



Full wwPDB EM Validation Report ⓘ

Aug 6, 2025 – 10:54 AM EDT

PDB ID : 9MSE / pdb_00009mse
EMDB ID : EMD-48586
Title : de novo SigN RNA polymerase transcription initiation intermediate with pre-catalytic bEBP state (RPI1 open ring)
Authors : Mueller, A.U.; Darst, S.A.
Deposited on : 2025-01-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.45.1

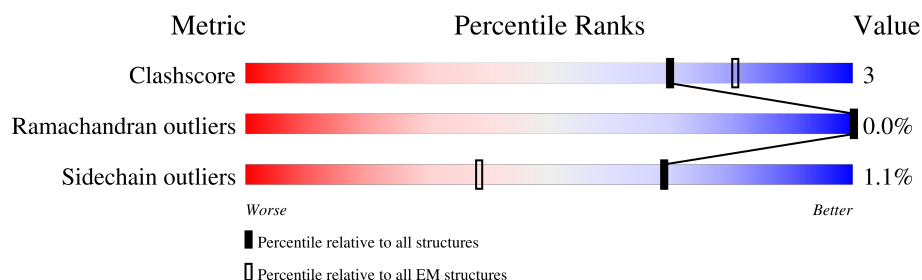
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.





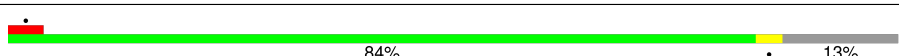
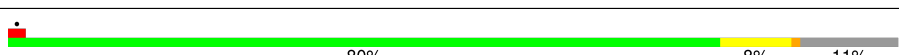


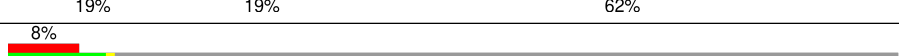
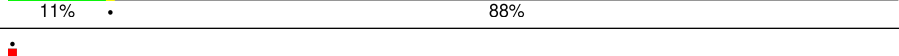
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	268	78% 14% 8%
1	B	268	84% 9% 8%
1	C	268	87% 6% 8%
1	D	268	84% 7% 8%
1	E	268	87% 6% 8%
1	F	268	83% 9% 8%
2	G	329	84% 7% 8%
2	H	329	60% 8% 32%

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Mol	Chain	Length	Quality of chain
3	I	1342	
4	J	1415	
5	K	91	
6	M	477	
7	S	90	
7	U	90	
8	T	90	
8	V	90	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43810 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 Transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	0
			1979	1278	333	364	4		
1	B	247	Total	C	N	O	S	0	0
			1979	1278	333	364	4		
1	C	247	Total	C	N	O	S	0	0
			1979	1278	333	364	4		
1	D	246	Total	C	N	O	S	0	0
			1972	1273	332	363	4		
1	E	247	Total	C	N	O	S	0	0
			1979	1278	333	364	4		
1	F	247	Total	C	N	O	S	0	0
			1979	1278	333	364	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	initiating methionine	UNP O67198
B	120	MET	-	initiating methionine	UNP O67198
C	120	MET	-	initiating methionine	UNP O67198
D	120	MET	-	initiating methionine	UNP O67198
E	120	MET	-	initiating methionine	UNP O67198
F	120	MET	-	initiating methionine	UNP O67198

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	302	Total	C	N	O	S	0	0
			2347	1470	414	455	8		
2	H	223	Total	C	N	O	S	0	0
			1718	1074	302	336	6		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	1352	Total	C	N	O	S	0	0
			10523	6613	1876	1984	50		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 6 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	423	Total	C	N	O	S	0	0
			3371	2109	587	664	11		

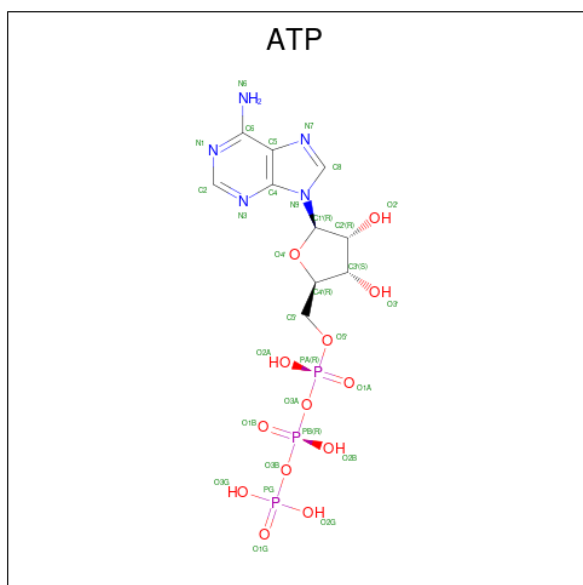
- Molecule 7 is a DNA chain called dhsU (-60 to +30) non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	13	Total	C	N	O	P	0	0
			276	130	56	77	13		
7	U	34	Total	C	N	O	P	0	0
			701	334	140	193	34		

- Molecule 8 is a DNA chain called dhsU (-60 to +30) template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	11	Total	C	N	O	P	0	0
			217	105	33	68	11		
8	V	34	Total	C	N	O	P	0	0
			693	335	109	215	34		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

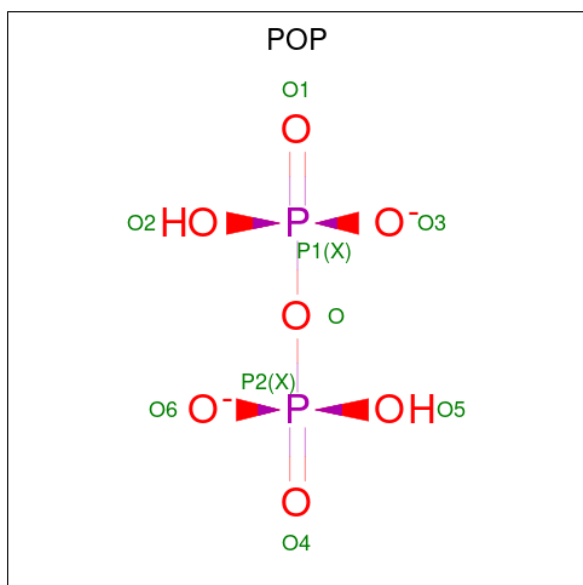
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
10	E	1	Total	Mg	0
			1	1	
10	J	1	Total	Mg	0
			1	1	

- Molecule 11 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			AltConf
11	I	1	Total	O	P	0
			9	7	2	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	J	2	Total	Zn	0
			2	2	

- Molecule 13 is water.


Mol	Chain	Residues	Atoms		AltConf
13	A	3	Total	O	0
			3	3	
13	B	3	Total	O	0
			3	3	
13	C	9	Total	O	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
13	D	11	Total 11	O 11	0
13	E	13	Total 13	O 13	0
13	F	5	Total 5	O 5	0
13	G	69	Total 69	O 69	0
13	H	28	Total 28	O 28	0
13	I	296	Total 296	O 296	0
13	J	205	Total 205	O 205	0
13	K	9	Total 9	O 9	0
13	M	30	Total 30	O 30	0
13	U	11	Total 11	O 11	0
13	V	11	Total 11	O 11	0

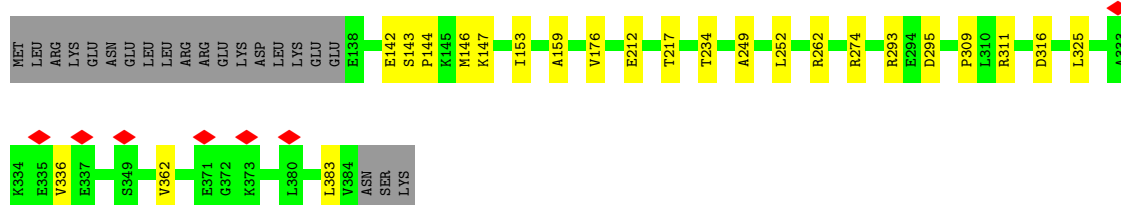
- Molecule 1: Transcriptional regulator (NtrC family)

Chain E:  87% 6% 8%




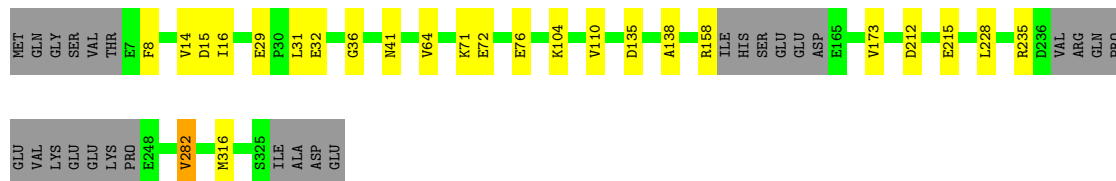
- Molecule 1: Transcriptional regulator (NtrC family)

Chain F:  83% 9% 8%



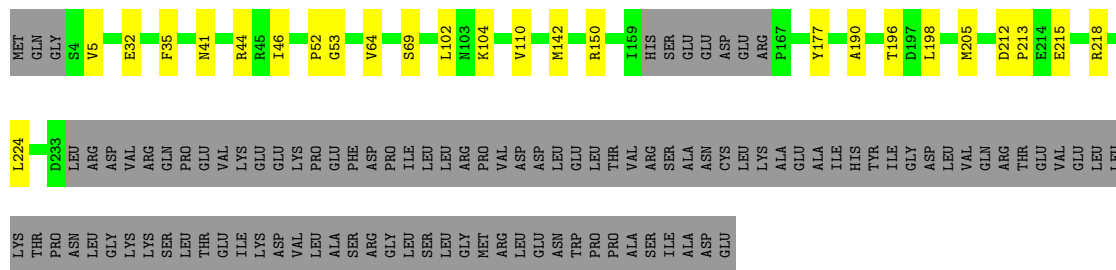
- Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain G:  84% 7% 8%




- Molecule 2: DNA-directed RNA polymerase subunit alpha

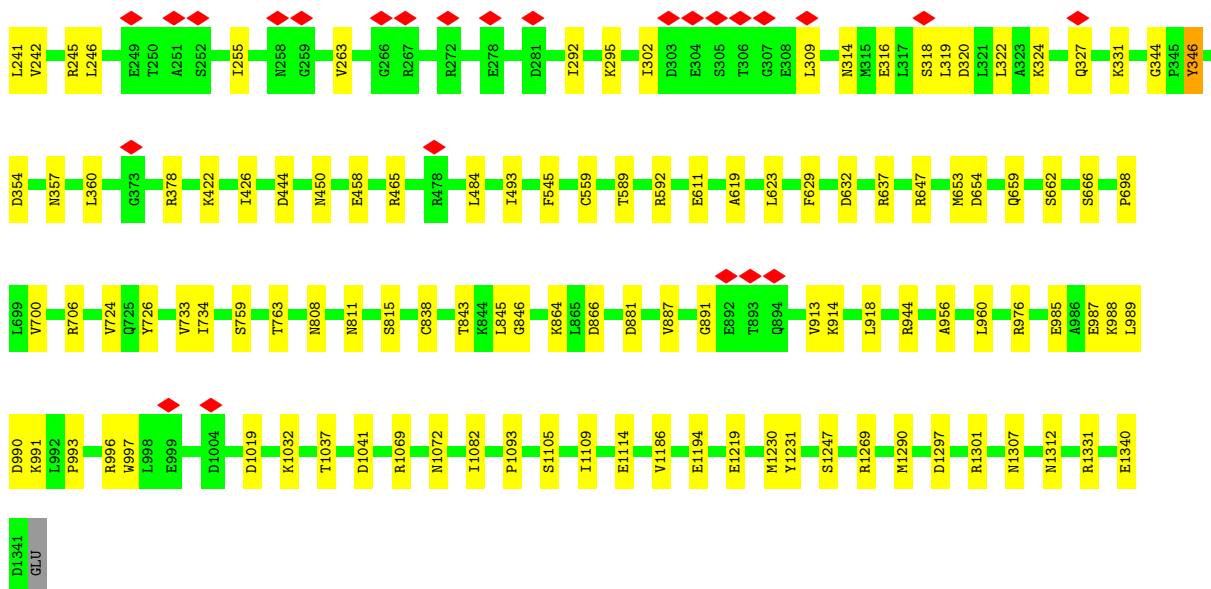
Chain H:  60% 8% 32%



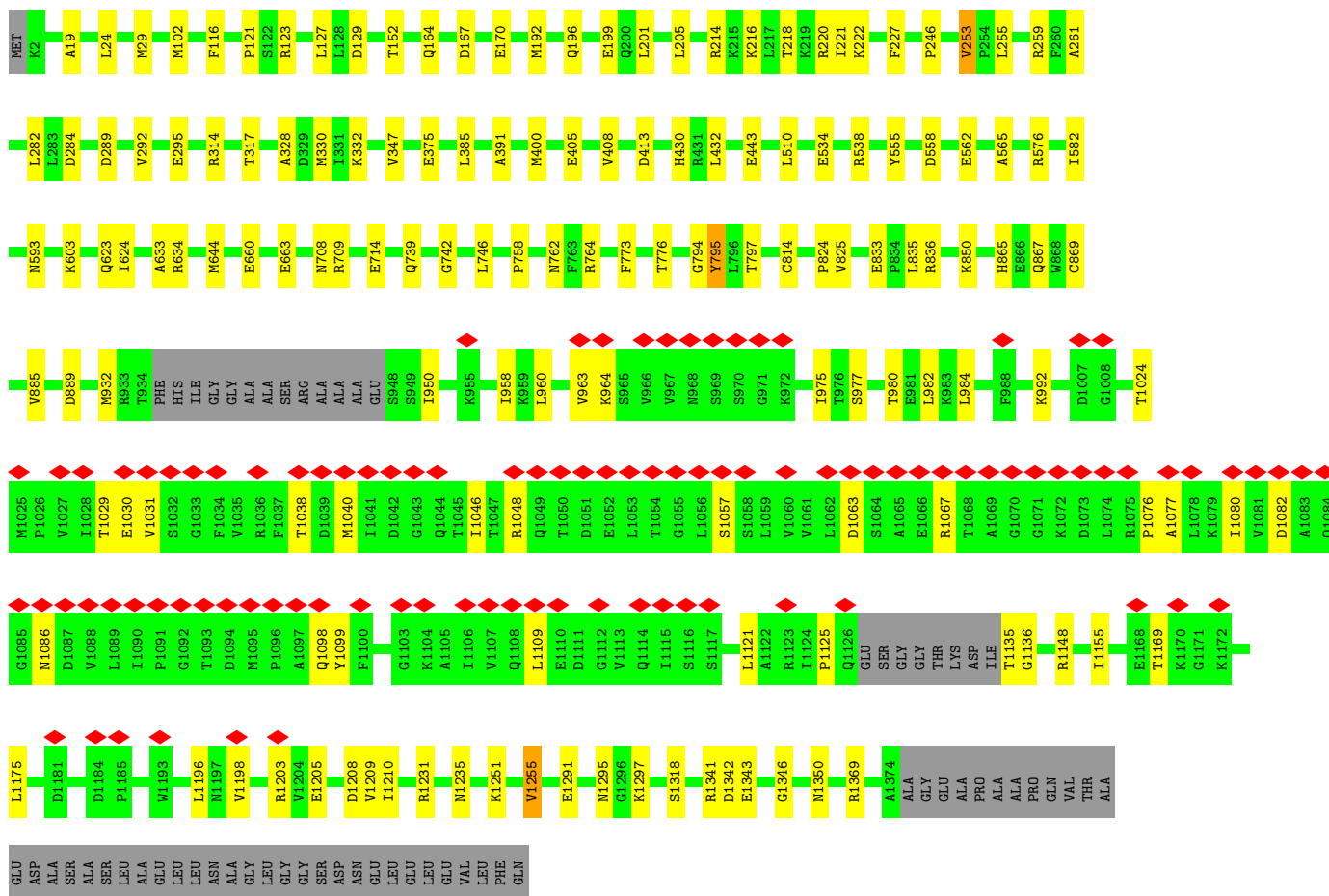
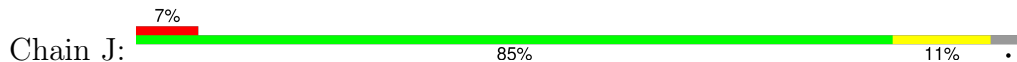
- Molecule 3: DNA-directed RNA polymerase subunit beta

Chain I:  90% 10%

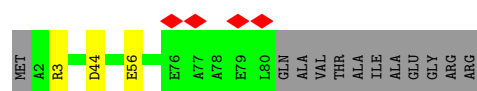




- Molecule 4: DNA-directed RNA polymerase subunit beta'



- Molecule 5: DNA-directed RNA polymerase subunit omega



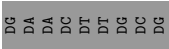
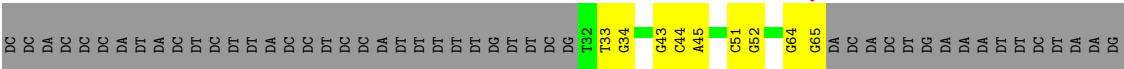
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- [illegible]

- [illegible]

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- The diagram shows a 1000 nm long optical waveguide. The waveguide is represented by a long horizontal grey bar. It is divided into sections labeled with codes: DC, DA, C4, C5, C6, A9, C10, T11, C12, T13, T14, and then a long sequence of DC, DA, DT, DG, and DA. Above the bar, red diamonds indicate input/output points. Below the bar, a sequence of codes (DC, DT, DG, DA) indicates the waveguide's configuration. A green box highlights the section from C4 to T14, and a yellow box highlights the section from C5 to C6.

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118561	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)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.796	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	385.28, 385.28, 385.28	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, POP, ZN

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	0.09	0/2013	0.23	0/2700
1	B	0.11	0/2013	0.25	0/2700
1	C	0.12	0/2013	0.26	0/2700
1	D	0.12	0/2006	0.24	0/2690
1	E	0.12	0/2013	0.25	0/2700
1	F	0.09	0/2013	0.23	0/2700
2	G	0.11	0/2376	0.28	0/3218
2	H	0.10	0/1738	0.27	0/2355
3	I	0.12	0/10736	0.27	0/14487
4	J	0.11	0/10681	0.26	0/14418
5	K	0.11	0/629	0.23	0/847
6	M	0.11	0/3422	0.25	0/4637
7	S	0.16	0/311	0.34	0/480
7	U	0.18	0/790	0.34	0/1216
8	T	0.13	0/240	0.31	0/366
8	V	0.19	0/772	0.39	0/1190
All	All	0.11	0/43766	0.26	0/59404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1979	0	2040	17	0
1	B	1979	0	2040	13	0
1	C	1979	0	2040	10	0
1	D	1972	0	2031	13	0
1	E	1979	0	2040	10	0
1	F	1979	0	2040	14	0
2	G	2347	0	2404	14	0
2	H	1718	0	1756	14	0
3	I	10567	0	10585	77	0
4	J	10523	0	10760	86	0
5	K	627	0	634	1	0
6	M	3371	0	3372	22	0
7	S	276	0	147	4	0
7	U	701	0	381	12	0
8	T	217	0	126	1	0
8	V	693	0	392	5	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0
9	D	31	0	12	0	0
9	E	31	0	12	0	0
9	F	31	0	12	0	0
10	A	1	0	0	0	0
10	E	1	0	0	0	0
10	J	1	0	0	0	0
11	I	9	0	0	0	0
12	J	2	0	0	0	0
13	A	3	0	0	0	0
13	B	3	0	0	0	0
13	C	9	0	0	1	0
13	D	11	0	0	1	0
13	E	13	0	0	0	0
13	F	5	0	0	0	0
13	G	69	0	0	4	0
13	H	28	0	0	0	0
13	I	296	0	0	5	0
13	J	205	0	0	1	0
13	K	9	0	0	0	0
13	M	30	0	0	1	0
13	U	11	0	0	1	0
13	V	11	0	0	0	0
All	All	43810	0	42860	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:158:ARG:NH2	2:G:173:VAL:O	2.23	0.71
3:I:985:GLU:HB3	3:I:988:LYS:HB2	1.73	0.71
4:J:644:MET:O	4:J:764:ARG:NH1	2.24	0.67
1:D:295:ASP:OD1	1:D:295:ASP:N	2.28	0.66
3:I:360:LEU:HD11	3:I:378:ARG:HG3	1.79	0.65
2:G:41:ASN:ND2	13:G:405:HOH:O	2.30	0.65
8:V:51:DC:H2'	8:V:52:DG:C8	2.34	0.63
1:F:142:GLU:O	1:F:147:LYS:NZ	2.29	0.62
3:I:302:ILE:HG22	3:I:309:LEU:HA	1.81	0.62
1:B:289:GLU:OE1	1:B:291:LYS:NZ	2.29	0.62
1:F:234:THR:HG22	1:F:274:ARG:HB3	1.80	0.61
4:J:958:ILE:HD12	4:J:982:LEU:HD11	1.82	0.61
3:I:221:LEU:HD11	3:I:314:ASN:HB2	1.83	0.60
1:F:143:SER:HB3	1:F:146:MET:HG2	1.83	0.60
6:M:41:LEU:HD23	6:M:47:LEU:HB3	1.83	0.60
4:J:205:LEU:HD11	4:J:214:ARG:HD3	1.84	0.60
3:I:866:ASP:OD2	3:I:944:ARG:NH1	2.35	0.60
4:J:1148:ARG:NH1	8:T:6:DC:OP1	2.35	0.60
4:J:1203:ARG:NH1	4:J:1205:GLU:OE1	2.35	0.59
1:A:174:GLU:OE2	1:A:178:ARG:NH1	2.35	0.59
1:F:309:PRO:HG2	1:F:311:ARG:HG2	1.83	0.59
1:B:365:ARG:NH1	1:C:302:VAL:O	2.36	0.59
4:J:255:LEU:HB2	4:J:259:ARG:HG3	1.84	0.59
1:A:159:ALA:O	1:A:274:ARG:NH1	2.36	0.58
4:J:1135:THR:OG1	4:J:1136:GLY:N	2.35	0.58
3:I:444:ASP:O	3:I:450:ASN:ND2	2.35	0.58
4:J:289:ASP:HA	4:J:292:VAL:HG22	1.85	0.58
1:B:343:ALA:HB1	1:B:380:LEU:HD21	1.86	0.57
4:J:510:LEU:HD11	4:J:624:ILE:HG23	1.85	0.57
4:J:314:ARG:HE	6:M:55:GLU:HG3	1.69	0.56
1:A:308:PRO:HG2	1:A:313:ARG:HD2	1.88	0.56
1:F:153:ILE:HD11	1:F:176:VAL:HG13	1.88	0.56
2:G:212:ASP:HB3	2:G:215:GLU:HG2	1.86	0.56
1:E:308:PRO:HG2	1:E:313:ARG:HD2	1.88	0.56
1:B:295:ASP:OD1	1:B:295:ASP:N	2.36	0.56
4:J:708:ASN:OD1	4:J:709:ARG:N	2.37	0.56
3:I:318:SER:OG	3:I:320:ASP:OD1	2.18	0.56
4:J:167:ASP:HA	4:J:170:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:385:THR:HG22	6:M:399:LEU:HD23	1.87	0.56
1:B:153:ILE:HD11	1:B:176:VAL:HG13	1.87	0.55
1:F:159:ALA:O	1:F:274:ARG:NH1	2.39	0.55
3:I:993:PRO:HG2	3:I:996:ARG:HG2	1.88	0.55
4:J:121:PRO:O	4:J:123:ARG:NH1	2.38	0.55
4:J:1341:ARG:NH1	4:J:1343:GLU:OE2	2.39	0.55
3:I:1269:ARG:NH1	13:I:1537:HOH:O	2.39	0.55
7:U:39:DC:H2'	7:U:40:DG:C8	2.42	0.55
6:M:316:SER:OG	6:M:320:ARG:NH1	2.40	0.55
3:I:17:LYS:NZ	3:I:1194:GLU:OE2	2.33	0.55
3:I:623:LEU:HD11	3:I:653:MET:HE1	1.88	0.55
7:U:57:DC:H2''	7:U:58:DA:C8	2.43	0.54
2:H:215:GLU:OE1	2:H:218:ARG:NH2	2.40	0.54
3:I:242:VAL:HB	3:I:245:ARG:HG2	1.89	0.54
2:G:104:LYS:HG2	2:G:110:VAL:HG22	1.88	0.54
3:I:324:LYS:O	3:I:327:GLN:NE2	2.40	0.54
1:E:326:LYS:O	1:E:330:ARG:HG2	2.08	0.54
4:J:282:LEU:HD11	6:M:45:PRO:HG3	1.90	0.54
3:I:843:THR:OG1	3:I:846:GLY:O	2.23	0.53
4:J:708:ASN:ND2	4:J:714:GLU:OE2	2.41	0.53
7:S:88:DT:H2'	7:S:89:DG:C8	2.44	0.53
1:A:156:ILE:HD12	1:A:303:ILE:HD13	1.89	0.53
3:I:887:VAL:HB	3:I:913:VAL:HB	1.90	0.53
4:J:1291:GLU:OE2	4:J:1295:ASN:ND2	2.41	0.53
1:E:239:GLU:HG3	1:E:242:GLU:HG2	1.90	0.53
3:I:956:ALA:HB1	3:I:1032:LYS:HD3	1.91	0.53
4:J:391:ALA:HB2	4:J:400:MET:HE2	1.91	0.53
1:F:362:VAL:HG13	1:F:383:LEU:HD22	1.92	0.52
3:I:122:VAL:HG11	3:I:493:ILE:HD11	1.92	0.52
6:M:378:GLU:N	6:M:378:GLU:OE1	2.43	0.52
1:A:162:PRO:HA	1:A:275:ILE:O	2.10	0.52
3:I:1331:ARG:NH1	13:I:1531:HOH:O	2.36	0.52
4:J:742:GLY:O	4:J:762:ASN:HB3	2.08	0.52
1:D:365:ARG:NH2	13:D:503:HOH:O	2.41	0.52
4:J:836:ARG:HG3	4:J:869:CYS:HB3	1.91	0.52
4:J:1077:ALA:HB3	4:J:1098:GLN:HE21	1.75	0.52
7:U:51:DT:H2''	7:U:52:DA:C8	2.44	0.52
3:I:1082:ILE:HD11	3:I:1093:PRO:HG2	1.92	0.51
3:I:706:ARG:NH1	13:I:1543:HOH:O	2.44	0.51
3:I:1219:GLU:OE1	4:J:634:ARG:NH2	2.44	0.51
7:U:28:DA:H2''	7:U:29:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:811:ASN:HA	3:I:815:SER:HB2	1.92	0.51
3:I:985:GLU:HB2	3:I:989:LEU:HB2	1.92	0.51
4:J:1109:LEU:HD22	4:J:1121:LEU:HD23	1.92	0.51
1:F:325:LEU:HD11	1:F:336:VAL:HG11	1.92	0.51
7:U:27:DC:H2"	7:U:28:DA:C8	2.45	0.51
2:H:46:ILE:HD11	2:H:224:LEU:HD13	1.93	0.51
2:G:282:VAL:HG13	2:G:316:MET:HB2	1.93	0.50
3:I:1069:ARG:NH2	3:I:1114:GLU:OE2	2.39	0.50
4:J:977:SER:OG	4:J:980:THR:OG1	2.26	0.50
1:C:195:ASN:HB2	1:D:253:ARG:HD3	1.93	0.50
4:J:1048:ARG:NH1	4:J:1057:SER:OG	2.45	0.50
1:A:195:ASN:HB2	1:B:253:ARG:HD3	1.93	0.50
4:J:1038:THR:O	4:J:1076:PRO:HA	2.12	0.50
6:M:377:HIS:HB2	8:V:43:DG:H5"	1.94	0.50
3:I:102:LEU:HB3	3:I:118:LYS:HG3	1.94	0.50
4:J:102:MET:HG2	4:J:246:PRO:HD3	1.92	0.50
6:M:33:LEU:HD23	6:M:295:PRO:HG2	1.94	0.50
2:G:72:GLU:O	13:G:401:HOH:O	2.19	0.49
7:U:55:DT:H2"	7:U:56:DA:C8	2.47	0.49
3:I:103:VAL:HG12	3:I:117:ILE:HG22	1.95	0.49
1:D:308:PRO:HG2	1:D:313:ARG:HD2	1.94	0.49
2:G:15:ASP:OD1	2:G:16:ILE:N	2.45	0.49
4:J:814:CYS:HB2	4:J:889:ASP:HB2	1.94	0.49
1:E:379:GLU:OE1	1:E:379:GLU:N	2.45	0.49
2:G:71:LYS:NZ	13:G:401:HOH:O	2.45	0.49
4:J:127:LEU:HG	4:J:192:MET:HE1	1.93	0.49
3:I:241:LEU:HD21	3:I:246:LEU:HD21	1.94	0.49
4:J:1251:LYS:O	4:J:1255:VAL:HG13	2.13	0.49
7:S:77:DA:H2"	7:S:78:DA:C8	2.47	0.49
1:B:209:PHE:HE1	1:B:254:VAL:HG11	1.77	0.49
1:D:153:ILE:HD11	1:D:176:VAL:HG13	1.95	0.49
3:I:960:LEU:HD11	3:I:1032:LYS:HD2	1.95	0.49
1:A:285:GLU:N	1:A:285:GLU:OE1	2.45	0.48
3:I:55:SER:OG	3:I:465:ARG:NH1	2.47	0.48
3:I:698:PRO:HA	3:I:1231:TYR:CE1	2.48	0.48
4:J:328:ALA:O	4:J:332:LYS:HG2	2.13	0.48
1:B:318:ILE:HG12	1:B:348:LEU:HD21	1.96	0.48
3:I:292:ILE:HB	3:I:322:LEU:HD11	1.96	0.48
1:C:293:ARG:NH1	13:C:503:HOH:O	2.46	0.48
4:J:1063:ASP:O	4:J:1067:ARG:HG3	2.13	0.48
3:I:838:CYS:HB2	3:I:918:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1082:ASP:OD1	4:J:1086:ASN:N	2.39	0.48
1:A:149:ILE:O	1:A:153:ILE:HG12	2.13	0.48
2:G:228:LEU:HD21	2:H:224:LEU:HB3	1.95	0.48
4:J:1040:MET:HB3	4:J:1046:ILE:HD13	1.96	0.48
1:F:249:ALA:HA	1:F:252:LEU:HD13	1.95	0.48
7:U:31:DA:H2''	7:U:32:DA:C8	2.49	0.48
4:J:825:VAL:HB	4:J:833:GLU:HB3	1.96	0.47
6:M:207:ASP:N	6:M:207:ASP:OD1	2.47	0.47
1:D:379:GLU:N	1:D:379:GLU:OE1	2.47	0.47
3:I:13:LYS:NZ	13:I:1550:HOH:O	2.47	0.47
4:J:950:ILE:HG21	4:J:982:LEU:HD23	1.96	0.47
1:A:186:ARG:NH1	1:A:232:GLY:O	2.47	0.47
2:H:102:LEU:HB3	2:H:142:MET:HG2	1.97	0.47
3:I:23:ASP:OD1	3:I:23:ASP:N	2.47	0.47
4:J:885:VAL:HG21	4:J:1255:VAL:HG12	1.95	0.47
4:J:1231:ARG:O	4:J:1235:ASN:ND2	2.35	0.47
8:V:33:DT:H2''	8:V:34:DG:C8	2.49	0.47
1:E:295:ASP:O	1:E:299:ARG:NH1	2.45	0.47
4:J:430:HIS:CE1	4:J:432:LEU:HB2	2.49	0.47
1:C:153:ILE:HD11	1:C:176:VAL:HG13	1.96	0.47
1:E:342:SER:HB2	1:E:377:ARG:HH11	1.79	0.46
2:H:196:THR:HG21	4:J:443:GLU:HG3	1.97	0.46
2:G:31:LEU:HD13	2:G:36:GLY:HA2	1.98	0.46
3:I:422:LYS:O	3:I:426:ILE:HG12	2.15	0.46
3:I:632:ASP:OD1	3:I:647:ARG:NH2	2.48	0.46
3:I:845:LEU:HD13	3:I:891:GLY:HA3	1.97	0.46
4:J:739:GLN:NE2	13:J:1639:HOH:O	2.44	0.46
6:M:455:ARG:NH1	13:M:504:HOH:O	2.38	0.46
1:A:176:VAL:HG21	1:A:307:ILE:HD11	1.98	0.46
2:H:104:LYS:HD2	2:H:110:VAL:HG22	1.97	0.46
6:M:318:PHE:O	6:M:322:ASN:ND2	2.30	0.46
3:I:192:ASP:HB3	3:I:346:TYR:HD1	1.80	0.46
6:M:268:GLU:HG3	6:M:269:PRO:HD2	1.98	0.46
3:I:344:GLY:HA3	3:I:346:TYR:CZ	2.51	0.46
6:M:149:ASP:OD1	6:M:151:THR:OG1	2.29	0.46
4:J:558:ASP:N	4:J:562:GLU:O	2.47	0.46
3:I:160:ASP:OD2	3:I:171:LEU:HB2	2.15	0.45
3:I:611:GLU:OE2	3:I:637:ARG:NH2	2.48	0.45
3:I:864:LYS:NZ	3:I:881:ASP:OD2	2.50	0.45
1:C:185:ASP:OD1	1:C:185:ASP:N	2.49	0.45
3:I:232:ILE:HB	3:I:331:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1297:ASP:O	3:I:1301:ARG:HG3	2.16	0.45
1:A:271:VAL:HG23	1:A:272:ASN:H	1.80	0.45
4:J:1024:THR:HG22	4:J:1125:PRO:HA	1.97	0.45
6:M:315:ASP:OD1	6:M:315:ASP:N	2.48	0.45
8:V:44:DC:H2"	8:V:45:DA:C8	2.52	0.45
2:G:8:PHE:HD2	2:G:32:GLU:HG3	1.80	0.45
6:M:144:ILE:HG12	6:M:161:ILE:HD13	1.97	0.45
3:I:987:GLU:HG2	3:I:991:LYS:HE3	1.97	0.45
4:J:773:PHE:O	4:J:776:THR:OG1	2.33	0.45
4:J:1196:LEU:HD11	4:J:1210:ILE:HG22	1.99	0.45
3:I:1072:ASN:HD21	3:I:1230:MET:HE1	1.81	0.45
3:I:1247:SER:HB2	4:J:375:GLU:O	2.17	0.45
1:A:252:LEU:HB2	1:A:296:LEU:HD13	1.98	0.45
2:H:64:VAL:HG13	2:H:69:SER:HB2	1.98	0.45
1:F:212:GLU:OE1	1:F:262:ARG:NH2	2.47	0.44
3:I:21:VAL:HG21	3:I:592:ARG:HD3	1.98	0.44
3:I:1307:ASN:HB3	3:I:1312:ASN:O	2.16	0.44
7:S:82:DT:H2"	7:S:83:DA:C8	2.52	0.44
3:I:211:ARG:CZ	3:I:357:ASN:HA	2.47	0.44
4:J:795:TYR:CZ	7:S:89:DG:H5'	2.52	0.44
1:C:251:LEU:O	1:C:255:ILE:HG12	2.17	0.44
7:U:34:DT:H2"	7:U:35:DG:C8	2.51	0.44
2:H:52:PRO:HG3	2:H:150:ARG:NH1	2.31	0.44
8:V:64:DG:H2"	8:V:65:DG:C8	2.53	0.44
6:M:302:HIS:CE1	6:M:306:MET:HE3	2.53	0.44
6:M:199:LEU:HB3	6:M:220:ILE:HD13	2.00	0.44
2:H:190:ALA:O	2:H:198:LEU:HB2	2.17	0.43
3:I:724:VAL:HA	3:I:734:ILE:HD13	1.99	0.43
4:J:534:GLU:O	4:J:538:ARG:HG2	2.18	0.43
2:H:32:GLU:HB2	2:H:35:PHE:CD1	2.53	0.43
3:I:1340:GLU:HB2	4:J:19:ALA:HB3	1.99	0.43
3:I:759:SER:OG	3:I:763:THR:OG1	2.29	0.43
4:J:282:LEU:HD22	4:J:295:GLU:HG3	2.00	0.43
1:D:228:GLU:OE2	1:D:262:ARG:NH1	2.51	0.43
3:I:808:ASN:H	4:J:633:ALA:HB2	1.82	0.43
3:I:196:VAL:HG23	3:I:206:ALA:HA	2.00	0.43
3:I:1290:MET:HG3	4:J:347:VAL:HG11	2.00	0.43
4:J:746:LEU:HD23	4:J:758:PRO:HB3	1.99	0.43
1:D:168:GLU:O	1:D:173:LYS:NZ	2.52	0.43
2:G:76:GLU:O	13:G:402:HOH:O	2.21	0.43
4:J:1208:ASP:OD1	4:J:1209:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:HG3	1:A:242:GLU:HG2	2.00	0.43
1:B:376:ASP:OD1	1:B:377:ARG:N	2.47	0.43
1:F:143:SER:HB2	1:F:316:ASP:OD1	2.18	0.43
3:I:65:ASN:O	3:I:105:TYR:N	2.39	0.43
4:J:960:LEU:HD13	4:J:963:VAL:HG21	2.01	0.43
4:J:964:LYS:HD3	4:J:977:SER:HB3	2.00	0.43
6:M:37:LEU:HD22	6:M:297:LEU:HD11	2.00	0.43
3:I:666:SER:HA	3:I:1186:VAL:HG11	2.01	0.43
6:M:278:VAL:HG22	6:M:287:VAL:HG22	2.00	0.43
1:E:196:VAL:HG21	1:E:240:ILE:HD12	2.01	0.43
3:I:179:TYR:OH	3:I:458:GLU:OE2	2.33	0.43
1:B:140:VAL:HG11	1:B:319:PRO:HB2	2.01	0.42
2:G:135:ASP:HB3	2:G:138:ALA:HB2	2.01	0.42
3:I:589:THR:OG1	3:I:659:GLN:OE1	2.36	0.42
4:J:24:LEU:HD21	4:J:116:PHE:CZ	2.54	0.42
4:J:218:THR:O	4:J:222:LYS:HG2	2.19	0.42
1:E:295:ASP:HB3	1:E:299:ARG:HH12	1.84	0.42
2:G:14:VAL:HG21	2:G:29:GLU:HB3	2.02	0.42
3:I:106:GLU:HB2	3:I:113:THR:HB	2.00	0.42
3:I:629:PHE:HB2	3:I:647:ARG:HD3	2.01	0.42
3:I:1072:ASN:OD1	3:I:1072:ASN:N	2.51	0.42
4:J:660:GLU:O	4:J:663:GLU:HG3	2.19	0.42
6:M:299:ILE:HD11	6:M:327:LYS:HG3	2.02	0.42
4:J:196:GLN:O	4:J:199:GLU:HG3	2.19	0.42
4:J:1040:MET:HE3	4:J:1046:ILE:HG21	2.02	0.42
3:I:1109:ILE:HD12	4:J:644:MET:HE1	2.01	0.42
4:J:1029:THR:HA	4:J:1099:TYR:CZ	2.54	0.42
4:J:1175:LEU:HD21	4:J:1198:VAL:HG21	2.00	0.42
1:C:314:LYS:NZ	1:C:348:LEU:O	2.38	0.42
4:J:576:ARG:HD3	4:J:593:ASN:HA	2.02	0.42
3:I:316:GLU:OE1	3:I:316:GLU:N	2.49	0.42
4:J:850:LYS:HB2	4:J:850:LYS:HE3	1.80	0.42
2:H:205:MET:HG3	2:H:213:PRO:HB3	2.02	0.42
3:I:255:ILE:HB	3:I:263:VAL:HB	2.01	0.42
1:D:195:ASN:HB2	1:E:253:ARG:HD3	2.02	0.42
2:H:53:GLY:HA3	2:H:177:TYR:O	2.20	0.42
1:A:185:ASP:OD1	1:A:185:ASP:N	2.52	0.41
3:I:698:PRO:C	3:I:700:VAL:H	2.28	0.41
1:D:318:ILE:HG12	1:D:348:LEU:HD21	2.02	0.41
1:D:342:SER:HB2	1:D:377:ARG:HE	1.84	0.41
4:J:317:THR:HB	6:M:56:ILE:HD11	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1031:VAL:HG23	4:J:1080:ILE:HG21	2.03	0.41
7:U:29:DG:H2"	7:U:30:DA:H8	1.85	0.41
1:C:322:ASN:O	1:C:326:LYS:HG2	2.20	0.41
2:H:205:MET:HE3	2:H:205:MET:HB2	1.90	0.41
4:J:129:ASP:OD2	4:J:220:ARG:NH1	2.54	0.41
1:F:144:PRO:HA	1:F:147:LYS:HE2	2.02	0.41
7:U:43:DA:N7	13:U:103:HOH:O	2.37	0.41
1:B:162:PRO:HA	1:B:275:ILE:O	2.20	0.41
1:B:195:ASN:HB2	1:C:253:ARG:HD3	2.02	0.41
4:J:984:LEU:HD23	4:J:992:LYS:HB2	2.02	0.41
7:U:31:DA:H2"	7:U:32:DA:H8	1.85	0.41
1:C:234:THR:HG22	1:C:274:ARG:HB3	2.02	0.41
4:J:201:LEU:HD11	4:J:220:ARG:HD3	2.01	0.41
4:J:794:GLY:HA2	4:J:797:THR:HG22	2.02	0.41
4:J:1030:GLU:N	4:J:1099:TYR:OH	2.43	0.41
4:J:1318:SER:OG	4:J:1342:ASP:OD2	2.35	0.41
1:A:163:VAL:HB	1:A:276:LEU:HD22	2.02	0.41
1:E:217:THR:O	1:F:217:THR:HG22	2.20	0.41
3:I:1041:ASP:OD1	3:I:1041:ASP:N	2.44	0.41
3:I:1105:SER:HB3	13:I:1631:HOH:O	2.21	0.41
4:J:385:LEU:HD13	4:J:400:MET:HE3	2.02	0.41
4:J:824:PRO:HD3	4:J:835:LEU:HD13	2.02	0.41
7:U:57:DC:H2"	7:U:58:DA:N7	2.36	0.41
4:J:164:GLN:HA	4:J:167:ASP:OD2	2.21	0.41
4:J:865:HIS:CE1	4:J:867:GLN:HB2	2.56	0.41
3:I:186:PHE:CD2	3:I:196:VAL:HG22	2.56	0.41
3:I:545:PHE:HZ	4:J:932:MET:HE1	1.86	0.41
3:I:726:TYR:HB3	3:I:733:VAL:HB	2.01	0.41
4:J:555:TYR:CE2	4:J:565:ALA:HB2	2.56	0.41
4:J:582:ILE:HD12	4:J:623:GLN:HB3	2.03	0.41
1:A:147:LYS:O	1:A:151:GLU:HG2	2.20	0.41
4:J:405:GLU:O	4:J:408:VAL:HG22	2.21	0.41
4:J:1346:GLY:O	4:J:1350:ASN:ND2	2.46	0.41
5:K:3:ARG:NH1	5:K:44:ASP:OD2	2.54	0.41
1:A:283:ILE:HD11	1:A:292:PHE:CD2	2.55	0.40
1:D:376:ASP:OD1	1:D:377:ARG:N	2.42	0.40
2:H:41:ASN:OD1	2:H:44:ARG:NH2	2.48	0.40
3:I:292:ILE:HA	3:I:295:LYS:HG2	2.03	0.40
3:I:484:LEU:H	3:I:484:LEU:HD22	1.86	0.40
4:J:1155:ILE:HB	4:J:1210:ILE:HB	2.03	0.40
3:I:559:CYS:HB2	3:I:662:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:253:VAL:HG23	4:J:261:ALA:HB3	2.04	0.40
1:D:143:SER:N	1:D:316:ASP:OD1	2.54	0.40
3:I:619:ALA:HB2	3:I:654:ASP:HB2	2.04	0.40
3:I:976:ARG:HB2	3:I:997:TRP:CZ3	2.57	0.40
1:B:324:PHE:CE2	1:B:360:LYS:HG2	2.57	0.40
1:F:252:LEU:HD21	1:F:293:ARG:HH21	1.87	0.40
4:J:216:LYS:HE3	4:J:216:LYS:HB2	1.84	0.40
6:M:15:MET:SD	6:M:15:MET:N	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	245/268 (91%)	237 (97%)	8 (3%)	0	100	100
1	B	245/268 (91%)	239 (98%)	6 (2%)	0	100	100
1	C	245/268 (91%)	240 (98%)	5 (2%)	0	100	100
1	D	244/268 (91%)	237 (97%)	7 (3%)	0	100	100
1	E	245/268 (91%)	238 (97%)	7 (3%)	0	100	100
1	F	245/268 (91%)	242 (99%)	3 (1%)	0	100	100
2	G	296/329 (90%)	290 (98%)	6 (2%)	0	100	100
2	H	219/329 (67%)	214 (98%)	5 (2%)	0	100	100
3	I	1338/1342 (100%)	1308 (98%)	30 (2%)	0	100	100
4	J	1346/1415 (95%)	1319 (98%)	27 (2%)	0	100	100
5	K	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
6	M	419/477 (88%)	409 (98%)	9 (2%)	1 (0%)	44	68
All	All	5164/5591 (92%)	5048 (98%)	115 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	20	GLN

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	212/233 (91%)	206 (97%)	6 (3%)	38	68
1	B	212/233 (91%)	211 (100%)	1 (0%)	86	95
1	C	212/233 (91%)	212 (100%)	0	100	100
1	D	211/233 (91%)	209 (99%)	2 (1%)	75	90
1	E	212/233 (91%)	212 (100%)	0	100	100
1	F	212/233 (91%)	211 (100%)	1 (0%)	86	95
2	G	261/286 (91%)	258 (99%)	3 (1%)	70	87
2	H	191/286 (67%)	189 (99%)	2 (1%)	73	89
3	I	1155/1157 (100%)	1145 (99%)	10 (1%)	75	90
4	J	1135/1176 (96%)	1120 (99%)	15 (1%)	65	85
5	K	67/75 (89%)	66 (98%)	1 (2%)	60	83
6	M	379/428 (89%)	371 (98%)	8 (2%)	48	76
All	All	4459/4806 (93%)	4410 (99%)	49 (1%)	69	87

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ILE
1	A	238	ASP
1	A	294	GLU
1	A	310	LEU
1	A	312	GLU
1	A	368	LEU
1	B	274	ARG
1	D	251	LEU

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Mol	Chain	Res	Type
1	D	295	ASP
1	F	295	ASP
2	G	64	VAL
2	G	235	ARG
2	G	282	VAL
2	H	5	VAL
2	H	212	ASP
3	I	122	VAL
3	I	207	THR
3	I	239	MET
3	I	319	LEU
3	I	346	TYR
3	I	354	ASP
3	I	914	LYS
3	I	990	ASP
3	I	1019	ASP
3	I	1037	THR
4	J	29	MET
4	J	152	THR
4	J	221	ILE
4	J	227	PHE
4	J	253	VAL
4	J	284	ASP
4	J	330	MET
4	J	413	ASP
4	J	603	LYS
4	J	795	TYR
4	J	975	ILE
4	J	1169	THR
4	J	1255	VAL
4	J	1297	LYS
4	J	1369	ARG
5	K	56	GLU
6	M	21	GLN
6	M	55	GLU
6	M	111	VAL
6	M	276	VAL
6	M	294	ILE
6	M	315	ASP
6	M	399	LEU
6	M	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	HIS
1	C	282	ASN
1	E	280	ASN
2	H	37	HIS
2	H	75	GLN
2	H	103	ASN
2	H	186	ASN
3	I	235	ASN
3	I	314	ASN
3	I	677	ASN
3	I	686	GLN
3	I	1013	GLN
3	I	1023	HIS
3	I	1116	HIS
3	I	1209	GLN
3	I	1288	GLN
4	J	157	GLN
4	J	424	ASN
4	J	488	ASN
4	J	623	GLN
4	J	669	GLN
4	J	720	ASN
4	J	739	GLN
4	J	1126	GLN
5	K	31	GLN
6	M	302	HIS
6	M	387	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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
9	ATP	A	401	10	28,33,33	0.70	0	34,52,52	0.79	2 (5%)
9	ATP	B	401	-	28,33,33	0.65	0	34,52,52	0.76	2 (5%)
9	ATP	E	401	10	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
11	POP	I	1401	-	6,8,8	0.78	0	12,13,13	0.95	0
9	ATP	D	401	-	28,33,33	0.64	0	34,52,52	0.63	1 (2%)
9	ATP	F	401	-	28,33,33	0.63	0	34,52,52	0.80	2 (5%)
9	ATP	C	401	-	28,33,33	0.65	0	34,52,52	0.67	1 (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
9	ATP	A	401	10	-	4/18/38/38	0/3/3/3
9	ATP	B	401	-	-	6/18/38/38	0/3/3/3
9	ATP	E	401	10	-	0/18/38/38	0/3/3/3
11	POP	I	1401	-	-	3/6/6/6	-
9	ATP	D	401	-	-	3/18/38/38	0/3/3/3
9	ATP	F	401	-	-	9/18/38/38	0/3/3/3
9	ATP	C	401	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	401	ATP	C4'-O4'-C1'	-3.02	107.16	109.92
9	A	401	ATP	C4'-O4'-C1'	-2.81	107.35	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	401	ATP	C4'-O4'-C1'	-2.57	107.57	109.92
9	D	401	ATP	C5-C6-N6	2.32	123.84	120.31
9	A	401	ATP	C5-C6-N6	2.31	123.83	120.31
9	B	401	ATP	C5-C6-N6	2.31	123.83	120.31
9	F	401	ATP	C5-C6-N6	2.29	123.80	120.31
9	E	401	ATP	C5-C6-N6	2.28	123.79	120.31
9	C	401	ATP	C5-C6-N6	2.27	123.76	120.31

There are no chirality outliers.

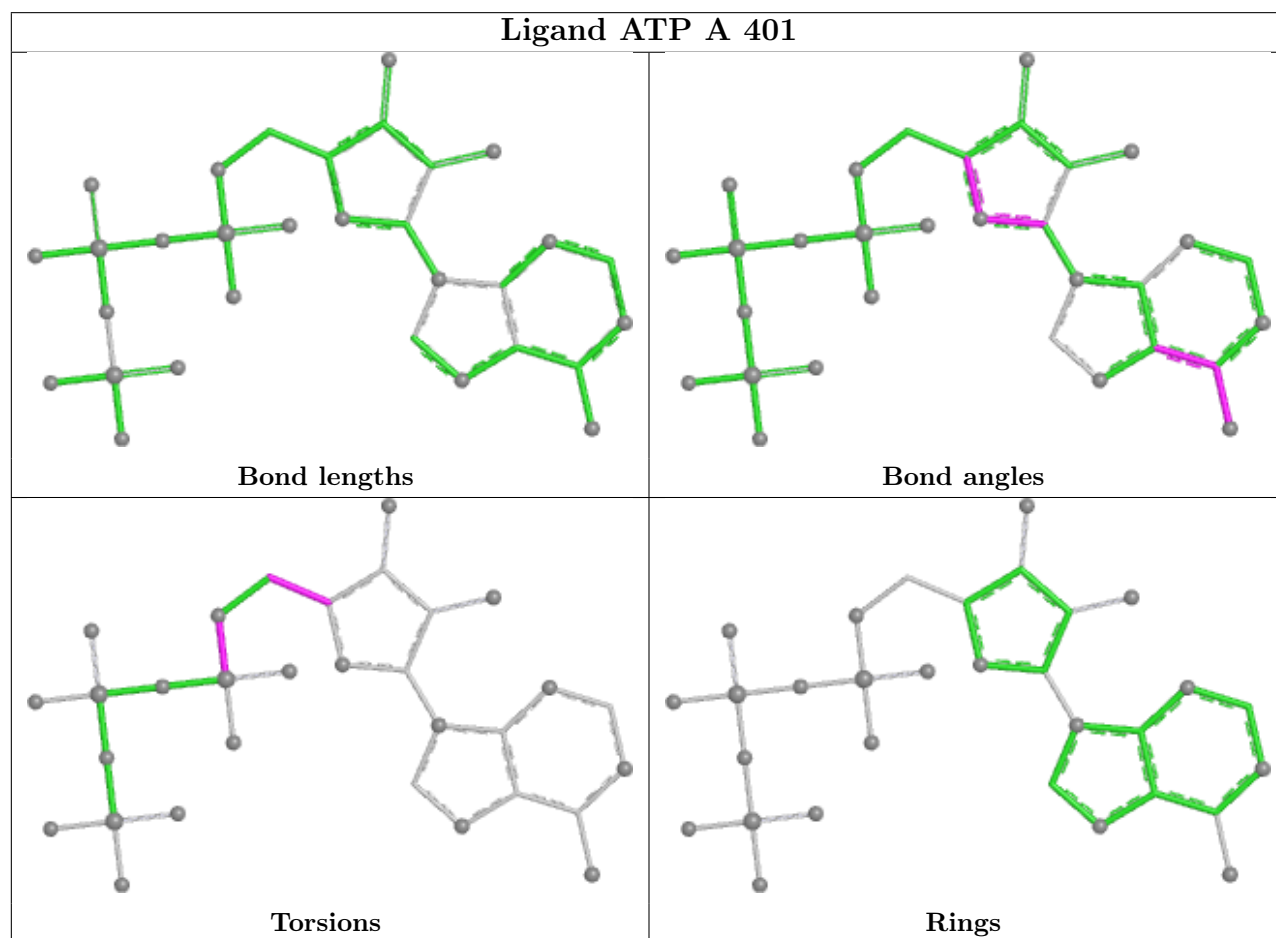
All (29) torsion outliers are listed below:

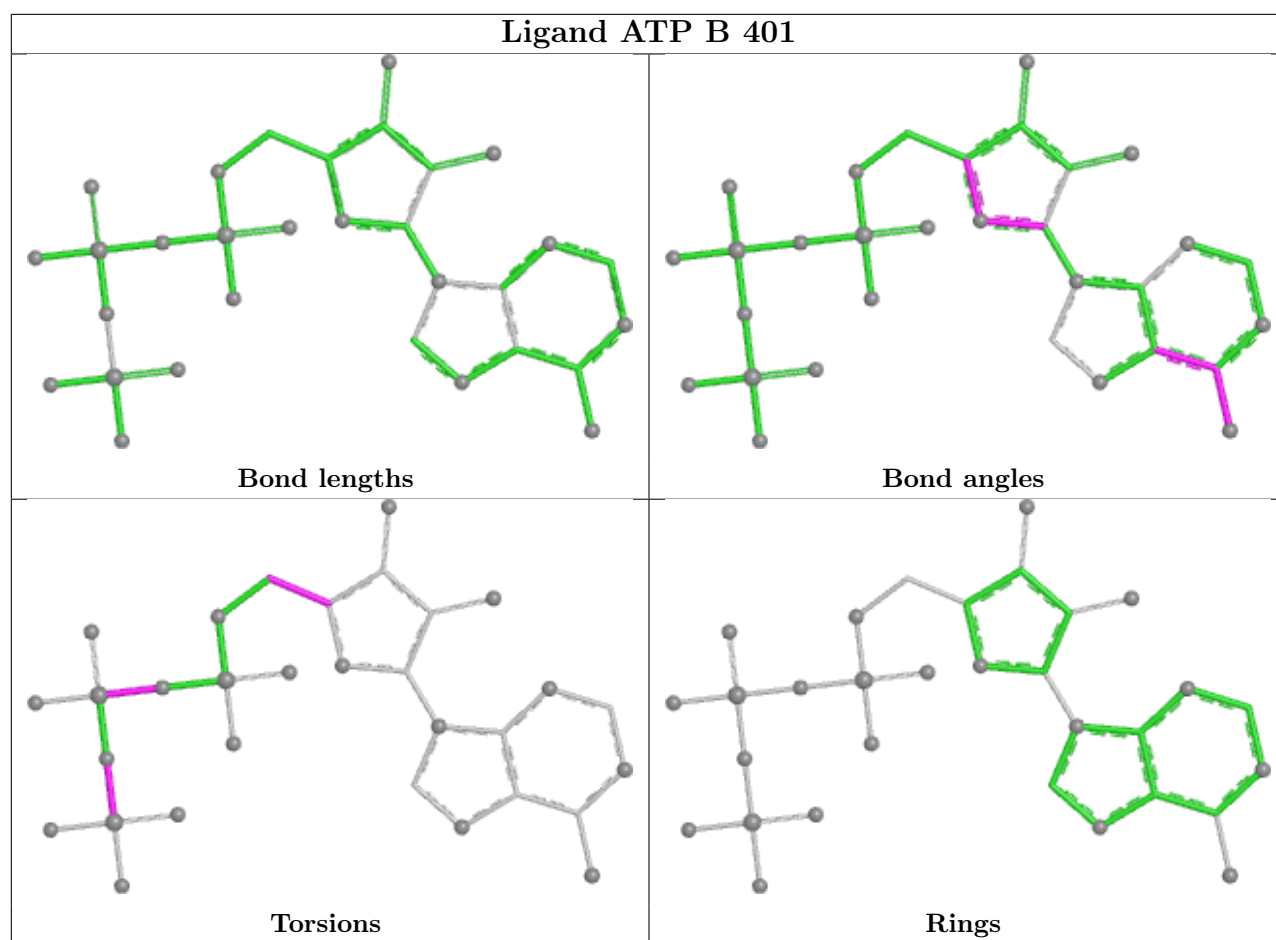
Mol	Chain	Res	Type	Atoms
9	A	401	ATP	C5'-O5'-PA-O2A
9	A	401	ATP	C5'-O5'-PA-O3A
9	B	401	ATP	PB-O3B-PG-O2G
9	C	401	ATP	PB-O3B-PG-O2G
9	D	401	ATP	PB-O3B-PG-O2G
9	F	401	ATP	C5'-O5'-PA-O1A
9	F	401	ATP	C5'-O5'-PA-O3A
9	A	401	ATP	O4'-C4'-C5'-O5'
9	B	401	ATP	C3'-C4'-C5'-O5'
9	A	401	ATP	C3'-C4'-C5'-O5'
9	B	401	ATP	O4'-C4'-C5'-O5'
9	B	401	ATP	PA-O3A-PB-O1B
9	F	401	ATP	O4'-C4'-C5'-O5'
11	I	1401	POP	P2-O-P1-O1
9	C	401	ATP	PB-O3B-PG-O3G
9	D	401	ATP	PB-O3B-PG-O3G
9	C	401	ATP	PA-O3A-PB-O1B
9	D	401	ATP	PA-O3A-PB-O1B
9	F	401	ATP	PG-O3B-PB-O1B
9	F	401	ATP	C4'-C5'-O5'-PA
9	F	401	ATP	PB-O3A-PA-O1A
9	B	401	ATP	PB-O3B-PG-O1G
9	B	401	ATP	PB-O3B-PG-O3G
11	I	1401	POP	P2-O-P1-O2
11	I	1401	POP	P2-O-P1-O3
9	F	401	ATP	PB-O3A-PA-O2A
9	C	401	ATP	PB-O3B-PG-O1G
9	F	401	ATP	C3'-C4'-C5'-O5'
9	F	401	ATP	PG-O3B-PB-O2B

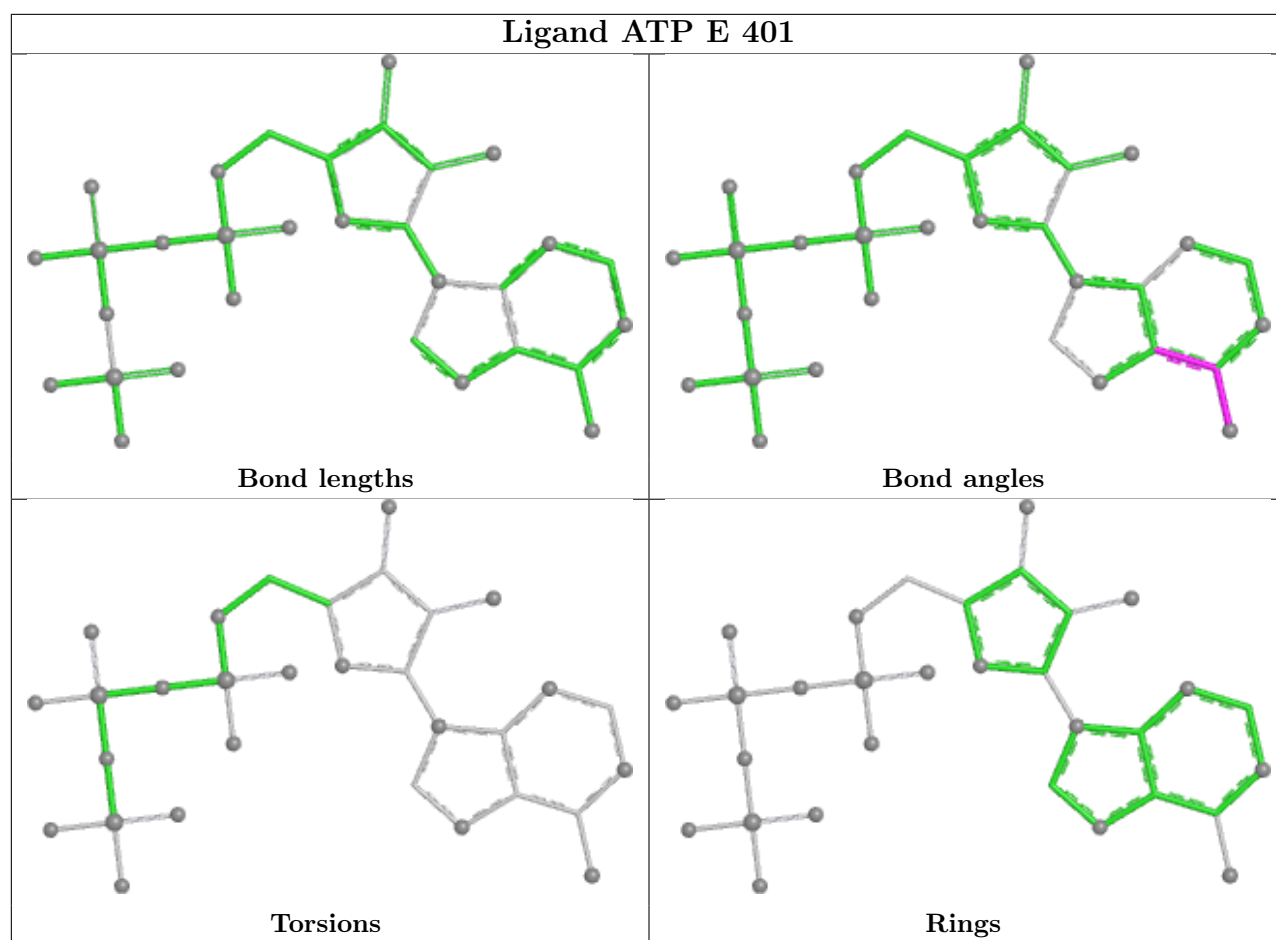
There are no ring outliers.

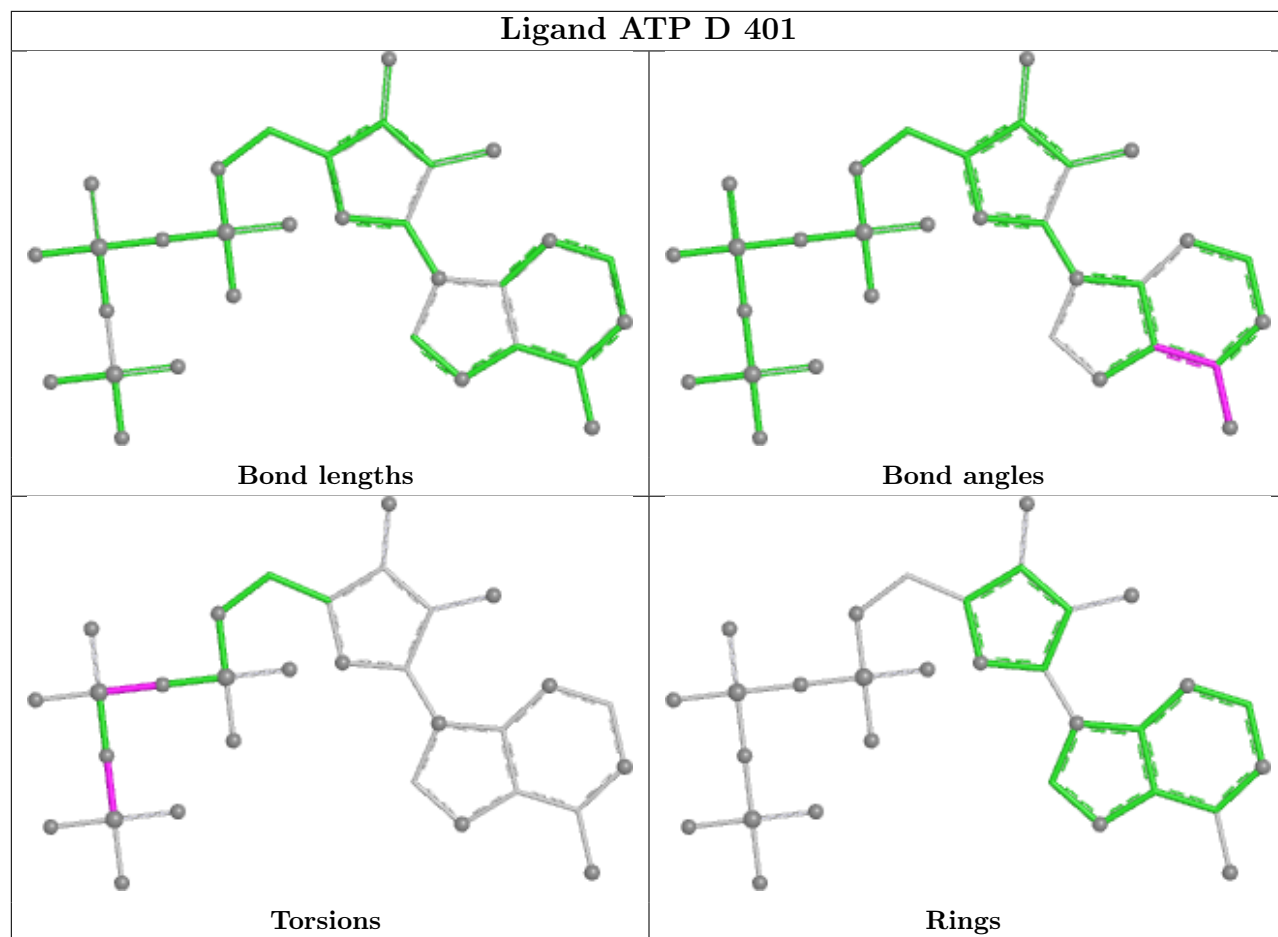
No monomer is involved in short contacts.

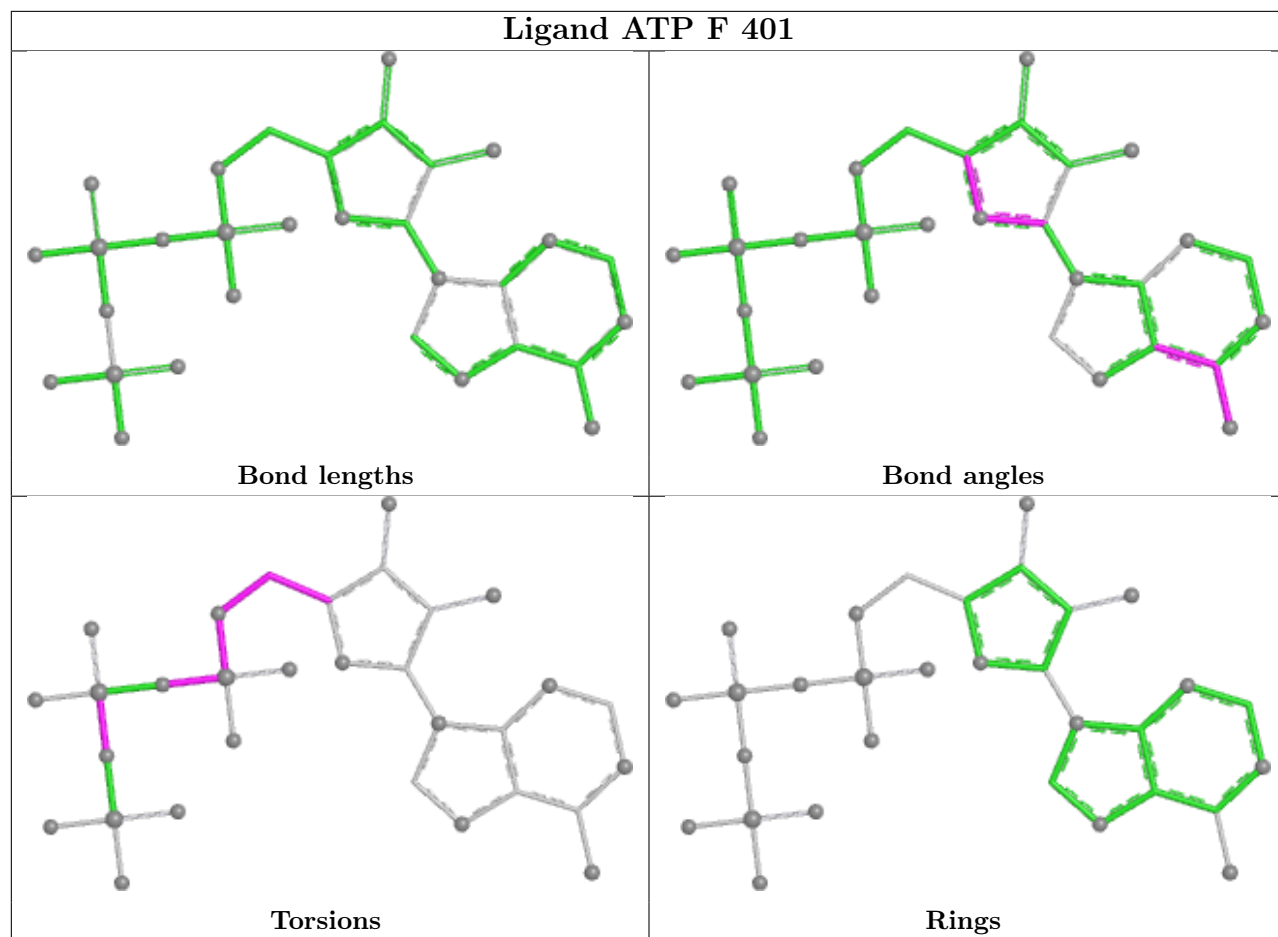
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

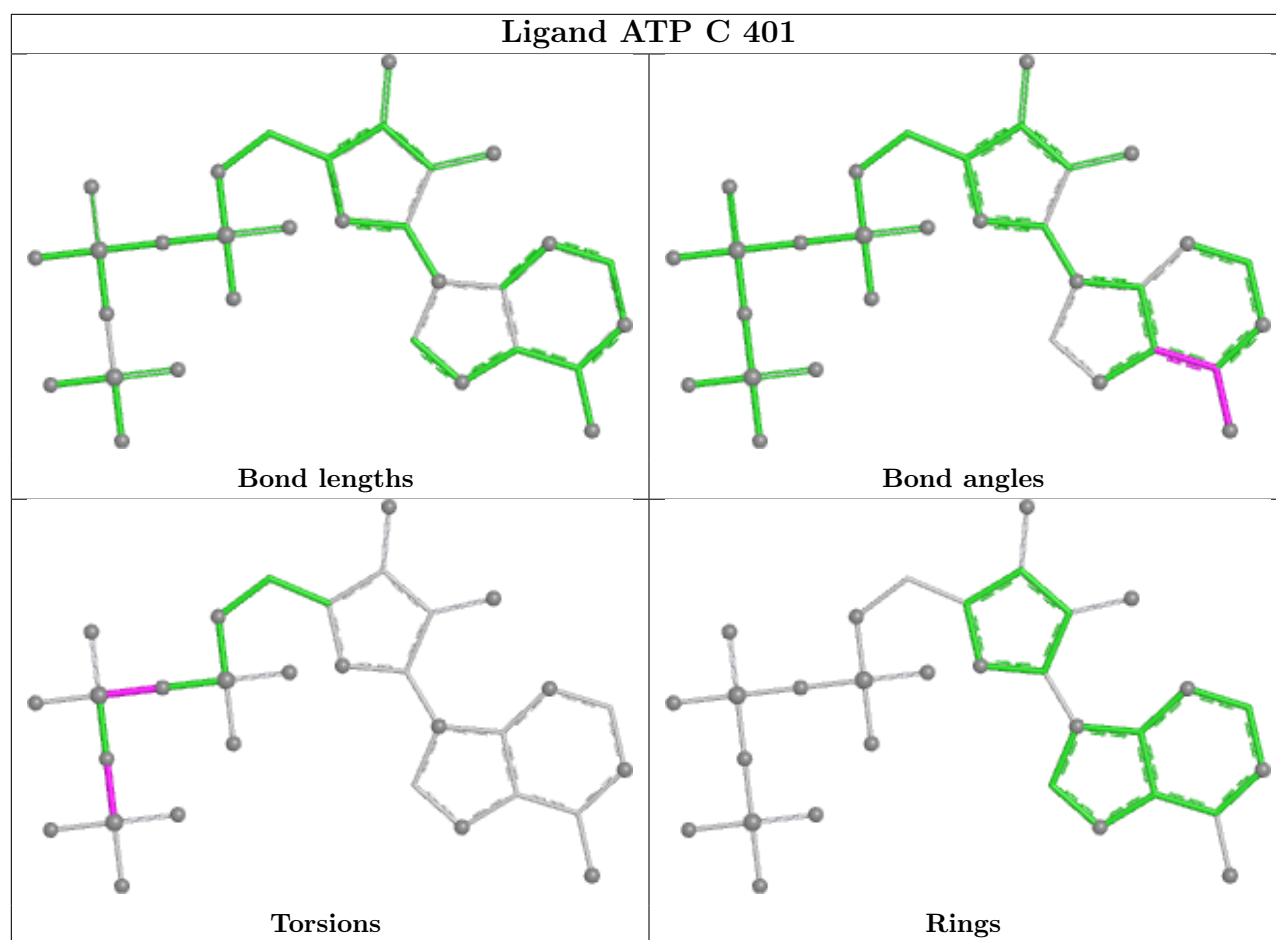












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

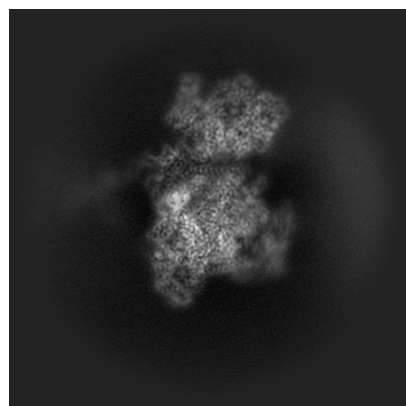
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48586. These allow visual inspection of the internal detail of the map and identification of artifacts.

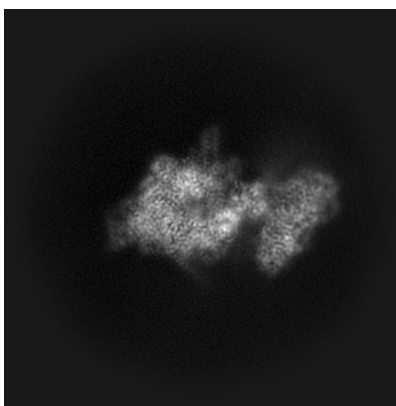
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

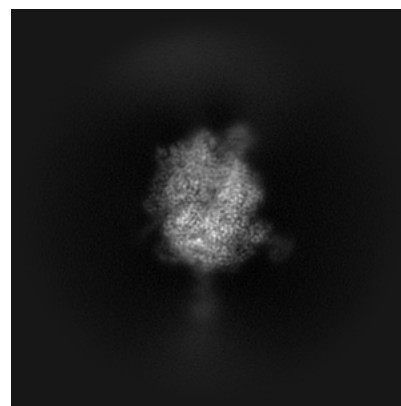
6.1.1 Primary map



X

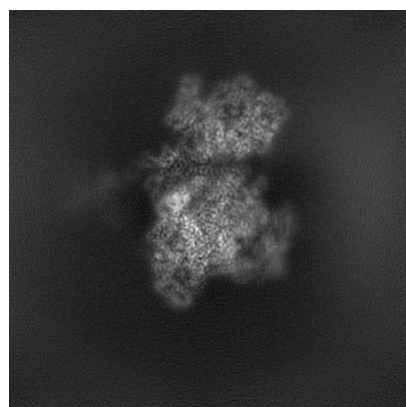


Y

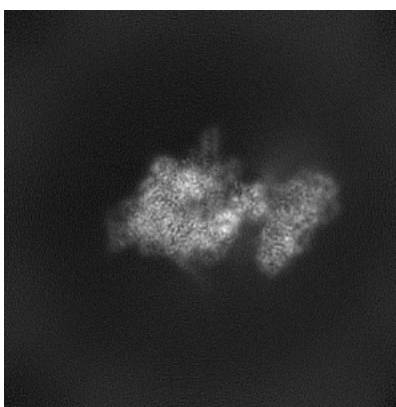


Z

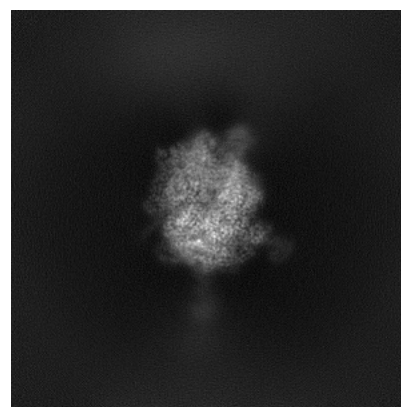
6.1.2 Raw map



X



Y

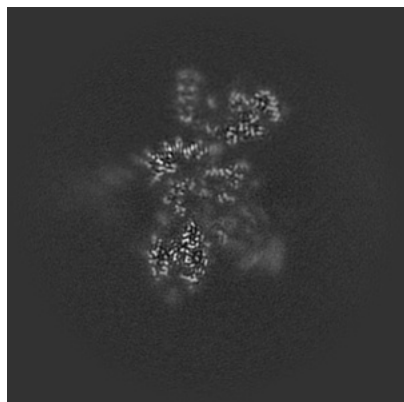


Z

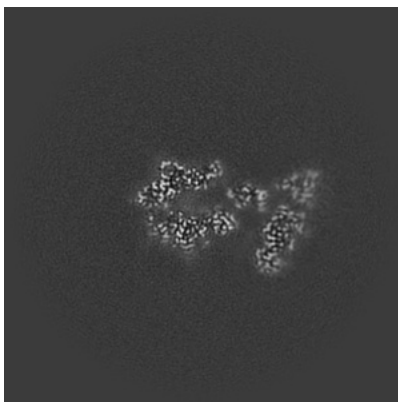
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

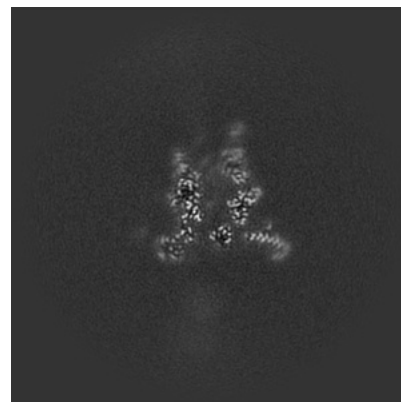
6.2.1 Primary map



X Index: 224



Y Index: 224

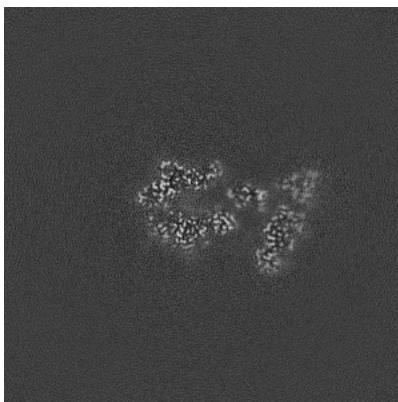


Z Index: 224

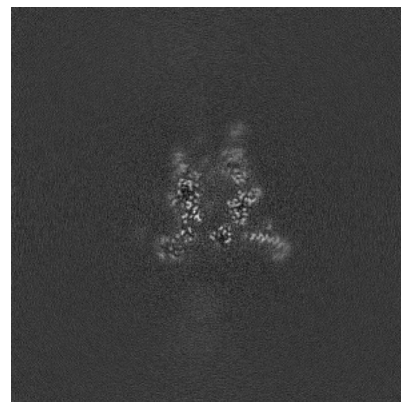
6.2.2 Raw map



X Index: 224



Y Index: 224

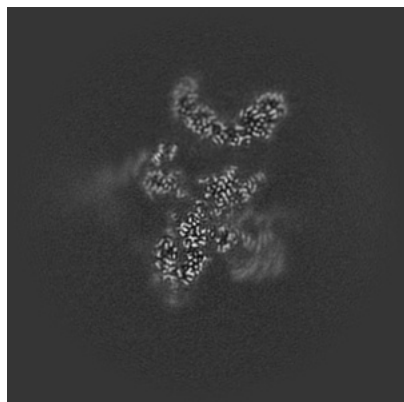


Z Index: 224

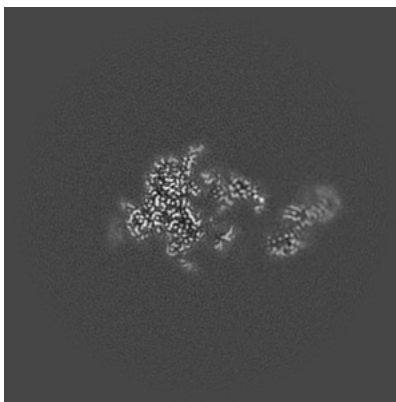
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

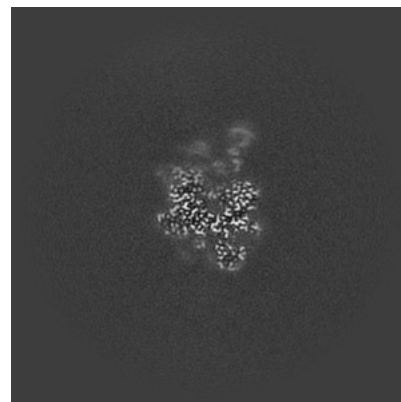
6.3.1 Primary map



X Index: 213

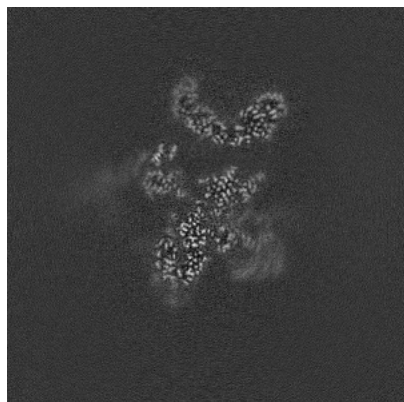


Y Index: 205

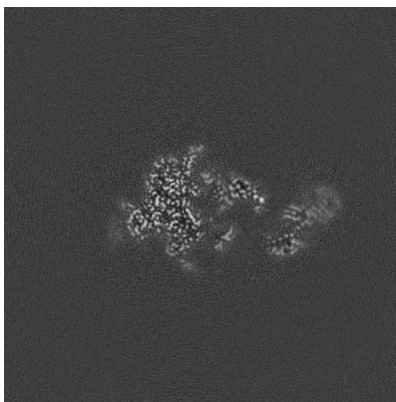


Z Index: 194

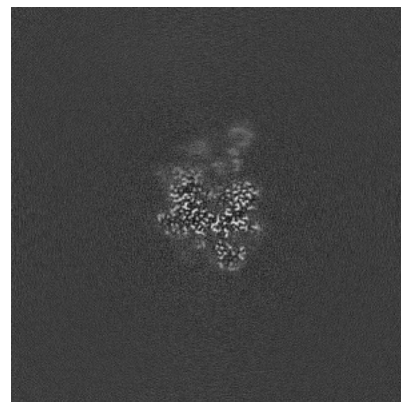
6.3.2 Raw map



X Index: 213



Y Index: 205

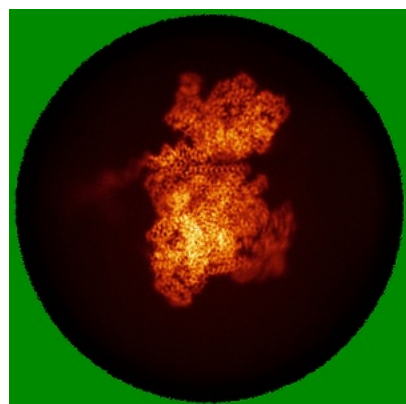


Z Index: 194

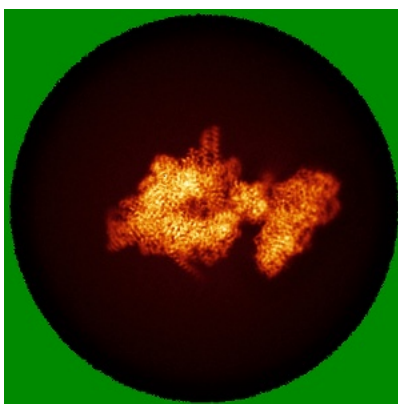
The images above show the largest variance slices of the map in three orthogonal directions.

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

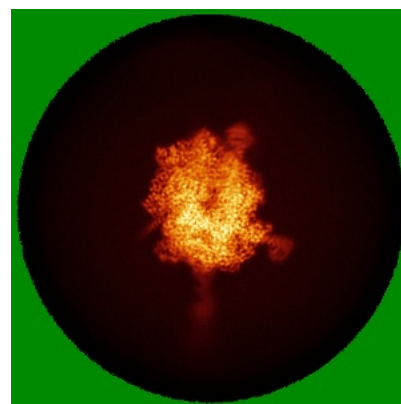
6.4.1 Primary map



X



Y

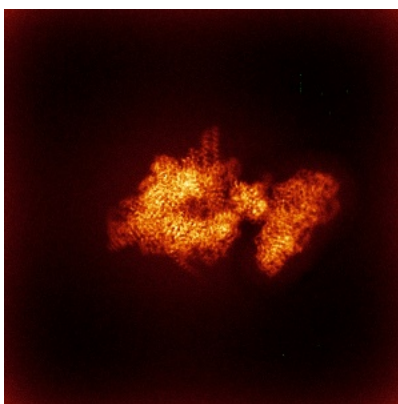


Z

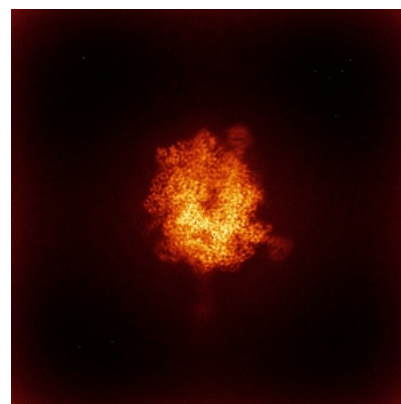
6.4.2 Raw map



X



Y

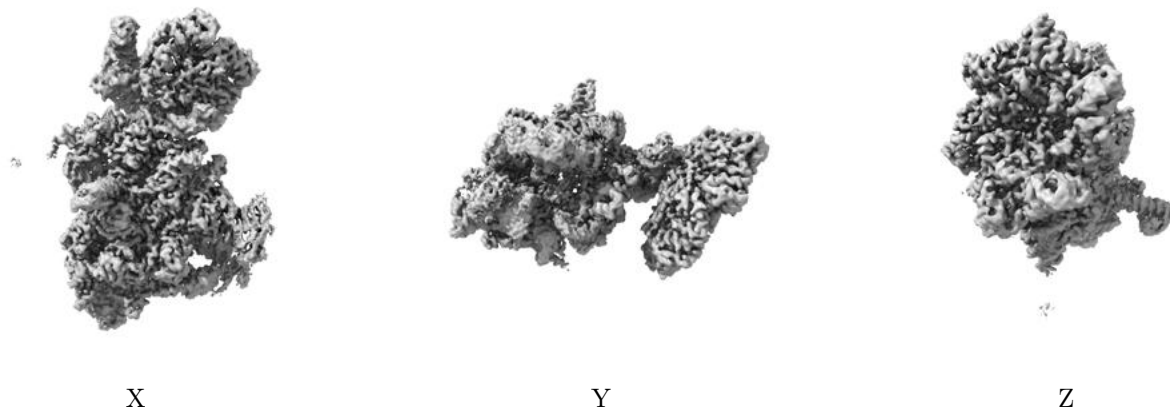


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

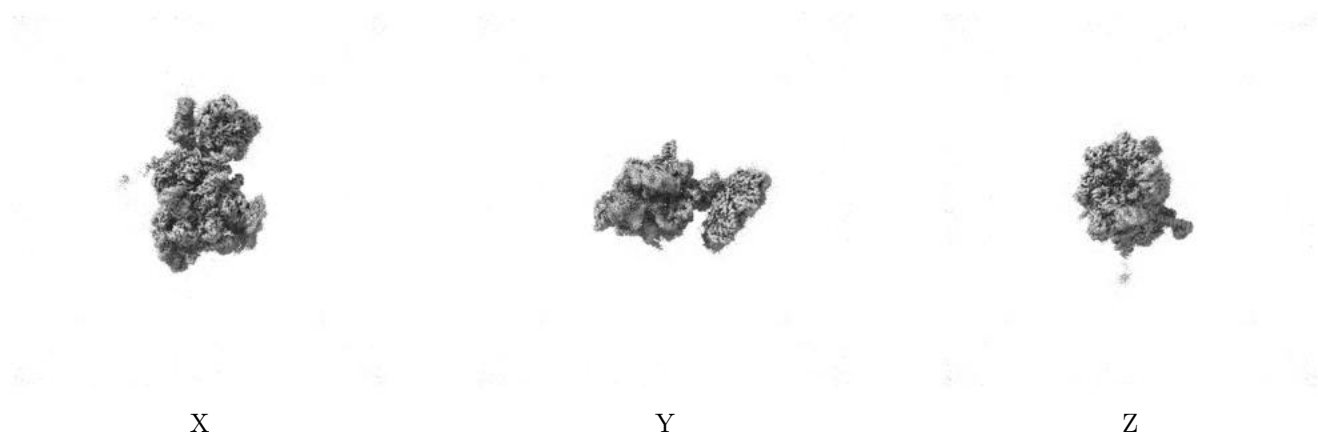
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

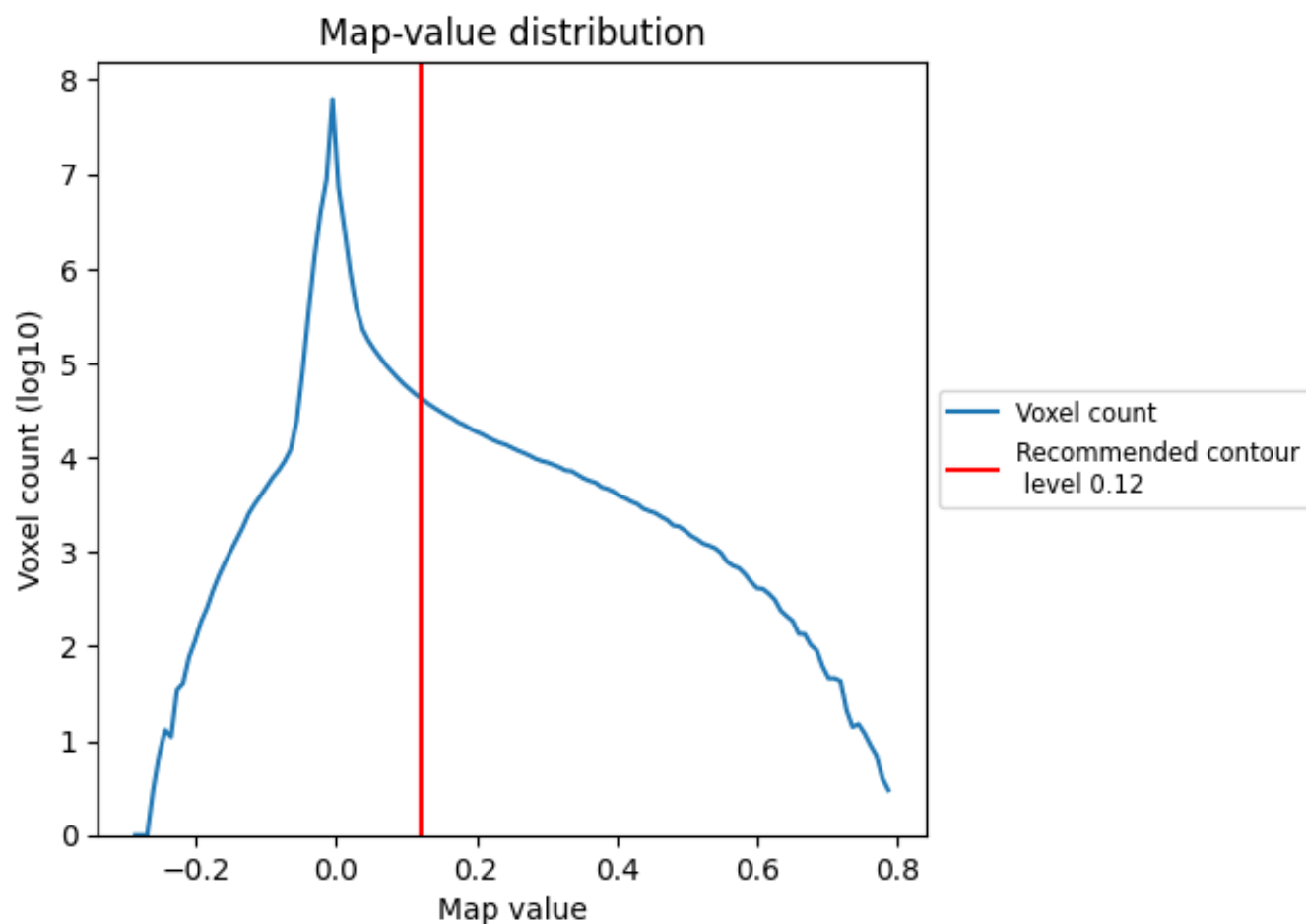
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

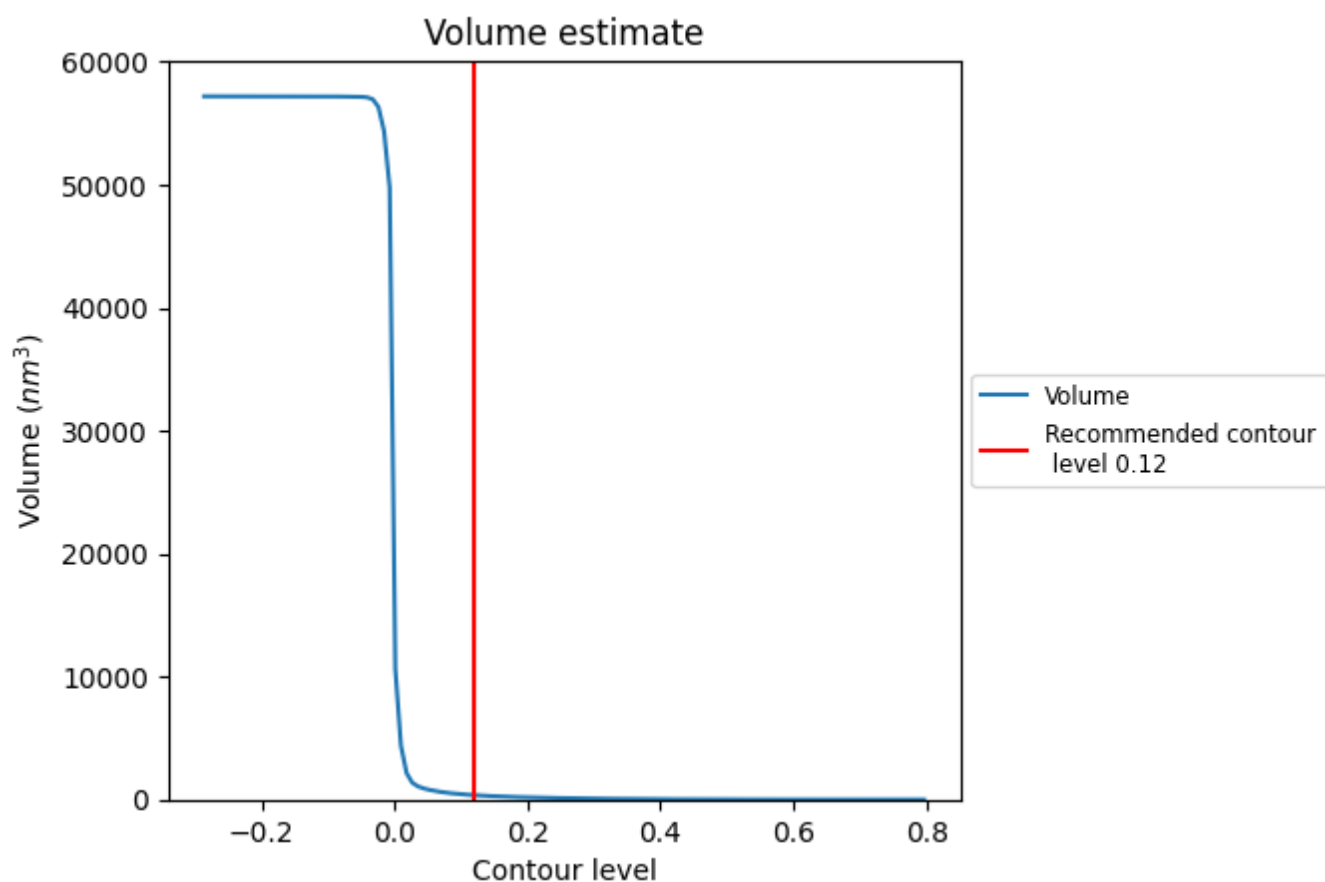
This section contains the results of statistical analysis of the map.

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.

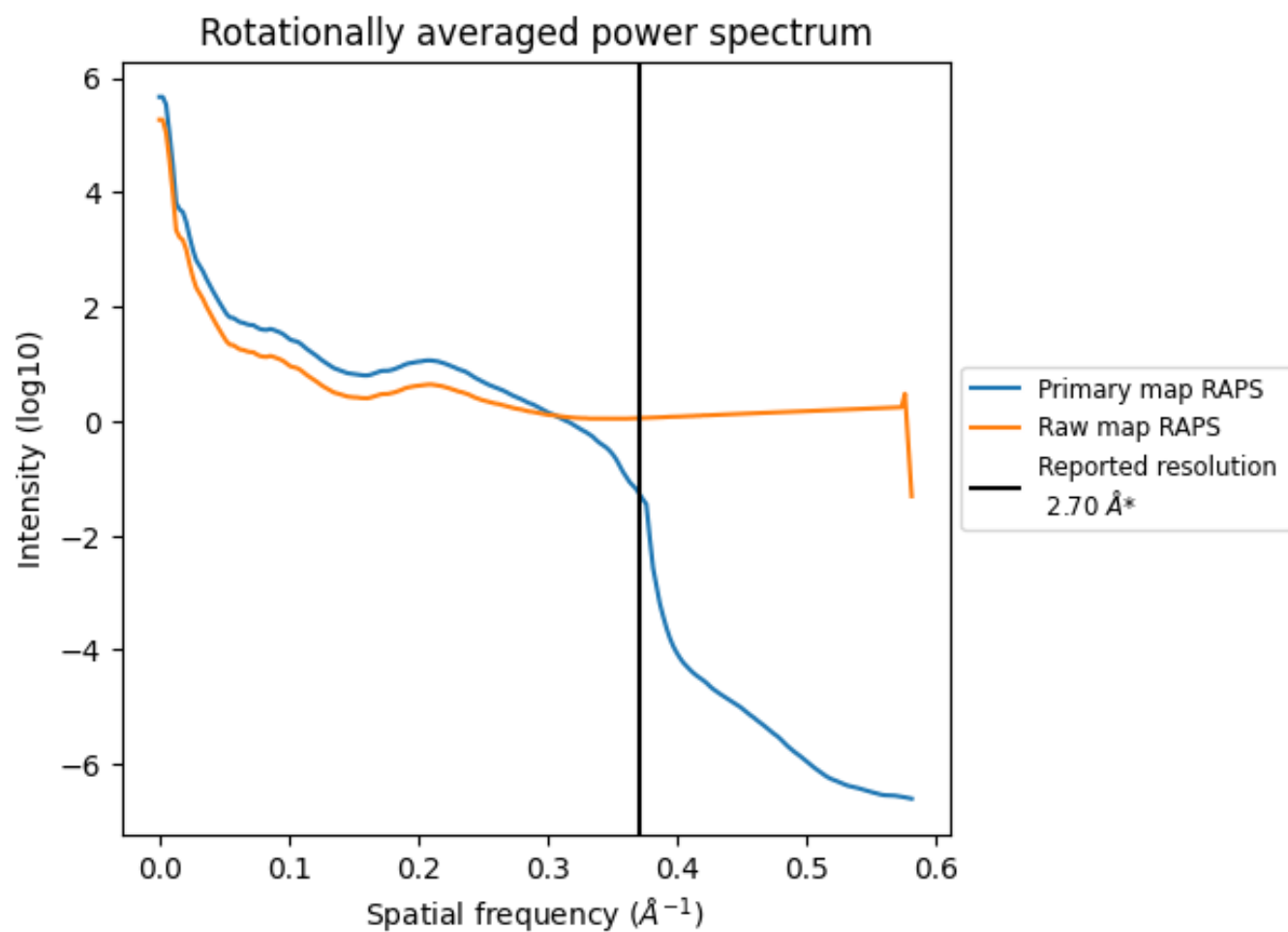
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm³; this corresponds to an approximate mass of 323 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 ⓘ

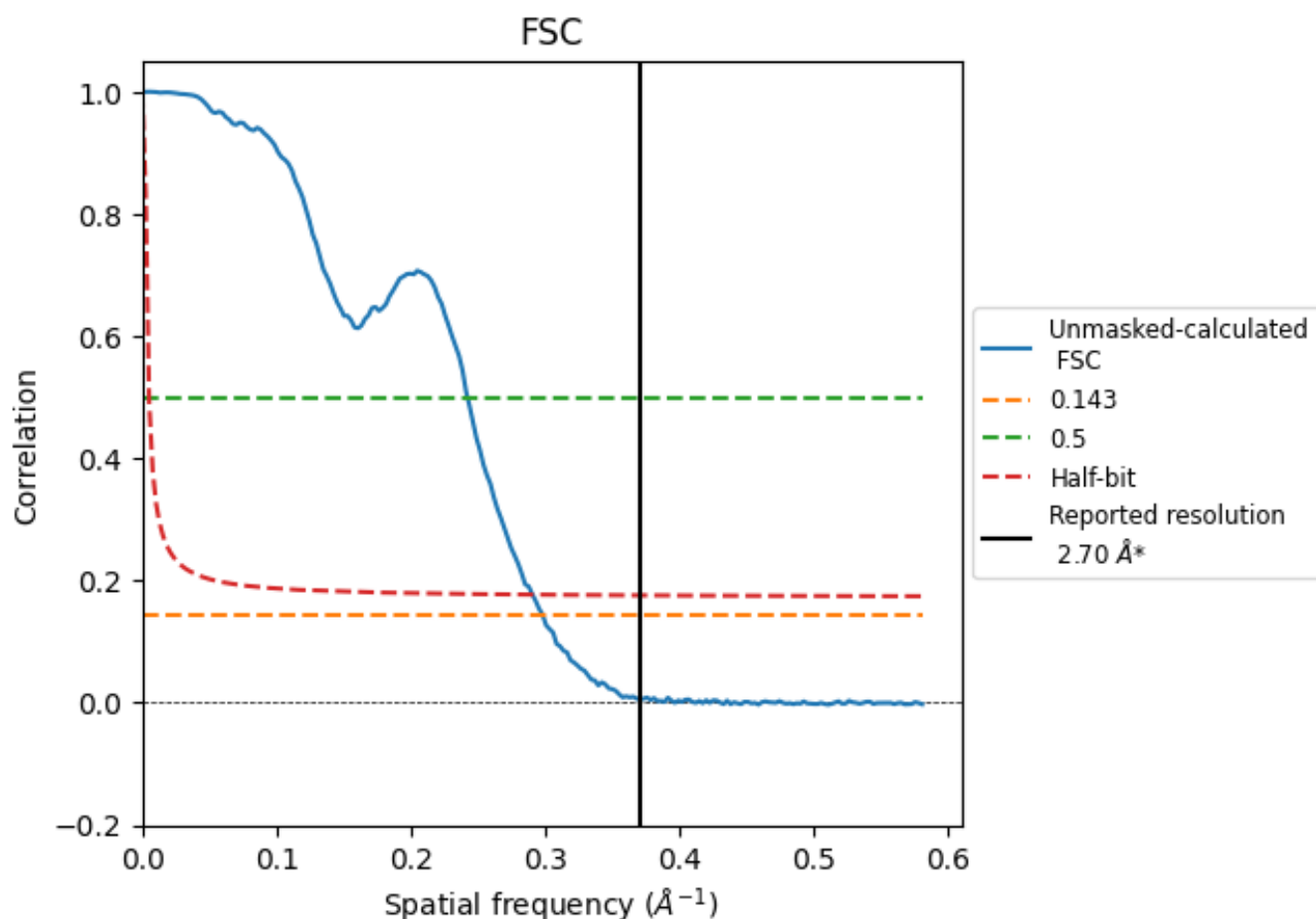


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

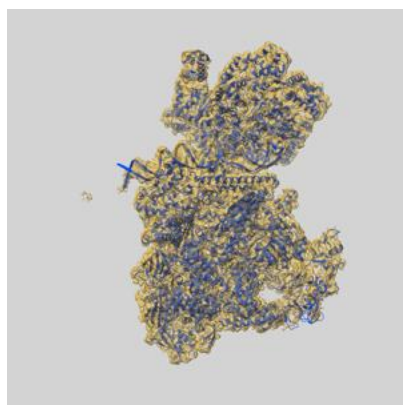
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.35	4.13	3.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.7 by more than 10 %

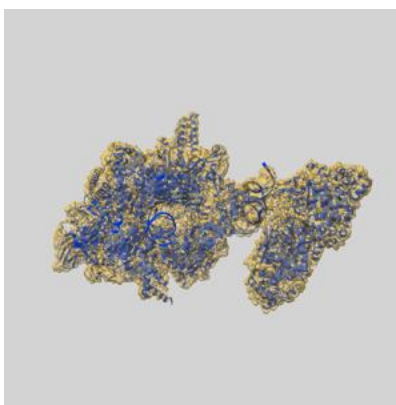
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48586 and PDB model 9MSE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

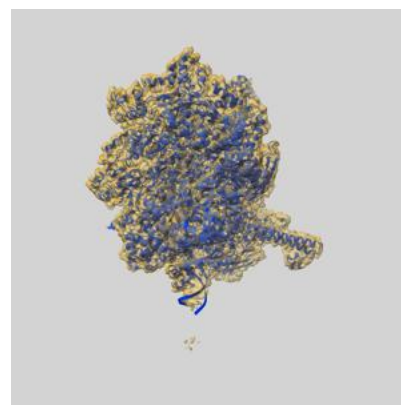
9.1 Map-model overlay [i](#)



X



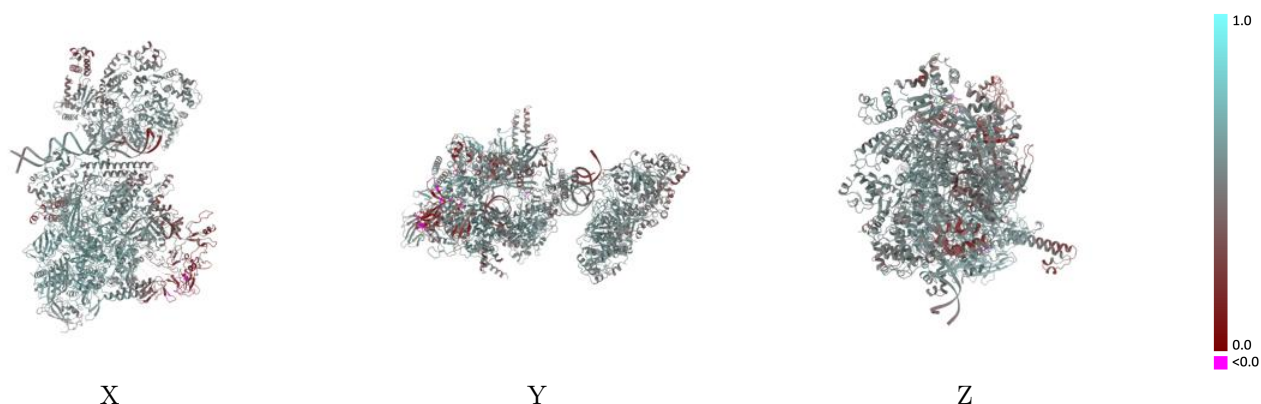
Y



Z

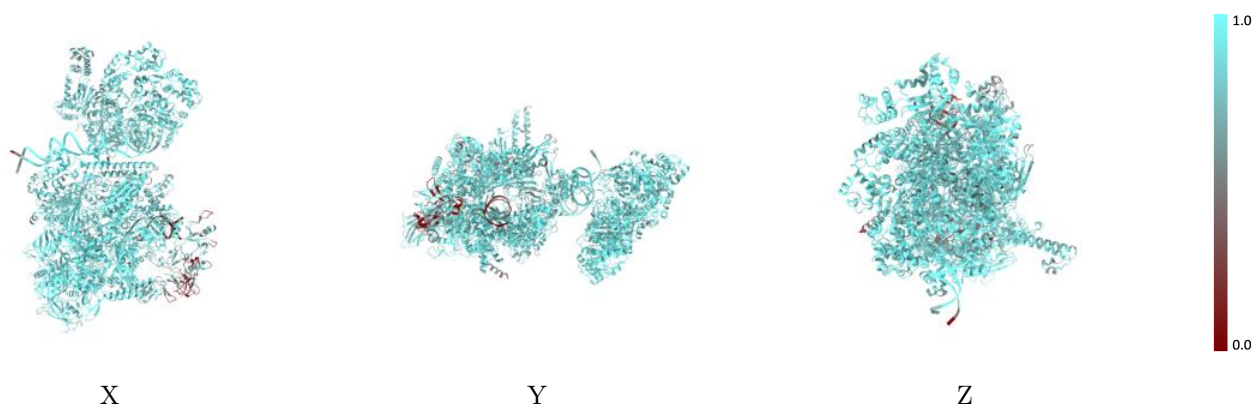
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



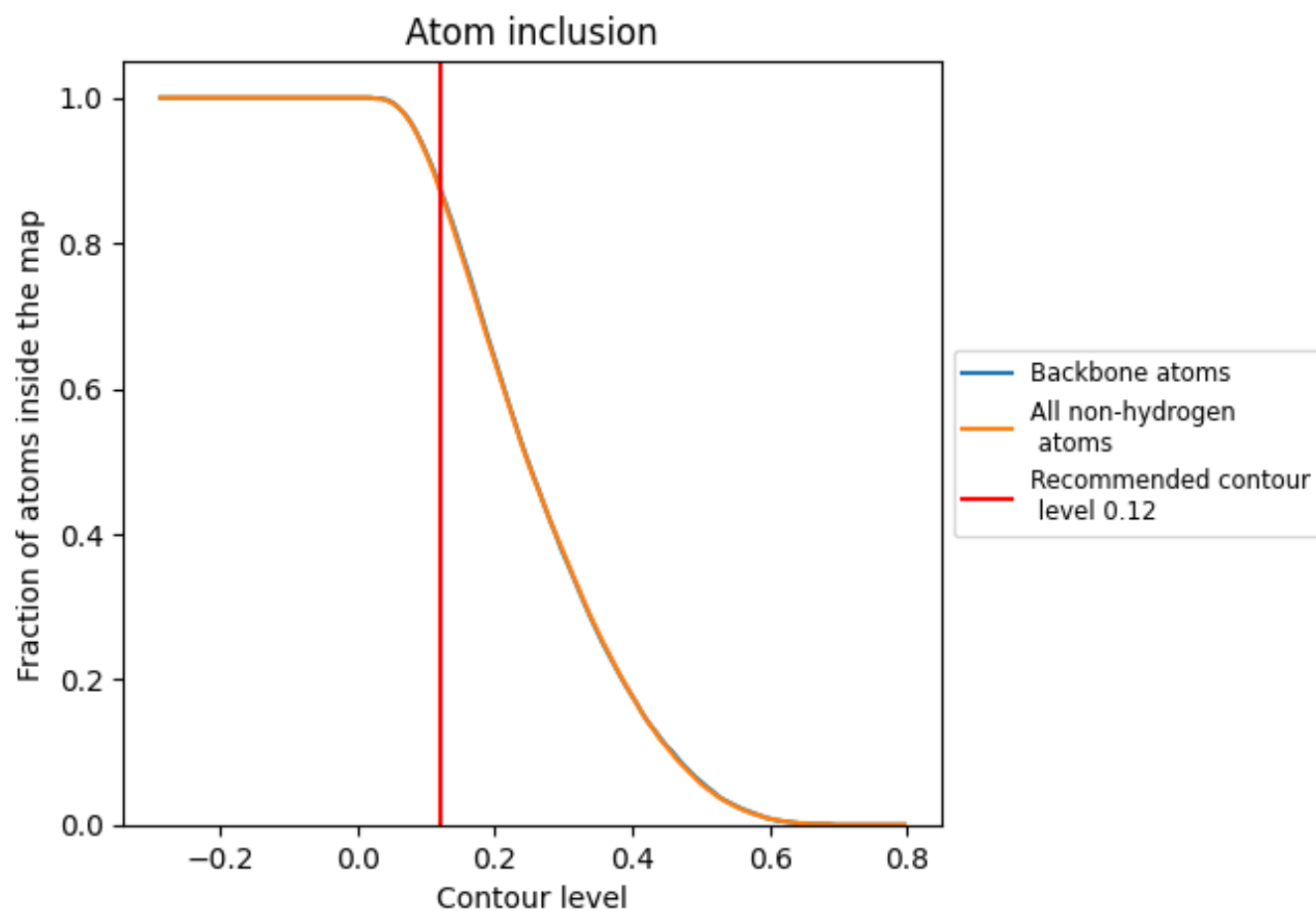
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5210
A	 0.8540	 0.4810
B	 0.8990	 0.5290
C	 0.9200	 0.5430
D	 0.9150	 0.5490
E	 0.9060	 0.5350
F	 0.8110	 0.4430
G	 0.9290	 0.5750
H	 0.9100	 0.5400
I	 0.8990	 0.5370
J	 0.8530	 0.5080
K	 0.8360	 0.5630
M	 0.9000	 0.5340
S	 0.3510	 0.3420
T	 0.2720	 0.3280
U	 0.9000	 0.4520
V	 0.8960	 0.4640

