



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:51 PM UTC

PDB ID : 8RAP / pdb_00008rap
EMDB ID : EMD-19022
Title : Structure of Sen1-ADP.BeF3 bound RNA Polymerase II pre-termination complex
Authors : Rengachari, S.; Lidscreiber, M.; Cramer, P.
Deposited on : 2023-12-01
Resolution : 4.30 Å(reported)
Based on initial models : 7NKX, ., 2XZO, 6I59

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

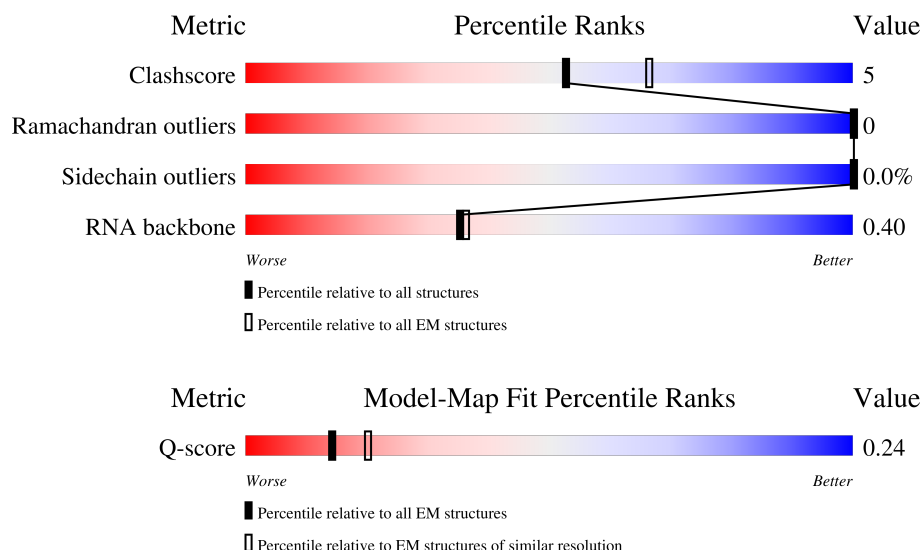
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 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	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	1733	
2	B	1224	
3	C	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	145	
14	N	58	
15	O	2231	
16	P	35	
17	T	58	
18	Y	102	
19	Z	1063	

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
23	BEF	O	3003	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 42924 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11020	6948	1929	2081	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1113	Total	C	N	O	S	0	0
			8839	5596	1553	1635	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			2078	1308	346	411	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	159	Total	C	N	O	S	0	0
			1270	788	223	257	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	85	Total	C	N	O	S	0	0
			688	439	116	130	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	118	Total	C	N	O	S	0	0
			964	592	178	184	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			343	211	69	59	4		

- Molecule 13 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	65	Total	C	N	O	S	0	0
			504	311	87	101	5		

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	27	Total	C	N	O	P	0	0
			547	262	98	160	27		

- Molecule 15 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	694	Total	C	N	O	S	0	0
			5557	3509	973	1044	31		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	25	Total	C	N	O	P	0	0
			540	240	101	174	25		

- Molecule 17 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			786	374	142	232	38		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	100	Total	C	N	O	S	0	0
			760	474	129	147	10		

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	426	Total	C	N	O	S	0	0
			3374	2136	599	630	9		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

Continued on next page...

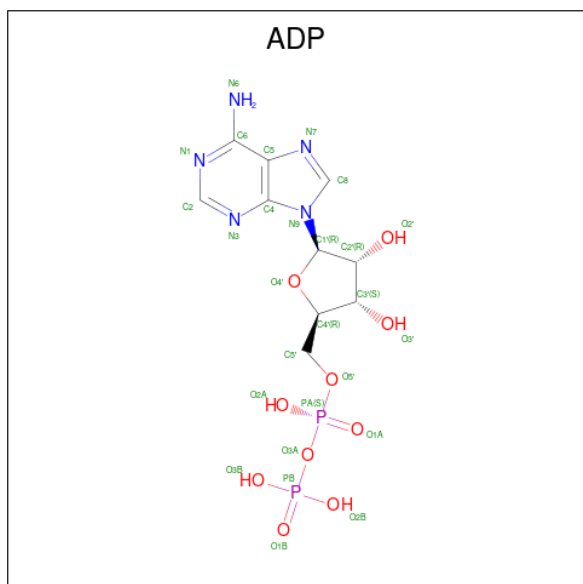
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	
20	M	1	Total	Zn	0
			1	1	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

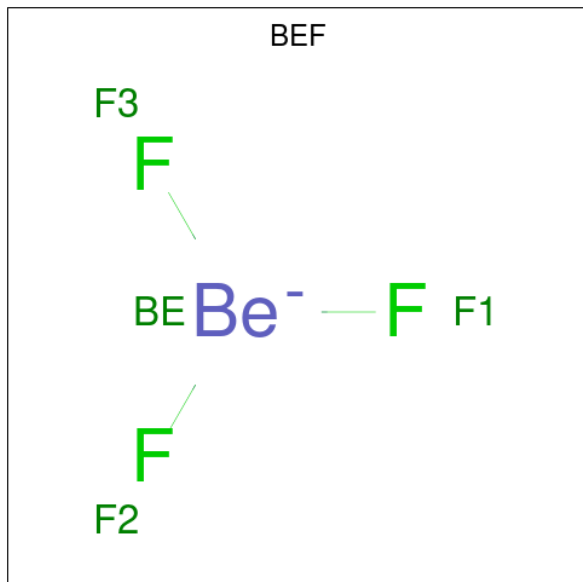
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	
21	O	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 23 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

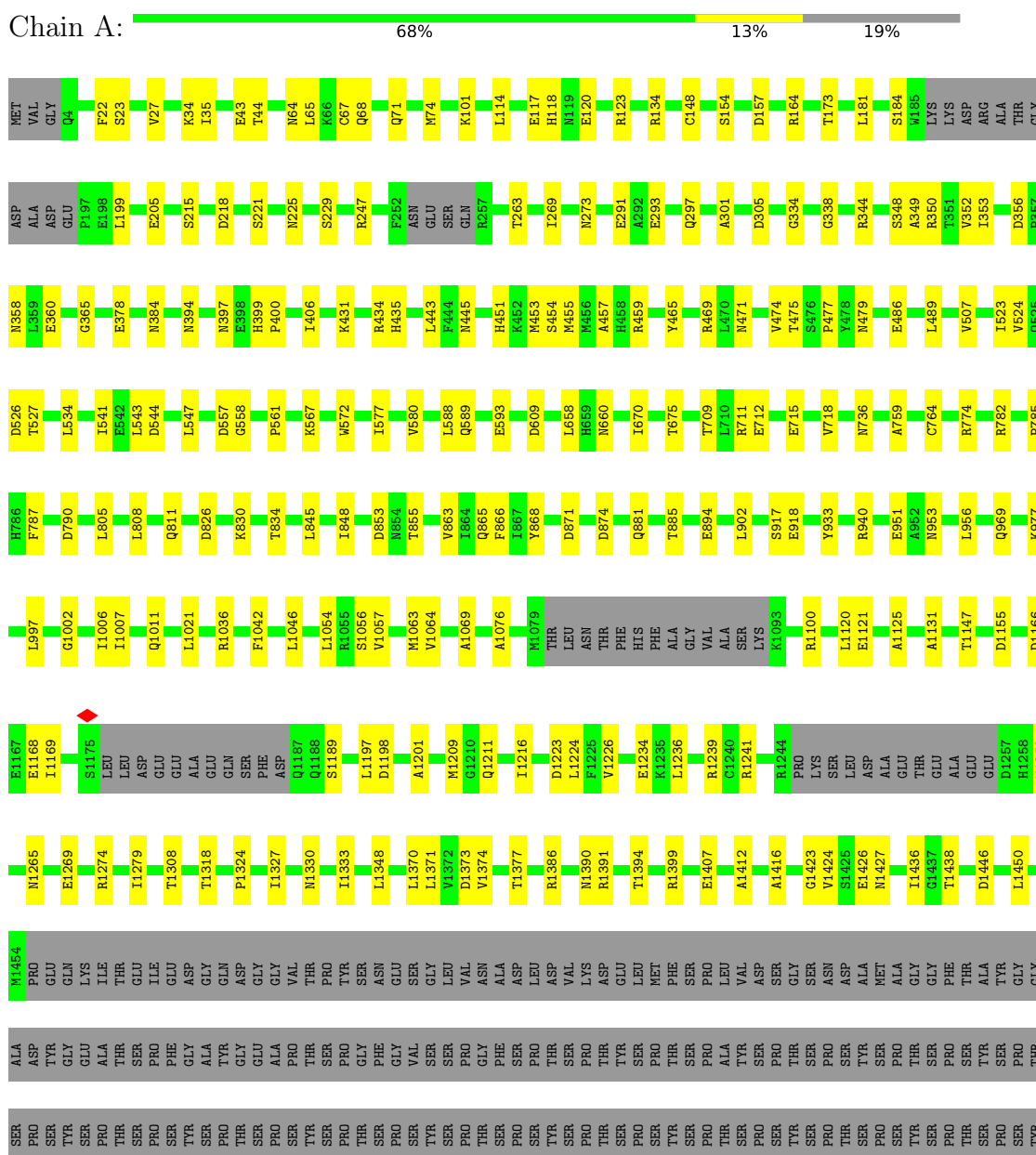


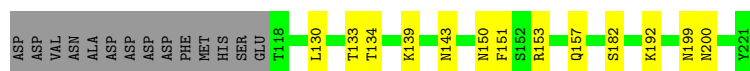
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
23	O	1	4	1	3	0

3 Residue-property plots

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: DNA-directed RNA polymerase II subunit RPB1





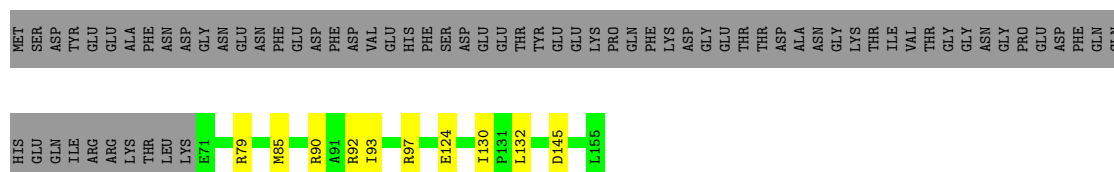
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 86% 14%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 48% 6% 45%



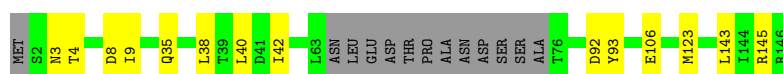
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 88% 12%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 82% 10% 9%



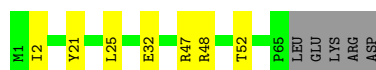
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 87% 10% 3%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 83% 10% 7%



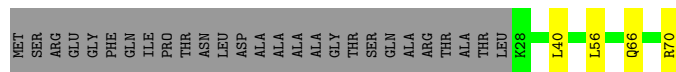
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:  78% 18% .



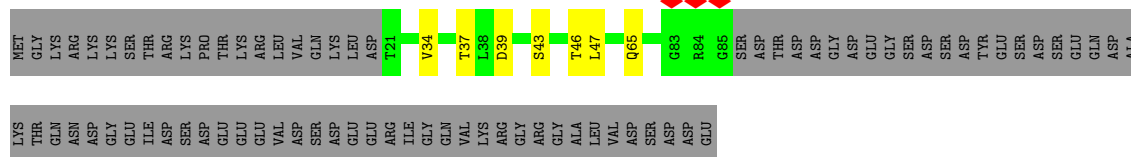
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  56% 6% 39%



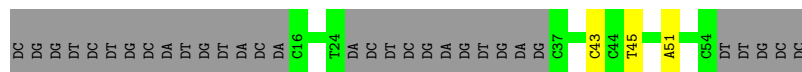
- Molecule 13: Transcription elongation factor 1

Chain M:  40% 5% 55%



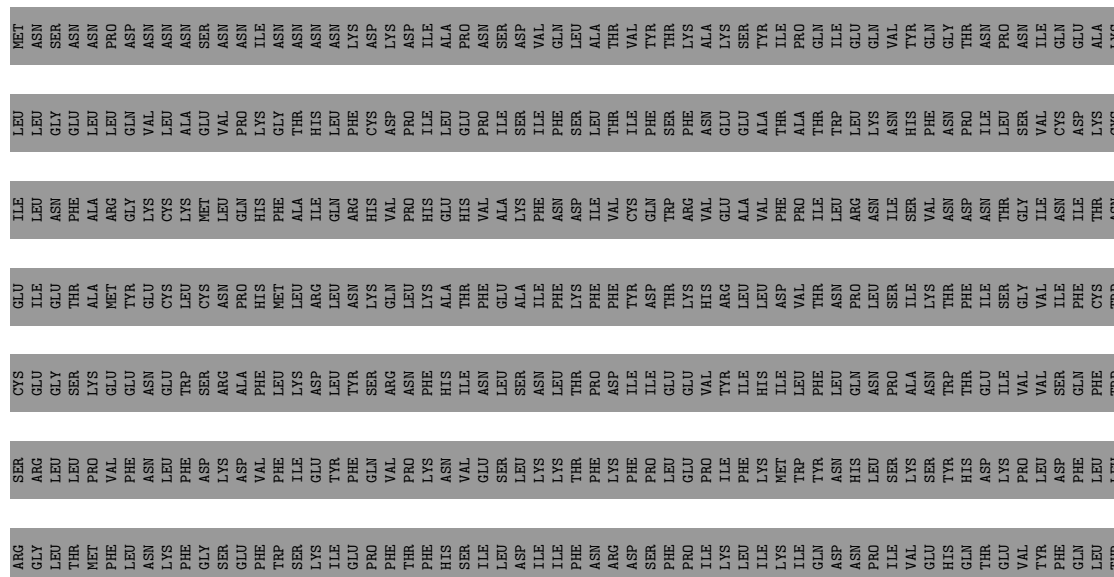
- Molecule 14: Non-template strand

Chain N:  41% 5% 53%

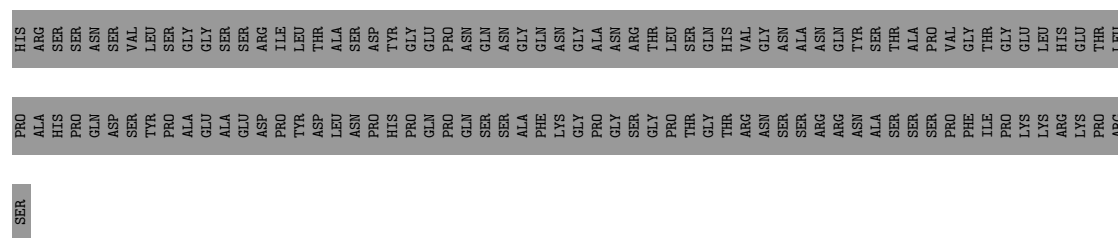


- Molecule 15: Helicase SEN1

Chain O:  28% 69%







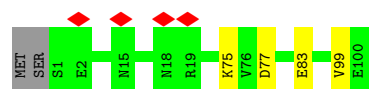
• Molecule 16: RNA



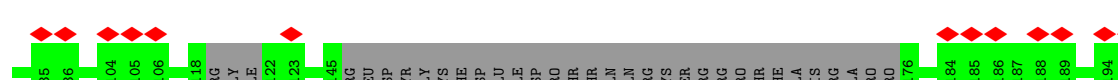
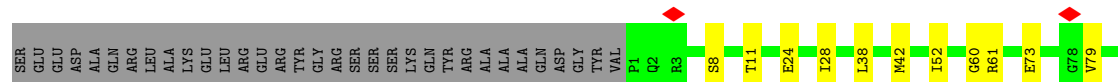
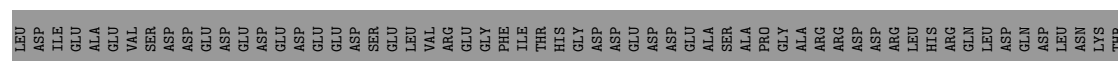
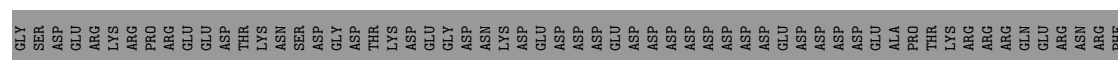
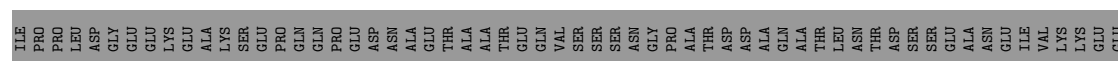
• Molecule 17: Template strand



• Molecule 18: Transcription elongation factor SPT4



• Molecule 19: Transcription elongation factor SPT5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9095	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 ($e^-/\text{\AA}^2$)	40.02	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.042	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.08	0/11217	0.21	0/15166
2	B	0.08	0/9011	0.22	0/12149
3	C	0.08	0/2116	0.20	0/2868
4	D	0.08	0/1279	0.19	0/1716
5	E	0.09	0/1788	0.21	0/2406
6	F	0.09	0/700	0.21	0/945
7	G	0.09	0/1368	0.20	0/1844
8	H	0.08	0/1086	0.24	0/1470
9	I	0.10	0/982	0.24	0/1321
10	J	0.11	0/541	0.22	0/727
11	K	0.10	0/938	0.19	0/1267
12	L	0.10	0/345	0.27	0/457
13	M	0.06	0/512	0.19	0/689
14	N	0.17	0/611	0.40	0/936
15	O	0.08	0/5659	0.20	0/7624
16	P	0.05	0/603	0.13	0/937
17	T	0.17	0/881	0.43	0/1360
18	Y	0.09	0/776	0.18	0/1050
19	Z	0.08	0/3419	0.21	0/4599
All	All	0.09	0/43832	0.22	0/59531

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	11020	0	11104	159	0
2	B	8839	0	8896	120	0
3	C	2078	0	2041	29	0
4	D	1270	0	1287	13	0
5	E	1752	0	1776	20	0
6	F	688	0	707	6	0
7	G	1340	0	1357	13	0
8	H	1068	0	1040	11	0
9	I	964	0	922	9	0
10	J	532	0	542	6	0
11	K	920	0	929	18	0
12	L	343	0	363	3	0
13	M	504	0	480	5	0
14	N	547	0	306	3	0
15	O	5557	0	5587	47	0
16	P	540	0	272	3	0
17	T	786	0	431	10	0
18	Y	760	0	741	3	0
19	Z	3374	0	3478	39	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
21	O	1	0	0	0	0
22	O	27	0	12	0	0
23	O	4	0	0	3	0
All	All	42924	0	42271	450	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 5.

All (450) 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:B:1177:HIS:CD2	19:Z:645:LEU:HD22	1.57	1.38
2:B:1177:HIS:CD2	19:Z:645:LEU:CD2	2.21	1.22
2:B:1177:HIS:NE2	19:Z:645:LEU:HD22	1.58	1.18
2:B:1177:HIS:HD2	19:Z:645:LEU:CD2	1.78	0.96
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.53	0.89
1:A:853:ASP:OD1	1:A:855:THR:OG1	1.94	0.85
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.58	0.85
2:B:1177:HIS:CD2	19:Z:645:LEU:HD23	2.11	0.83
19:Z:849:ASN:ND2	19:Z:869:PRO:O	2.15	0.80
2:B:1177:HIS:NE2	19:Z:645:LEU:CD2	2.33	0.80
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.00	0.80
1:A:344:ARG:NH1	17:T:27:DT:OP1	2.15	0.79
4:D:22:GLU:OE1	4:D:28:GLN:NE2	2.15	0.79
1:A:811:GLN:NE2	2:B:705:MET:SD	2.56	0.78
1:A:885:THR:O	1:A:940:ARG:NH1	2.17	0.78
1:A:350:ARG:NH1	1:A:486:GLU:OE1	2.17	0.78
15:O:1654:GLN:NE2	15:O:1676:ASP:OD1	2.16	0.78
2:B:287:ARG:NH1	2:B:292:ILE:O	2.16	0.78
15:O:1191:VAL:O	15:O:1266:ARG:NH2	2.17	0.78
1:A:134:ARG:NH1	1:A:221:SER:O	2.17	0.77
15:O:1125:TYR:O	15:O:1173:ARG:NH1	2.18	0.77
2:B:906:SER:OG	19:Z:830:GLU:OE1	2.03	0.77
2:B:822:ASN:O	10:J:48:ARG:NH1	2.18	0.76
11:K:11:LEU:O	11:K:37:LYS:NZ	2.18	0.76
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.67	0.76
7:G:97:HIS:NE2	19:Z:622:GLU:OE2	2.19	0.75
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.21	0.74
13:M:37:THR:OG1	13:M:46:THR:OG1	2.05	0.74
2:B:315:LYS:NZ	2:B:319:GLU:OE2	2.19	0.74
7:G:25:TYR:O	7:G:28:THR:OG1	2.05	0.74
1:A:215:SER:OG	1:A:218:ASP:OD1	2.05	0.74
2:B:971:THR:OG1	3:C:61:GLU:OE1	2.03	0.74
1:A:567:LYS:NZ	8:H:93:TYR:O	2.21	0.73
2:B:101:MET:O	2:B:169:ARG:NH2	2.20	0.73
2:B:39:ARG:NH2	2:B:665:GLU:OE1	2.21	0.73
7:G:129:SER:OG	7:G:137:ILE:O	2.07	0.73
2:B:26:THR:OG1	2:B:29:ASP:OD1	2.06	0.72
19:Z:626:THR:OG1	19:Z:629:ASN:OD1	2.07	0.72
1:A:782:ARG:NH2	1:A:785:PRO:O	2.22	0.72
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.23	0.72
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.23	0.71
1:A:1100:ARG:NH2	1:A:1330:ASN:OD1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:SG	1:A:164:ARG:NH2	2.64	0.70
1:A:360:GLU:OE1	1:A:459:ARG:NH2	2.24	0.70
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.25	0.70
8:H:8:ASP:OD1	8:H:9:ILE:N	2.24	0.70
2:B:857:ARG:NH1	2:B:858:SER:O	2.25	0.70
2:B:98:THR:O	2:B:126:SER:OG	2.05	0.69
18:Y:75:LYS:NZ	18:Y:77:ASP:OD1	2.25	0.69
9:I:19:ASP:O	9:I:23:ASN:N	2.24	0.69
1:A:291:GLU:N	1:A:291:GLU:OE1	2.25	0.69
1:A:711:ARG:NH1	9:I:95:THR:O	2.26	0.69
1:A:291:GLU:OE2	19:Z:61:ARG:NH2	2.26	0.69
2:B:53:GLN:NE2	2:B:547:VAL:O	2.26	0.69
2:B:341:LEU:HD22	19:Z:73:GLU:OE1	1.93	0.69
1:A:1386:ARG:O	1:A:1391:ARG:NH1	2.26	0.68
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.27	0.68
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.27	0.68
4:D:139:LYS:O	4:D:143:ASN:ND2	2.27	0.68
4:D:153:ARG:NH2	4:D:182:SER:O	2.26	0.68
2:B:805:THR:OG1	2:B:1041:GLU:OE2	2.12	0.68
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.27	0.67
17:T:41:DT:OP2	19:Z:216:ARG:NH1	2.28	0.67
2:B:1177:HIS:NE2	19:Z:645:LEU:HB2	2.09	0.67
1:A:881:GLN:HB2	1:A:956:LEU:HD12	1.77	0.67
2:B:649:LYS:NZ	2:B:737:THR:O	2.27	0.67
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.27	0.67
1:A:951:GLU:OE1	1:A:953:ASN:N	2.28	0.66
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.13	0.66
1:A:114:LEU:O	1:A:164:ARG:NH1	2.29	0.66
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.29	0.66
3:C:226:ASP:OD1	3:C:227:THR:N	2.28	0.66
7:G:85:GLU:N	7:G:85:GLU:OE1	2.28	0.65
15:O:1668:GLU:O	15:O:1671:GLN:NE2	2.30	0.65
1:A:43:GLU:O	1:A:44:THR:OG1	2.14	0.65
2:B:328:GLU:N	2:B:328:GLU:OE1	2.30	0.65
8:H:3:ASN:OD1	8:H:4:THR:N	2.30	0.65
2:B:496:ARG:NH2	2:B:540:SER:O	2.29	0.64
2:B:711:GLU:N	2:B:711:GLU:OE1	2.29	0.64
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.30	0.64
1:A:1155:ASP:OD2	1:A:1239:ARG:NH2	2.31	0.64
15:O:1293:ARG:NH1	15:O:1570:SER:O	2.30	0.63
19:Z:28:ILE:CD1	19:Z:52:ILE:HG22	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.31	0.63
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.31	0.63
1:A:1390:ASN:OD1	1:A:1391:ARG:NH2	2.32	0.63
2:B:287:ARG:NE	2:B:324:ILE:O	2.31	0.63
3:C:4:GLU:OE2	11:K:104:ASN:ND2	2.31	0.62
2:B:995:ARG:NH2	11:K:39:ASP:OD2	2.32	0.62
2:B:125:SER:O	2:B:169:ARG:NH2	2.33	0.62
19:Z:38:LEU:HB3	19:Z:42:MET:HE2	1.80	0.62
2:B:776:GLN:OE1	16:P:33:A:O2'	2.15	0.62
2:B:868:MET:O	2:B:869:SER:OG	2.17	0.62
2:B:1177:HIS:HD2	19:Z:645:LEU:HD23	1.51	0.62
9:I:90:GLN:OE1	9:I:92:ARG:NH1	2.33	0.61
2:B:908:GLU:N	2:B:908:GLU:OE1	2.33	0.61
2:B:639:ILE:HD12	2:B:688:GLY:O	2.00	0.61
1:A:154:SER:OG	1:A:157:ASP:O	2.18	0.61
19:Z:854:GLU:N	19:Z:854:GLU:OE1	2.33	0.61
2:B:310:MET:HG3	2:B:386:LEU:HD13	1.83	0.61
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.34	0.61
1:A:1318:THR:HG23	5:E:141:VAL:HG11	1.83	0.61
19:Z:8:SER:HG	19:Z:11:THR:HG1	1.49	0.60
2:B:816:GLU:N	2:B:816:GLU:OE1	2.34	0.60
4:D:41:GLN:OE1	4:D:41:GLN:N	2.34	0.60
15:O:1127:ARG:NE	15:O:1129:SER:OG	2.34	0.60
1:A:1168:GLU:N	1:A:1168:GLU:OE1	2.35	0.60
2:B:499:ASN:OD1	2:B:500:THR:N	2.35	0.59
19:Z:860:GLU:N	19:Z:860:GLU:OE1	2.34	0.59
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.36	0.59
2:B:904:ARG:NH1	2:B:905:VAL:O	2.35	0.59
15:O:1699:PHE:O	15:O:1854:ALA:N	2.35	0.59
1:A:22:PHE:CE2	1:A:27:VAL:HG22	2.38	0.59
2:B:733:HIS:O	2:B:733:HIS:ND1	2.35	0.59
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.02	0.59
4:D:150:ASN:OD1	4:D:151:PHE:N	2.36	0.59
5:E:40:GLU:OE1	5:E:43:LYS:NZ	2.35	0.59
2:B:399:ASP:OD2	2:B:510:LYS:NZ	2.35	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.85	0.58
2:B:262:GLU:OE1	2:B:267:ARG:NH2	2.36	0.58
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.34	0.58
3:C:90:ASP:OD1	19:Z:848:TYR:OH	2.22	0.58
1:A:173:THR:OG1	1:A:184:SER:OG	2.22	0.58
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:O	1:A:273:ASN:ND2	2.36	0.58
19:Z:870:GLN:OE1	19:Z:870:GLN:N	2.36	0.58
5:E:36:GLU:OE1	5:E:36:GLU:N	2.37	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.57
1:A:871:ASP:OD1	5:E:204:THR:OG1	2.18	0.57
2:B:567:GLU:N	2:B:567:GLU:OE1	2.38	0.57
1:A:43:GLU:OE1	1:A:43:GLU:N	2.36	0.57
1:A:68:GLN:N	1:A:68:GLN:OE1	2.38	0.57
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.37	0.57
2:B:570:VAL:O	2:B:570:VAL:HG13	2.04	0.57
15:O:1770:MET:N	15:O:1770:MET:SD	2.78	0.57
1:A:293:GLU:OE2	1:A:297:GLN:NE2	2.39	0.56
1:A:808:LEU:O	2:B:728:ARG:NH2	2.39	0.56
2:B:1129:ARG:NE	17:T:26:DG:OP1	2.35	0.56
5:E:33:GLU:N	5:E:33:GLU:OE1	2.38	0.56
11:K:36:GLU:OE1	11:K:70:ARG:NE	2.38	0.56
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.38	0.56
1:A:205:GLU:N	1:A:205:GLU:OE1	2.38	0.56
7:G:117:GLN:N	7:G:117:GLN:OE1	2.39	0.56
4:D:199:ASN:OD1	4:D:200:ASN:N	2.35	0.56
1:A:588:LEU:HD23	1:A:589:GLN:N	2.21	0.56
1:A:917:SER:OG	1:A:918:GLU:OE1	2.21	0.56
13:M:39:ASP:O	13:M:43:SER:N	2.39	0.56
5:E:85:GLU:N	5:E:85:GLU:OE1	2.38	0.56
1:A:365:GLY:N	1:A:469:ARG:O	2.34	0.56
1:A:660:ASN:O	2:B:1082:MET:N	2.39	0.56
15:O:1591:GLU:OE2	23:O:3003:BEF:F1	2.14	0.56
1:A:1169:ILE:HG21	1:A:1239:ARG:HD3	1.87	0.56
15:O:1246:LYS:NZ	15:O:1292:GLU:OE2	2.20	0.55
11:K:64:GLU:OE1	11:K:64:GLU:N	2.39	0.55
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.36	0.55
2:B:357:GLN:NE2	2:B:368:GLU:OE1	2.39	0.55
1:A:451:HIS:NE2	1:A:477:PRO:O	2.36	0.55
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.87	0.55
2:B:468:GLU:N	2:B:468:GLU:OE1	2.38	0.55
11:K:79:GLU:OE1	11:K:79:GLU:N	2.38	0.55
2:B:1177:HIS:NE2	19:Z:645:LEU:CB	2.69	0.55
15:O:1253:THR:HG22	15:O:1254:LYS:H	1.71	0.55
1:A:67:CYS:O	1:A:71:GLN:N	2.39	0.55
4:D:157:GLN:N	4:D:157:GLN:OE1	2.40	0.54
1:A:344:ARG:NE	2:B:1120:GLU:OE1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD11	2:B:658:ILE:HG13	1.88	0.54
2:B:872:GLU:N	2:B:872:GLU:OE1	2.38	0.54
2:B:996:ARG:CZ	3:C:38:ILE:HD11	2.37	0.54
1:A:1223:ASP:C	1:A:1224:LEU:HD12	2.33	0.54
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.89	0.54
2:B:610:ASN:O	2:B:613:VAL:HG12	2.08	0.54
3:C:215:GLU:OE1	3:C:215:GLU:N	2.40	0.54
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.40	0.54
7:G:22:MET:SD	7:G:23:LYS:N	2.81	0.54
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.89	0.53
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.90	0.53
5:E:185:ALA:O	5:E:189:GLY:N	2.40	0.53
18:Y:99:VAL:HG12	18:Y:99:VAL:O	2.09	0.53
11:K:38:GLU:OE1	11:K:42:LEU:HD12	2.08	0.53
15:O:1431:GLN:OE1	15:O:1431:GLN:N	2.39	0.53
1:A:577:ILE:O	1:A:580:VAL:HG22	2.08	0.53
18:Y:83:GLU:OE1	18:Y:83:GLU:N	2.39	0.53
19:Z:24:GLU:OE1	19:Z:24:GLU:N	2.40	0.53
15:O:1776:ASP:OD1	15:O:1777:PHE:N	2.41	0.53
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.44	0.53
15:O:1191:VAL:HG23	15:O:1194:PHE:HB2	1.90	0.53
1:A:593:GLU:OE1	1:A:593:GLU:N	2.41	0.53
8:H:106:GLU:OE1	8:H:106:GLU:N	2.41	0.53
1:A:348:SER:HB2	2:B:1128:LEU:HD22	1.91	0.52
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.25	0.52
2:B:760:ASP:OD1	2:B:761:HIS:ND1	2.42	0.52
3:C:11:ARG:NH1	3:C:12:GLU:OE2	2.42	0.52
2:B:322:PHE:O	2:B:325:GLN:NE2	2.40	0.52
1:A:1189:SER:O	1:A:1241:ARG:NH1	2.41	0.52
3:C:259:LEU:HD21	11:K:91:CYS:HB2	1.91	0.52
5:E:90:VAL:HG23	14:N:51:DA:OP1	2.08	0.52
2:B:564:GLU:N	2:B:564:GLU:OE1	2.40	0.52
15:O:1707:GLN:N	15:O:1707:GLN:OE1	2.42	0.52
2:B:762:ASN:OD1	2:B:763:GLN:N	2.42	0.52
5:E:168:TYR:HB3	5:E:170:LEU:HD13	1.91	0.52
15:O:1820:ARG:NH2	23:O:3003:BEF:F3	2.32	0.52
1:A:863:VAL:O	1:A:863:VAL:HG23	2.10	0.52
3:C:58:LEU:HD11	10:J:2:ILE:HD11	1.92	0.52
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.27	0.52
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.52
1:A:1211:GLN:OE1	1:A:1274:ARG:NH1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ILE:HD11	7:G:29:LYS:HD3	1.92	0.51
2:B:1174:LYS:O	2:B:1178:ASN:N	2.43	0.51
5:E:138:ALA:O	5:E:141:VAL:HG12	2.09	0.51
1:A:790:ASP:OD2	9:I:87:GLN:N	2.43	0.51
1:A:1412:ALA:O	1:A:1416:ALA:N	2.44	0.51
3:C:111:THR:HG23	15:O:1266:ARG:HH22	1.76	0.51
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.51
15:O:1619:GLN:NE2	23:O:3003:BEF:F3	2.34	0.51
3:C:47:ASP:OD1	12:L:70:ARG:NH1	2.44	0.51
1:A:394:ASN:ND2	1:A:400:PRO:O	2.41	0.50
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.42	0.50
5:E:48:ASP:OD1	5:E:51:GLY:N	2.44	0.50
3:C:17:ASN:OD1	3:C:231:ASN:ND2	2.42	0.50
19:Z:801:LEU:HD23	19:Z:802:GLY:N	2.26	0.50
1:A:874:ASP:N	1:A:1056:SER:O	2.38	0.50
1:A:101:LYS:NZ	14:N:43:DC:OP1	2.37	0.50
1:A:526:ASP:OD2	2:B:835:GLN:NE2	2.44	0.50
2:B:786:ASN:O	2:B:967:ARG:NH2	2.45	0.50
1:A:406:ILE:N	1:A:431:LYS:O	2.45	0.50
19:Z:24:GLU:OE2	19:Z:60:GLY:N	2.39	0.50
1:A:845:LEU:HD23	1:A:848:ILE:HD12	1.94	0.50
1:A:1324:PRO:O	1:A:1327:ILE:HG22	2.12	0.50
7:G:11:ILE:HD13	7:G:26:LEU:HG	1.94	0.50
14:N:45:DT:O2	17:T:16:DG:N2	2.45	0.50
19:Z:711:ILE:HD12	19:Z:711:ILE:C	2.36	0.50
2:B:120:ARG:NH2	2:B:956:THR:O	2.45	0.50
2:B:1035:ALA:O	2:B:1039:GLY:N	2.44	0.50
15:O:1183:ILE:HG22	15:O:1201:VAL:HG22	1.94	0.50
2:B:766:ARG:NH2	2:B:985:GLY:O	2.45	0.49
9:I:60:GLN:OE1	9:I:60:GLN:N	2.41	0.49
15:O:1332:SER:OG	15:O:1430:LYS:O	2.16	0.49
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.47	0.49
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.93	0.49
1:A:544:ASP:O	11:K:47:ARG:NH2	2.45	0.49
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.44	0.49
15:O:1441:ARG:NH1	15:O:1442:VAL:O	2.45	0.49
8:H:92:ASP:O	8:H:145:ARG:NH2	2.45	0.49
19:Z:732:PHE:CD1	19:Z:746:VAL:HG22	2.48	0.49
4:D:34:GLN:N	4:D:34:GLN:OE1	2.46	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.53	0.49
15:O:1127:ARG:NH2	15:O:1134:ASP:OD1	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.43	0.49
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.45	0.49
3:C:258:ILE:HD11	11:K:42:LEU:HD13	1.93	0.49
9:I:68:LEU:O	9:I:70:ARG:NH1	2.45	0.49
1:A:23:SER:O	1:A:27:VAL:HG23	2.12	0.49
1:A:443:LEU:CD1	1:A:455:MET:HE2	2.39	0.49
1:A:1042:PHE:CE1	1:A:1046:LEU:HD11	2.48	0.49
1:A:782:ARG:NE	1:A:787:PHE:O	2.42	0.48
17:T:35:DA:H2'	17:T:35:DA:N3	2.28	0.48
2:B:481:GLN:NE2	16:P:32:C:OP1	2.47	0.48
1:A:349:ALA:O	2:B:1128:LEU:HD21	2.13	0.48
2:B:364:ILE:CD1	2:B:365:THR:HG22	2.44	0.48
1:A:74:MET:O	2:B:1116:ARG:NH1	2.47	0.48
1:A:334:GLY:O	1:A:338:GLY:N	2.46	0.48
15:O:1702:ILE:O	15:O:1830:HIS:ND1	2.45	0.48
1:A:1216:ILE:HG21	1:A:1226:VAL:HG21	1.96	0.48
2:B:618:ASP:O	2:B:622:LYS:N	2.47	0.48
2:B:1176:ASN:OD1	2:B:1177:HIS:CD2	2.67	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.44	0.48
2:B:824:ILE:N	2:B:824:ILE:HD12	2.28	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:CG2	2.43	0.48
2:B:566:LEU:HD22	2:B:586:TRP:O	2.14	0.48
17:T:8:DT:H2'	17:T:9:DT:H71	1.96	0.47
19:Z:28:ILE:HD13	19:Z:52:ILE:HG22	1.95	0.47
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.97	0.47
15:O:1339:GLN:NE2	15:O:1361:THR:O	2.46	0.47
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.95	0.47
11:K:37:LYS:N	11:K:69:ALA:O	2.46	0.47
15:O:1408:ILE:HD12	15:O:1408:ILE:N	2.30	0.47
1:A:894:GLU:OE2	1:A:933:TYR:OH	2.30	0.47
3:C:38:ILE:HB	3:C:176:ILE:HD12	1.97	0.47
1:A:475:THR:O	1:A:479:ASN:N	2.47	0.47
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.45	0.47
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.97	0.47
15:O:1731:TYR:OH	15:O:1735:LYS:NZ	2.32	0.47
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.96	0.47
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.47
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.96	0.47
1:A:247:ARG:NH2	1:A:263:THR:OG1	2.43	0.46
1:A:557:ASP:OD1	1:A:558:GLY:N	2.46	0.46
2:B:640:VAL:HG12	2:B:649:LYS:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1362:GLY:O	15:O:1366:THR:N	2.43	0.46
19:Z:699:ASP:OD1	19:Z:703:ASN:N	2.49	0.46
1:A:1234:GLU:OE1	1:A:1234:GLU:N	2.40	0.46
2:B:364:ILE:HD12	2:B:365:THR:HG22	1.96	0.46
2:B:806:THR:HG23	2:B:1045:SER:HA	1.96	0.46
8:H:40:LEU:HD21	8:H:42:ILE:HD11	1.97	0.46
4:D:133:THR:O	4:D:134:THR:OG1	2.30	0.46
15:O:1641:ARG:O	15:O:1645:ASN:ND2	2.43	0.46
15:O:1749:ILE:HD11	15:O:1793:ILE:HG12	1.96	0.46
6:F:79:ARG:NH1	6:F:145:ASP:O	2.49	0.46
1:A:356:ASP:OD1	11:K:65:HIS:NE2	2.47	0.46
1:A:68:GLN:O	1:A:71:GLN:NE2	2.49	0.46
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.16	0.46
19:Z:860:GLU:O	19:Z:864:ARG:N	2.45	0.46
3:C:101:LEU:HD23	3:C:102:GLN:N	2.31	0.45
1:A:830:LYS:O	1:A:834:THR:HG23	2.17	0.45
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.46	0.45
9:I:21:GLU:OE1	9:I:21:GLU:N	2.45	0.45
1:A:457:ALA:O	1:A:507:VAL:HG23	2.17	0.45
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.38	0.45
6:F:85:MET:HE2	6:F:90:ARG:HA	1.98	0.45
15:O:1309:GLN:O	15:O:1313:ALA:N	2.50	0.45
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.99	0.45
1:A:453:MET:SD	1:A:453:MET:N	2.90	0.45
1:A:709:THR:HG23	1:A:712:GLU:H	1.82	0.45
2:B:773:MET:SD	2:B:987:LYS:NZ	2.81	0.45
3:C:234:SER:OG	3:C:238:ILE:O	2.12	0.45
7:G:39:THR:O	7:G:43:GLY:N	2.50	0.45
1:A:1450:LEU:HD23	1:A:1450:LEU:O	2.17	0.45
2:B:120:ARG:HE	2:B:122:LEU:HD11	1.81	0.45
2:B:326:ASP:OD1	2:B:327:ARG:N	2.50	0.45
2:B:337:ARG:NH1	13:M:65:GLN:OE1	2.50	0.45
1:A:1147:THR:HG22	1:A:1197:LEU:CD2	2.47	0.45
1:A:1318:THR:CG2	5:E:141:VAL:HG11	2.47	0.44
2:B:22:SER:O	2:B:654:ARG:NH1	2.50	0.44
3:C:111:THR:HG23	15:O:1266:ARG:NH2	2.32	0.44
15:O:1354:LEU:HD21	15:O:1642:MET:HB2	1.99	0.44
1:A:445:ASN:ND2	1:A:454:SER:O	2.51	0.44
2:B:417:PHE:O	2:B:418:LYS:C	2.59	0.44
4:D:45:GLU:OE1	4:D:45:GLU:N	2.49	0.44
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1167:GLN:NE2	16:P:2:G:O6	2.50	0.44
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.82	0.44
1:A:1386:ARG:NH2	17:T:21:DA:N3	2.65	0.44
12:L:40:LEU:HD21	12:L:56:LEU:HD21	1.98	0.44
15:O:1212:SER:HG	15:O:1215:ASP:CG	2.26	0.44
2:B:619:ILE:N	2:B:619:ILE:HD12	2.32	0.44
8:H:143:LEU:N	8:H:143:LEU:HD12	2.32	0.44
19:Z:616:SER:O	19:Z:620:SER:N	2.49	0.44
11:K:60:ALA:O	11:K:73:LEU:HD12	2.17	0.44
15:O:1315:PRO:HG3	15:O:1642:MET:HE3	2.00	0.44
2:B:310:MET:CG	2:B:386:LEU:HD13	2.48	0.44
3:C:36:VAL:HG13	11:K:41:THR:HG21	1.99	0.44
15:O:1137:ILE:N	15:O:1137:ILE:HD12	2.33	0.44
15:O:1733:PHE:O	15:O:1737:ASP:N	2.51	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.82	0.44
3:C:37:MET:SD	3:C:244:VAL:HG12	2.57	0.44
1:A:526:ASP:OD1	1:A:527:THR:N	2.50	0.44
2:B:228:LYS:O	2:B:261:ARG:NH1	2.51	0.44
15:O:1686:ARG:NE	15:O:1789:GLU:OE2	2.45	0.44
2:B:255:GLN:N	2:B:255:GLN:OE1	2.50	0.44
3:C:121:VAL:HA	15:O:1276:LEU:HD12	1.99	0.44
1:A:471:ASN:O	1:A:474:VAL:HG22	2.18	0.43
2:B:183:GLU:N	2:B:183:GLU:OE1	2.51	0.43
2:B:785:TYR:O	2:B:967:ARG:NH1	2.50	0.43
1:A:118:HIS:O	1:A:123:ARG:NH1	2.51	0.43
1:A:352:VAL:HG12	1:A:353:ILE:N	2.33	0.43
1:A:834:THR:HG21	1:A:1076:ALA:O	2.18	0.43
15:O:1779:THR:O	15:O:1783:PHE:N	2.50	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
13:M:34:VAL:HG13	13:M:47:LEU:HD21	2.00	0.43
17:T:9:DT:H2'	17:T:10:DT:H71	2.01	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
11:K:49:GLU:OE2	11:K:93:SER:OG	2.35	0.43
12:L:66:GLN:HE21	19:Z:816:LEU:HG	1.84	0.43
1:A:718:VAL:HG11	1:A:774:ARG:NH1	2.33	0.43
1:A:465:TYR:HB3	2:B:976:ILE:HD11	2.00	0.43
1:A:523:ILE:HG22	1:A:524:VAL:N	2.34	0.43
1:A:1169:ILE:HG21	1:A:1239:ARG:CD	2.49	0.43
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.43	0.43
8:H:38:LEU:C	8:H:38:LEU:HD23	2.44	0.43
2:B:581:PHE:O	2:B:626:ILE:N	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ARG:O	2:B:331:LEU:HD23	2.18	0.42
19:Z:625:ILE:HG22	19:Z:626:THR:N	2.35	0.42
1:A:225:ASN:O	1:A:229:SER:OG	2.33	0.42
1:A:715:GLU:OE1	1:A:774:ARG:NE	2.51	0.42
1:A:759:ALA:O	1:A:764:CYS:N	2.41	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.54	0.42
1:A:117:GLU:O	1:A:123:ARG:NH1	2.50	0.42
2:B:301:ILE:HD12	2:B:382:ILE:HG21	2.00	0.42
13:M:47:LEU:C	13:M:47:LEU:HD23	2.45	0.42
1:A:301:ALA:O	1:A:305:ASP:N	2.41	0.42
1:A:609:ASP:OD2	1:A:969:GLN:NE2	2.52	0.42
1:A:1209:MET:HE3	1:A:1236:LEU:HB3	2.00	0.42
3:C:35:ARG:NE	11:K:41:THR:OG1	2.42	0.42
4:D:192:LYS:NZ	4:D:199:ASN:O	2.50	0.42
8:H:35:GLN:OE1	8:H:35:GLN:N	2.41	0.42
15:O:1815:ASN:O	15:O:1819:THR:HG23	2.20	0.42
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.47	0.42
4:D:130:LEU:O	4:D:130:LEU:HD23	2.19	0.42
7:G:12:THR:OG1	7:G:69:GLU:OE1	2.20	0.42
19:Z:79:VAL:HG11	19:Z:82:ILE:HD12	2.01	0.42
1:A:543:LEU:HD13	1:A:572:TRP:CH2	2.54	0.42
9:I:54:GLU:OE2	9:I:118:ARG:NH2	2.52	0.42
1:A:199:LEU:N	1:A:199:LEU:HD12	2.35	0.42
15:O:1843:LEU:C	15:O:1843:LEU:HD23	2.45	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG21	2.01	0.42
6:F:130:ILE:HG22	6:F:132:LEU:H	1.85	0.42
3:C:260:LEU:HD23	3:C:260:LEU:O	2.20	0.41
5:E:165:LEU:O	5:E:169:ARG:N	2.52	0.41
15:O:1169:LEU:C	15:O:1169:LEU:HD23	2.45	0.41
1:A:181:LEU:HD12	1:A:181:LEU:O	2.20	0.41
7:G:119:LEU:HD23	7:G:120:THR:N	2.35	0.41
17:T:8:DT:C2'	17:T:9:DT:H71	2.49	0.41
1:A:658:LEU:HD23	1:A:658:LEU:O	2.19	0.41
1:A:1373:ASP:O	1:A:1377:THR:N	2.54	0.41
2:B:90:ILE:N	2:B:90:ILE:HD12	2.36	0.41
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.54	0.41
3:C:53:THR:OG1	3:C:154:LYS:NZ	2.53	0.41
15:O:1187:ASN:OD1	15:O:1188:ARG:N	2.54	0.41
17:T:34:DC:H4'	17:T:35:DA:H5'	2.02	0.41
1:A:35:ILE:HD12	1:A:35:ILE:N	2.35	0.41
1:A:64:ASN:C	1:A:65:LEU:HD12	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:229:SER:N	2.53	0.41
1:A:826:ASP:O	1:A:830:LYS:HG2	2.21	0.41
1:A:1259:MET:HE2	1:A:1259:MET:HA	2.01	0.41
2:B:269:ILE:HD12	2:B:269:ILE:N	2.35	0.41
2:B:845:SER:HB3	2:B:850:LEU:HD22	2.03	0.41
1:A:534:LEU:HD11	1:A:541:ILE:HD11	2.02	0.41
1:A:561:PRO:O	1:A:572:TRP:NE1	2.42	0.41
1:A:1121:GLU:O	1:A:1125:ALA:N	2.54	0.41
2:B:952:VAL:HG23	2:B:966:VAL:HG22	2.02	0.41
5:E:68:SER:O	5:E:72:PHE:N	2.45	0.41
5:E:50:MET:SD	5:E:52:ARG:NH2	2.91	0.41
7:G:103:VAL:O	7:G:103:VAL:HG13	2.19	0.41
19:Z:8:SER:OG	19:Z:11:THR:OG1	2.20	0.41
1:A:489:LEU:HD23	1:A:489:LEU:C	2.45	0.41
1:A:902:LEU:HD23	1:A:902:LEU:O	2.21	0.41
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.21	0.41
3:C:155:LEU:HD12	3:C:155:LEU:C	2.45	0.41
4:D:27:LEU:N	4:D:27:LEU:HD22	2.36	0.41
9:I:19:ASP:O	9:I:23:ASN:CA	2.69	0.41
1:A:349:ALA:C	2:B:1128:LEU:HD21	2.45	0.41
2:B:861:ASP:OD1	2:B:862:GLN:N	2.53	0.41
5:E:128:PRO:N	5:E:129:PRO:HD2	2.35	0.41
15:O:1216:LEU:HD12	15:O:1245:ALA:O	2.21	0.41
15:O:1574:HIS:ND1	15:O:1576:VAL:HG12	2.35	0.41
1:A:866:PHE:N	5:E:208:TYR:OH	2.53	0.40
1:A:1006:ILE:N	1:A:1006:ILE:HD12	2.36	0.40
1:A:1348:LEU:O	1:A:1348:LEU:HD23	2.21	0.40
2:B:1168:LEU:HD11	2:B:1208:MET:SD	2.61	0.40
3:C:33:LEU:HD13	3:C:248:ILE:CD1	2.50	0.40
1:A:34:LYS:C	1:A:35:ILE:HD12	2.46	0.40
19:Z:711:ILE:HD13	19:Z:752:VAL:CG1	2.51	0.40
1:A:399:HIS:O	1:A:435:HIS:ND1	2.53	0.40
1:A:397:ASN:HB3	19:Z:839:THR:HG21	2.02	0.40
1:A:1318:THR:O	1:A:1318:THR:HG22	2.20	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.44	0.40
19:Z:806:ARG:CZ	19:Z:816:LEU:HD21	2.51	0.40
1:A:1002:GLY:N	1:A:1007:ILE:HG21	2.37	0.40
3:C:260:LEU:HD23	3:C:260:LEU:C	2.47	0.40
15:O:1253:THR:HG22	15:O:1254:LYS:N	2.34	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	1388/1733 (80%)	1345 (97%)	43 (3%)	0	100	100
2	B	1099/1224 (90%)	1077 (98%)	22 (2%)	0	100	100
3	C	262/318 (82%)	251 (96%)	11 (4%)	0	100	100
4	D	155/221 (70%)	153 (99%)	2 (1%)	0	100	100
5	E	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
6	F	83/155 (54%)	82 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	169 (100%)	0	0	100	100
8	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
9	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	63 (100%)	0	0	100	100
11	K	113/120 (94%)	113 (100%)	0	0	100	100
12	L	41/70 (59%)	41 (100%)	0	0	100	100
13	M	63/145 (43%)	63 (100%)	0	0	100	100
15	O	688/2231 (31%)	675 (98%)	13 (2%)	0	100	100
18	Y	98/102 (96%)	98 (100%)	0	0	100	100
19	Z	412/1063 (39%)	406 (98%)	6 (2%)	0	100	100
All	All	5091/8106 (63%)	4981 (98%)	110 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1225/1520 (81%)	1225 (100%)	0	100	100
2	B	964/1061 (91%)	964 (100%)	0	100	100
3	C	232/274 (85%)	231 (100%)	1 (0%)	84	82
4	D	141/200 (70%)	141 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	112/116 (97%)	112 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	60/131 (46%)	60 (100%)	0	100	100
15	O	618/2010 (31%)	618 (100%)	0	100	100
18	Y	85/87 (98%)	85 (100%)	0	100	100
19	Z	374/876 (43%)	374 (100%)	0	100	100
All	All	4548/7113 (64%)	4547 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	169	ASN
1	A	576	GLN
1	A	953	ASN
1	A	1059	HIS
2	B	52	ASN
2	B	481	GLN
2	B	538	ASN
2	B	951	GLN
3	C	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	23	ASN
4	D	37	GLN
7	G	57	GLN
7	G	71	ASN
13	M	29	ASN
13	M	42	ASN
15	O	1241	HIS
15	O	1267	ASN
15	O	1738	ASN
19	Z	102	ASN
19	Z	835	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	23/35 (65%)	8 (34%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	3	U
16	P	4	C
16	P	5	G
16	P	6	U
16	P	9	G
16	P	21	G
16	P	23	G
16	P	25	G

There are no RNA pucker outliers to report.

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

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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
22	ADP	O	3001	21	28,29,29	1.43	4 (14%)	43,45,45	1.90	11 (25%)
23	BEF	O	3003	-	0,3,3	-	-	-		

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
22	ADP	O	3001	21	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	3001	ADP	C5-C4	4.76	1.47	1.39
22	O	3001	ADP	C5-C6	2.82	1.48	1.41
22	O	3001	ADP	C8-N7	2.47	1.36	1.31
22	O	3001	ADP	C5-N7	-2.31	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	3001	ADP	C5-C4-N3	-6.02	118.42	126.72
22	O	3001	ADP	N3-C4-N9	4.65	135.08	127.17
22	O	3001	ADP	C2-N3-C4	3.95	121.47	111.83
22	O	3001	ADP	N3-C2-N1	-3.69	123.00	128.58
22	O	3001	ADP	C4-C5-N7	-3.66	106.39	110.58
22	O	3001	ADP	C5-N7-C8	2.79	107.84	103.45
22	O	3001	ADP	C3'-C2'-C1'	2.55	106.28	101.46
22	O	3001	ADP	C4-N9-C8	2.52	108.39	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	3001	ADP	C6-C5-N7	2.17	136.28	132.09
22	O	3001	ADP	N9-C8-N7	-2.15	110.88	113.94
22	O	3001	ADP	C2-N1-C6	2.13	122.22	118.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

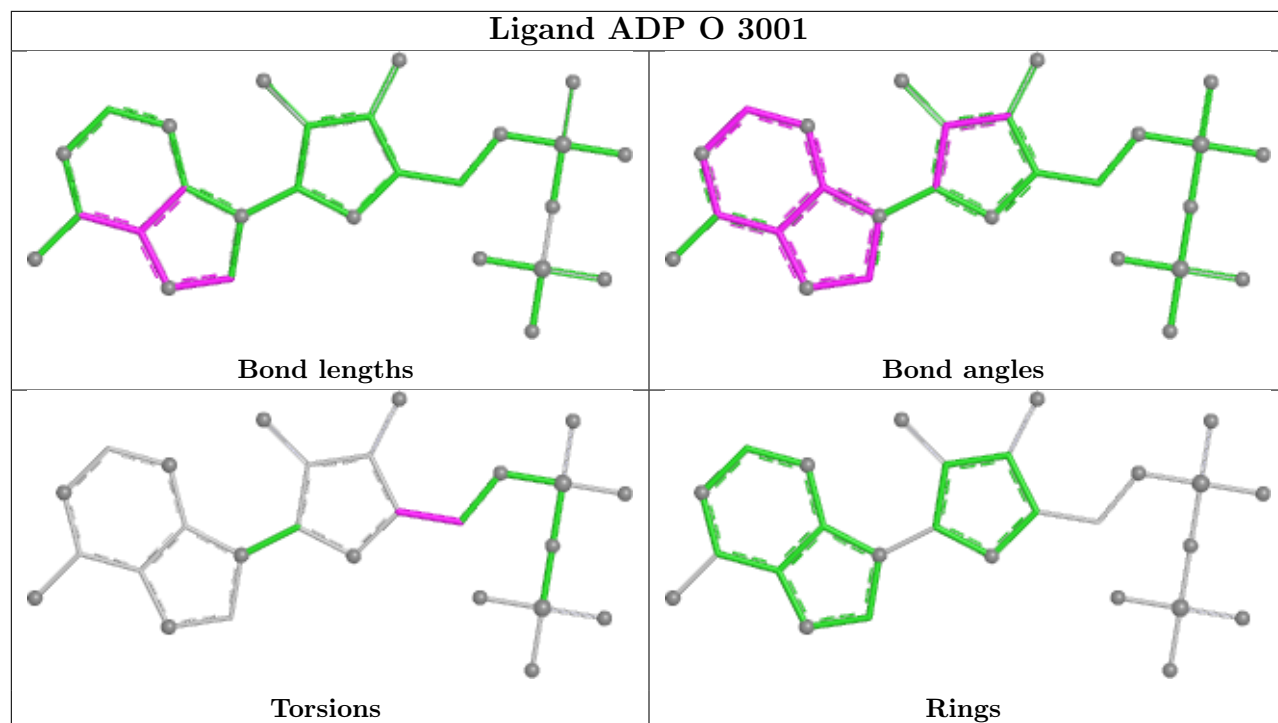
Mol	Chain	Res	Type	Atoms
22	O	3001	ADP	O4'-C4'-C5'-O5'
22	O	3001	ADP	C3'-C4'-C5'-O5'

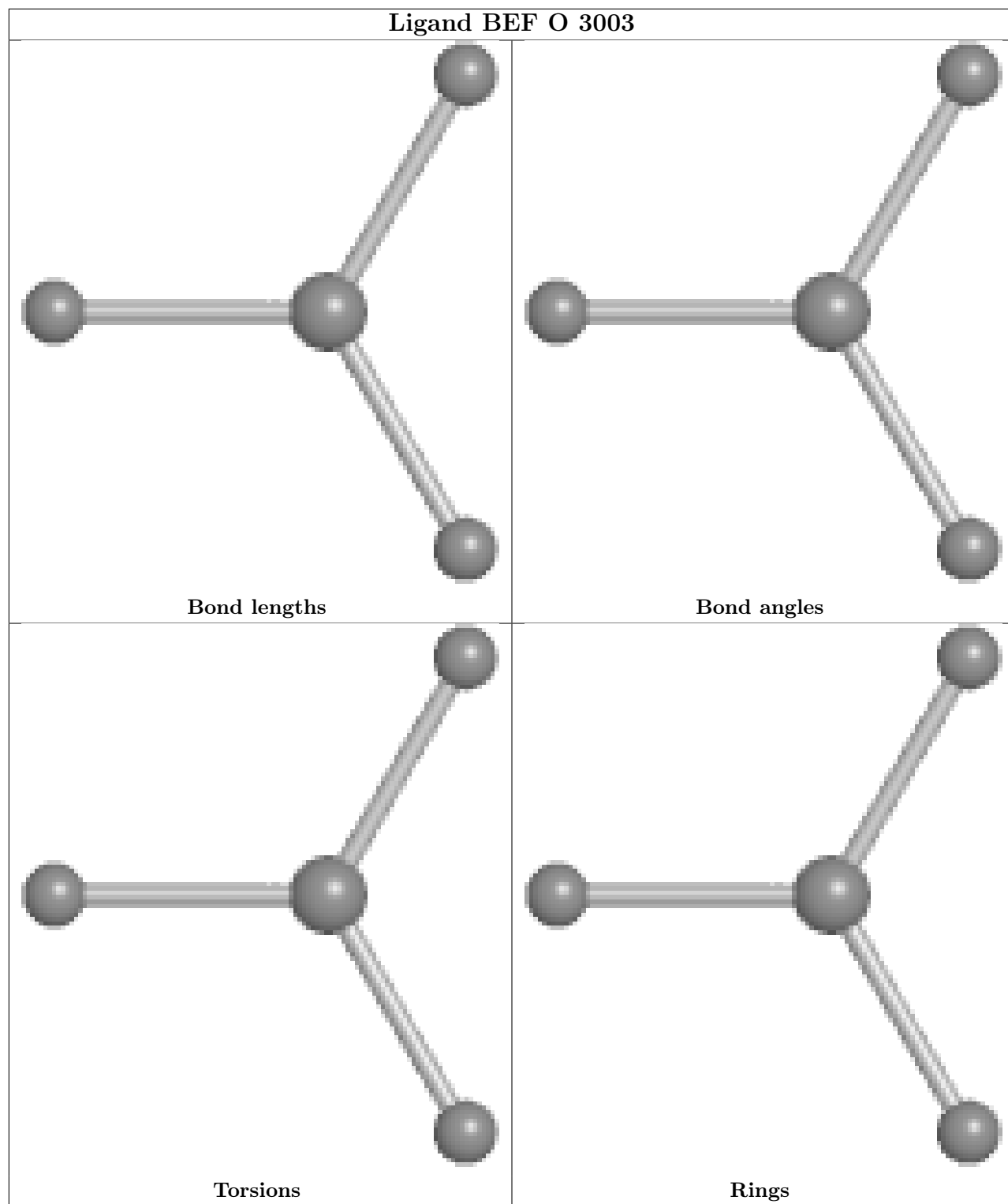
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	3003	BEF	3	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 ⓘ

There are no chain breaks in this entry.

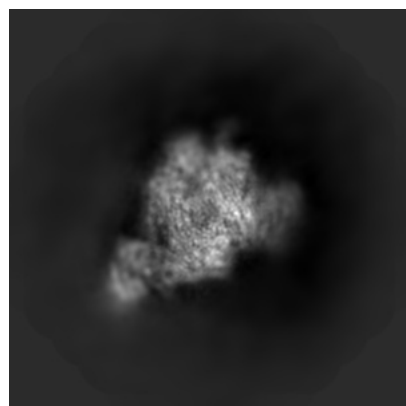
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19022. These allow visual inspection of the internal detail of the map and identification of artifacts.

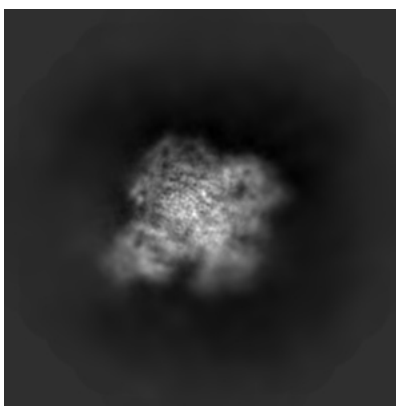
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

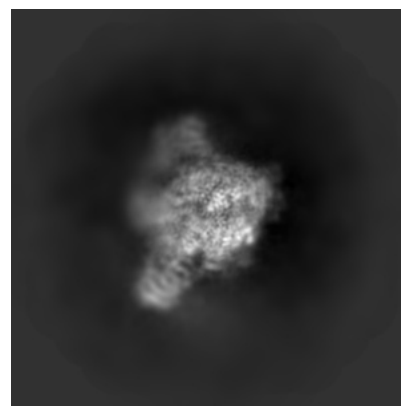
6.1.1 Primary map



X

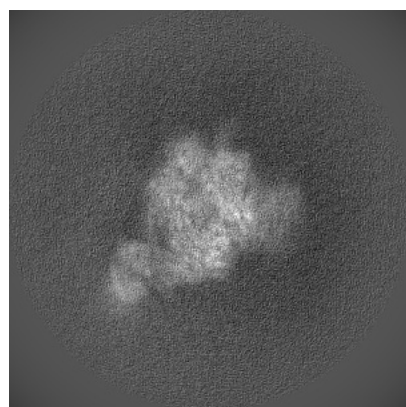


Y

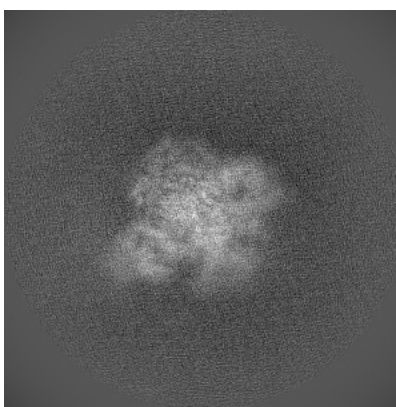


Z

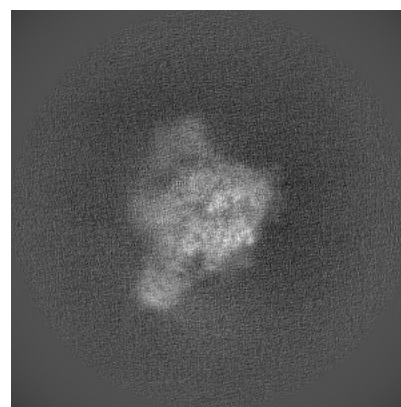
6.1.2 Raw map



X



Y

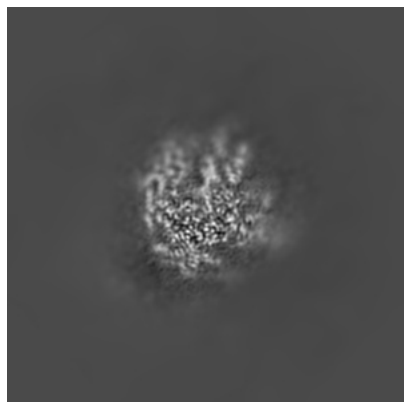


Z

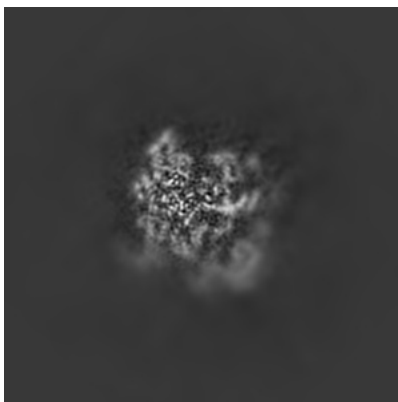
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

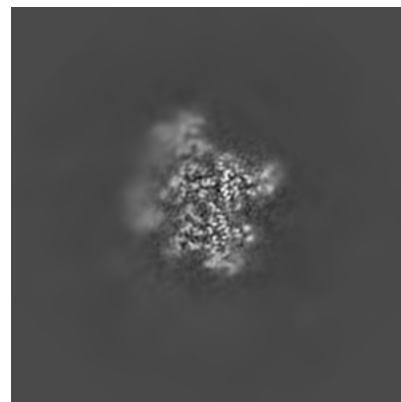
6.2.1 Primary map



X Index: 180

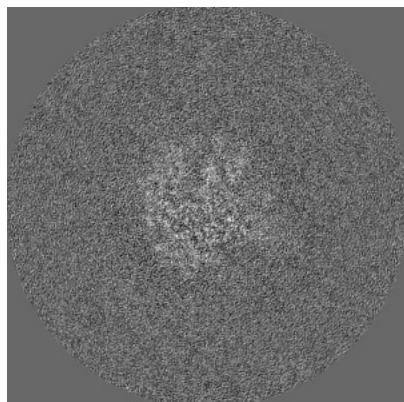


Y Index: 180

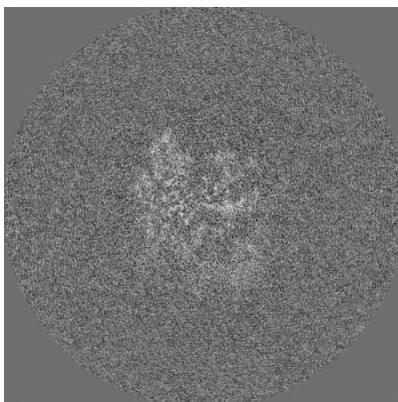


Z Index: 180

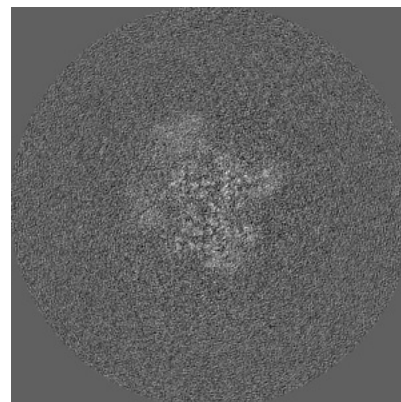
6.2.2 Raw map



X Index: 180



Y Index: 180

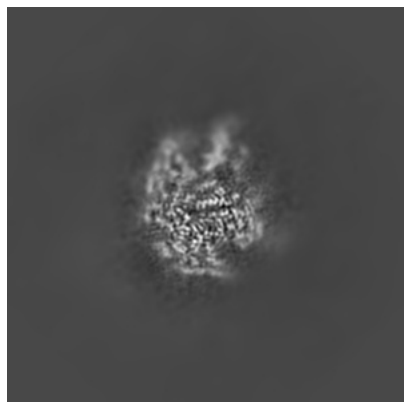


Z Index: 180

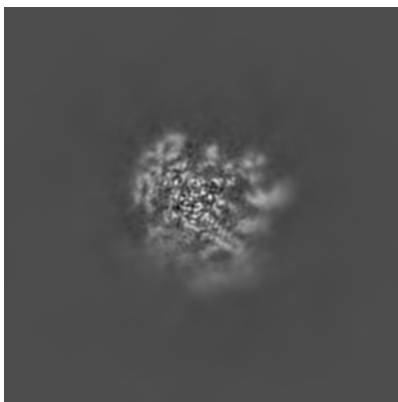
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

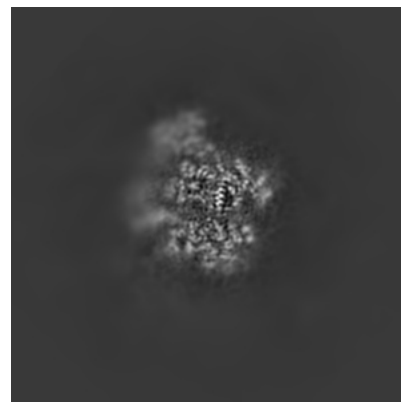
6.3.1 Primary map



X Index: 186

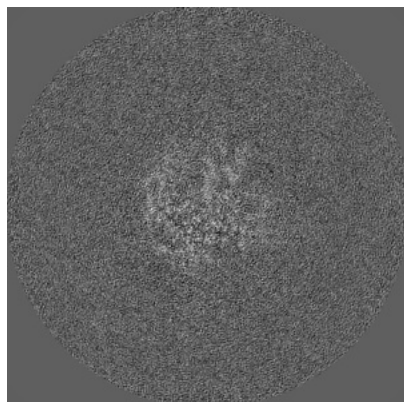


Y Index: 190

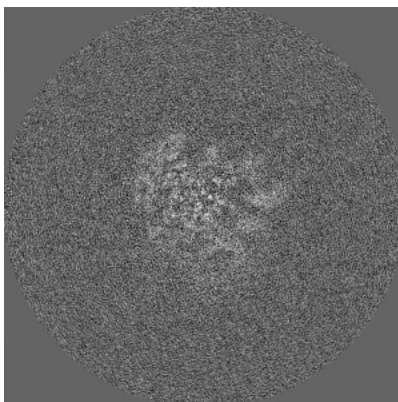


Z Index: 185

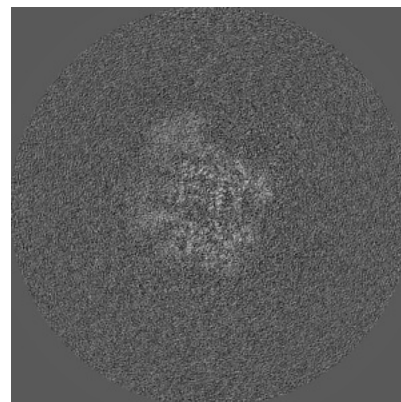
6.3.2 Raw map



X Index: 179



Y Index: 190

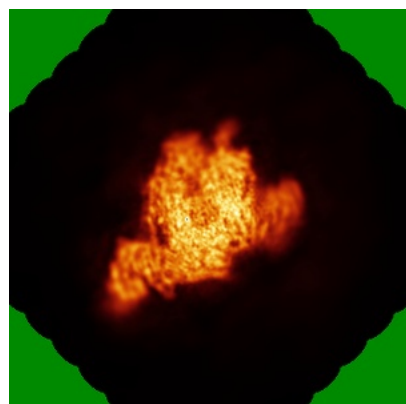


Z Index: 185

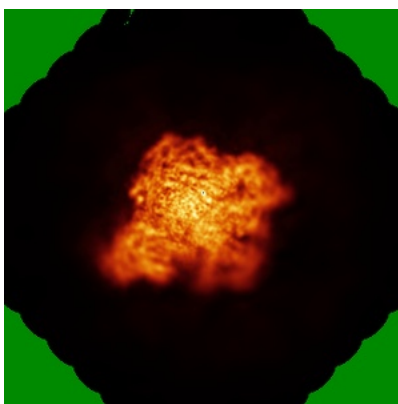
The images above show the largest variance slices of the map in three orthogonal directions.

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

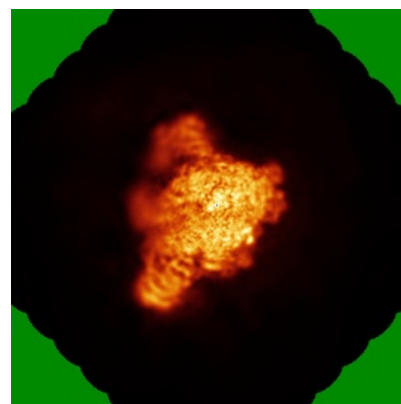
6.4.1 Primary map



X

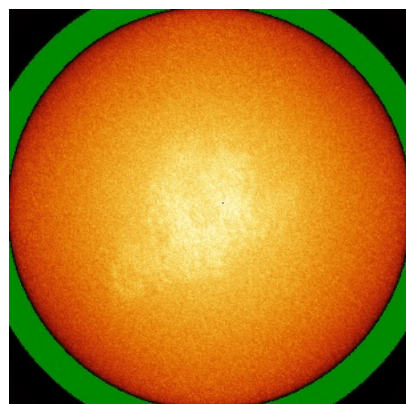


Y

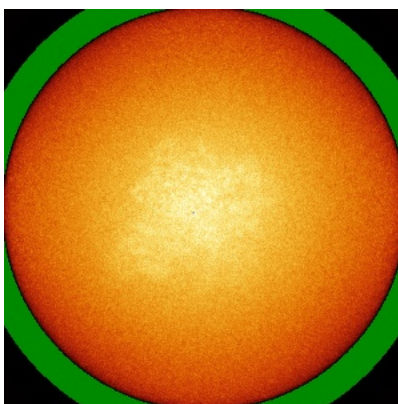


Z

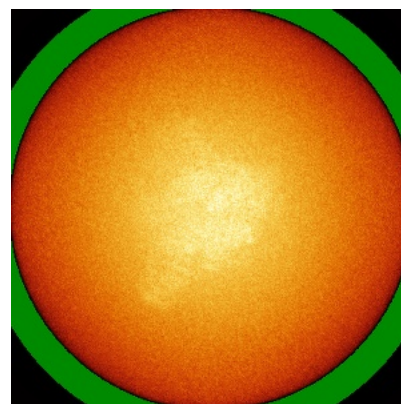
6.4.2 Raw map



X



Y

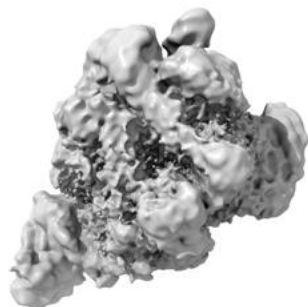


Z

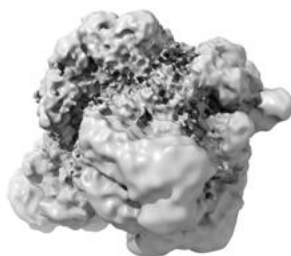
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

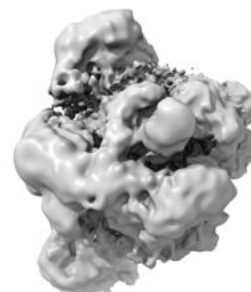
6.5.1 Primary map



X



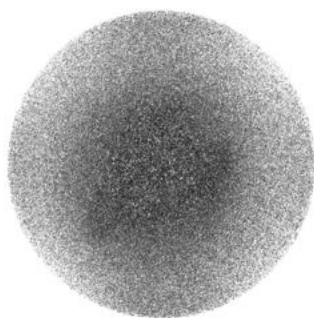
Y



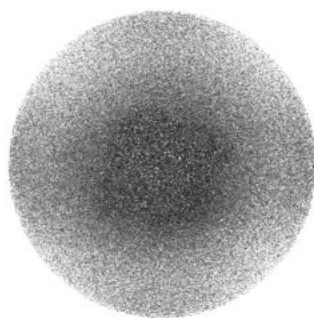
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

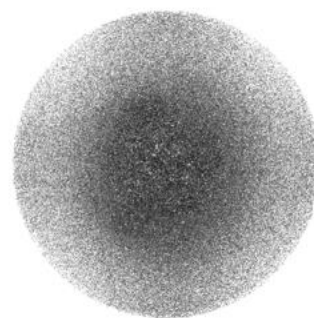
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

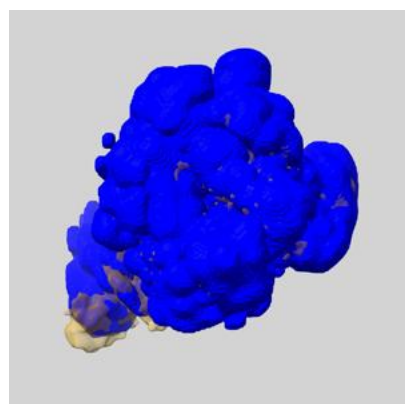
6.6 Mask visualisation [i](#)

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

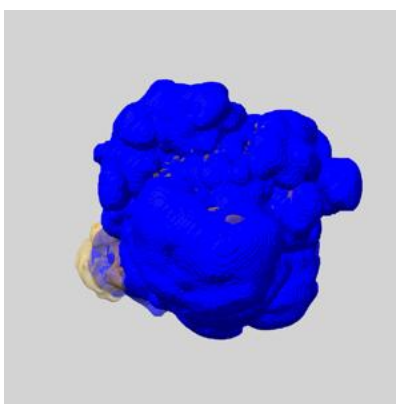
A mask typically either:

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

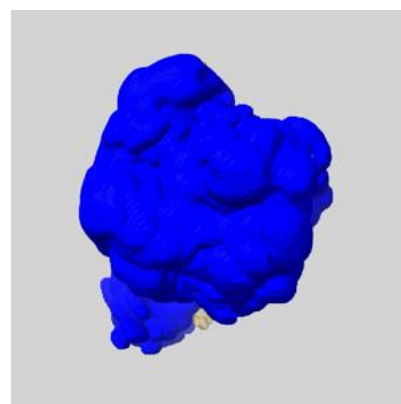
6.6.1 emd_19022_msk_1.map [i](#)



X



Y

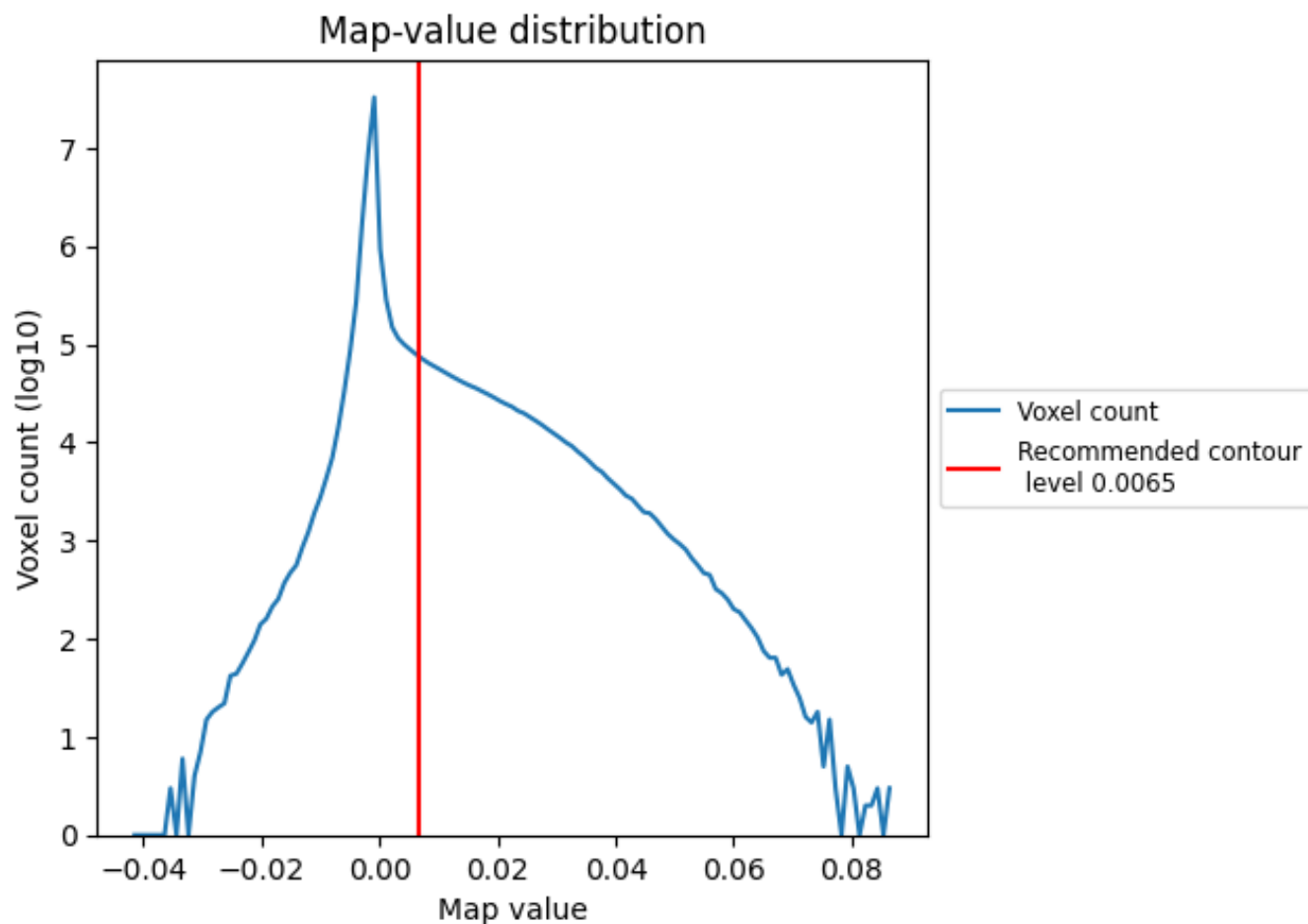


Z

7 Map analysis [i](#)

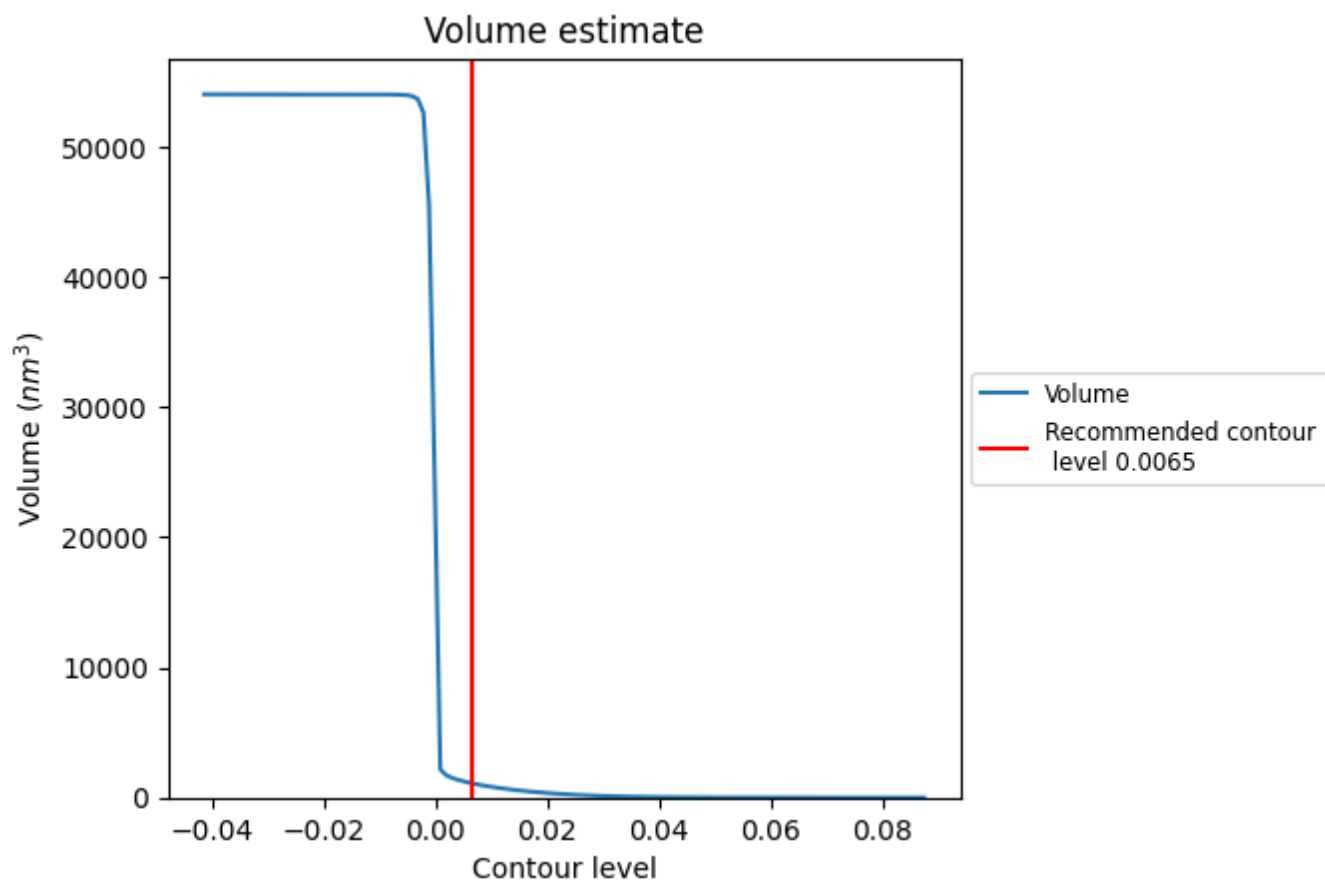
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

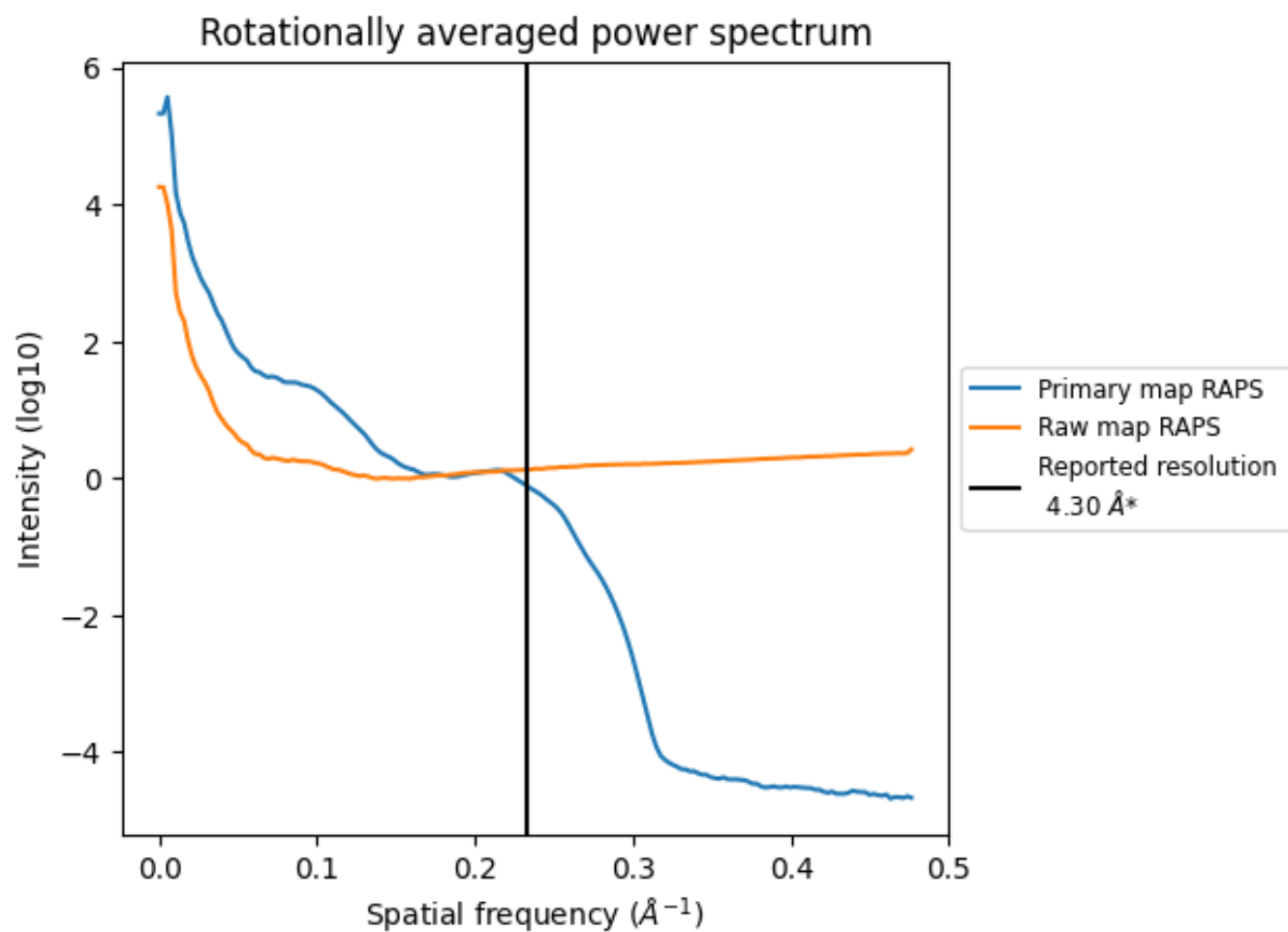
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1093 nm^3 ; this corresponds to an approximate mass of 987 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 ⓘ

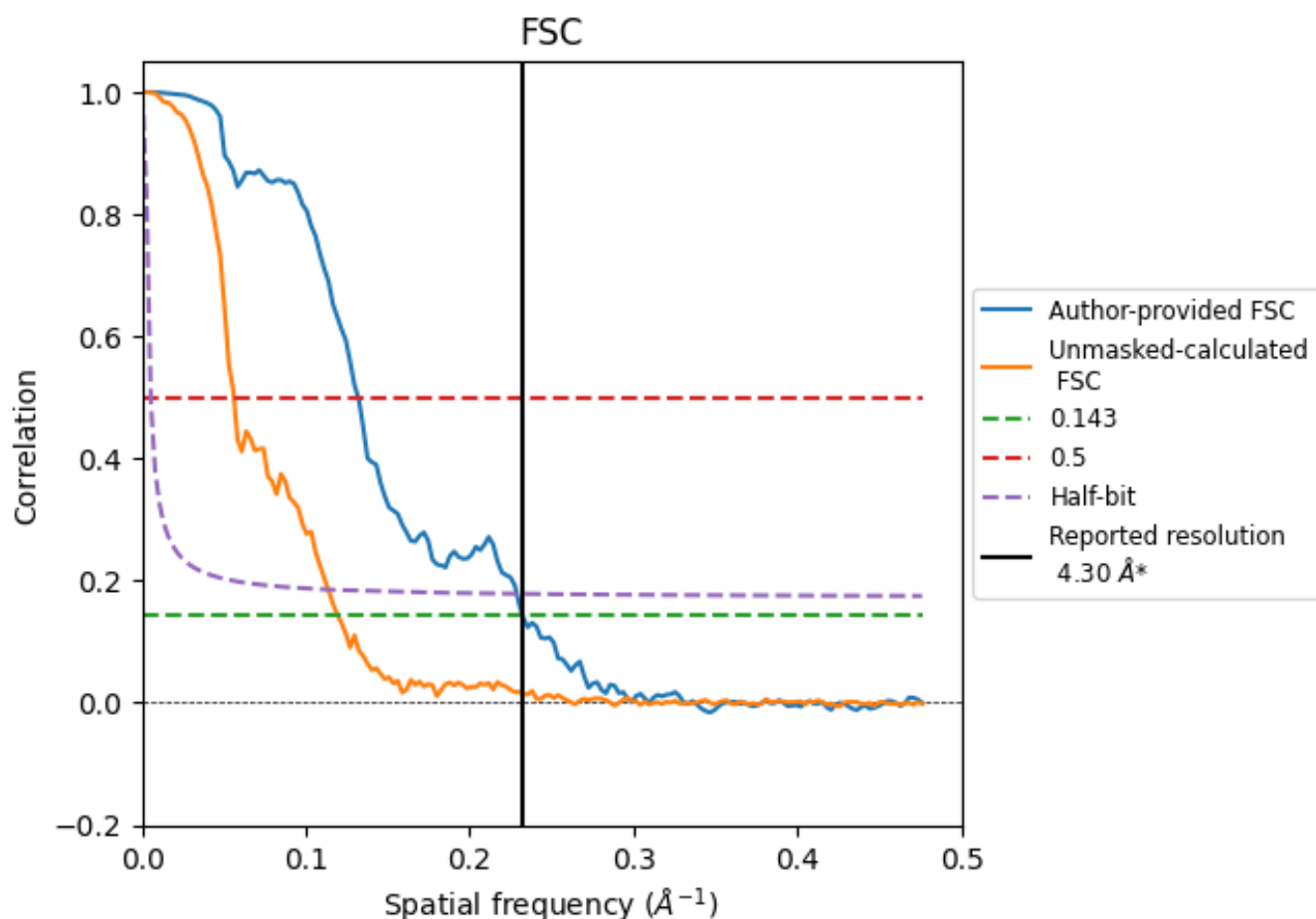


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

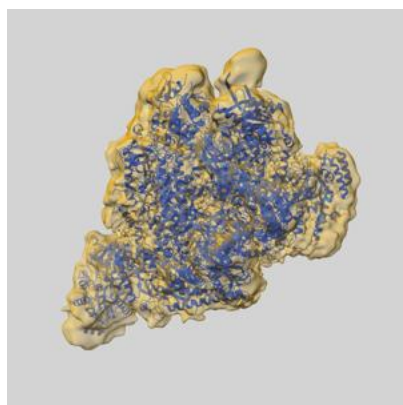
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.31	7.58	4.37
Unmasked-calculated*	8.38	17.89	8.80

*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 8.38 differs from the reported value 4.3 by more than 10 %

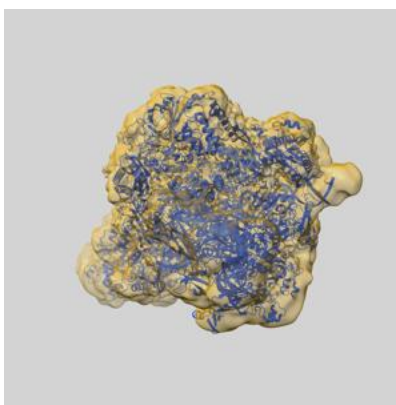
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19022 and PDB model 8RAP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

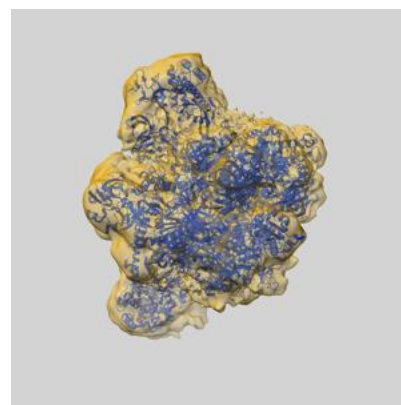
9.1 Map-model overlay [i](#)



X



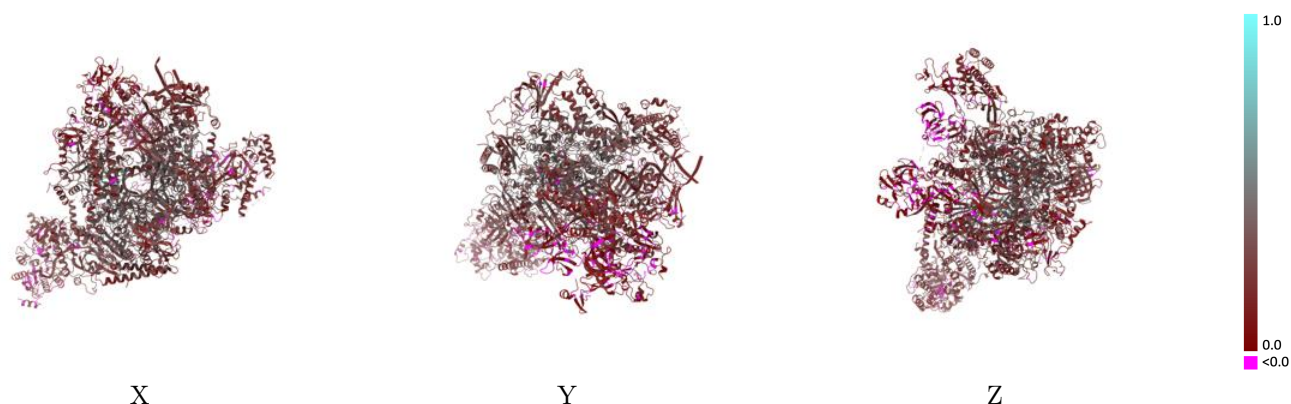
Y



Z

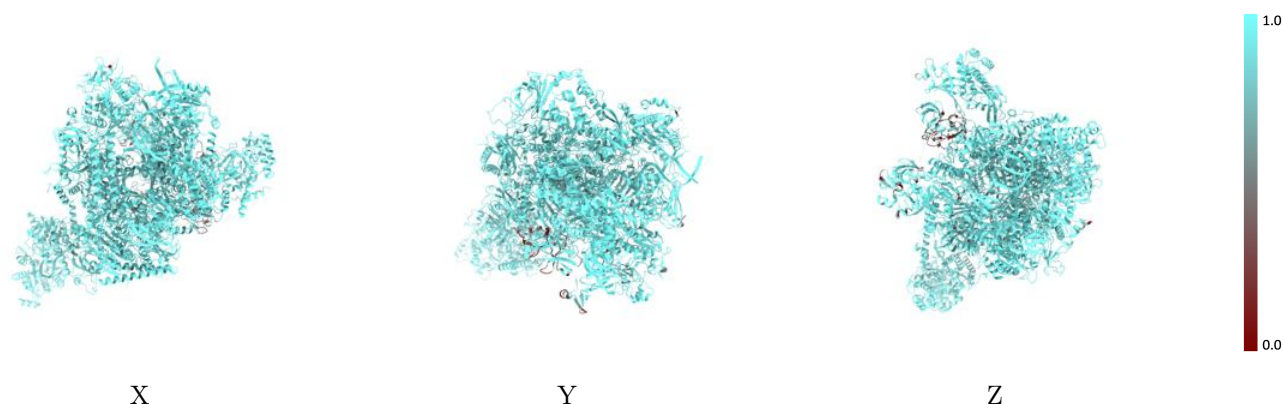
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



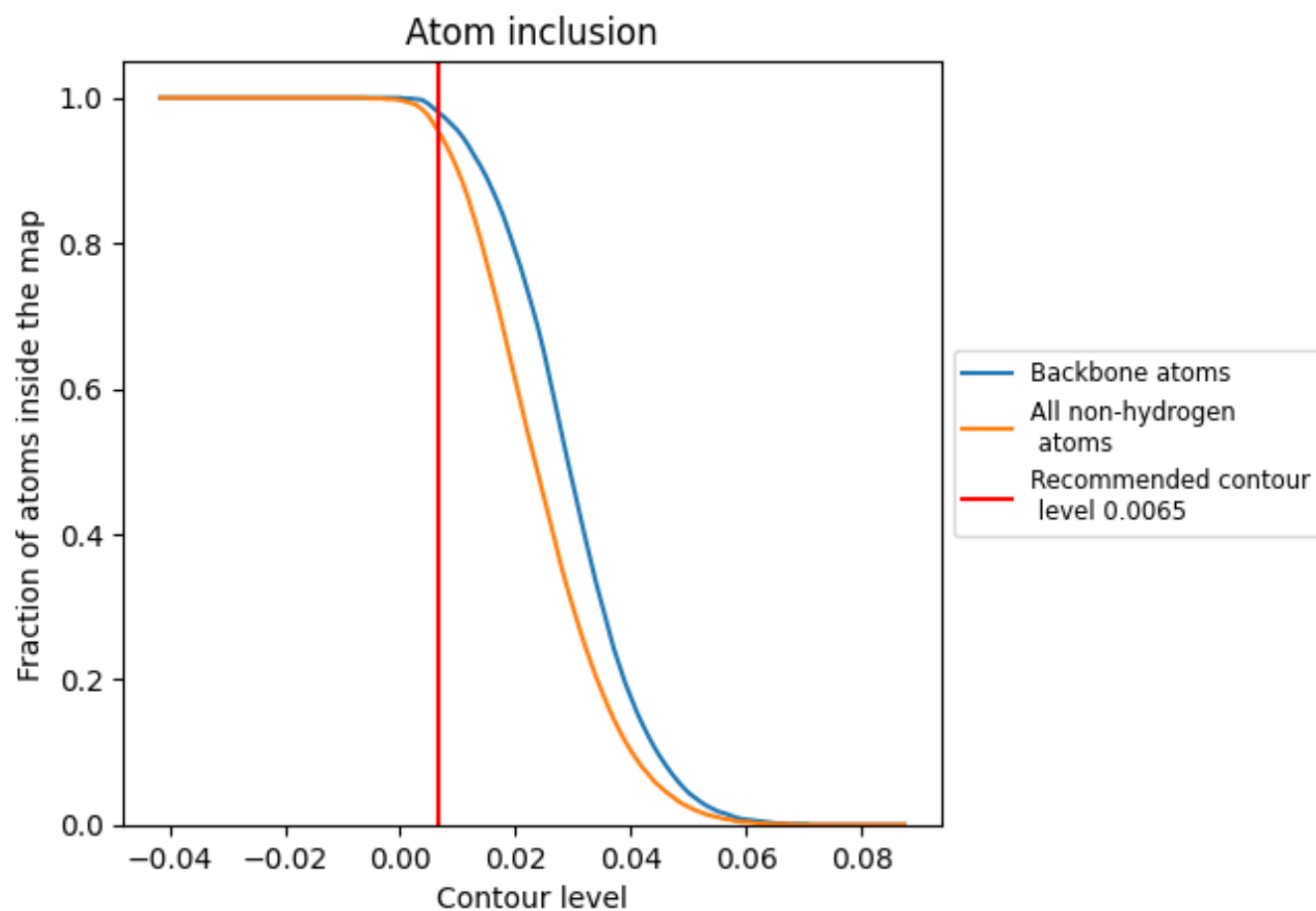
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.2400
A	 0.9660	 0.2910
B	 0.9660	 0.3020
C	 0.9660	 0.3130
D	 0.9830	 0.1600
E	 0.9820	 0.2750
F	 0.9790	 0.2940
G	 0.9750	 0.1620
H	 0.9820	 0.2430
I	 0.9820	 0.1500
J	 0.9590	 0.3350
K	 0.9800	 0.2720
L	 0.9550	 0.2900
M	 0.8980	 0.1210
N	 0.9820	 0.1840
O	 0.9760	 0.1680
P	 0.9870	 0.2190
T	 0.9820	 0.2400
Y	 0.9290	 0.0720
Z	 0.7950	 0.0850

