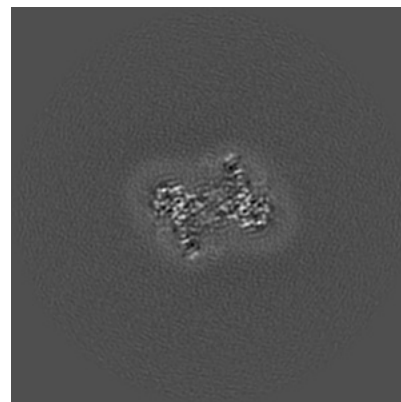
6.2.1 Primary map



X Index: 160

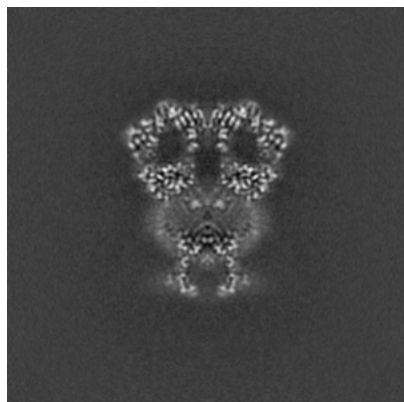


Y Index: 160

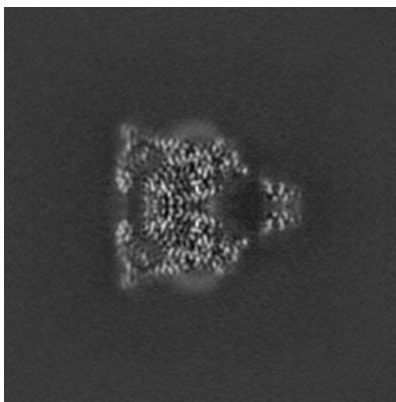


Z Index: 160

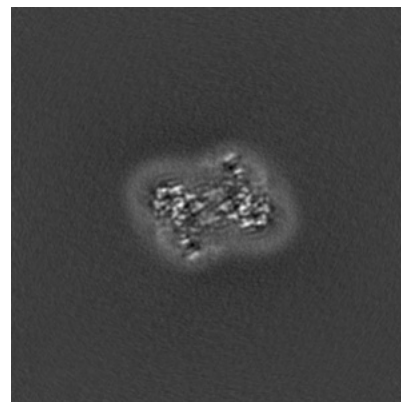
6.2.2 Raw map



X Index: 160



Y Index: 160

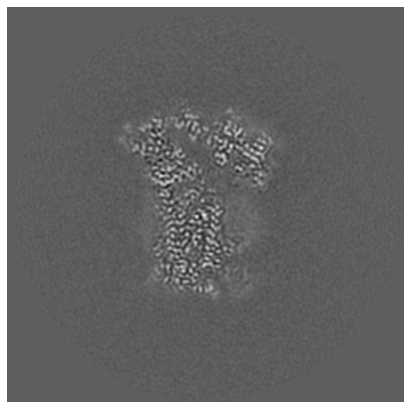


Z Index: 160

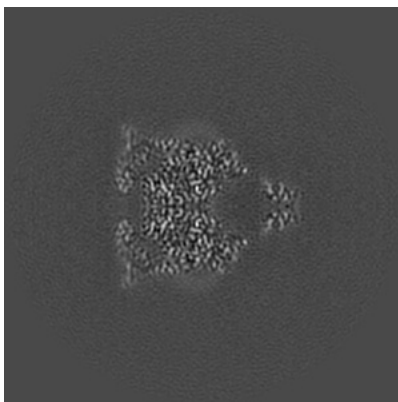
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

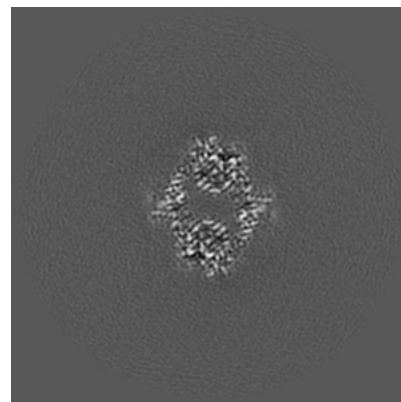
6.3.1 Primary map



X Index: 143

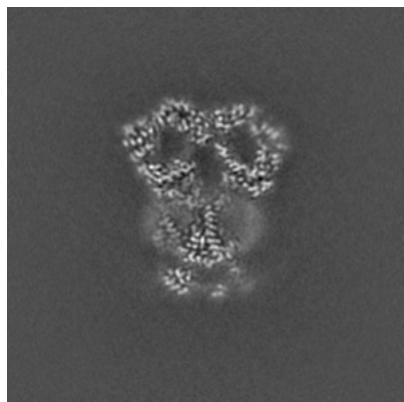


Y Index: 160

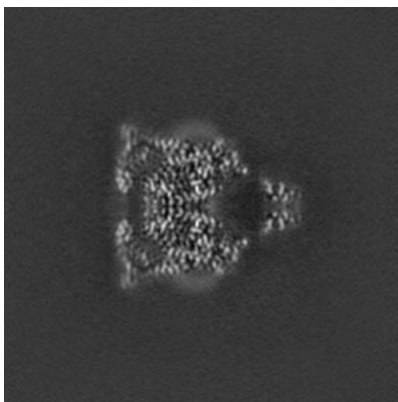


Z Index: 184

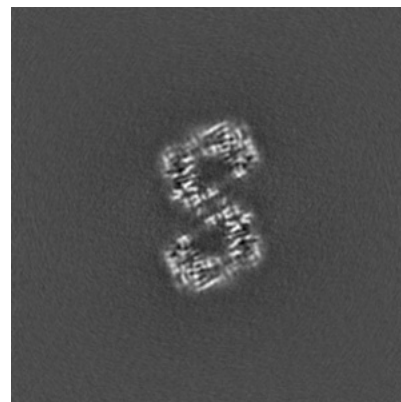
6.3.2 Raw map



X Index: 153



Y Index: 160

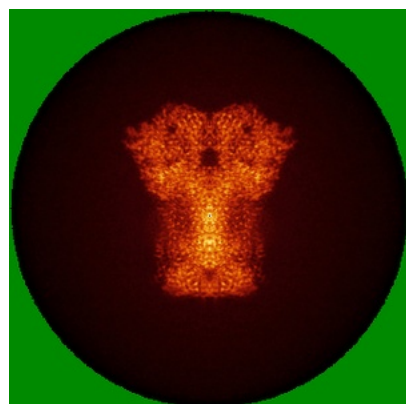


Z Index: 209

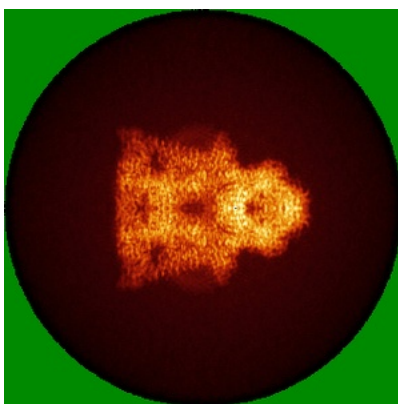
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

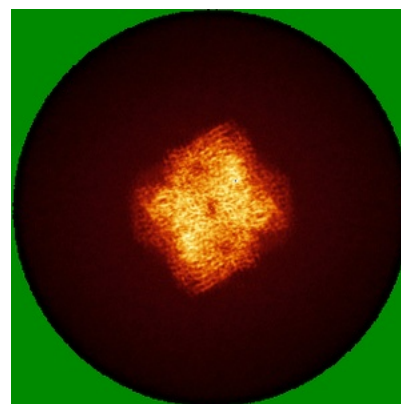
6.4.1 Primary map



X

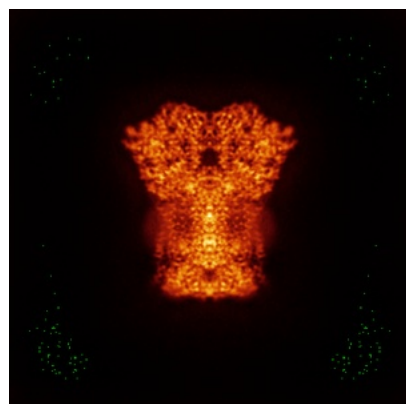


Y

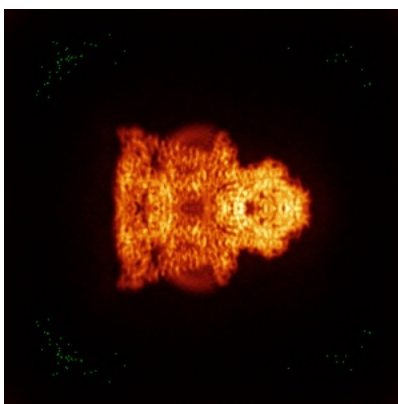


Z

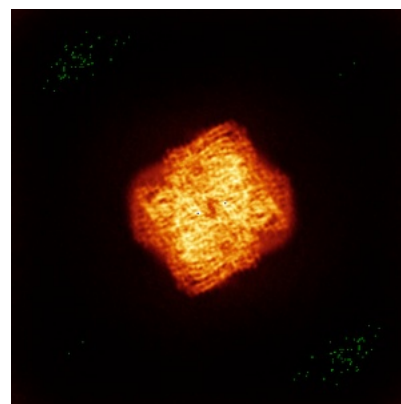
6.4.2 Raw map



X



Y

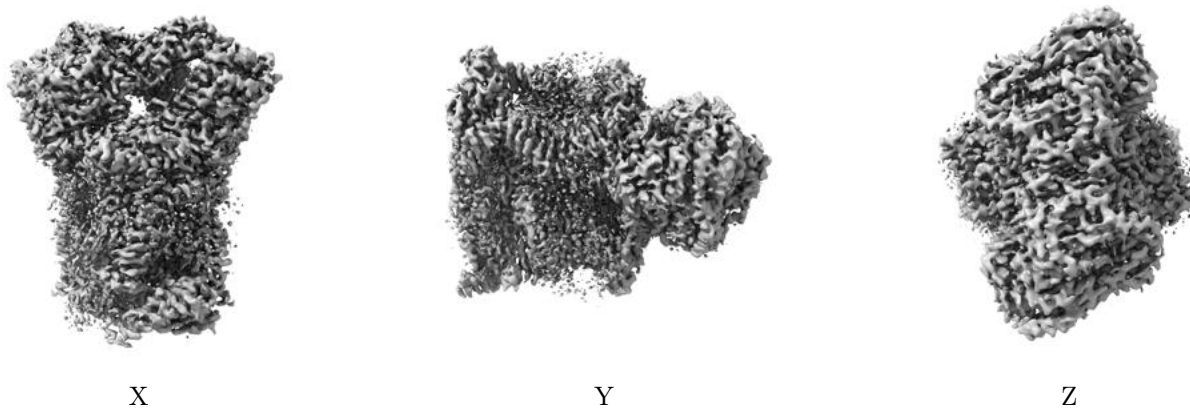


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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.

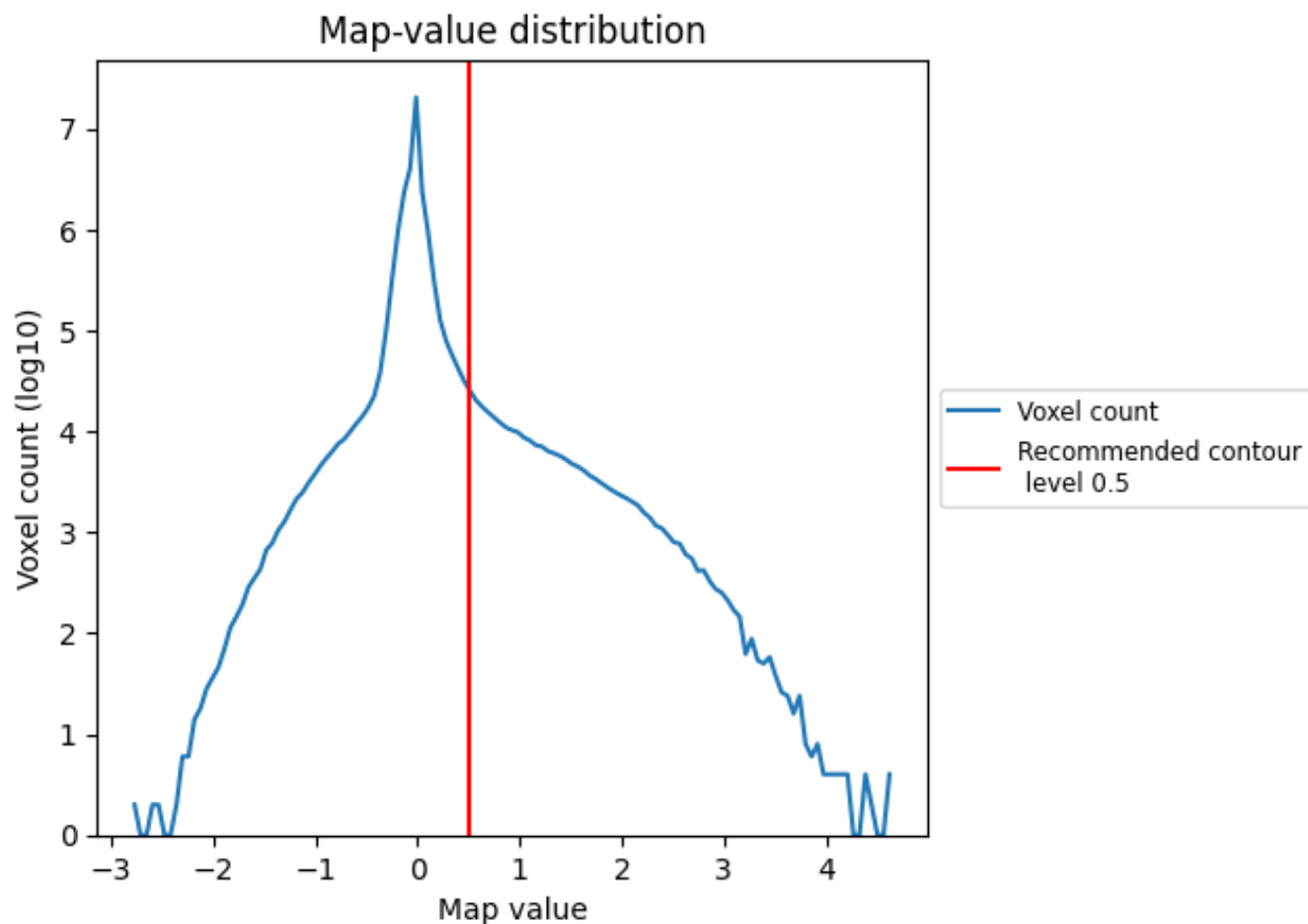
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

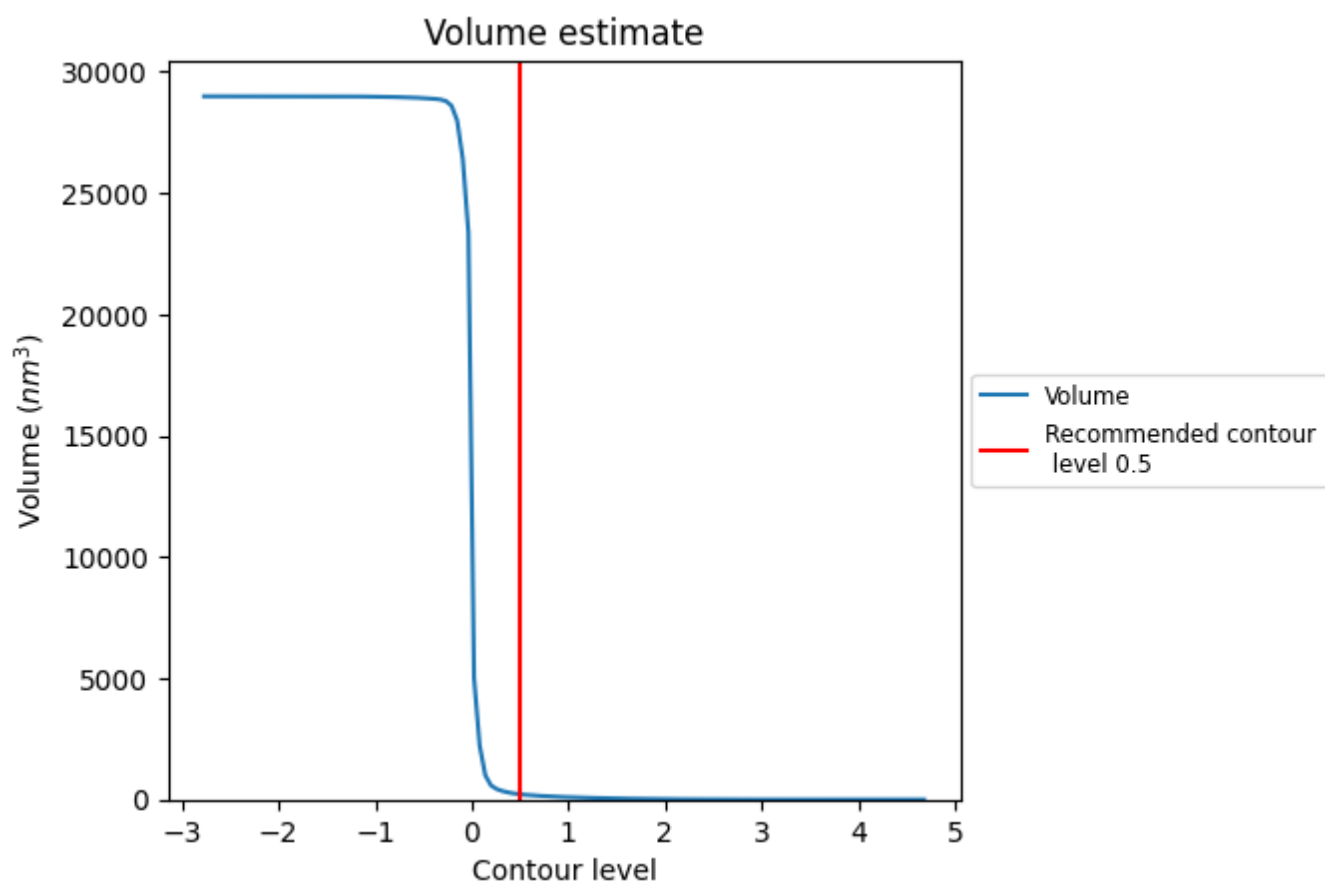
This section contains the results of statistical analysis of the map.

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.

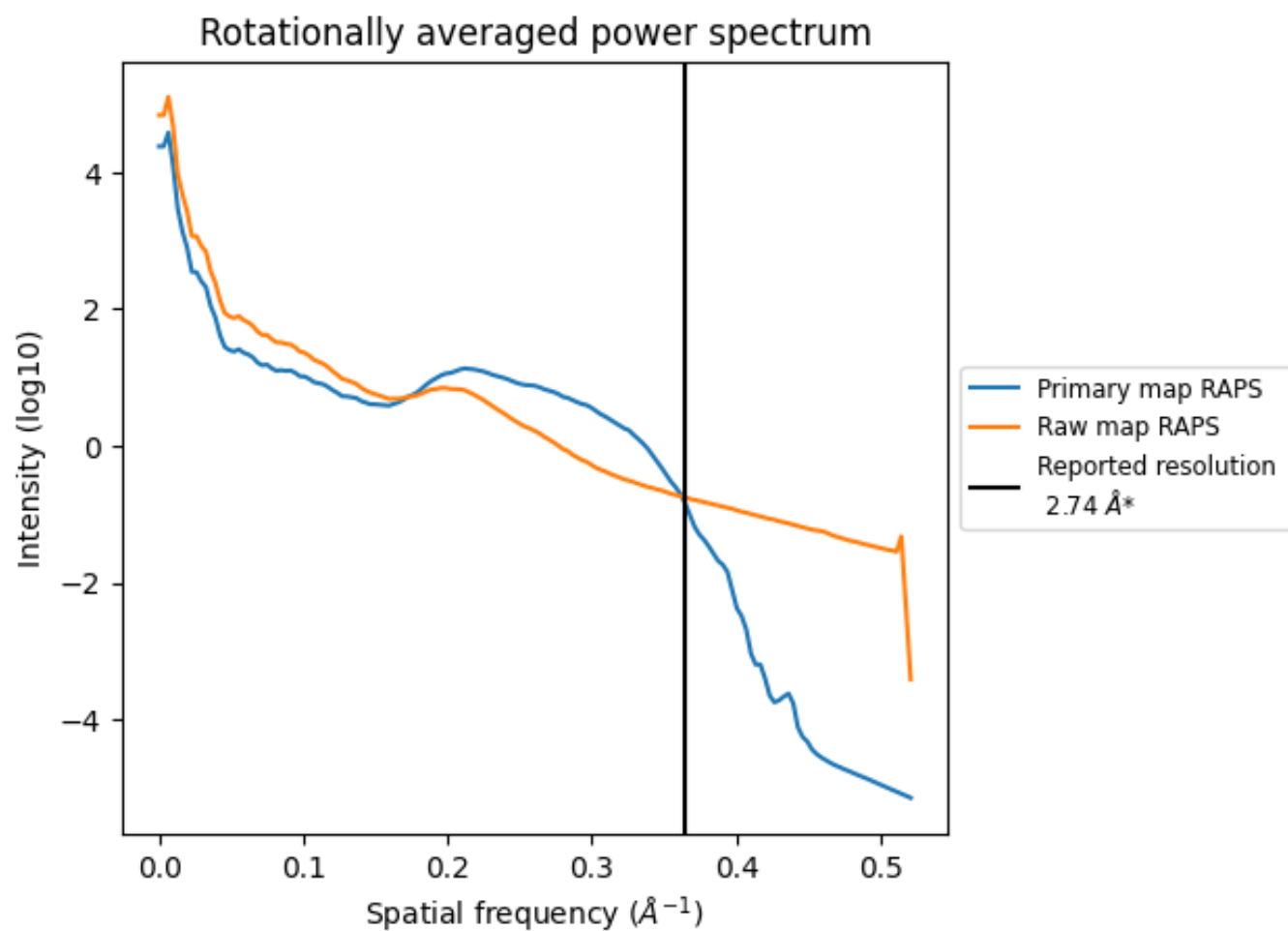
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm³; this corresponds to an approximate mass of 197 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 ⓘ

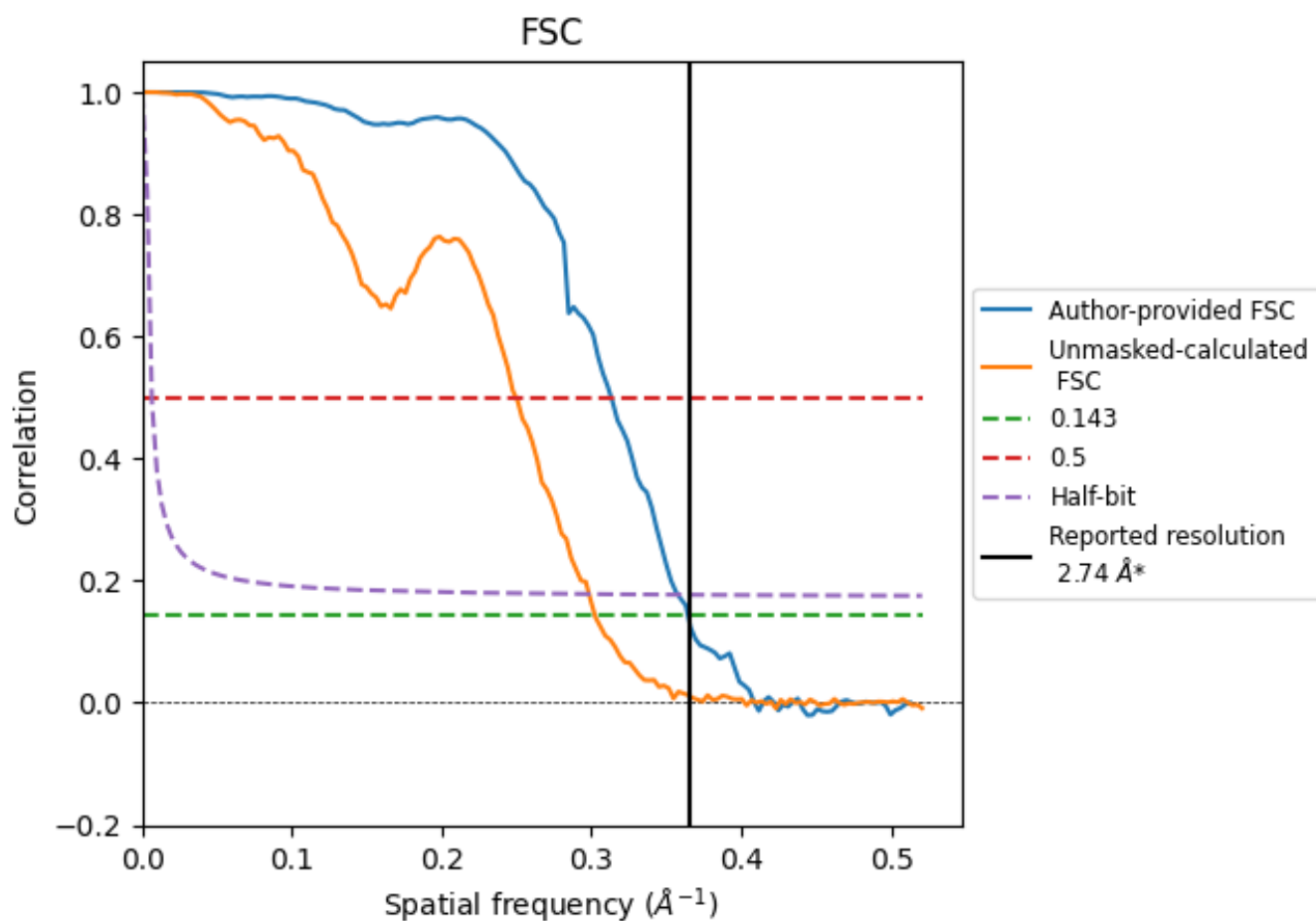


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

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 0.365 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

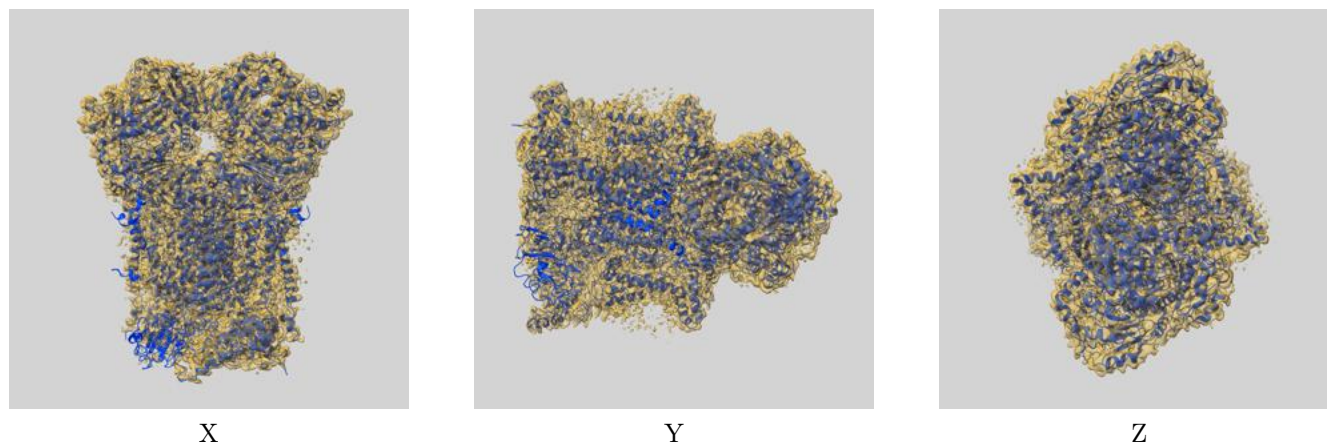
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.19	2.79
Unmasked-calculated*	3.31	4.01	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

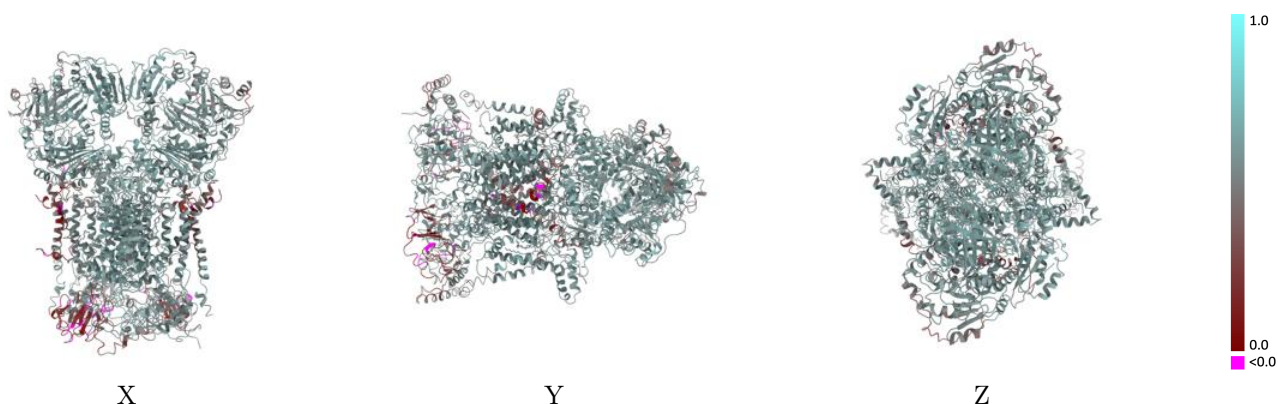
This section contains information regarding the fit between EMDB map EMD-39323 and PDB model 8YIN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



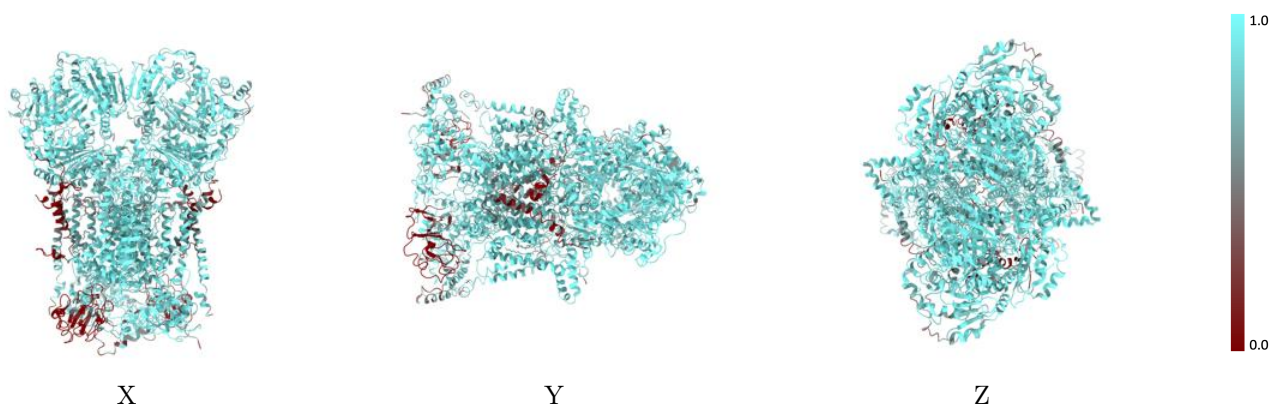
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



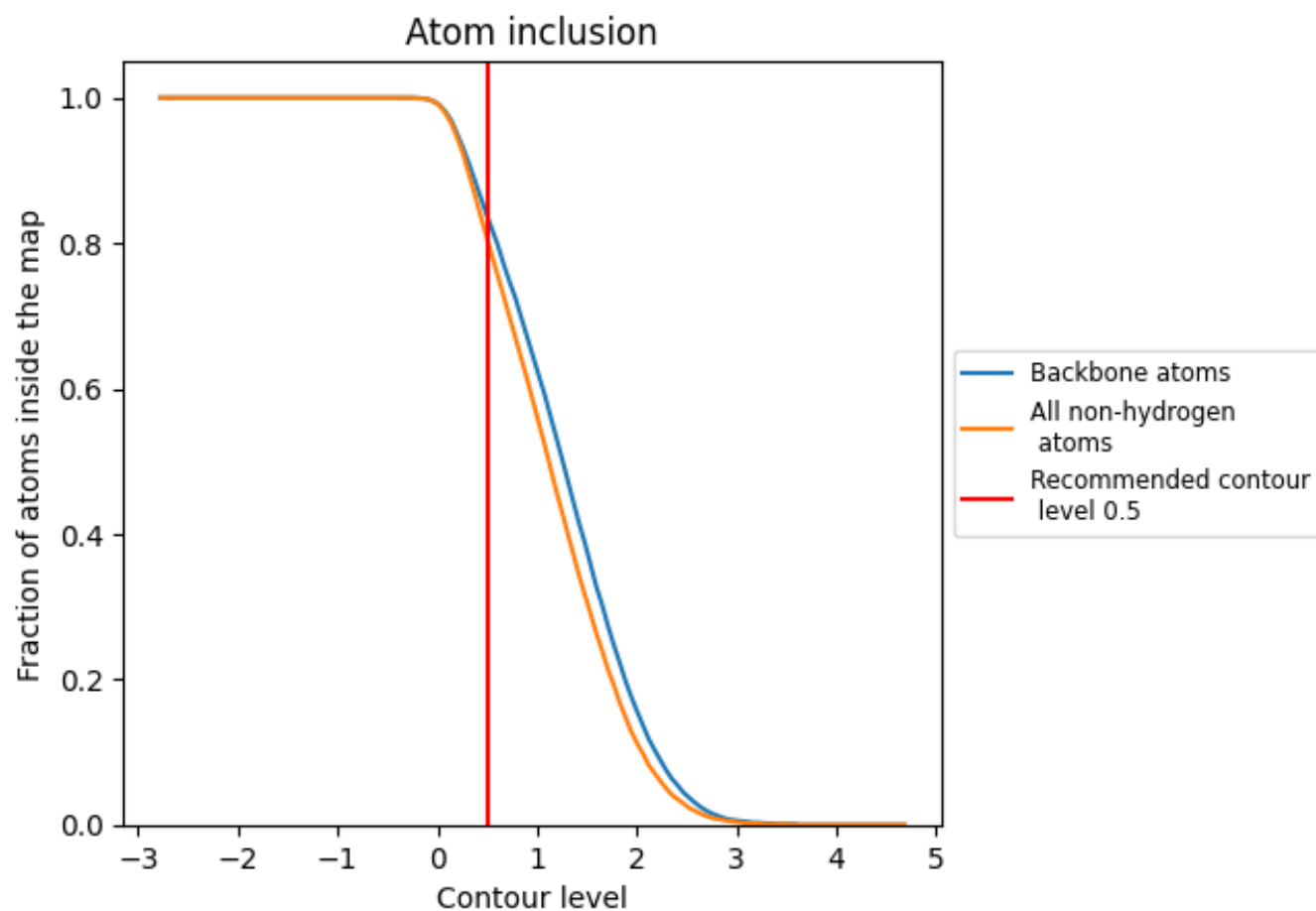
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.5300
A	 0.8790	 0.5530
B	 0.9190	 0.5780
C	 0.9200	 0.5930
D	 0.9160	 0.5710
E	 0.3060	 0.3200
F	 0.6650	 0.4440
G	 0.8860	 0.5710
H	 0.7290	 0.5050
I	 0.5550	 0.4030
L	 0.8860	 0.5530
M	 0.9200	 0.5790
N	 0.9300	 0.5930
O	 0.9140	 0.5660
P	 0.2970	 0.3410
Q	 0.6510	 0.4440
R	 0.8880	 0.5710
S	 0.7330	 0.5040
T	 0.5520	 0.4100
U	 0.0560	 0.2050
V	 0.0530	 0.2100

