



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 05:14 AM JST

PDB ID : 9XAB / pdb_00009xab
EMDB ID : EMD-66681
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 WT) from *Chaetomium thermophilum*, state Tsr1-3
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.20 Å (reported)
Based on initial model : 6G18

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

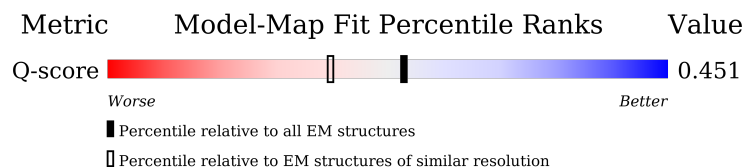
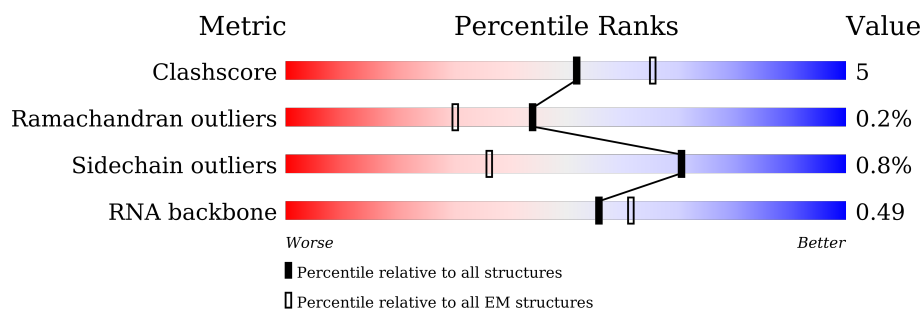
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



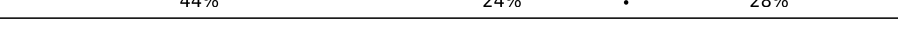
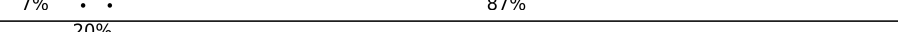
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	D	285	
2	E	255	
3	F	263	

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Mol	Chain	Length	Quality of chain
4	H	264	 88% 11%
5	J	239	 81% 16%
6	K	203	 79% 17%
7	L	202	 84% 16%
8	M	190	 82% 13% 6%
9	O	161	 81% 12% 7%
10	Q	151	 93% 7%
11	R	150	 71% 19% 10%
12	U	143	 6% 22% 77%
13	Y	98	 71% 16% 12%
14	Z	130	 84% 15%
15	a	145	 77% 16% 7%
16	b	136	 86% 11%
17	e	82	 88% 11%
18	h	62	 27% 5% 68%
19	A	1796	 44% 24% 28%
20	1	282	 7% 87%
21	2	830	 20% 64% 16% 20%
22	3	259	 56% 15% 29%

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 56332 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	208	Total	C	N	O	S	0	0
			1641	1051	289	295	6		

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	213	Total	C	N	O	S	0	0
			1723	1096	319	303	5		

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	207	Total	C	N	O	S	0	0
			1598	1032	275	288	3		

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	261	Total	C	N	O	S	0	0
			2072	1314	389	362	7		

- Molecule 5 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	232	Total	C	N	O	S	0	0
			1875	1171	376	323	5		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	195	Total	C	N	O	0	0
			1562	983	300	279		

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 8 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 9 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 10 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 11 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	135	Total	C	N	O	S	0	0
			1002	614	199	184	5		

- Molecule 12 is a protein called 40S ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	33	Total	C	N	O	S	0	0
			255	161	40	53	1		

- Molecule 13 is a protein called 40S ribosomal protein S21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	86	Total	C	N	O	S	0	0
			664	408	124	128	4		

- Molecule 14 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 15 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	135	Total	C	N	O	S	0	0
			1048	663	202	181	2		

- Molecule 16 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	132	Total	C	N	O	S	0	0
			1061	668	209	182	2		

- Molecule 17 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 18 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	h	20	Total	C	N	O	0	0
			172	112	37	23		

- Molecule 19 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	1286	Total	C	N	O	P	0	0
			27436	12263	4904	8983	1286		

- Molecule 20 is a protein called Methyltransferase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	37	Total	C	N	O	S	0	0
			307	195	62	49	1		

- Molecule 21 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	667	Total	C	N	O	S	0	0
			5319	3348	970	983	18		

- Molecule 22 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	184	Total	C	N	O	S	0	0
			1451	921	267	256	7		

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

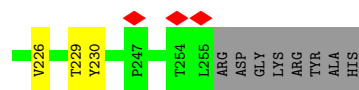
Mol	Chain	Residues	Atoms		AltConf
23	a	1	Total	Mg	0
			1	1	
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	e	1	Total	Zn	0
			1	1	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	4	Total	O	0
			4	4	



- Molecule 4: 40S ribosomal protein S4

Chain H: 88% 11%



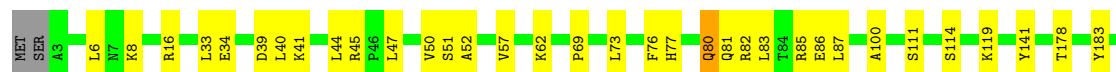
- Molecule 5: 40S ribosomal protein S6

Chain J: 81% 16%



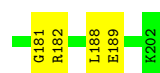
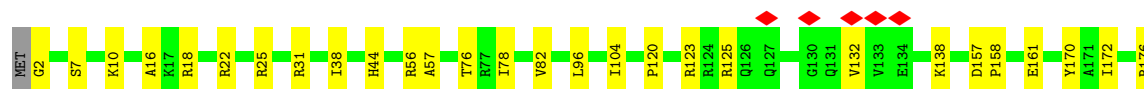
- Molecule 6: 40S ribosomal protein S7

Chain K: 79% 17%



- Molecule 7: 40S ribosomal protein S8

Chain L: 84% 16%



- Molecule 8: 40S ribosomal protein s9-like protein

Chain M: 82% 13% 6%



- Molecule 9: 40S ribosomal protein S11-like protein

Chain O:  81% 12% 7%



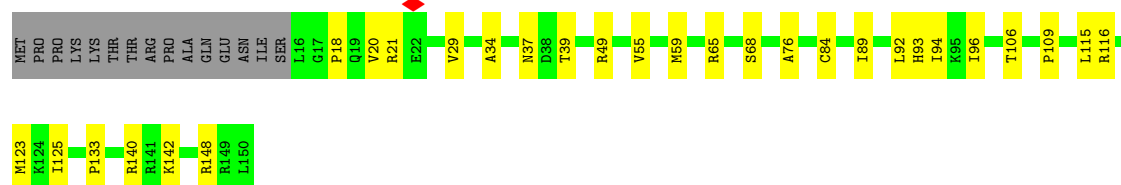
- Molecule 10: 40S ribosomal protein S13-like protein

Chain Q:  93% 7%



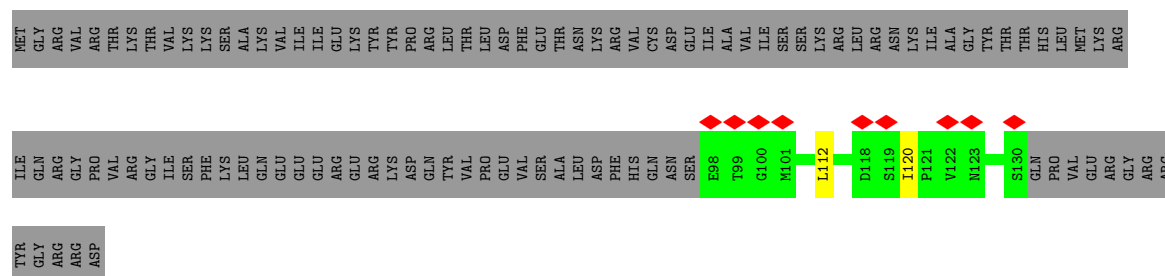
- Molecule 11: 40S ribosomal protein S14-like protein

Chain R:  71% 19% 10%



- Molecule 12: 40S ribosomal protein S17-like protein

Chain U:  6% 22% 77%



- Molecule 13: 40S ribosomal protein S21-like protein

Chain Y:  71% 16% 12%



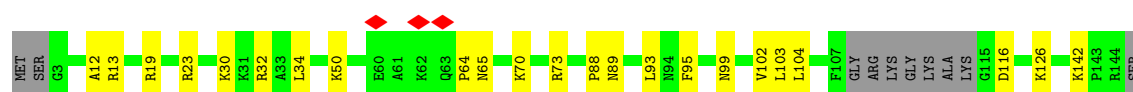
- Molecule 14: 40S ribosomal protein S22-like protein

Chain Z:  84% 15%



- Molecule 15: 40S ribosomal protein s23-like protein

Chain a: 



- Molecule 16: Small ribosomal subunit protein eS24

Chain b: 



- Molecule 17: Ribosomal protein s27-like protein

Chain e: 



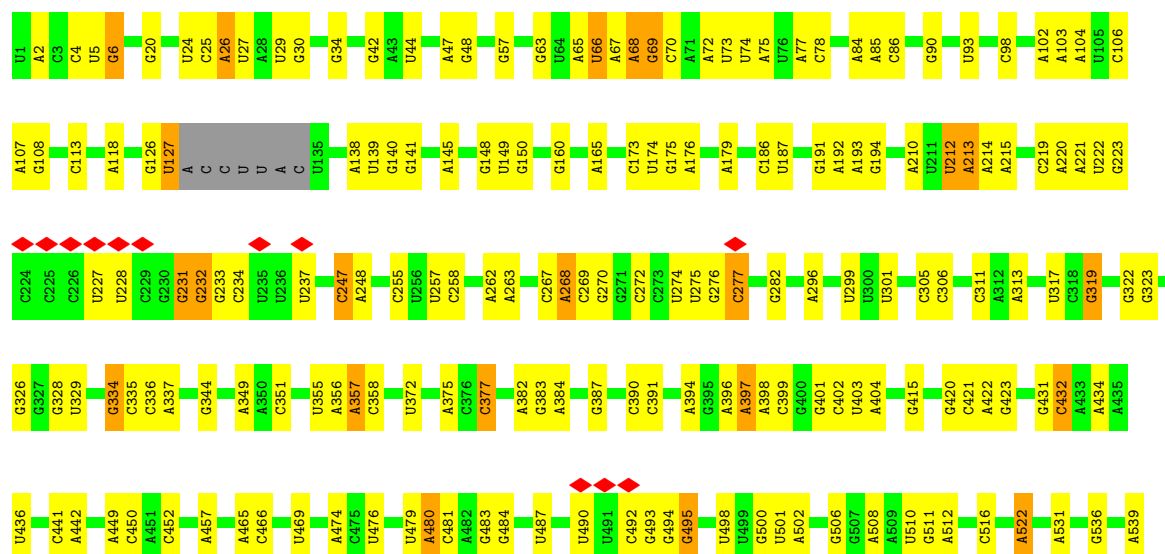
- Molecule 18: 40S ribosomal protein S30

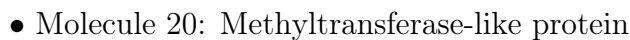
Chain h: 



- Molecule 19: 18S rRNA

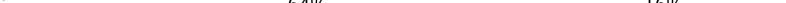
Chain A: 



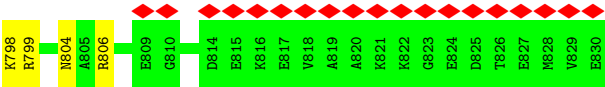


[illegible]

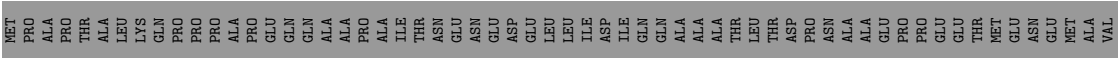
GLY	K246	S249	K250	K255	E258	Q259	M260	E261	R262	K263	G264	K265	I266	V267	K268	P280	K281	F282
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Chain 2: 

L726	G643	S622	G643	T727	S644	E527	G648	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797
L727	G644	E527	D648	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797				
G728	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797					
G729	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797					
G730	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797					
G731	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797					
G732	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497	A616	S617	I618	S622	E623	M624	R632	A707	T708	N636	P637	L712	T716	A721	K722	R723	A724	I725	S795	L796	V797					
G733	S644	E527	V649	E533	W537	K651	Y652	G653	R654	L541	R542	I543	P544	D545	R547	A471	D473	M474	R475	A476	L477	A478	A479	Y480	R481	K482	L483	K484	R485	L575	T486	E487	A488	E489	D490	D491	R492	E493	F494	P495	A603	L607	E497																										



• Molecule 22: Pre-rRNA-processing protein PNO1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.477	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	412.56, 412.56, 412.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	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, 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	D	0.22	0/1683	0.52	0/2299
2	E	0.21	0/1752	0.54	0/2361
3	F	0.33	0/1628	0.64	0/2203
4	H	0.16	0/2112	0.43	0/2842
5	J	0.17	0/1906	0.44	0/2547
6	K	0.22	0/1587	0.58	0/2140
7	L	0.16	0/1654	0.41	0/2213
8	M	0.16	0/1489	0.44	0/1993
9	O	0.15	0/1249	0.39	0/1678
10	Q	0.16	0/1205	0.43	0/1627
11	R	0.23	0/1014	0.62	0/1361
12	U	0.17	0/258	0.43	0/350
13	Y	0.18	0/671	0.50	0/900
14	Z	0.20	0/1055	0.53	0/1416
15	a	0.25	0/1064	0.55	0/1422
16	b	0.15	0/1075	0.42	0/1431
17	e	0.20	0/623	0.53	0/843
18	h	0.42	0/175	0.64	0/230
19	A	0.22	0/30689	0.38	5/47813 (0.0%)
20	1	0.91	0/311	1.22	3/403 (0.7%)
21	2	0.24	0/5432	0.50	0/7349
22	3	0.28	0/1475	0.57	0/1982
All	All	0.23	0/60107	0.45	8/87403 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1763	G	C2'-C3'-O3'	-10.52	97.91	113.70
19	A	1763	G	C1'-O4'-C4'	-6.81	103.09	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	552	A	C2'-C3'-O3'	6.52	123.48	113.70
20	1	262	ARG	N-CA-C	-6.42	104.37	111.36
19	A	1763	G	C4'-C3'-O3'	6.09	122.14	113.00
19	A	1763	G	C4'-C3'-C2'	-5.39	97.21	102.60
20	1	280	PRO	N-CA-CB	-5.23	97.76	103.25
20	1	261	GLU	N-CA-C	-5.06	106.27	112.90

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	D	1641	0	1650	22	0
2	E	1723	0	1804	13	0
3	F	1598	0	1698	24	0
4	H	2072	0	2155	20	0
5	J	1875	0	1983	28	0
6	K	1562	0	1641	22	0
7	L	1621	0	1645	23	0
8	M	1466	0	1582	19	0
9	O	1222	0	1289	16	0
10	Q	1182	0	1264	6	0
11	R	1002	0	1034	23	0
12	U	255	0	255	2	0
13	Y	664	0	662	14	0
14	Z	1037	0	1076	13	0
15	a	1048	0	1105	17	0
16	b	1061	0	1150	8	0
17	e	611	0	632	6	0
18	h	172	0	201	2	0
19	A	27436	0	13822	233	0
20	1	307	0	346	8	0
21	2	5319	0	5354	78	0
22	3	1451	0	1524	21	0
23	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	1	0	0	0	0
24	e	1	0	0	0	0
25	A	4	0	0	0	0
All	All	56332	0	43872	527	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 (527) 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)
21:2:263:VAL:HA	21:2:274:ILE:O	1.32	1.21
3:F:92:LYS:HA	20:1:264:GLY:HA3	1.22	1.21
19:A:214:A:N6	19:A:828:U:H3	1.59	1.01
19:A:824:U:H3	19:A:844:G:H1	1.09	0.97
19:A:214:A:H62	19:A:828:U:H3	1.03	0.95
19:A:1762:A:H2'	19:A:1763:G:H1'	1.49	0.95
19:A:1661:U:H3	19:A:1732:G:H1	1.17	0.87
19:A:1763:G:H2'	19:A:1764:G:C8	2.14	0.82
19:A:652:G:H1	19:A:673:U:H3	1.29	0.81
19:A:709:G:H1	19:A:722:U:H3	1.25	0.80
14:Z:83:LEU:O	14:Z:86:LEU:HB3	1.82	0.80
19:A:702:A:H62	19:A:731:G:N2	1.82	0.77
19:A:866:G:H1	19:A:958:U:H3	1.33	0.77
3:F:92:LYS:HA	20:1:264:GLY:CA	2.11	0.74
19:A:220:A:N1	19:A:835:G:C6	2.55	0.73
6:K:73:LEU:HD22	6:K:100:ALA:HB2	1.71	0.72
21:2:201:GLN:HA	21:2:204:ARG:HD3	1.73	0.71
14:Z:2:VAL:N	19:A:1032:C:HO2'	1.89	0.70
19:A:219:C:N4	19:A:220:A:N6	2.41	0.69
21:2:256:SER:HB3	21:2:593:SER:HB3	1.72	0.69
19:A:1078:A:H62	19:A:1088:A:H62	1.41	0.68
19:A:214:A:N7	19:A:828:U:O2	2.29	0.66
15:a:50:LYS:HG3	19:A:432:C:H5'	1.76	0.66
21:2:215:ILE:O	21:2:219:HIS:N	2.28	0.66
5:J:231:LYS:HD2	5:J:232:ARG:HG2	1.79	0.65
6:K:41:LYS:HB3	6:K:45:ARG:HH22	1.59	0.65
21:2:537:TRP:HE1	21:2:716:THR:HB	1.62	0.65
19:A:702:A:N6	19:A:731:G:N2	2.45	0.64
21:2:96:ILE:HG22	21:2:142:LEU:HD21	1.79	0.63
7:L:138:LYS:NZ	19:A:186:C:OP2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:80:VAL:O	9:O:125:GLY:N	2.31	0.62
21:2:125:VAL:HG22	21:2:140:ILE:HG12	1.79	0.62
9:O:74:ARG:NH1	19:A:301:U:O2	2.32	0.62
3:F:172:SER:HB2	19:A:1083:A:H5'	1.81	0.61
7:L:182:ARG:NH1	19:A:255:C:O2	2.33	0.61
2:E:179:CYS:HB3	2:E:183:GLN:HB2	1.84	0.60
4:H:51:ARG:NH1	4:H:109:PHE:O	2.35	0.60
4:H:87:MET:HE1	4:H:235:ILE:HD13	1.84	0.60
15:a:99:ASN:O	21:2:250:ARG:NH2	2.34	0.60
5:J:160:ARG:HH12	19:A:68:A:H5'	1.67	0.60
19:A:565:G:N2	19:A:572:C:C2	2.70	0.60
19:A:1143:G:H3'	19:A:1144:A:H8	1.66	0.60
21:2:90:PRO:HD2	21:2:278:VAL:HG11	1.83	0.60
4:H:12:LEU:HD11	8:M:3:PRO:HG3	1.83	0.59
15:a:73:ARG:NH2	19:A:1645:C:O2'	2.36	0.59
8:M:77:ARG:NH1	19:A:761:A:OP1	2.34	0.59
19:A:1686:G:N2	19:A:1708:A:N7	2.51	0.59
9:O:82:SER:HB3	9:O:90:ILE:HB	1.86	0.58
21:2:163:LEU:HB2	21:2:192:VAL:HG22	1.84	0.58
7:L:78:ILE:HG12	7:L:104:ILE:HG22	1.85	0.58
21:2:260:ILE:HD12	21:2:275:VAL:HB	1.86	0.58
15:a:73:ARG:HH22	19:A:1646:U:H5'	1.68	0.58
15:a:95:PHE:O	15:a:142:LYS:NZ	2.34	0.57
19:A:1688:G:N1	19:A:1706:U:N3	2.53	0.57
19:A:869:A:H2'	19:A:870:G:C8	2.40	0.57
1:D:59:LYS:NZ	13:Y:70:ASN:OD1	2.38	0.57
11:R:59:MET:HE1	19:A:897:G:H4'	1.85	0.57
8:M:134:VAL:HG22	8:M:154:ILE:HG12	1.87	0.57
9:O:107:LYS:O	15:a:13:ARG:NH2	2.38	0.57
1:D:44:ARG:HH12	1:D:48:VAL:HG22	1.70	0.56
21:2:635:ILE:HG23	21:2:637:PRO:HD3	1.87	0.56
19:A:442:A:H1'	19:A:522:A:H5''	1.86	0.56
21:2:255:ARG:NH2	21:2:671:THR:OG1	2.38	0.56
21:2:737:ILE:HD12	21:2:769:LYS:HZ1	1.70	0.56
6:K:6:LEU:O	6:K:16:ARG:NH1	2.38	0.56
22:3:84:LYS:HB3	22:3:121:ARG:HD3	1.87	0.56
22:3:148:MET:HE1	22:3:166:ILE:HG21	1.86	0.56
2:E:64:ARG:HG2	11:R:49:ARG:HD3	1.86	0.56
19:A:798:U:H2'	19:A:799:G:H8	1.71	0.56
13:Y:17:CYS:HB2	13:Y:56:SER:HB3	1.88	0.56
11:R:37:ASN:ND2	19:A:900:G:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:189:ARG:NH1	22:3:235:LEU:O	2.39	0.55
2:E:146:ARG:HD3	2:E:147:PRO:HD2	1.88	0.55
3:F:226:VAL:O	3:F:229:THR:OG1	2.24	0.55
21:2:540:LEU:HD22	21:2:602:THR:HA	1.88	0.55
3:F:88:VAL:HA	3:F:110:VAL:HG23	1.88	0.55
19:A:487:U:H3	19:A:494:G:H1	1.55	0.55
19:A:824:U:O4	19:A:844:G:O6	2.25	0.55
16:b:15:PHE:HZ	16:b:24:LYS:HD2	1.71	0.55
19:A:974:G:N1	19:A:1021:A:O2'	2.33	0.55
1:D:170:ARG:NH1	1:D:207:TYR:O	2.36	0.55
19:A:484:G:N1	19:A:498:U:C2	2.75	0.55
8:M:76:ARG:NH1	19:A:762:U:OP1	2.37	0.55
19:A:67:A:O2'	19:A:69:G:OP1	2.23	0.55
19:A:702:A:N6	19:A:731:G:C2	2.75	0.55
2:E:26:ARG:HH21	2:E:50:ARG:HB2	1.72	0.55
5:J:49:ILE:HG23	5:J:114:VAL:HB	1.87	0.55
5:J:58:LYS:HA	5:J:107:SER:HB2	1.89	0.54
7:L:56:ARG:NH2	19:A:329:U:OP1	2.37	0.54
9:O:104:ARG:HG3	15:a:12:ALA:HB2	1.89	0.54
19:A:707:A:N1	19:A:724:U:O2'	2.40	0.54
6:K:119:LYS:NZ	19:A:816:C:OP1	2.39	0.54
1:D:187:LEU:HD12	13:Y:45:ALA:HB2	1.89	0.54
19:A:638:G:O6	19:A:690:U:O4	2.26	0.54
21:2:798:LYS:NZ	21:2:799:ARG:O	2.41	0.54
15:a:103:LEU:HB3	15:a:126:LYS:HB2	1.90	0.54
22:3:83:ARG:NH1	22:3:137:GLN:OE1	2.41	0.54
11:R:29:VAL:HG12	11:R:93:HIS:HB2	1.89	0.53
1:D:21:LEU:HD11	12:U:112:LEU:HD21	1.90	0.53
16:b:123:GLY:O	16:b:128:LYS:NZ	2.41	0.53
19:A:1625:G:H3'	21:2:15:THR:H	1.73	0.53
8:M:15:ARG:HH22	19:A:20:G:H22	1.56	0.53
21:2:103:ASP:O	21:2:193:GLN:NE2	2.42	0.53
6:K:34:GLU:HB3	6:K:44:LEU:HD11	1.91	0.53
15:a:30:LYS:HE2	15:a:34:LEU:HD11	1.91	0.53
19:A:215:A:N1	19:A:840:C:N3	2.56	0.53
19:A:945:C:H2'	19:A:946:G:H8	1.73	0.53
7:L:16:ALA:HB2	19:A:351:C:H5''	1.90	0.53
21:2:155:VAL:HB	21:2:590:PRO:HB3	1.90	0.53
4:H:50:ASN:O	4:H:53:LYS:NZ	2.42	0.53
19:A:1650:G:H2'	19:A:1651:A:H8	1.74	0.53
8:M:2:ALA:N	19:A:377:C:N3	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:103:GLU:O	10:Q:106:ARG:NH1	2.42	0.53
19:A:1703:C:H2'	19:A:1704:A:H8	1.73	0.53
1:D:193:ASN:HB3	1:D:196:THR:HG22	1.91	0.53
5:J:13:GLN:OE1	19:A:148:G:N2	2.39	0.53
19:A:1626:U:H3'	19:A:1627:A:H8	1.74	0.53
14:Z:90:VAL:HG13	14:Z:94:LEU:HD12	1.91	0.52
1:D:75:ASP:O	1:D:119:LYS:NZ	2.41	0.52
5:J:72:ARG:HH22	19:A:415:G:HO2'	1.56	0.52
21:2:772:LEU:HD22	21:2:779:LYS:HG3	1.90	0.52
5:J:177:ARG:HG3	19:A:77:A:H2	1.75	0.52
6:K:33:LEU:HD11	6:K:40:LEU:HD12	1.91	0.52
3:F:61:MET:HE3	3:F:80:PHE:HB2	1.90	0.52
4:H:98:ASN:ND2	4:H:116:ASP:OD1	2.42	0.52
6:K:69:PRO:O	6:K:73:LEU:N	2.39	0.52
14:Z:18:GLU:HG3	14:Z:69:LEU:HD22	1.91	0.52
19:A:160:G:OP2	19:A:160:G:N2	2.33	0.52
21:2:303:ILE:HG12	21:2:570:VAL:HG22	1.92	0.52
19:A:708:U:O2	19:A:723:G:O6	2.27	0.52
17:e:23:THR:OG1	17:e:25:VAL:O	2.28	0.52
1:D:10:PHE:HA	1:D:194:ARG:HH12	1.74	0.52
1:D:77:CYS:SG	1:D:78:VAL:N	2.82	0.52
16:b:11:ARG:HD2	19:A:778:U:H2'	1.90	0.52
21:2:484:LYS:HA	21:2:487:GLU:HG3	1.90	0.52
16:b:129:GLY:O	16:b:132:ALA:HB3	2.10	0.52
19:A:871:U:O4	19:A:952:G:O6	2.28	0.51
19:A:991:A:H62	19:A:1009:G:H21	1.59	0.51
2:E:45:LYS:NZ	11:R:18:PRO:O	2.43	0.51
10:Q:38:CYS:SG	10:Q:78:ASN:ND2	2.83	0.51
1:D:121:PRO:HG2	1:D:144:ILE:HG13	1.93	0.51
2:E:133:TYR:HD2	2:E:181:LEU:HD13	1.73	0.51
7:L:189:GLU:O	9:O:22:ASN:ND2	2.43	0.51
1:D:145:PRO:HG3	13:Y:32:CYS:HB2	1.93	0.51
19:A:871:U:O4	19:A:951:G:O6	2.27	0.51
21:2:618:ILE:HB	21:2:656:LEU:HB3	1.92	0.51
3:F:107:LYS:HA	3:F:125:THR:HA	1.92	0.51
19:A:484:G:C2	19:A:498:U:O2	2.64	0.51
4:H:191:ARG:NH2	4:H:212:ASP:OD2	2.43	0.51
19:A:214:A:N7	19:A:828:U:C2	2.79	0.51
17:e:64:CYS:HB3	17:e:73:LEU:HD23	1.92	0.51
21:2:575:LEU:HD12	21:2:576:PRO:HD2	1.93	0.51
5:J:199:ARG:NH2	19:A:282:G:OP1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:80:VAL:O	9:O:125:GLY:CA	2.60	0.50
21:2:299:GLN:OE1	21:2:334:ARG:NH2	2.44	0.50
21:2:305:ALA:HB3	21:2:325:GLN:HB3	1.91	0.50
8:M:146:VAL:HG11	8:M:154:ILE:HD11	1.92	0.50
11:R:34:ALA:HA	11:R:39:THR:HA	1.92	0.50
11:R:55:VAL:HG23	11:R:59:MET:HG3	1.93	0.50
15:a:32:ARG:NH2	19:A:372:U:OP1	2.44	0.50
19:A:922:A:H2'	19:A:923:G:C8	2.46	0.50
5:J:180:ARG:NH2	19:A:140:G:O6	2.45	0.50
15:a:64:PRO:HB3	20:1:246:LYS:HE2	1.93	0.50
19:A:874:G:O6	19:A:933:U:O4	2.29	0.50
19:A:604:G:H21	19:A:611:A:H5''	1.76	0.50
19:A:874:G:O6	19:A:933:U:C4	2.64	0.50
19:A:1661:U:O2	19:A:1732:G:N2	2.38	0.50
21:2:513:TYR:HB3	21:2:796:LEU:HB3	1.93	0.50
21:2:651:LYS:HE2	21:2:723:ARG:HD3	1.94	0.50
4:H:19:LEU:HD22	19:A:786:A:H2'	1.93	0.50
9:O:71:ILE:HG21	9:O:145:LEU:HD11	1.94	0.50
5:J:165:LYS:HD2	19:A:70:C:H5'	1.94	0.50
3:F:46:VAL:O	3:F:51:ARG:NH2	2.44	0.50
5:J:15:LEU:HD22	19:A:150:G:H4'	1.93	0.50
5:J:159:ARG:HE	5:J:175:ALA:HB2	1.77	0.50
11:R:65:ARG:NH1	19:A:902:G:O2'	2.45	0.50
19:A:951:G:H2'	19:A:952:G:C8	2.47	0.50
3:F:123:ILE:HG12	3:F:216:GLU:HG3	1.93	0.50
13:Y:74:GLN:OE1	13:Y:82:VAL:N	2.44	0.50
19:A:355:U:O2'	19:A:357:A:OP1	2.30	0.49
19:A:469:U:O2'	19:A:768:A:N3	2.40	0.49
19:A:651:C:H2'	19:A:652:G:H8	1.77	0.49
19:A:1645:C:OP1	21:2:547:ARG:NH2	2.45	0.49
1:D:159:VAL:O	13:Y:65:SER:OG	2.30	0.49
18:h:31:LYS:HA	18:h:35:LYS:HB2	1.93	0.49
22:3:248:LEU:HA	22:3:251:ILE:HG22	1.94	0.49
2:E:32:ILE:HA	2:E:96:CYS:HB2	1.93	0.49
11:R:106:THR:HG21	22:3:168:SER:HB2	1.94	0.49
5:J:159:ARG:NH2	19:A:78:C:OP1	2.45	0.49
7:L:44:HIS:ND1	19:A:1672:U:OP1	2.46	0.49
14:Z:42:GLN:NE2	14:Z:48:GLY:O	2.43	0.49
11:R:18:PRO:HB2	11:R:20:VAL:HG12	1.93	0.49
17:e:17:ARG:O	19:A:1067:U:O2'	2.30	0.49
7:L:57:ALA:HB2	7:L:181:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:219:C:C4	19:A:220:A:N6	2.79	0.49
19:A:247:C:H2'	19:A:248:A:H8	1.77	0.49
21:2:135:GLN:HG3	21:2:242:CYS:HB3	1.95	0.49
21:2:285:LYS:NZ	21:2:556:GLU:O	2.46	0.49
21:2:339:ASP:HB3	21:2:601:ARG:HD3	1.94	0.49
21:2:516:LEU:HD12	21:2:522:SER:HB2	1.95	0.49
1:D:56:THR:HA	1:D:164:PRO:HD2	1.93	0.49
4:H:151:ASP:OD2	5:J:218:ARG:NH2	2.44	0.49
21:2:171:GLU:OE2	21:2:700:THR:OG1	2.29	0.49
21:2:301:GLU:HG3	21:2:573:LYS:HG2	1.94	0.49
6:K:39:ASP:OD2	6:K:82:ARG:NH1	2.39	0.49
19:A:820:U:H3	19:A:848:G:H1	1.61	0.49
21:2:783:ASP:N	21:2:783:ASP:OD1	2.45	0.49
5:J:2:LYS:HB2	5:J:108:VAL:HG22	1.96	0.48
8:M:8:LYS:NZ	19:A:24:U:OP1	2.38	0.48
11:R:148:ARG:NH2	19:A:901:U:OP1	2.46	0.48
19:A:5:U:H2'	19:A:6:G:C8	2.48	0.48
2:E:138:PHE:O	2:E:213:ARG:N	2.46	0.48
19:A:5:U:H2'	19:A:6:G:H8	1.78	0.48
19:A:834:U:O4	19:A:835:G:O6	2.31	0.48
19:A:978:G:H4'	19:A:1772:A:H4'	1.94	0.48
6:K:76:PHE:O	6:K:80:GLN:N	2.41	0.48
9:O:45:LEU:HD13	9:O:75:ILE:HD11	1.94	0.48
21:2:622:SER:OG	21:2:624:MET:SD	2.69	0.48
4:H:251:ARG:NH1	4:H:252:ASP:OD1	2.47	0.48
5:J:183:THR:HG23	5:J:186:ARG:H	1.79	0.48
9:O:130:VAL:HG12	9:O:144:VAL:HA	1.96	0.48
14:Z:23:ARG:HD3	17:e:4:ALA:HB2	1.95	0.48
19:A:1654:G:H3'	19:A:1655:A:H8	1.78	0.48
5:J:79:GLU:HG3	5:J:86:PRO:HG3	1.95	0.48
19:A:954:U:OP1	19:A:1069:C:O2'	2.32	0.48
11:R:116:ARG:NH2	22:3:141:ASP:OD2	2.46	0.48
3:F:150:GLY:N	3:F:161:SER:O	2.45	0.48
4:H:19:LEU:HD11	4:H:108:ARG:HD2	1.94	0.48
7:L:31:ARG:NH1	19:A:329:U:OP1	2.46	0.47
22:3:172:LYS:NZ	22:3:178:LEU:O	2.47	0.47
8:M:16:PRO:O	8:M:21:ARG:NH2	2.47	0.47
21:2:92:ASN:HB3	21:2:156:ALA:HA	1.95	0.47
21:2:343:GLU:HG2	21:2:347:MET:HE1	1.95	0.47
9:O:139:THR:OG1	19:A:322:G:OP1	2.31	0.47
19:A:173:C:N4	19:A:263:A:OP2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:603:ALA:HA	21:2:667:MET:HA	1.97	0.47
4:H:141:THR:OG1	4:H:143:ASP:OD1	2.26	0.47
5:J:176:PRO:O	19:A:77:A:O2'	2.26	0.47
7:L:158:PRO:HA	7:L:161:GLU:HB2	1.97	0.47
19:A:484:G:C2	19:A:498:U:C2	3.02	0.47
1:D:179:MET:HE1	1:D:182:ARG:HH21	1.79	0.47
2:E:88:VAL:HA	2:E:98:THR:HA	1.95	0.47
11:R:84:CYS:HB2	11:R:89:ILE:HB	1.96	0.47
14:Z:31:SER:HB3	19:A:633:A:H5''	1.97	0.47
15:a:30:LYS:NZ	19:A:1129:A:OP1	2.42	0.47
19:A:595:U:H2'	19:A:596:A:H8	1.78	0.47
19:A:843:G:H2'	19:A:844:G:H8	1.77	0.47
21:2:259:LEU:O	21:2:277:GLY:HA3	2.15	0.47
22:3:201:ILE:HD13	22:3:248:LEU:HD21	1.96	0.47
22:3:255:MET:HE1	22:3:258:ARG:HH21	1.79	0.47
8:M:107:LEU:HB2	8:M:144:PHE:HB3	1.96	0.47
15:a:65:ASN:ND2	15:a:116:ASP:OD2	2.43	0.47
19:A:550:G:H3'	19:A:551:C:H2'	1.96	0.47
19:A:1644:A:N6	19:A:1749:A:N1	2.62	0.47
5:J:160:ARG:NE	19:A:66:U:O2	2.44	0.47
19:A:215:A:N6	19:A:840:C:H42	2.12	0.47
21:2:58:LYS:HA	21:2:61:ARG:HE	1.80	0.47
21:2:97:PRO:HA	21:2:162:VAL:HB	1.96	0.47
22:3:255:MET:HE3	22:3:259:TRP:CD1	2.49	0.47
6:K:83:LEU:HD12	6:K:87:LEU:HD23	1.97	0.47
13:Y:4:ASP:OD1	13:Y:4:ASP:N	2.46	0.47
14:Z:25:VAL:HB	14:Z:63:VAL:HB	1.97	0.47
21:2:689:ASP:N	21:2:689:ASP:OD1	2.47	0.47
5:J:7:HIS:HD2	5:J:113:ILE:HD12	1.79	0.47
19:A:140:G:H2'	19:A:141:G:C8	2.50	0.47
21:2:533:GLU:OE2	21:2:538:GLN:NE2	2.43	0.47
1:D:62:LEU:HD13	13:Y:79:LEU:HD23	1.97	0.46
9:O:82:SER:OG	19:A:344:G:OP1	2.29	0.46
19:A:948:C:H2'	19:A:949:A:C8	2.50	0.46
21:2:275:VAL:HG23	21:2:570:VAL:HB	1.97	0.46
22:3:109:CYS:HB3	22:3:135:ALA:HB1	1.96	0.46
8:M:34:LEU:HA	8:M:124:ARG:HH12	1.80	0.46
2:E:75:LYS:HB3	2:E:75:LYS:HE3	1.75	0.46
19:A:921:A:H2'	19:A:922:A:C8	2.50	0.46
11:R:37:ASN:HA	11:R:68:SER:HB3	1.98	0.46
13:Y:74:GLN:NE2	13:Y:83:TRP:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:124:LYS:NZ	19:A:746:C:O2'	2.48	0.46
22:3:209:ILE:HD13	22:3:232:ILE:HD11	1.96	0.46
3:F:230:TYR:HE2	13:Y:25:LYS:HA	1.81	0.46
19:A:231:G:H2'	19:A:232:G:C8	2.50	0.46
10:Q:104:ARG:HH22	19:A:948:C:H1'	1.79	0.46
13:Y:40:ASP:HB3	13:Y:46:ILE:HD11	1.97	0.46
17:e:35:VAL:HA	17:e:78:SER:O	2.16	0.46
19:A:29:U:H2'	19:A:30:G:H8	1.79	0.46
19:A:44:U:OP2	19:A:434:A:N6	2.46	0.46
6:K:44:LEU:HA	6:K:47:LEU:HD13	1.96	0.46
11:R:96:ILE:HD11	11:R:115:LEU:HD22	1.98	0.46
3:F:90:LYS:HB2	3:F:90:LYS:HE3	1.68	0.46
7:L:76:THR:HG21	7:L:104:ILE:HD12	1.97	0.46
1:D:44:ARG:HD2	1:D:47:GLY:HA3	1.98	0.46
4:H:151:ASP:HB3	4:H:154:ILE:HG13	1.98	0.46
7:L:22:ARG:NH1	19:A:382:A:OP1	2.44	0.46
19:A:213:A:N1	19:A:841:U:O2'	2.42	0.46
19:A:1039:G:H2'	19:A:1040:G:C8	2.50	0.46
8:M:34:LEU:HD13	8:M:39:GLU:HB2	1.98	0.45
11:R:94:ILE:HG21	11:R:115:LEU:HD13	1.97	0.45
19:A:510:U:H2'	19:A:511:G:C8	2.51	0.45
21:2:145:ASP:OD1	21:2:145:ASP:N	2.46	0.45
4:H:11:ARG:NH1	4:H:21:ASP:O	2.45	0.45
6:K:81:GLN:NE2	6:K:82:ARG:HG2	2.31	0.45
3:F:53:VAL:HG11	3:F:76:ILE:HG12	1.99	0.45
15:a:102:VAL:HG12	15:a:104:LEU:HD12	1.99	0.45
21:2:147:THR:HG23	21:2:632:ARG:HH22	1.81	0.45
7:L:2:GLY:N	19:A:390:C:OP2	2.49	0.45
19:A:597:U:H2'	19:A:598:A:H8	1.82	0.45
7:L:172:ILE:HG13	7:L:188:LEU:HD23	1.97	0.45
19:A:220:A:C6	19:A:835:G:C6	3.05	0.45
19:A:735:C:H2'	19:A:736:A:H8	1.81	0.45
19:A:798:U:H2'	19:A:799:G:C8	2.51	0.45
19:A:844:G:H2'	19:A:845:A:C8	2.52	0.45
6:K:51:SER:OG	6:K:52:ALA:N	2.50	0.45
6:K:57:VAL:HG12	6:K:62:LYS:HA	1.97	0.45
7:L:120:PRO:HB2	7:L:123:ARG:HG3	1.99	0.45
19:A:905:A:O2'	19:A:995:G:O2'	2.31	0.45
1:D:119:LYS:NZ	1:D:121:PRO:HA	2.32	0.45
5:J:195:ALA:HA	5:J:198:ARG:HD3	1.98	0.45
19:A:1645:C:H2'	19:A:1646:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:HIS:HB3	1:D:53:LEU:HD21	1.99	0.45
3:F:178:ILE:HB	3:F:205:TYR:HB2	1.98	0.45
6:K:57:VAL:HG21	6:K:178:THR:HA	1.99	0.45
7:L:157:ASP:OD1	7:L:157:ASP:N	2.50	0.45
14:Z:87:GLU:OE1	14:Z:117:ARG:NH2	2.50	0.45
19:A:810:A:H4'	19:A:811:U:H3'	1.99	0.45
8:M:15:ARG:HA	8:M:15:ARG:HD3	1.68	0.45
11:R:92:LEU:HG	11:R:123:MET:HE2	1.99	0.45
19:A:139:U:H2'	19:A:140:G:H8	1.82	0.45
1:D:91:LYS:O	1:D:95:HIS:ND1	2.42	0.44
4:H:61:THR:O	4:H:65:MET:HG2	2.17	0.44
13:Y:85:ALA:HB1	17:e:6:ASP:H	1.81	0.44
19:A:483:G:H1	19:A:498:U:H3	1.65	0.44
19:A:977:A:H4'	19:A:1782:G:N2	2.32	0.44
19:A:1040:G:H22	19:A:1073:A:H2	1.64	0.44
19:A:1708:A:H4'	19:A:1708:A:OP1	2.17	0.44
5:J:20:ASP:HB3	5:J:23:LYS:HE2	1.98	0.44
9:O:138:LYS:HB2	19:A:334:G:H3'	1.99	0.44
19:A:215:A:H61	19:A:840:C:N4	2.15	0.44
19:A:1005:C:H2'	19:A:1006:G:H8	1.82	0.44
20:1:267:VAL:HB	20:1:268:LYS:H	1.63	0.44
21:2:89:ALA:HB2	21:2:565:GLY:HA2	2.00	0.44
21:2:804:ASN:O	21:2:806:ARG:NH1	2.50	0.44
3:F:87:GLU:HG2	3:F:194:ARG:HH21	1.83	0.44
21:2:192:VAL:HG21	21:2:211:LEU:HD13	2.00	0.44
4:H:197:HIS:HB3	19:A:735:C:H5''	2.00	0.44
7:L:176:ARG:NH2	19:A:328:G:N7	2.64	0.44
19:A:1625:G:H2'	21:2:15:THR:HG23	2.00	0.44
6:K:111:SER:HB3	6:K:114:SER:HB3	1.99	0.44
3:F:43:TRP:CD2	3:F:75:GLN:HG2	2.52	0.44
14:Z:76:SER:HB2	19:A:1098:G:H5''	2.00	0.44
19:A:500:G:H2'	19:A:501:U:C6	2.52	0.44
21:2:503:LYS:HA	21:2:503:LYS:HD3	1.79	0.44
21:2:684:PRO:HG3	21:2:704:THR:HB	1.98	0.44
19:A:276:G:H8	19:A:277:C:H4'	1.82	0.44
19:A:856:G:OP2	19:A:856:G:N2	2.38	0.44
2:E:51:THR:HG23	2:E:56:ASN:HA	1.99	0.44
11:R:55:VAL:HG13	11:R:76:ALA:HB1	2.00	0.44
19:A:148:G:H2'	19:A:149:U:C6	2.53	0.44
22:3:96:LYS:HA	22:3:96:LYS:HD2	1.77	0.44
7:L:38:ILE:HD11	7:L:96:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:48:G:OP2	21:2:62:ARG:NH2	2.51	0.44
19:A:487:U:N3	19:A:495:G:N1	2.66	0.44
19:A:706:C:H2'	19:A:707:A:C8	2.53	0.44
19:A:1654:G:H3'	19:A:1655:A:C8	2.53	0.44
3:F:188:ALA:HB3	3:F:193:LYS:HB2	2.00	0.43
19:A:102:A:H4'	19:A:104:A:C8	2.53	0.43
19:A:574:G:H3'	19:A:575:U:H4'	1.99	0.43
11:R:142:LYS:HB3	19:A:988:C:H5'	2.00	0.43
22:3:223:GLU:O	22:3:227:MET:HG3	2.18	0.43
7:L:10:LYS:NZ	19:A:319:G:O2'	2.51	0.43
8:M:128:ARG:HA	8:M:128:ARG:HD2	1.77	0.43
10:Q:48:SER:OG	19:A:866:G:N2	2.51	0.43
19:A:643:U:H3	19:A:683:G:H1	1.65	0.43
19:A:923:G:H2'	19:A:924:A:C8	2.53	0.43
21:2:303:ILE:HB	21:2:328:ASP:HB3	2.00	0.43
9:O:91:ILE:HD11	9:O:112:LEU:HD22	2.01	0.43
11:R:92:LEU:HB2	11:R:125:ILE:HG22	2.01	0.43
19:A:90:G:OP1	19:A:394:A:N6	2.48	0.43
19:A:267:C:H2'	19:A:268:A:H8	1.83	0.43
19:A:883:G:H2'	19:A:884:U:C6	2.54	0.43
19:A:952:G:H2'	19:A:953:A:C8	2.54	0.43
21:2:642:PRO:HD3	21:2:662:ALA:HA	2.01	0.43
1:D:20:LEU:HD13	1:D:53:LEU:HD12	2.00	0.43
6:K:82:ARG:O	6:K:86:GLU:HG2	2.18	0.43
6:K:183:TYR:O	6:K:187:THR:OG1	2.34	0.43
9:O:83:THR:HA	9:O:89:ILE:HG22	1.99	0.43
19:A:692:C:H4'	19:A:693:U:H5'	2.01	0.43
19:A:834:U:C4	19:A:835:G:O6	2.72	0.43
21:2:154:SER:HB2	21:2:183:GLN:HE22	1.84	0.43
3:F:84:LEU:HD23	3:F:114:ASP:HB3	2.00	0.43
10:Q:29:THR:OG1	10:Q:31:GLU:OE1	2.35	0.43
19:A:992:G:H2'	19:A:993:A:C8	2.54	0.43
21:2:472:GLU:OE1	21:2:475:ARG:NH2	2.52	0.43
21:2:607:LEU:HB2	21:2:712:LEU:HD11	1.99	0.43
4:H:211:LYS:HE2	4:H:211:LYS:HB2	1.88	0.43
6:K:77:HIS:O	6:K:141:TYR:OH	2.30	0.43
7:L:125:ARG:HE	7:L:132:VAL:HG12	1.83	0.43
18:h:31:LYS:HE2	19:A:542:A:H2'	2.01	0.43
19:A:479:U:H2'	19:A:480:A:H8	1.84	0.43
19:A:727:C:H2'	19:A:728:G:C8	2.53	0.43
21:2:175:LEU:HD11	21:2:705:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:52:ARG:O	8:M:56:ILE:HG12	2.19	0.43
19:A:1766:C:N3	19:A:1767:U:C4	2.87	0.43
21:2:90:PRO:HB3	21:2:136:LYS:HG3	2.00	0.43
5:J:169:LYS:NZ	19:A:72:A:OP2	2.52	0.43
19:A:1650:G:H2'	19:A:1651:A:C8	2.53	0.43
19:A:587:C:H2'	19:A:588:A:C8	2.54	0.42
19:A:1043:C:H2'	19:A:1044:G:H8	1.84	0.42
19:A:1142:U:H2'	19:A:1143:G:H8	1.84	0.42
19:A:106:C:H2'	19:A:107:A:H8	1.84	0.42
19:A:992:G:H2'	19:A:993:A:H8	1.83	0.42
1:D:6:LEU:HD22	13:Y:79:LEU:HA	2.02	0.42
5:J:63:MET:HG2	5:J:98:ARG:HG3	2.02	0.42
15:a:19:ARG:O	15:a:23:ARG:HB2	2.19	0.42
19:A:835:G:H2'	19:A:836:G:C8	2.54	0.42
21:2:74:ARG:O	21:2:78:LYS:HE3	2.19	0.42
19:A:834:U:H2'	19:A:835:G:C8	2.54	0.42
19:A:945:C:H2'	19:A:946:G:C8	2.53	0.42
19:A:1778:A:H3'	19:A:1779:C:O4'	2.19	0.42
21:2:601:ARG:HA	21:2:668:GLY:O	2.19	0.42
22:3:88:PRO:O	22:3:92:MET:N	2.51	0.42
4:H:199:GLU:OE2	19:A:797:A:O2'	2.35	0.42
19:A:24:U:O2'	19:A:26:A:OP1	2.37	0.42
19:A:487:U:N3	19:A:495:G:C6	2.88	0.42
19:A:1629:A:H3'	19:A:1630:C:H6	1.85	0.42
19:A:118:A:H1'	19:A:394:A:C5	2.55	0.42
19:A:336:C:H2'	19:A:337:A:H8	1.84	0.42
19:A:1731:C:H2'	19:A:1732:G:C8	2.55	0.42
21:2:193:GLN:HA	21:2:228:LEU:HD13	2.01	0.42
21:2:289:LEU:HD22	21:2:297:THR:HG22	2.00	0.42
5:J:14:LYS:HE2	5:J:124:LEU:HB2	2.02	0.42
6:K:50:VAL:HG23	6:K:69:PRO:HD3	2.01	0.42
12:U:112:LEU:HD12	12:U:120:ILE:HG13	2.02	0.42
19:A:980:U:H2'	19:A:981:A:C8	2.55	0.42
20:1:249:SER:O	20:1:250:LYS:C	2.63	0.42
21:2:683:ASP:OD1	21:2:683:ASP:N	2.50	0.42
22:3:103:PRO:HA	22:3:106:VAL:HG22	2.02	0.42
8:M:64:ASP:HB3	8:M:67:ARG:HB3	2.01	0.42
11:R:109:PRO:HB3	22:3:165:TYR:HB3	2.00	0.42
19:A:698:G:H2'	19:A:699:A:C8	2.55	0.42
19:A:1084:A:H2'	19:A:1085:A:C8	2.54	0.42
19:A:1112:U:H2'	19:A:1113:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1142:U:H2'	19:A:1143:G:C8	2.55	0.42
21:2:127:ARG:HG2	21:2:138:GLN:OE1	2.20	0.42
21:2:260:ILE:HB	21:2:589:LEU:HB3	2.01	0.42
2:E:124:ASN:HA	2:E:137:LEU:O	2.19	0.42
3:F:74:TYR:CD2	3:F:138:ILE:HD12	2.55	0.42
6:K:8:LYS:NZ	6:K:44:LEU:O	2.50	0.42
19:A:694:U:H2'	19:A:695:C:C6	2.55	0.42
2:E:90:GLU:HB3	2:E:97:LEU:HB2	2.02	0.42
7:L:25:ARG:HA	19:A:397:A:H5''	2.01	0.42
19:A:561:G:N2	19:A:577:A:H8	2.18	0.42
19:A:923:G:H2'	19:A:924:A:H8	1.85	0.42
19:A:1700:G:H2'	19:A:1701:A:H8	1.85	0.42
5:J:27:PHE:HE2	5:J:41:LEU:HD21	1.85	0.41
10:Q:62:GLN:HB2	10:Q:65:VAL:HG22	2.02	0.41
11:R:133:PRO:HB3	19:A:885:A:H5''	2.01	0.41
19:A:561:G:H21	19:A:577:A:H8	1.68	0.41
19:A:220:A:N1	19:A:835:G:O6	2.53	0.41
19:A:322:G:H2'	19:A:323:G:H8	1.85	0.41
19:A:674:G:H2'	19:A:675:G:C8	2.55	0.41
19:A:1689:A:H2'	19:A:1690:G:H8	1.84	0.41
21:2:108:ILE:HG21	21:2:126:PHE:HZ	1.85	0.41
22:3:91:ARG:HG2	22:3:147:ALA:HA	2.02	0.41
11:R:140:ARG:HD2	11:R:140:ARG:HA	1.86	0.41
14:Z:25:VAL:O	14:Z:62:VAL:HA	2.21	0.41
15:a:64:PRO:HB3	20:1:246:LYS:HB2	2.02	0.41
19:A:139:U:H2'	19:A:140:G:C8	2.55	0.41
19:A:227:U:O2	19:A:231:G:C6	2.73	0.41
19:A:403:U:H2'	19:A:404:A:C8	2.55	0.41
3:F:111:LEU:HA	3:F:121:LEU:HA	2.01	0.41
4:H:3:ARG:HG2	19:A:396:A:H4'	2.02	0.41
4:H:102:ILE:HD12	4:H:238:PRO:HD3	2.02	0.41
8:M:51:ARG:NH1	8:M:55:ARG:HH12	2.17	0.41
19:A:84:A:N3	19:A:145:A:O2'	2.43	0.41
19:A:390:C:H2'	19:A:391:C:C6	2.55	0.41
19:A:882:A:H2'	19:A:883:G:C8	2.55	0.41
19:A:1739:U:H2'	19:A:1740:A:H8	1.85	0.41
1:D:63:ALA:O	1:D:67:ILE:HG12	2.20	0.41
16:b:102:LYS:NZ	16:b:103:VAL:O	2.53	0.41
19:A:85:A:H2'	19:A:86:C:H6	1.86	0.41
21:2:151:ASP:HB2	21:2:590:PRO:HG3	2.03	0.41
3:F:107:LYS:HG3	3:F:125:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:82:VAL:HG21	7:L:170:TYR:HE1	1.85	0.41
16:b:63:LEU:HD23	16:b:74:GLY:HA3	2.01	0.41
19:A:107:A:H2'	19:A:108:G:C8	2.55	0.41
19:A:214:A:N6	19:A:828:U:N3	2.31	0.41
19:A:383:G:H2'	19:A:384:A:C8	2.56	0.41
19:A:841:U:H2'	19:A:842:A:H8	1.86	0.41
20:1:255:LYS:O	20:1:258:GLU:HG3	2.20	0.41
9:O:80:VAL:O	9:O:125:GLY:HA2	2.19	0.41
19:A:29:U:H2'	19:A:30:G:C8	2.54	0.41
3:F:136:ALA:HA	3:F:139:ILE:HG12	2.03	0.41
3:F:176:ARG:HD3	3:F:178:ILE:HD11	2.03	0.41
19:A:1625:G:H5'	21:2:15:THR:OG1	2.21	0.41
21:2:496:ASP:HA	21:2:654:ARG:HH22	1.86	0.41
7:L:7:SER:O	7:L:18:ARG:NH1	2.54	0.41
16:b:32:HIS:HB2	16:b:35:ARG:HB2	2.02	0.41
19:A:212:U:O2'	19:A:828:U:O3'	2.35	0.41
19:A:648:C:H2'	19:A:649:G:C8	2.56	0.41
22:3:134:GLU:O	22:3:138:MET:HG3	2.20	0.41
19:A:1049:G:H2'	19:A:1050:C:C6	2.56	0.41
19:A:1054:U:H2'	19:A:1055:A:C8	2.56	0.41
4:H:45:ILE:HG13	4:H:61:THR:HG21	2.03	0.40
14:Z:103:ILE:HD11	14:Z:129:PHE:HE1	1.86	0.40
19:A:893:G:H2'	19:A:894:U:C6	2.56	0.40
19:A:1040:G:H2'	19:A:1041:A:H8	1.86	0.40
20:1:263:LYS:HB3	20:1:264:GLY:H	1.66	0.40
21:2:602:THR:O	21:2:667:MET:HA	2.21	0.40
21:2:682:ARG:HA	21:2:682:ARG:HD3	1.95	0.40
6:K:82:ARG:HD2	6:K:85:ARG:HH22	1.86	0.40
13:Y:32:CYS:HB3	13:Y:60:ARG:HH11	1.86	0.40
15:a:70:LYS:HB3	15:a:93:LEU:HD11	2.03	0.40
16:b:57:GLN:HE21	16:b:81:SER:HA	1.85	0.40
19:A:126:G:H4'	19:A:127:U:H3'	2.03	0.40
19:A:1783:C:H2'	19:A:1784:G:C8	2.56	0.40
21:2:637:PRO:HB2	21:2:664:ALA:HB1	2.02	0.40
19:A:98:C:OP2	19:A:375:A:O2'	2.30	0.40
21:2:109:LYS:HG3	21:2:121:VAL:HG11	2.02	0.40
3:F:194:ARG:HD2	3:F:194:ARG:HA	1.98	0.40
8:M:51:ARG:HH11	8:M:55:ARG:HH12	1.68	0.40
19:A:106:C:H2'	19:A:107:A:C8	2.57	0.40
19:A:604:G:N2	19:A:611:A:H5''	2.35	0.40
19:A:1658:G:H4'	21:2:63:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:92:ARG:O	19:A:402:C:O2'	2.28	0.40
5:J:193:ARG:HD3	5:J:193:ARG:HA	1.88	0.40
8:M:118:LYS:HG3	19:A:476:U:H4'	2.03	0.40
19:A:623:U:H2'	19:A:624:C:H6	1.86	0.40
22:3:76:PRO:HB2	22:3:77:ILE:H	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	206/285 (72%)	190 (92%)	16 (8%)	0	100	100
2	E	211/255 (83%)	200 (95%)	11 (5%)	0	100	100
3	F	203/263 (77%)	195 (96%)	7 (3%)	1 (0%)	24	59
4	H	259/264 (98%)	248 (96%)	11 (4%)	0	100	100
5	J	230/239 (96%)	222 (96%)	8 (4%)	0	100	100
6	K	193/203 (95%)	180 (93%)	12 (6%)	1 (0%)	24	59
7	L	199/202 (98%)	191 (96%)	8 (4%)	0	100	100
8	M	177/190 (93%)	172 (97%)	5 (3%)	0	100	100
9	O	148/161 (92%)	145 (98%)	3 (2%)	0	100	100
10	Q	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
11	R	133/150 (89%)	121 (91%)	11 (8%)	1 (1%)	16	50
12	U	31/143 (22%)	29 (94%)	2 (6%)	0	100	100
13	Y	84/98 (86%)	81 (96%)	3 (4%)	0	100	100
14	Z	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
15	a	131/145 (90%)	124 (95%)	7 (5%)	0	100	100
16	b	130/136 (96%)	125 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	e	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
18	h	18/62 (29%)	17 (94%)	1 (6%)	0	100	100
20	1	35/282 (12%)	24 (69%)	8 (23%)	3 (9%)	0	3
21	2	659/830 (79%)	630 (96%)	28 (4%)	1 (0%)	43	73
22	3	182/259 (70%)	179 (98%)	3 (2%)	0	100	100
All	All	3583/4530 (79%)	3412 (95%)	164 (5%)	7 (0%)	44	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	K	80	GLN
11	R	21	ARG
20	1	250	LYS
20	1	280	PRO
20	1	267	VAL
21	2	17	LYS
3	F	93	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	178/225 (79%)	178 (100%)	0	100	100
2	E	187/223 (84%)	187 (100%)	0	100	100
3	F	174/206 (84%)	166 (95%)	8 (5%)	24	58
4	H	219/221 (99%)	219 (100%)	0	100	100
5	J	198/204 (97%)	198 (100%)	0	100	100
6	K	169/177 (96%)	169 (100%)	0	100	100
7	L	163/164 (99%)	163 (100%)	0	100	100
8	M	154/162 (95%)	154 (100%)	0	100	100
9	O	133/143 (93%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Q	129/130 (99%)	129 (100%)	0	100	100
11	R	102/117 (87%)	102 (100%)	0	100	100
12	U	31/131 (24%)	31 (100%)	0	100	100
13	Y	69/80 (86%)	69 (100%)	0	100	100
14	Z	112/113 (99%)	112 (100%)	0	100	100
15	a	109/116 (94%)	107 (98%)	2 (2%)	51	74
16	b	112/115 (97%)	112 (100%)	0	100	100
17	e	70/71 (99%)	70 (100%)	0	100	100
18	h	18/52 (35%)	17 (94%)	1 (6%)	19	52
20	1	32/227 (14%)	24 (75%)	8 (25%)	0	3
21	2	576/714 (81%)	572 (99%)	4 (1%)	76	83
22	3	155/215 (72%)	153 (99%)	2 (1%)	61	78
All	All	3090/3806 (81%)	3065 (99%)	25 (1%)	70	82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	90	LYS
3	F	92	LYS
3	F	94	VAL
3	F	105	ARG
3	F	125	THR
3	F	126	SER
3	F	128	GLU
3	F	129	VAL
15	a	88	PRO
15	a	89	ASN
18	h	26	LYS
20	1	255	LYS
20	1	259	GLN
20	1	261	GLU
20	1	265	LYS
20	1	266	ILE
20	1	267	VAL
20	1	268	LYS
20	1	281	LYS
21	2	17	LYS
21	2	21	LYS

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Mol	Chain	Res	Type
21	2	24	LYS
21	2	30	LYS
22	3	246	ASN
22	3	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	24	GLN
2	E	58	ASN
2	E	209	ASN
4	H	36	HIS
4	H	57	ASN
5	J	7	HIS
5	J	10	ASN
5	J	81	HIS
5	J	188	GLN
7	L	52	ASN
10	Q	69	ASN
10	Q	105	ASN
12	U	114	HIS
14	Z	15	ASN
14	Z	39	GLN
14	Z	70	ASN
15	a	94	ASN
16	b	18	ASN
16	b	57	GLN
21	2	10	HIS
21	2	92	ASN
21	2	183	GLN
21	2	203	GLN
21	2	217	HIS
21	2	236	ASN
21	2	597	HIS
22	3	203	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	A	1278/1796 (71%)	272 (21%)	11 (0%)

All (272) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	A	2	A
19	A	4	C
19	A	6	G
19	A	25	C
19	A	26	A
19	A	27	U
19	A	34	G
19	A	42	G
19	A	47	A
19	A	57	G
19	A	63	G
19	A	65	A
19	A	66	U
19	A	68	A
19	A	69	G
19	A	73	U
19	A	74	U
19	A	75	A
19	A	93	U
19	A	103	A
19	A	113	C
19	A	127	U
19	A	138	A
19	A	165	A
19	A	174	U
19	A	175	G
19	A	176	A
19	A	179	A
19	A	187	U
19	A	191	G
19	A	192	A
19	A	193	A
19	A	194	G
19	A	210	A
19	A	212	U
19	A	213	A
19	A	221	A
19	A	222	U
19	A	223	G
19	A	228	U
19	A	231	G
19	A	232	G

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Mol	Chain	Res	Type
19	A	234	C
19	A	237	U
19	A	247	C
19	A	257	U
19	A	258	C
19	A	262	A
19	A	268	A
19	A	269	C
19	A	270	G
19	A	272	C
19	A	274	U
19	A	275	U
19	A	277	C
19	A	296	A
19	A	299	U
19	A	305	C
19	A	306	C
19	A	311	C
19	A	313	A
19	A	317	U
19	A	319	G
19	A	326	G
19	A	334	G
19	A	335	C
19	A	349	A
19	A	356	A
19	A	357	A
19	A	358	C
19	A	377	C
19	A	387	G
19	A	397	A
19	A	398	A
19	A	399	C
19	A	401	G
19	A	420	G
19	A	421	C
19	A	422	A
19	A	423	G
19	A	431	G
19	A	432	C
19	A	436	U
19	A	441	C

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Mol	Chain	Res	Type
19	A	449	A
19	A	450	C
19	A	452	C
19	A	457	A
19	A	465	A
19	A	466	C
19	A	474	A
19	A	480	A
19	A	481	C
19	A	490	U
19	A	492	C
19	A	493	G
19	A	495	G
19	A	502	A
19	A	506	G
19	A	508	A
19	A	512	A
19	A	516	C
19	A	522	A
19	A	531	A
19	A	536	G
19	A	539	A
19	A	551	C
19	A	552	A
19	A	553	A
19	A	555	U
19	A	556	C
19	A	558	G
19	A	562	C
19	A	563	C
19	A	573	G
19	A	574	G
19	A	575	U
19	A	576	A
19	A	577	A
19	A	578	U
19	A	579	U
19	A	581	C
19	A	591	A
19	A	592	G
19	A	607	G
19	A	608	U

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Mol	Chain	Res	Type
19	A	611	A
19	A	616	A
19	A	617	A
19	A	619	A
19	A	620	A
19	A	621	G
19	A	636	U
19	A	677	U
19	A	678	G
19	A	679	G
19	A	680	G
19	A	683	G
19	A	686	C
19	A	690	U
19	A	691	C
19	A	693	U
19	A	705	G
19	A	709	G
19	A	710	C
19	A	724	U
19	A	725	G
19	A	726	U
19	A	727	C
19	A	729	G
19	A	730	G
19	A	731	G
19	A	732	A
19	A	742	U
19	A	754	A
19	A	764	G
19	A	765	C
19	A	773	A
19	A	774	G
19	A	777	C
19	A	779	A
19	A	780	U
19	A	781	G
19	A	787	A
19	A	792	U
19	A	793	U
19	A	809	A
19	A	810	A

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Mol	Chain	Res	Type
19	A	812	A
19	A	813	G
19	A	818	U
19	A	819	G
19	A	823	U
19	A	828	U
19	A	829	U
19	A	830	U
19	A	832	G
19	A	850	C
19	A	861	A
19	A	871	U
19	A	874	G
19	A	884	U
19	A	895	C
19	A	896	A
19	A	897	G
19	A	901	U
19	A	911	G
19	A	912	G
19	A	930	A
19	A	931	A
19	A	932	C
19	A	933	U
19	A	940	G
19	A	957	U
19	A	958	U
19	A	964	A
19	A	990	A
19	A	991	A
19	A	994	C
19	A	998	C
19	A	999	A
19	A	1001	A
19	A	1014	C
19	A	1019	C
19	A	1024	A
19	A	1026	C
19	A	1028	A
19	A	1029	U
19	A	1030	G
19	A	1037	A

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Mol	Chain	Res	Type
19	A	1050	C
19	A	1051	G
19	A	1056	U
19	A	1057	U
19	A	1059	U
19	A	1060	U
19	A	1073	A
19	A	1077	U
19	A	1078	A
19	A	1089	A
19	A	1093	G
19	A	1094	U
19	A	1095	U
19	A	1097	G
19	A	1106	G
19	A	1135	A
19	A	1143	G
19	A	1145	C
19	A	1146	G
19	A	1147	G
19	A	1150	G
19	A	1152	G
19	A	1155	C
19	A	1613	U
19	A	1615	C
19	A	1618	G
19	A	1625	G
19	A	1626	U
19	A	1627	A
19	A	1630	C
19	A	1631	A
19	A	1643	U
19	A	1644	A
19	A	1653	U
19	A	1654	G
19	A	1655	A
19	A	1658	G
19	A	1676	G
19	A	1684	C
19	A	1699	C
19	A	1708	A
19	A	1711	G

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Mol	Chain	Res	Type
19	A	1712	C
19	A	1742	A
19	A	1746	A
19	A	1749	A
19	A	1762	A
19	A	1763	G
19	A	1765	U
19	A	1766	C
19	A	1768	C
19	A	1771	U
19	A	1776	G
19	A	1777	A
19	A	1778	A
19	A	1779	C
19	A	1782	G
19	A	1788	G
19	A	1789	G
19	A	1790	A
19	A	1791	U
19	A	1795	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	A	222	U
19	A	231	G
19	A	233	G
19	A	269	C
19	A	449	A
19	A	552	A
19	A	577	A
19	A	678	G
19	A	792	U
19	A	1787	G
19	A	1790	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

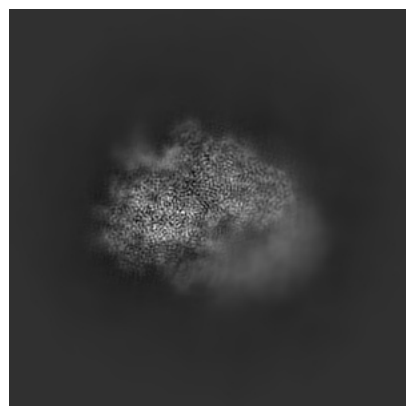
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66681. These allow visual inspection of the internal detail of the map and identification of artifacts.

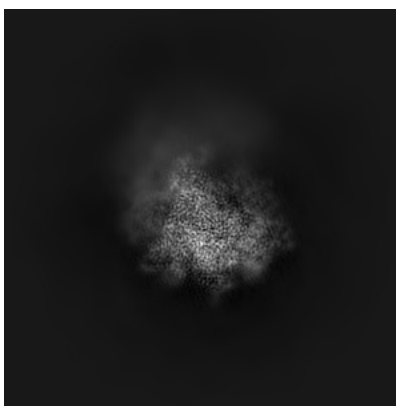
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

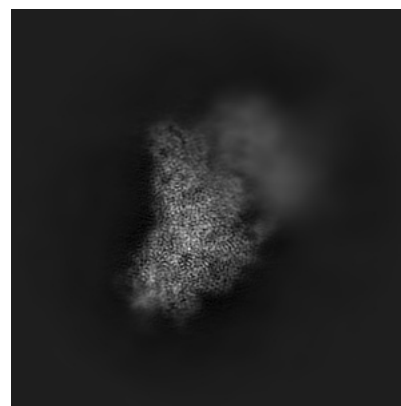
6.1.1 Primary map



X

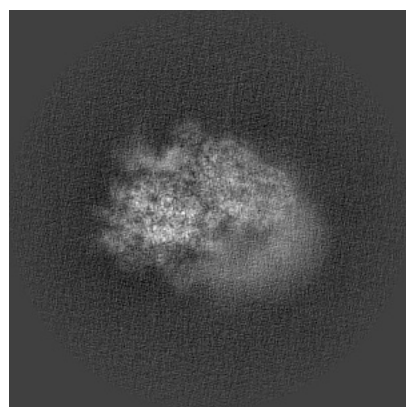


Y

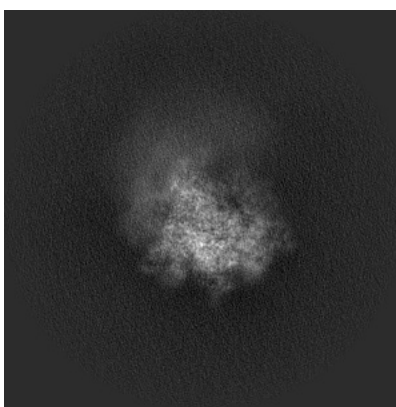


Z

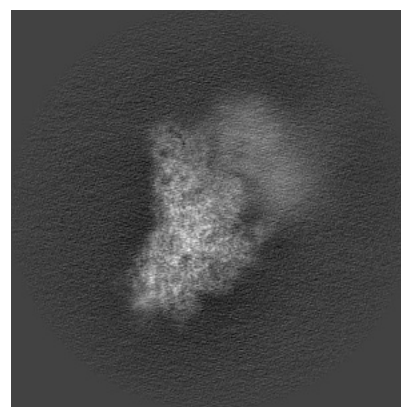
6.1.2 Raw map



X



Y

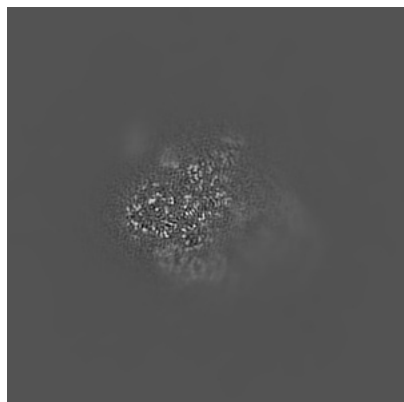


Z

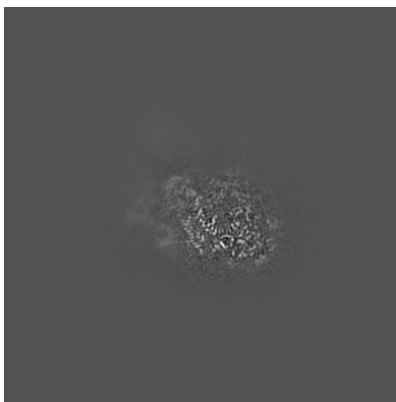
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

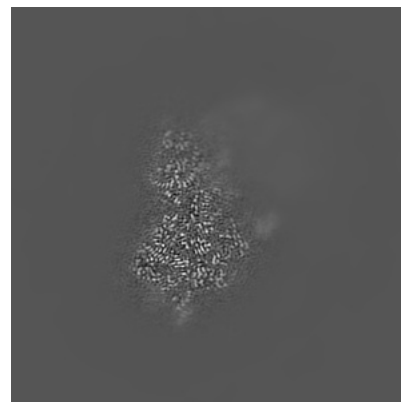
6.2.1 Primary map



X Index: 180

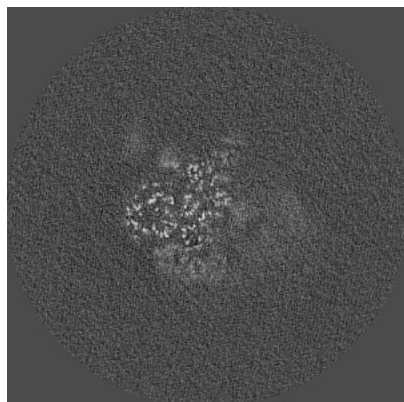


Y Index: 180

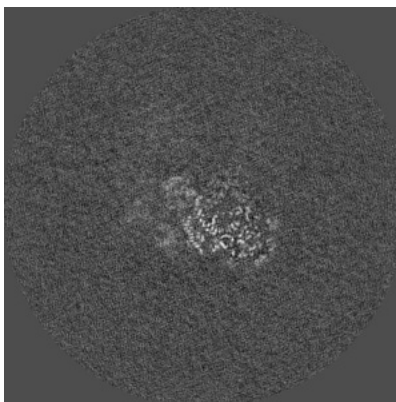


Z Index: 180

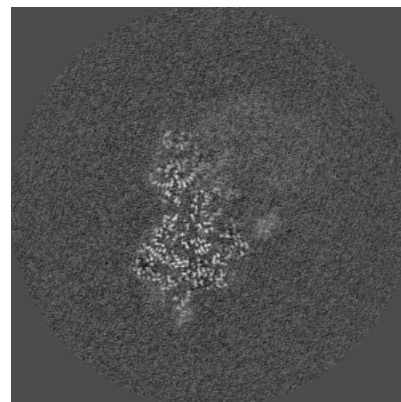
6.2.2 Raw map



X Index: 180



Y Index: 180

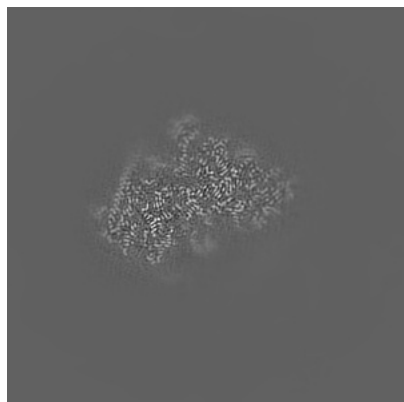


Z Index: 180

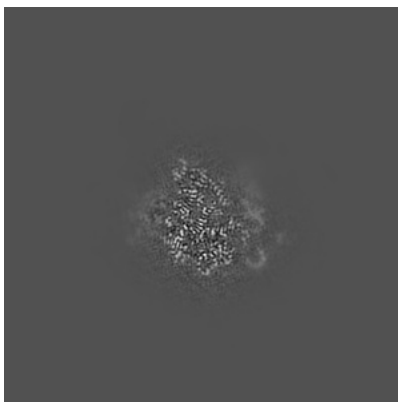
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

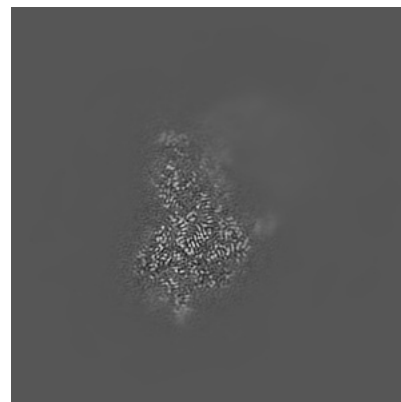
6.3.1 Primary map



X Index: 148

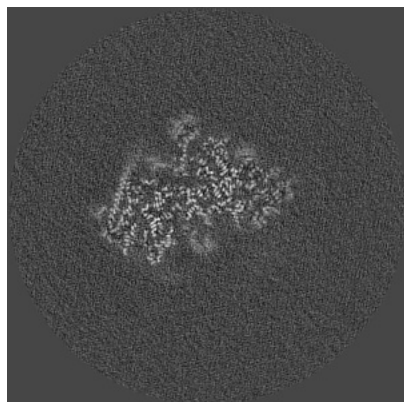


Y Index: 145

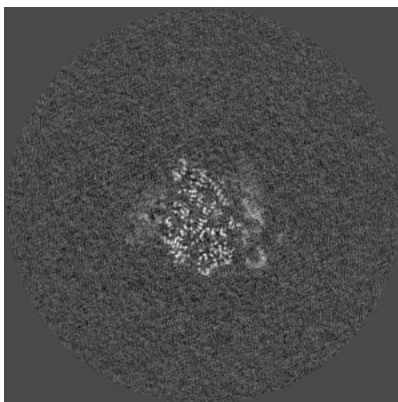


Z Index: 177

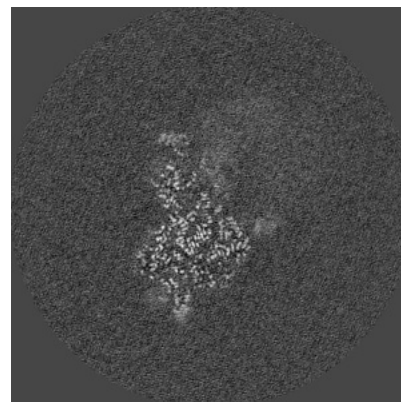
6.3.2 Raw map



X Index: 148



Y Index: 145

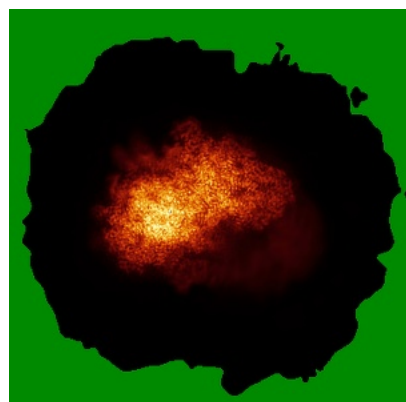


Z Index: 177

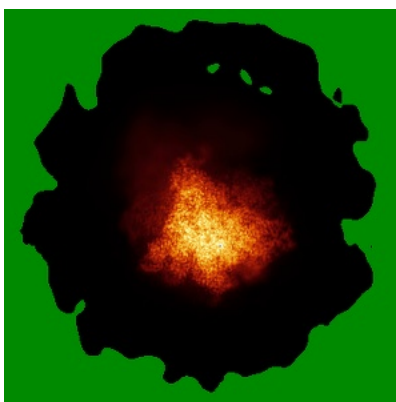
The images above show the largest variance slices of the map in three orthogonal directions.

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

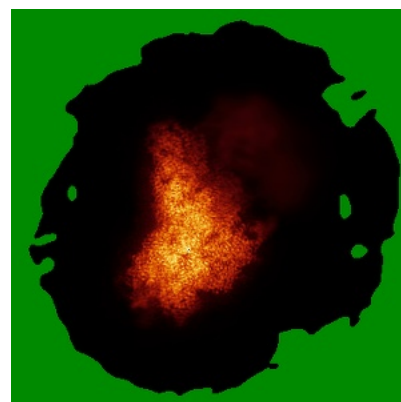
6.4.1 Primary map



X

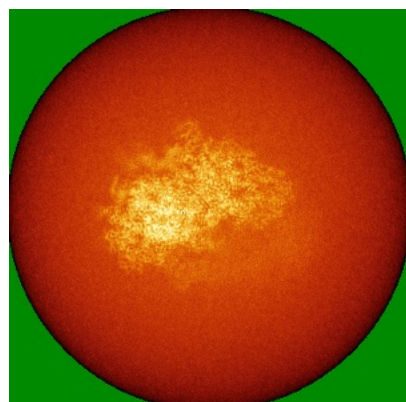


Y

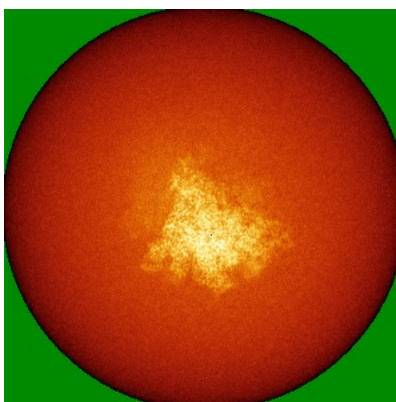


Z

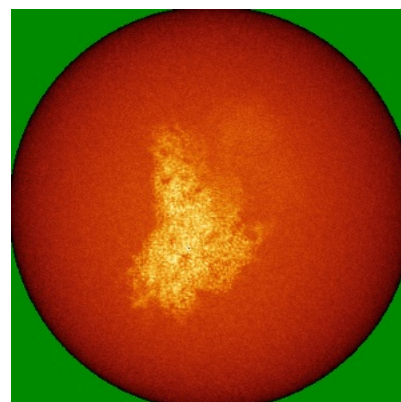
6.4.2 Raw map



X



Y

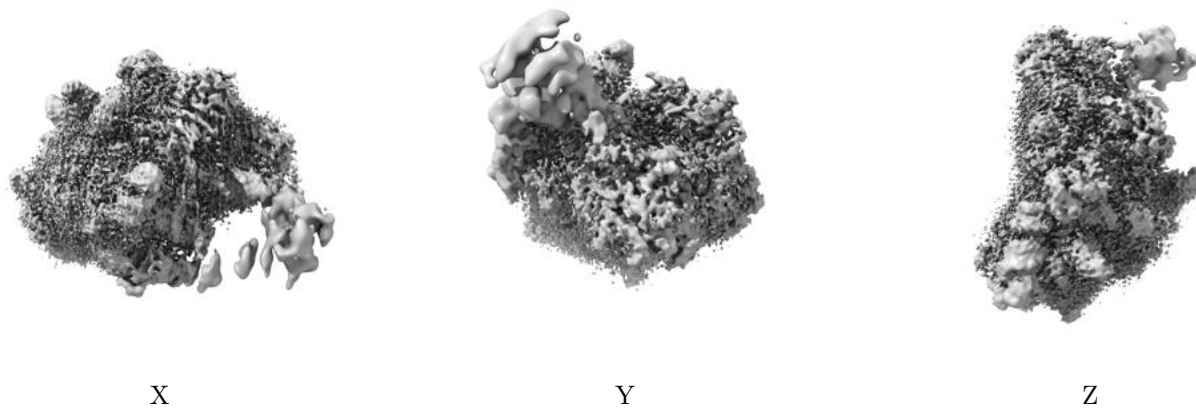


Z

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.

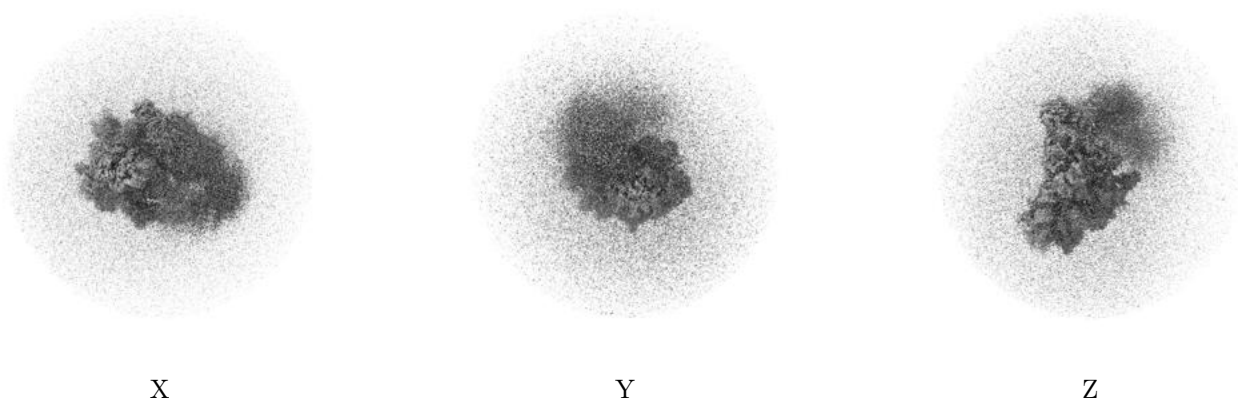
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

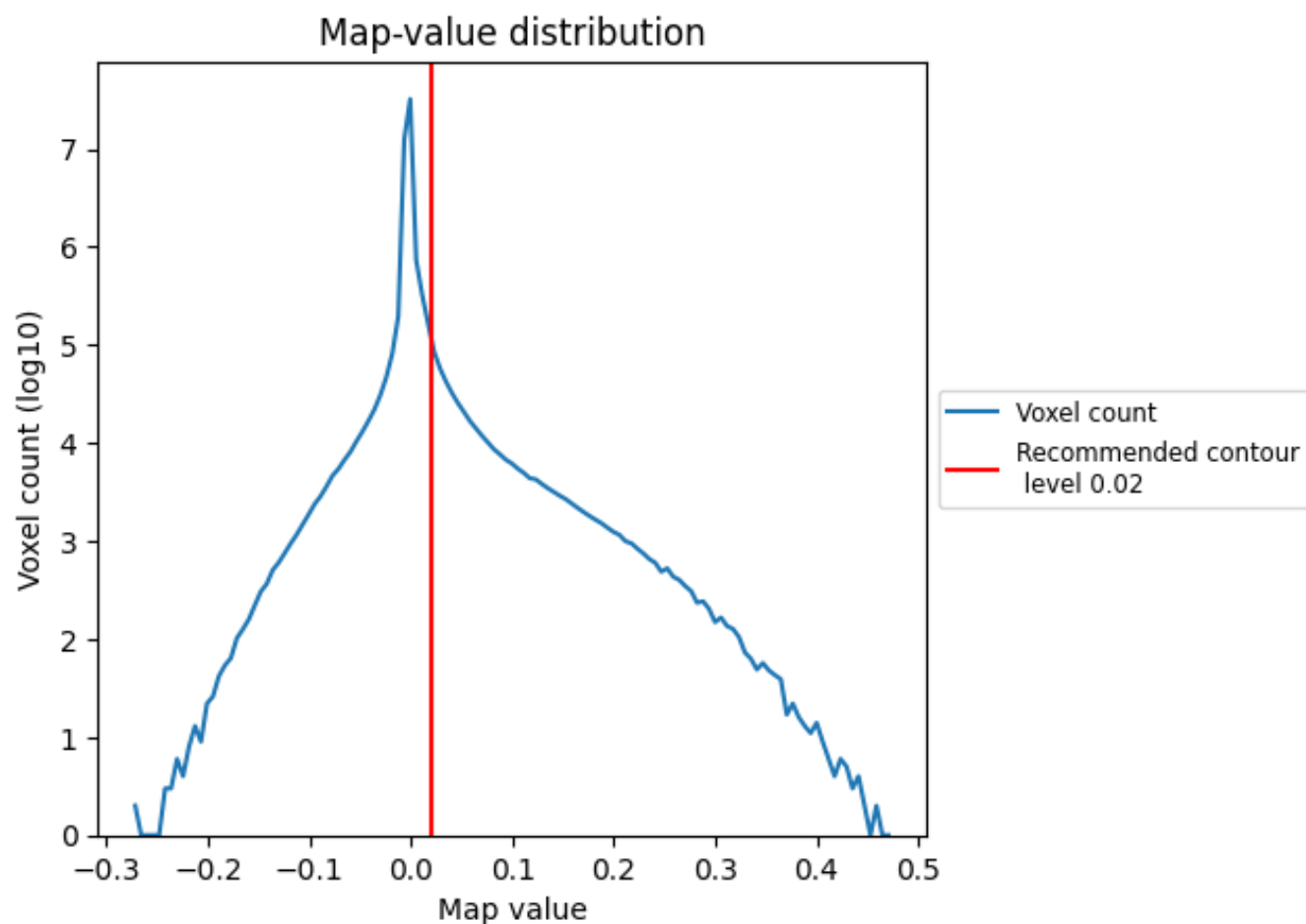
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

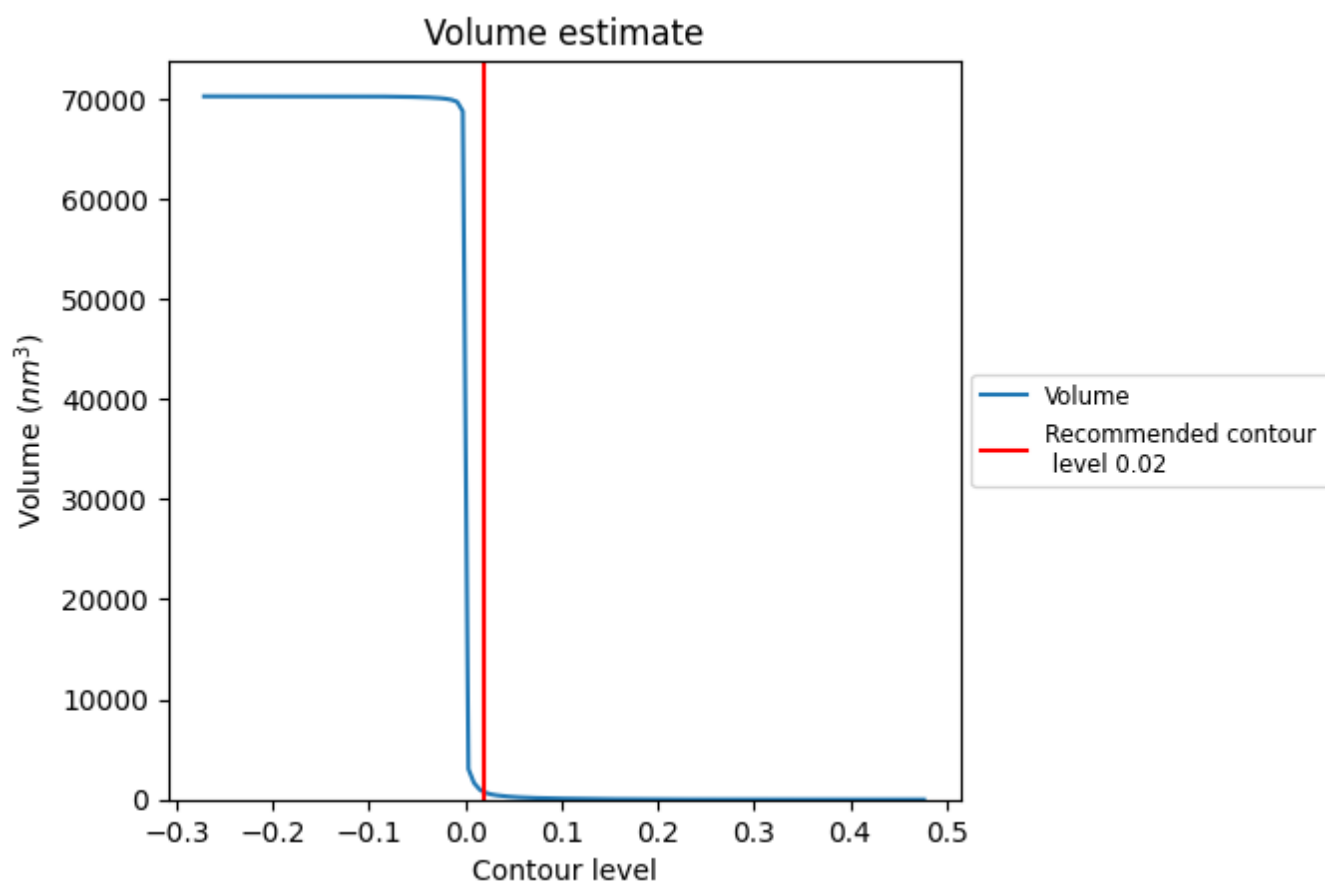
This section contains the results of statistical analysis of the map.

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.

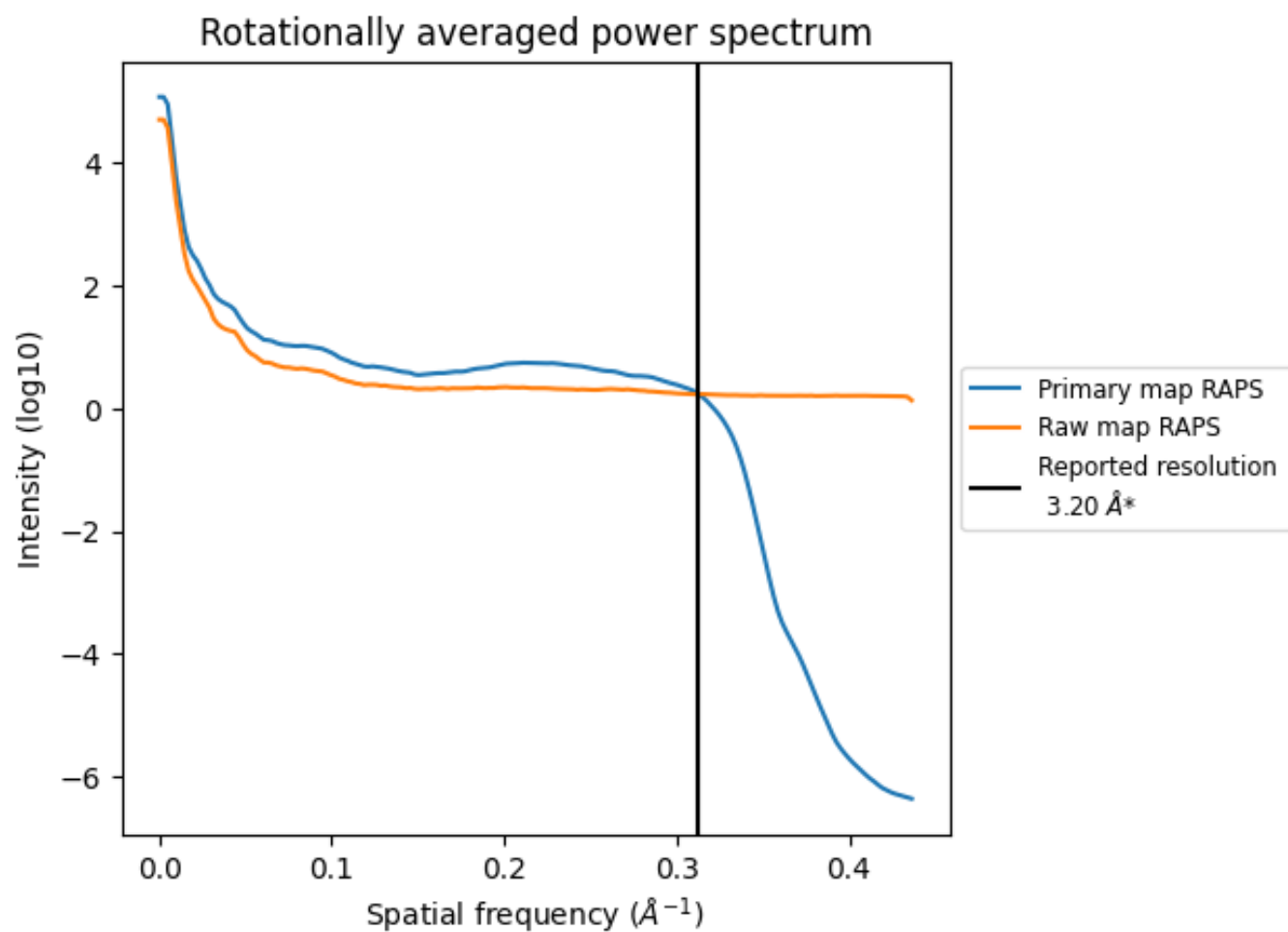
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 658 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 ⓘ

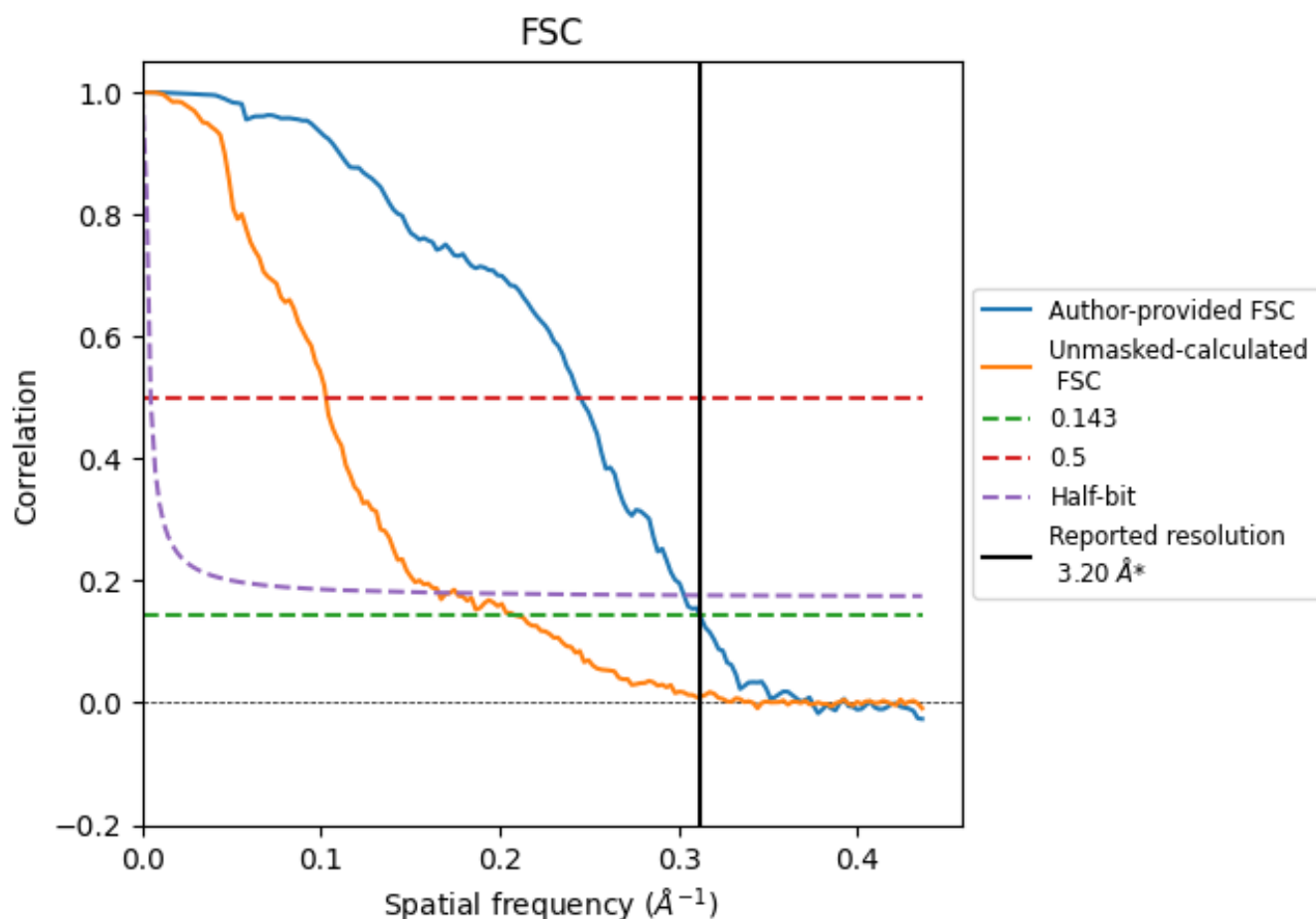


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

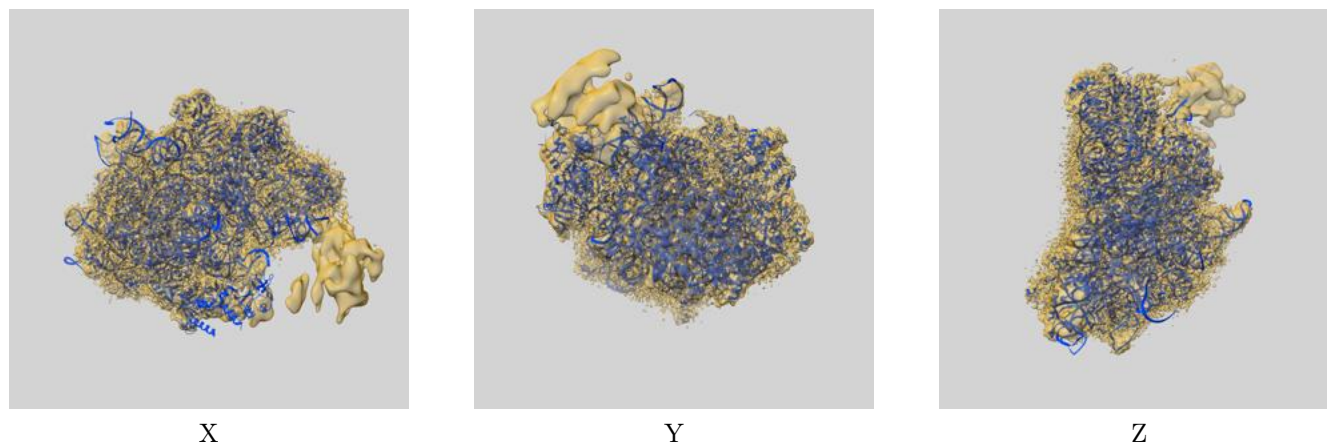
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	4.08	3.30
Unmasked-calculated*	4.79	9.73	6.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.79 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

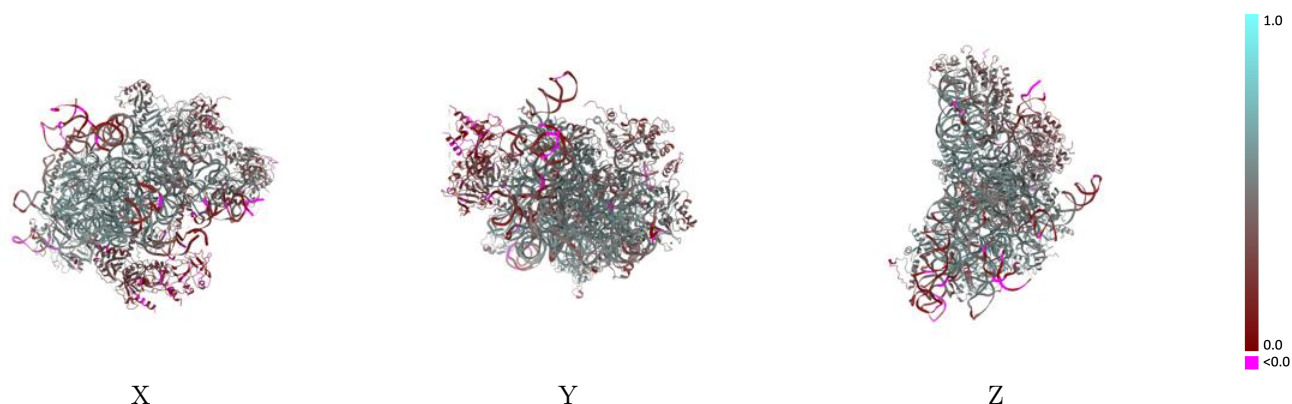
This section contains information regarding the fit between EMDB map EMD-66681 and PDB model 9XAB. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



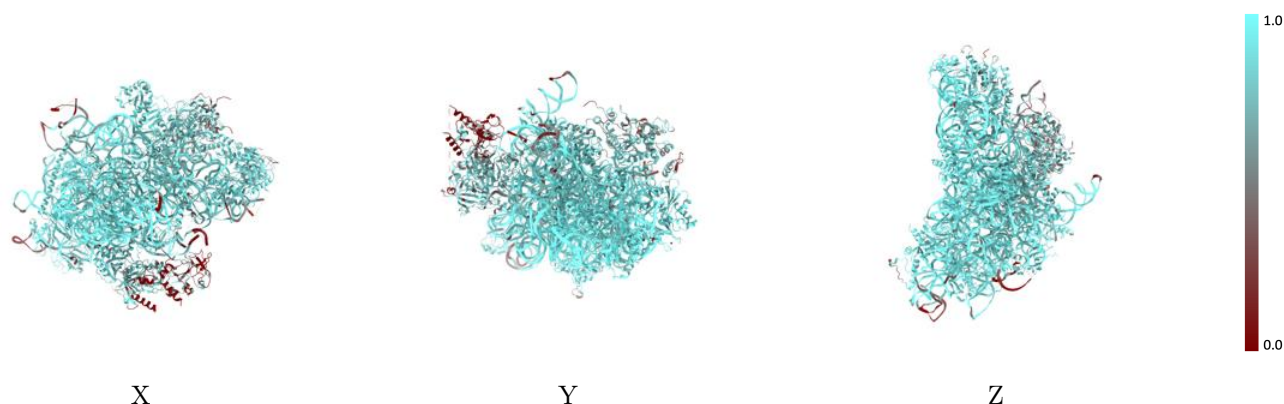
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



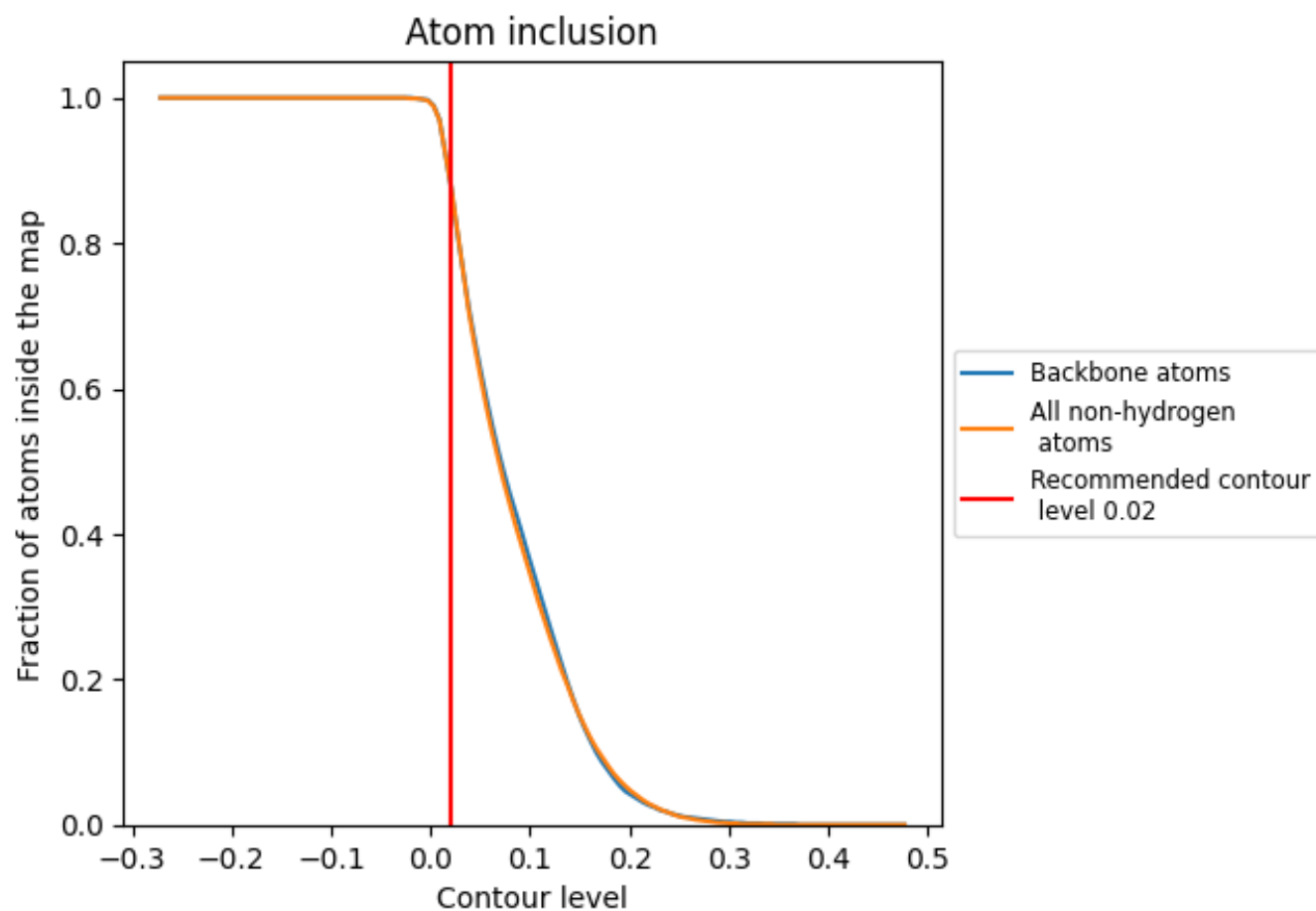
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.4510
1	 0.7810	 0.3450
2	 0.6150	 0.2410
3	 0.8290	 0.4060
A	 0.9230	 0.4570
D	 0.6800	 0.3720
E	 0.9370	 0.4890
F	 0.8010	 0.4510
H	 0.9750	 0.5750
J	 0.9510	 0.4910
K	 0.9340	 0.4600
L	 0.9470	 0.5280
M	 0.9590	 0.5430
O	 0.9640	 0.5680
Q	 0.9640	 0.5420
R	 0.8690	 0.4450
U	 0.5490	 0.3240
Y	 0.7910	 0.4540
Z	 0.9730	 0.5730
a	 0.9180	 0.5230
b	 0.9300	 0.5130
e	 0.9550	 0.5210
h	 0.9390	 0.5310

