



Full wwPDB EM Validation Report ⓘ

May 12, 2025 – 04:20 PM JST

PDB ID : 8ZJC / pdb_00008zjc
EMDB ID : EMD-60140
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-05-14
Resolution : 2.50 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

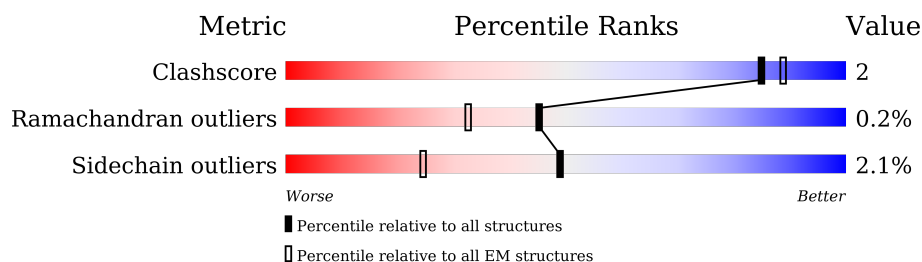
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 6% 99% .
1	L	431	 6% 100% .
2	B	352	 98% .
2	M	352	 98% ..
3	C	385	 98% .
3	N	385	 98% .
4	D	248	 98% .
4	O	248	 99% .

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Mol	Chain	Length	Quality of chain
5	E	185	
5	P	185	
6	F	75	
6	Q	75	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	55	
9	T	55	
10	U	52	
10	V	52	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	FES	E	301	-	-	X	-
17	FES	P	301	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 32311 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
			3083	2076	484	502	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.

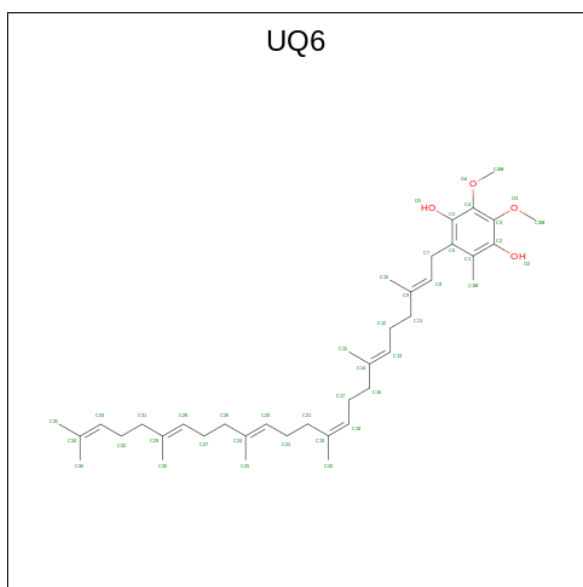
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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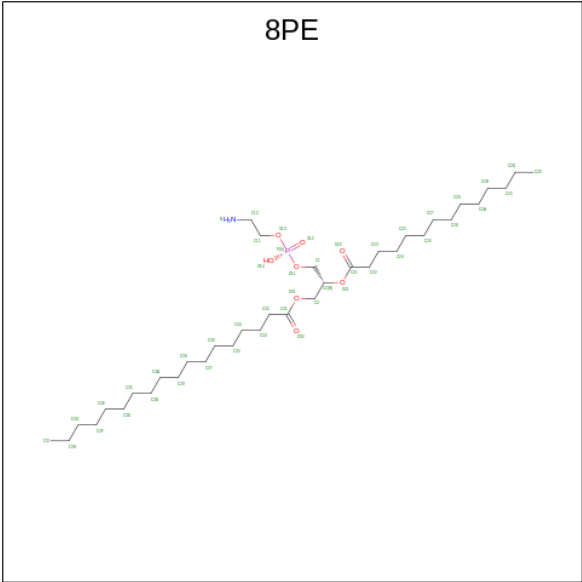
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is 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: $C_{39}H_{60}O_4$).



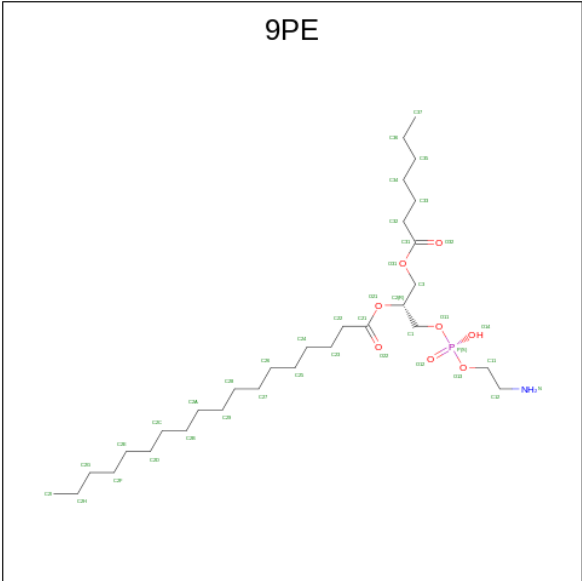
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			43	39	4	
11	N	1	Total	C	O	0
			43	39	4	

- Molecule 12 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
12	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
12	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

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



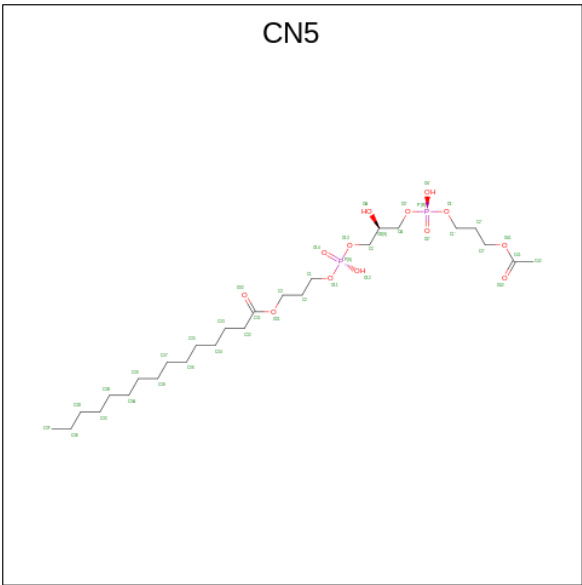
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

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

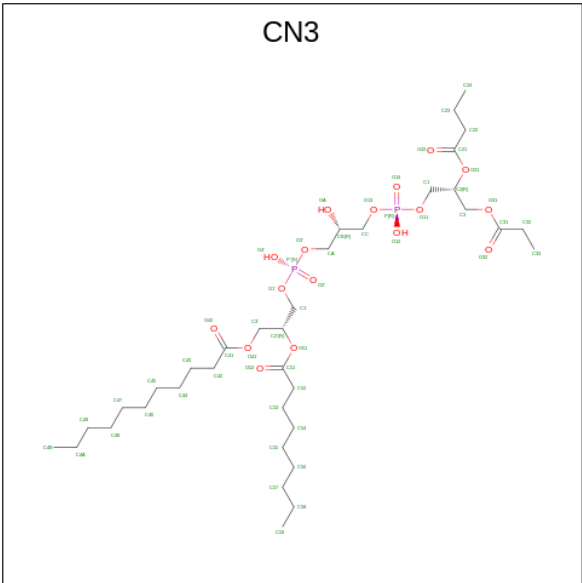
- # HEM

- 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: $C_{26}H_{52}O_{13}P_2$).



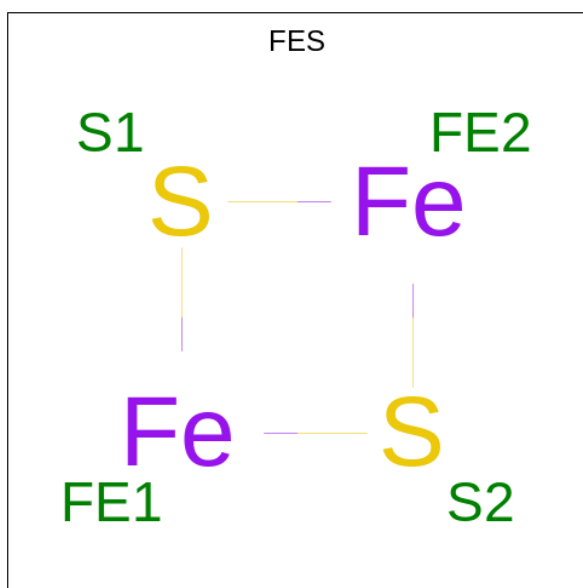
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 16 is (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).



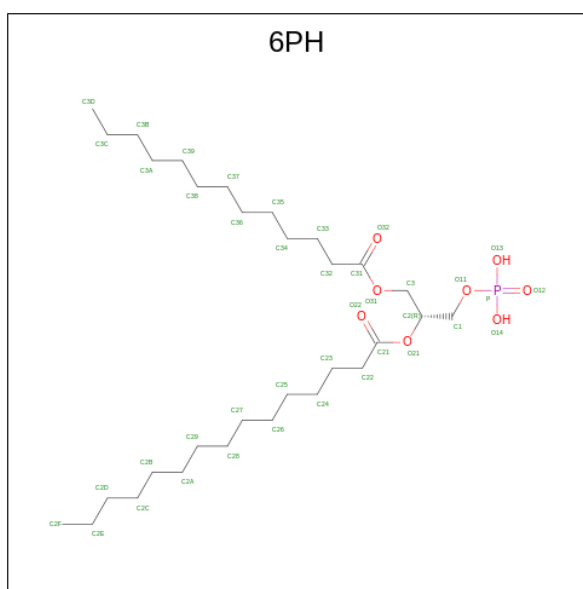
Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total	C	O	P	0
			55	36	17	2	
16	N	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 18 is (1R)-2-(phosphonooxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: $\text{C}_{31}\text{H}_{61}\text{O}_8\text{P}$).

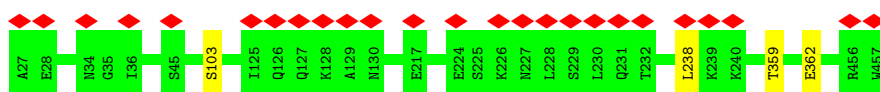


Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	O	P	0
			40	31	8	1	
18	P	1	Total	C	O	P	0
			40	31	8	1	

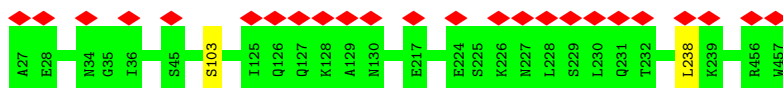
3 Residue-property plots [i](#)

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.

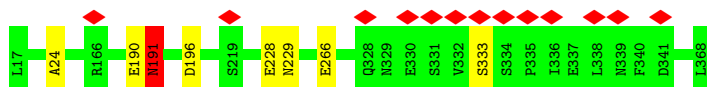
- Molecule 1: COR1 isoform 1



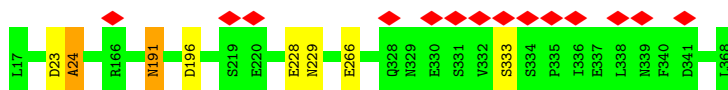
- Molecule 1: COR1 isoform 1



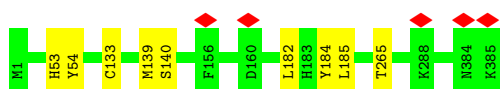
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



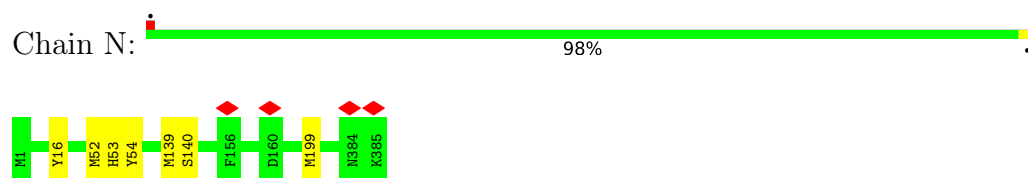
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



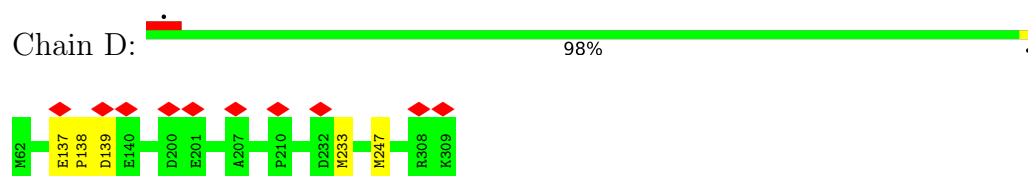
- Molecule 3: Cytochrome b



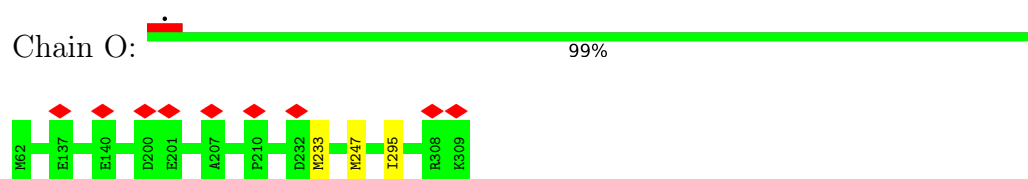
- Molecule 3: Cytochrome b



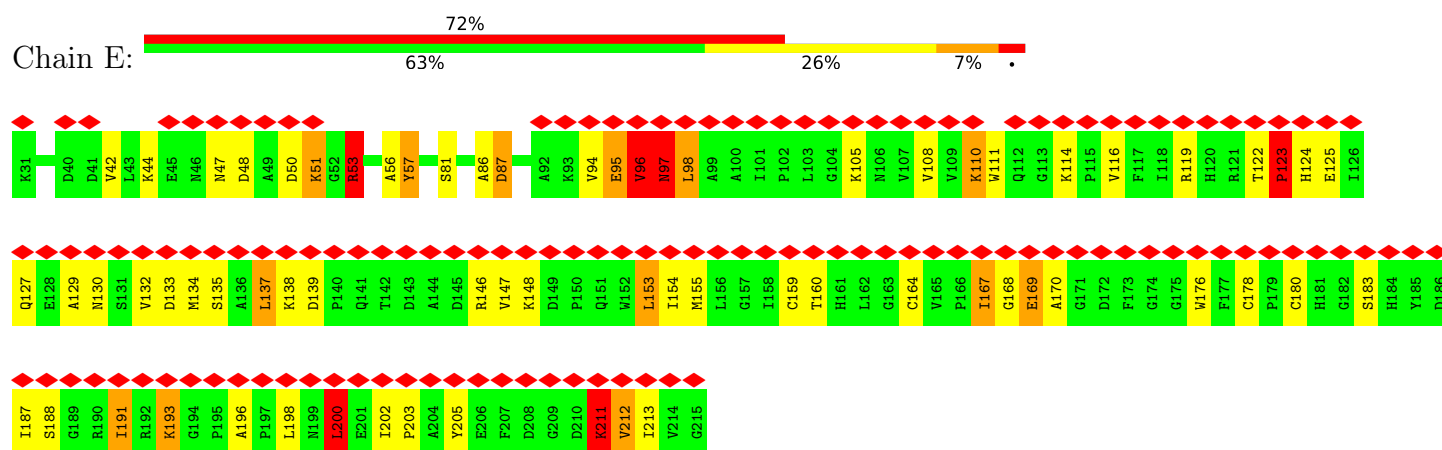
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



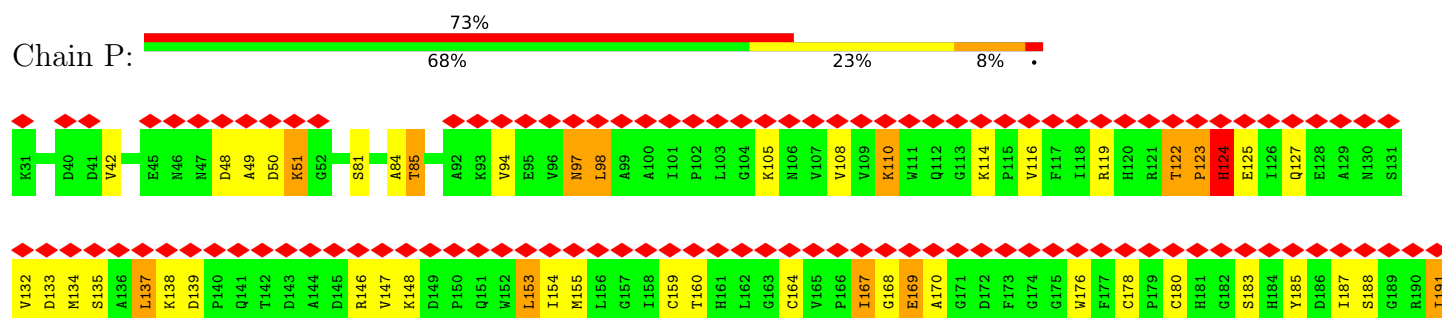
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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

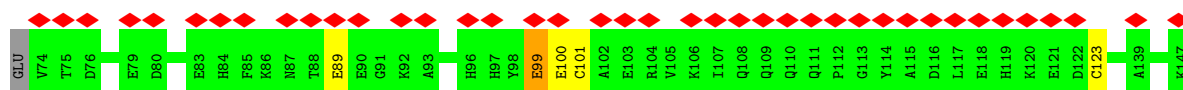
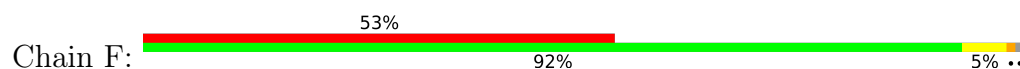


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

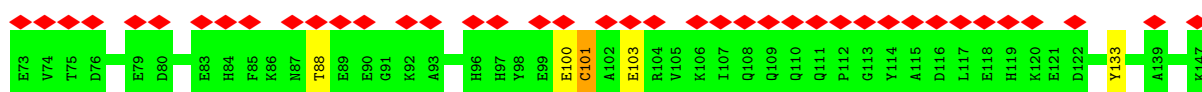




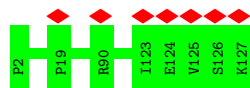
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



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



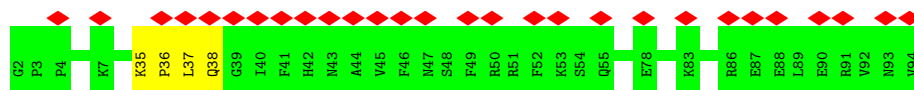
- Molecule 7: Cytochrome b-c1 complex subunit 7



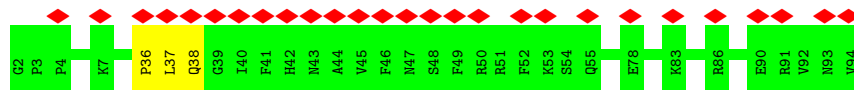
- Molecule 7: Cytochrome b-c1 complex subunit 7



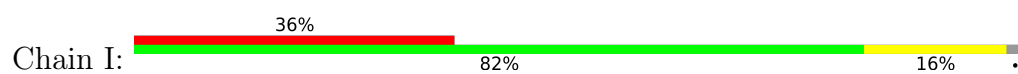
- Molecule 8: Cytochrome b-c1 complex subunit 8



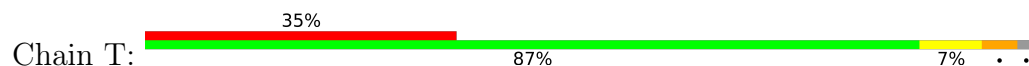
- Molecule 8: Cytochrome b-c1 complex subunit 8



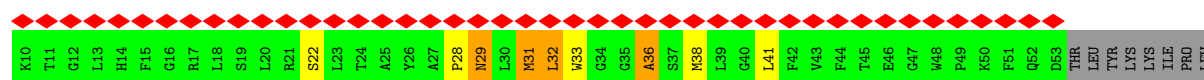
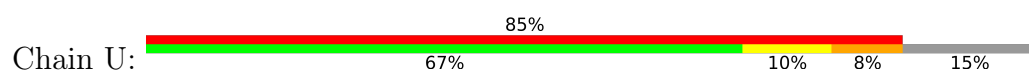
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



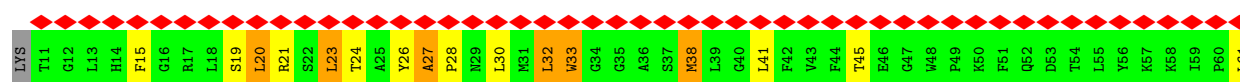
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



- 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	451636	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 ($e^-/\text{\AA}^2$)	49.04	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.847	Depositor
Minimum map value	-4.510	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.231	Depositor
Recommended contour level	0.906	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PH, CN5, UQ6, 8PE, FES, 9PE, CN3, 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	0.31	0/3405	0.49	0/4615
1	L	0.31	0/3405	0.49	0/4615
2	B	0.43	3/2781 (0.1%)	0.55	3/3764 (0.1%)
2	M	0.39	2/2781 (0.1%)	0.56	5/3764 (0.1%)
3	C	0.54	4/3192 (0.1%)	0.57	3/4354 (0.1%)
3	N	0.54	3/3184 (0.1%)	0.58	5/4344 (0.1%)
4	D	0.50	2/2022 (0.1%)	0.54	1/2751 (0.0%)
4	O	0.32	0/2022	0.49	0/2751
5	E	0.82	6/1444 (0.4%)	1.29	21/1957 (1.1%)
5	P	0.84	7/1444 (0.5%)	1.16	16/1957 (0.8%)
6	F	0.32	0/638	0.59	0/858
6	Q	0.32	0/647	0.67	1/870 (0.1%)
7	G	0.32	0/1040	0.52	0/1408
7	R	0.45	1/1040 (0.1%)	0.64	1/1408 (0.1%)
8	H	0.69	1/804 (0.1%)	0.74	4/1088 (0.4%)
8	S	0.73	1/804 (0.1%)	0.61	1/1088 (0.1%)
9	I	0.29	0/455	0.51	0/614
9	T	0.52	2/456 (0.4%)	0.78	2/615 (0.3%)
10	U	0.49	1/358 (0.3%)	1.27	6/483 (1.2%)
10	V	0.91	2/419 (0.5%)	1.24	3/567 (0.5%)
All	All	0.50	35/32341 (0.1%)	0.67	72/43871 (0.2%)

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
2	B	0	2
2	M	0	1
5	E	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	P	0	7
6	F	0	1
9	T	0	1
10	U	0	3
10	V	0	2
All	All	0	27

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	54	TYR	C-N	18.72	1.59	1.33
8	S	36	PRO	C-N	18.30	1.57	1.33
5	P	137	LEU	C-N	16.99	1.54	1.33
8	H	36	PRO	C-N	16.89	1.57	1.33
3	C	54	TYR	C-N	16.64	1.56	1.33
5	E	86	ALA	C-N	14.69	1.57	1.33
4	D	138	PRO	C-N	14.49	1.53	1.33
10	V	27	ALA	C-N	13.89	1.51	1.33
2	B	191	ASN	C-N	13.82	1.53	1.33
5	P	98	LEU	C-N	9.93	1.44	1.33
4	D	137	GLU	C-N	9.43	1.45	1.33
2	M	23	ASP	C-N	-9.25	1.23	1.33
3	C	133	CYS	C-N	8.62	1.45	1.33
2	M	228	GLU	C-N	8.51	1.44	1.33
5	E	87	ASP	C-N	-8.23	1.22	1.33
3	C	139	MET	C-N	-7.83	1.23	1.33
3	C	140	SER	C-N	7.49	1.44	1.33
7	R	83	LEU	C-O	-7.42	1.14	1.24
2	B	229	ASN	C-N	7.17	1.43	1.33
9	T	19	GLY	C-N	6.75	1.43	1.34
5	E	57	TYR	C-N	6.66	1.42	1.34
5	P	138	LYS	C-N	6.60	1.47	1.33
5	E	169	GLU	C-N	6.36	1.41	1.33
5	P	168	GLY	C-N	6.33	1.41	1.33
5	P	84	ALA	C-N	-6.17	1.25	1.33
9	T	20	THR	C-N	-6.16	1.26	1.33
5	E	168	GLY	C-N	6.11	1.41	1.33
5	P	94	VAL	C-N	-6.06	1.24	1.33
10	V	23	LEU	C-N	5.93	1.43	1.33
3	N	140	SER	C-O	-5.70	1.17	1.24
5	P	203	PRO	C-N	-5.69	1.26	1.33
10	U	29	ASN	C-N	5.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	228	GLU	C-N	5.35	1.40	1.33
5	E	203	PRO	C-N	-5.16	1.27	1.33
3	N	140	SER	CA-CB	-5.00	1.45	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	57	TYR	O-C-N	-17.05	102.27	122.22
10	U	36	ALA	O-C-N	14.17	140.65	122.23
4	D	138	PRO	O-C-N	-11.18	109.38	122.91
8	H	37	LEU	O-C-N	-10.14	109.10	122.59
5	E	137	LEU	O-C-N	-9.62	111.67	122.92
2	B	190	GLU	CA-C-N	9.30	136.13	122.74
2	B	190	GLU	C-N-CA	9.30	136.13	122.74
5	P	85	THR	O-C-N	-9.26	112.49	122.96
5	E	87	ASP	O-C-N	-8.76	108.31	122.42
10	V	27	ALA	O-C-N	8.56	131.16	121.32
5	P	85	THR	CA-C-N	8.52	132.06	120.38
5	P	85	THR	C-N-CA	8.52	132.06	120.38
8	H	36	PRO	O-C-N	8.44	131.98	123.03
5	P	123	PRO	N-CA-C	-7.96	103.72	113.98
2	M	229	ASN	O-C-N	7.86	132.28	123.48
3	N	53	HIS	O-C-N	7.80	131.41	122.20
9	T	13	ARG	CA-CB-CG	7.67	129.45	114.10
5	P	138	LYS	O-C-N	-7.49	114.06	122.08
10	U	36	ALA	CA-C-N	-7.24	109.73	122.26
10	U	36	ALA	C-N-CA	-7.24	109.73	122.26
2	B	190	GLU	O-C-N	-7.19	114.74	123.30
5	E	138	LYS	O-C-N	7.09	132.02	122.59
3	C	53	HIS	O-C-N	6.95	130.40	122.20
10	U	29	ASN	O-C-N	-6.92	114.13	122.22
8	S	37	LEU	O-C-N	-6.85	114.64	122.86
5	P	122	THR	O-C-N	-6.75	116.72	121.65
5	E	57	TYR	CA-C-N	6.63	129.82	120.28
5	E	57	TYR	C-N-CA	6.63	129.82	120.28
10	V	38	MET	CB-CG-SD	-6.56	93.02	112.70
5	E	202	ILE	CA-C-N	6.53	126.56	119.90
5	E	202	ILE	C-N-CA	6.53	126.56	119.90
10	V	38	MET	CA-CB-CG	6.50	127.09	114.10
3	N	53	HIS	CA-C-N	-6.48	109.04	122.07
3	N	53	HIS	C-N-CA	-6.48	109.04	122.07
8	H	37	LEU	CA-C-N	6.42	133.31	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	37	LEU	C-N-CA	6.42	133.31	122.65
5	E	193	LYS	CD-CE-NZ	6.34	132.18	111.90
5	P	193	LYS	CD-CE-NZ	6.33	132.15	111.90
5	E	86	ALA	CA-C-N	-6.24	109.83	122.31
5	E	86	ALA	C-N-CA	-6.24	109.83	122.31
5	P	204	ALA	CA-C-N	6.17	131.24	122.72
5	P	204	ALA	C-N-CA	6.17	131.24	122.72
5	E	51	LYS	N-CA-C	-6.07	106.42	113.88
2	M	24	ALA	CA-C-N	6.00	127.33	119.84
2	M	24	ALA	C-N-CA	6.00	127.33	119.84
2	M	24	ALA	O-C-N	-5.95	115.92	122.17
5	E	137	LEU	CA-C-N	5.85	132.72	121.54
5	E	137	LEU	C-N-CA	5.85	132.72	121.54
5	E	123	PRO	N-CA-C	-5.81	100.50	112.47
6	Q	101	CYS	CA-CB-SG	-5.77	101.14	114.40
3	N	139	MET	CA-C-N	5.62	128.37	120.28
3	N	139	MET	C-N-CA	5.62	128.37	120.28
9	T	13	ARG	N-CA-CB	-5.54	102.75	110.29
5	E	53	ARG	N-CA-C	-5.47	106.65	113.38
3	C	53	HIS	CA-C-N	-5.44	111.14	122.07
3	C	53	HIS	C-N-CA	-5.44	111.14	122.07
2	M	191	ASN	CB-CA-C	5.42	118.76	111.82
5	P	110	LYS	CA-CB-CG	5.31	124.71	114.10
5	E	110	LYS	CA-CB-CG	5.29	124.67	114.10
5	E	98	LEU	N-CA-C	-5.29	108.59	114.62
5	P	169	GLU	CA-CB-CG	5.23	124.56	114.10
5	E	169	GLU	CA-CB-CG	5.22	124.54	114.10
7	R	82	GLU	N-CA-CB	-5.18	102.54	110.26
5	P	211	LYS	CB-CG-CD	5.18	123.22	111.30
5	E	211	LYS	CB-CG-CD	5.18	123.21	111.30
5	E	110	LYS	CB-CG-CD	5.07	122.95	111.30
5	P	110	LYS	CB-CG-CD	5.04	122.90	111.30
5	P	94	VAL	CA-C-N	5.03	131.08	121.87
5	P	94	VAL	C-N-CA	5.03	131.08	121.87
10	U	33	TRP	CA-C-N	-5.03	114.36	119.94
10	U	33	TRP	C-N-CA	-5.03	114.36	119.94
5	P	124	HIS	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	ASN	Mainchain
2	B	333	SER	Peptide
5	E	105	LYS	Peptide
5	E	127	GLN	Peptide
5	E	160	THR	Peptide
5	E	167	ILE	Peptide
5	E	191	ILE	Peptide
5	E	200	LEU	Peptide
5	E	53	ARG	Sidechain
5	E	56	ALA	Mainchain
5	E	57	TYR	Mainchain
5	E	87	ASP	Mainchain
6	F	99	GLU	Mainchain
2	M	333	SER	Peptide
5	P	105	LYS	Peptide
5	P	127	GLN	Peptide
5	P	160	THR	Peptide
5	P	167	ILE	Peptide
5	P	191	ILE	Peptide
5	P	200	LEU	Peptide
5	P	85	THR	Mainchain
9	T	14	ASN	Peptide
10	U	22	SER	Peptide
10	U	38	MET	Peptide
10	U	41	LEU	Peptide
10	V	20	LEU	Peptide
10	V	38	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3323	6	0
1	L	3344	0	3323	0	0
2	B	2735	0	2774	1	0
2	M	2735	0	2774	1	0
3	C	3090	0	3129	4	0
3	N	3083	0	3119	3	0
4	D	1961	0	1890	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1961	0	1890	3	0
5	E	1411	0	1390	31	0
5	P	1411	0	1390	29	0
6	F	624	0	583	2	0
6	Q	633	0	589	2	0
7	G	1019	0	1034	0	0
7	R	1019	0	1034	3	0
8	H	773	0	736	2	0
8	S	773	0	736	1	0
9	I	442	0	440	14	0
9	T	443	0	440	7	0
10	U	347	0	345	5	0
10	V	406	0	414	21	0
11	C	43	0	60	0	0
11	N	43	0	60	4	0
12	C	47	0	73	0	0
12	N	47	0	73	0	0
13	C	80	0	118	0	0
14	C	86	0	60	2	0
14	D	43	0	30	0	0
14	N	86	0	60	2	0
14	O	43	0	30	2	0
15	C	41	0	50	5	0
16	C	55	0	66	0	0
16	N	55	0	66	0	0
17	E	4	0	0	5	0
17	P	4	0	0	3	0
18	L	40	0	59	0	0
18	P	40	0	59	0	0
All	All	32311	0	32217	133	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 (133) 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)
9:I:17:PHE:HA	9:I:20:THR:HG22	1.38	1.05
15:C:406:CN5:H2	15:C:406:CN5:H37	1.42	1.00
9:T:17:PHE:HA	9:T:20:THR:HG22	1.45	0.96
5:E:183:SER:HB2	17:E:301:FES:S1	2.04	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:178:CYS:SG	5:P:185:TYR:HE1	1.89	0.95
5:E:178:CYS:SG	17:E:301:FES:S2	2.68	0.91
5:E:122:THR:C	5:E:124:HIS:H	1.83	0.87
5:E:196:ALA:HB2	17:E:301:FES:S1	2.16	0.85
5:E:122:THR:C	5:E:124:HIS:N	2.31	0.84
1:A:359:THR:HG23	1:A:362:GLU:H	1.45	0.81
9:I:17:PHE:HA	9:I:20:THR:CG2	2.10	0.81
5:P:183:SER:HB2	17:P:301:FES:S1	2.21	0.81
5:E:122:THR:HB	5:E:124:HIS:HB2	1.63	0.81
2:B:24:ALA:HB3	2:B:191:ASN:OD1	1.81	0.79
1:A:359:THR:CG2	1:A:362:GLU:HG3	2.14	0.77
10:V:20:LEU:HA	10:V:23:LEU:HB3	1.66	0.76
5:P:178:CYS:SG	5:P:185:TYR:CE1	2.78	0.73
9:I:17:PHE:CA	9:I:20:THR:HG22	2.17	0.73
5:P:122:THR:HG22	5:P:123:PRO:HD2	1.75	0.69
5:P:98:LEU:HD11	5:P:211:LYS:HA	1.75	0.68
4:O:295:ILE:HG22	7:R:83:LEU:HD11	1.76	0.68
10:U:28:PRO:O	10:U:32:LEU:HG	1.94	0.68
9:I:30:THR:HG21	10:V:61:LEU:HA	1.78	0.66
5:E:196:ALA:CB	17:E:301:FES:S1	2.82	0.66
1:A:359:THR:HG22	1:A:362:GLU:HG3	1.76	0.66
5:E:183:SER:CB	17:E:301:FES:S1	2.84	0.66
5:P:164:CYS:SG	5:P:180:CYS:HB2	2.36	0.66
5:P:178:CYS:HG	5:P:185:TYR:HE1	1.43	0.65
5:E:164:CYS:SG	5:E:180:CYS:HB2	2.36	0.64
9:I:13:ARG:HB2	9:I:16:VAL:HG13	1.79	0.64
1:A:359:THR:HG22	1:A:362:GLU:CG	2.28	0.64
9:I:13:ARG:NH1	10:V:32:LEU:HD23	2.13	0.63
5:P:147:VAL:HG21	5:P:205:TYR:OH	1.99	0.62
10:V:32:LEU:C	10:V:32:LEU:HD12	2.24	0.62
5:P:122:THR:C	5:P:124:HIS:N	2.54	0.61
14:O:401:HEM:HBC2	14:O:401:HEM:HHD	1.83	0.61
9:I:13:ARG:HH11	10:V:32:LEU:HD23	1.65	0.60
9:I:15:ALA:HB2	10:V:33:TRP:HB2	1.83	0.60
5:P:122:THR:C	5:P:124:HIS:H	2.09	0.60
14:O:401:HEM:HMB1	14:O:401:HEM:HBB2	1.83	0.59
5:E:147:VAL:HG21	5:E:205:TYR:OH	2.03	0.59
10:V:41:LEU:O	10:V:45:THR:HG22	2.02	0.59
5:P:183:SER:CB	17:P:301:FES:S1	2.90	0.58
1:A:359:THR:HG22	1:A:362:GLU:OE1	2.02	0.58
5:P:167:ILE:HG22	5:P:176:TRP:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:196:ALA:HB2	17:P:301:FES:S1	2.44	0.58
5:E:167:ILE:HG22	5:E:176:TRP:HA	1.84	0.58
14:N:402:HEM:HBC2	14:N:402:HEM:HHD	1.85	0.57
9:I:16:VAL:HG23	9:I:17:PHE:HB2	1.86	0.57
5:E:122:THR:HG22	5:E:123:PRO:HD2	1.87	0.56
9:T:17:PHE:HA	9:T:20:THR:CG2	2.27	0.56
5:E:95:GLU:HB3	5:E:212:VAL:O	2.06	0.56
5:E:94:VAL:HG12	5:E:111:TRP:HD1	1.72	0.55
10:V:20:LEU:HG	10:V:23:LEU:HD23	1.88	0.55
5:P:167:ILE:CD1	5:P:170:ALA:HB3	2.38	0.54
5:E:167:ILE:CD1	5:E:170:ALA:HB3	2.38	0.54
5:P:97:ASN:CG	5:P:98:LEU:H	2.15	0.54
5:E:94:VAL:HG12	5:E:111:TRP:CD1	2.43	0.53
5:E:97:ASN:C	5:E:98:LEU:HD12	2.34	0.53
9:T:13:ARG:C	9:T:16:VAL:HG12	2.35	0.51
4:O:295:ILE:CG2	7:R:83:LEU:HD11	2.39	0.51
10:U:29:ASN:HA	10:U:32:LEU:HD12	1.93	0.51
9:I:13:ARG:HH11	10:V:32:LEU:CD2	2.23	0.51
2:M:24:ALA:O	2:M:191:ASN:ND2	2.43	0.51
10:V:32:LEU:HD12	10:V:32:LEU:O	2.10	0.51
15:C:406:CN5:C2	15:C:406:CN5:H34	2.40	0.50
9:T:16:VAL:HG13	9:T:17:PHE:HB2	1.94	0.50
5:P:48:ASP:O	5:P:49:ALA:HB3	2.11	0.50
15:C:406:CN5:H34	15:C:406:CN5:H2A	1.94	0.49
5:E:53:ARG:NH1	9:I:7:TYR:CE2	2.81	0.49
3:C:182:LEU:HD23	11:N:405:UQ6:C34	2.43	0.49
4:D:233:MET:HG2	4:D:247:MET:HE1	1.94	0.49
3:C:265:THR:HG21	5:P:164:CYS:HA	1.95	0.49
4:O:233:MET:HG2	4:O:247:MET:HE1	1.94	0.48
5:P:122:THR:HG22	5:P:123:PRO:CD	2.43	0.48
10:V:27:ALA:HB3	10:V:28:PRO:HD3	1.95	0.48
6:F:101:CYS:HG	6:F:123:CYS:HG	0.54	0.48
10:V:23:LEU:O	10:V:27:ALA:HB2	2.14	0.47
6:F:99:GLU:C	6:F:101:CYS:N	2.66	0.47
5:E:167:ILE:HD11	5:E:170:ALA:HB3	1.97	0.47
5:E:42:VAL:HA	8:H:38:GLN:HE21	1.79	0.47
5:P:167:ILE:HD11	5:P:170:ALA:HB3	1.97	0.47
10:U:28:PRO:O	10:U:31:MET:HB3	2.15	0.47
6:Q:88:THR:HG21	6:Q:133:TYR:OH	2.15	0.47
5:P:119:ARG:HB2	5:P:153:LEU:HB2	1.97	0.46
10:U:29:ASN:HA	10:U:32:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:122:THR:CG2	5:E:123:PRO:HD2	2.46	0.46
10:V:15:PHE:HB3	10:V:19:SER:HA	1.98	0.46
10:V:20:LEU:HG	10:V:23:LEU:CD2	2.46	0.46
9:T:17:PHE:CA	9:T:20:THR:HG22	2.32	0.46
5:E:116:VAL:HG22	5:E:154:ILE:HG23	1.98	0.46
6:Q:100:GLU:O	6:Q:103:GLU:HG2	2.15	0.46
5:E:98:LEU:HD11	5:E:211:LYS:HA	1.97	0.45
10:V:30:LEU:HA	10:V:33:TRP:HD1	1.81	0.45
1:A:359:THR:HG22	1:A:362:GLU:CD	2.41	0.45
3:N:52:MET:HE2	11:N:405:UQ6:H362	1.98	0.45
5:E:119:ARG:HB2	5:E:153:LEU:HB2	1.97	0.45
5:P:116:VAL:HG22	5:P:154:ILE:HG23	1.98	0.45
3:C:184:TYR:CE1	14:C:405:HEM:HBC1	2.53	0.44
15:C:406:CN5:H36A	15:C:406:CN5:H39A	1.57	0.44
5:E:95:GLU:O	5:E:97:ASN:N	2.50	0.44
10:V:24:THR:HA	10:V:27:ALA:HB2	1.98	0.44
5:P:42:VAL:HA	8:S:38:GLN:HE21	1.82	0.44
15:C:406:CN5:H36	3:N:199:MET:HG2	1.99	0.44
5:P:203:PRO:O	5:P:205:TYR:HD1	2.01	0.44
9:T:13:ARG:O	9:T:16:VAL:HG12	2.18	0.44
10:V:45:THR:O	10:V:45:THR:HG23	2.18	0.43
5:P:97:ASN:CG	5:P:98:LEU:N	2.76	0.43
5:E:159:CYS:HA	5:E:200:LEU:HD11	2.01	0.43
5:P:48:ASP:HB3	5:P:51:LYS:CB	2.49	0.42
3:C:185:LEU:HD22	11:N:405:UQ6:C35	2.48	0.42
5:P:159:CYS:HA	5:P:200:LEU:HD11	2.01	0.42
10:V:19:SER:HB2	10:V:21:ARG:HB3	2.01	0.42
10:V:33:TRP:CD1	10:V:33:TRP:C	2.98	0.42
9:I:17:PHE:C	9:I:20:THR:HG22	2.44	0.42
10:V:30:LEU:HA	10:V:33:TRP:CD1	2.55	0.42
9:I:14:ASN:O	9:I:18:VAL:HG12	2.19	0.42
5:P:167:ILE:HD13	5:P:170:ALA:HB3	2.01	0.42
9:T:13:ARG:HD3	9:T:16:VAL:HB	2.02	0.42
5:E:95:GLU:O	5:E:96:VAL:C	2.62	0.42
3:N:16:TYR:O	11:N:405:UQ6:H4M2	2.19	0.42
5:E:167:ILE:HD13	5:E:170:ALA:HB3	2.01	0.42
5:P:122:THR:HB	5:P:124:HIS:HB2	2.01	0.42
5:P:122:THR:CG2	5:P:123:PRO:HD2	2.49	0.41
5:E:44:LYS:CG	8:H:35:LYS:HA	2.51	0.41
5:E:122:THR:O	5:E:124:HIS:N	2.54	0.41
14:C:408:HEM:HMB1	14:C:408:HEM:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:403:HEM:HMB1	14:N:403:HEM:HBB2	2.01	0.41
7:R:81:THR:HG22	7:R:86:HIS:O	2.21	0.41
10:U:32:LEU:O	10:U:36:ALA:N	2.54	0.41
9:I:13:ARG:C	9:I:16:VAL:HG22	2.45	0.40
5:E:129:ALA:C	5:E:130:ASN:HD22	2.30	0.40
10:V:26:TYR:CD2	10:V:30:LEU:HD23	2.57	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%)	410 (96%)	18 (4%)	1 (0%)	44	64
1	L	429/431 (100%)	410 (96%)	18 (4%)	1 (0%)	44	64
2	B	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
2	M	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	C	383/385 (100%)	374 (98%)	9 (2%)	0	100	100
3	N	383/385 (100%)	374 (98%)	9 (2%)	0	100	100
4	D	246/248 (99%)	240 (98%)	5 (2%)	1 (0%)	30	49
4	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
5	E	183/185 (99%)	143 (78%)	36 (20%)	4 (2%)	5	9
5	P	183/185 (99%)	144 (79%)	38 (21%)	1 (0%)	25	44
6	F	72/75 (96%)	67 (93%)	4 (6%)	1 (1%)	9	17
6	Q	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
7	G	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
8	H	91/93 (98%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
9	I	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
9	T	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
10	U	42/52 (81%)	35 (83%)	7 (17%)	0	100	100
10	V	49/52 (94%)	40 (82%)	9 (18%)	0	100	100
All	All	3952/4004 (99%)	3741 (95%)	202 (5%)	9 (0%)	45	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	96	VAL
5	E	97	ASN
5	P	97	ASN
5	E	48	ASP
6	F	89	GLU
1	A	238	LEU
1	L	238	LEU
4	D	139	ASP
5	E	123	PRO

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%)	369 (100%)	1 (0%)	91	97
1	L	370/370 (100%)	369 (100%)	1 (0%)	91	97
2	B	301/301 (100%)	299 (99%)	2 (1%)	81	93
2	M	301/301 (100%)	299 (99%)	2 (1%)	81	93
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	336/338 (99%)	336 (100%)	0	100	100
4	D	206/206 (100%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	206/206 (100%)	206 (100%)	0	100	100
5	E	151/151 (100%)	120 (80%)	31 (20%)	1	2
5	P	151/151 (100%)	123 (82%)	28 (18%)	1	2
6	F	67/68 (98%)	66 (98%)	1 (2%)	60	82
6	Q	68/68 (100%)	67 (98%)	1 (2%)	60	82
7	G	110/110 (100%)	110 (100%)	0	100	100
7	R	110/110 (100%)	109 (99%)	1 (1%)	75	90
8	H	77/77 (100%)	77 (100%)	0	100	100
8	S	77/77 (100%)	77 (100%)	0	100	100
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%)	17	35
10	V	42/43 (98%)	40 (95%)	2 (5%)	21	43
All	All	3405/3418 (100%)	3333 (98%)	72 (2%)	49	74

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	SER
2	B	196	ASP
2	B	266	GLU
5	E	47	ASN
5	E	50	ASP
5	E	51	LYS
5	E	81	SER
5	E	95	GLU
5	E	96	VAL
5	E	97	ASN
5	E	108	VAL
5	E	110	LYS
5	E	114	LYS
5	E	125	GLU
5	E	132	VAL
5	E	133	ASP
5	E	134	MET
5	E	135	SER
5	E	137	LEU

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Mol	Chain	Res	Type
5	E	139	ASP
5	E	146	ARG
5	E	148	LYS
5	E	153	LEU
5	E	155	MET
5	E	169	GLU
5	E	187	ILE
5	E	188	SER
5	E	191	ILE
5	E	193	LYS
5	E	198	LEU
5	E	200	LEU
5	E	211	LYS
5	E	212	VAL
5	E	213	ILE
6	F	100	GLU
1	L	103	SER
2	M	196	ASP
2	M	266	GLU
5	P	50	ASP
5	P	51	LYS
5	P	81	SER
5	P	108	VAL
5	P	110	LYS
5	P	114	LYS
5	P	124	HIS
5	P	125	GLU
5	P	132	VAL
5	P	133	ASP
5	P	134	MET
5	P	135	SER
5	P	137	LEU
5	P	139	ASP
5	P	146	ARG
5	P	148	LYS
5	P	153	LEU
5	P	155	MET
5	P	169	GLU
5	P	187	ILE
5	P	188	SER
5	P	191	ILE
5	P	193	LYS

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Mol	Chain	Res	Type
5	P	198	LEU
5	P	200	LEU
5	P	211	LYS
5	P	212	VAL
5	P	213	ILE
6	Q	101	CYS
7	R	83	LEU
10	U	31	MET
10	U	32	LEU
10	V	32	LEU
10	V	33	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	345	HIS
2	B	36	HIS
3	C	57	ASN
3	C	177	GLN
3	C	183	HIS
3	C	249	ASN
5	E	97	ASN
5	E	161	HIS
5	E	181	HIS
5	E	199	ASN
6	F	84	HIS
7	G	34	ASN
7	G	85	HIS
9	I	29	GLN
1	L	47	HIS
1	L	213	ASN
1	L	221	ASN
1	L	271	ASN
1	L	345	HIS
2	M	36	HIS
2	M	339	ASN
3	N	141	HIS
3	N	183	HIS
3	N	249	ASN
4	O	303	ASN
5	P	181	HIS

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Mol	Chain	Res	Type
5	P	199	ASN
7	R	34	ASN
7	R	122	ASN
10	V	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
16	CN3	N	401	-	54,54,54	1.16	8 (14%)	60,66,66	1.18	5 (8%)
14	HEM	N	403	3	41,50,50	1.42	3 (7%)	45,82,82	1.19	4 (8%)
15	CN5	C	406	-	40,40,40	0.33	0	44,48,48	0.59	0
16	CN3	C	407	-	54,54,54	1.19	8 (14%)	60,66,66	1.03	4 (6%)
11	UQ6	C	401	-	43,43,43	1.62	11 (25%)	51,55,55	1.59	12 (23%)
14	HEM	C	405	3	41,50,50	1.51	4 (9%)	45,82,82	1.29	6 (13%)
13	9PE	C	404	-	39,39,39	0.94	3 (7%)	42,44,44	0.82	2 (4%)
11	UQ6	N	405	-	43,43,43	1.63	9 (20%)	51,55,55	1.64	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	9PE	C	403	-	39,39,39	0.98	2 (5%)	42,44,44	1.00	2 (4%)
12	8PE	C	402	-	46,46,46	0.89	3 (6%)	49,51,51	0.99	2 (4%)
18	6PH	P	302	-	39,39,39	0.95	4 (10%)	43,44,44	1.08	2 (4%)
12	8PE	N	404	-	46,46,46	0.90	4 (8%)	49,51,51	1.00	2 (4%)
17	FES	E	301	5	0,4,4	-	-	-	-	-
17	FES	P	301	5	0,4,4	-	-	-	-	-
14	HEM	O	401	4	41,50,50	1.48	3 (7%)	45,82,82	1.27	4 (8%)
14	HEM	C	408	3	41,50,50	1.42	3 (7%)	45,82,82	1.15	4 (8%)
18	6PH	L	501	-	39,39,39	0.93	4 (10%)	43,44,44	1.01	2 (4%)
14	HEM	N	402	3	41,50,50	1.55	3 (7%)	45,82,82	1.39	6 (13%)
14	HEM	D	401	4	41,50,50	1.47	5 (12%)	45,82,82	1.33	5 (11%)

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
16	CN3	N	401	-	-	27/65/65/65	-
14	HEM	N	403	3	-	4/12/54/54	-
15	CN5	C	406	-	-	20/44/44/44	-
16	CN3	C	407	-	-	42/65/65/65	-
11	UQ6	C	401	-	-	9/39/39/39	0/1/1/1
14	HEM	C	405	3	-	5/12/54/54	-
13	9PE	C	404	-	-	26/43/43/43	-
11	UQ6	N	405	-	-	7/39/39/39	0/1/1/1
13	9PE	C	403	-	-	28/43/43/43	-
12	8PE	C	402	-	-	23/50/50/50	-
18	6PH	P	302	-	-	21/41/41/41	-
12	8PE	N	404	-	-	23/50/50/50	-
17	FES	E	301	5	-	-	0/1/1/1
17	FES	P	301	5	-	-	0/1/1/1
14	HEM	O	401	4	-	2/12/54/54	-
14	HEM	C	408	3	-	2/12/54/54	-
18	6PH	L	501	-	-	15/41/41/41	-
14	HEM	N	402	3	-	5/12/54/54	-
14	HEM	D	401	4	-	1/12/54/54	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	402	HEM	C3C-C2C	-5.40	1.32	1.40
14	C	405	HEM	C3C-C2C	-4.82	1.33	1.40
11	N	405	UQ6	C7-C6	4.82	1.56	1.51
14	O	401	HEM	C3C-C2C	-4.78	1.33	1.40
11	C	401	UQ6	C7-C6	4.64	1.56	1.51
14	D	401	HEM	C3C-C2C	-4.54	1.34	1.40
14	C	408	HEM	C3C-C2C	-4.35	1.34	1.40
14	N	403	HEM	C3C-C2C	-4.35	1.34	1.40
11	C	401	UQ6	C16-C14	3.90	1.59	1.51
14	O	401	HEM	C3C-CAC	3.68	1.55	1.47
11	N	405	UQ6	C16-C14	3.61	1.58	1.51
14	C	408	HEM	C3C-CAC	3.38	1.54	1.47
14	N	403	HEM	C3C-CAC	3.37	1.54	1.47
14	N	402	HEM	C3C-CAC	3.20	1.54	1.47
14	D	401	HEM	C3C-CAC	3.16	1.54	1.47
14	C	405	HEM	C3C-CAC	3.12	1.54	1.47
11	C	401	UQ6	C11-C9	2.86	1.57	1.51
14	O	401	HEM	CAB-C3B	2.85	1.55	1.47
11	N	405	UQ6	C11-C9	2.82	1.57	1.51
14	N	403	HEM	CAB-C3B	2.79	1.55	1.47
14	C	408	HEM	CAB-C3B	2.76	1.55	1.47
12	C	402	8PE	O21-C2	-2.74	1.39	1.46
14	C	405	HEM	CAB-C3B	2.74	1.54	1.47
14	N	402	HEM	CAB-C3B	2.72	1.54	1.47
13	C	403	9PE	O21-C2	-2.66	1.39	1.46
18	P	302	6PH	O21-C2	-2.65	1.40	1.46
11	C	401	UQ6	C12-C13	2.65	1.59	1.50
11	N	405	UQ6	C26-C24	2.64	1.56	1.51
11	N	405	UQ6	C12-C13	2.60	1.58	1.50
14	D	401	HEM	CAB-C3B	2.60	1.54	1.47
13	C	403	9PE	O31-C31	2.59	1.40	1.33
12	N	404	8PE	O31-C3	-2.57	1.39	1.45
18	P	302	6PH	O31-C31	2.52	1.40	1.33
12	C	402	8PE	O31-C3	-2.47	1.39	1.45
16	C	407	CN3	O51-C2'	-2.46	1.40	1.46
16	C	407	CN3	O21-C2	-2.46	1.40	1.46
18	L	501	6PH	O31-C31	2.44	1.40	1.33
16	N	401	CN3	O51-C2'	-2.43	1.40	1.46
16	N	401	CN3	O41-C41	2.42	1.40	1.33
12	N	404	8PE	O21-C2	-2.39	1.40	1.46
16	C	407	CN3	O41-C3'	-2.39	1.39	1.45
16	C	407	CN3	O31-C31	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	401	UQ6	C26-C24	2.36	1.56	1.51
18	L	501	6PH	O21-C2	-2.35	1.40	1.46
13	C	404	9PE	O21-C2	-2.33	1.40	1.46
16	N	401	CN3	O41-C3'	-2.32	1.39	1.45
16	N	401	CN3	O31-C3	-2.29	1.39	1.45
16	C	407	CN3	O21-C21	2.28	1.40	1.34
16	N	401	CN3	O51-C51	2.26	1.40	1.34
18	L	501	6PH	O21-C21	2.25	1.40	1.34
13	C	404	9PE	O31-C31	2.25	1.39	1.33
11	C	401	UQ6	C31-C29	2.24	1.55	1.51
14	C	405	HEM	FE-NB	2.24	2.07	1.96
16	N	401	CN3	O21-C2	-2.23	1.41	1.46
12	N	404	8PE	O21-C21	2.22	1.40	1.34
16	N	401	CN3	O31-C31	2.22	1.39	1.33
16	N	401	CN3	O21-C21	2.21	1.40	1.34
11	N	405	UQ6	C31-C29	2.18	1.55	1.51
16	C	407	CN3	O41-C41	2.18	1.39	1.33
13	C	404	9PE	O31-C3	-2.17	1.40	1.45
11	N	405	UQ6	O3-C3	2.17	1.42	1.38
11	N	405	UQ6	O4-C4	2.16	1.42	1.38
16	C	407	CN3	O31-C3	-2.14	1.40	1.45
14	D	401	HEM	CMB-C2B	2.14	1.55	1.50
11	C	401	UQ6	O4-C4	2.14	1.42	1.38
16	C	407	CN3	O51-C51	2.13	1.40	1.34
11	C	401	UQ6	O3-C3	2.11	1.42	1.38
11	C	401	UQ6	C7-C8	2.10	1.55	1.50
11	N	405	UQ6	C7-C8	2.10	1.55	1.50
18	L	501	6PH	O31-C3	-2.10	1.40	1.45
14	D	401	HEM	CAA-C2A	2.10	1.55	1.52
18	P	302	6PH	O31-C3	-2.09	1.40	1.45
12	N	404	8PE	O31-C31	2.04	1.39	1.33
12	C	402	8PE	O31-C31	2.04	1.39	1.33
18	P	302	6PH	O21-C21	2.03	1.40	1.34
11	C	401	UQ6	C17-C18	2.03	1.57	1.50
11	C	401	UQ6	C22-C23	2.00	1.56	1.50

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	401	CN3	O51-C51-C52	4.81	121.86	111.50
14	N	402	HEM	C4C-CHD-C1D	4.17	128.06	122.56
18	P	302	6PH	O21-C21-C22	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	404	8PE	O21-C21-C22	3.92	119.94	111.50
16	C	407	CN3	O51-C51-C52	3.89	119.89	111.50
11	C	401	UQ6	C6-C7-C8	-3.72	106.27	112.17
11	C	401	UQ6	C10-C9-C8	-3.70	114.18	123.68
11	N	405	UQ6	C10-C9-C8	-3.56	114.54	123.68
11	N	405	UQ6	C30-C29-C31	3.50	121.15	115.27
18	L	501	6PH	O21-C21-C22	3.49	119.03	111.50
11	C	401	UQ6	C10-C9-C11	3.46	121.09	115.27
16	C	407	CN3	O31-C31-C32	3.30	120.03	111.38
13	C	403	9PE	O21-C21-C22	3.29	118.58	111.50
12	C	402	8PE	O21-C21-C22	3.27	118.55	111.50
11	N	405	UQ6	C6-C7-C8	-3.27	106.99	112.17
11	N	405	UQ6	C10-C9-C11	3.17	120.61	115.27
18	P	302	6PH	O31-C31-C32	3.14	121.77	111.91
11	C	401	UQ6	C15-C14-C16	3.13	120.53	115.27
13	C	403	9PE	O31-C31-C32	3.04	121.46	111.91
11	N	405	UQ6	C20-C19-C21	3.04	120.39	115.27
14	N	402	HEM	C4A-C3A-C2A	3.04	109.11	107.00
11	N	405	UQ6	C25-C24-C26	2.97	120.27	115.27
16	N	401	CN3	O31-C31-C32	2.93	119.07	111.38
14	O	401	HEM	C4B-CHC-C1C	2.92	126.41	122.56
14	D	401	HEM	C1B-NB-C4B	2.89	108.05	105.07
16	C	407	CN3	O21-C21-C22	2.83	117.59	111.50
11	C	401	UQ6	C12-C13-C14	-2.82	120.87	127.66
16	N	401	CN3	O21-C21-C22	2.81	117.56	111.50
11	N	405	UQ6	C15-C14-C16	2.81	119.99	115.27
11	N	405	UQ6	C12-C13-C14	-2.80	120.91	127.66
14	C	405	HEM	C4A-C3A-C2A	2.78	108.93	107.00
14	N	403	HEM	C4B-CHC-C1C	2.76	126.20	122.56
11	N	405	UQ6	C17-C18-C19	-2.76	121.02	127.66
13	C	404	9PE	O21-C21-C22	2.74	117.42	111.50
16	N	401	CN3	O41-C41-C42	2.72	120.45	111.91
14	C	408	HEM	C4B-CHC-C1C	2.71	126.13	122.56
11	C	401	UQ6	C1M-C1-C6	2.69	124.33	120.42
11	C	401	UQ6	C1M-C1-C2	-2.69	115.94	120.50
12	C	402	8PE	O31-C31-C32	2.69	120.34	111.91
14	O	401	HEM	C4C-CHD-C1D	2.58	125.97	122.56
11	C	401	UQ6	C30-C29-C31	2.58	119.61	115.27
14	C	405	HEM	C4D-ND-C1D	2.57	107.73	105.07
14	C	408	HEM	CMC-C2C-C3C	2.54	129.43	124.68
14	N	403	HEM	CMC-C2C-C3C	2.54	129.42	124.68
14	C	408	HEM	C4D-ND-C1D	2.49	107.64	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	403	HEM	C4D-ND-C1D	2.47	107.62	105.07
11	C	401	UQ6	C20-C19-C21	2.44	119.38	115.27
11	N	405	UQ6	C1M-C1-C2	-2.43	116.37	120.50
14	N	402	HEM	C1B-NB-C4B	2.43	107.58	105.07
14	O	401	HEM	C4D-ND-C1D	2.41	107.57	105.07
14	D	401	HEM	C4D-ND-C1D	2.39	107.55	105.07
14	D	401	HEM	C4C-CHD-C1D	2.32	125.61	122.56
11	C	401	UQ6	C17-C18-C19	-2.31	122.09	127.66
14	D	401	HEM	CAD-CBD-CGD	-2.31	108.64	113.60
14	N	403	HEM	C1B-NB-C4B	2.29	107.44	105.07
13	C	404	9PE	O31-C31-C32	2.29	119.09	111.91
12	N	404	8PE	O31-C31-C32	2.29	119.09	111.91
11	N	405	UQ6	C1M-C1-C6	2.28	123.74	120.42
14	C	405	HEM	C4C-CHD-C1D	2.26	125.54	122.56
14	C	408	HEM	C1B-NB-C4B	2.26	107.41	105.07
14	D	401	HEM	C4B-CHC-C1C	2.20	125.46	122.56
14	N	402	HEM	C4B-CHC-C1C	2.19	125.44	122.56
14	O	401	HEM	C1B-NB-C4B	2.18	107.33	105.07
16	C	407	CN3	O41-C41-C42	2.17	118.72	111.91
11	N	405	UQ6	C27-C28-C29	-2.17	122.44	127.66
18	L	501	6PH	O31-C31-C32	2.16	118.68	111.91
14	C	405	HEM	C2C-C3C-C4C	2.16	108.41	106.90
14	N	402	HEM	CBA-CAA-C2A	-2.14	108.97	112.62
14	C	405	HEM	CBA-CAA-C2A	-2.11	109.02	112.62
11	C	401	UQ6	C36-C34-C35	2.09	119.21	114.60
14	N	402	HEM	C2C-C3C-C4C	2.08	108.35	106.90
16	N	401	CN3	O51-C51-O52	-2.07	118.69	123.70
14	C	405	HEM	C1B-NB-C4B	2.04	107.18	105.07
11	C	401	UQ6	C36-C34-C33	-2.03	116.78	122.65

There are no chirality outliers.

All (260) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	UQ6	C9-C11-C12-C13
11	N	405	UQ6	C9-C11-C12-C13
12	C	402	8PE	C1-O11-P-O12
12	C	402	8PE	C11-O13-P-O12
12	C	402	8PE	O13-C11-C12-N
12	C	402	8PE	O11-C1-C2-O21
12	C	402	8PE	O22-C21-O21-C2
12	C	402	8PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
12	N	404	8PE	C11-O13-P-O11
12	N	404	8PE	C11-O13-P-O12
12	N	404	8PE	C11-O13-P-O14
13	C	403	9PE	C11-O13-P-O12
13	C	403	9PE	O13-C11-C12-N
13	C	403	9PE	O22-C21-O21-C2
13	C	403	9PE	C22-C21-O21-C2
15	C	406	CN5	CC-O13-P-O14
15	C	406	CN5	C1'-O1'-P'-O3'
15	C	406	CN5	O1'-C1'-C2'-C3'
16	C	407	CN3	C1-O11-P-O12
16	C	407	CN3	CC-O13-P-O12
16	C	407	CN3	C1'-O1'-P'-O2'
16	C	407	CN3	C1'-O1'-P'-O4'
16	C	407	CN3	CA-O3'-P'-O2'
16	C	407	CN3	O52-C51-O51-C2'
16	C	407	CN3	C52-C51-O51-C2'
16	N	401	CN3	O52-C51-O51-C2'
16	N	401	CN3	CA-CB-CC-O13
18	P	302	6PH	O21-C2-C3-O31
18	P	302	6PH	O22-C21-O21-C2
18	P	302	6PH	C22-C21-O21-C2
15	C	406	CN5	O32-C31-O31-C3
16	N	401	CN3	O32-C31-O31-C3
12	N	404	8PE	C32-C31-O31-C3
15	C	406	CN5	C32-C31-O31-C3
16	C	407	CN3	C42-C41-O41-C3'
16	N	401	CN3	C32-C31-O31-C3
16	N	401	CN3	C52-C51-O51-C2'
15	C	406	CN5	C1'-C2'-C3'-O41
12	N	404	8PE	O32-C31-O31-C3
16	C	407	CN3	O42-C41-O41-C3'
15	C	406	CN5	C3A-C3B-C3C-C3D
15	C	406	CN5	C36-C37-C38-C39
15	C	406	CN5	O42-C41-O41-C3'
11	C	401	UQ6	C14-C16-C17-C18
11	N	405	UQ6	C29-C31-C32-C33
15	C	406	CN5	C42-C41-O41-C3'
12	C	402	8PE	C32-C31-O31-C3
16	C	407	CN3	C32-C31-O31-C3
16	C	407	CN3	OA-CB-CC-O13
16	N	401	CN3	OA-CB-CC-O13

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Mol	Chain	Res	Type	Atoms
12	N	404	8PE	C22-C21-O21-C2
12	C	402	8PE	O32-C31-O31-C3
16	C	407	CN3	O32-C31-O31-C3
16	C	407	CN3	C41-C42-C43-C44
18	L	501	6PH	C31-C32-C33-C34
13	C	403	9PE	C31-C32-C33-C34
13	C	404	9PE	C31-C32-C33-C34
18	L	501	6PH	C21-C22-C23-C24
11	C	401	UQ6	C24-C26-C27-C28
18	P	302	6PH	C31-C32-C33-C34
16	C	407	CN3	O3'-CA-CB-OA
13	C	403	9PE	C1-O11-P-O13
13	C	403	9PE	C11-O13-P-O11
13	C	404	9PE	C1-O11-P-O13
13	C	404	9PE	C11-O13-P-O11
16	C	407	CN3	C1-O11-P-O13
16	C	407	CN3	CC-O13-P-O11
16	C	407	CN3	C1'-O1'-P'-O3'
16	N	401	CN3	C1'-O1'-P'-O3'
16	N	401	CN3	CA-O3'-P'-O1'
16	C	407	CN3	C51-C52-C53-C54
16	C	407	CN3	O3'-CA-CB-CC
12	N	404	8PE	O22-C21-O21-C2
18	P	302	6PH	C32-C31-O31-C3
12	N	404	8PE	C33-C34-C35-C36
16	N	401	CN3	C44-C45-C46-C47
13	C	404	9PE	C24-C25-C26-C27
13	C	404	9PE	C27-C28-C29-C2A
18	L	501	6PH	C38-C39-C3A-C3B
12	N	404	8PE	C35-C36-C37-C38
13	C	404	9PE	C2A-C2B-C2C-C2D
12	C	402	8PE	C32-C33-C34-C35
13	C	404	9PE	C29-C2A-C2B-C2C
16	C	407	CN3	C44-C45-C46-C47
18	P	302	6PH	C35-C36-C37-C38
12	N	404	8PE	C27-C28-C29-C2A
18	L	501	6PH	C27-C28-C29-C2A
13	C	404	9PE	O13-C11-C12-N
13	C	404	9PE	C26-C27-C28-C29
18	P	302	6PH	C39-C3A-C3B-C3C
18	P	302	6PH	O32-C31-O31-C3
13	C	403	9PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	C	403	9PE	C32-C33-C34-C35
13	C	404	9PE	C2C-C2D-C2E-C2F
18	L	501	6PH	C23-C24-C25-C26
18	P	302	6PH	C25-C26-C27-C28
16	C	407	CN3	C21-C22-C23-C24
13	C	403	9PE	C2-C1-O11-P
13	C	403	9PE	C2C-C2D-C2E-C2F
18	P	302	6PH	C28-C29-C2A-C2B
18	L	501	6PH	C24-C25-C26-C27
18	P	302	6PH	C24-C25-C26-C27
15	C	406	CN5	C32-C33-C34-C35
18	P	302	6PH	C26-C27-C28-C29
16	C	407	CN3	C46-C47-C48-C49
15	C	406	CN5	C37-C38-C39-C3A
12	N	404	8PE	O21-C2-C3-O31
12	C	402	8PE	C34-C35-C36-C37
16	C	407	CN3	C42-C43-C44-C45
12	C	402	8PE	C3D-C3E-C3F-C3G
12	C	402	8PE	C11-O13-P-O11
16	C	407	CN3	CA-O3'-P'-O1'
16	N	401	CN3	CC-O13-P-O11
16	C	407	CN3	CB-CC-O13-P
18	L	501	6PH	C2-C1-O11-P
13	C	403	9PE	C2E-C2F-C2G-C2H
13	C	404	9PE	O11-C1-C2-C3
18	P	302	6PH	C2B-C2C-C2D-C2E
12	C	402	8PE	C39-C3A-C3B-C3C
15	C	406	CN5	C35-C36-C37-C38
13	C	404	9PE	C23-C24-C25-C26
16	C	407	CN3	C1-C2-C3-O31
16	C	407	CN3	C1'-C2'-C3'-O41
18	P	302	6PH	C1-C2-C3-O31
16	N	401	CN3	C56-C57-C58-C59
18	P	302	6PH	O31-C31-C32-C33
13	C	403	9PE	C2F-C2G-C2H-C2I
13	C	404	9PE	C3-C2-O21-C21
13	C	403	9PE	C33-C34-C35-C36
13	C	403	9PE	C29-C2A-C2B-C2C
16	N	401	CN3	C42-C41-O41-C3'
18	L	501	6PH	C29-C2A-C2B-C2C
12	N	404	8PE	C3A-C3B-C3C-C3D
12	C	402	8PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
12	N	404	8PE	C1-C2-C3-O31
13	C	403	9PE	C2B-C2C-C2D-C2E
15	C	406	CN5	CC-O13-P-O11
12	C	402	8PE	C36-C37-C38-C39
18	P	302	6PH	C34-C35-C36-C37
16	N	401	CN3	O42-C41-O41-C3'
16	C	407	CN3	C56-C57-C58-C59
13	C	404	9PE	C22-C21-O21-C2
18	L	501	6PH	C2B-C2C-C2D-C2E
12	C	402	8PE	C2-C1-O11-P
15	C	406	CN5	C1-C2-C3-O31
12	C	402	8PE	O11-C1-C2-C3
16	N	401	CN3	C54-C55-C56-C57
16	C	407	CN3	C54-C55-C56-C57
13	C	404	9PE	O22-C21-O21-C2
13	C	404	9PE	C34-C35-C36-C37
12	C	402	8PE	C25-C26-C27-C28
12	N	404	8PE	C3E-C3F-C3G-C3H
16	N	401	CN3	C47-C48-C49-C4A
16	C	407	CN3	C2-C1-O11-P
13	C	403	9PE	O11-C1-C2-O21
13	C	403	9PE	C27-C28-C29-C2A
18	P	302	6PH	C22-C23-C24-C25
16	C	407	CN3	O21-C2-C3-O31
16	C	407	CN3	O51-C2'-C3'-O41
11	C	401	UQ6	C25-C24-C26-C27
13	C	403	9PE	C2A-C2B-C2C-C2D
12	N	404	8PE	C39-C3A-C3B-C3C
15	C	406	CN5	CB-CA-O3'-P'
12	C	402	8PE	C11-O13-P-O14
13	C	403	9PE	C1-O11-P-O12
13	C	403	9PE	C1-O11-P-O14
13	C	403	9PE	C11-O13-P-O14
13	C	404	9PE	C1-O11-P-O12
13	C	404	9PE	C11-O13-P-O14
15	C	406	CN5	C1'-O1'-P'-O4'
16	C	407	CN3	CA-O3'-P'-O4'
16	N	401	CN3	C1'-O1'-P'-O2'
16	N	401	CN3	C1'-O1'-P'-O4'
16	N	401	CN3	CA-O3'-P'-O4'
13	C	403	9PE	C21-C22-C23-C24
13	C	403	9PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	N	401	CN3	C52-C53-C54-C55
16	C	407	CN3	C22-C21-O21-C2
12	N	404	8PE	C12-C11-O13-P
13	C	403	9PE	C12-C11-O13-P
11	C	401	UQ6	C15-C14-C16-C17
13	C	404	9PE	O11-C1-C2-O21
13	C	404	9PE	C33-C34-C35-C36
16	C	407	CN3	O22-C21-O21-C2
12	N	404	8PE	C32-C33-C34-C35
11	N	405	UQ6	C24-C26-C27-C28
16	C	407	CN3	CA-CB-CC-O13
18	L	501	6PH	O32-C31-O31-C3
11	C	401	UQ6	C23-C24-C26-C27
12	C	402	8PE	C1-O11-P-O13
12	N	404	8PE	C1-O11-P-O13
15	C	406	CN5	C1-O11-P-O13
15	C	406	CN5	CA-O3'-P'-O1'
16	N	401	CN3	C48-C49-C4A-C4B
13	C	404	9PE	C2F-C2G-C2H-C2I
18	L	501	6PH	C32-C31-O31-C3
16	N	401	CN3	C21-C22-C23-C24
18	P	302	6PH	O32-C31-C32-C33
16	N	401	CN3	C55-C56-C57-C58
13	C	404	9PE	C25-C26-C27-C28
11	N	405	UQ6	C6-C7-C8-C9
16	N	401	CN3	C1-C2-O21-C21
14	C	405	HEM	CAD-CBD-CGD-O1D
14	N	402	HEM	CAD-CBD-CGD-O1D
16	N	401	CN3	O1'-C1'-C2'-O51
12	N	404	8PE	C24-C25-C26-C27
14	N	402	HEM	CAD-CBD-CGD-O2D
14	C	405	HEM	CAD-CBD-CGD-O2D
14	C	405	HEM	CAA-CBA-CGA-O2A
15	C	406	CN5	C3C-C3D-C3E-C3F
11	N	405	UQ6	C30-C29-C31-C32
16	N	401	CN3	O1'-C1'-C2'-C3'
12	C	402	8PE	C38-C39-C3A-C3B
13	C	404	9PE	O21-C2-C3-O31
14	C	405	HEM	CAA-CBA-CGA-O1A
16	C	407	CN3	O41-C41-C42-C43
12	N	404	8PE	C23-C24-C25-C26
18	P	302	6PH	C1-O11-P-O13

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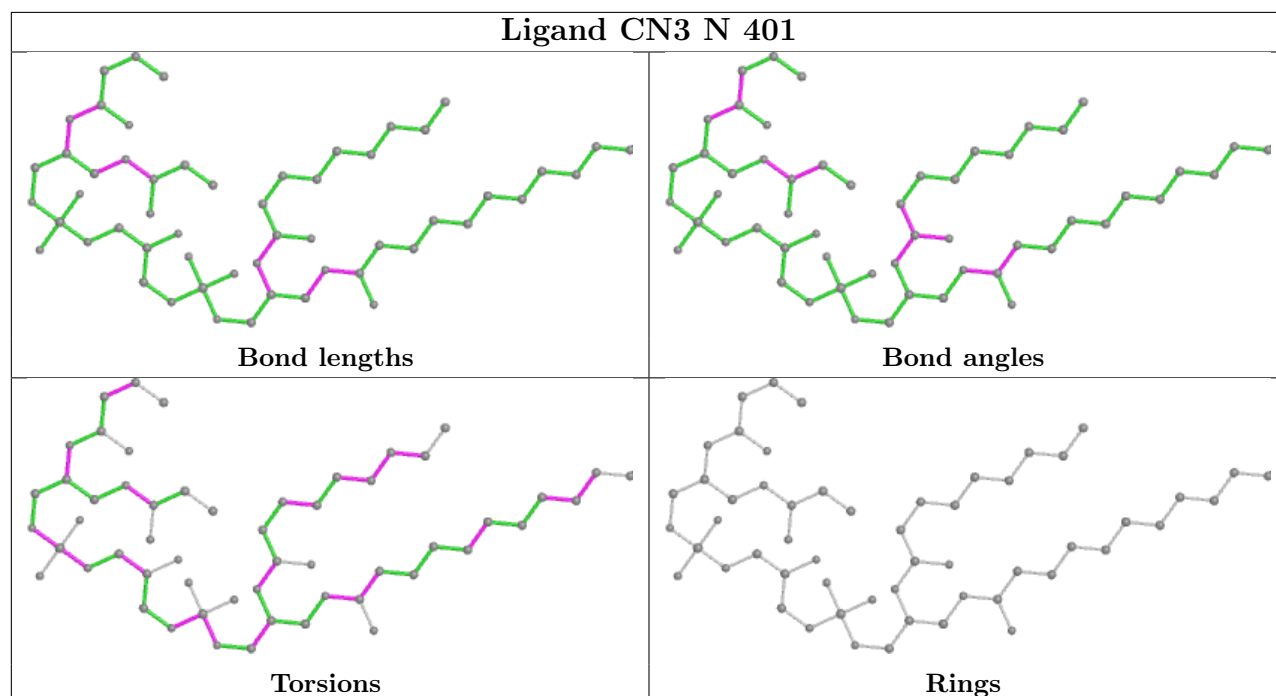
Mol	Chain	Res	Type	Atoms
11	N	405	UQ6	C15-C14-C16-C17
11	C	401	UQ6	C13-C14-C16-C17
16	C	407	CN3	C3-C2-O21-C21
16	C	407	CN3	C3'-C2'-O51-C51
14	C	408	HEM	CAA-CBA-CGA-O2A
12	N	404	8PE	O31-C31-C32-C33
13	C	403	9PE	C1-C2-C3-O31
14	N	402	HEM	CAA-CBA-CGA-O2A
12	C	402	8PE	C2B-C2C-C2D-C2E
14	N	402	HEM	CAA-CBA-CGA-O1A
14	C	408	HEM	CAA-CBA-CGA-O1A
14	C	405	HEM	C3D-CAD-CBD-CGD
14	N	402	HEM	C3D-CAD-CBD-CGD
16	C	407	CN3	O11-C1-C2-C3
14	N	403	HEM	CAA-CBA-CGA-O2A
13	C	403	9PE	O21-C2-C3-O31
13	C	404	9PE	C32-C33-C34-C35
18	P	302	6PH	C36-C37-C38-C39
14	N	403	HEM	CAA-CBA-CGA-O1A
12	N	404	8PE	O32-C31-C32-C33
18	L	501	6PH	O31-C31-C32-C33
11	C	401	UQ6	C6-C7-C8-C9
18	L	501	6PH	C34-C35-C36-C37
11	C	401	UQ6	C11-C12-C13-C14
18	L	501	6PH	O32-C31-C32-C33
16	C	407	CN3	O42-C41-C42-C43
14	O	401	HEM	CAD-CBD-CGD-O2D
12	N	404	8PE	C1-O11-P-O12
13	C	404	9PE	C11-O13-P-O12
16	C	407	CN3	C1-O11-P-O14
16	N	401	CN3	C1-O11-P-O14
14	D	401	HEM	CAA-CBA-CGA-O2A
13	C	403	9PE	O31-C31-C32-C33
13	C	404	9PE	C12-C11-O13-P
18	P	302	6PH	C32-C33-C34-C35
11	N	405	UQ6	C28-C29-C31-C32
16	N	401	CN3	O41-C41-C42-C43
18	L	501	6PH	O21-C21-C22-C23
14	O	401	HEM	CAD-CBD-CGD-O1D
12	C	402	8PE	O21-C21-C22-C23
14	N	403	HEM	CAD-CBD-CGD-O2D
14	N	403	HEM	CAD-CBD-CGD-O1D

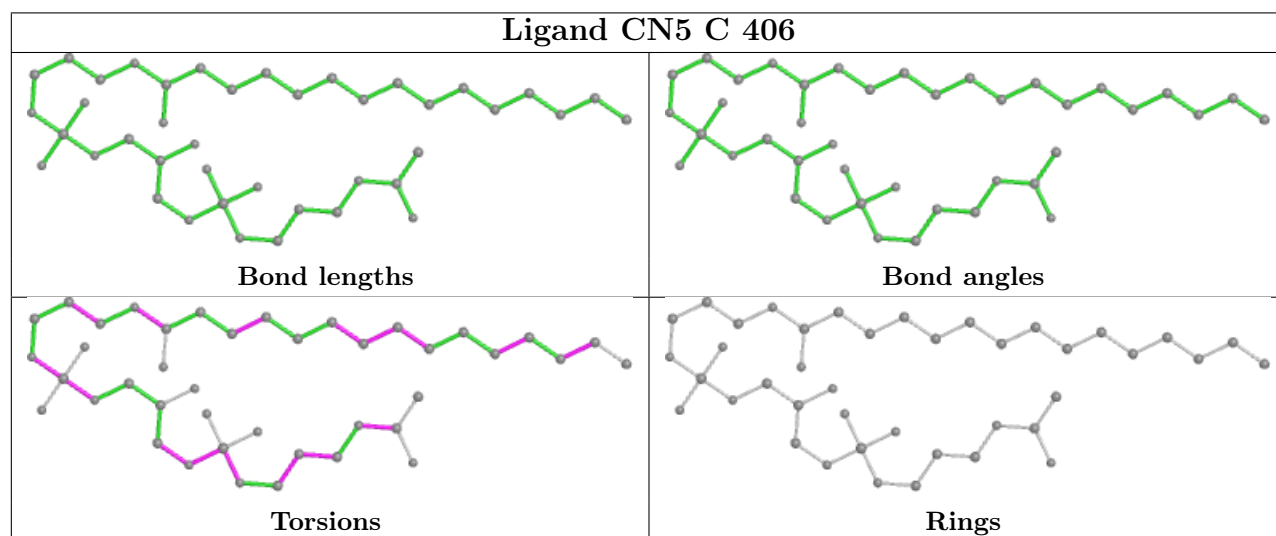
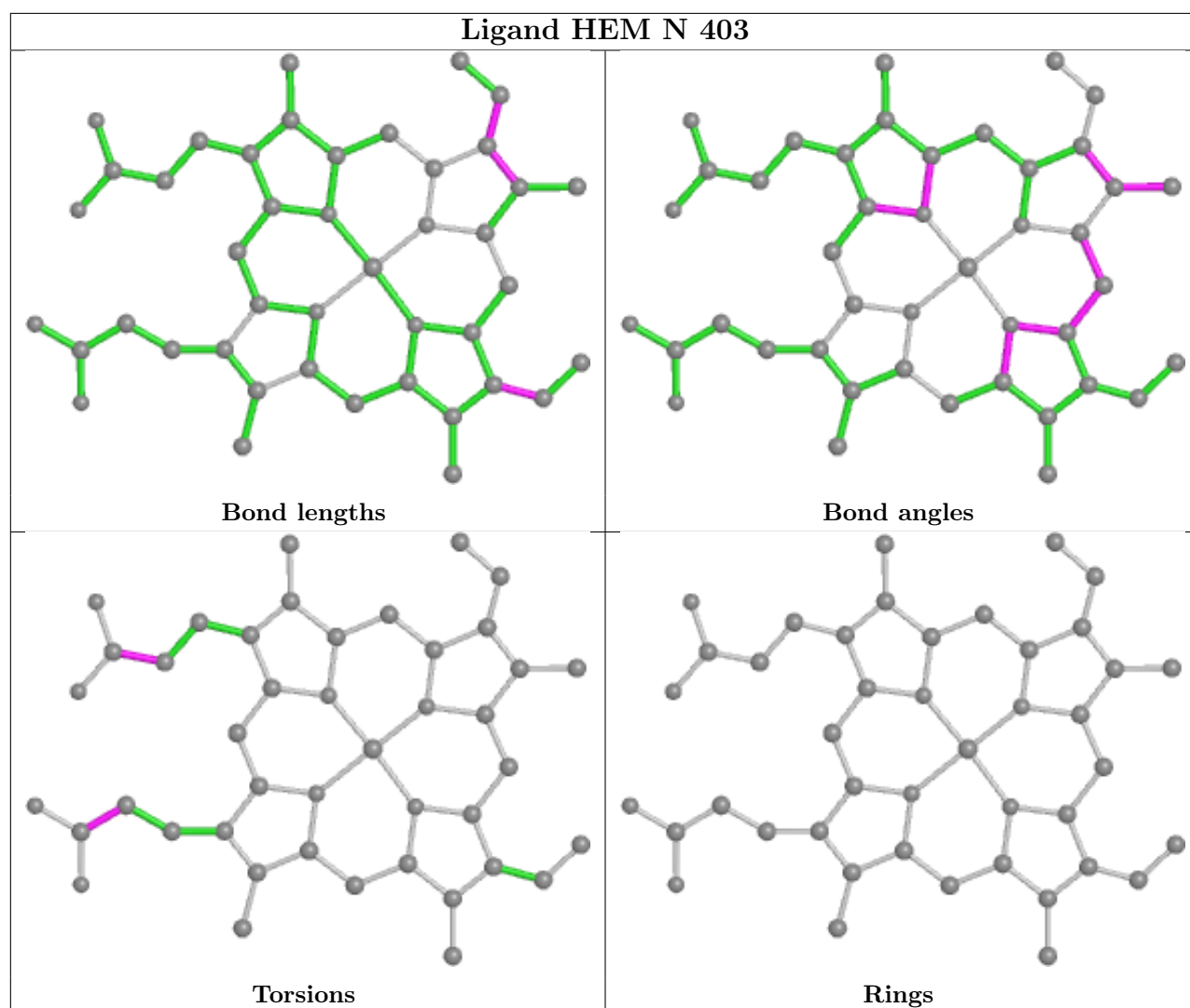
There are no ring outliers.

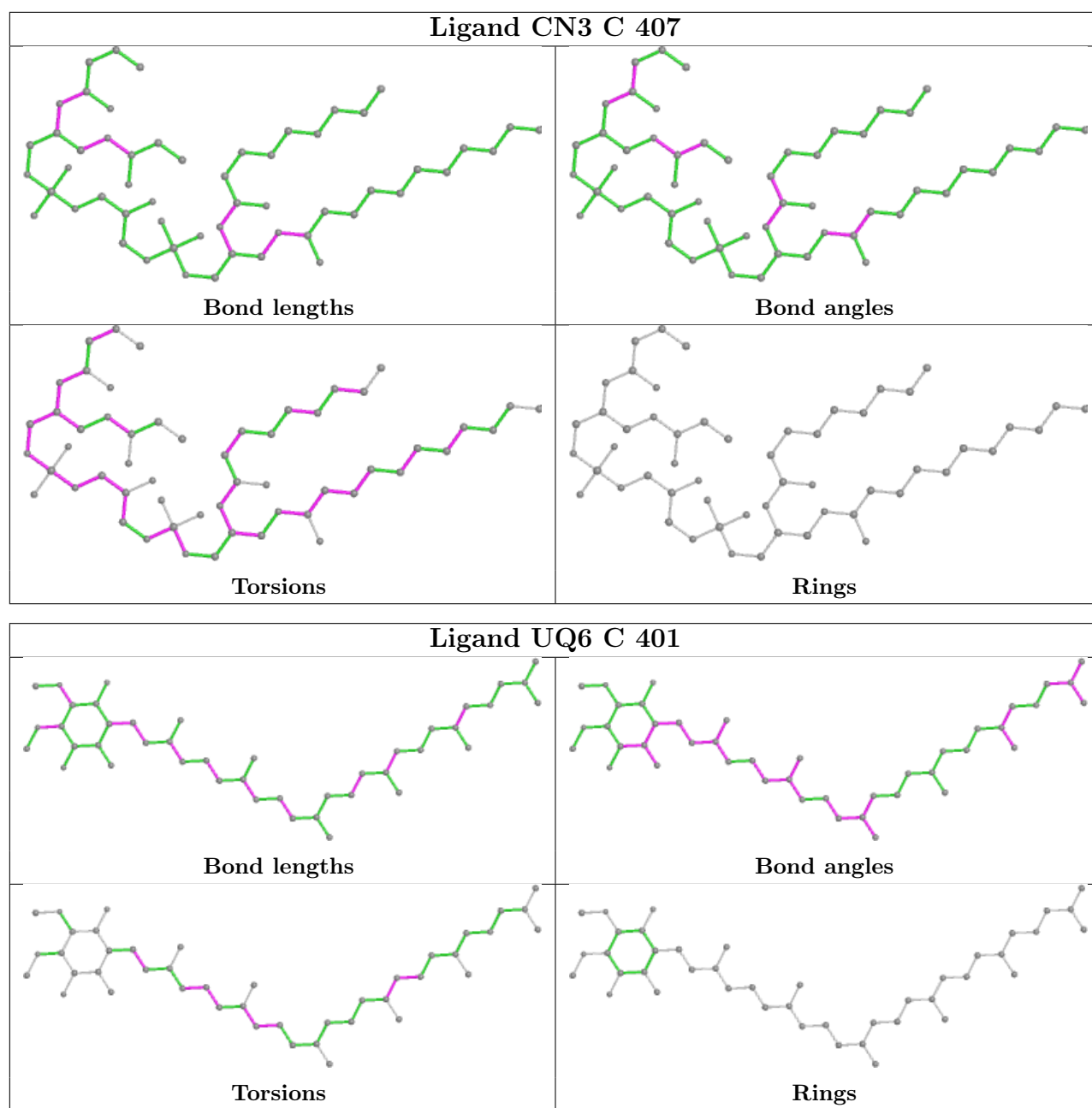
9 monomers are involved in 23 short contacts:

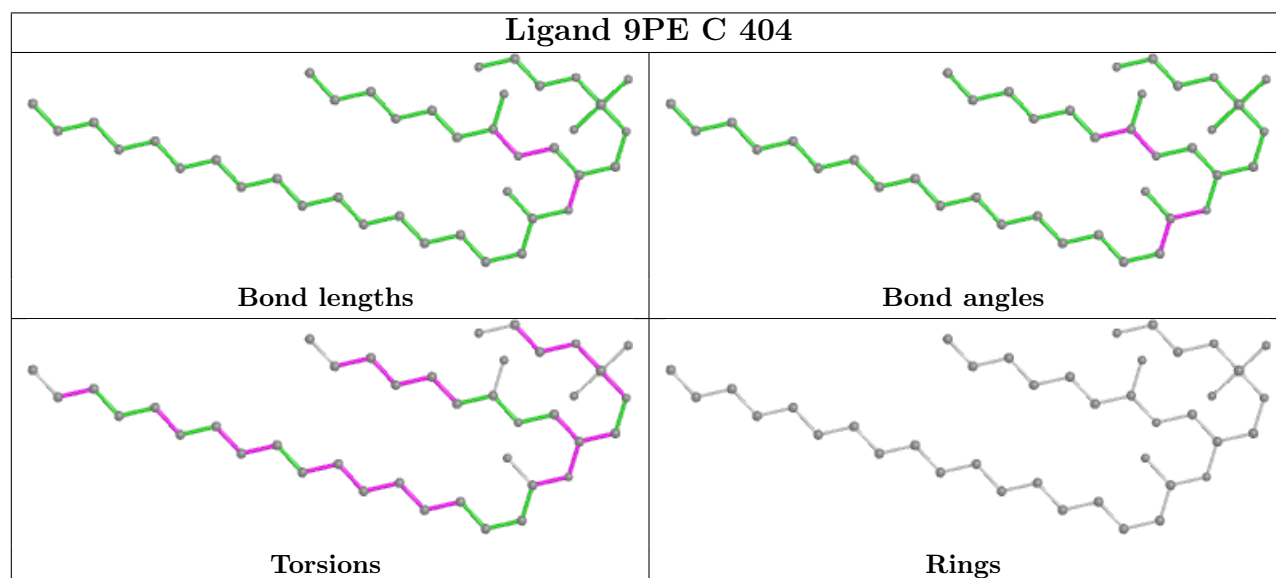
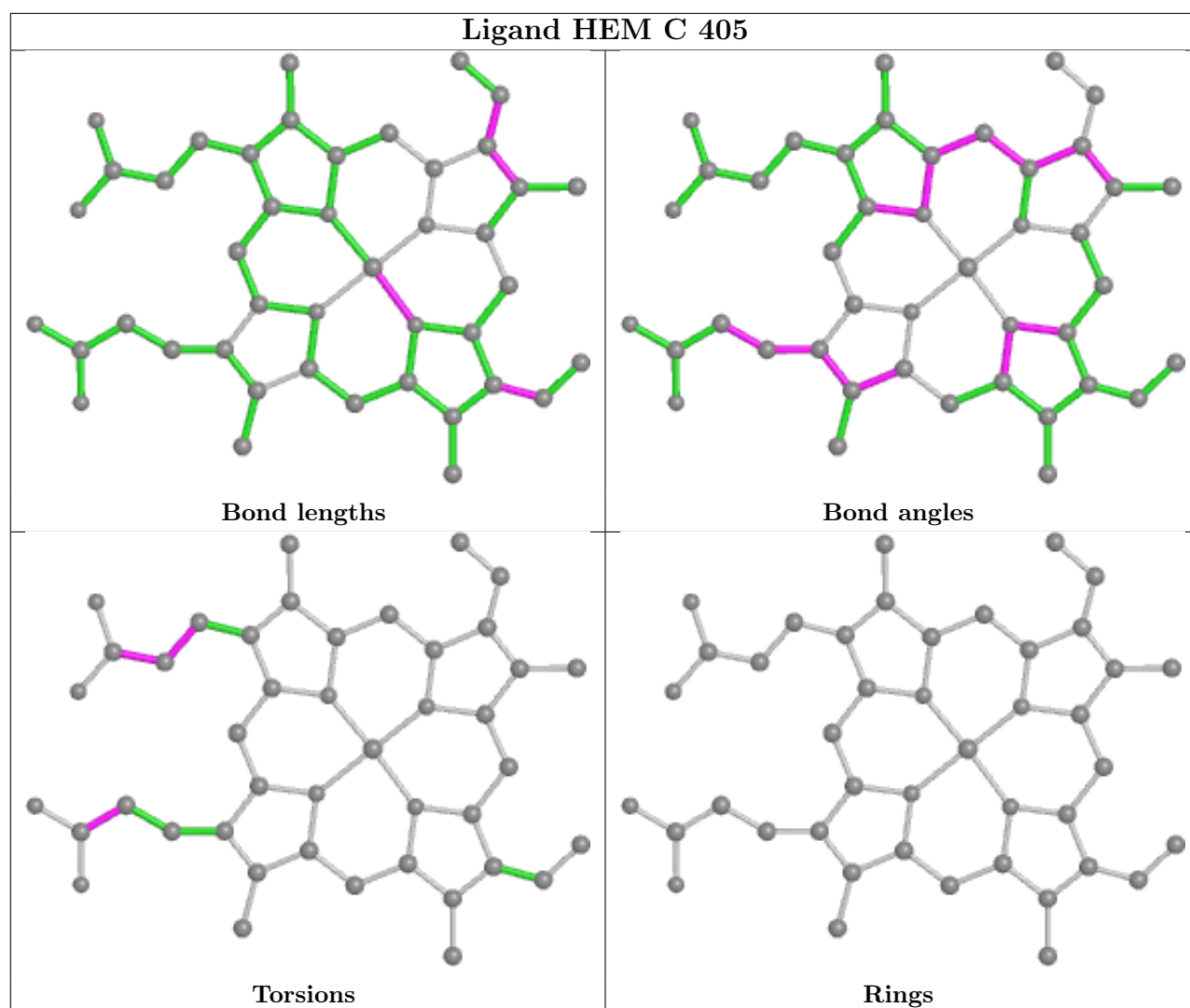
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	403	HEM	1	0
15	C	406	CN5	5	0
14	C	405	HEM	1	0
11	N	405	UQ6	4	0
17	E	301	FES	5	0
17	P	301	FES	3	0
14	O	401	HEM	2	0
14	C	408	HEM	1	0
14	N	402	HEM	1	0

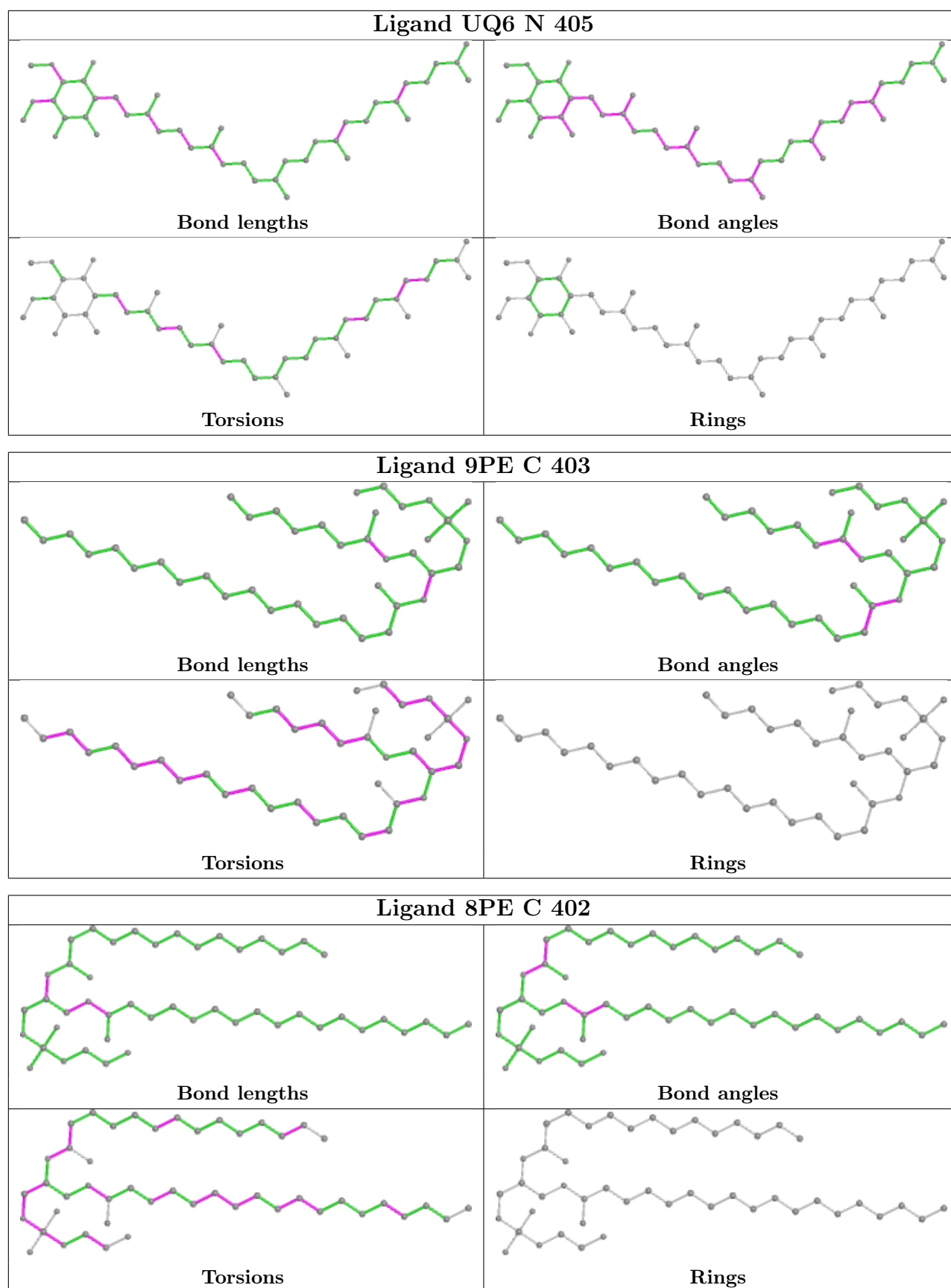
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

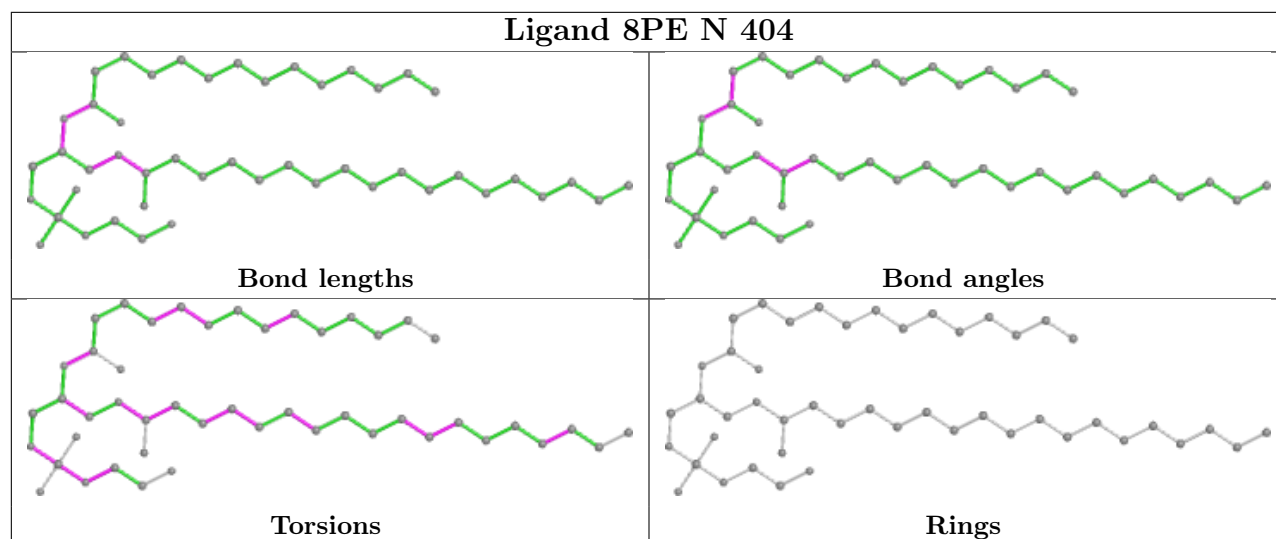
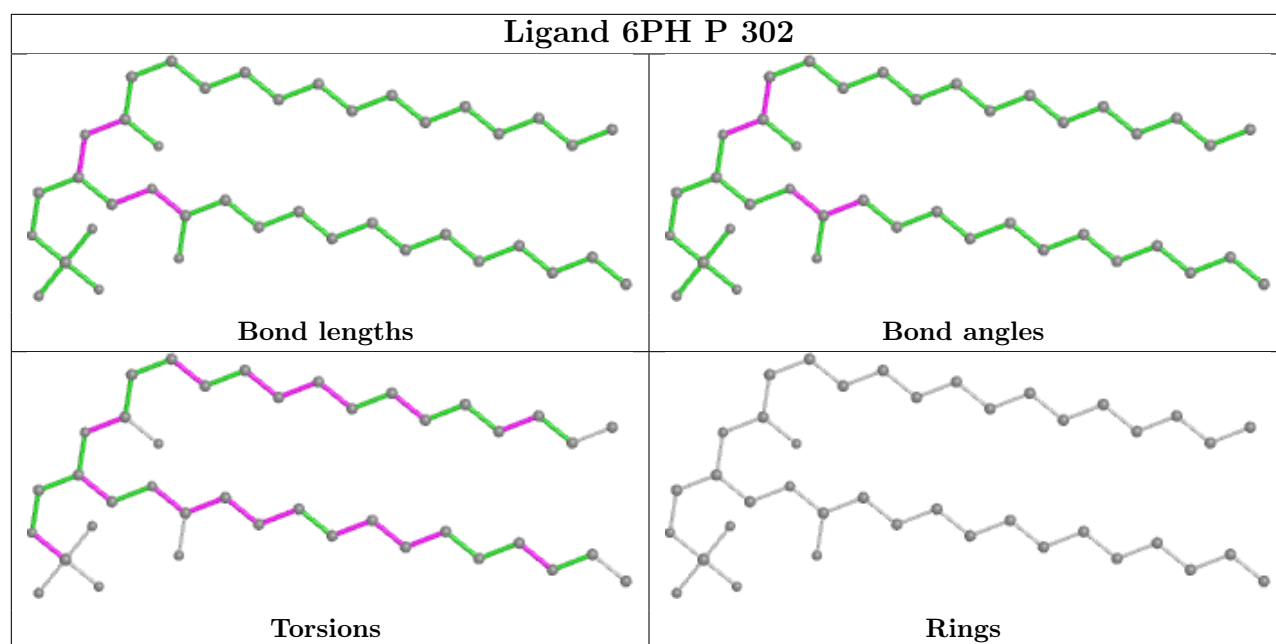


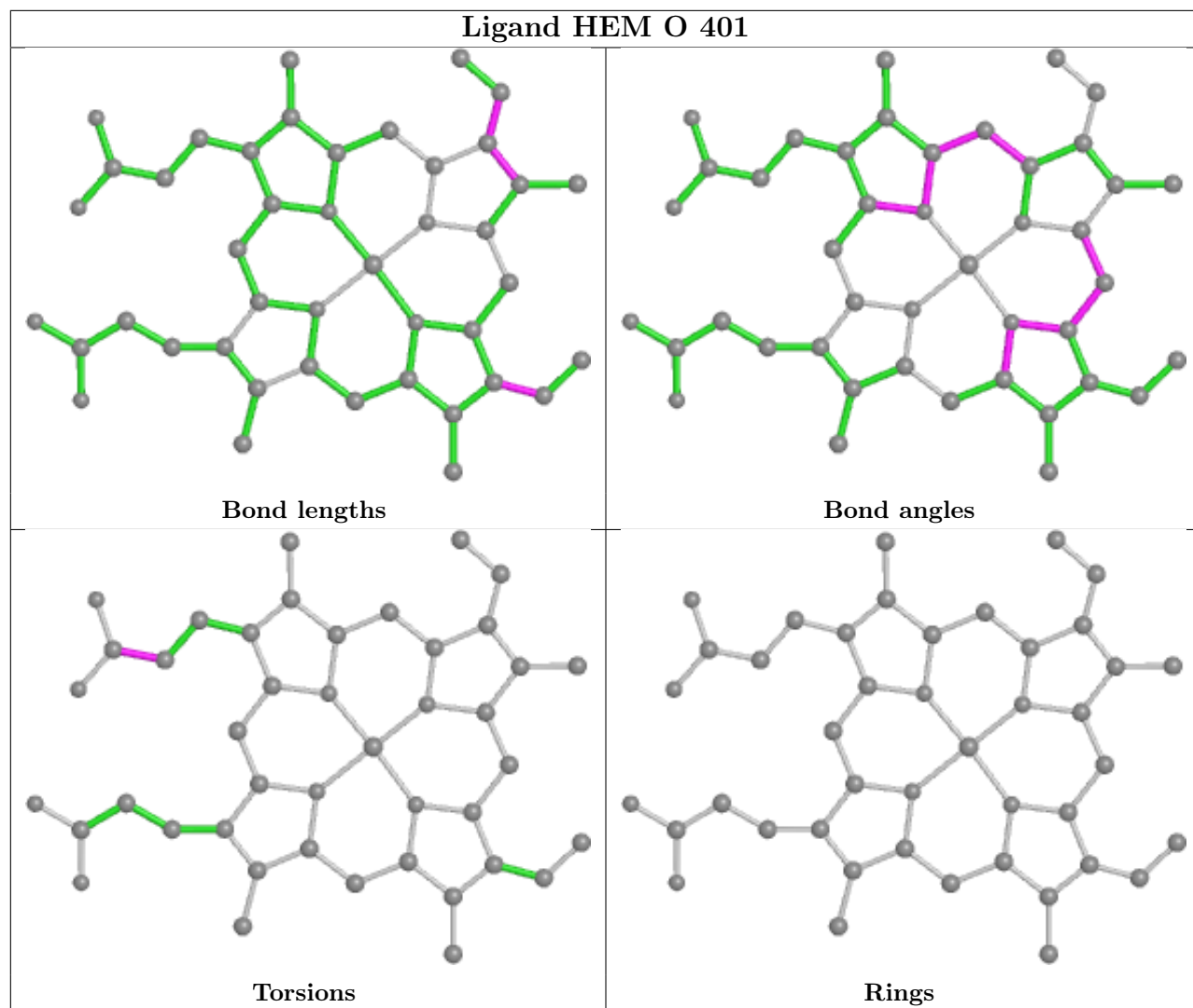


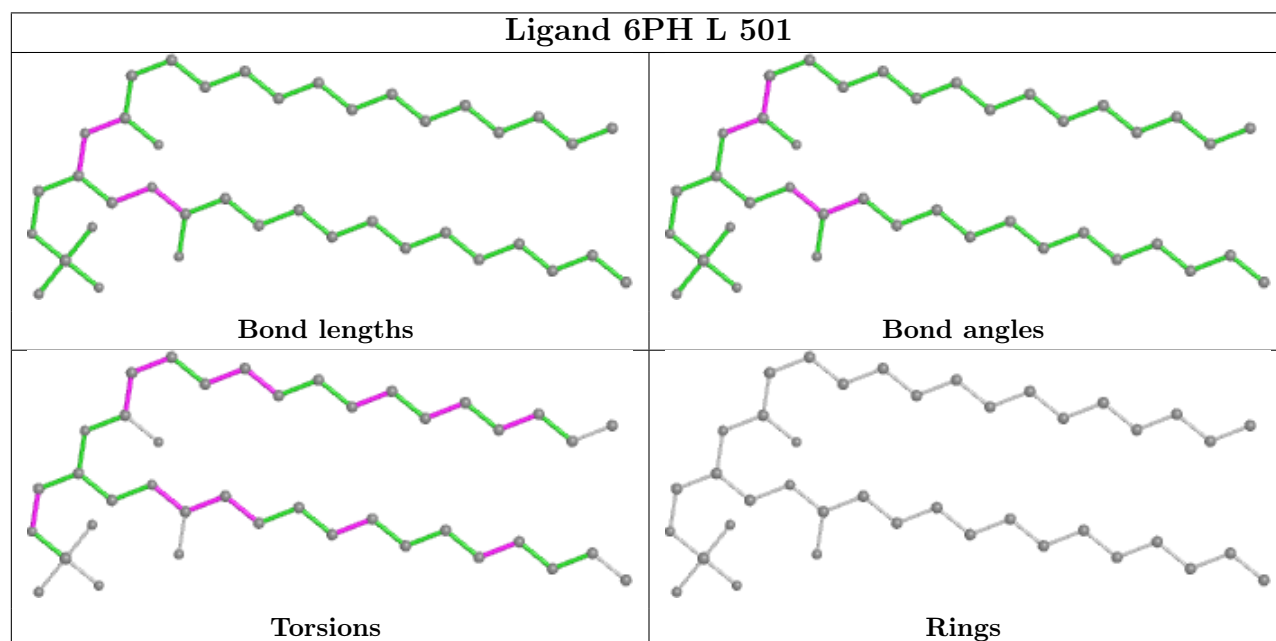
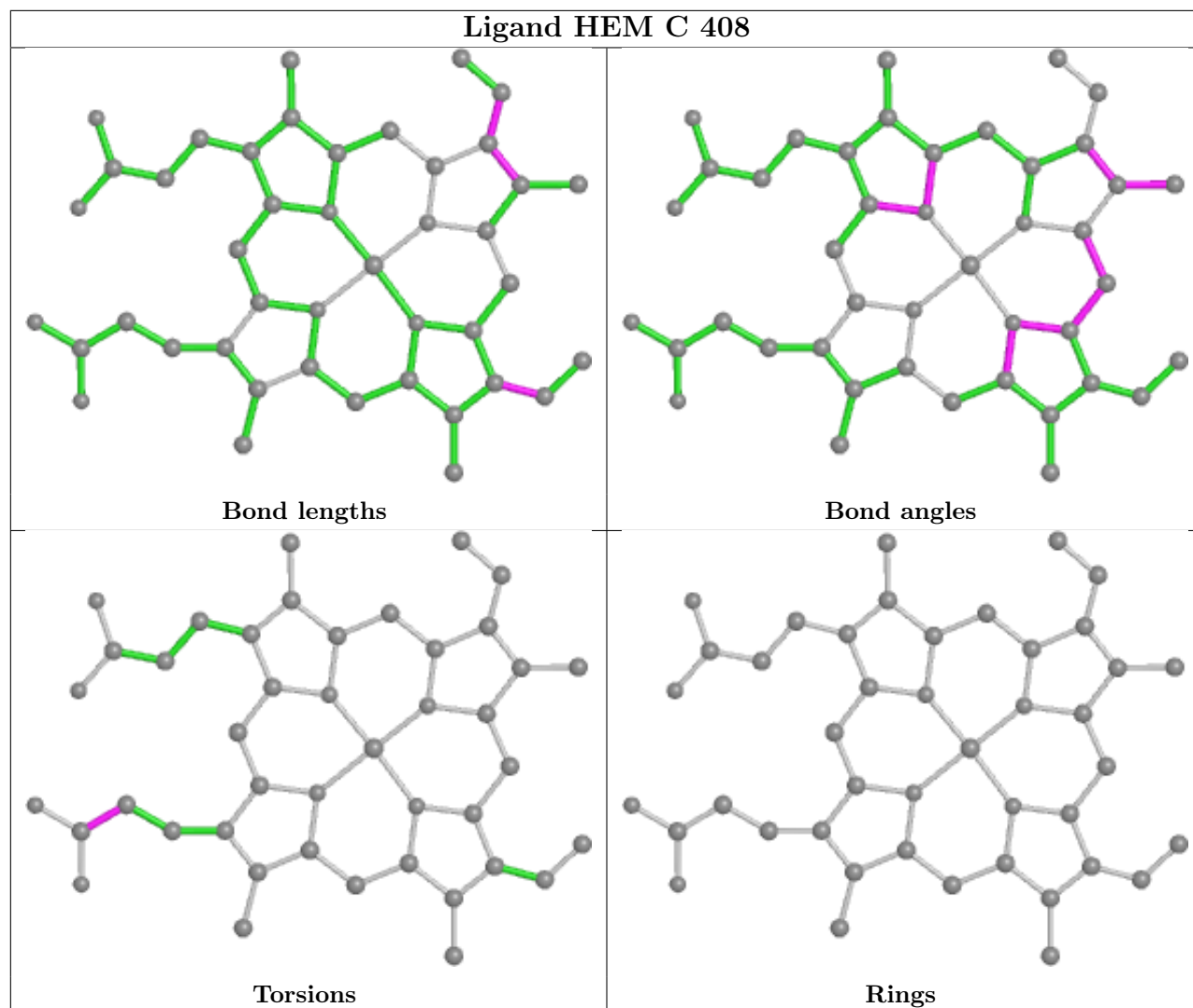


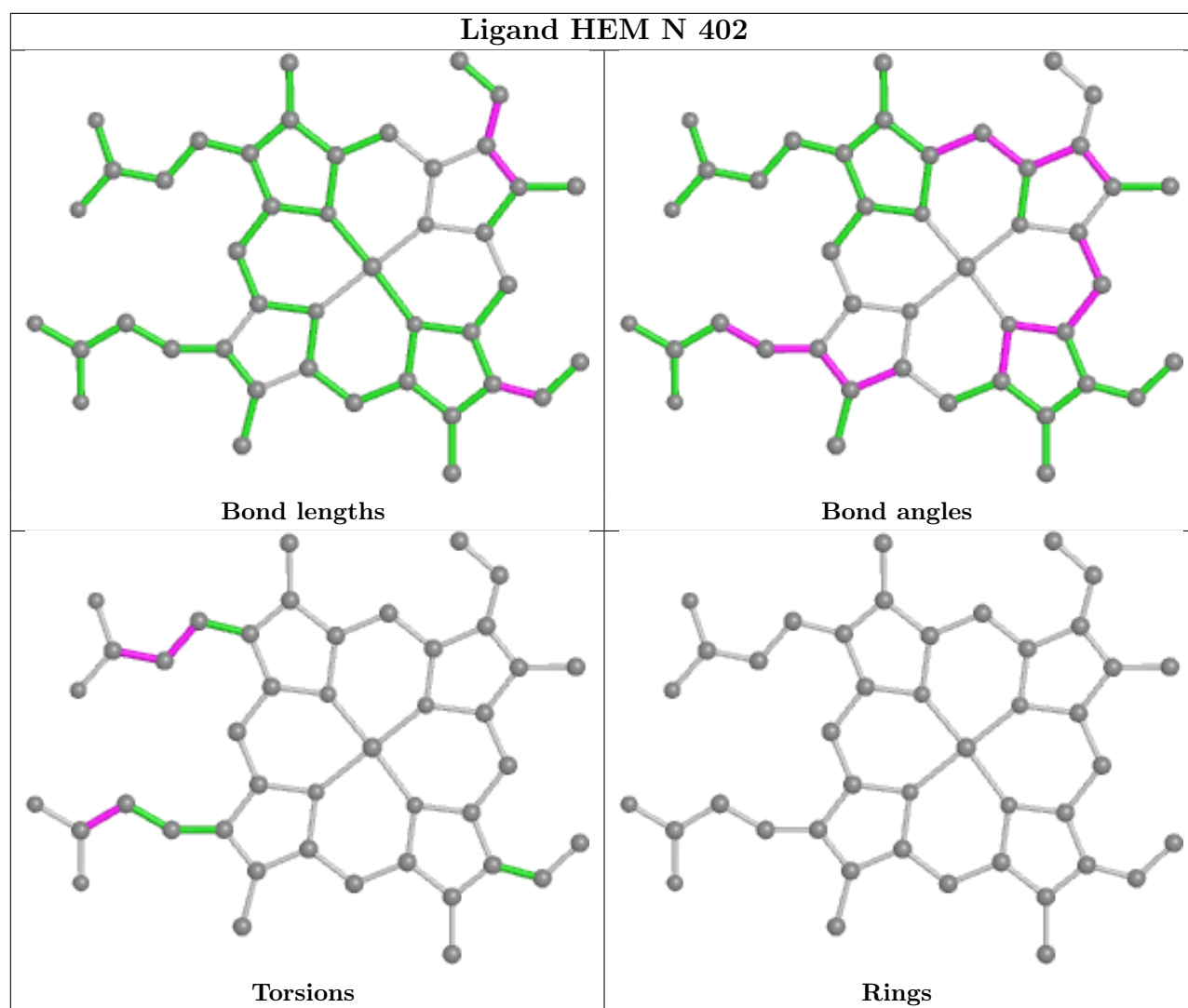


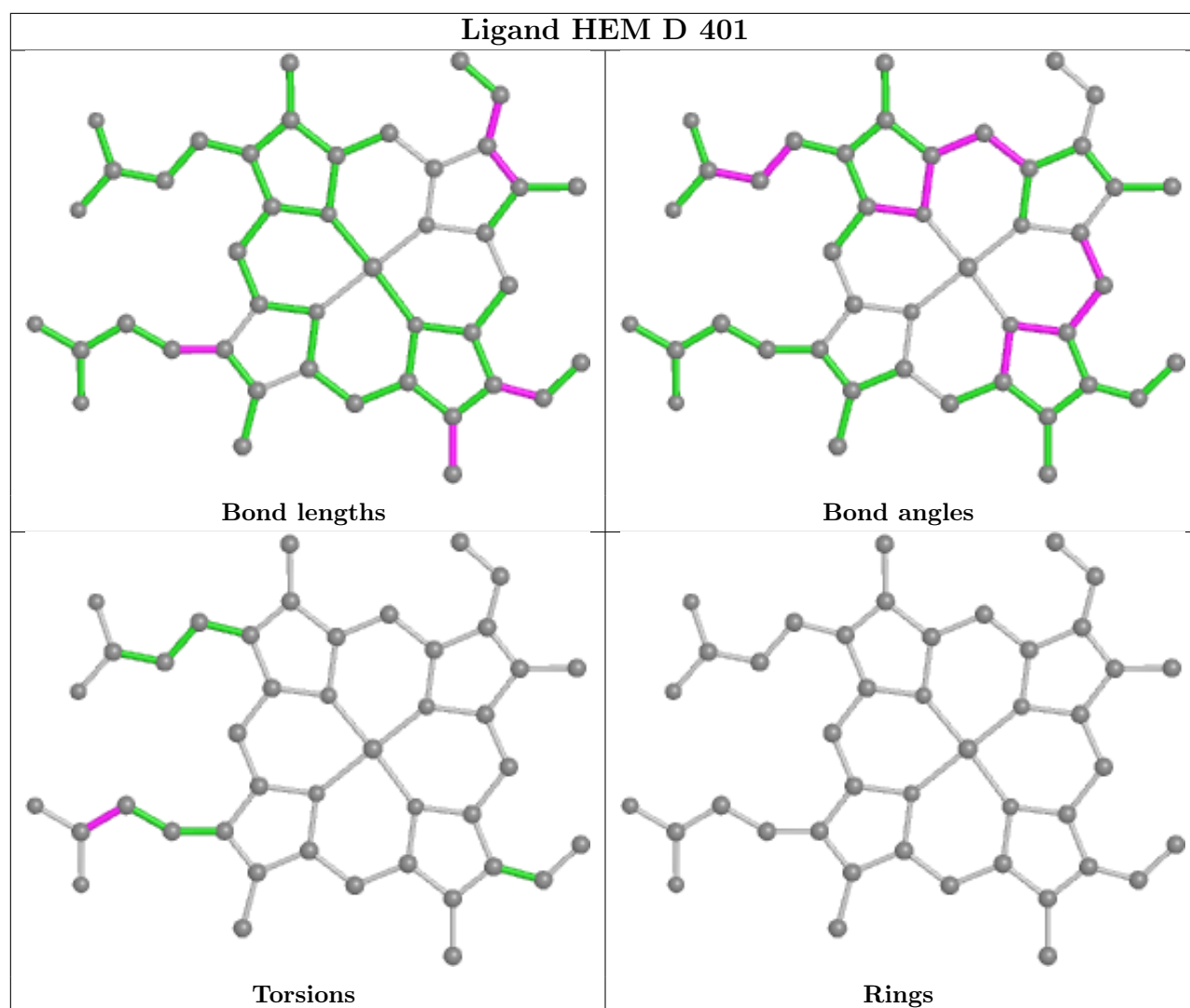












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

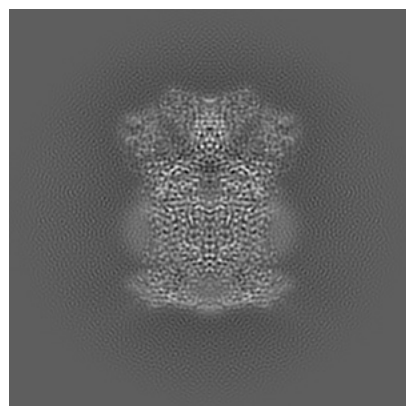
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60140. These allow visual inspection of the internal detail of the map and identification of artifacts.

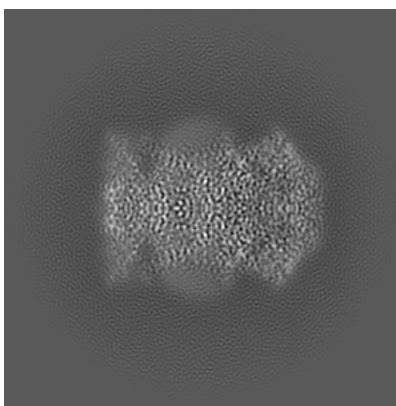
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

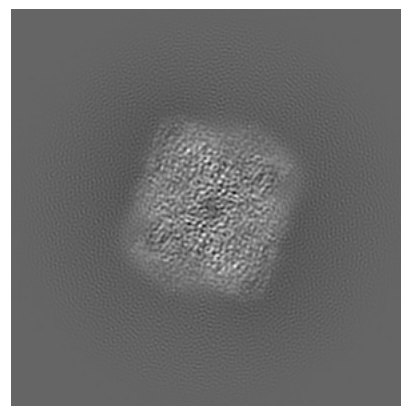
6.1.1 Primary map



X

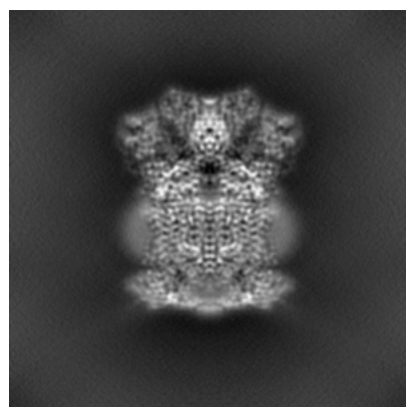


Y

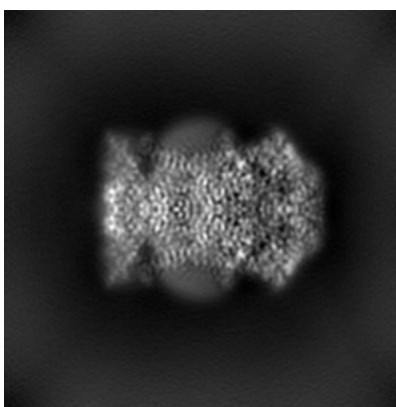


Z

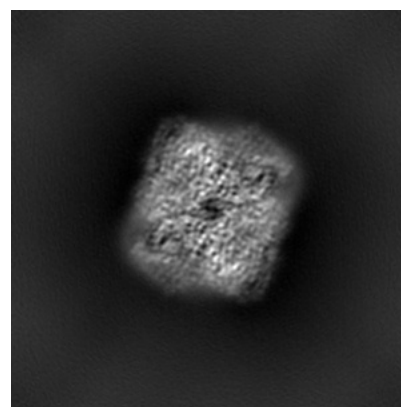
6.1.2 Raw map



X



Y

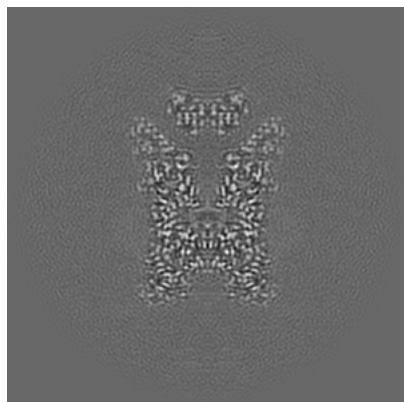


Z

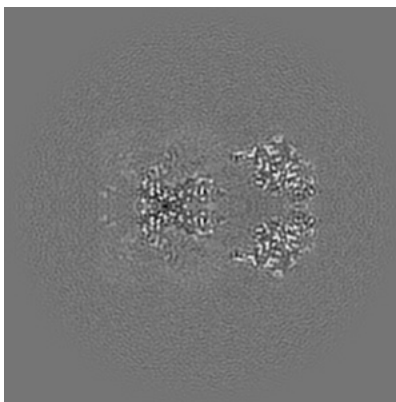
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

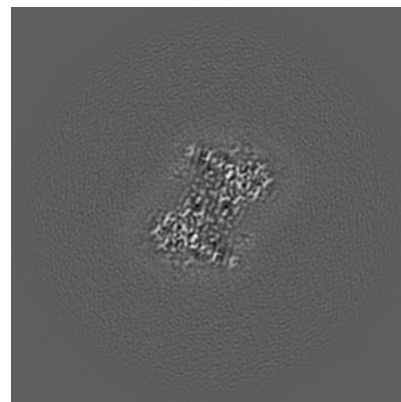
6.2.1 Primary map



X Index: 140

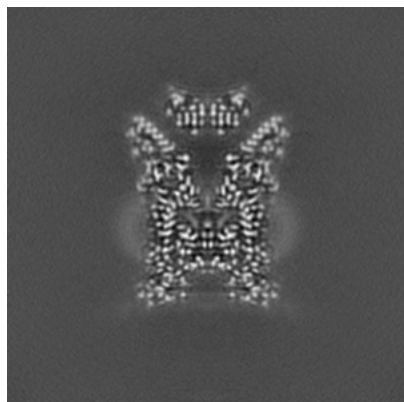


Y Index: 140

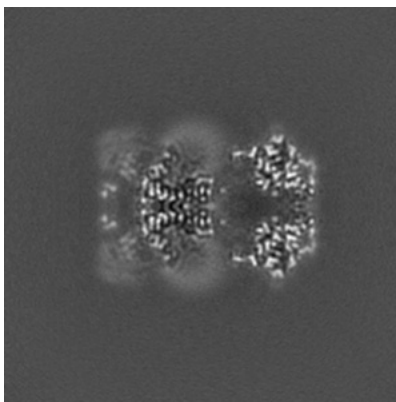


Z Index: 140

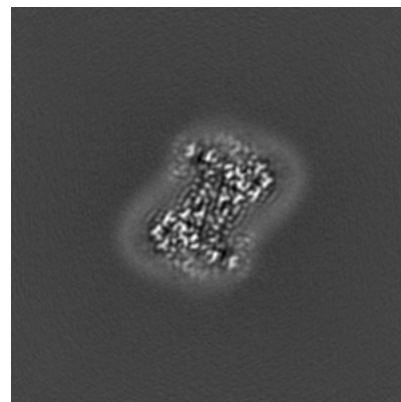
6.2.2 Raw map



X Index: 140



Y Index: 140

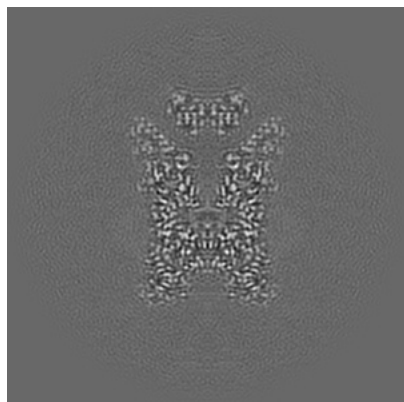


Z Index: 140

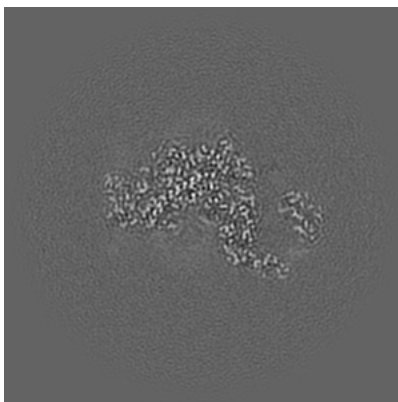
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

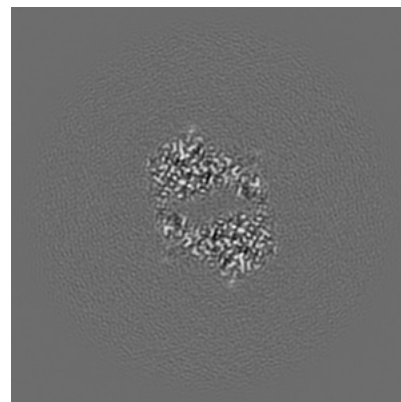
6.3.1 Primary map



X Index: 140

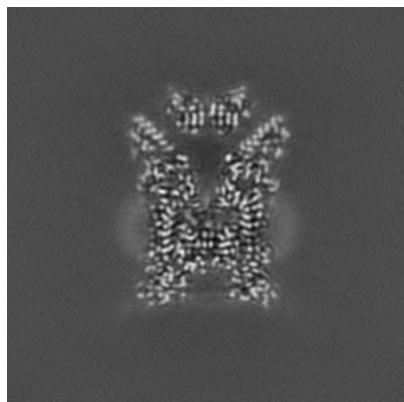


Y Index: 158

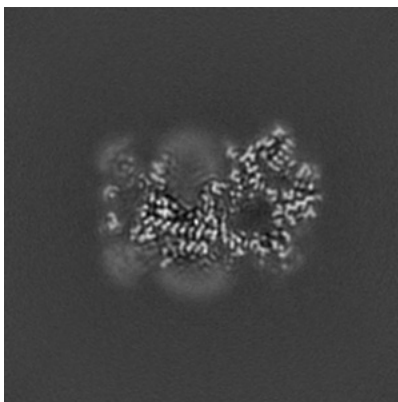


Z Index: 167

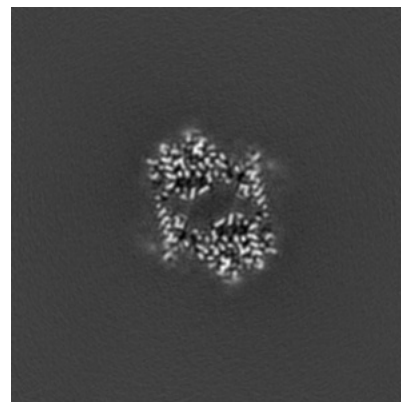
6.3.2 Raw map



X Index: 139



Y Index: 131

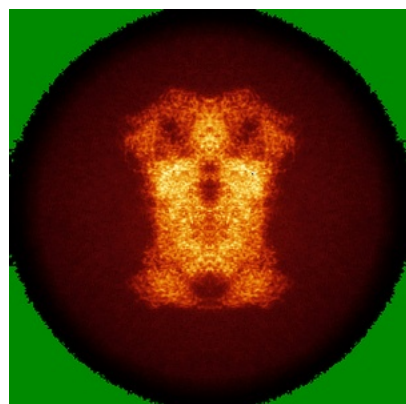


Z Index: 165

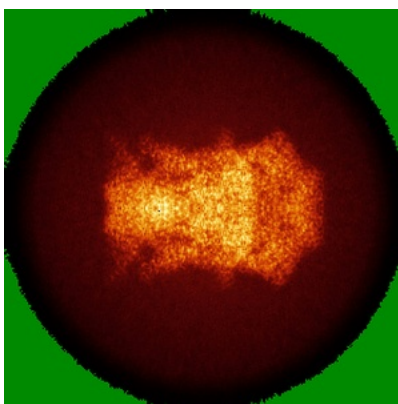
The images above show the largest variance slices of the map in three orthogonal directions.

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

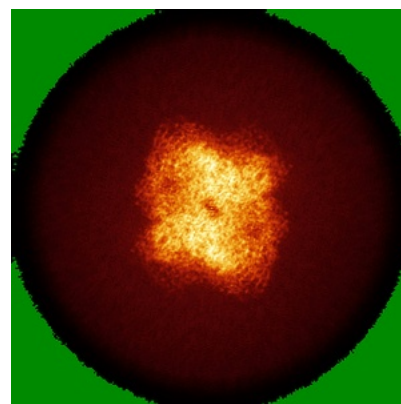
6.4.1 Primary map



X

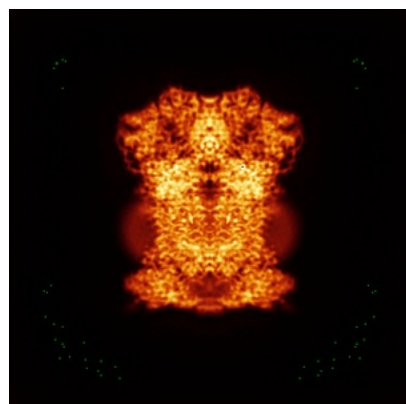


Y

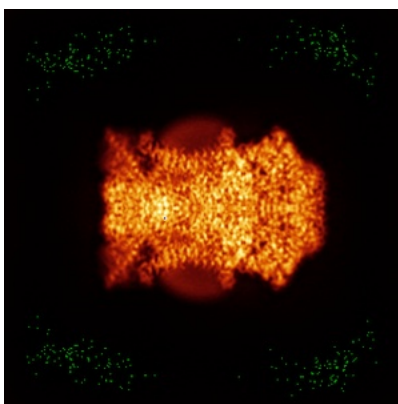


Z

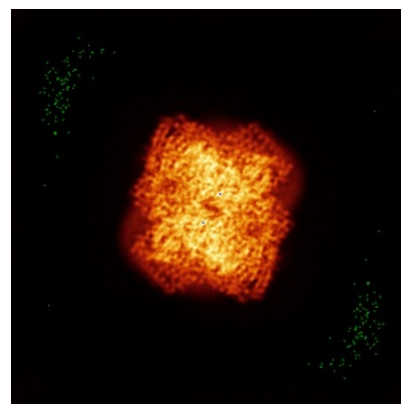
6.4.2 Raw map



X



Y

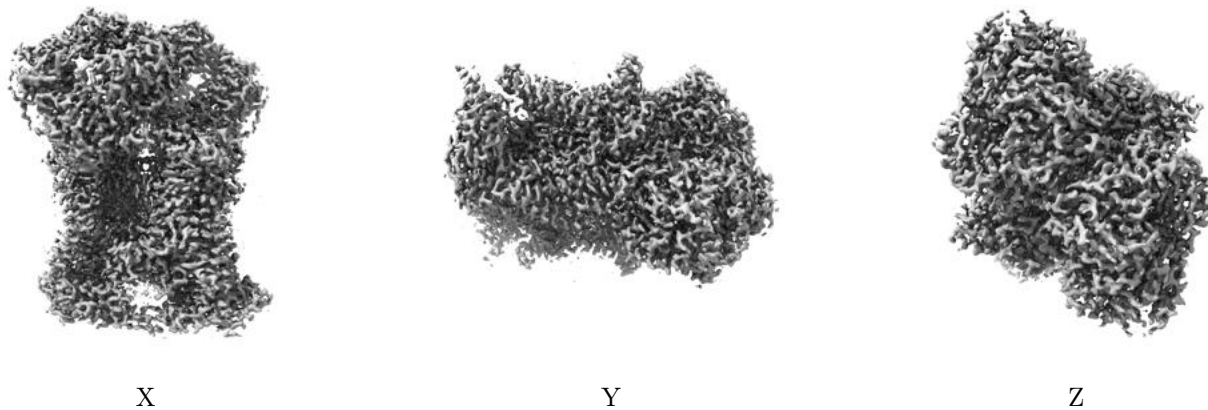


Z

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.

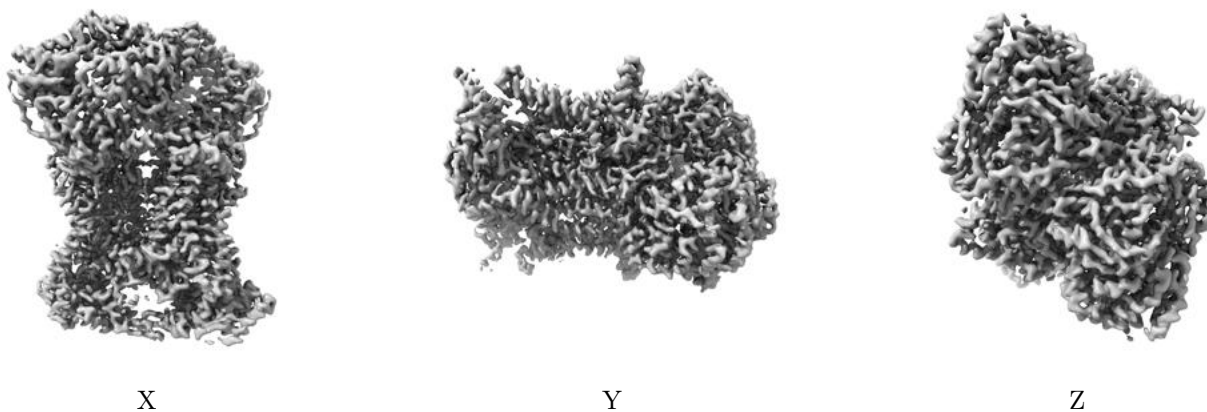
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.906. 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.

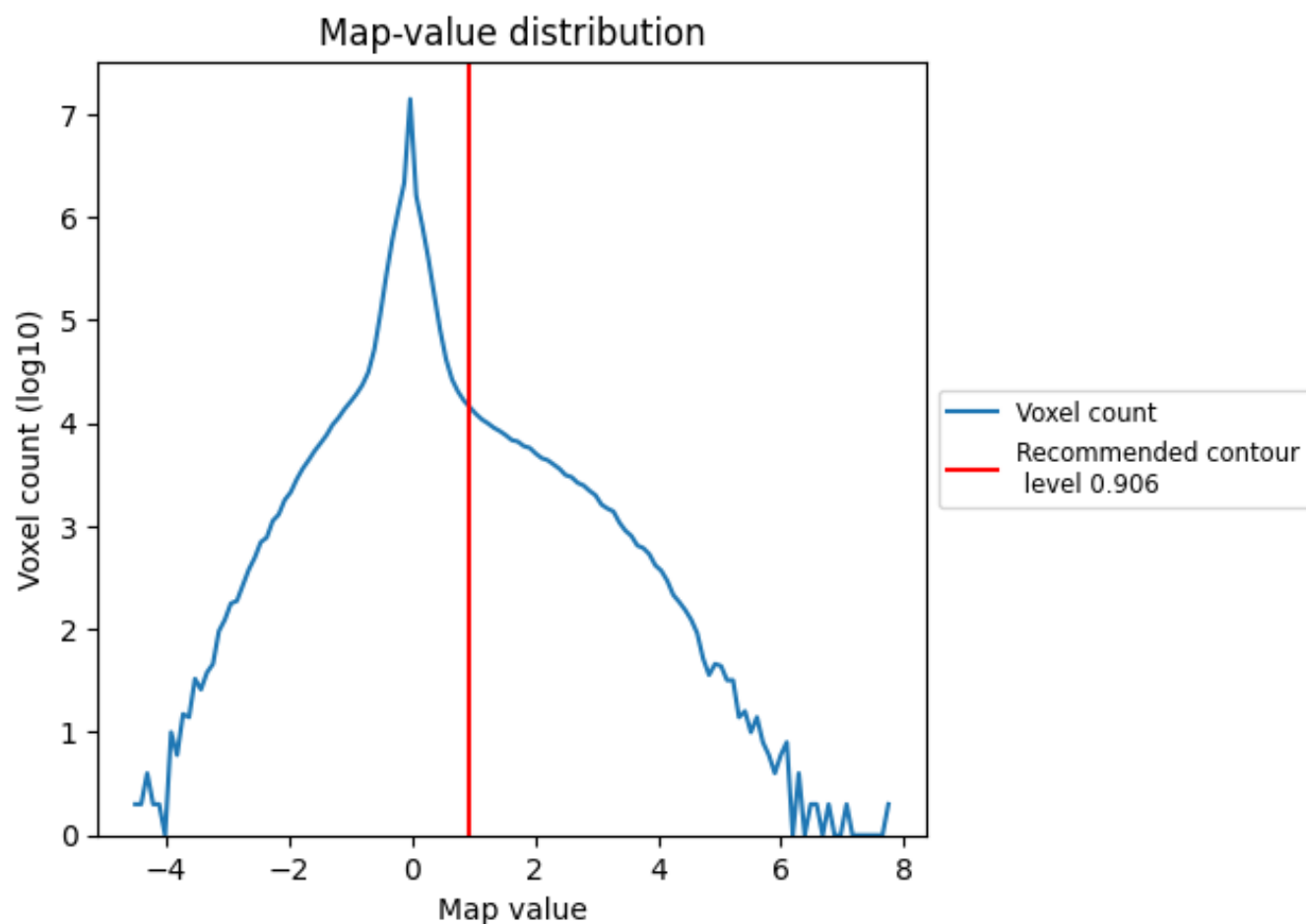
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

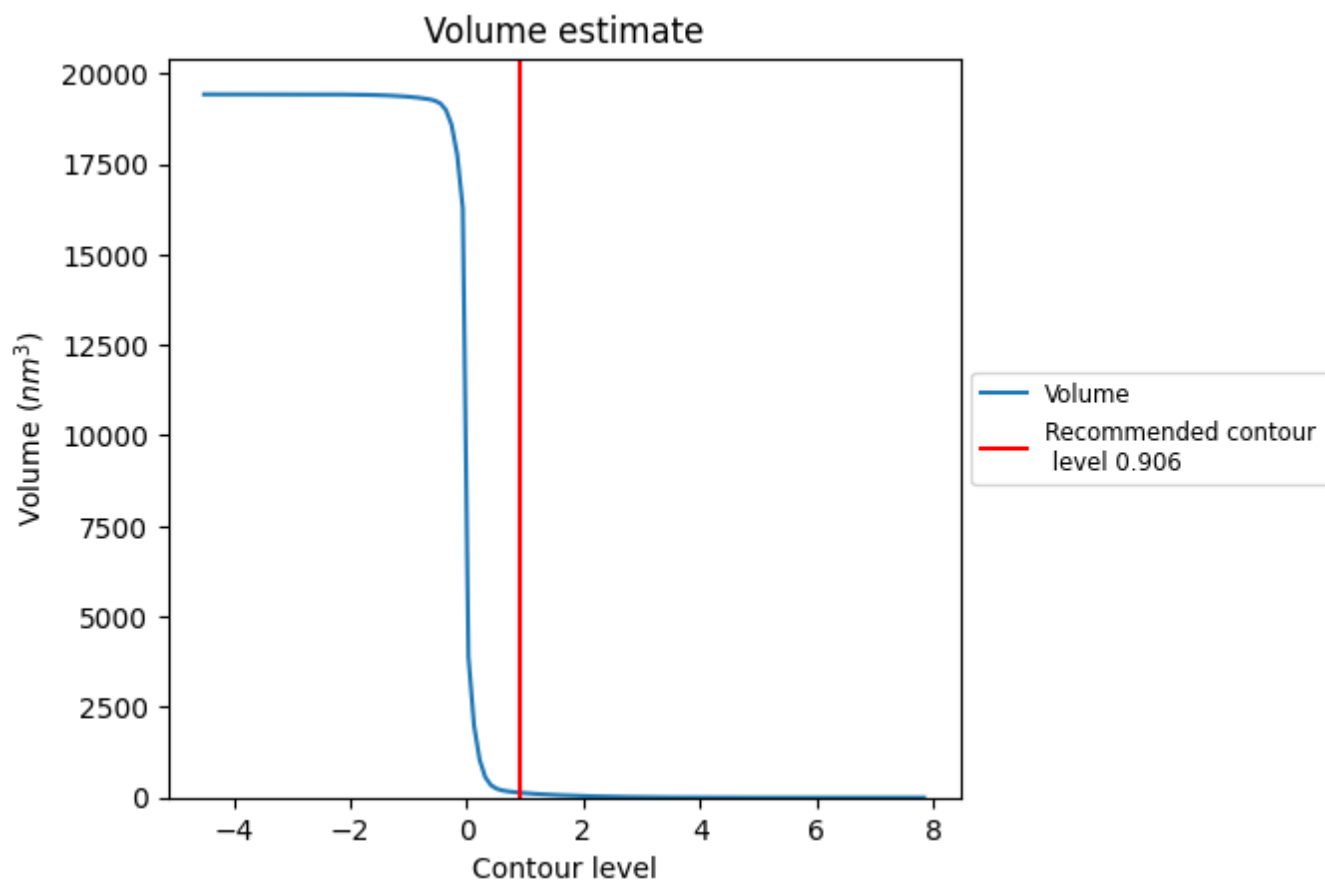
This section contains the results of statistical analysis of the map.

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.

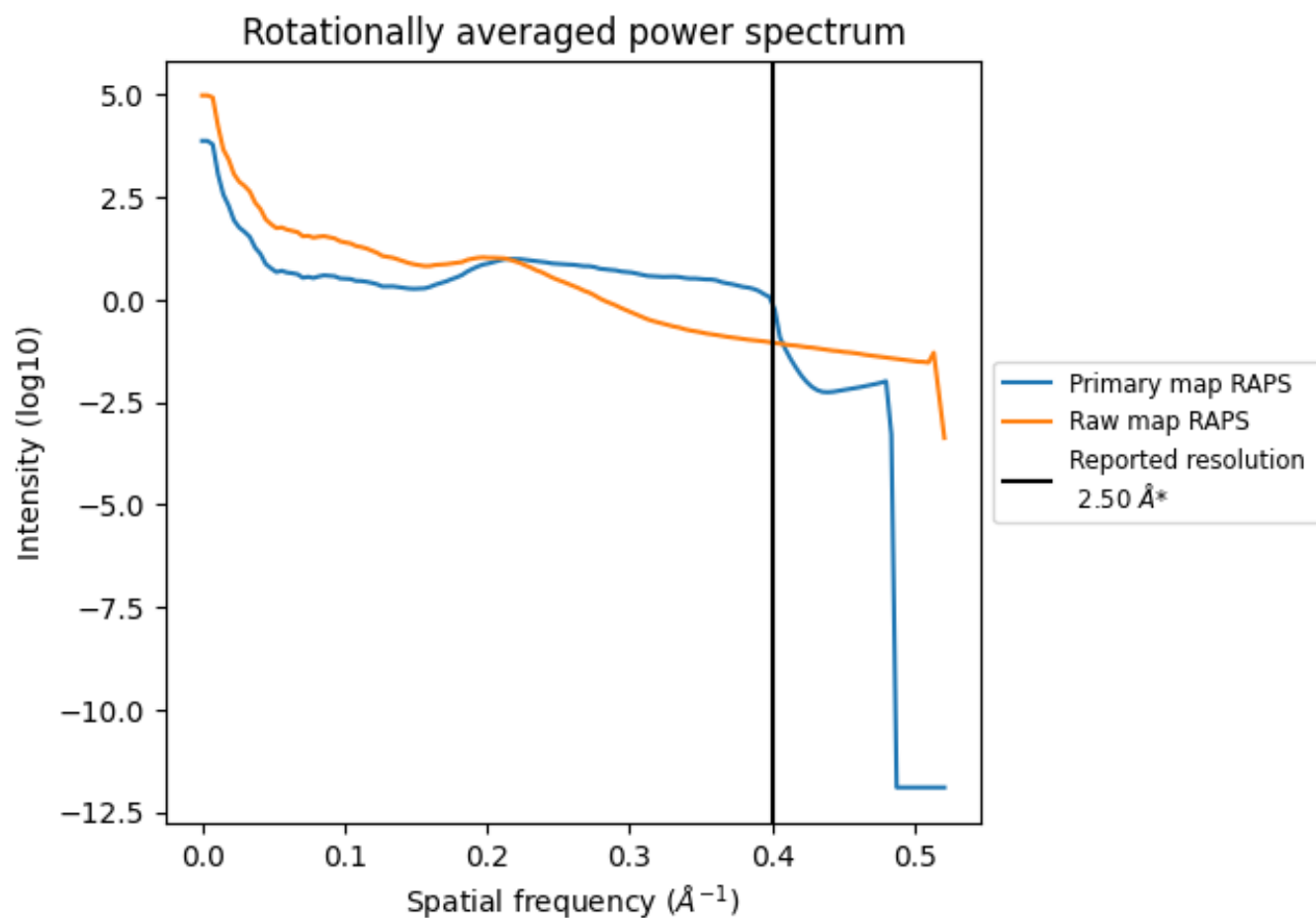
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

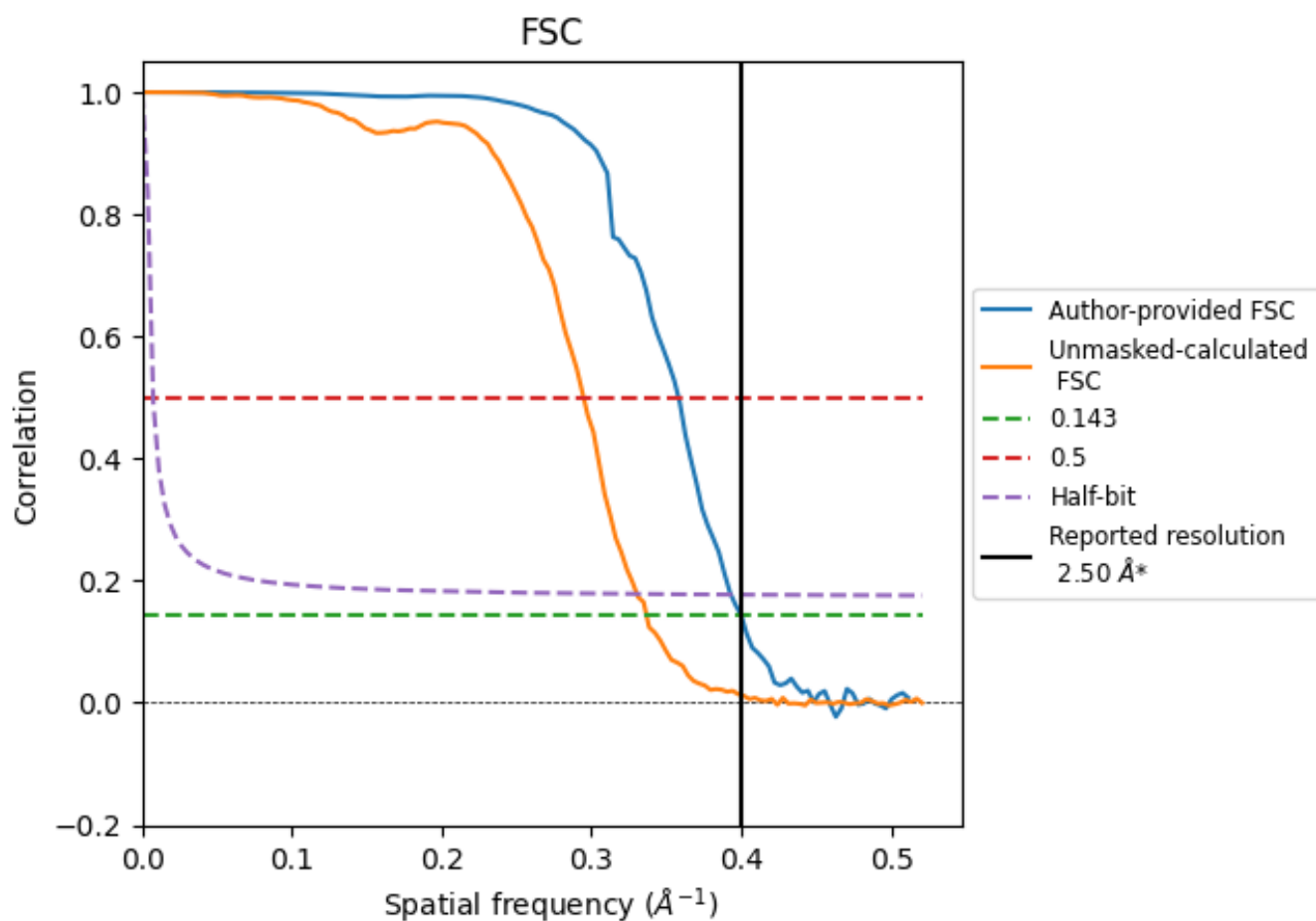


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

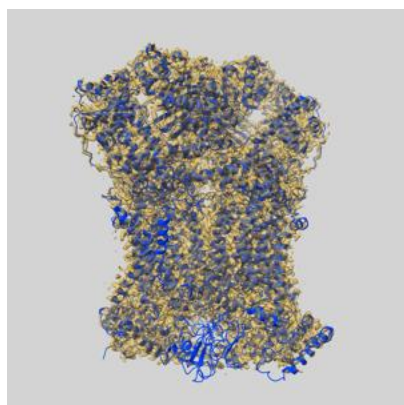
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.79	2.54
Unmasked-calculated*	2.97	3.39	3.03

*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 2.97 differs from the reported value 2.5 by more than 10 %

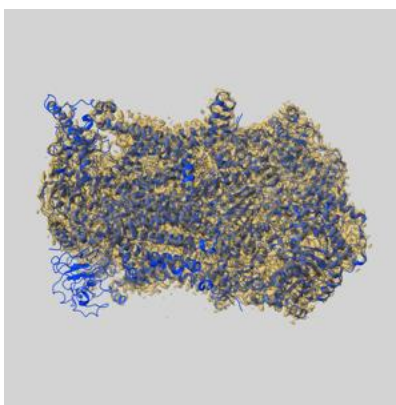
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60140 and PDB model 8ZJC. Per-residue inclusion information can be found in section [3](#) on page [12](#).

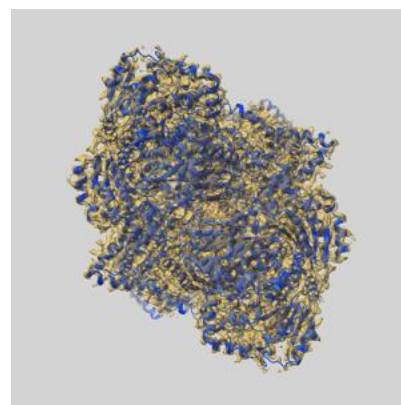
9.1 Map-model overlay [i](#)



X



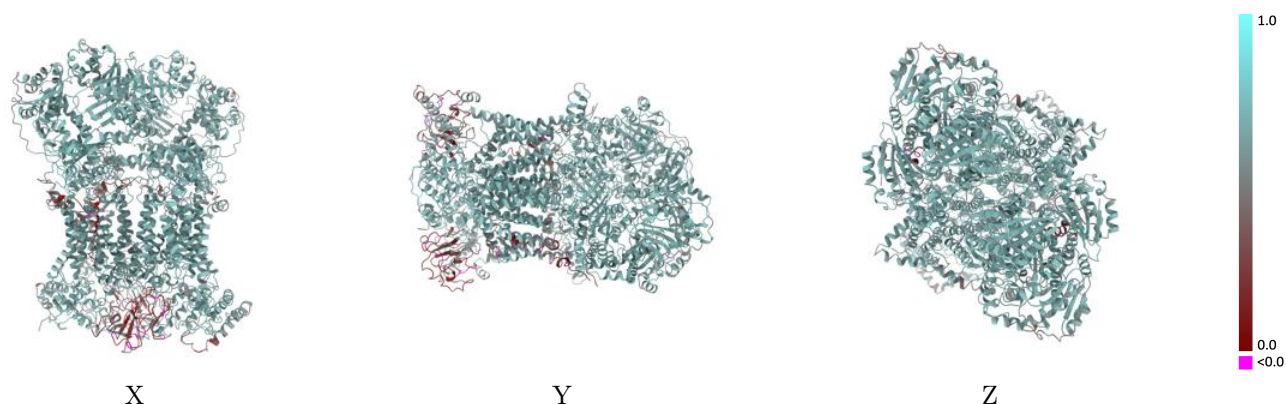
Y



Z

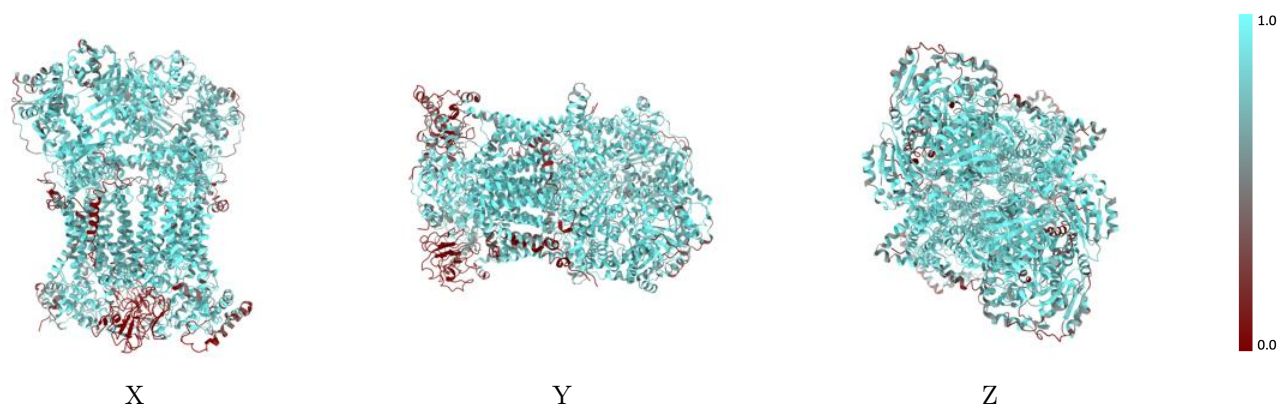
The images above show the 3D surface view of the map at the recommended contour level 0.906 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



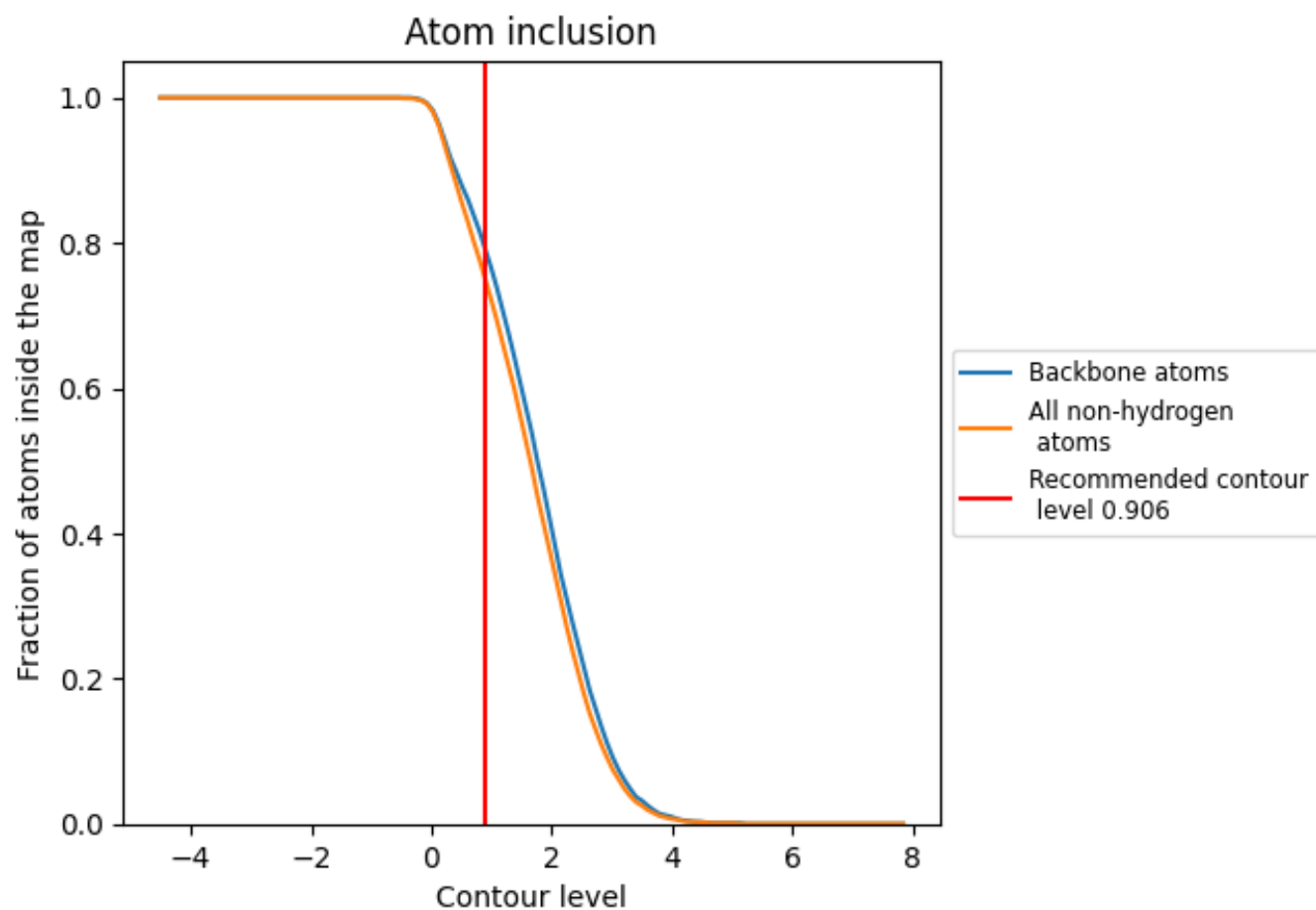
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.906).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (0.906) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.5990
A	 0.8290	 0.6440
B	 0.8390	 0.6470
C	 0.9050	 0.6540
D	 0.8450	 0.6450
E	 0.2460	 0.3410
F	 0.4280	 0.5360
G	 0.8410	 0.6330
H	 0.6570	 0.5950
I	 0.5110	 0.4990
L	 0.8270	 0.6450
M	 0.8420	 0.6470
N	 0.9220	 0.6620
O	 0.8430	 0.6440
P	 0.2500	 0.3410
Q	 0.4200	 0.5160
R	 0.8460	 0.6350
S	 0.6610	 0.5950
T	 0.5060	 0.5120
U	 0.0030	 0.2310
V	 0.0030	 0.1850

