



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 08:32 PM UTC

PDB ID : 7RJE / pdb_00007rje
EMDB ID : EMD-24486
Title : Complex III2 from Candida albicans, Inz-5 bound
Authors : Di Trani, J.M.; Rubinstein, J.L.
Deposited on : 2021-07-20
Resolution : 3.30 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

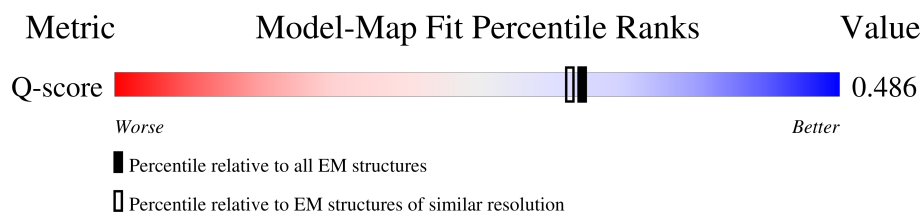
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	15087 (2.80 - 3.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 57440 atoms, of which 28132 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	K	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		
1	T	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		

- Molecule 2 is a protein called Ubiquinol--cytochrome-c reductase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		
2	E	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		
3	L	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		

- Molecule 4 is a protein called Ubiquinol--cytochrome-c reductase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		
4	N	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	122	Total	C	H	N	O	S	0	0
			1978	629	1002	161	183	3		
5	P	122	Total	C	H	N	O	S	0	0
			1978	629	1002	161	183	3		

- Molecule 6 is a protein called Ubiquinol--cytochrome-c reductase subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	88	Total	C	H	N	O	S	0	0
			1410	472	687	124	126	1		
6	O	88	Total	C	H	N	O	S	0	0
			1410	472	687	124	126	1		

- Molecule 7 is a protein called Ubiquinol--cytochrome-c reductase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	72	Total	C	H	N	O	S	0	0
			1104	363	522	105	108	6		
7	Q	72	Total	C	H	N	O	S	0	0
			1104	363	522	105	108	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	47	GLU	ASP	conflict	UNP A0A1D8PJT8
Q	47	GLU	ASP	conflict	UNP A0A1D8PJT8

- Molecule 8 is a protein called Ubiquinol--cytochrome-c reductase subunit 9.

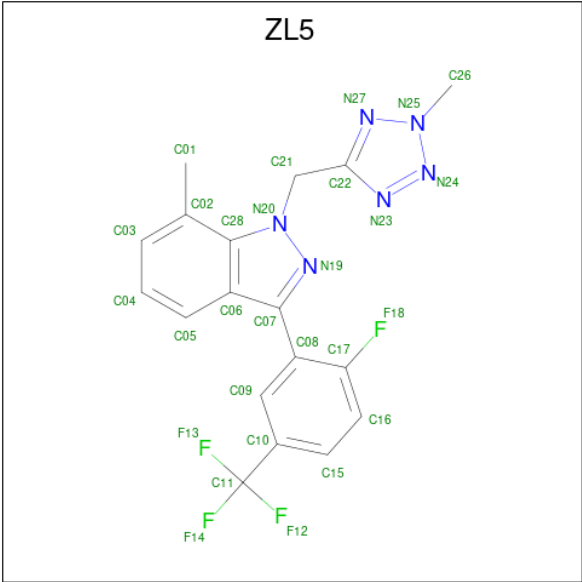
Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	38	Total	C	H	N	O		0	0
			613	211	300	53	49			
8	R	38	Total	C	H	N	O		0	0
			613	211	300	53	49			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		
9	M	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		

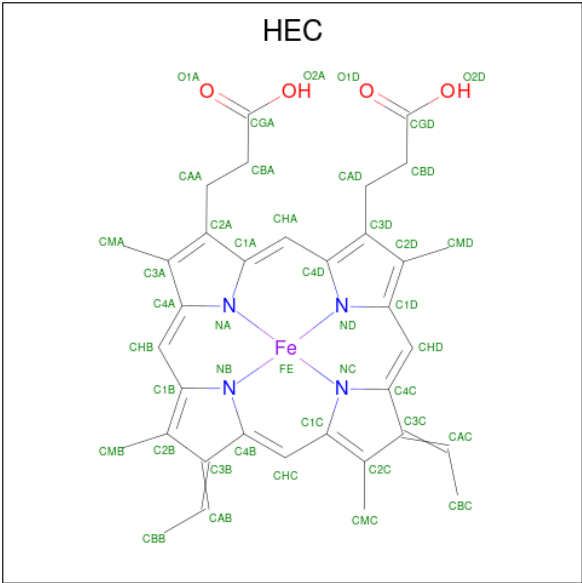
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- The diagram illustrates the chemical structure of HEM (heme). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (CH=CH₂), methyl groups (CH₃), and ethyl groups (CH₂CH₃). The central iron atom is also coordinated by a proximal histidine residue (His F8) and a distal water molecule (H₂O). The structure is labeled with various atoms and groups, including O1A, O2A, O1D, O2D, C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, 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- Molecule 11 is 3-[2-fluoro-5-(trifluoromethyl)phenyl]-7-methyl-1-[(2-methyl-2H-tetrazol-5-yl)methyl]-1H-indazole (CCD ID: ZL5) (formula: C₁₈H₁₄F₄N₆) (labeled as "Ligand of Interest" by depositor).



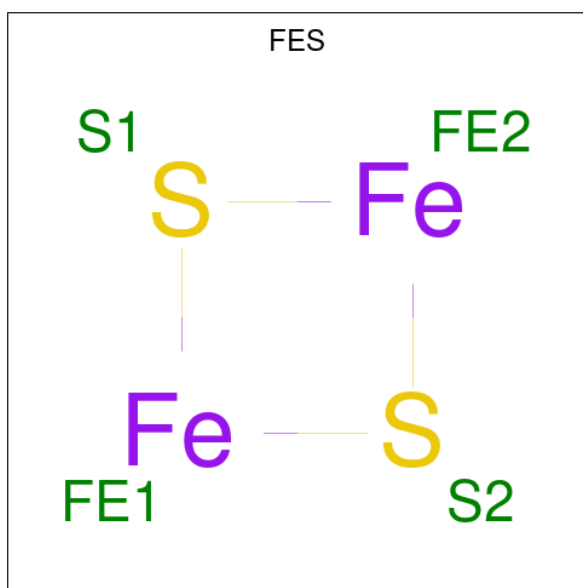
Mol	Chain	Residues	Atoms					AltConf
11	K	1	Total	C	F	H	N	0
			42	18	4	14	6	
11	T	1	Total	C	F	H	N	0
			42	18	4	14	6	

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
12	D	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
12	N	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total 4	Fe 2	S 2	0
13	M	1	Total 4	Fe 2	S 2	0

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3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.718	Depositor
Minimum map value	-2.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.52	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	FES	C	301	9	0,4,4	-	-	-		
10	HEM	T	402	1	50,50,50	1.40	6 (12%)	67,82,82	1.16	6 (8%)
12	HEC	D	301	4	46,50,50	1.86	6 (13%)	58,82,82	1.09	3 (5%)
13	FES	M	301	9	0,4,4	-	-	-		
10	HEM	K	402	1	50,50,50	1.39	6 (12%)	67,82,82	1.16	6 (8%)
11	ZL5	T	403	-	31,31,31	4.86	16 (51%)	41,47,47	2.90	14 (34%)
11	ZL5	K	403	-	31,31,31	4.87	16 (51%)	41,47,47	2.92	15 (36%)
12	HEC	N	301	4	46,50,50	1.86	6 (13%)	58,82,82	1.09	3 (5%)
10	HEM	K	401	1	50,50,50	1.35	6 (12%)	67,82,82	1.02	2 (2%)
10	HEM	T	401	1	50,50,50	1.35	7 (14%)	67,82,82	1.03	2 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FES	C	301	9	-	-	0/1/1/1
10	HEM	T	402	1	-	4/14/54/54	-
12	HEC	D	301	4	-	2/14/54/54	-
13	FES	M	301	9	-	-	0/1/1/1
10	HEM	K	402	1	-	2/14/54/54	-
11	ZL5	T	403	-	-	3/14/14/14	0/4/4/4
11	ZL5	K	403	-	-	3/14/14/14	0/4/4/4
12	HEC	N	301	4	-	2/14/54/54	-
10	HEM	K	401	1	-	5/14/54/54	-
10	HEM	T	401	1	-	4/14/54/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	403	ZL5	C28-N20	14.84	1.48	1.37
11	T	403	ZL5	C28-N20	14.73	1.48	1.37
11	T	403	ZL5	C08-C17	10.59	1.53	1.38
11	K	403	ZL5	C08-C17	10.58	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	403	ZL5	C09-C10	9.03	1.52	1.39
11	K	403	ZL5	C09-C10	8.94	1.52	1.39
11	K	403	ZL5	C16-C15	8.70	1.52	1.38
11	T	403	ZL5	C16-C15	8.61	1.52	1.38
11	T	403	ZL5	C07-N19	-8.50	1.23	1.33
11	K	403	ZL5	C07-N19	-8.50	1.23	1.33
12	N	301	HEC	CAC-C3C	6.24	1.55	1.35
12	D	301	HEC	CAC-C3C	6.23	1.55	1.35
12	D	301	HEC	CAB-C3B	6.13	1.54	1.35
12	N	301	HEC	CAB-C3B	6.07	1.54	1.35
11	K	403	ZL5	C09-C08	-5.09	1.31	1.39
11	T	403	ZL5	C09-C08	-5.02	1.32	1.39
11	T	403	ZL5	C21-C22	4.79	1.52	1.49
11	K	403	ZL5	N25-N27	4.72	1.39	1.33
11	K	403	ZL5	C06-C28	4.69	1.48	1.41
11	T	403	ZL5	N25-N27	4.67	1.39	1.33
11	T	403	ZL5	C06-C28	4.64	1.48	1.41
11	K	403	ZL5	C21-C22	4.63	1.52	1.49
11	K	403	ZL5	C15-C10	-4.60	1.31	1.39
11	T	403	ZL5	C15-C10	-4.54	1.31	1.39
12	N	301	HEC	CBB-CAB	-4.31	1.33	1.49
12	D	301	HEC	CBB-CAB	-4.25	1.33	1.49
12	D	301	HEC	CBC-CAC	-4.15	1.34	1.49
12	N	301	HEC	CBC-CAC	-4.12	1.34	1.49
10	T	402	HEM	FE-ND	3.74	2.06	1.94
11	K	403	ZL5	N25-N24	3.63	1.36	1.31
11	T	403	ZL5	N25-N24	3.63	1.36	1.31
10	K	402	HEM	FE-ND	3.61	2.06	1.94
10	K	401	HEM	FE-ND	3.26	2.04	1.94
10	T	402	HEM	FE-NB	3.22	2.04	1.94
10	K	401	HEM	FE-NB	3.17	2.04	1.94
10	K	402	HEM	FE-NB	3.12	2.04	1.94
10	T	401	HEM	FE-NB	3.09	2.04	1.94
10	T	401	HEM	FE-ND	3.06	2.04	1.94
10	T	401	HEM	FE-NC	3.00	2.05	1.95
11	K	403	ZL5	C16-C17	-2.95	1.31	1.37
11	T	403	ZL5	C16-C17	-2.95	1.31	1.37
10	K	402	HEM	CAB-C3B	2.89	1.55	1.47
10	T	402	HEM	CAB-C3B	2.88	1.55	1.47
10	T	402	HEM	CAC-C3C	2.88	1.55	1.47
10	K	401	HEM	FE-NC	2.86	2.04	1.95
10	T	401	HEM	CAB-C3B	2.85	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	401	HEM	CAB-C3B	2.83	1.54	1.47
10	K	402	HEM	CAC-C3C	2.83	1.54	1.47
11	K	403	ZL5	C06-C07	-2.79	1.40	1.47
10	K	402	HEM	FE-NA	2.78	2.04	1.95
10	T	402	HEM	FE-NA	2.75	2.04	1.95
11	T	403	ZL5	C06-C07	-2.75	1.40	1.47
10	T	401	HEM	CAC-C3C	2.71	1.54	1.47
10	K	401	HEM	CAC-C3C	2.57	1.54	1.47
11	T	403	ZL5	C08-C07	2.48	1.53	1.49
11	K	403	ZL5	C08-C07	2.39	1.53	1.49
12	N	301	HEC	C3B-C2B	-2.28	1.33	1.41
12	D	301	HEC	C3B-C2B	-2.23	1.33	1.41
11	K	403	ZL5	N20-N19	-2.19	1.32	1.36
10	T	401	HEM	FE-NA	2.18	2.02	1.95
12	D	301	HEC	C3C-C2C	-2.15	1.33	1.41
12	N	301	HEC	C3C-C2C	-2.13	1.34	1.41
11	T	403	ZL5	N20-N19	-2.10	1.32	1.36
11	K	403	ZL5	C22-N27	2.10	1.35	1.32
11	T	403	ZL5	C22-N27	2.09	1.35	1.32
10	K	401	HEM	CMC-C2C	2.06	1.55	1.50
10	T	401	HEM	CMC-C2C	2.03	1.54	1.50
10	K	402	HEM	C2A-C3A	-2.02	1.33	1.38
10	T	402	HEM	C2A-C3A	-2.01	1.33	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	403	ZL5	N27-N25-N24	-10.19	108.37	114.35
11	K	403	ZL5	C06-C07-N19	10.10	119.14	110.60
11	T	403	ZL5	N27-N25-N24	-10.07	108.44	114.35
11	T	403	ZL5	C06-C07-N19	10.03	119.08	110.60
11	K	403	ZL5	C26-N25-N24	5.21	126.19	122.51
11	T	403	ZL5	C26-N25-N24	5.15	126.15	122.51
11	K	403	ZL5	C28-N20-N19	4.22	113.64	111.71
11	T	403	ZL5	C28-N20-N19	4.15	113.61	111.71
11	K	403	ZL5	C02-C28-N20	3.33	139.83	129.69
11	T	403	ZL5	C02-C28-N20	3.29	139.69	129.69
11	K	403	ZL5	N25-N24-N23	3.25	107.81	106.10
11	T	403	ZL5	N25-N24-N23	3.19	107.78	106.10
11	K	403	ZL5	C26-N25-N27	2.84	125.43	122.38
12	N	301	HEC	CBB-CAB-C3B	-2.83	121.77	127.43
11	T	403	ZL5	C26-N25-N27	2.82	125.41	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	301	HEC	CBB-CAB-C3B	-2.81	121.82	127.43
12	N	301	HEC	CBC-CAC-C3C	-2.78	121.88	127.43
12	D	301	HEC	CBC-CAC-C3C	-2.77	121.90	127.43
11	K	403	ZL5	C16-C17-C08	-2.70	120.16	123.07
11	T	403	ZL5	C22-N23-N24	2.68	108.56	106.31
11	K	403	ZL5	C22-N23-N24	2.66	108.55	106.31
11	T	403	ZL5	C16-C17-C08	-2.62	120.25	123.07
10	T	402	HEM	C3B-C2B-C1B	2.58	108.35	106.41
10	K	402	HEM	C3B-C2B-C1B	2.52	108.30	106.41
11	T	403	ZL5	C05-C06-C07	2.51	139.31	132.41
11	K	403	ZL5	C05-C06-C07	2.48	139.24	132.41
11	K	403	ZL5	C21-C22-N23	2.45	125.37	122.78
11	T	403	ZL5	C21-C22-N23	2.45	125.37	122.78
10	K	402	HEM	C4D-ND-C1D	2.44	108.09	105.21
10	T	402	HEM	C4D-ND-C1D	2.36	108.00	105.21
11	T	403	ZL5	N27-C22-N23	-2.35	108.95	111.86
11	K	403	ZL5	N27-C22-N23	-2.34	108.95	111.86
10	K	402	HEM	CBD-CAD-C3D	-2.30	106.17	112.53
10	K	402	HEM	CHC-C1C-NC	2.22	126.87	124.45
10	T	402	HEM	C1B-NB-C4B	2.22	107.83	105.21
11	K	403	ZL5	C09-C08-C17	2.21	119.58	116.83
10	K	402	HEM	C1B-NB-C4B	2.19	107.81	105.21
10	T	401	HEM	C4D-ND-C1D	2.18	107.79	105.21
10	K	401	HEM	C2A-C1A-NA	-2.15	107.76	110.15
10	K	402	HEM	C3D-C4D-ND	-2.15	107.81	110.17
11	T	403	ZL5	C09-C08-C17	2.13	119.47	116.83
10	T	401	HEM	C2A-C1A-NA	-2.13	107.79	110.15
11	T	403	ZL5	C21-N20-C28	-2.12	126.44	129.39
10	T	402	HEM	CHC-C1C-NC	2.12	126.76	124.45
10	T	402	HEM	C3D-C4D-ND	-2.10	107.86	110.17
10	T	402	HEM	CBD-CAD-C3D	-2.08	106.78	112.53
11	K	403	ZL5	C21-N20-C28	-2.04	126.56	129.39
10	K	401	HEM	C4D-ND-C1D	2.03	107.61	105.21
11	K	403	ZL5	C08-C07-C06	-2.01	123.78	128.81
12	D	301	HEC	C2A-C1A-NA	-2.00	108.39	110.32
12	N	301	HEC	C2A-C1A-NA	-2.00	108.39	110.32

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	403	ZL5	C22-C21-N20-C28

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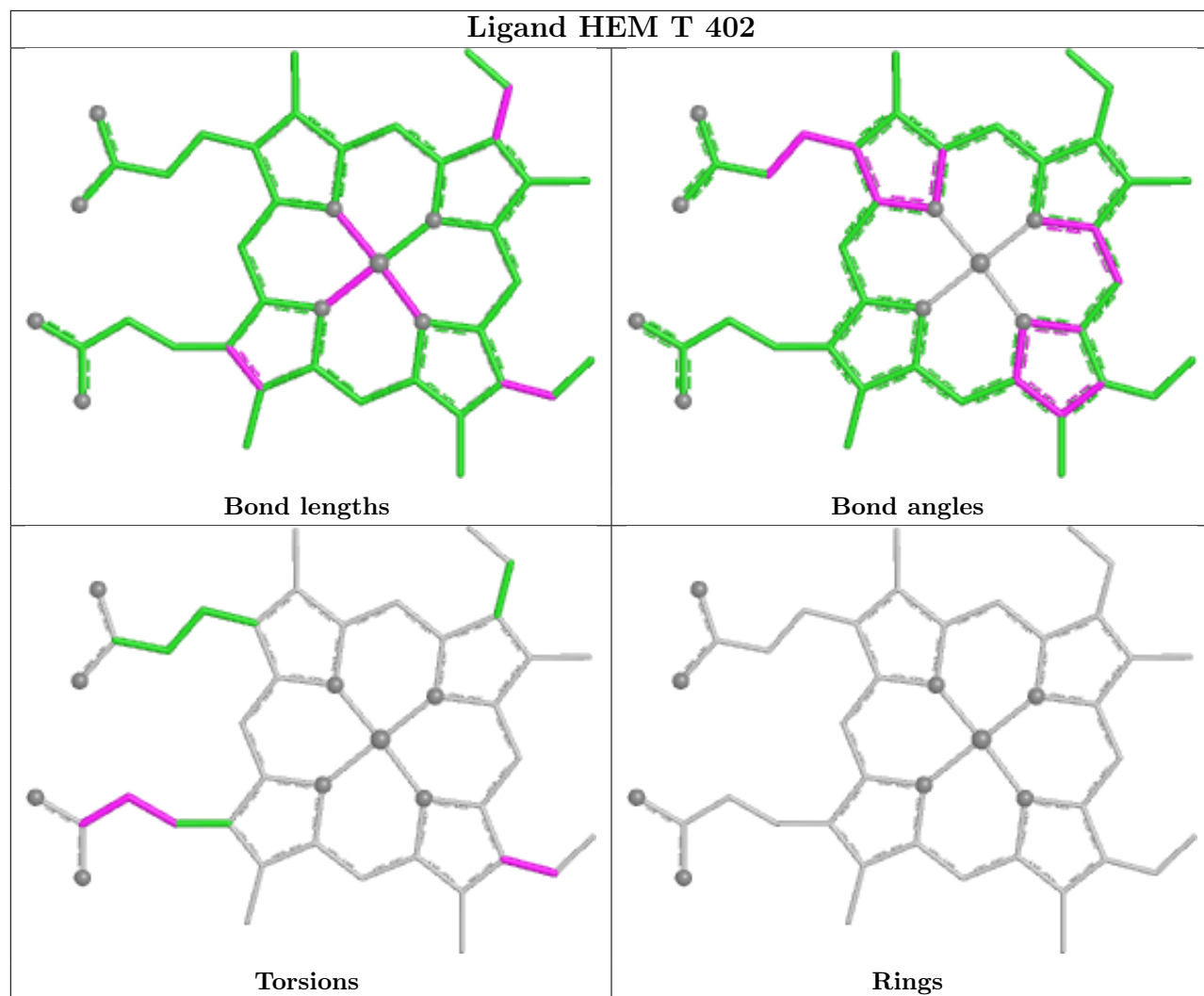
Continued from previous page...

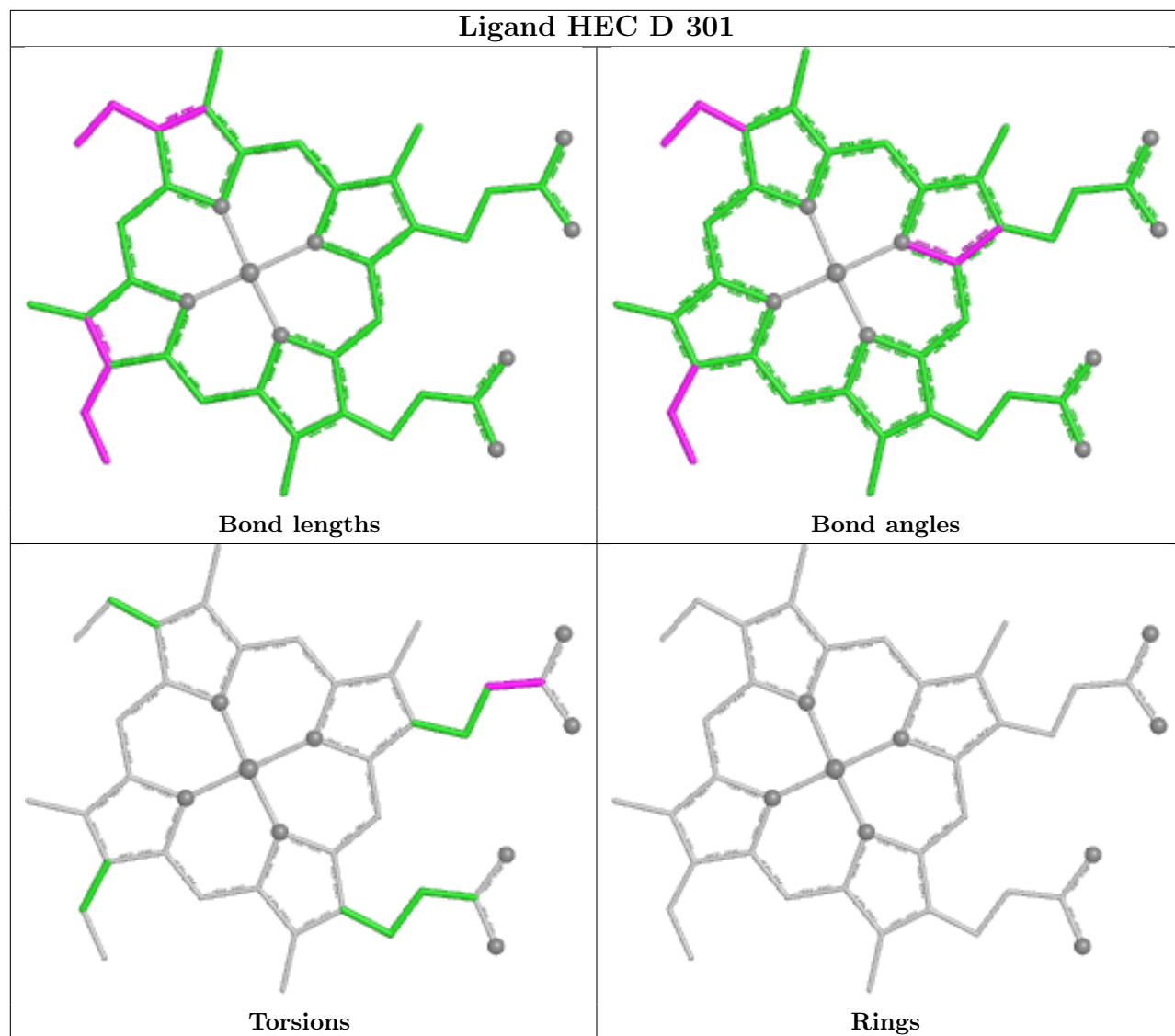
Mol	Chain	Res	Type	Atoms
11	T	403	ZL5	C22-C21-N20-C28
10	K	401	HEM	C3D-CAD-CBD-CGD
10	T	401	HEM	C3D-CAD-CBD-CGD
10	K	401	HEM	C2D-C3D-CAD-CBD
10	T	401	HEM	C2D-C3D-CAD-CBD
10	K	401	HEM	C4D-C3D-CAD-CBD
10	K	402	HEM	C4C-C3C-CAC-CBC
10	T	401	HEM	C4D-C3D-CAD-CBD
11	K	403	ZL5	C06-C07-C08-C09
11	T	403	ZL5	C06-C07-C08-C09
10	K	401	HEM	C1A-C2A-CAA-CBA
10	K	402	HEM	C4B-C3B-CAB-CBB
10	T	402	HEM	C4B-C3B-CAB-CBB
11	K	403	ZL5	C06-C07-C08-C17
11	T	403	ZL5	C06-C07-C08-C17
10	T	401	HEM	C1A-C2A-CAA-CBA
12	D	301	HEC	CAA-CBA-CGA-O2A
10	T	402	HEM	C2A-CAA-CBA-CGA
12	D	301	HEC	CAA-CBA-CGA-O1A
12	N	301	HEC	CAA-CBA-CGA-O2A
10	T	402	HEM	CAA-CBA-CGA-O1A
10	T	402	HEM	CAA-CBA-CGA-O2A
12	N	301	HEC	CAA-CBA-CGA-O1A
10	K	401	HEM	CAD-CBD-CGD-O2D

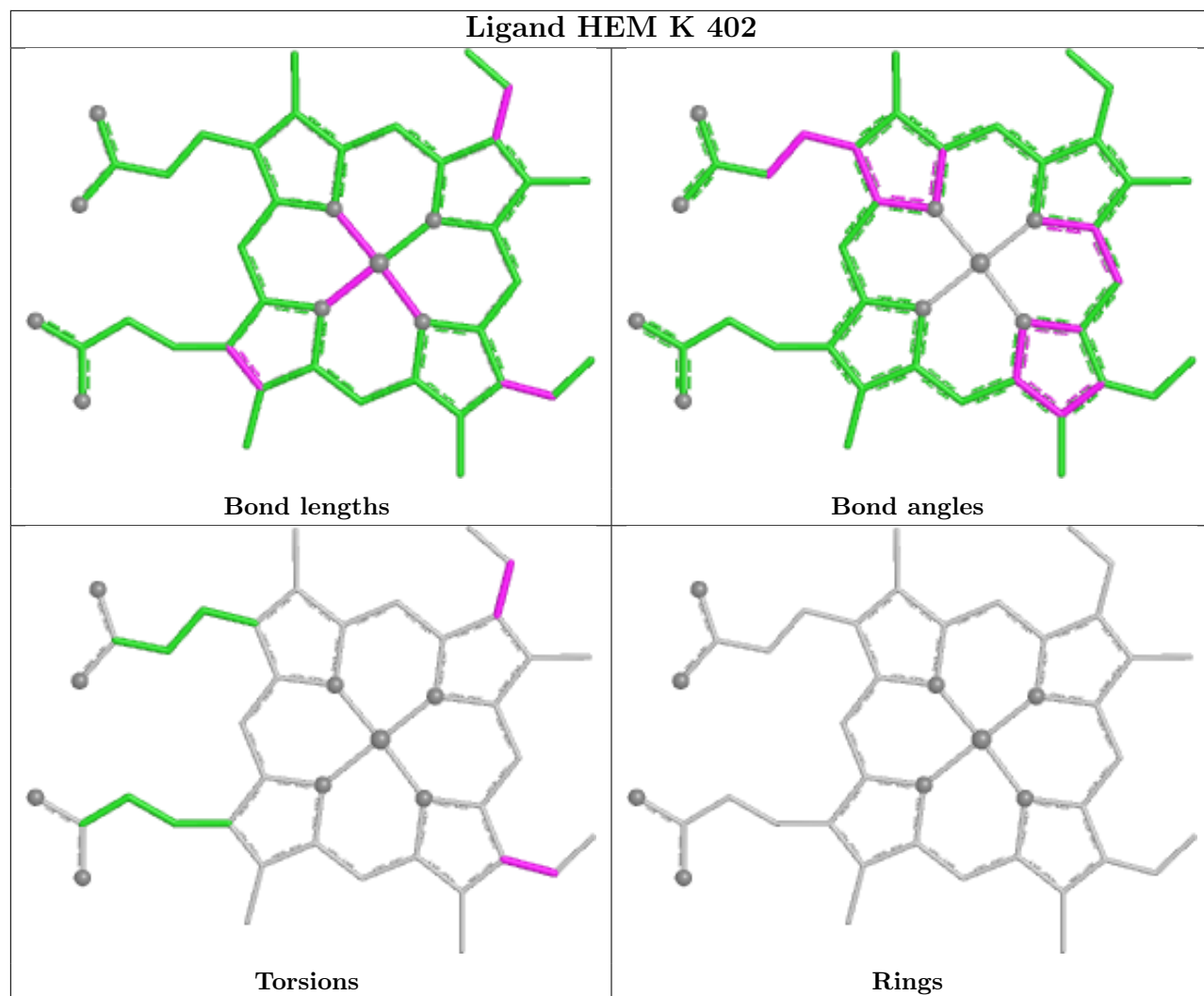
There are no ring outliers.

No monomer is involved in short contacts.

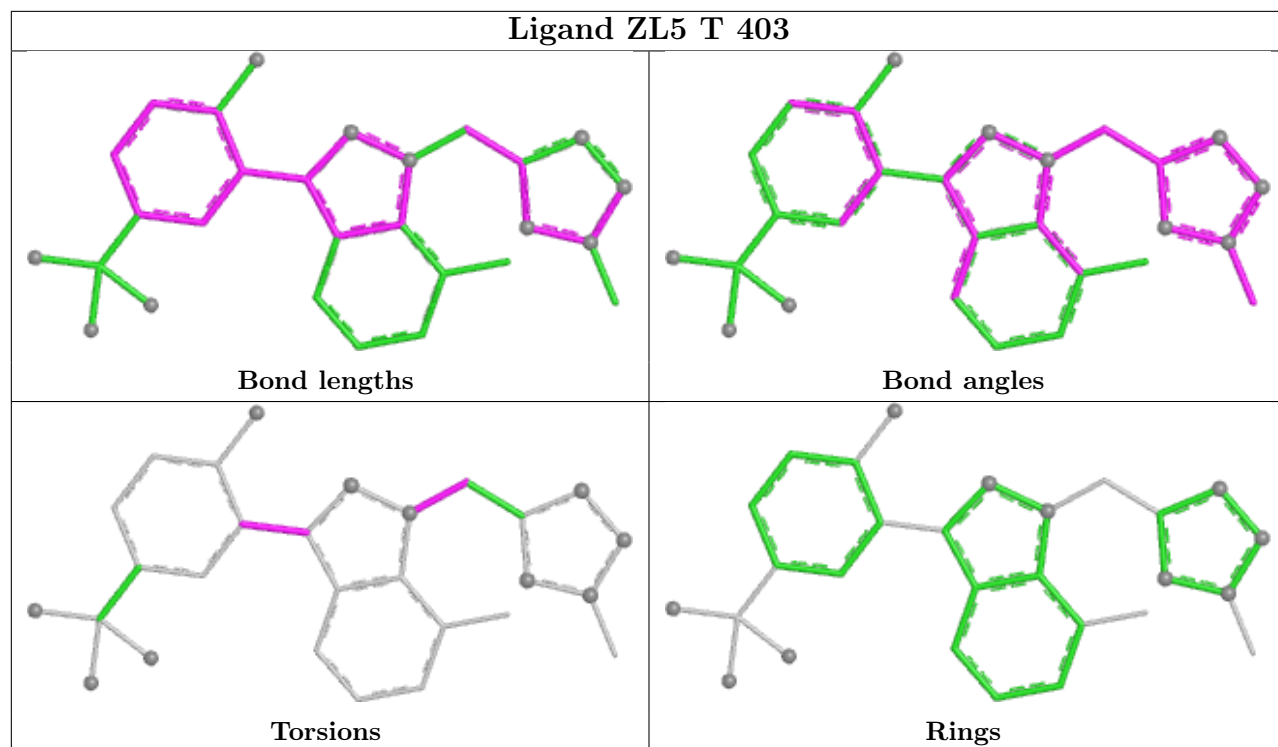
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



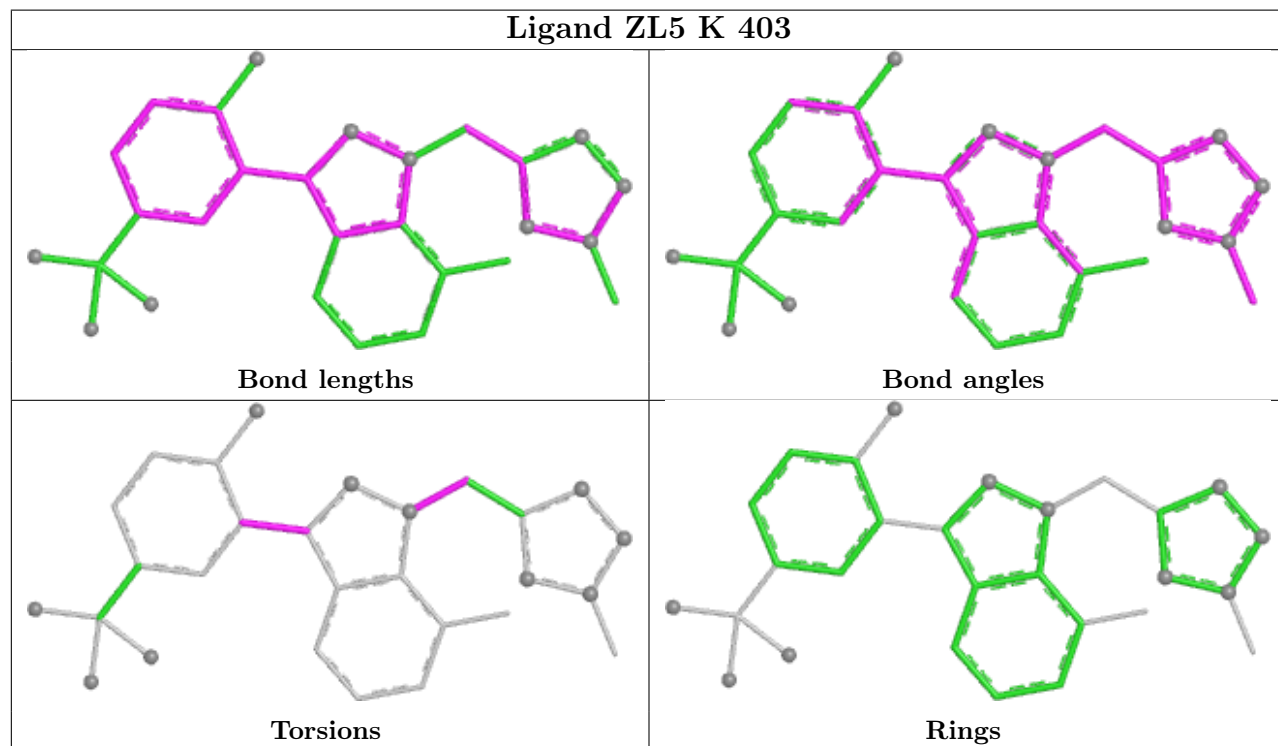


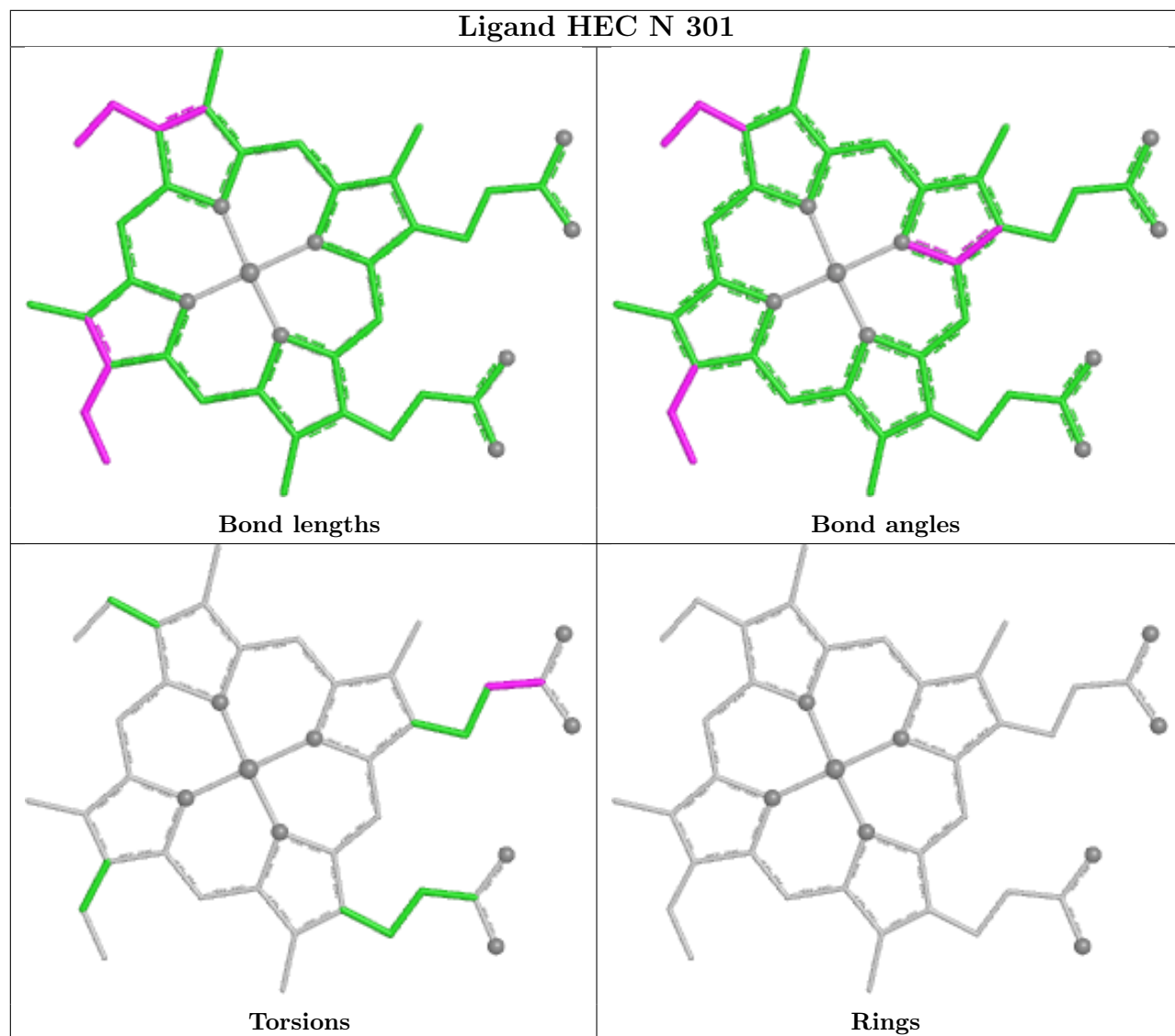


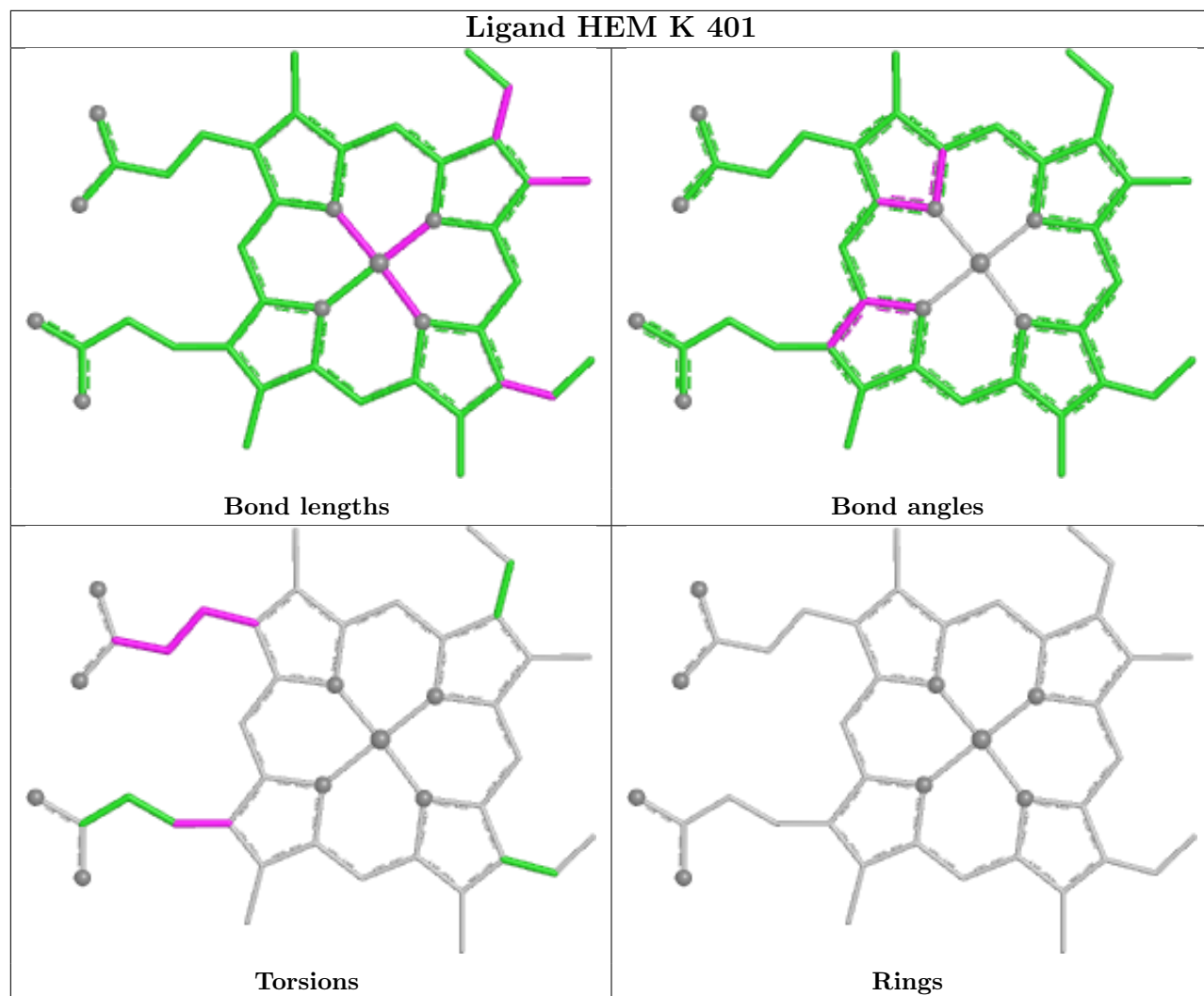
Ligand ZL5 T 403

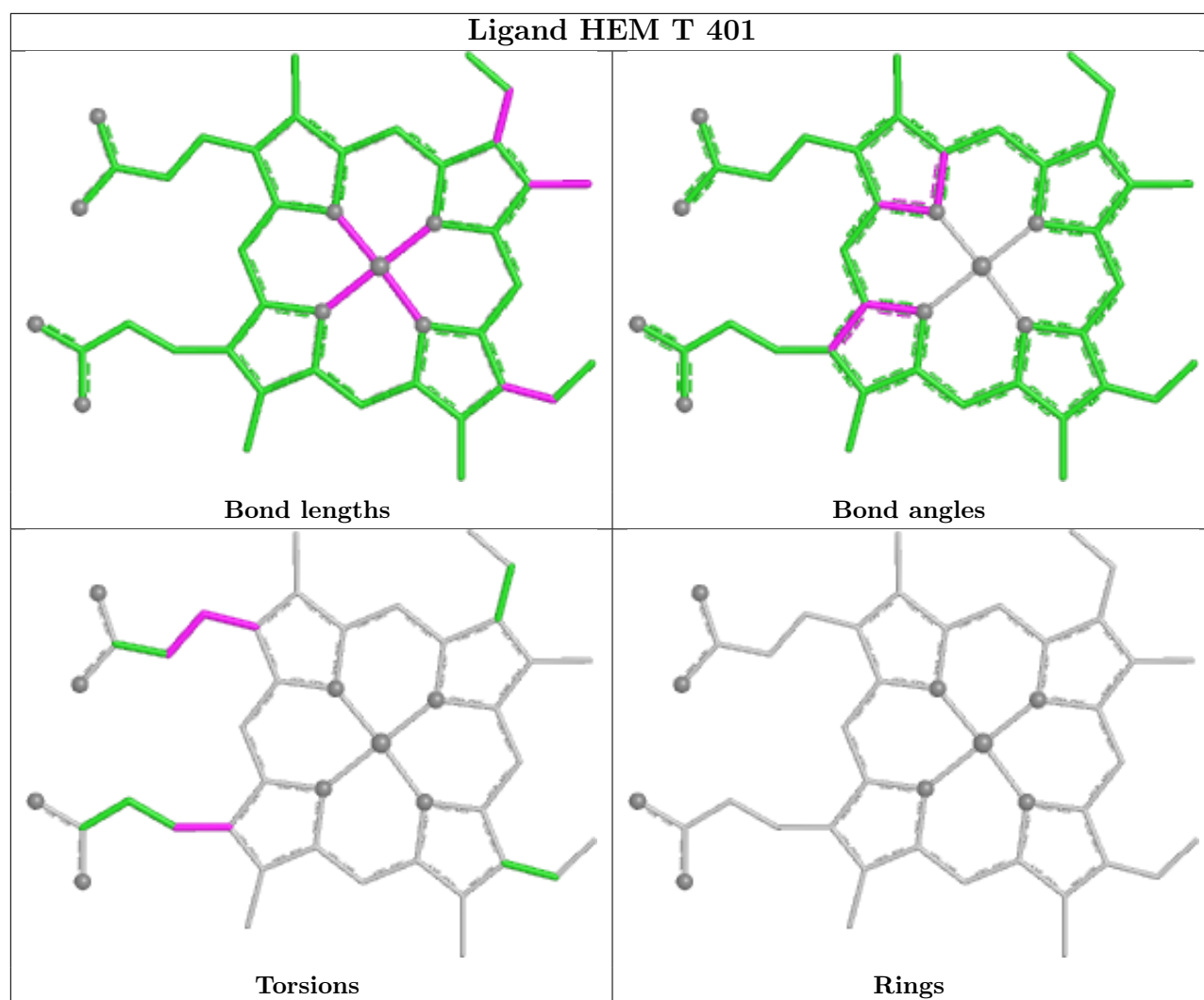


Ligand ZL5 K 403









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

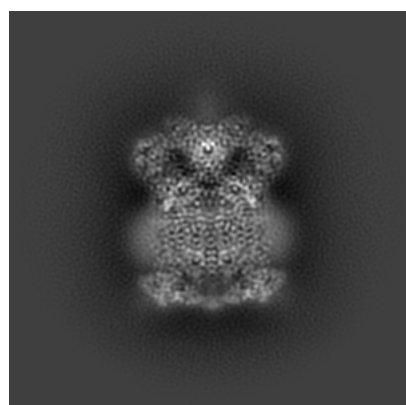
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24486. These allow visual inspection of the internal detail of the map and identification of artifacts.

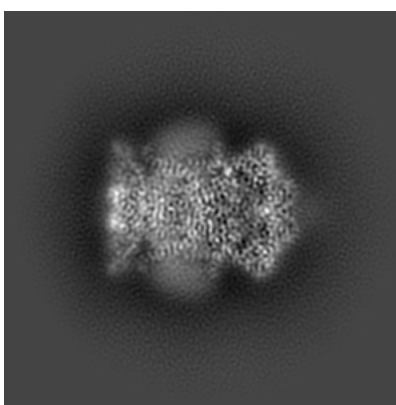
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

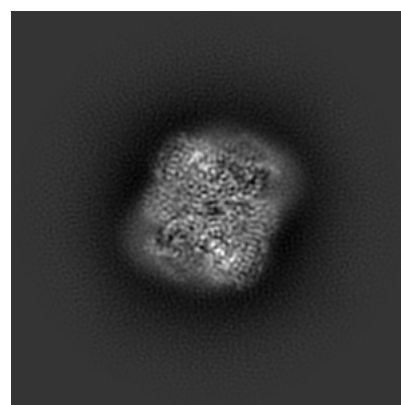
5.1.1 Primary map



X



Y

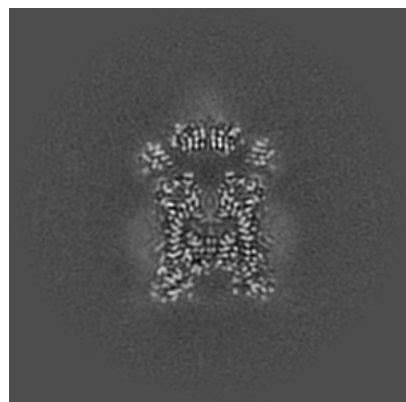


Z

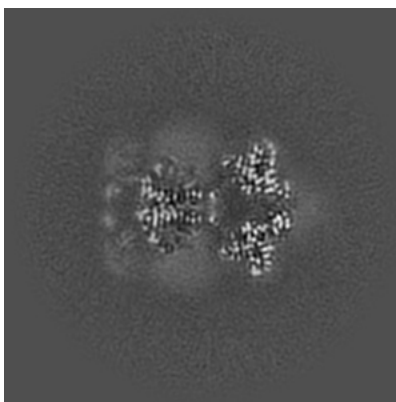
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

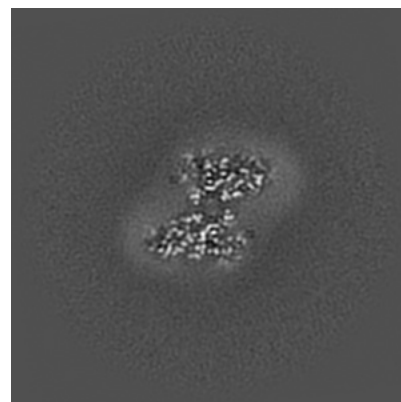
5.2.1 Primary map



X Index: 144



Y Index: 144

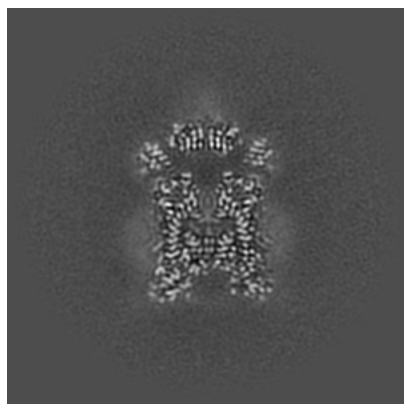


Z Index: 144

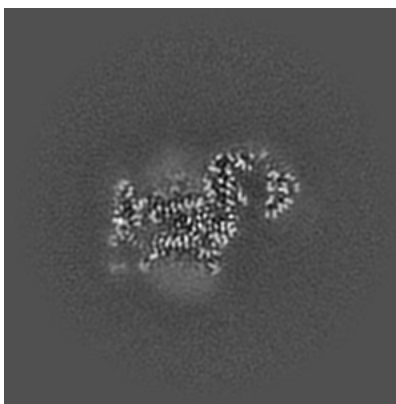
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

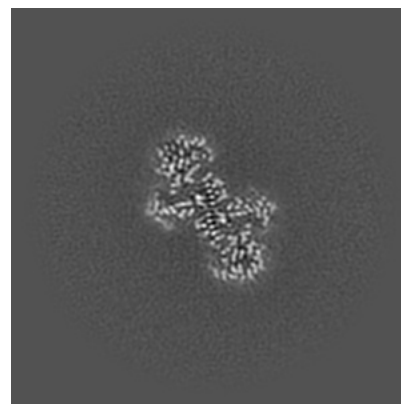
5.3.1 Primary map



X Index: 144



Y Index: 122

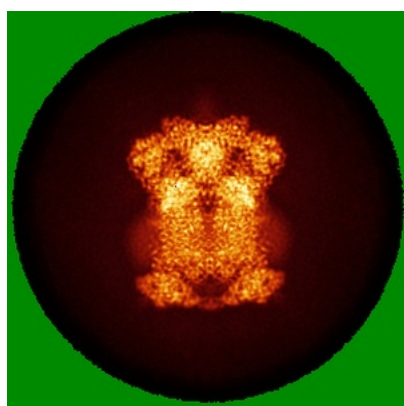


Z Index: 191

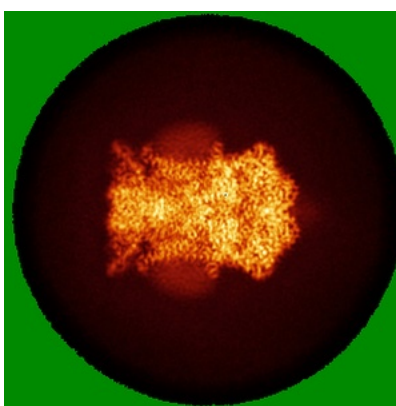
The images above show the largest variance slices of the map in three orthogonal directions.

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

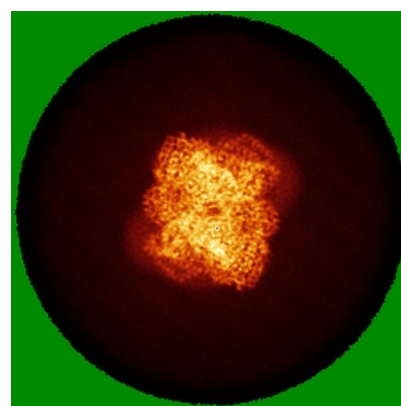
5.4.1 Primary map



X



Y

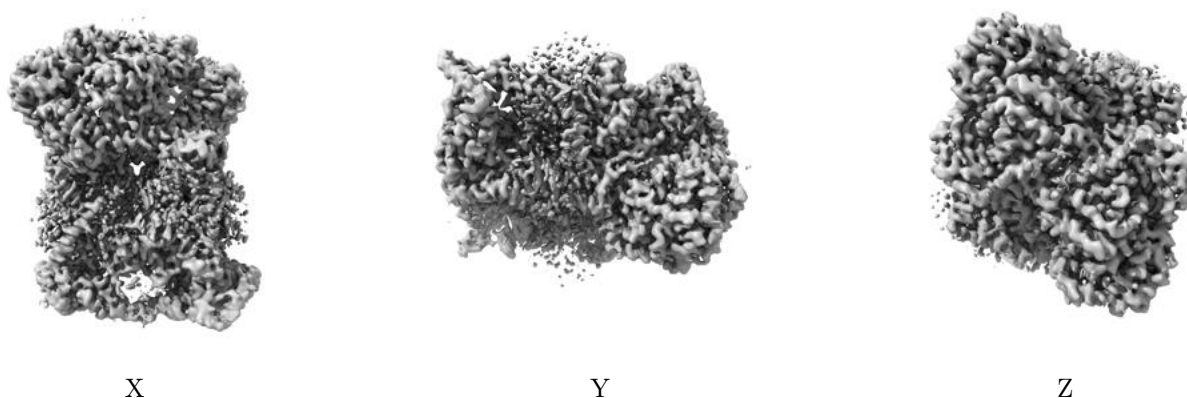


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

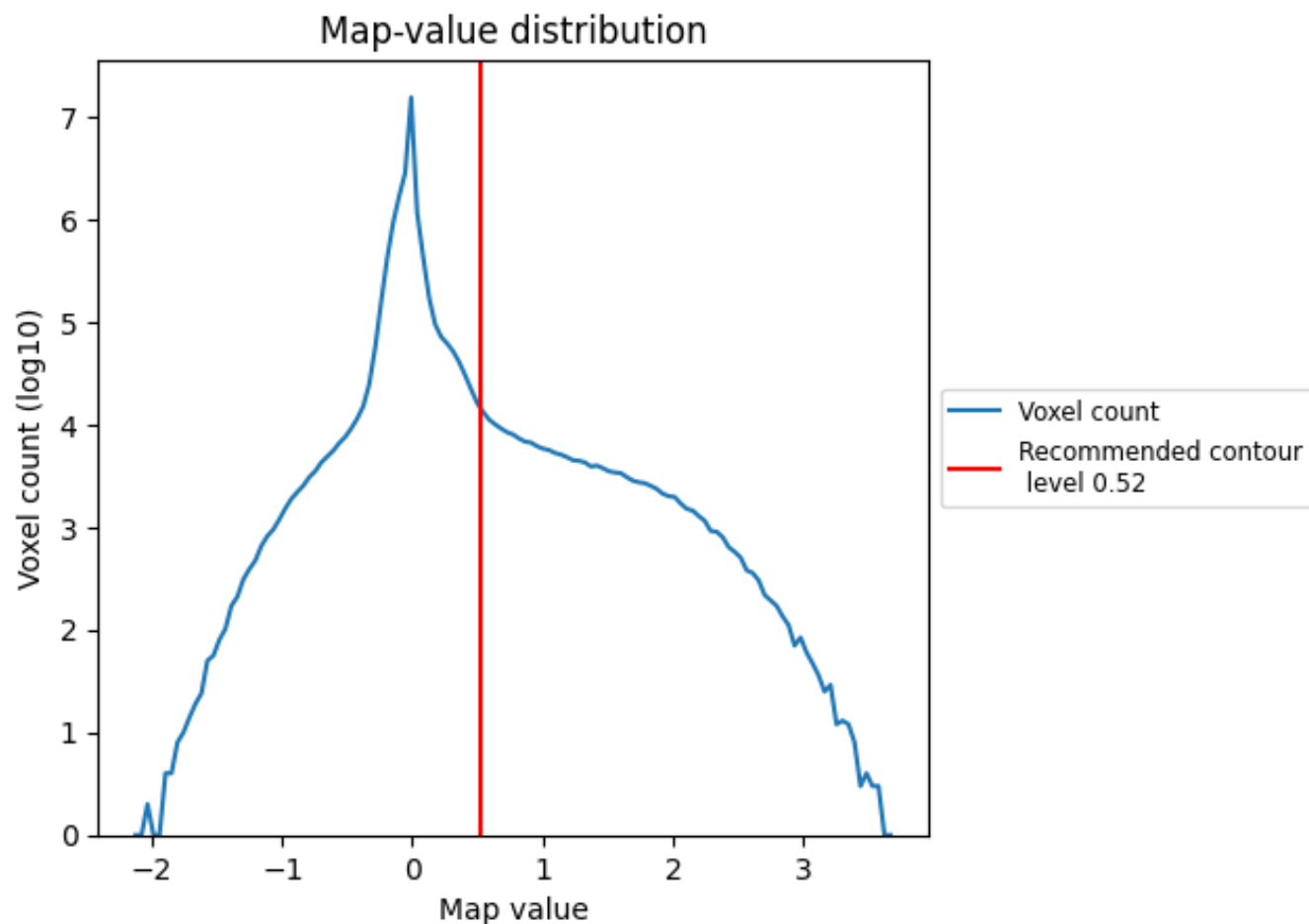
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

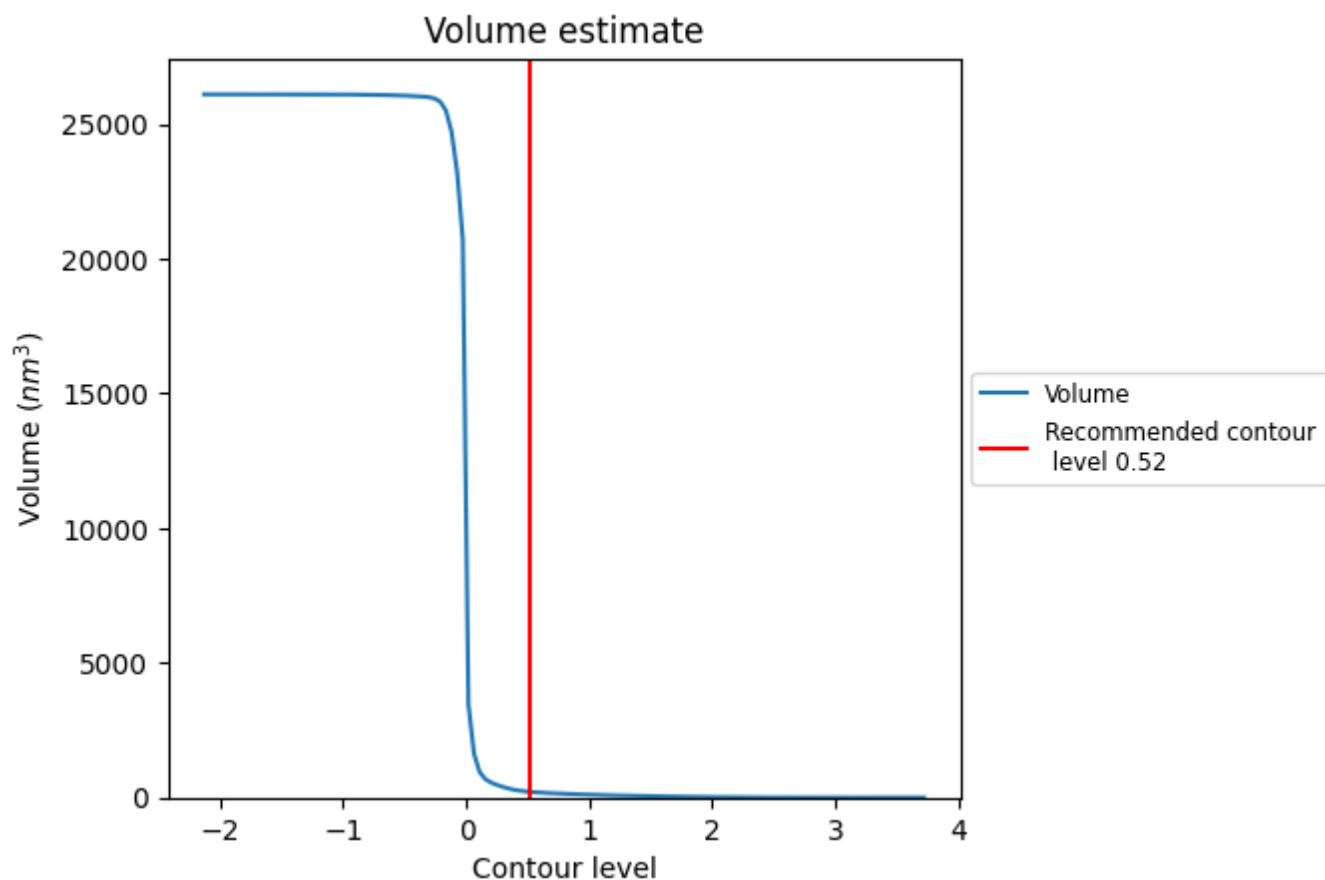
This section contains the results of statistical analysis of the map.

6.1 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.

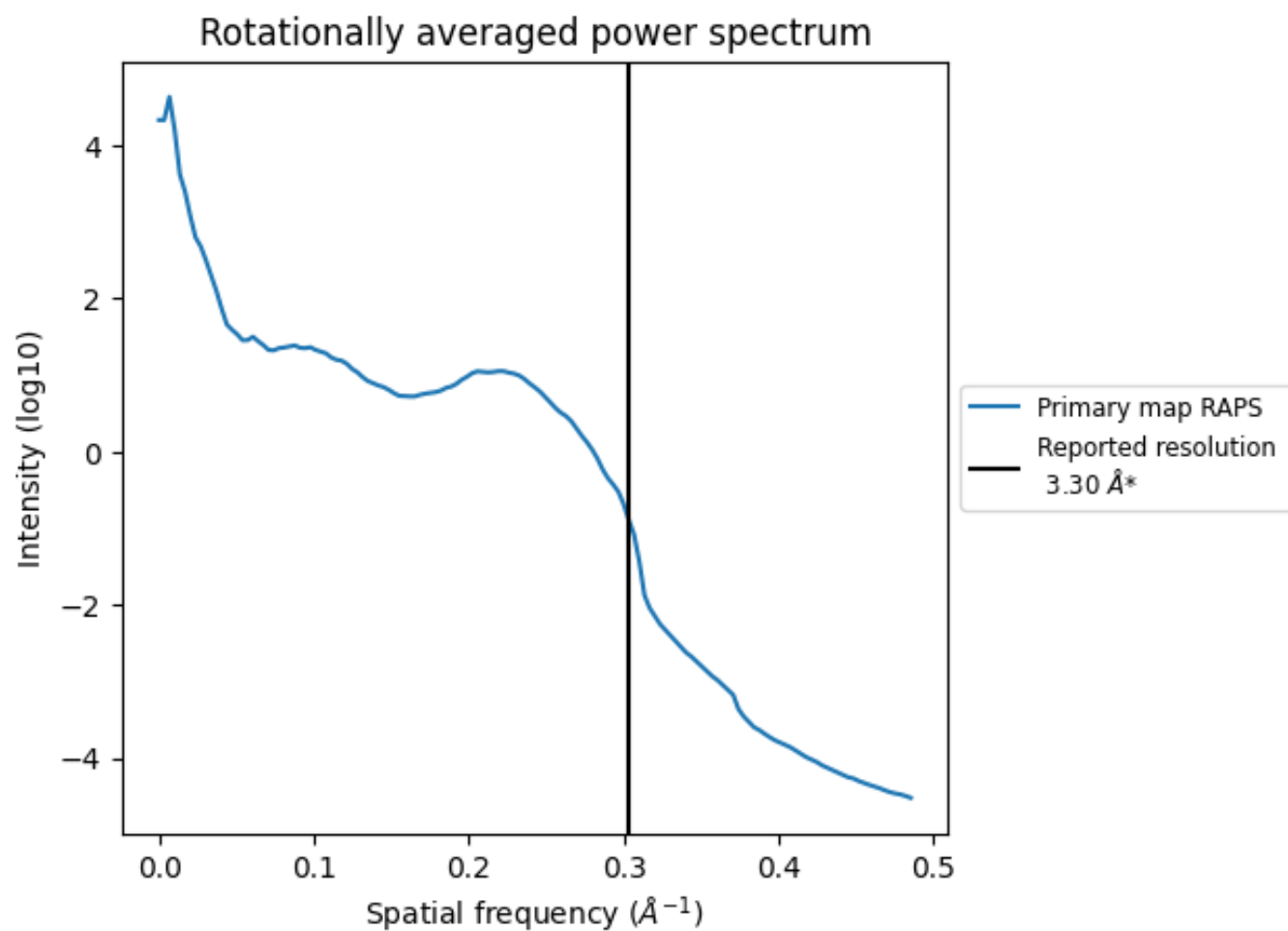
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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.

6.3 Rotationally averaged power spectrum ⓘ

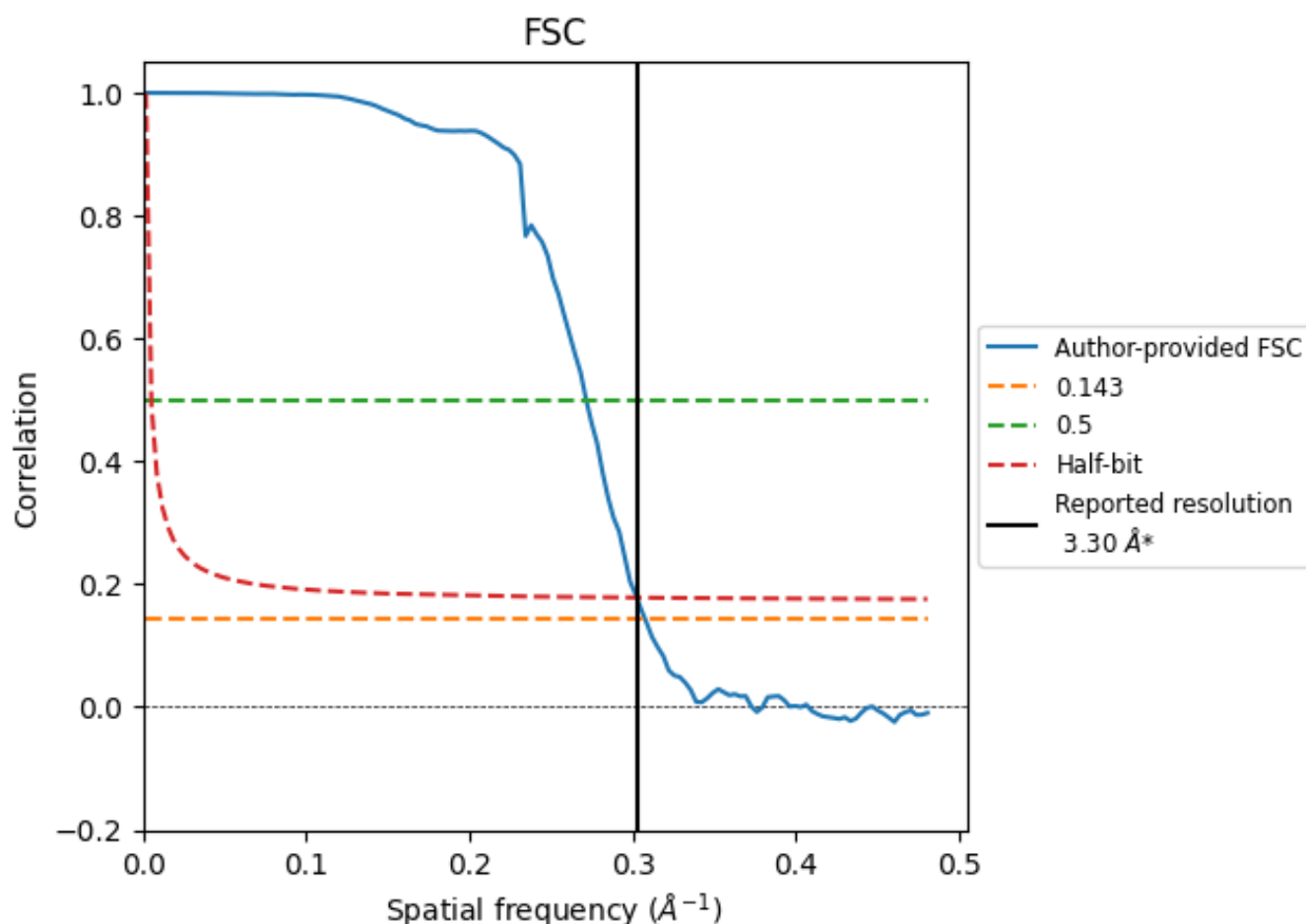


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

7.2 Resolution estimates [i](#)

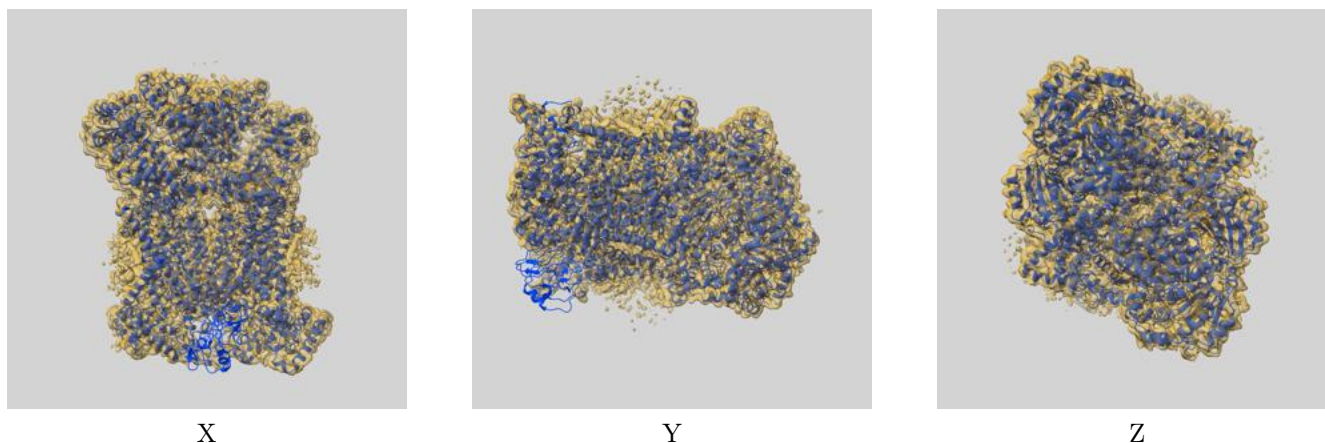
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.68	3.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

8 Map-model fit [i](#)

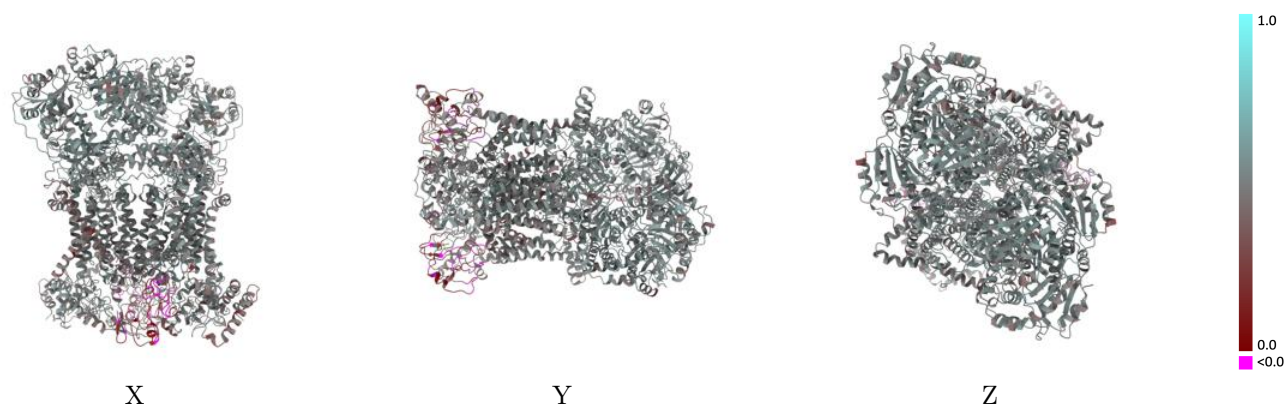
This section contains information regarding the fit between EMDB map EMD-24486 and PDB model 7RJE. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



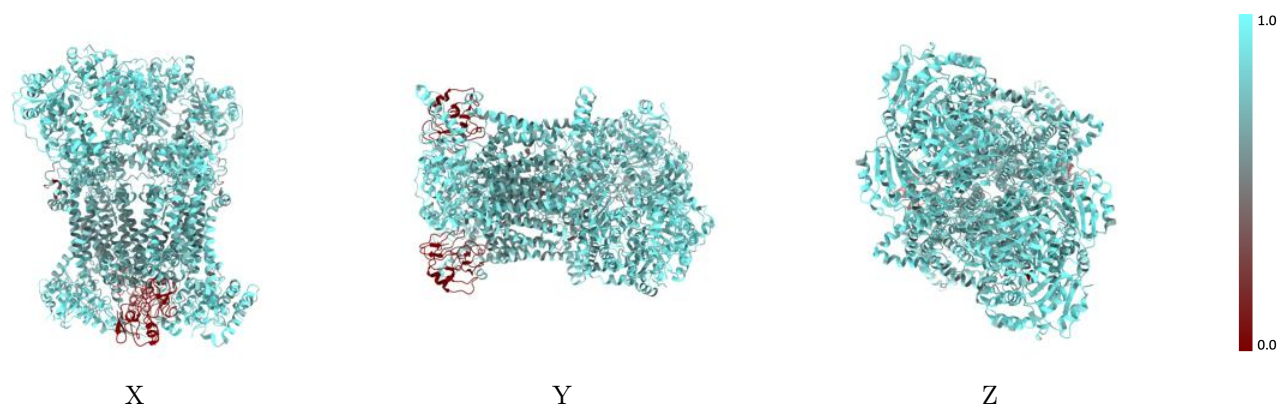
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



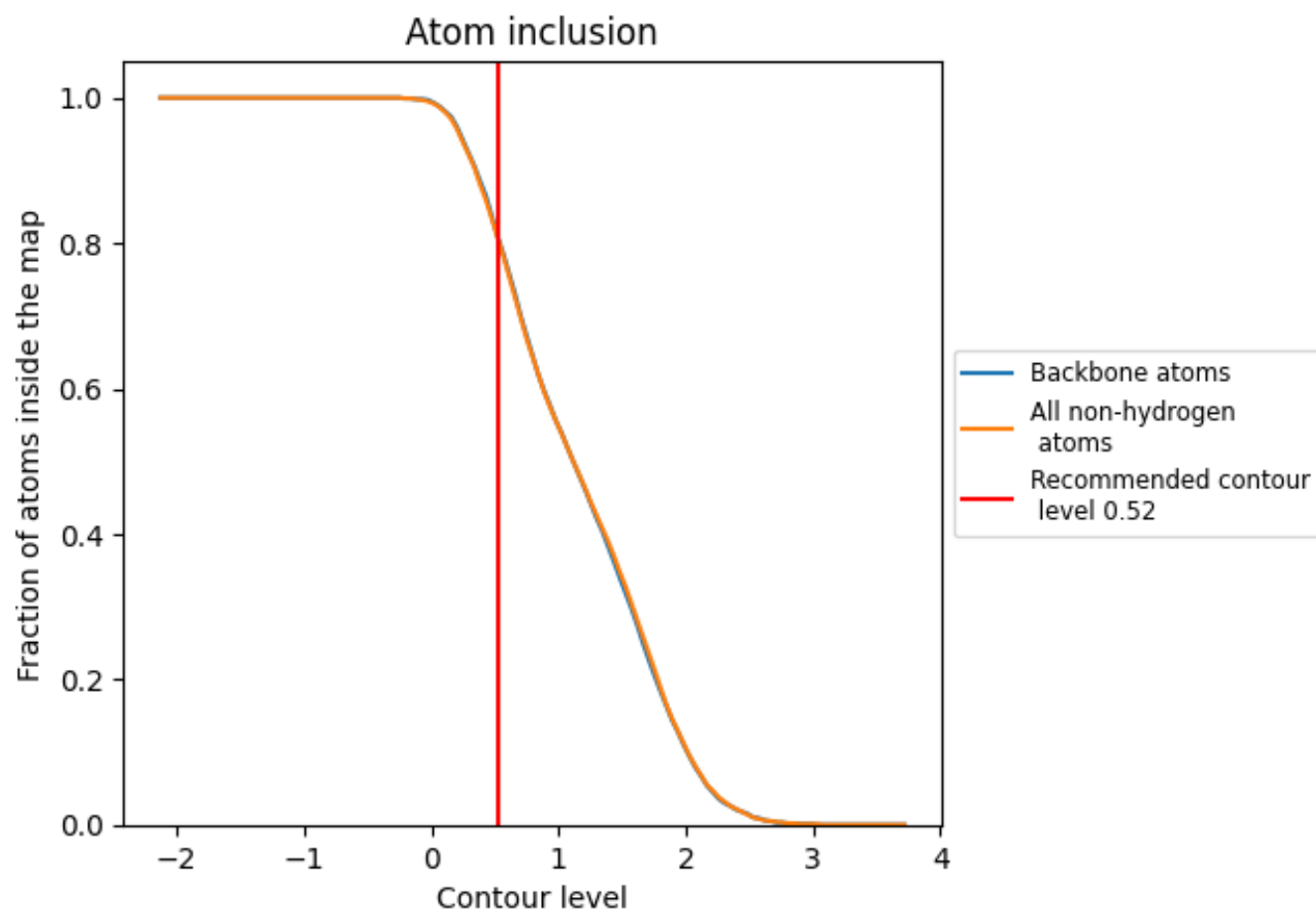
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.52).

8.4 Atom inclusion [i](#)



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

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.4860
A	 0.8740	 0.5170
B	 0.8720	 0.5130
C	 0.2810	 0.2890
D	 0.8650	 0.4920
E	 0.8740	 0.5150
F	 0.8080	 0.4760
G	 0.8460	 0.5090
H	 0.8290	 0.4320
I	 0.8000	 0.4520
K	 0.8140	 0.5000
L	 0.8720	 0.5140
M	 0.2680	 0.2890
N	 0.8740	 0.4940
O	 0.8210	 0.4810
P	 0.8370	 0.5060
Q	 0.8240	 0.4260
R	 0.8100	 0.4550
T	 0.8190	 0.5020

