



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:39 AM JST

PDB ID : 8ZMT / pdb_00008zmt
EMDB ID : EMD-60256
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex in Metyltetrapr
ole-bound state
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-05-23
Resolution : 2.52 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.dev133
Mogul : 1.8.5 (274361), 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

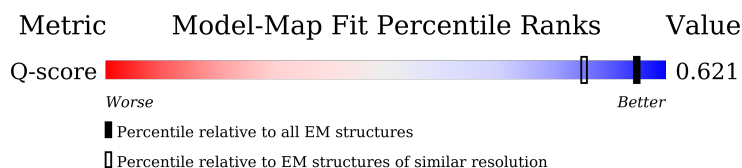
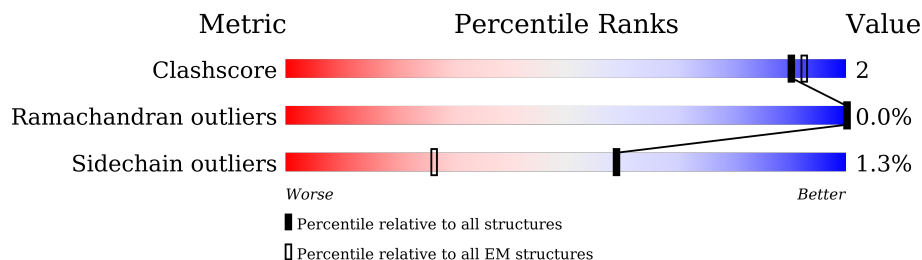
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

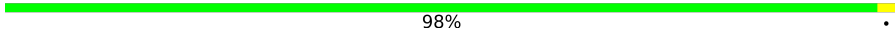
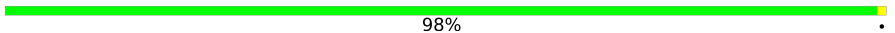
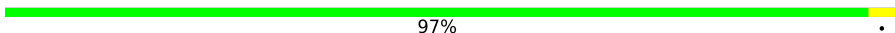
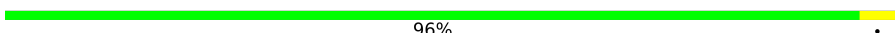
The reported resolution of this entry is 2.52 Å.

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.



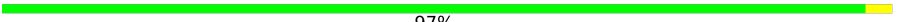
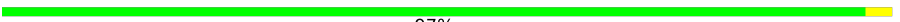
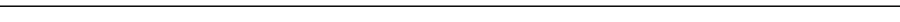
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

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	 98% .
1	L	431	 98% .
2	B	352	 97% .
2	M	352	 96% .

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Mol	Chain	Length	Quality of chain
3	C	385	 97% .
3	N	385	 97% .
4	D	248	 100%
4	O	248	 99% .
5	E	185	 31% 81% 16% ..
5	P	185	 30% 81% 16% ..
6	F	75	 96% ..
6	Q	75	 97% .
7	G	126	 98% .
7	R	126	 98% .
8	H	93	 99% .
8	S	93	 99% .
9	I	55	 95% ..
9	T	55	 85% 11% ..
10	U	52	 71% 65% 15% .. 15%
10	V	52	 87% 77% 19% ..

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32414 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-c1 complex subunit 2, mitochondrial.

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

- Molecule 3 is a protein called Cytochrome b.

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

- 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 6, mitochondrial.

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

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

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

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

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

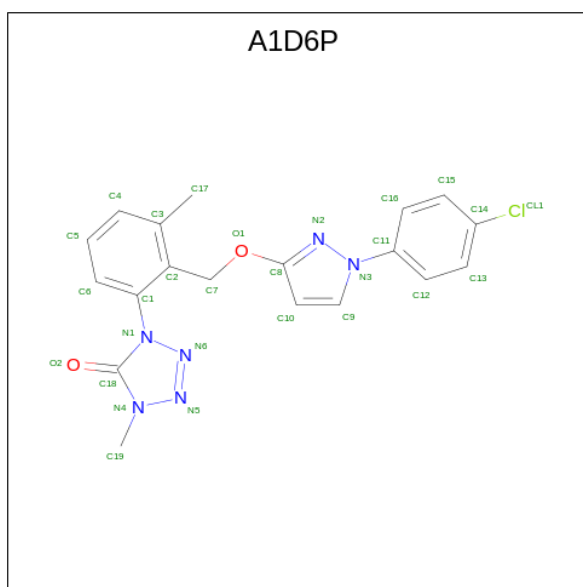
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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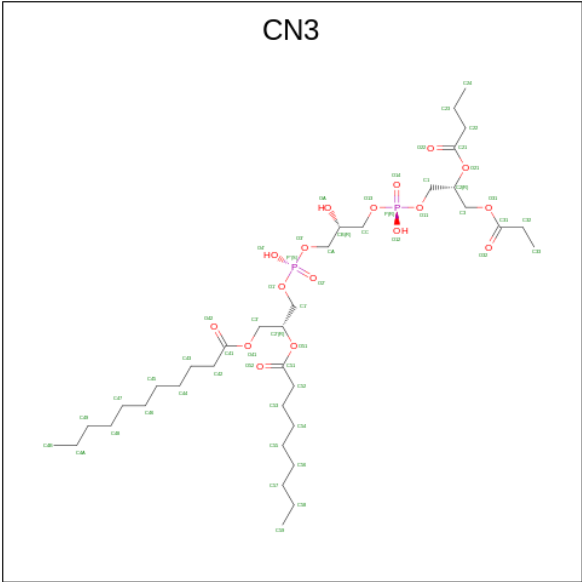
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is 1-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (CCD ID: A1D6P) (formula: C₁₉H₁₇ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



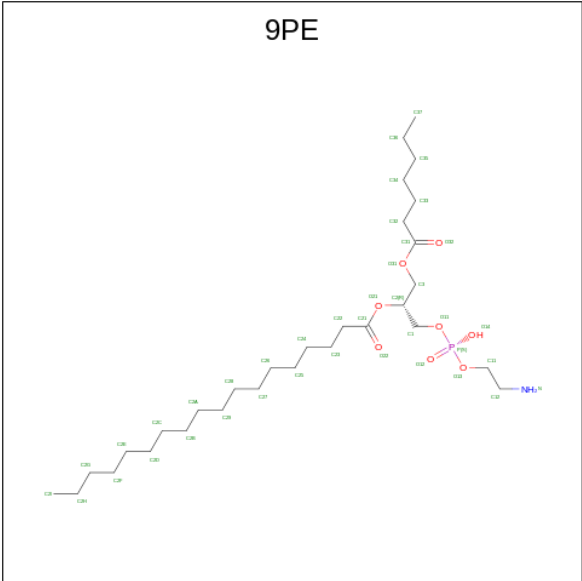
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
11	N	1	Total	C	Cl	N	O	0
			28	19	1	6	2	

- 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-diphosphanonadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



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).



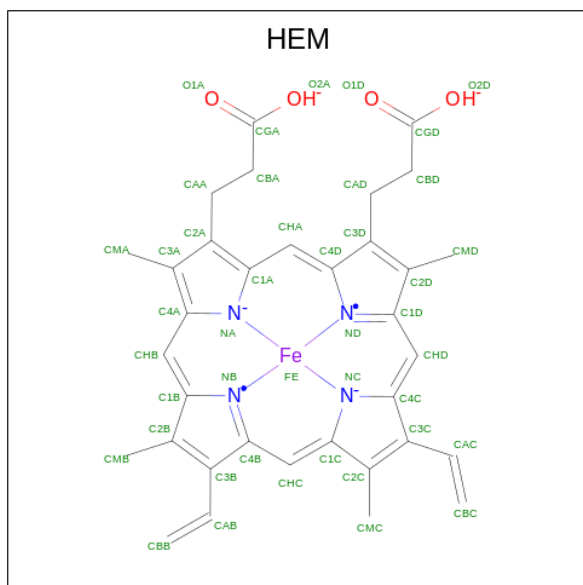
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

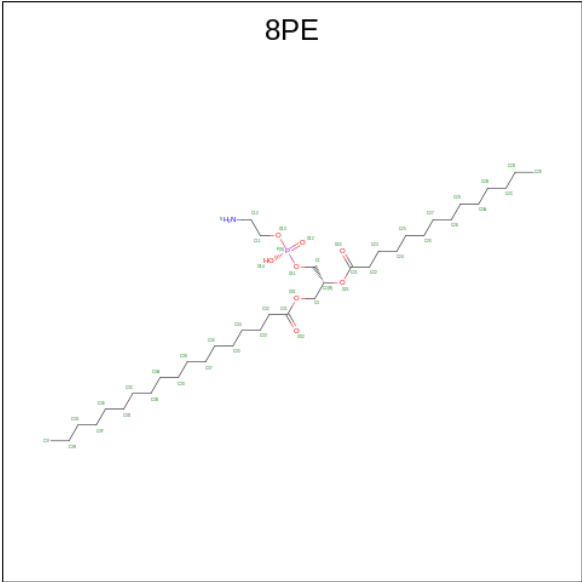
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Mol	Chain	Residues	Atoms					AltConf
13	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

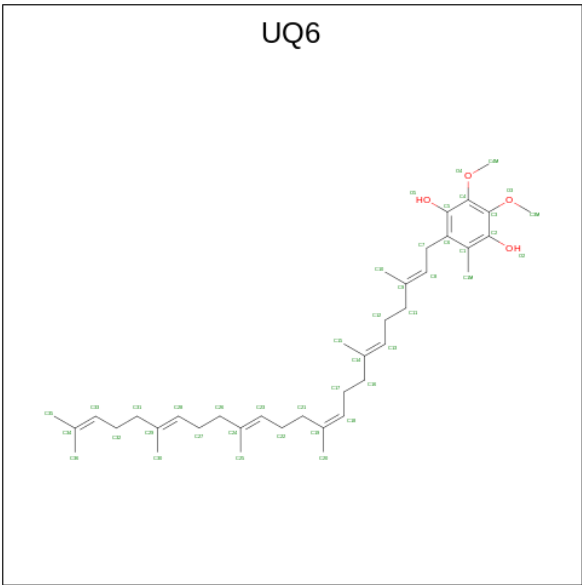
- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
15	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

- 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).



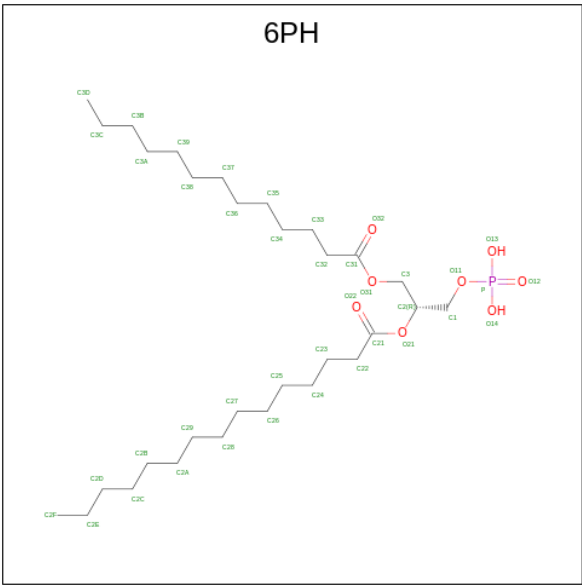
Mol	Chain	Residues	Atoms			AltConf
16	C	1	Total	C	O	0
			43	39	4	

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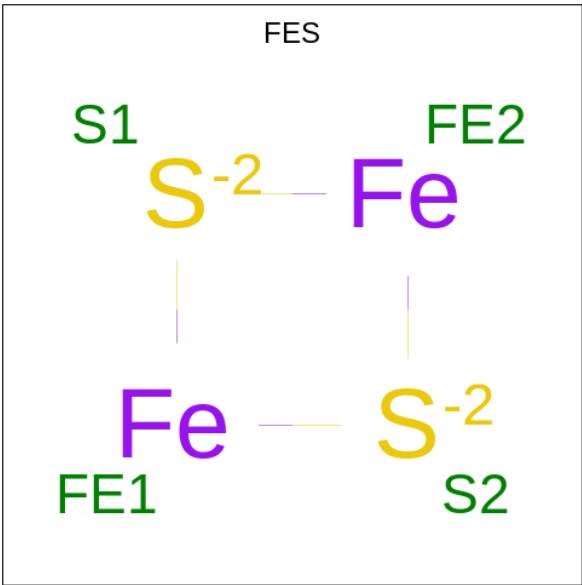
Mol	Chain	Residues	Atoms			AltConf
16	N	1	Total	C	O	0
			43	39	4	

- Molecule 17 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



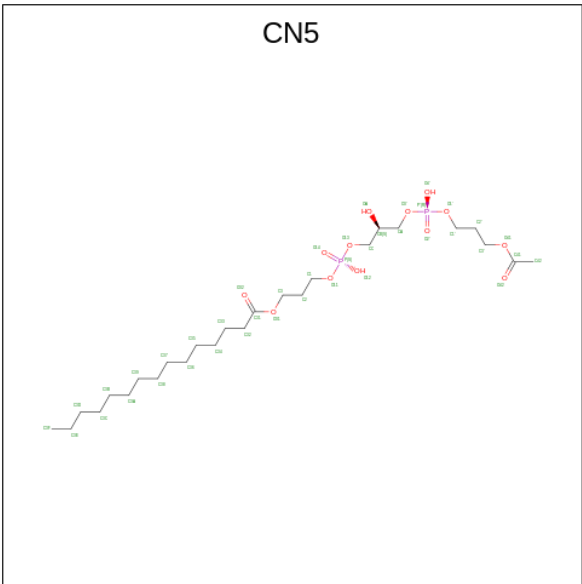
Mol	Chain	Residues	Atoms				AltConf
17	D	1	Total	C	O	P	0
			40	31	8	1	
17	E	1	Total	C	O	P	0
			40	31	8	1	
17	L	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 19 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).

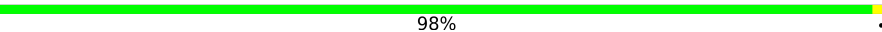


Mol	Chain	Residues	Atoms				AltConf
19	N	1	Total	C	O	P	0
			41	26	13	2	

3 Residue-property plots [i](#)

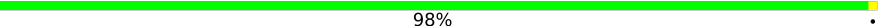
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A:  98%

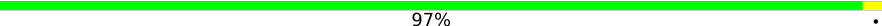


- Molecule 1: COR1 isoform 1

Chain L:  98%



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

Chain B:  97%

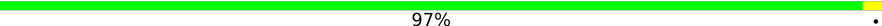


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  96%

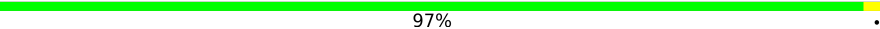


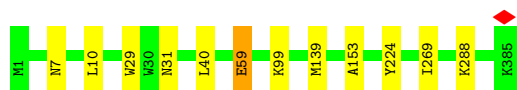
- Molecule 3: Cytochrome b

Chain C:  97%

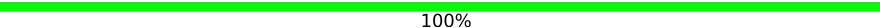


- Molecule 3: Cytochrome b

Chain N:  97% .

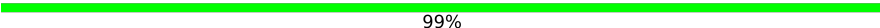


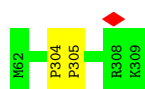
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  100%



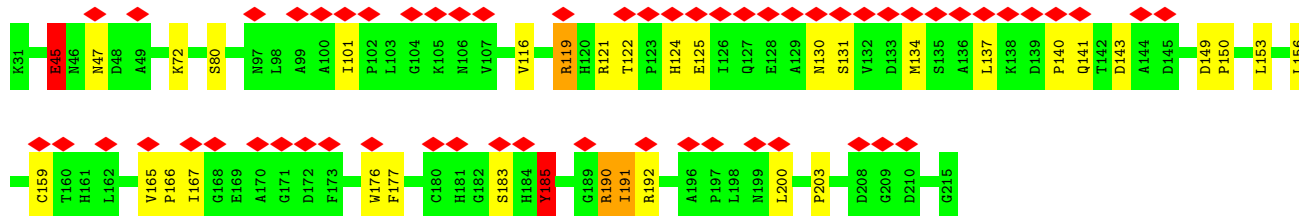
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:  99% .



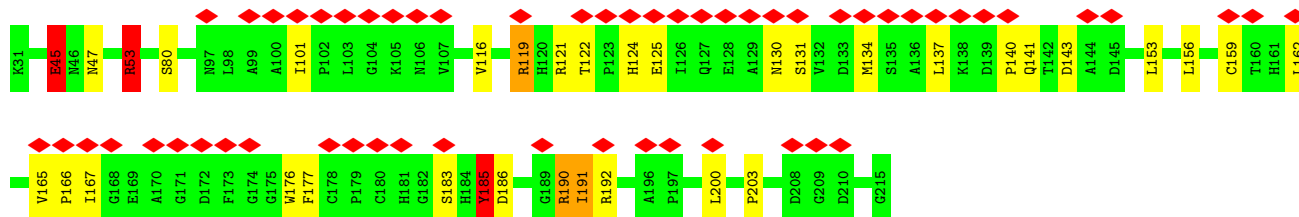
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:  31% 81% 16% ..

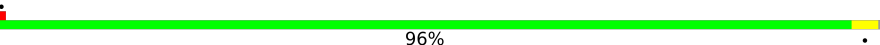


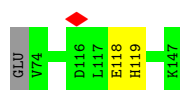
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:  30% 81% 16% ..

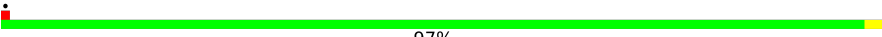


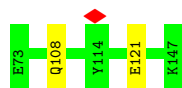
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain F:  96% ..

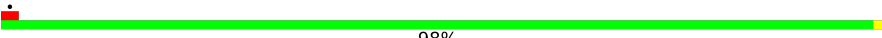


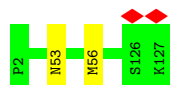
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Q:  97%

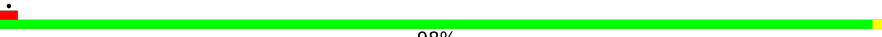


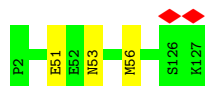
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G:  98%

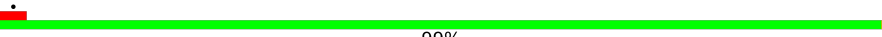


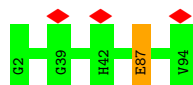
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:  98%

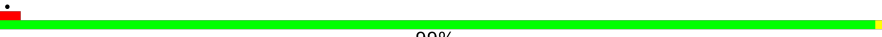


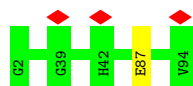
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:  99%



- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:  99%



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

Chain I:  95%



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

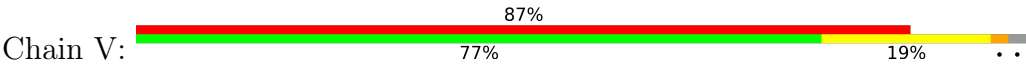
Chain T:  85% 11%



● 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	420119	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 ($e^-/\text{\AA}^2$)	49.40	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	4.311	Depositor
Minimum map value	-2.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.25	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: A1D6P, CN3, 9PE, 6PH, 8PE, FES, HEM, CN5, UQ6

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	0.26	0/3405	0.49	0/4615
1	L	0.25	0/3405	0.49	0/4615
2	B	0.24	0/2781	0.48	2/3764 (0.1%)
2	M	0.24	0/2781	0.48	2/3764 (0.1%)
3	C	0.28	0/3192	0.51	3/4354 (0.1%)
3	N	0.28	0/3192	0.51	3/4354 (0.1%)
4	D	0.24	0/2022	0.42	0/2751
4	O	0.24	0/2022	0.43	0/2751
5	E	0.33	0/1444	0.79	8/1957 (0.4%)
5	P	0.33	0/1444	0.79	8/1957 (0.4%)
6	F	0.23	0/638	0.54	0/858
6	Q	0.22	0/647	0.50	0/870
7	G	0.27	0/1040	0.56	0/1408
7	R	0.27	0/1040	0.56	0/1408
8	H	0.21	0/804	0.45	0/1088
8	S	0.21	0/804	0.46	0/1088
9	I	0.18	0/455	0.52	2/614 (0.3%)
9	T	0.21	0/456	0.71	2/615 (0.3%)
10	U	0.49	1/358 (0.3%)	1.21	6/483 (1.2%)
10	V	0.76	2/419 (0.5%)	1.06	4/567 (0.7%)
All	All	0.28	3/32349 (0.0%)	0.55	40/43881 (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
5	E	0	1
5	P	0	2
9	T	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	U	0	1
10	V	0	2
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	V	33	TRP	C-N	9.19	1.46	1.34
10	V	28	PRO	C-N	7.17	1.43	1.33
10	U	30	LEU	C-N	5.71	1.42	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	32	LEU	N-CA-C	-9.42	101.21	112.89
10	U	32	LEU	O-C-N	-9.14	109.84	122.46
5	E	125	GLU	CA-CB-CG	8.52	131.14	114.10
5	P	125	GLU	CA-CB-CG	8.49	131.08	114.10
3	C	59	GLU	CA-CB-CG	7.76	129.63	114.10
3	N	59	GLU	CA-CB-CG	7.75	129.59	114.10
10	U	31	MET	N-CA-C	-6.71	105.24	113.50
9	T	16	VAL	CA-C-N	6.69	134.31	121.54
9	T	16	VAL	C-N-CA	6.69	134.31	121.54
10	V	33	TRP	N-CA-C	-6.42	104.36	111.36
5	E	185	TYR	CA-CB-CG	6.33	125.30	113.90
5	P	185	TYR	CA-CB-CG	6.32	125.27	113.90
5	P	119	ARG	NE-CZ-NH2	6.15	124.73	119.20
5	E	119	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	M	190	GLU	CB-CG-CD	6.07	122.92	112.60
5	P	125	GLU	CB-CG-CD	6.05	122.89	112.60
2	B	190	GLU	CB-CG-CD	6.03	122.85	112.60
5	E	125	GLU	CB-CG-CD	5.99	122.78	112.60
2	B	190	GLU	CA-CB-CG	5.76	125.61	114.10
10	U	25	ALA	CA-C-N	5.75	131.21	121.14
10	U	25	ALA	C-N-CA	5.75	131.21	121.14
2	M	190	GLU	CA-CB-CG	5.72	125.54	114.10
10	U	33	TRP	N-CA-C	-5.57	106.44	113.18
5	E	177	PHE	CA-C-N	5.53	140.08	121.27
5	E	177	PHE	C-N-CA	5.53	140.08	121.27
5	P	177	PHE	CA-C-N	5.53	140.06	121.27
5	P	177	PHE	C-N-CA	5.53	140.06	121.27
10	V	28	PRO	CA-C-N	5.44	131.96	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	28	PRO	C-N-CA	5.44	131.96	121.18
3	N	59	GLU	CB-CG-CD	5.41	121.80	112.60
3	C	59	GLU	CB-CG-CD	5.39	121.76	112.60
10	V	33	TRP	O-C-N	5.25	128.14	122.15
9	I	11	PHE	CA-C-N	5.17	131.42	121.54
9	I	11	PHE	C-N-CA	5.17	131.42	121.54
5	E	141	GLN	CA-C-N	5.16	131.40	121.54
5	E	141	GLN	C-N-CA	5.16	131.40	121.54
5	P	141	GLN	CA-C-N	5.16	131.39	121.54
5	P	141	GLN	C-N-CA	5.16	131.39	121.54
3	N	31	ASN	CA-CB-CG	5.16	117.75	112.60
3	C	31	ASN	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	45	GLU	Peptide
5	P	45	GLU	Peptide
5	P	53	ARG	Sidechain
9	T	16	VAL	Peptide
9	T	7	TYR	Peptide
10	U	32	LEU	Mainchain
10	V	31	MET	Peptide
10	V	34	GLY	Mainchain

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	A	3344	0	3323	6	0
1	L	3344	0	3323	4	0
2	B	2735	0	2774	4	0
2	M	2735	0	2774	11	0
3	C	3090	0	3129	8	0
3	N	3090	0	3129	6	0
4	D	1961	0	1890	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1961	0	1890	1	0
5	E	1411	0	1390	21	0
5	P	1411	0	1390	22	0
6	F	624	0	581	1	0
6	Q	633	0	587	1	0
7	G	1019	0	1034	2	0
7	R	1019	0	1034	3	0
8	H	773	0	736	1	0
8	S	773	0	736	0	0
9	I	442	0	440	1	0
9	T	443	0	440	3	0
10	U	347	0	345	3	0
10	V	406	0	414	6	0
11	C	28	0	0	0	0
11	N	28	0	0	0	0
12	C	55	0	66	0	0
12	N	55	0	66	0	0
13	C	40	0	59	1	0
13	N	40	0	59	0	0
14	C	86	0	60	1	0
14	D	43	0	30	0	0
14	N	86	0	60	1	0
14	O	43	0	30	1	0
15	C	47	0	73	0	0
15	N	47	0	73	0	0
16	C	43	0	60	4	0
16	N	43	0	60	4	0
17	D	40	0	59	0	0
17	E	40	0	59	3	0
17	L	40	0	59	2	0
18	E	4	0	0	0	0
18	P	4	0	0	0	0
19	N	41	0	50	4	0
All	All	32414	0	32282	111	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 2.

All (111) 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:M:134:ALA:HB1	2:M:140:LYS:HE2	1.60	0.83
2:M:134:ALA:HB1	2:M:140:LYS:CE	2.11	0.80
2:M:134:ALA:CB	2:M:140:LYS:HE2	2.12	0.78
5:E:121:ARG:HD2	5:E:153:LEU:HB2	1.66	0.77
5:P:121:ARG:HD2	5:P:153:LEU:HB2	1.66	0.76
5:P:121:ARG:CD	5:P:153:LEU:HB2	2.15	0.76
10:U:29:ASN:HA	10:U:32:LEU:HB2	1.69	0.75
5:E:121:ARG:CD	5:E:153:LEU:HB2	2.15	0.75
2:M:134:ALA:HB1	2:M:140:LYS:HD3	1.70	0.74
2:M:134:ALA:HB1	2:M:140:LYS:CD	2.19	0.73
17:L:501:6PH:H38	19:N:406:CN5:H35	1.70	0.73
2:B:332:VAL:HG13	2:B:334:SER:H	1.55	0.71
2:M:332:VAL:HG13	2:M:334:SER:H	1.55	0.70
10:U:15:PHE:HB2	10:U:18:LEU:HB2	1.74	0.68
10:V:57:LYS:HG3	10:V:58:LYS:HG3	1.78	0.66
5:E:72:LYS:HG3	10:V:44:PHE:HA	1.76	0.65
5:P:121:ARG:HG3	5:P:153:LEU:HB2	1.78	0.65
5:E:121:ARG:HG3	5:E:153:LEU:HB2	1.78	0.64
5:P:121:ARG:CG	5:P:153:LEU:HB2	2.27	0.63
5:E:121:ARG:CG	5:E:153:LEU:HB2	2.27	0.62
10:V:20:LEU:HA	10:V:23:LEU:HB2	1.83	0.61
5:E:137:LEU:HG	5:E:192:ARG:HB3	1.83	0.60
5:P:121:ARG:HD2	5:P:153:LEU:HD13	1.83	0.60
5:E:121:ARG:HD2	5:E:153:LEU:HD13	1.82	0.59
5:P:137:LEU:HG	5:P:192:ARG:HB3	1.83	0.59
6:Q:108:GLN:HE22	6:Q:121:GLU:HB3	1.67	0.59
3:C:7:ASN:HD22	3:C:10:LEU:H	1.50	0.58
3:N:7:ASN:HD22	3:N:10:LEU:H	1.50	0.58
5:P:159:CYS:HA	5:P:200:LEU:HD11	1.87	0.56
5:E:159:CYS:HA	5:E:200:LEU:HD11	1.88	0.56
1:A:456:ARG:HA	10:V:33:TRP:HZ2	1.71	0.55
3:N:29:TRP:HB3	3:N:99:LYS:HG3	1.89	0.54
9:I:31:VAL:HG13	10:V:61:LEU:HD12	1.89	0.54
3:C:29:TRP:HB3	3:C:99:LYS:HG3	1.89	0.54
16:N:402:UQ6:H3M2	14:N:408:HEM:HAA2	1.90	0.53
2:B:336:ILE:HG13	2:B:338:LEU:HD13	1.91	0.53
3:C:153:ALA:HB2	3:C:288:LYS:HE2	1.91	0.53
2:M:336:ILE:HG13	2:M:338:LEU:HD13	1.91	0.53
1:A:172:THR:HG21	1:A:242:ALA:HA	1.92	0.52
1:L:172:THR:CG2	1:L:242:ALA:HA	2.40	0.51
3:C:40:LEU:HD23	16:C:407:UQ6:H151	1.92	0.51
19:N:406:CN5:O2'	19:N:406:CN5:H2'A	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:CG2	1:A:242:ALA:HA	2.40	0.51
3:N:153:ALA:HB2	3:N:288:LYS:HE2	1.91	0.51
1:L:172:THR:HG21	1:L:242:ALA:HA	1.93	0.50
3:C:139:MET:HE1	3:C:269:ILE:HA	1.94	0.50
3:N:139:MET:HE1	3:N:269:ILE:HA	1.94	0.50
5:E:130:ASN:HD21	5:E:143:ASP:HB2	1.78	0.49
14:C:405:HEM:HAA2	16:C:407:UQ6:H3M3	1.95	0.49
5:E:156:LEU:HD23	5:E:203:PRO:HG3	1.95	0.49
6:F:118:GLU:O	6:F:119:HIS:HD2	1.94	0.49
5:P:121:ARG:HH21	5:P:153:LEU:HD22	1.79	0.48
5:P:130:ASN:HD22	5:P:190:ARG:HH22	1.61	0.48
3:C:269:ILE:HD12	5:P:162:LEU:HD22	1.95	0.48
5:E:130:ASN:HD22	5:E:190:ARG:HH22	1.62	0.48
5:E:121:ARG:HH21	5:E:153:LEU:HD22	1.79	0.48
5:P:156:LEU:HD23	5:P:203:PRO:HG3	1.95	0.48
5:P:130:ASN:HD21	5:P:143:ASP:HB2	1.78	0.48
10:U:23:LEU:HG	10:U:27:ALA:HB2	1.96	0.47
1:A:341:ASP:OD2	3:C:5:LYS:NZ	2.44	0.47
5:P:45:GLU:H	5:P:45:GLU:HG3	1.31	0.47
5:P:53:ARG:HH12	9:T:13:ARG:NH1	2.13	0.47
3:N:40:LEU:HD23	16:N:402:UQ6:H161	1.97	0.47
5:P:134:MET:HE3	5:P:190:ARG:HD2	1.97	0.46
5:E:134:MET:HE3	5:E:190:ARG:HD2	1.97	0.46
1:L:166:SER:HA	1:L:175:SER:HB2	1.98	0.46
17:E:302:6PH:H2D	17:E:302:6PH:H2A	1.66	0.46
19:N:406:CN5:H33	19:N:406:CN5:H36	1.39	0.46
7:G:53:ASN:ND2	7:G:56:MET:HB2	2.31	0.46
16:N:402:UQ6:H301	16:N:402:UQ6:H321	1.73	0.45
7:G:53:ASN:HD21	7:G:56:MET:HB2	1.82	0.45
5:P:130:ASN:ND2	5:P:143:ASP:HB2	2.32	0.45
9:T:4:SER:HB2	9:T:6:LEU:HD23	1.99	0.45
1:A:166:SER:HA	1:A:175:SER:HB2	1.98	0.45
5:E:134:MET:HE2	5:E:140:PRO:HA	2.00	0.44
7:R:53:ASN:HD21	7:R:56:MET:HB2	1.83	0.44
3:C:229:ASP:HB3	17:E:302:6PH:H2B	1.98	0.44
5:E:130:ASN:ND2	5:E:143:ASP:HB2	2.32	0.44
5:P:134:MET:HE2	5:P:140:PRO:HA	2.00	0.44
16:C:407:UQ6:H151	16:C:407:UQ6:H172	1.75	0.43
17:L:501:6PH:H3AA	19:N:406:CN5:H34	2.01	0.43
7:R:53:ASN:ND2	7:R:56:MET:HB2	2.32	0.43
9:T:16:VAL:HG12	9:T:20:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:444:ASP:OD2	3:N:224:TYR:HE1	2.02	0.43
16:C:407:UQ6:H201	16:C:407:UQ6:H222	1.76	0.43
2:B:267:LEU:HD22	2:B:304:ILE:HD13	2.01	0.43
16:N:402:UQ6:H1M1	16:N:402:UQ6:H71	1.79	0.43
4:O:304:PRO:HA	4:O:305:PRO:HD3	1.88	0.42
5:P:116:VAL:HA	5:P:156:LEU:HA	2.02	0.42
5:E:45:GLU:H	5:E:45:GLU:HG3	1.31	0.42
5:E:116:VAL:HA	5:E:156:LEU:HA	2.02	0.42
2:M:267:LEU:HD22	2:M:304:ILE:HD13	2.01	0.42
17:E:302:6PH:H2FA	17:E:302:6PH:H59	1.83	0.42
13:C:403:9PE:H33	13:C:403:9PE:H22	2.02	0.42
14:O:401:HEM:HBC2	14:O:401:HEM:HHD	2.02	0.41
2:M:134:ALA:HB2	2:M:140:LYS:HE2	1.96	0.41
8:H:87:GLU:H	8:H:87:GLU:HG2	1.72	0.41
5:P:122:THR:HG22	5:P:124:HIS:H	1.85	0.41
5:P:185:TYR:CD1	5:P:191:ILE:HG12	2.56	0.41
1:A:53:VAL:HG23	1:A:120:LEU:HD21	2.02	0.41
5:E:166:PRO:HB2	5:E:176:TRP:HB3	2.02	0.41
2:B:132:ALA:HA	2:B:135:GLU:HG2	2.02	0.41
2:M:115:LYS:HD3	2:M:115:LYS:HA	1.89	0.41
5:E:122:THR:HG22	5:E:124:HIS:H	1.85	0.41
5:E:185:TYR:CD1	5:E:191:ILE:HG12	2.56	0.41
5:P:166:PRO:HB2	5:P:176:TRP:HB3	2.02	0.41
7:R:51:GLU:HA	7:R:56:MET:HG2	2.03	0.41
10:V:23:LEU:HG	10:V:27:ALA:HB2	2.02	0.41
5:E:149:ASP:HA	5:E:150:PRO:HD3	1.98	0.40
5:P:185:TYR:HB2	5:P:186:ASP:H	1.75	0.40
2:M:132:ALA:HA	2:M:135:GLU:HG2	2.02	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%)	411 (96%)	18 (4%)	0	100	100
1	L	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
2	B	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
2	M	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	C	383/385 (100%)	377 (98%)	6 (2%)	0	100	100
3	N	383/385 (100%)	377 (98%)	6 (2%)	0	100	100
4	D	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
4	O	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
5	E	183/185 (99%)	150 (82%)	33 (18%)	0	100	100
5	P	183/185 (99%)	149 (81%)	34 (19%)	0	100	100
6	F	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
6	Q	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
7	G	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
7	R	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
8	S	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
9	I	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
9	T	52/55 (94%)	46 (88%)	5 (10%)	1 (2%)	6	10
10	U	42/52 (81%)	35 (83%)	7 (17%)	0	100	100
10	V	49/52 (94%)	42 (86%)	7 (14%)	0	100	100
All	All	3952/4004 (99%)	3762 (95%)	189 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	T	17	PHE

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%)	366 (99%)	4 (1%)	65	83
1	L	370/370 (100%)	367 (99%)	3 (1%)	73	88
2	B	301/301 (100%)	298 (99%)	3 (1%)	68	85
2	M	301/301 (100%)	298 (99%)	3 (1%)	68	85
3	C	338/338 (100%)	337 (100%)	1 (0%)	86	94
3	N	338/338 (100%)	337 (100%)	1 (0%)	86	94
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	206/206 (100%)	206 (100%)	0	100	100
5	E	151/151 (100%)	139 (92%)	12 (8%)	11	22
5	P	151/151 (100%)	138 (91%)	13 (9%)	10	19
6	F	67/68 (98%)	67 (100%)	0	100	100
6	Q	68/68 (100%)	68 (100%)	0	100	100
7	G	110/110 (100%)	110 (100%)	0	100	100
7	R	110/110 (100%)	110 (100%)	0	100	100
8	H	77/77 (100%)	76 (99%)	1 (1%)	61	81
8	S	77/77 (100%)	76 (99%)	1 (1%)	61	81
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	36
10	V	42/43 (98%)	42 (100%)	0	100	100
All	All	3407/3418 (100%)	3363 (99%)	44 (1%)	59	81

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	172	THR
1	A	444	ASP
1	A	456	ARG
2	B	54	PHE
2	B	190	GLU
2	B	281	ASP
3	C	59	GLU
5	E	45	GLU
5	E	47	ASN
5	E	80	SER

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Mol	Chain	Res	Type
5	E	101	ILE
5	E	119	ARG
5	E	131	SER
5	E	165	VAL
5	E	167	ILE
5	E	183	SER
5	E	185	TYR
5	E	190	ARG
5	E	191	ILE
8	H	87	GLU
1	L	113	THR
1	L	172	THR
1	L	456	ARG
2	M	54	PHE
2	M	190	GLU
2	M	281	ASP
3	N	59	GLU
5	P	45	GLU
5	P	47	ASN
5	P	53	ARG
5	P	80	SER
5	P	101	ILE
5	P	119	ARG
5	P	131	SER
5	P	165	VAL
5	P	167	ILE
5	P	183	SER
5	P	185	TYR
5	P	190	ARG
5	P	191	ILE
8	S	87	GLU
10	U	31	MET
10	U	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	154	ASN
1	A	199	ASN
1	A	271	ASN
1	A	274	ASN

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	298	GLN
1	A	317	HIS
1	A	352	ASN
1	A	385	ASN
2	B	52	ASN
2	B	157	ASN
2	B	325	ASN
2	B	339	ASN
3	C	7	ASN
3	C	222	HIS
3	C	316	ASN
3	C	332	ASN
4	D	79	ASN
4	D	87	HIS
4	D	127	ASN
4	D	161	ASN
4	D	256	ASN
5	E	120	HIS
5	E	130	ASN
5	E	181	HIS
5	E	184	HIS
6	F	87	ASN
6	F	96	HIS
7	G	30	ASN
7	G	34	ASN
7	G	53	ASN
7	G	79	HIS
7	G	85	HIS
8	H	72	ASN
1	L	122	GLN
1	L	154	ASN
1	L	199	ASN
1	L	274	ASN
1	L	283	GLN
1	L	298	GLN
1	L	317	HIS
1	L	352	ASN
1	L	385	ASN
2	M	52	ASN
2	M	157	ASN
2	M	325	ASN

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Mol	Chain	Res	Type
3	N	7	ASN
3	N	73	HIS
3	N	222	HIS
3	N	316	ASN
3	N	332	ASN
4	O	79	ASN
4	O	87	HIS
4	O	127	ASN
4	O	161	ASN
4	O	256	ASN
5	P	120	HIS
5	P	130	ASN
5	P	181	HIS
5	P	184	HIS
6	Q	77	GLN
6	Q	84	HIS
6	Q	96	HIS
6	Q	108	GLN
6	Q	119	HIS
7	R	30	ASN
7	R	34	ASN
7	R	53	ASN
7	R	79	HIS
8	S	47	ASN
8	S	72	ASN
9	T	14	ASN
9	T	44	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

22 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$
17	6PH	D	402	-	39,39,39	0.93	4 (10%)	43,44,44	1.17	2 (4%)
12	CN3	N	407	-	54,54,54	1.16	8 (14%)	60,66,66	1.18	4 (6%)
15	8PE	C	406	-	46,46,46	0.90	4 (8%)	49,51,51	1.12	2 (4%)
12	CN3	C	402	-	54,54,54	1.19	8 (14%)	60,66,66	1.25	4 (6%)
14	HEM	N	405	3	50,50,50	1.46	7 (14%)	66,82,82	1.61	14 (21%)
11	A1D6P	N	401	-	31,31,31	1.68	6 (19%)	34,44,44	2.13	4 (11%)
13	9PE	C	403	-	39,39,39	0.94	4 (10%)	42,44,44	1.15	2 (4%)
14	HEM	O	401	4	50,50,50	1.35	7 (14%)	66,82,82	1.40	12 (18%)
14	HEM	C	405	3	50,50,50	1.41	8 (16%)	66,82,82	1.38	10 (15%)
14	HEM	C	404	3	50,50,50	1.47	7 (14%)	66,82,82	1.57	14 (21%)
18	FES	E	301	-	0,4,4	-	-	-	-	-
16	UQ6	C	407	-	43,43,43	1.54	6 (13%)	51,55,55	1.89	14 (27%)
16	UQ6	N	402	-	43,43,43	1.55	7 (16%)	51,55,55	1.73	14 (27%)
14	HEM	D	401	4	50,50,50	1.32	6 (12%)	66,82,82	1.25	8 (12%)
18	FES	P	301	-	0,4,4	-	-	-	-	-
17	6PH	E	302	-	39,39,39	0.93	3 (7%)	43,44,44	1.17	2 (4%)
11	A1D6P	C	401	-	31,31,31	1.67	5 (16%)	34,44,44	2.12	4 (11%)
15	8PE	N	403	-	46,46,46	0.89	4 (8%)	49,51,51	1.17	2 (4%)
19	CN5	N	406	-	40,40,40	0.33	0	44,48,48	0.40	0
17	6PH	L	501	-	39,39,39	0.94	4 (10%)	43,44,44	1.15	2 (4%)
13	9PE	N	404	-	39,39,39	0.93	3 (7%)	42,44,44	1.06	3 (7%)
14	HEM	N	408	3	50,50,50	1.43	7 (14%)	66,82,82	1.43	10 (15%)

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
17	6PH	D	402	-	-	19/41/41/41	-
12	CN3	N	407	-	-	29/65/65/65	-
15	8PE	C	406	-	-	18/50/50/50	-
12	CN3	C	402	-	-	11/65/65/65	-
14	HEM	N	405	3	-	4/14/54/54	-
11	A1D6P	N	401	-	-	0/13/13/13	0/4/4/4
13	9PE	C	403	-	-	23/43/43/43	-
14	HEM	O	401	4	-	1/14/54/54	-
14	HEM	C	405	3	-	7/14/54/54	-
14	HEM	C	404	3	-	6/14/54/54	-
18	FES	E	301	-	-	-	0/1/1/1
16	UQ6	C	407	-	-	14/39/39/39	0/1/1/1
16	UQ6	N	402	-	-	14/39/39/39	0/1/1/1
14	HEM	D	401	4	-	2/14/54/54	-
18	FES	P	301	-	-	-	0/1/1/1
17	6PH	E	302	-	-	19/41/41/41	-
11	A1D6P	C	401	-	-	0/13/13/13	0/4/4/4
15	8PE	N	403	-	-	21/50/50/50	-
19	CN5	N	406	-	-	23/44/44/44	-
17	6PH	L	501	-	-	14/41/41/41	-
13	9PE	N	404	-	-	23/43/43/43	-
14	HEM	N	408	3	-	4/14/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	401	A1D6P	O1-C8	4.72	1.40	1.35
11	C	401	A1D6P	O1-C8	4.66	1.40	1.35
14	N	408	HEM	FE-ND	4.39	2.08	1.94
14	C	404	HEM	FE-ND	4.20	2.07	1.94
14	N	405	HEM	FE-ND	4.17	2.07	1.94
16	C	407	UQ6	C7-C6	4.09	1.56	1.51
16	N	402	UQ6	C7-C6	4.02	1.56	1.51
11	N	401	A1D6P	N3-N2	-3.99	1.32	1.37
14	C	405	HEM	FE-ND	3.97	2.07	1.94
11	C	401	A1D6P	N3-N2	-3.91	1.32	1.37
14	N	405	HEM	FE-NB	3.52	2.05	1.94
14	C	404	HEM	FE-NB	3.50	2.05	1.94
14	C	405	HEM	FE-NA	3.29	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	401	HEM	FE-NA	3.25	2.06	1.95
14	N	405	HEM	CAC-C3C	3.17	1.56	1.47
14	C	404	HEM	CAC-C3C	3.17	1.56	1.47
11	C	401	A1D6P	C9-N3	-3.12	1.31	1.35
14	N	408	HEM	CAC-C3C	3.10	1.55	1.47
11	N	401	A1D6P	C9-N3	-3.10	1.31	1.35
14	D	401	HEM	CAC-C3C	3.07	1.55	1.47
14	C	405	HEM	CAB-C3B	3.07	1.55	1.47
14	O	401	HEM	FE-NB	3.06	2.04	1.94
14	C	405	HEM	CAC-C3C	3.03	1.55	1.47
14	N	405	HEM	CAB-C3B	3.02	1.55	1.47
14	C	404	HEM	CAB-C3B	3.01	1.55	1.47
14	D	401	HEM	CAB-C3B	3.00	1.55	1.47
14	O	401	HEM	CAB-C3B	2.97	1.55	1.47
14	D	401	HEM	FE-NB	2.92	2.03	1.94
16	C	407	UQ6	O3-C3	2.91	1.43	1.38
16	N	402	UQ6	O3-C3	2.90	1.43	1.38
14	N	408	HEM	FE-NA	2.85	2.04	1.95
14	O	401	HEM	CAC-C3C	2.82	1.55	1.47
14	D	401	HEM	FE-NA	2.82	2.04	1.95
14	C	404	HEM	FE-NC	2.81	2.04	1.95
14	N	405	HEM	FE-NC	2.81	2.04	1.95
12	N	407	CN3	O21-C2	-2.73	1.39	1.46
14	C	405	HEM	FE-NC	2.72	2.04	1.95
14	N	408	HEM	FE-NB	2.71	2.03	1.94
15	C	406	8PE	O21-C2	-2.68	1.39	1.46
14	N	408	HEM	CAB-C3B	2.67	1.54	1.47
17	E	302	6PH	O21-C2	-2.62	1.40	1.46
17	L	501	6PH	O21-C2	-2.62	1.40	1.46
15	N	403	8PE	O21-C2	-2.61	1.40	1.46
12	N	407	CN3	O51-C2'	-2.55	1.40	1.46
17	D	402	6PH	O21-C2	-2.54	1.40	1.46
14	D	401	HEM	FE-ND	2.50	2.02	1.94
16	N	402	UQ6	C26-C24	2.46	1.56	1.51
15	C	406	8PE	O31-C3	-2.44	1.39	1.45
17	E	302	6PH	O31-C31	2.43	1.40	1.33
12	C	402	CN3	O41-C41	2.43	1.40	1.33
11	C	401	A1D6P	O2-C18	-2.42	1.18	1.22
12	C	402	CN3	O51-C2'	-2.41	1.40	1.46
17	L	501	6PH	O31-C31	2.41	1.40	1.33
12	C	402	CN3	O21-C2	-2.38	1.40	1.46
14	O	401	HEM	FE-NC	2.38	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	402	CN3	O51-C51	2.38	1.41	1.34
11	N	401	A1D6P	O2-C18	-2.37	1.18	1.22
13	N	404	9PE	O21-C21	2.37	1.41	1.34
16	C	407	UQ6	C26-C24	2.37	1.56	1.51
12	C	402	CN3	O31-C31	2.36	1.40	1.33
12	N	407	CN3	O41-C41	2.36	1.40	1.33
11	N	401	A1D6P	O1-C7	-2.35	1.40	1.45
11	C	401	A1D6P	O1-C7	-2.35	1.40	1.45
13	C	403	9PE	O21-C21	2.31	1.40	1.34
12	C	402	CN3	O21-C21	2.29	1.40	1.34
12	N	407	CN3	O41-C3'	-2.29	1.39	1.45
14	O	401	HEM	FE-ND	2.29	2.01	1.94
15	N	403	8PE	O31-C3	-2.28	1.40	1.45
12	C	402	CN3	O41-C3'	-2.28	1.40	1.45
16	C	407	UQ6	C16-C14	2.27	1.56	1.51
12	N	407	CN3	O51-C51	2.27	1.40	1.34
17	D	402	6PH	O31-C31	2.26	1.39	1.33
16	C	407	UQ6	C21-C19	2.25	1.56	1.51
15	N	403	8PE	O31-C31	2.25	1.39	1.33
15	C	406	8PE	O31-C31	2.24	1.39	1.33
12	N	407	CN3	O31-C3	-2.24	1.40	1.45
16	N	402	UQ6	C21-C19	2.24	1.55	1.51
13	C	403	9PE	O31-C3	-2.23	1.40	1.45
13	C	403	9PE	O31-C31	2.22	1.39	1.33
16	N	402	UQ6	C13-C14	2.22	1.38	1.33
17	D	402	6PH	O31-C3	-2.22	1.40	1.45
12	N	407	CN3	O31-C31	2.20	1.39	1.33
14	N	408	HEM	C3B-C2B	-2.20	1.32	1.37
17	E	302	6PH	O31-C3	-2.18	1.40	1.45
13	N	404	9PE	O31-C31	2.17	1.39	1.33
17	L	501	6PH	O31-C3	-2.17	1.40	1.45
13	N	404	9PE	O31-C3	-2.16	1.40	1.45
15	C	406	8PE	O21-C21	2.16	1.40	1.34
16	C	407	UQ6	C13-C14	2.10	1.38	1.33
14	O	401	HEM	C3C-C2C	-2.09	1.33	1.37
14	C	405	HEM	C2A-C3A	-2.09	1.33	1.38
16	N	402	UQ6	C16-C14	2.08	1.55	1.51
14	N	405	HEM	CMB-C2B	2.07	1.55	1.50
16	N	402	UQ6	C11-C9	2.07	1.55	1.51
12	N	407	CN3	O21-C21	2.06	1.40	1.34
17	L	501	6PH	O21-C21	2.06	1.40	1.34
14	C	405	HEM	FE-NB	2.05	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	403	8PE	O21-C21	2.05	1.40	1.34
12	C	402	CN3	O31-C3	-2.04	1.40	1.45
14	N	405	HEM	FE-NA	2.04	2.02	1.95
17	D	402	6PH	O21-C21	2.04	1.40	1.34
14	N	408	HEM	FE-NC	2.04	2.02	1.95
14	C	404	HEM	FE-NA	2.03	2.02	1.95
14	C	404	HEM	CMB-C2B	2.03	1.55	1.50
11	N	401	A1D6P	C14-CL1	2.03	1.78	1.74
14	D	401	HEM	CMB-C2B	2.03	1.55	1.50
13	C	403	9PE	O21-C2	-2.02	1.41	1.46
14	C	405	HEM	CMB-C2B	2.02	1.55	1.50

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	401	A1D6P	C10-C8-N2	-9.91	106.01	113.53
11	C	401	A1D6P	C10-C8-N2	-9.87	106.03	113.53
16	C	407	UQ6	C6-C7-C8	6.70	122.77	112.17
14	N	405	HEM	CAD-C3D-C4D	4.91	133.25	124.66
14	C	404	HEM	CAD-C3D-C4D	4.90	133.23	124.66
14	N	405	HEM	CAD-C3D-C2D	-4.37	119.74	127.88
14	C	404	HEM	CAD-C3D-C2D	-4.35	119.78	127.88
12	C	402	CN3	O21-C21-C22	4.29	120.75	111.50
15	N	403	8PE	O21-C21-C22	4.10	120.34	111.50
12	C	402	CN3	O51-C51-C52	4.06	120.25	111.50
12	N	407	CN3	O51-C51-C52	3.90	119.90	111.50
12	C	402	CN3	O31-C31-C32	3.86	121.51	111.38
17	E	302	6PH	O21-C21-C22	3.82	119.72	111.50
17	D	402	6PH	O21-C21-C22	3.80	119.68	111.50
12	N	407	CN3	O21-C21-C22	3.72	119.51	111.50
17	L	501	6PH	O21-C21-C22	3.71	119.50	111.50
16	N	402	UQ6	C3M-O3-C3	3.70	124.92	114.78
13	C	403	9PE	O21-C21-C22	3.65	119.36	111.50
11	C	401	A1D6P	C1-N1-N6	3.64	126.96	120.39
11	N	401	A1D6P	C1-N1-N6	3.64	126.96	120.39
14	N	408	HEM	C1B-NB-C4B	3.55	108.74	105.07
16	N	402	UQ6	C30-C29-C31	3.53	121.21	115.27
15	C	406	8PE	O21-C21-C22	3.53	119.10	111.50
12	N	407	CN3	O31-C31-C32	3.44	120.40	111.38
16	N	402	UQ6	C7-C8-C9	-3.42	121.93	127.24
14	N	408	HEM	C4C-NC-C1C	3.38	108.66	105.35
16	C	407	UQ6	C15-C14-C16	3.37	120.94	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	401	HEM	C4C-NC-C1C	3.26	108.55	105.35
16	C	407	UQ6	C12-C13-C14	-3.26	119.81	127.66
16	N	402	UQ6	C20-C19-C21	3.22	120.69	115.27
16	C	407	UQ6	C30-C29-C31	3.15	120.57	115.27
16	C	407	UQ6	C20-C19-C21	3.12	120.53	115.27
14	C	405	HEM	C4A-NA-C1A	3.06	108.34	105.35
14	C	404	HEM	C4D-ND-C1D	3.05	108.22	105.07
13	N	404	9PE	O21-C21-C22	3.05	118.07	111.50
14	N	405	HEM	C4A-NA-C1A	3.05	108.33	105.35
16	N	402	UQ6	C25-C24-C26	3.04	120.38	115.27
14	O	401	HEM	C4D-ND-C1D	3.02	108.19	105.07
14	N	405	HEM	C4D-ND-C1D	3.01	108.18	105.07
14	D	401	HEM	CAA-CBA-CGA	-2.97	107.22	113.60
16	N	402	UQ6	O3-C3-C4	2.95	127.21	120.39
14	C	404	HEM	C4A-NA-C1A	2.95	108.23	105.35
14	D	401	HEM	C4D-ND-C1D	2.93	108.10	105.07
14	N	408	HEM	CAB-C3B-C2B	-2.90	119.06	128.60
14	N	408	HEM	C3B-C2B-C1B	2.90	108.64	106.49
14	O	401	HEM	CAA-CBA-CGA	-2.89	107.39	113.60
13	C	403	9PE	O31-C31-C32	2.88	120.94	111.91
15	N	403	8PE	O31-C31-C32	2.87	120.92	111.91
14	O	401	HEM	CAC-C3C-C4C	2.83	131.74	124.90
14	C	405	HEM	C1B-NB-C4B	2.81	107.97	105.07
14	C	405	HEM	CAA-C2A-C1A	2.80	130.40	124.89
14	C	405	HEM	C4C-NC-C1C	2.79	108.08	105.35
11	C	401	A1D6P	C19-N4-N5	2.78	126.08	121.14
12	N	407	CN3	O41-C41-C42	2.78	120.63	111.91
11	N	401	A1D6P	C19-N4-N5	2.77	126.06	121.14
14	C	405	HEM	C4D-ND-C1D	2.76	107.93	105.07
16	C	407	UQ6	C22-C23-C24	-2.73	121.08	127.66
17	E	302	6PH	O31-C31-C32	2.71	120.43	111.91
17	L	501	6PH	O31-C31-C32	2.70	120.38	111.91
14	N	405	HEM	CHA-C4D-C3D	2.67	130.33	125.33
17	D	402	6PH	O31-C31-C32	2.66	120.25	111.91
14	N	405	HEM	C1B-NB-C4B	2.66	107.82	105.07
16	C	407	UQ6	C2-C1-C6	2.65	121.62	118.75
14	C	404	HEM	CHA-C4D-C3D	2.64	130.28	125.33
14	C	404	HEM	C1B-NB-C4B	2.64	107.80	105.07
14	N	408	HEM	C4D-ND-C1D	2.62	107.78	105.07
14	C	405	HEM	CMB-C2B-C1B	-2.62	121.05	125.04
16	N	402	UQ6	C12-C13-C14	-2.62	121.36	127.66
14	O	401	HEM	CMB-C2B-C1B	-2.61	121.07	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	405	HEM	CBA-CAA-C2A	2.59	119.82	112.63
16	C	407	UQ6	C3M-O3-C3	2.59	121.87	114.78
14	D	401	HEM	CMB-C2B-C1B	-2.58	121.11	125.04
16	C	407	UQ6	C25-C24-C26	2.57	119.60	115.27
14	N	408	HEM	CHB-C1B-NB	2.56	127.53	124.37
16	N	402	UQ6	C17-C18-C19	-2.55	121.52	127.66
16	N	402	UQ6	C15-C14-C16	2.53	119.53	115.27
16	C	407	UQ6	O3-C3-C2	2.52	124.42	119.00
14	C	405	HEM	C2A-C1A-NA	-2.51	107.34	110.15
16	N	402	UQ6	C27-C28-C29	-2.50	121.64	127.66
16	C	407	UQ6	C27-C28-C29	-2.49	121.66	127.66
14	N	408	HEM	CAC-C3C-C4C	-2.48	118.90	124.90
16	N	402	UQ6	C6-C7-C8	2.47	116.08	112.17
14	O	401	HEM	CAC-C3C-C2C	-2.44	120.56	128.60
14	N	405	HEM	CBA-CAA-C2A	-2.44	105.86	112.63
12	C	402	CN3	O41-C41-C42	2.44	119.56	111.91
14	N	408	HEM	CHC-C4B-C3B	2.43	130.36	125.13
14	C	404	HEM	CBA-CAA-C2A	-2.42	105.91	112.63
16	C	407	UQ6	C12-C11-C9	-2.42	105.03	112.98
16	N	402	UQ6	C36-C34-C35	2.40	119.90	114.60
14	N	405	HEM	C2A-C1A-NA	-2.38	107.49	110.15
14	C	404	HEM	C2A-C1A-NA	-2.37	107.50	110.15
14	C	404	HEM	CBD-CAD-C3D	2.36	119.20	112.63
14	C	405	HEM	CAA-C2A-C3A	-2.36	121.67	127.07
15	C	406	8PE	O31-C31-C32	2.35	119.29	111.91
14	N	405	HEM	CBD-CAD-C3D	2.35	119.16	112.63
16	C	407	UQ6	C17-C18-C19	-2.35	122.01	127.66
14	D	401	HEM	C4C-NC-C1C	2.34	107.64	105.35
14	D	401	HEM	C1B-NB-C4B	2.33	107.48	105.07
14	D	401	HEM	C4A-NA-C1A	2.33	107.63	105.35
14	O	401	HEM	CHD-C4C-C3C	2.33	129.24	125.26
14	C	404	HEM	C3D-C4D-ND	-2.32	107.58	110.17
13	N	404	9PE	O31-C31-C32	2.29	119.11	111.91
14	N	405	HEM	C3D-C4D-ND	-2.29	107.62	110.17
14	O	401	HEM	C1B-NB-C4B	2.26	107.41	105.07
14	O	401	HEM	CHC-C1C-NC	2.24	126.86	124.44
14	N	408	HEM	CHD-C4C-NC	2.21	126.83	124.44
14	N	405	HEM	CAD-CBD-CGD	-2.21	108.84	113.60
16	N	402	UQ6	O3-C3-C2	-2.21	114.23	119.00
14	D	401	HEM	C3D-C4D-ND	-2.21	107.71	110.17
14	O	401	HEM	C3D-C4D-ND	-2.19	107.73	110.17
14	C	404	HEM	CAD-CBD-CGD	-2.18	108.91	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	408	HEM	C4A-NA-C1A	2.15	107.46	105.35
16	N	402	UQ6	C22-C23-C24	-2.14	122.50	127.66
14	O	401	HEM	C4A-NA-C1A	2.13	107.44	105.35
14	O	401	HEM	C3C-C2C-C1C	2.13	109.11	107.08
14	C	404	HEM	C1D-C2D-C3D	2.11	109.18	106.96
11	N	401	A1D6P	N1-N6-N5	2.11	109.48	107.01
14	N	405	HEM	CAC-C3C-C4C	-2.09	119.84	124.90
14	N	405	HEM	C1D-C2D-C3D	2.07	109.14	106.96
11	C	401	A1D6P	N1-N6-N5	2.07	109.43	107.01
14	C	404	HEM	CAC-C3C-C4C	-2.05	119.95	124.90
14	N	405	HEM	CMB-C2B-C1B	-2.05	121.92	125.04
16	C	407	UQ6	C36-C34-C35	2.03	119.09	114.60
14	C	405	HEM	CAC-C3C-C4C	-2.03	120.00	124.90
14	D	401	HEM	CAC-C3C-C4C	-2.03	120.00	124.90
14	C	404	HEM	CMB-C2B-C1B	-2.02	121.96	125.04
13	N	404	9PE	C2-O21-C21	2.01	122.75	117.79

There are no chirality outliers.

All (252) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	402	CN3	CC-O13-P-O14
12	C	402	CN3	CA-O3'-P'-O1'
12	C	402	CN3	CA-O3'-P'-O2'
12	C	402	CN3	CA-O3'-P'-O4'
12	N	407	CN3	CC-O13-P-O11
12	N	407	CN3	CC-O13-P-O12
12	N	407	CN3	CC-O13-P-O14
12	N	407	CN3	CA-O3'-P'-O1'
12	N	407	CN3	CA-O3'-P'-O2'
12	N	407	CN3	CA-O3'-P'-O4'
13	C	403	9PE	C11-O13-P-O12
13	N	404	9PE	C1-O11-P-O14
13	N	404	9PE	C11-O13-P-O12
13	N	404	9PE	C11-O13-P-O14
13	N	404	9PE	O13-C11-C12-N
14	C	404	HEM	C2D-C3D-CAD-CBD
14	C	404	HEM	C4D-C3D-CAD-CBD
14	C	405	HEM	C1A-C2A-CAA-CBA
14	N	405	HEM	C2D-C3D-CAD-CBD
14	N	405	HEM	C4D-C3D-CAD-CBD
15	N	403	8PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
15	N	403	8PE	C11-O13-P-O12
15	N	403	8PE	C11-O13-P-O14
15	N	403	8PE	C22-C21-O21-C2
16	C	407	UQ6	C1-C6-C7-C8
16	C	407	UQ6	C15-C14-C16-C17
16	C	407	UQ6	C28-C29-C31-C32
16	C	407	UQ6	C30-C29-C31-C32
16	N	402	UQ6	C1-C6-C7-C8
17	D	402	6PH	C1-O11-P-O13
17	D	402	6PH	C1-O11-P-O14
17	D	402	6PH	C22-C21-O21-C2
17	E	302	6PH	C22-C21-O21-C2
19	N	406	CN5	CC-O13-P-O14
19	N	406	CN5	C2-C1-O11-P
17	E	302	6PH	O32-C31-O31-C3
17	E	302	6PH	C32-C31-O31-C3
12	C	402	CN3	O32-C31-O31-C3
15	N	403	8PE	O22-C21-O21-C2
17	D	402	6PH	O22-C21-O21-C2
17	E	302	6PH	O22-C21-O21-C2
16	N	402	UQ6	C15-C14-C16-C17
16	N	402	UQ6	C13-C14-C16-C17
12	C	402	CN3	C32-C31-O31-C3
13	C	403	9PE	C32-C31-O31-C3
19	N	406	CN5	OA-CB-CC-O13
13	C	403	9PE	C22-C21-O21-C2
19	N	406	CN5	C33-C34-C35-C36
16	C	407	UQ6	C20-C19-C21-C22
16	N	402	UQ6	C20-C19-C21-C22
16	N	402	UQ6	C30-C29-C31-C32
16	C	407	UQ6	C13-C14-C16-C17
16	C	407	UQ6	C18-C19-C21-C22
16	N	402	UQ6	C18-C19-C21-C22
16	N	402	UQ6	C28-C29-C31-C32
13	C	403	9PE	O32-C31-O31-C3
16	N	402	UQ6	C9-C11-C12-C13
16	N	402	UQ6	C14-C16-C17-C18
19	N	406	CN5	O3'-CA-CB-CC
13	C	403	9PE	O22-C21-O21-C2
12	N	407	CN3	C51-C52-C53-C54
19	N	406	CN5	O11-C1-C2-C3
15	N	403	8PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
15	N	403	8PE	C21-C22-C23-C24
14	C	405	HEM	C3A-C2A-CAA-CBA
16	C	407	UQ6	C9-C11-C12-C13
16	C	407	UQ6	C24-C26-C27-C28
16	N	402	UQ6	C29-C31-C32-C33
19	N	406	CN5	O3'-CA-CB-OA
15	N	403	8PE	O32-C31-O31-C3
12	C	402	CN3	CC-O13-P-O11
12	N	407	CN3	C1'-O1'-P'-O3'
13	N	404	9PE	C1-O11-P-O13
15	C	406	8PE	C11-O13-P-O11
15	N	403	8PE	C11-O13-P-O11
19	N	406	CN5	C1-O11-P-O13
19	N	406	CN5	CC-O13-P-O11
17	D	402	6PH	C32-C31-O31-C3
19	N	406	CN5	CA-CB-CC-O13
16	N	402	UQ6	C25-C24-C26-C27
12	N	407	CN3	C45-C46-C47-C48
13	C	403	9PE	C21-C22-C23-C24
17	D	402	6PH	C27-C28-C29-C2A
17	L	501	6PH	C38-C39-C3A-C3B
17	D	402	6PH	C28-C29-C2A-C2B
13	N	404	9PE	C2A-C2B-C2C-C2D
17	L	501	6PH	C37-C38-C39-C3A
15	N	403	8PE	C35-C36-C37-C38
13	C	403	9PE	C2E-C2F-C2G-C2H
15	C	406	8PE	C2A-C2B-C2C-C2D
19	N	406	CN5	C34-C35-C36-C37
17	L	501	6PH	C2B-C2C-C2D-C2E
15	C	406	8PE	O13-C11-C12-N
15	N	403	8PE	O13-C11-C12-N
19	N	406	CN5	C31-C32-C33-C34
17	D	402	6PH	O32-C31-O31-C3
17	L	501	6PH	C36-C37-C38-C39
13	C	403	9PE	C22-C23-C24-C25
17	D	402	6PH	C23-C24-C25-C26
17	L	501	6PH	C25-C26-C27-C28
13	N	404	9PE	C22-C21-O21-C2
17	L	501	6PH	C22-C21-O21-C2
17	E	302	6PH	C32-C33-C34-C35
13	N	404	9PE	C24-C25-C26-C27
13	N	404	9PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
17	D	402	6PH	C37-C38-C39-C3A
12	N	407	CN3	C43-C44-C45-C46
15	N	403	8PE	C25-C26-C27-C28
17	D	402	6PH	C26-C27-C28-C29
13	N	404	9PE	O22-C21-O21-C2
13	C	403	9PE	C27-C28-C29-C2A
15	C	406	8PE	C3C-C3D-C3E-C3F
15	N	403	8PE	C26-C27-C28-C29
15	N	403	8PE	C33-C34-C35-C36
17	D	402	6PH	O21-C2-C3-O31
16	N	402	UQ6	C23-C24-C26-C27
17	L	501	6PH	O22-C21-O21-C2
13	N	404	9PE	C11-O13-P-O11
12	N	407	CN3	C42-C41-O41-C3'
15	C	406	8PE	O11-C1-C2-C3
17	D	402	6PH	C2A-C2B-C2C-C2D
17	L	501	6PH	C35-C36-C37-C38
15	N	403	8PE	C36-C37-C38-C39
13	N	404	9PE	C22-C23-C24-C25
19	N	406	CN5	C1-C2-C3-O31
12	N	407	CN3	C54-C55-C56-C57
13	N	404	9PE	C29-C2A-C2B-C2C
13	C	403	9PE	C2F-C2G-C2H-C2I
17	E	302	6PH	C25-C26-C27-C28
19	N	406	CN5	C32-C33-C34-C35
12	N	407	CN3	O42-C41-O41-C3'
17	L	501	6PH	C2C-C2D-C2E-C2F
17	D	402	6PH	C29-C2A-C2B-C2C
12	C	402	CN3	C2-C1-O11-P
17	D	402	6PH	C1-O11-P-O12
17	E	302	6PH	C34-C35-C36-C37
19	N	406	CN5	C39-C3A-C3B-C3C
13	C	403	9PE	O11-C1-C2-O21
17	E	302	6PH	O11-C1-C2-O21
14	C	405	HEM	C2A-CAA-CBA-CGA
12	N	407	CN3	O21-C2-C3-O31
17	L	501	6PH	O21-C2-C3-O31
13	C	403	9PE	C2D-C2E-C2F-C2G
16	N	402	UQ6	C2-C3-O3-C3M
17	E	302	6PH	O11-C1-C2-C3
17	L	501	6PH	C2-C1-O11-P
13	N	404	9PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
17	E	302	6PH	C33-C34-C35-C36
17	E	302	6PH	C1-C2-C3-O31
17	L	501	6PH	C1-C2-C3-O31
17	E	302	6PH	C23-C24-C25-C26
17	D	402	6PH	C36-C37-C38-C39
15	N	403	8PE	C1-O11-P-O13
12	N	407	CN3	O51-C51-C52-C53
13	C	403	9PE	O21-C2-C3-O31
16	C	407	UQ6	C29-C31-C32-C33
17	L	501	6PH	C33-C34-C35-C36
16	C	407	UQ6	C6-C7-C8-C9
15	C	406	8PE	C23-C24-C25-C26
13	C	403	9PE	C29-C2A-C2B-C2C
13	C	403	9PE	C3-C2-O21-C21
12	N	407	CN3	C1-C2-C3-O31
17	D	402	6PH	C1-C2-C3-O31
14	O	401	HEM	C4C-C3C-CAC-CBC
17	E	302	6PH	O21-C2-C3-O31
13	N	404	9PE	O32-C31-O31-C3
17	E	302	6PH	C28-C29-C2A-C2B
13	N	404	9PE	C33-C34-C35-C36
17	D	402	6PH	C39-C3A-C3B-C3C
13	C	403	9PE	C11-O13-P-O11
12	C	402	CN3	CC-O13-P-O12
12	N	407	CN3	C1'-O1'-P'-O4'
13	N	404	9PE	C1-O11-P-O12
15	C	406	8PE	C1-O11-P-O12
15	C	406	8PE	C11-O13-P-O12
15	C	406	8PE	C11-O13-P-O14
15	N	403	8PE	C1-O11-P-O14
19	N	406	CN5	C1-O11-P-O14
19	N	406	CN5	CC-O13-P-O12
13	C	403	9PE	O11-C1-C2-C3
13	N	404	9PE	C23-C24-C25-C26
19	N	406	CN5	O1'-C1'-C2'-C3'
15	N	403	8PE	C3D-C3E-C3F-C3G
15	C	406	8PE	O11-C1-C2-O21
15	N	403	8PE	C31-C32-C33-C34
15	C	406	8PE	C3B-C3C-C3D-C3E
13	C	403	9PE	C1-C2-C3-O31
12	N	407	CN3	C53-C54-C55-C56
13	C	403	9PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
13	N	404	9PE	C2E-C2F-C2G-C2H
12	N	407	CN3	C56-C57-C58-C59
15	C	406	8PE	C35-C36-C37-C38
17	E	302	6PH	C2B-C2C-C2D-C2E
13	N	404	9PE	C3-C2-O21-C21
12	C	402	CN3	C1-O11-P-O13
13	C	403	9PE	C1-O11-P-O13
19	N	406	CN5	C1'-O1'-P'-O3'
13	C	403	9PE	C31-C32-C33-C34
15	C	406	8PE	O22-C21-O21-C2
17	E	302	6PH	C2A-C2B-C2C-C2D
13	C	403	9PE	C2-C1-O11-P
12	N	407	CN3	CA-CB-CC-O13
14	N	408	HEM	CAA-CBA-CGA-O1A
17	E	302	6PH	C35-C36-C37-C38
19	N	406	CN5	C3B-C3C-C3D-C3E
12	N	407	CN3	C44-C45-C46-C47
14	C	405	HEM	CAA-CBA-CGA-O1A
15	C	406	8PE	C1-C2-C3-O31
14	C	405	HEM	CAA-CBA-CGA-O2A
14	N	405	HEM	CAA-CBA-CGA-O1A
14	N	405	HEM	CAA-CBA-CGA-O2A
16	N	402	UQ6	C4-C3-O3-C3M
14	N	408	HEM	CAA-CBA-CGA-O2A
15	C	406	8PE	O21-C2-C3-O31
15	C	406	8PE	C22-C21-O21-C2
19	N	406	CN5	C2'-C1'-O1'-P'
14	C	404	HEM	CAA-CBA-CGA-O2A
15	C	406	8PE	O31-C31-C32-C33
16	C	407	UQ6	C14-C16-C17-C18
13	N	404	9PE	C2C-C2D-C2E-C2F
12	N	407	CN3	O31-C31-C32-C33
12	N	407	CN3	C21-C22-C23-C24
17	L	501	6PH	C1-O11-P-O13
14	C	404	HEM	CAA-CBA-CGA-O1A
13	C	403	9PE	C25-C26-C27-C28
12	N	407	CN3	O41-C41-C42-C43
14	C	404	HEM	CAD-CBD-CGD-O1D
14	C	404	HEM	CAD-CBD-CGD-O2D
17	D	402	6PH	C25-C26-C27-C28
13	N	404	9PE	C27-C28-C29-C2A
16	C	407	UQ6	C4-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
12	N	407	CN3	O52-C51-C52-C53
15	N	403	8PE	O21-C21-C22-C23
16	C	407	UQ6	C19-C21-C22-C23
19	N	406	CN5	C3C-C3D-C3E-C3F
17	E	302	6PH	O21-C21-C22-C23
12	N	407	CN3	OA-CB-CC-O13
14	C	405	HEM	CAD-CBD-CGD-O2D
12	N	407	CN3	C1'-O1'-P'-O2'
12	N	407	CN3	O42-C41-C42-C43
14	D	401	HEM	CAA-CBA-CGA-O2A
14	N	408	HEM	CAD-CBD-CGD-O2D
15	N	403	8PE	O22-C21-C22-C23
14	N	408	HEM	CAD-CBD-CGD-O1D
14	C	405	HEM	CAD-CBD-CGD-O1D
12	N	407	CN3	C42-C43-C44-C45
19	N	406	CN5	C35-C36-C37-C38
13	N	404	9PE	O31-C31-C32-C33
12	C	402	CN3	C56-C57-C58-C59
17	E	302	6PH	O22-C21-C22-C23
15	C	406	8PE	C25-C26-C27-C28
14	D	401	HEM	CAA-CBA-CGA-O1A

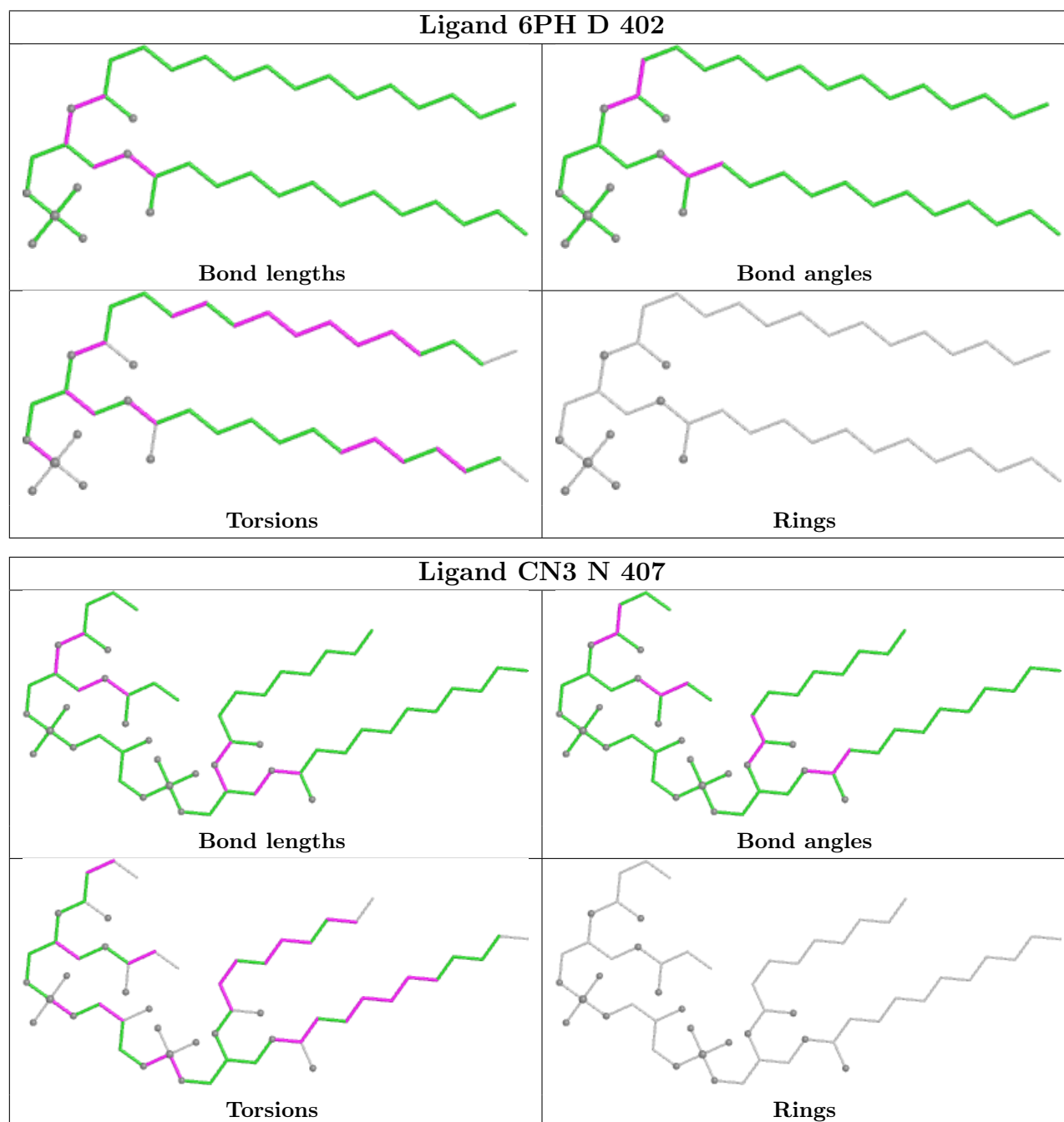
There are no ring outliers.

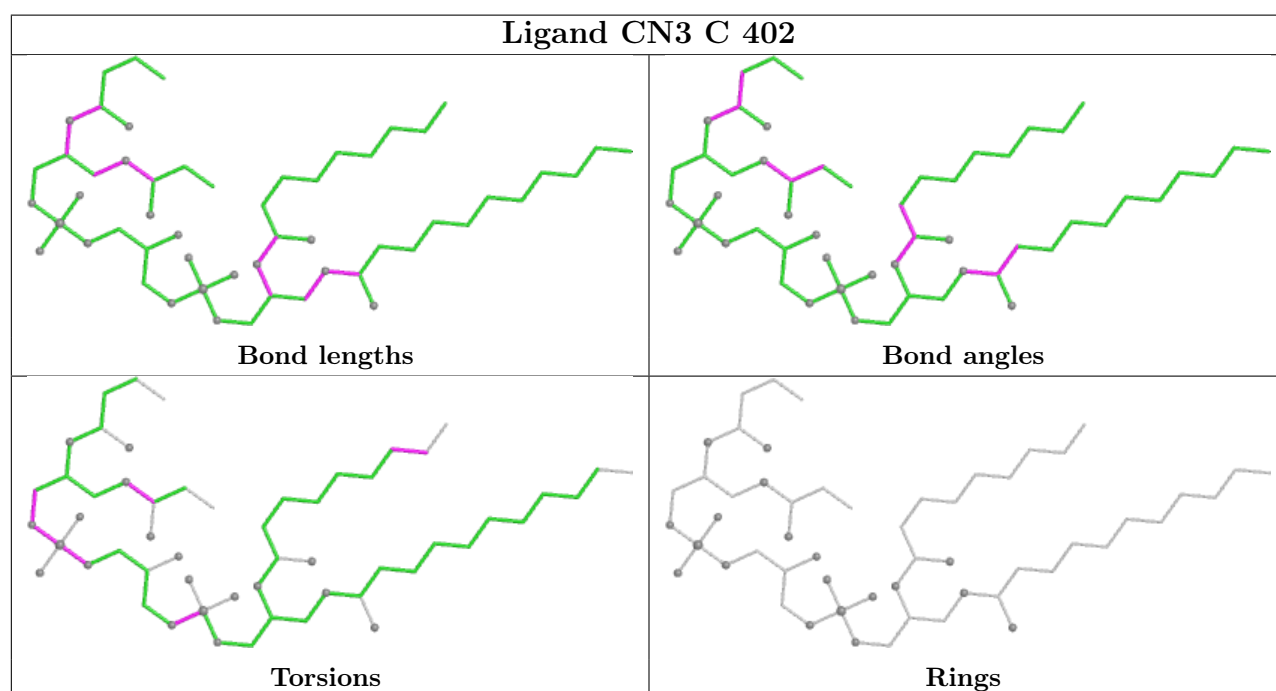
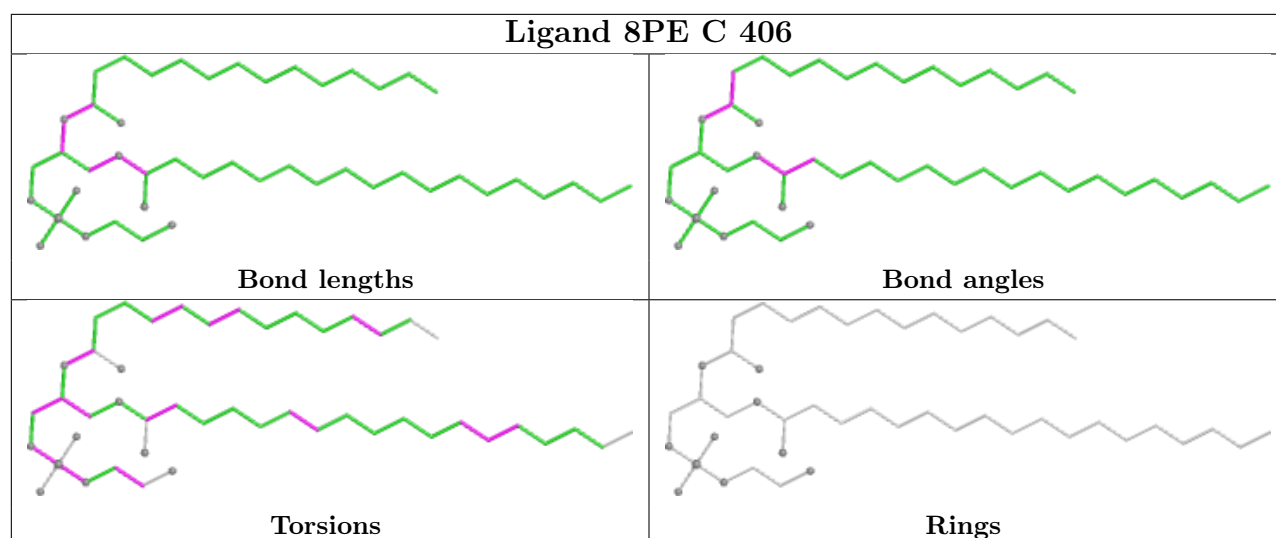
9 monomers are involved in 17 short contacts:

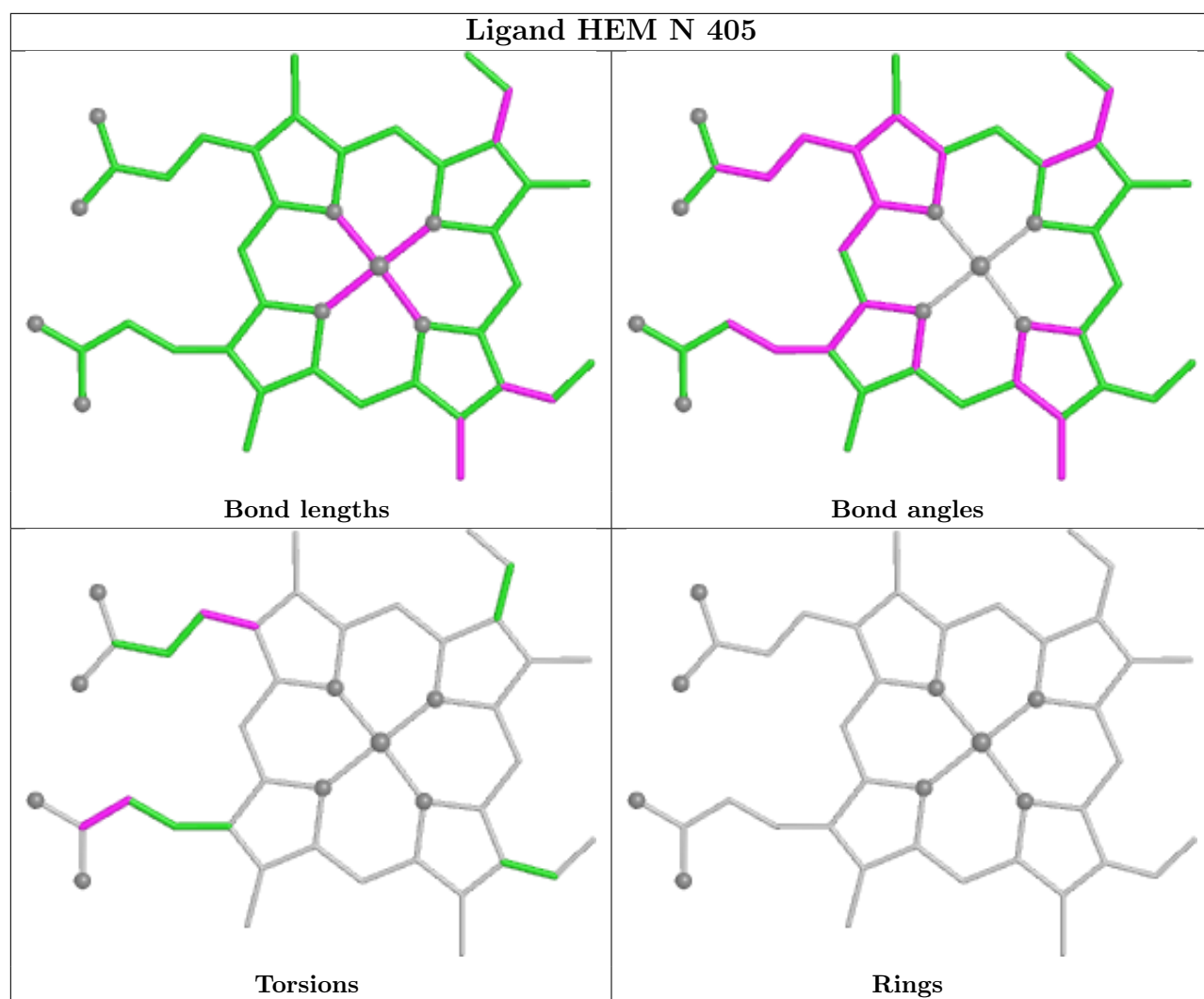
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	403	9PE	1	0
14	O	401	HEM	1	0
14	C	405	HEM	1	0
16	C	407	UQ6	4	0
16	N	402	UQ6	4	0
17	E	302	6PH	3	0
19	N	406	CN5	4	0
17	L	501	6PH	2	0
14	N	408	HEM	1	0

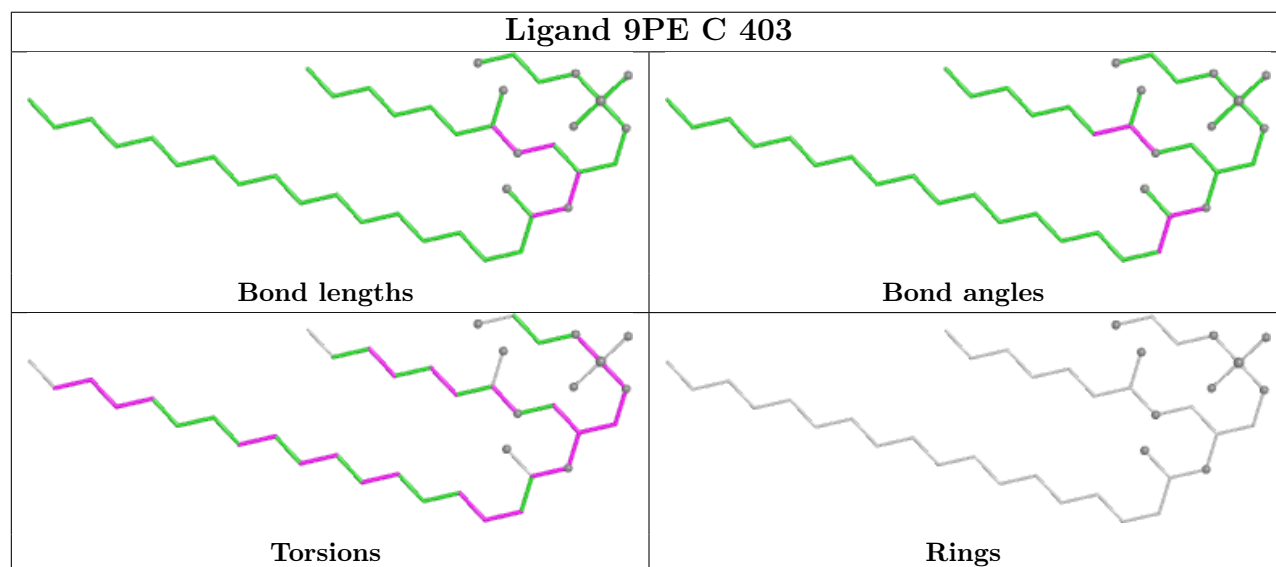
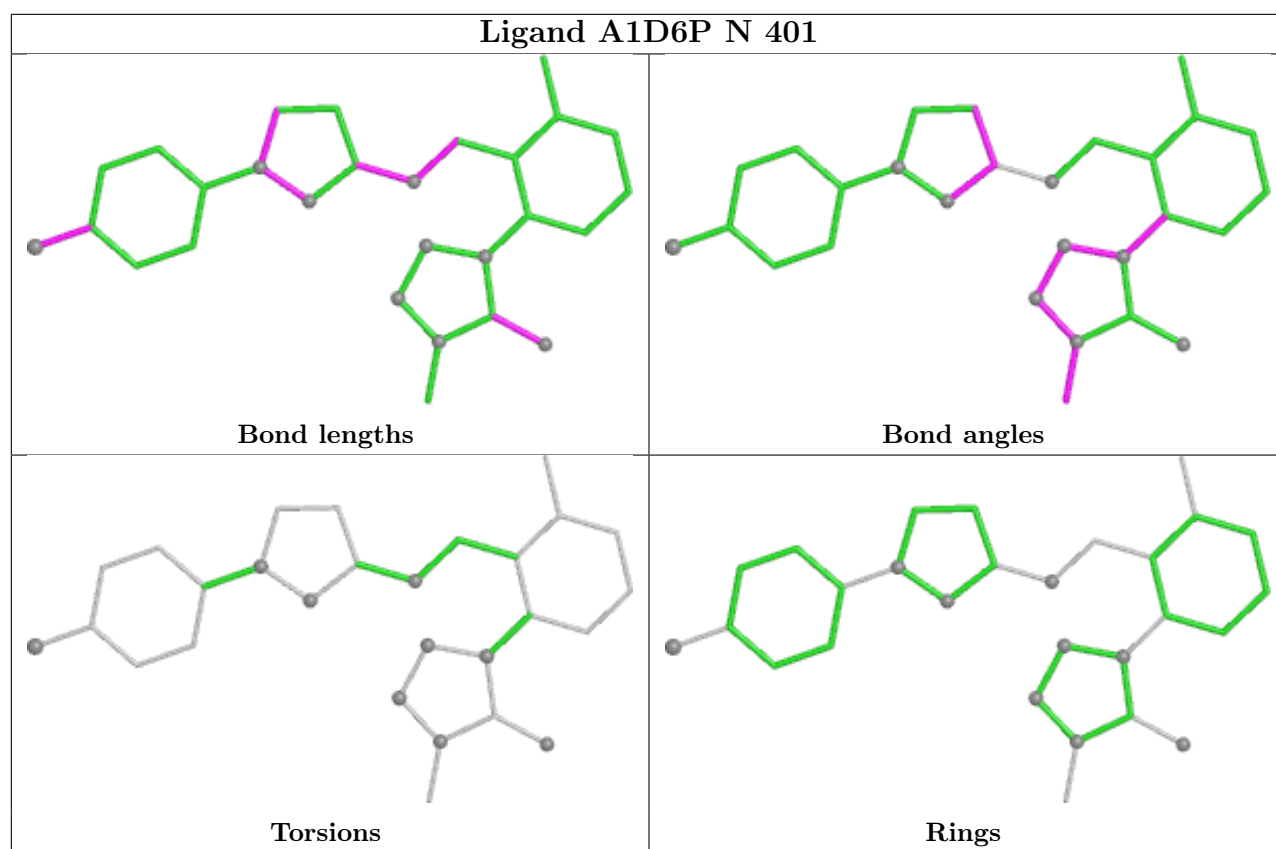
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

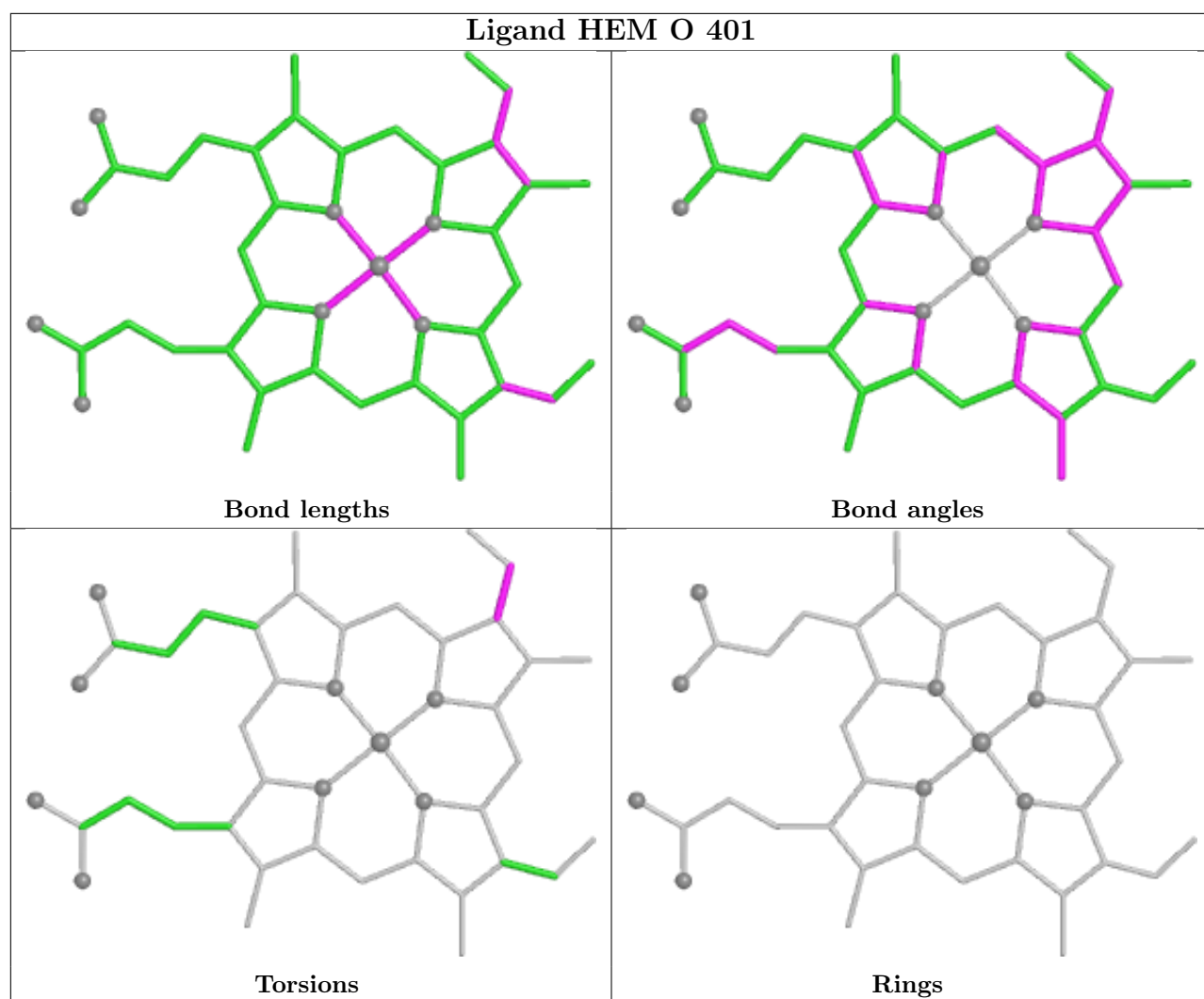
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

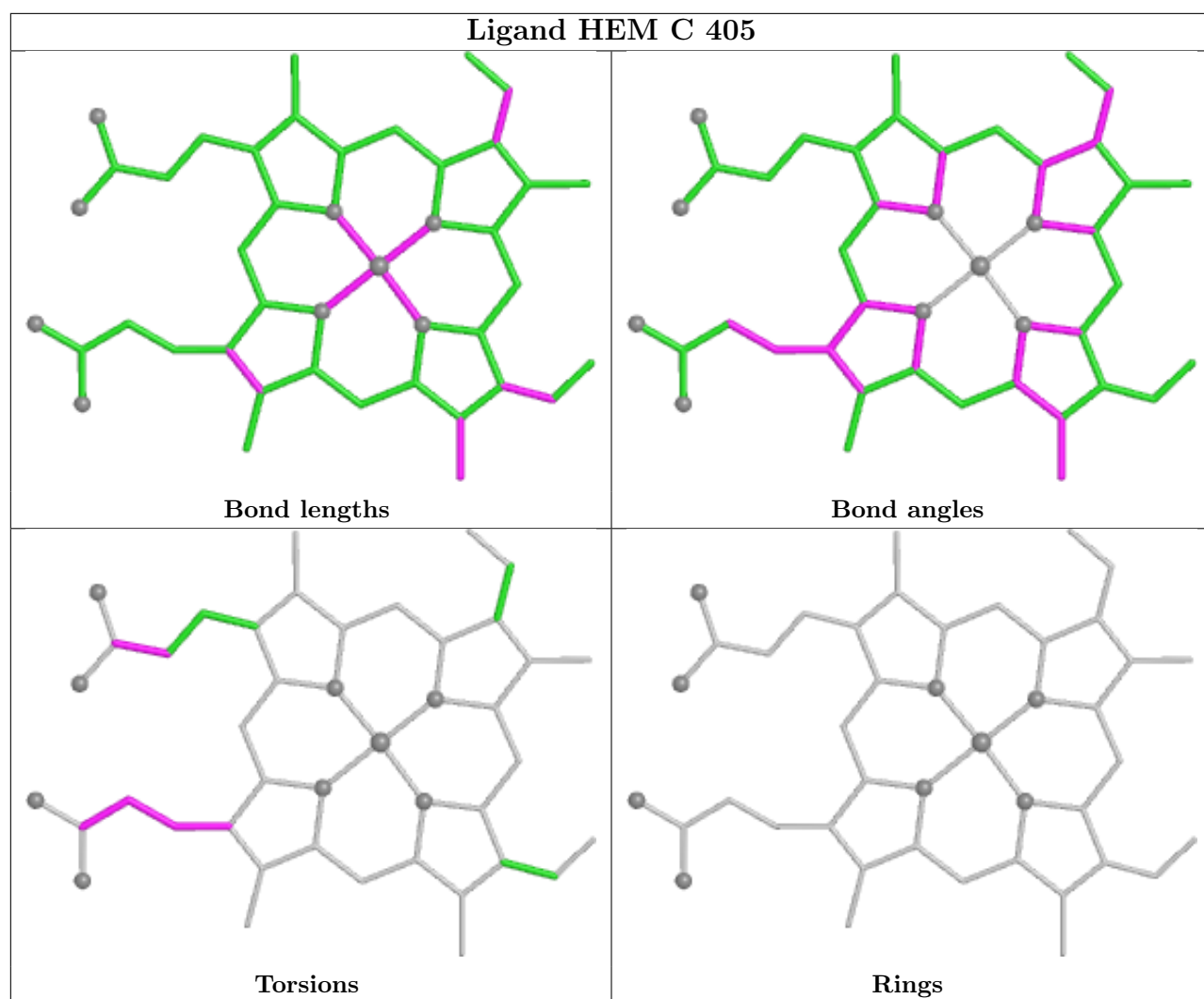


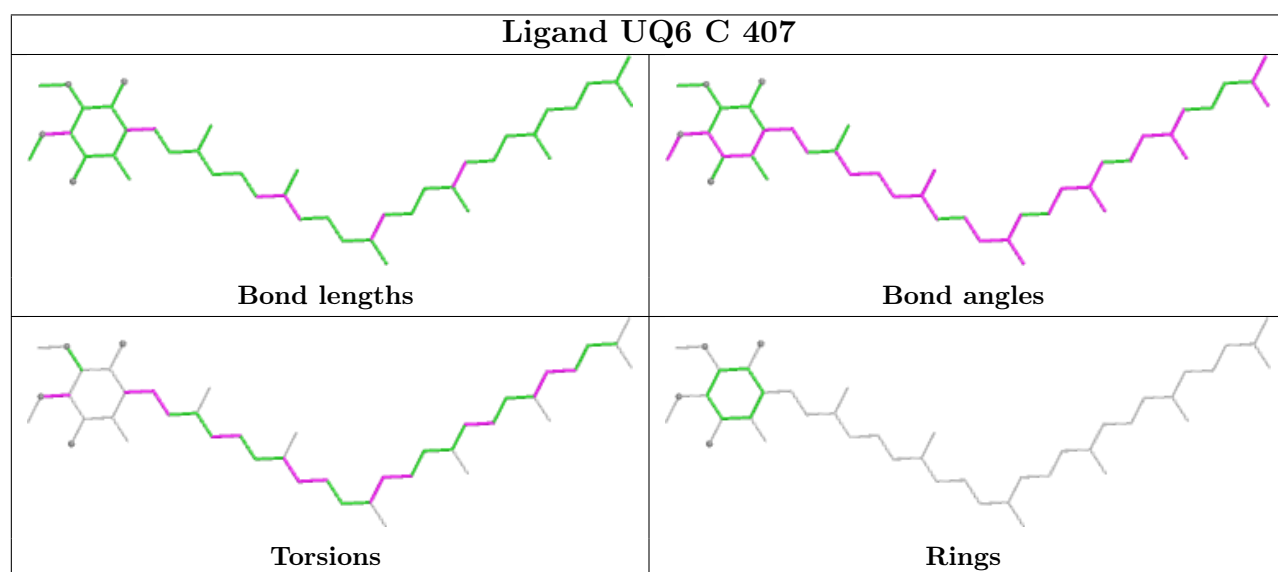
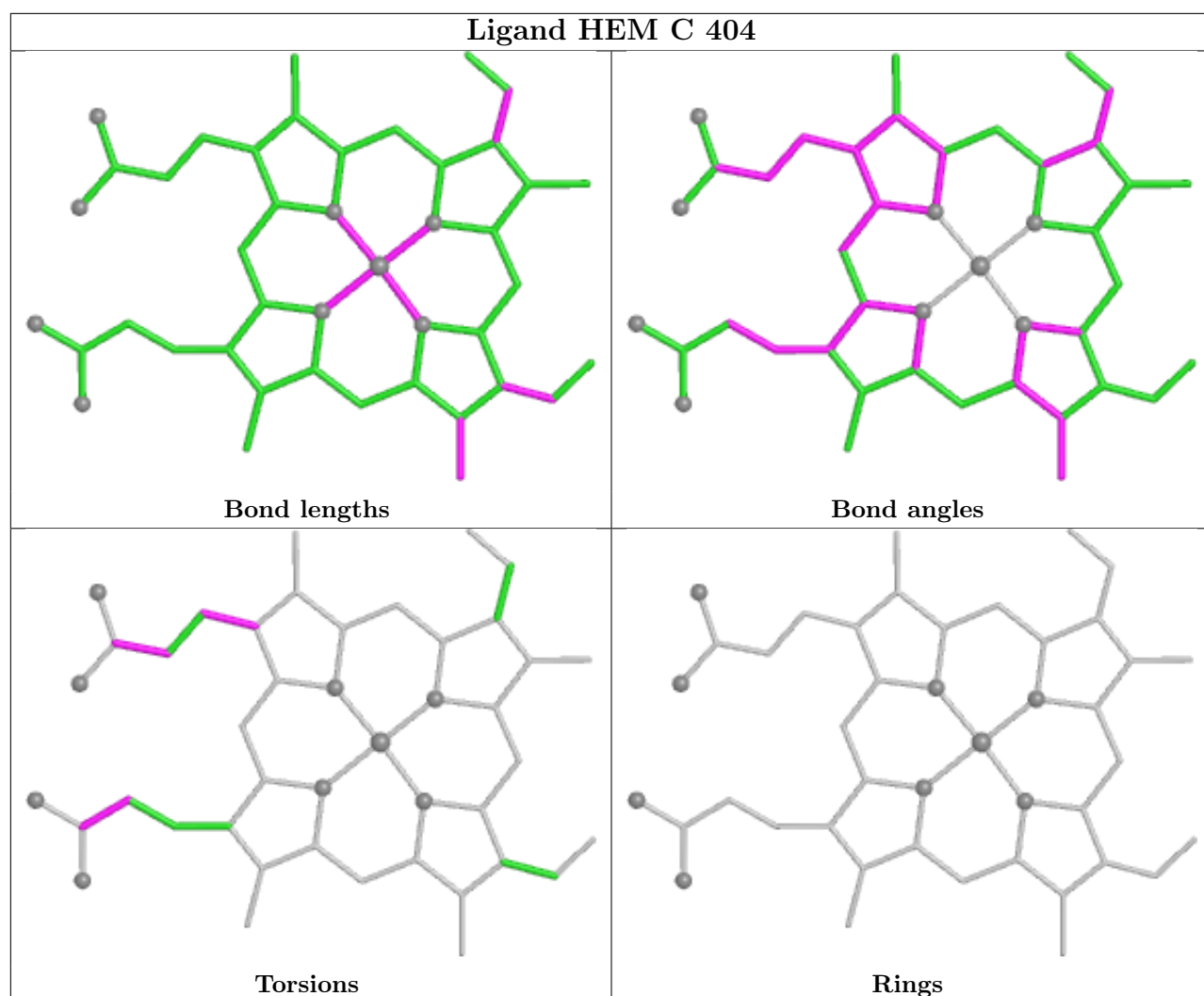


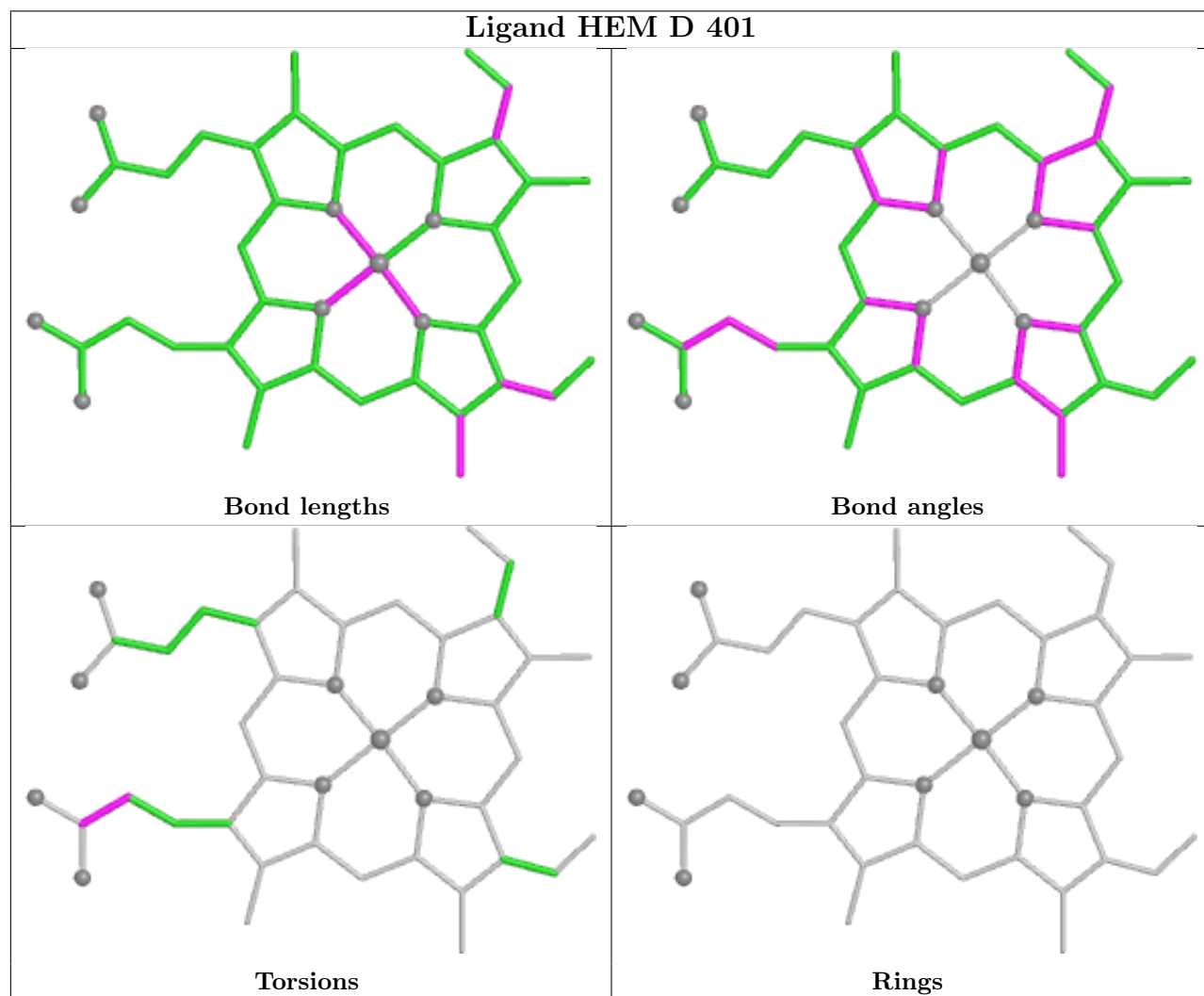
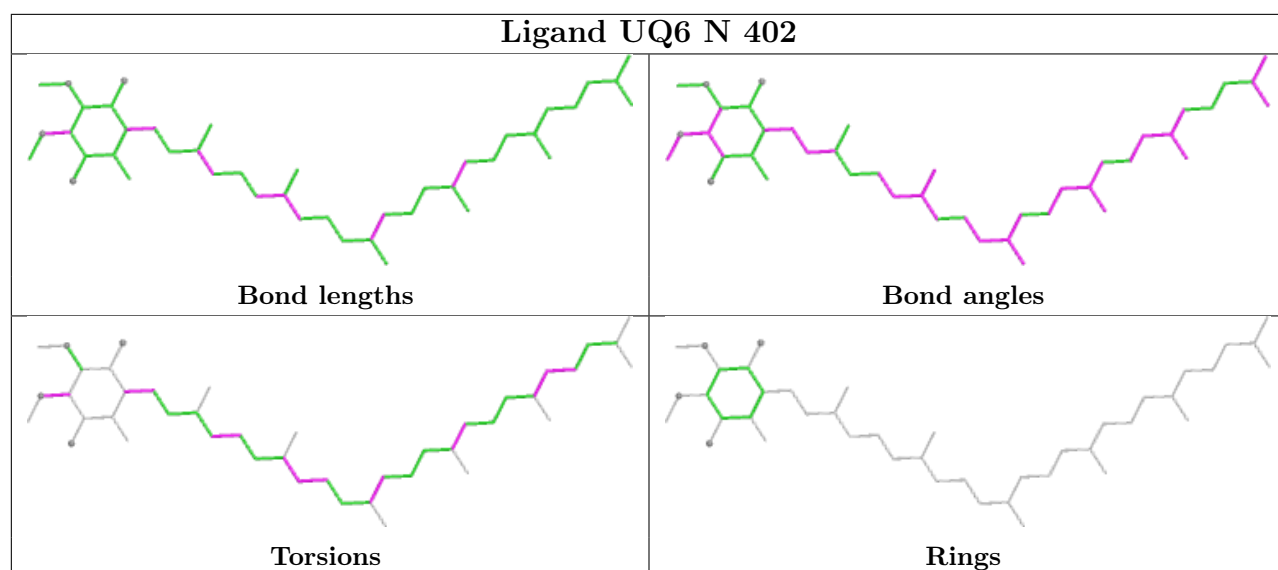


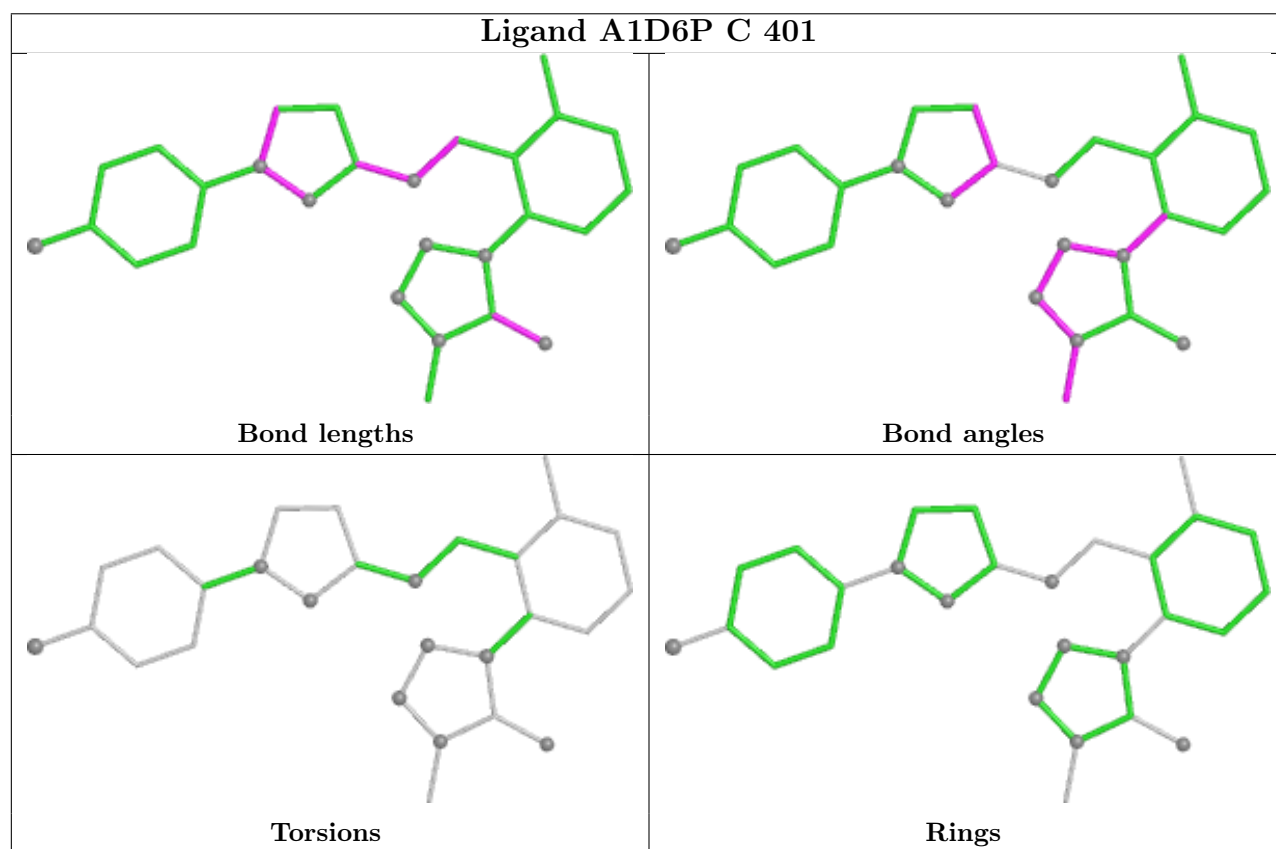
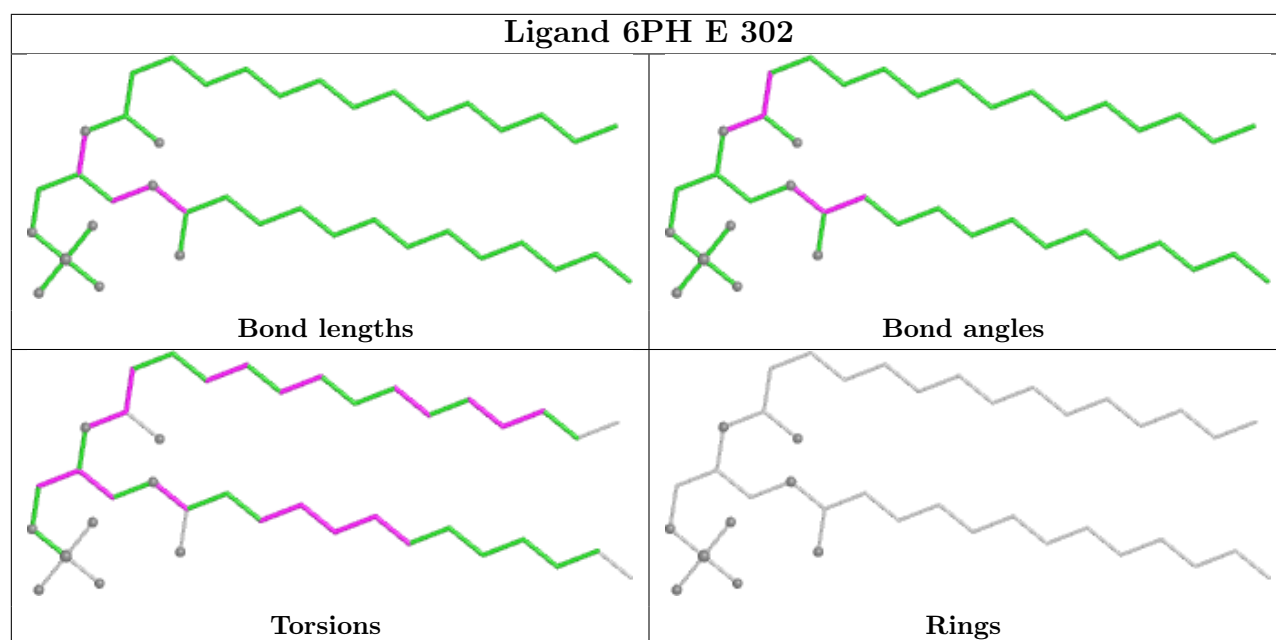


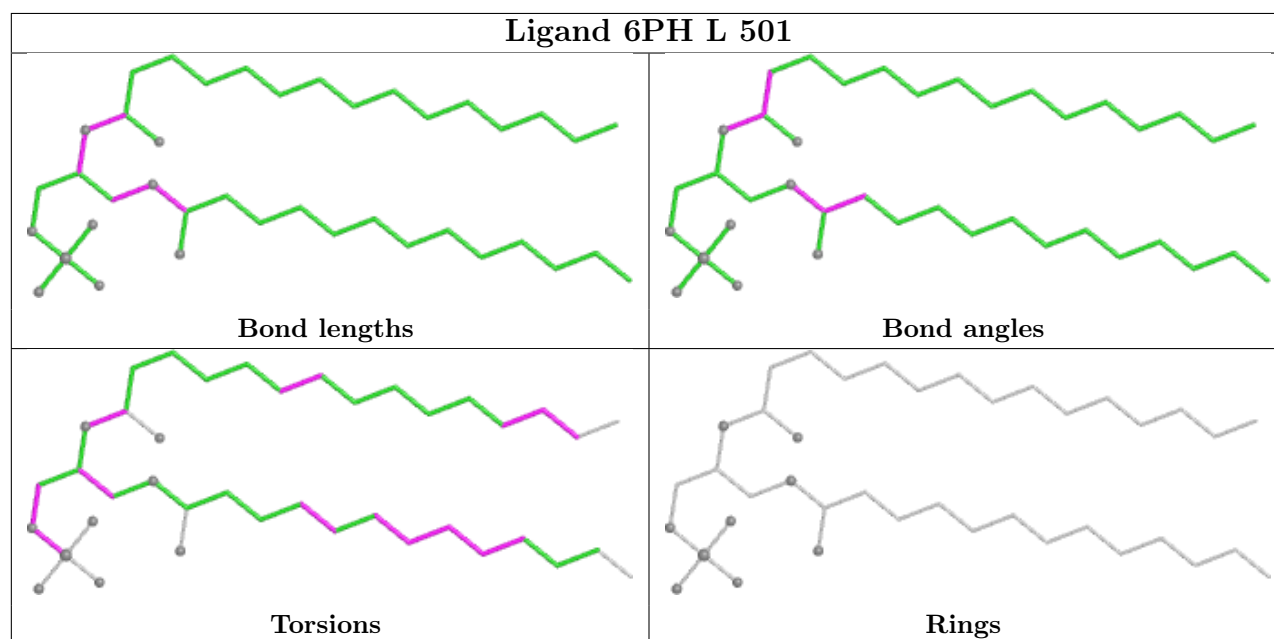
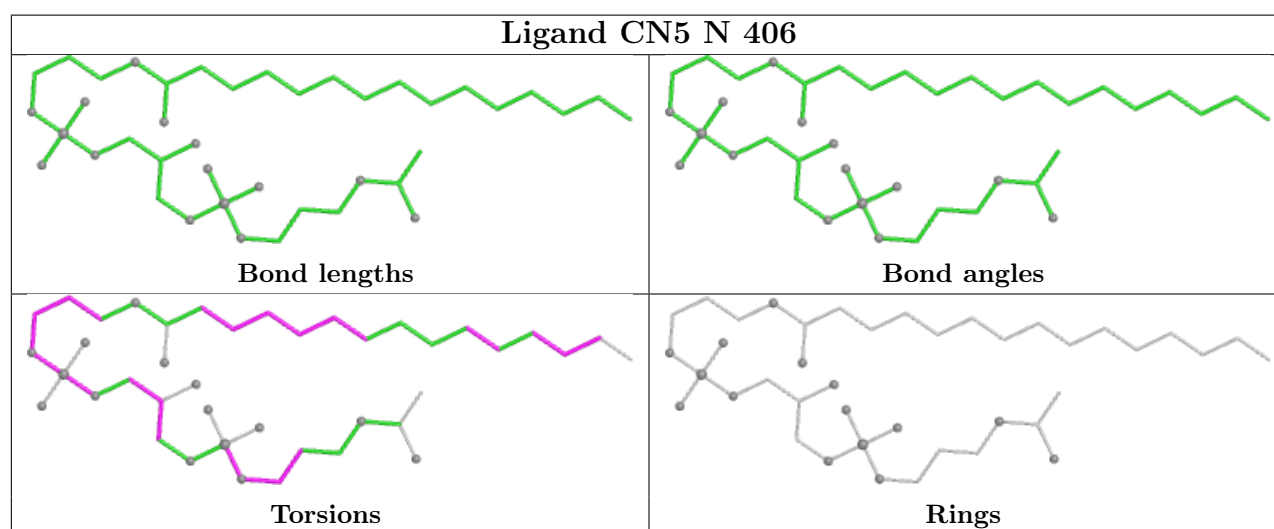
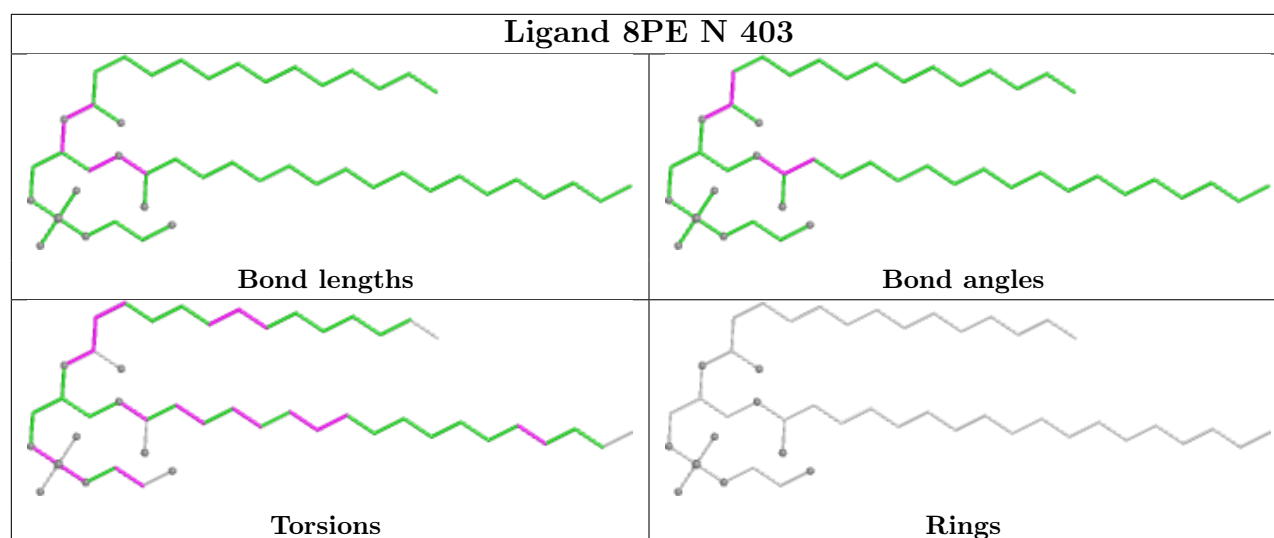


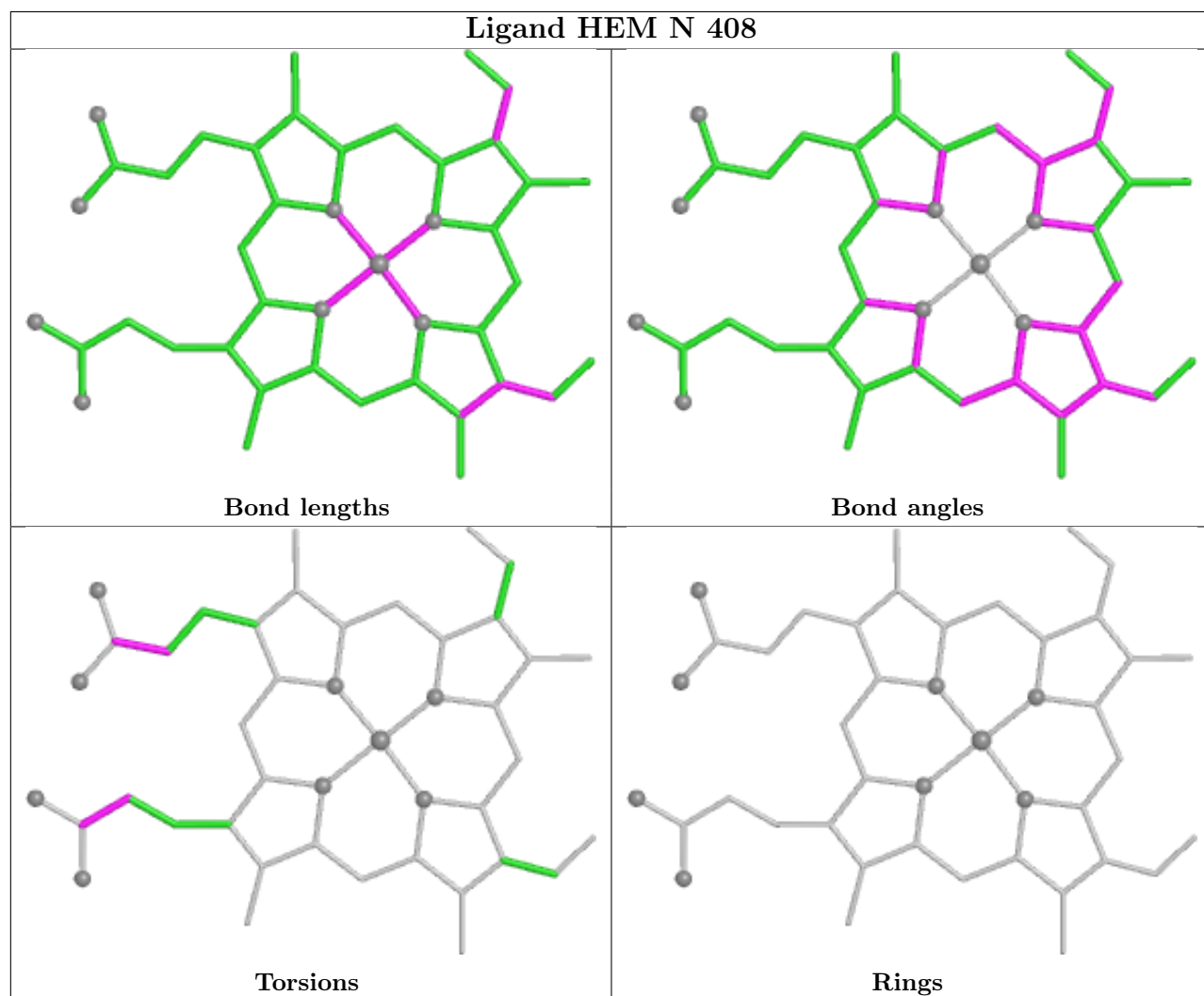
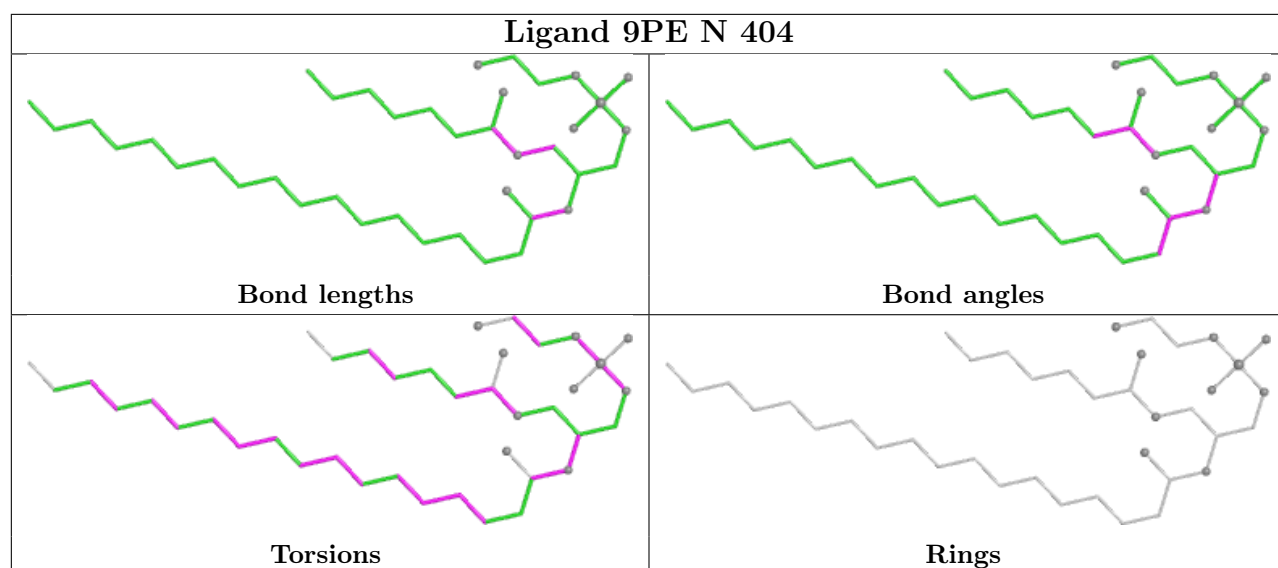












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

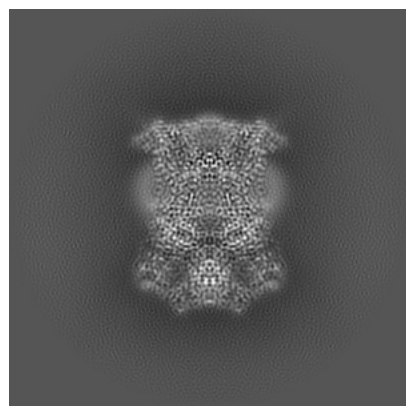
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60256. These allow visual inspection of the internal detail of the map and identification of artifacts.

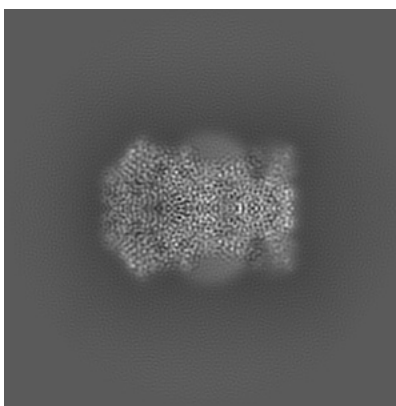
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

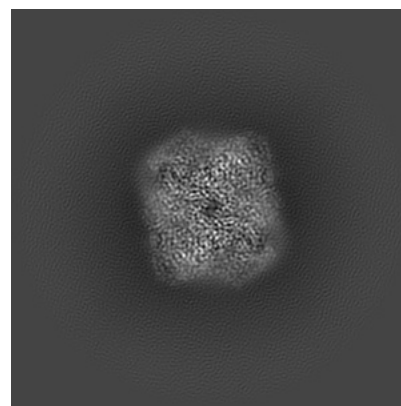
6.1.1 Primary map



X

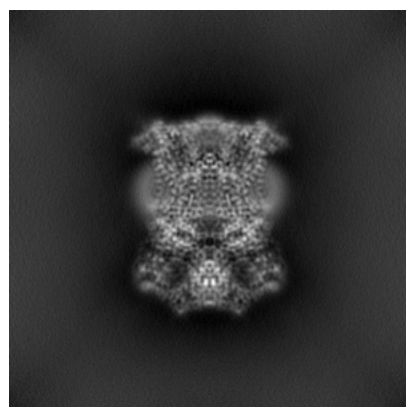


Y

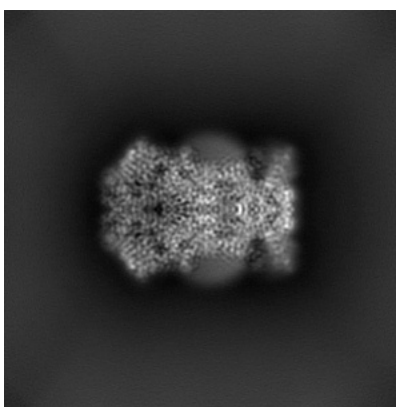


Z

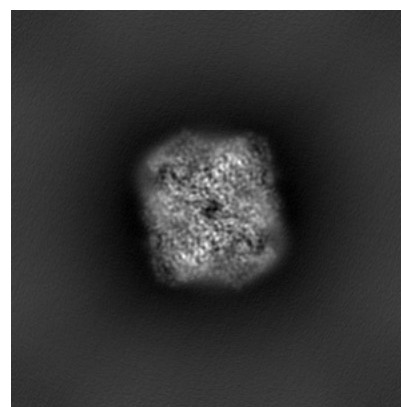
6.1.2 Raw map



X



Y

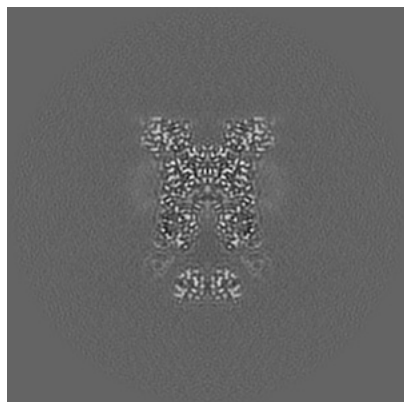


Z

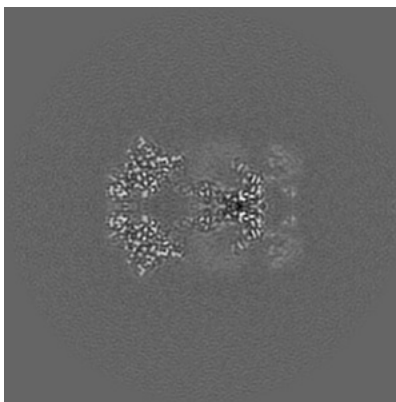
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

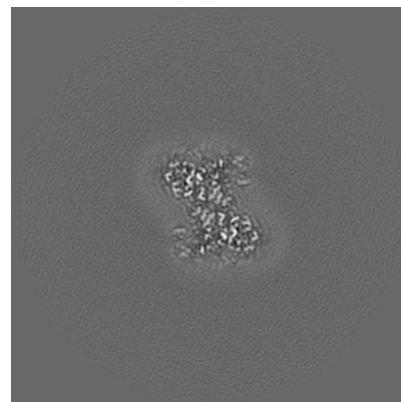
6.2.1 Primary map



X Index: 160

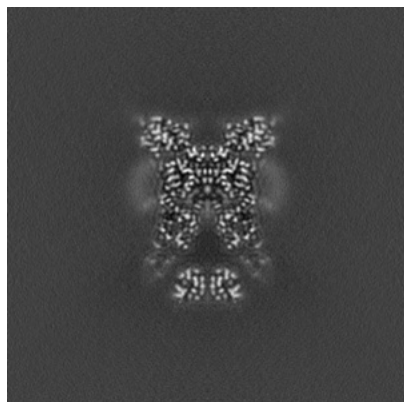


Y Index: 160

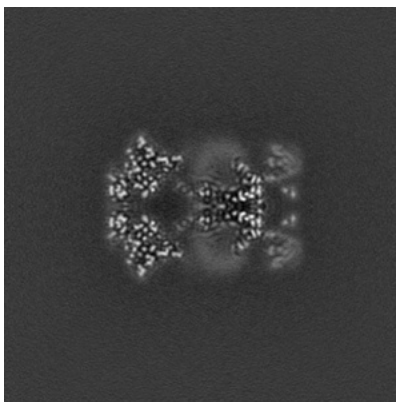


Z Index: 160

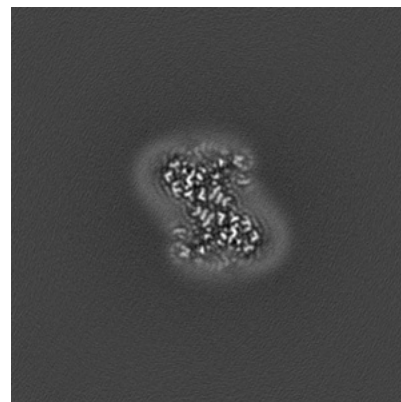
6.2.2 Raw map



X Index: 160



Y Index: 160

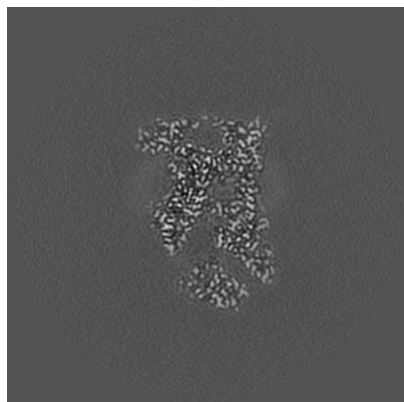


Z Index: 160

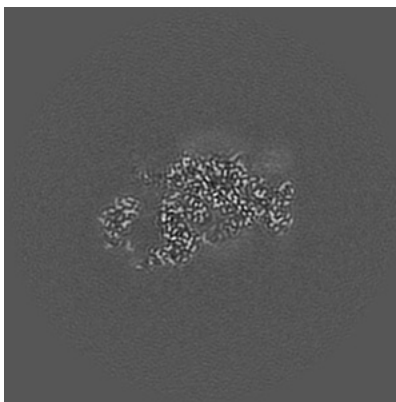
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

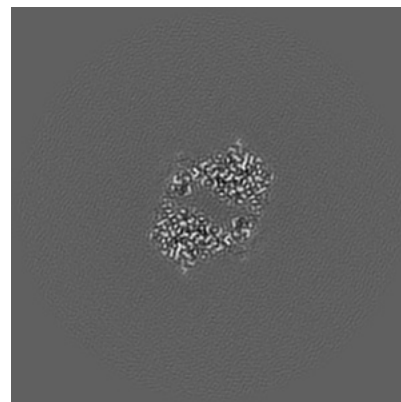
6.3.1 Primary map



X Index: 168

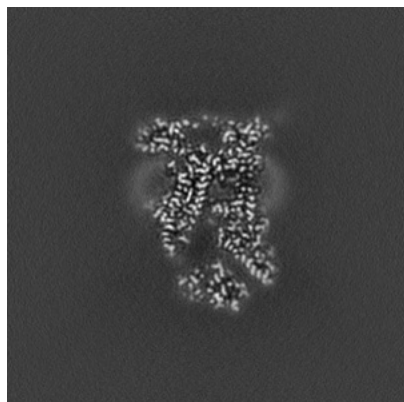


Y Index: 141

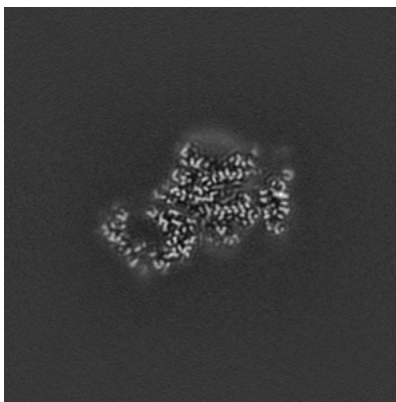


Z Index: 134

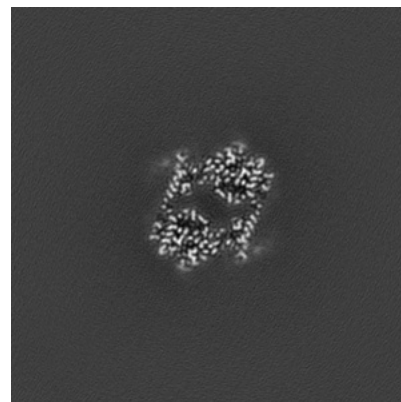
6.3.2 Raw map



X Index: 167



Y Index: 132

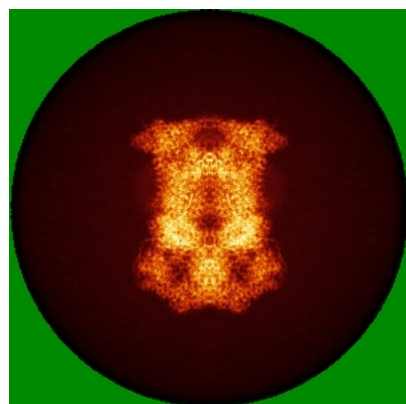


Z Index: 136

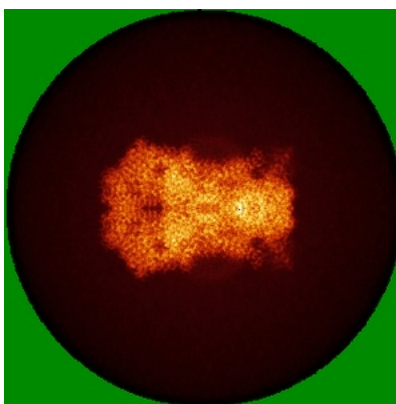
The images above show the largest variance slices of the map in three orthogonal directions.

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

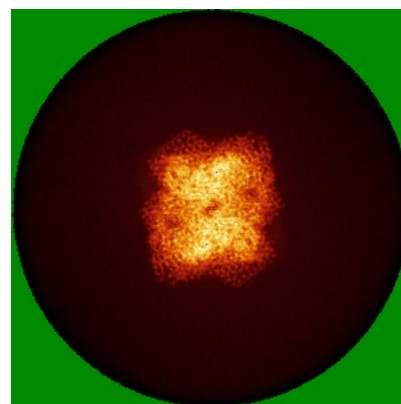
6.4.1 Primary map



X

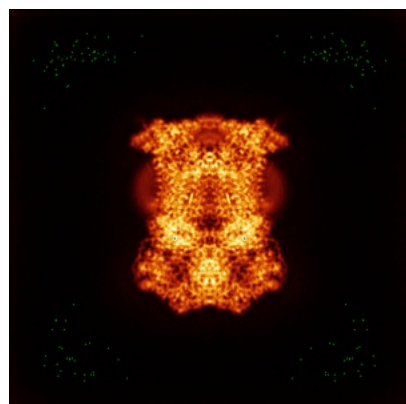


Y

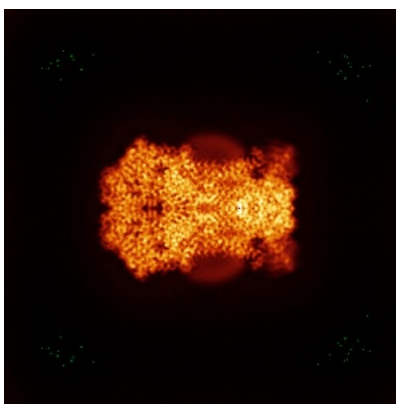


Z

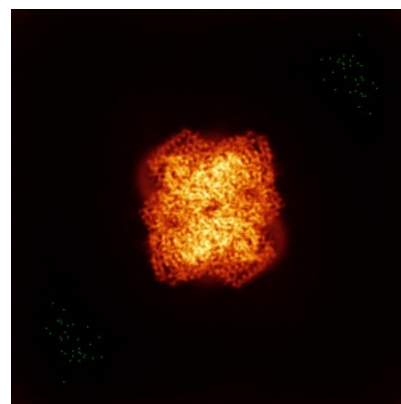
6.4.2 Raw map



X



Y

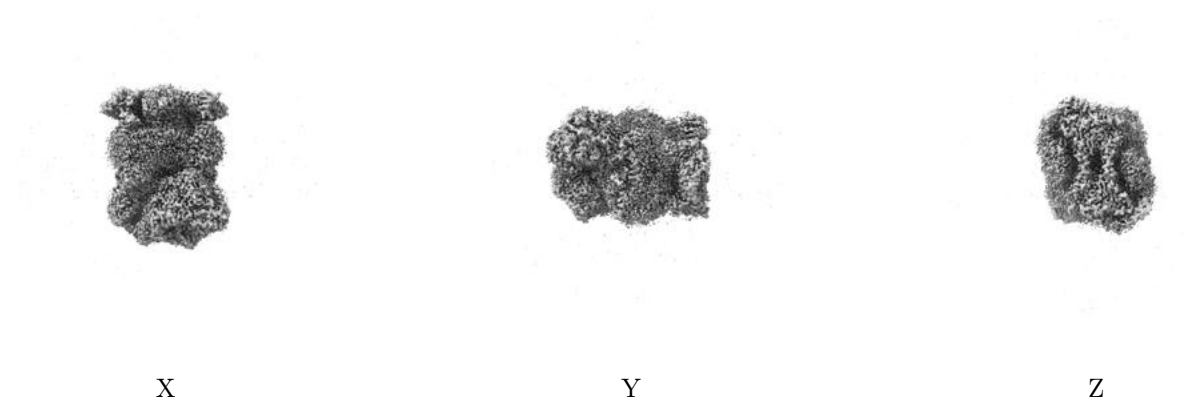


Z

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.

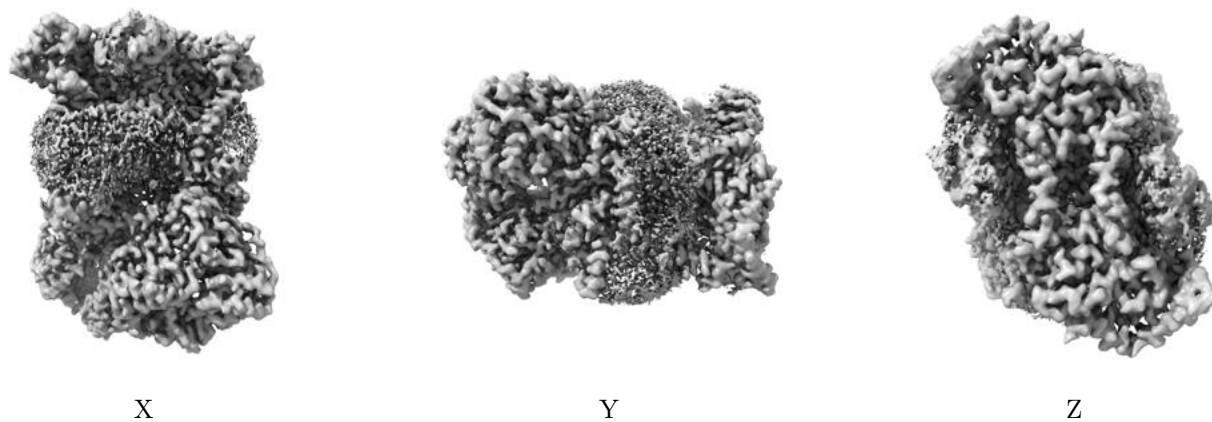
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

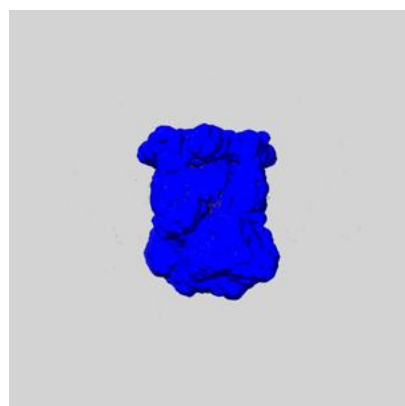
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

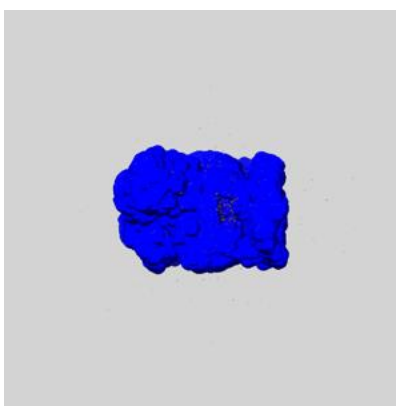
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

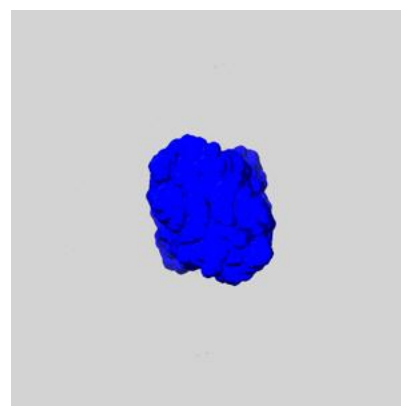
6.6.1 emd_60256_msk_1.map [i](#)



X



Y

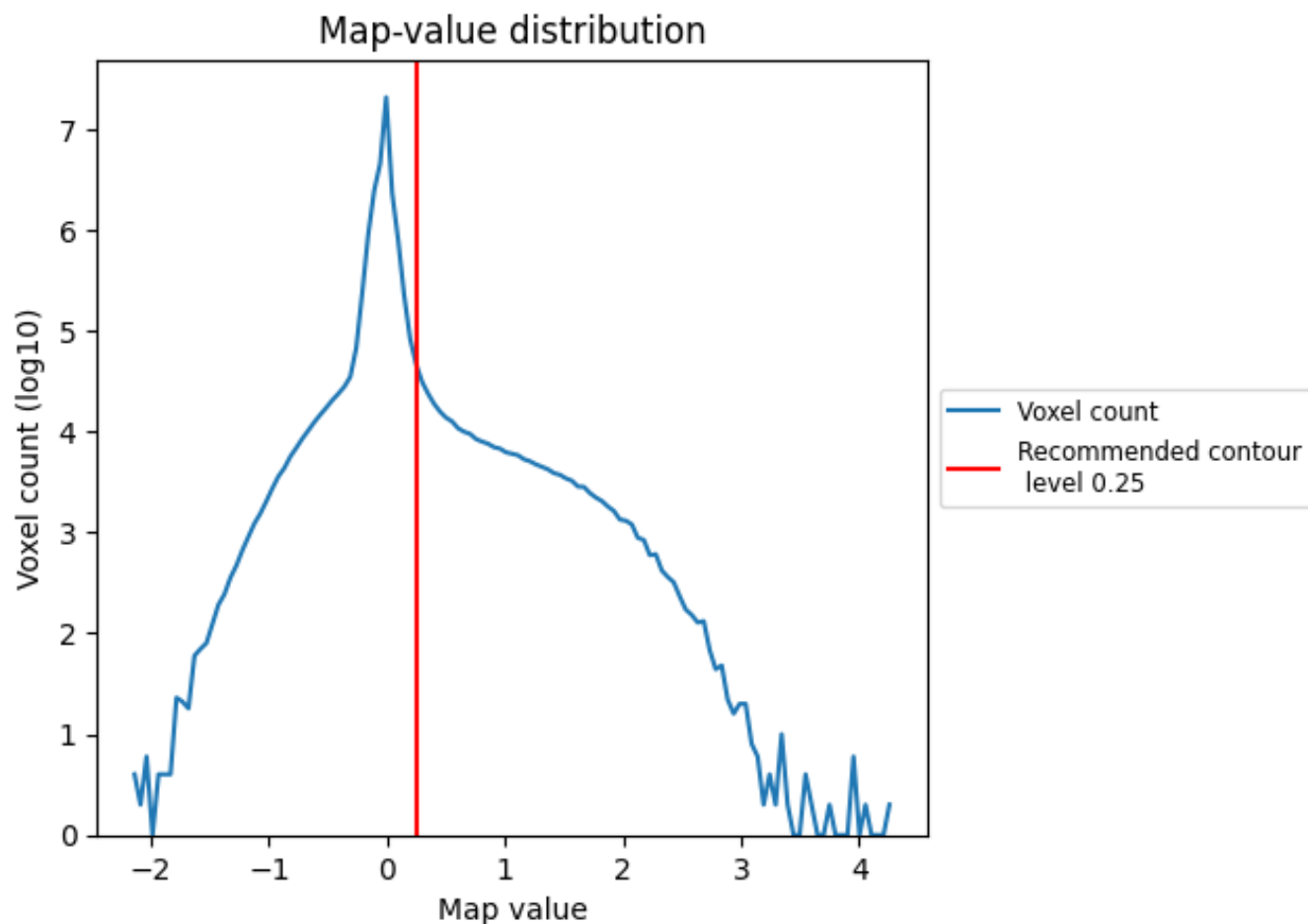


Z

7 Map analysis [i](#)

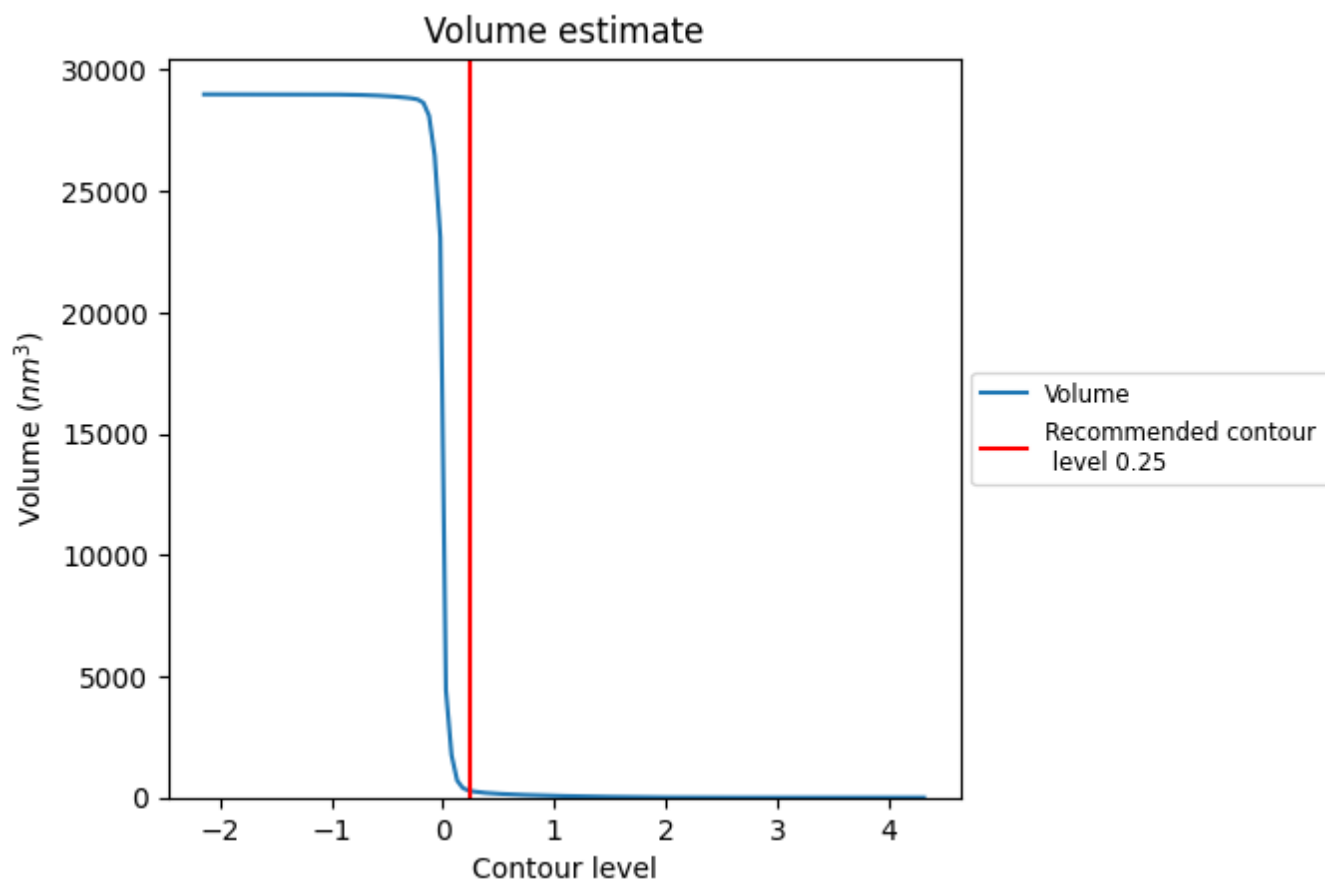
This section contains the results of statistical analysis of the map.

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.

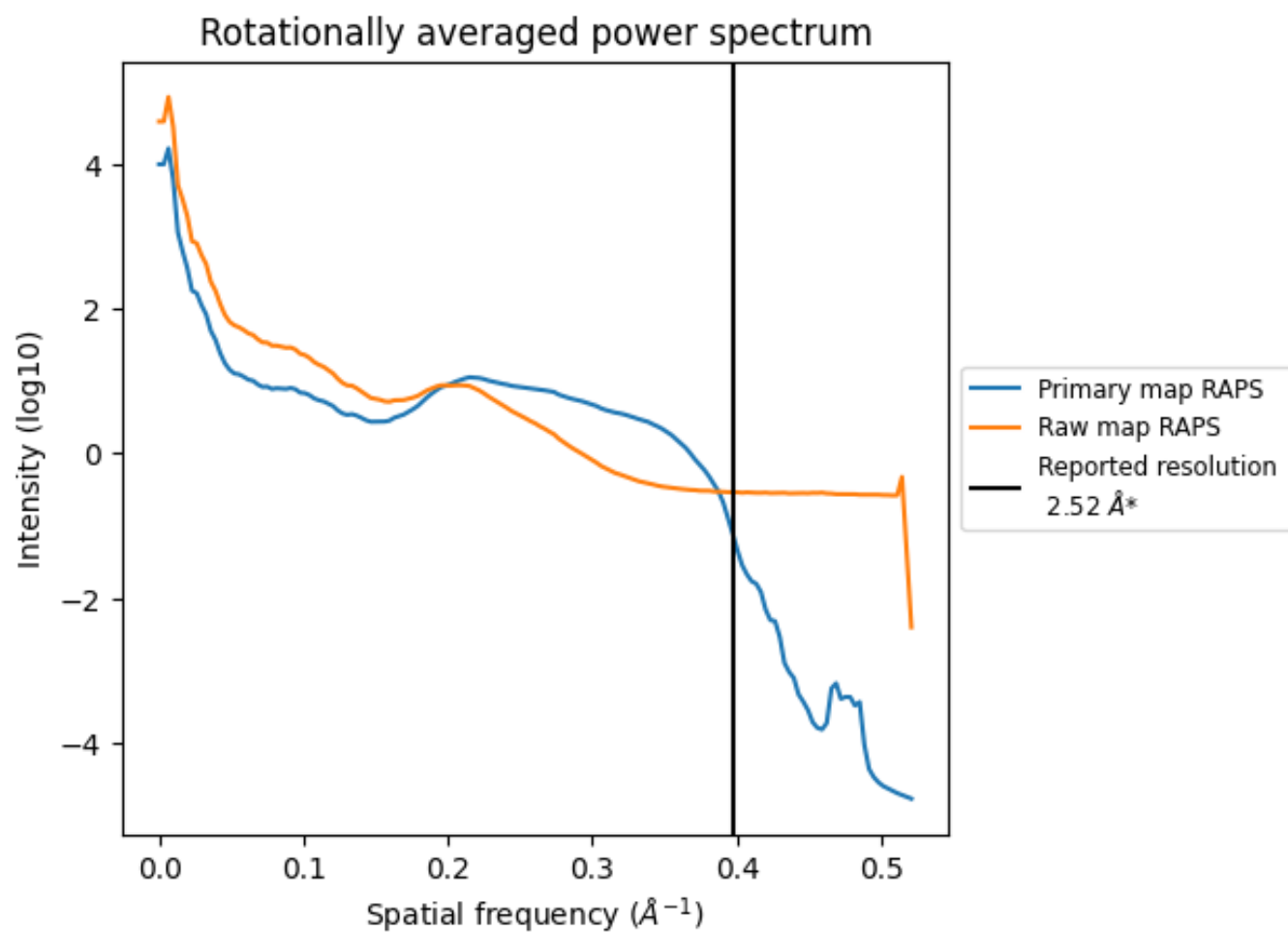
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 249 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 ⓘ

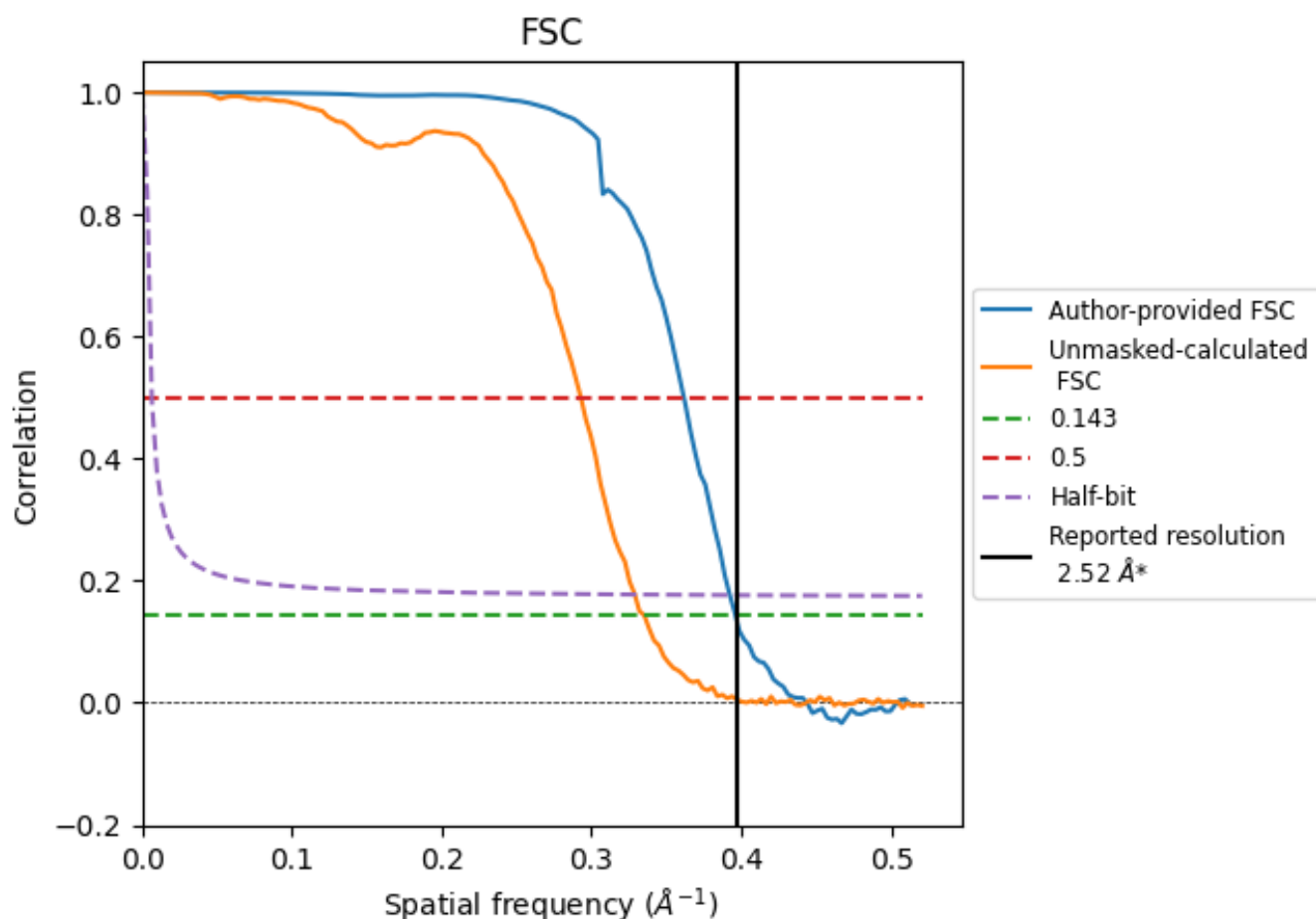


*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

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 0.397 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

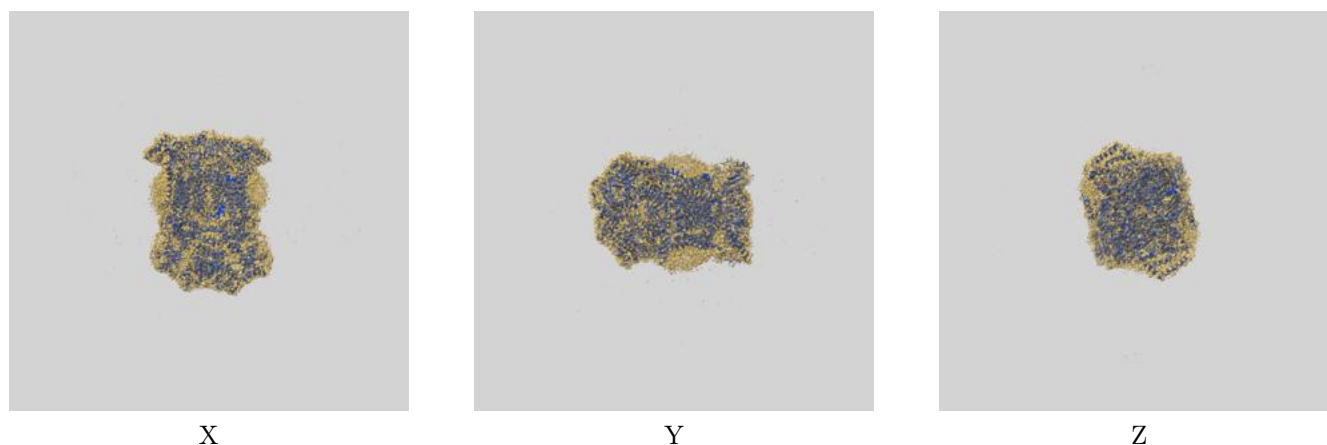
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.52	2.76	2.55
Unmasked-calculated*	2.98	3.41	3.04

*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 2.98 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

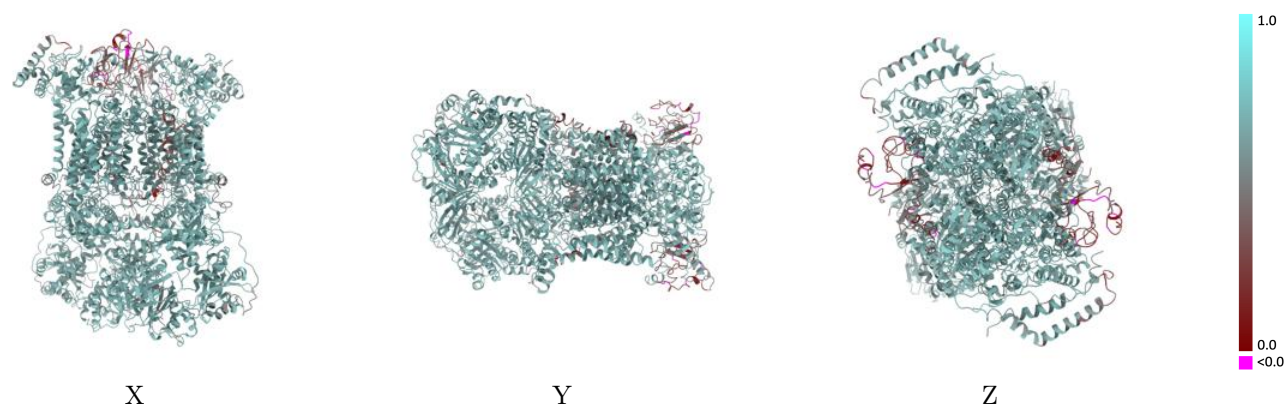
This section contains information regarding the fit between EMDB map EMD-60256 and PDB model 8ZMT. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



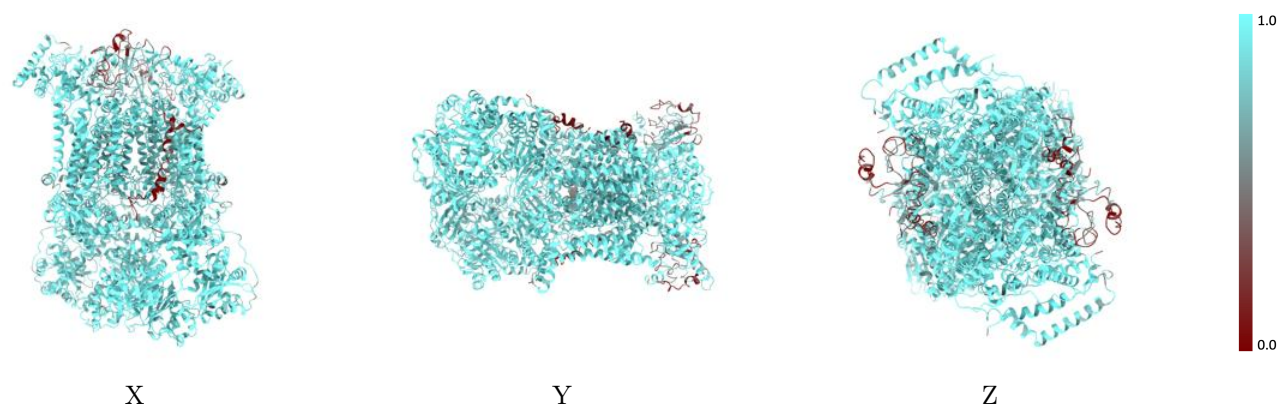
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



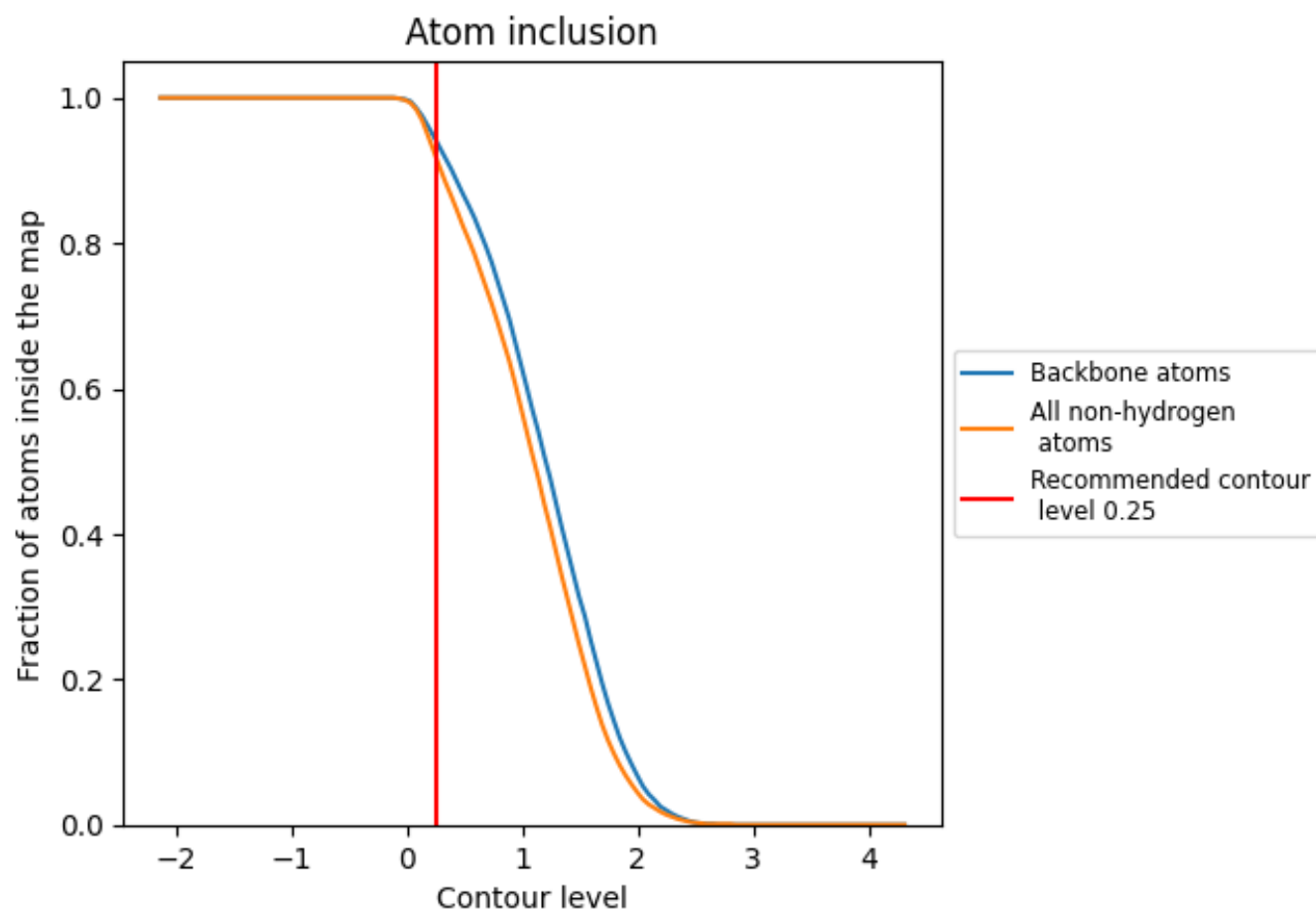
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.6210
A	 0.9690	 0.6520
B	 0.9680	 0.6500
C	 0.9920	 0.6740
D	 0.9760	 0.6570
E	 0.6250	 0.4140
F	 0.9020	 0.5930
G	 0.9550	 0.6500
H	 0.9240	 0.6170
I	 0.9170	 0.6240
L	 0.9690	 0.6520
M	 0.9680	 0.6480
N	 0.9880	 0.6730
O	 0.9770	 0.6570
P	 0.6140	 0.4160
Q	 0.8880	 0.5660
R	 0.9550	 0.6500
S	 0.9200	 0.6160
T	 0.9170	 0.6110
U	 0.1680	 0.2590
V	 0.1360	 0.2690

