



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:42 AM UTC

PDB ID : 9ZE2 / pdb_00009ze2
EMDB ID : EMD-74089
Title : Cryo-EM structure of the endogenous U2/branchpoint spliceosomal complex (core)
Authors : Liu, S.; Su, T.; Zhou, Z.H.
Deposited on : 2025-11-27
Resolution : 3.26 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

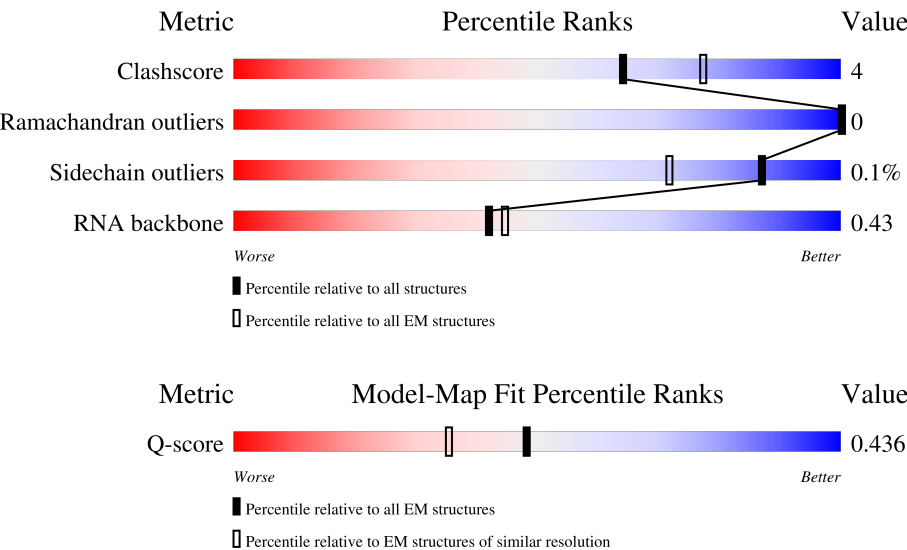
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.26 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.



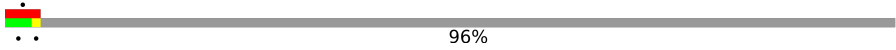





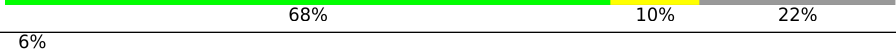
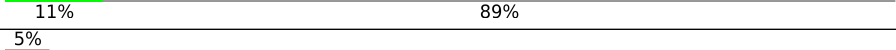
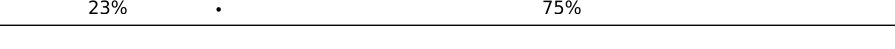
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	2	37	
2	H	110	
3	R	42	

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Mol	Chain	Length	Quality of chain
4	A	824	
5	B1	1304	
6	B2	895	
7	B3	1217	
8	B4	424	
9	B5	86	
10	B6	125	
11	A2	464	
12	A3	501	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 24516 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	37	Total	C	N	O	P	0	0
			781	352	127	265	37		

- Molecule 2 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	103	Total	C	N	O	S	0	0
			794	490	142	148	14		

- Molecule 3 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	32	Total	C	N	O	P	0	0
			642	289	69	252	32		

- Molecule 4 is a protein called RNA-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	29	Total	C	N	O	S	0	0
			258	161	50	45	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	MET	-	expression tag	UNP P52756
A	817	ASP	-	expression tag	UNP P52756
A	818	TYR	-	expression tag	UNP P52756
A	819	LYS	-	expression tag	UNP P52756
A	820	ASP	-	expression tag	UNP P52756
A	821	ASP	-	expression tag	UNP P52756
A	822	ASP	-	expression tag	UNP P52756
A	823	ASP	-	expression tag	UNP P52756
A	824	LYS	-	expression tag	UNP P52756

- Molecule 5 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B1	895	Total	C	N	O	S	0	0
			7142	4581	1225	1295	41		

- Molecule 6 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B2	250	Total	C	N	O	S	0	0
			1960	1260	348	345	7		

- Molecule 7 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B3	1198	Total	C	N	O	S	0	0
			9396	5959	1598	1794	45		

- Molecule 8 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B4	89	Total	C	N	O	S	0	0
			698	446	117	131	4		

- Molecule 9 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B5	75	Total	C	N	O	S	0	0
			616	390	108	113	5		

- Molecule 10 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B6	98	Total	C	N	O	S	0	0
			805	515	144	142	4		

- Molecule 11 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A2	51	Total	C	N	O	S	0	0
			407	252	77	75	3		

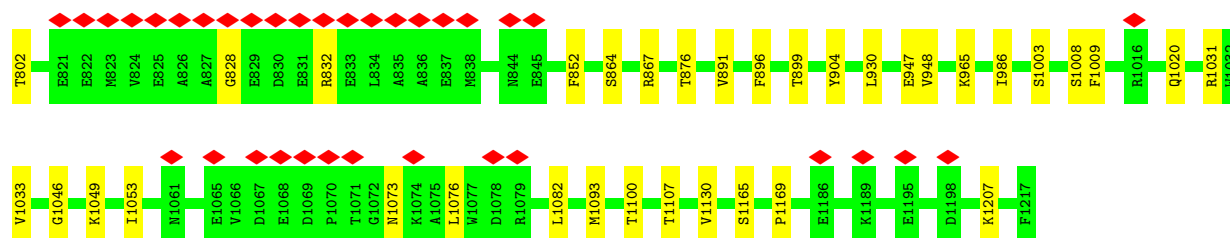
- Molecule 12 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A3	123	Total	C	N	O	S	0	0
			1014	646	181	183	4		

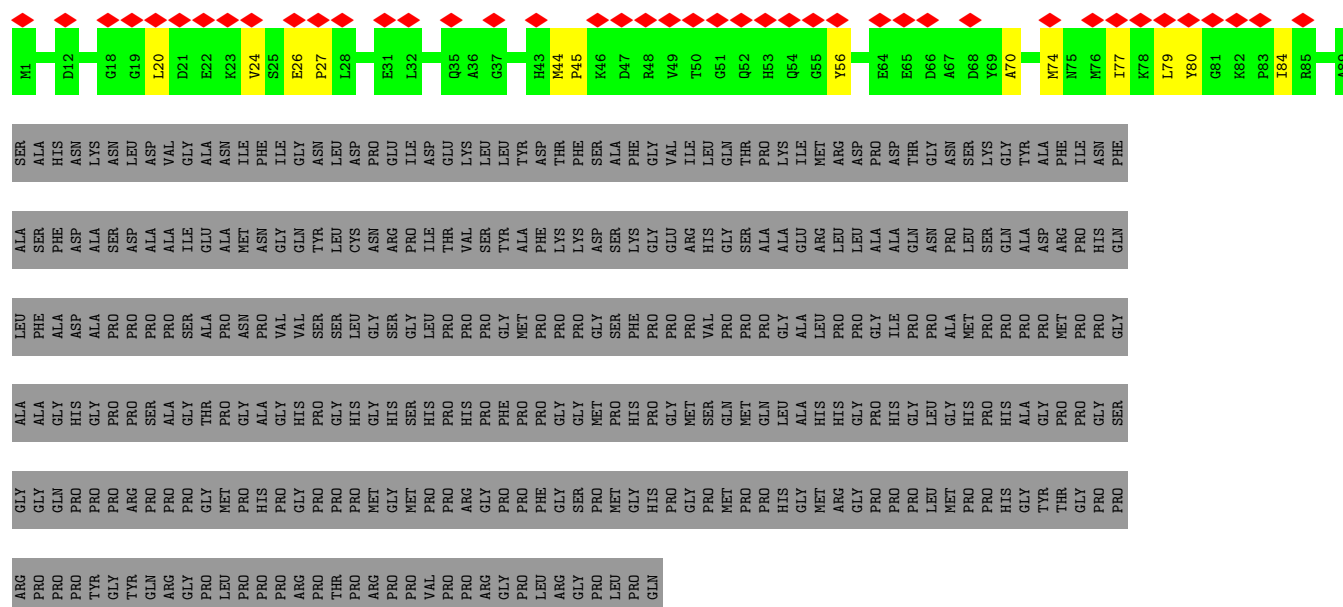
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	H	3	Total	Zn	0
			3	3	

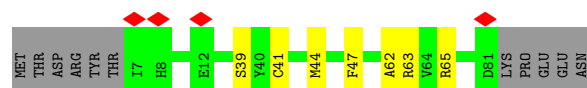
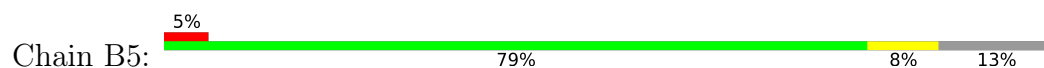




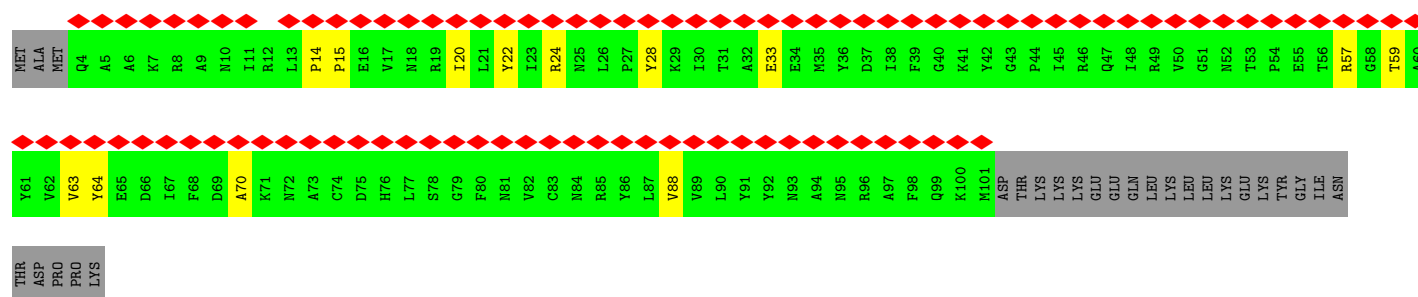
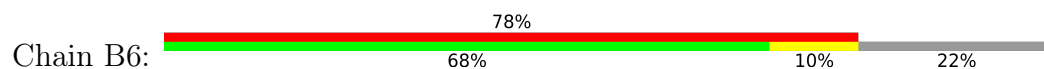
• Molecule 8: Splicing factor 3B subunit 4



• Molecule 9: Splicing factor 3B subunit 5



• Molecule 10: Splicing factor 3B subunit 6





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128413	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.200	Depositor
Minimum map value	-2.717	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.72	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OMC, PSU

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	2	0.17	0/625	0.33	0/972
2	H	0.09	0/807	0.28	0/1082
3	R	0.25	0/706	0.44	0/1089
4	A	0.07	0/261	0.16	0/342
5	B1	0.10	0/7284	0.26	0/9868
6	B2	0.18	0/2017	0.30	0/2735
7	B3	0.09	0/9590	0.28	0/13015
8	B4	0.08	0/713	0.26	0/964
9	B5	0.08	0/634	0.20	0/857
10	B6	0.07	0/823	0.21	0/1114
11	A2	0.06	0/415	0.16	0/555
12	A3	0.08	0/1045	0.25	0/1416
All	All	0.11	0/24920	0.28	0/34009

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	781	0	398	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	794	0	775	5	0
3	R	642	0	324	7	0
4	A	258	0	251	7	0
5	B1	7142	0	7319	62	0
6	B2	1960	0	1911	15	0
7	B3	9396	0	9309	79	0
8	B4	698	0	694	8	0
9	B5	616	0	579	6	0
10	B6	805	0	802	7	0
11	A2	407	0	397	1	0
12	A3	1014	0	974	9	0
13	H	3	0	0	0	0
All	All	24516	0	23733	198	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 4.

All (198) 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)
5:B1:460:PRO:HD3	5:B1:467:LEU:HD11	1.65	0.79
5:B1:731:LEU:HD22	5:B1:750:ILE:HD13	1.70	0.74
5:B1:1017:LEU:HD21	5:B1:1042:ILE:HG21	1.69	0.73
5:B1:501:LEU:HD21	5:B1:535:ILE:HG12	1.75	0.67
7:B3:704:VAL:HG11	7:B3:754:ILE:HG22	1.75	0.67
2:H:58:CYS:HB3	2:H:62:GLY:H	1.62	0.65
5:B1:1140:GLU:HB2	5:B1:1143:VAL:HG22	1.79	0.64
6:B2:630:PRO:HD2	6:B2:633:LEU:HD22	1.79	0.64
7:B3:474:ILE:HG13	7:B3:487:ILE:HD11	1.80	0.63
7:B3:674:LEU:HD11	7:B3:701:LEU:HD21	1.80	0.63
5:B1:790:LYS:HG3	5:B1:794:GLN:HE21	1.64	0.63
7:B3:828:GLY:HA2	7:B3:832:ARG:HD3	1.81	0.62
8:B4:26:GLU:HG3	8:B4:44:MET:HG3	1.81	0.62
6:B2:536:MET:HE1	6:B2:566:ILE:HB	1.83	0.61
5:B1:1103:VAL:HG13	5:B1:1105:GLU:H	1.67	0.60
1:2:47:OMC:H5	12:A3:383:LEU:HD11	1.65	0.60
7:B3:506:LEU:HG	7:B3:521:PRO:HD3	1.82	0.60
7:B3:500:LEU:HB2	7:B3:525:ARG:HH12	1.67	0.60
7:B3:423:LEU:HB2	7:B3:438:LEU:HB2	1.82	0.60
7:B3:117:PRO:HD3	7:B3:138:GLN:HE21	1.68	0.59
5:B1:1223:SER:HB2	5:B1:1226:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B2:605:LYS:HD2	6:B2:606:PRO:HD2	1.85	0.58
7:B3:428:GLY:HA3	7:B3:433:SER:HA	1.85	0.58
6:B2:452:LYS:HG3	6:B2:455:ARG:HH21	1.68	0.58
6:B2:474:VAL:HG11	6:B2:492:LYS:HB3	1.85	0.58
5:B1:732:TRP:CH2	5:B1:750:ILE:HD11	2.39	0.58
7:B3:606:ALA:HB1	7:B3:640:LEU:HD22	1.86	0.57
1:2:33:G:H1	3:R:1:U:H3	1.51	0.57
7:B3:947:GLU:HG3	7:B3:948:VAL:H	1.68	0.57
7:B3:118:GLY:HA2	7:B3:132:ILE:HD11	1.87	0.57
7:B3:545:VAL:HG22	7:B3:546:LYS:HE2	1.87	0.57
7:B3:520:TYR:HE1	7:B3:525:ARG:HG3	1.71	0.56
1:2:41:PSU:H2'	1:2:42:G:C8	2.40	0.56
7:B3:389:PRO:HB2	7:B3:852:PHE:HE2	1.70	0.55
7:B3:604:PHE:HB3	7:B3:616:ILE:HD11	1.89	0.55
7:B3:867:ARG:HH11	7:B3:876:THR:HG21	1.71	0.55
5:B1:665:ILE:HG23	5:B1:690:ILE:HD12	1.88	0.55
7:B3:61:VAL:HG12	9:B5:47:PHE:HE1	1.71	0.55
12:A3:392:ILE:HG13	12:A3:393:PRO:HD2	1.89	0.54
5:B1:380:PRO:HB3	5:B1:543:THR:HB	1.90	0.54
7:B3:633:LEU:HD12	7:B3:637:PRO:HG3	1.90	0.54
6:B2:588:GLY:HA3	7:B3:1082:LEU:HD11	1.90	0.54
6:B2:605:LYS:HG3	6:B2:607:GLY:H	1.73	0.54
2:H:30:CYS:SG	2:H:33:CYS:HB2	2.48	0.53
5:B1:460:PRO:HA	5:B1:479:LEU:HA	1.89	0.53
7:B3:65:LEU:HD12	7:B3:80:VAL:HG12	1.90	0.53
5:B1:1281:ILE:HD13	9:B5:39:SER:HA	1.92	0.52
2:H:96:THR:HG22	5:B1:588:TYR:HD2	1.75	0.52
5:B1:668:VAL:HG21	5:B1:690:ILE:HD11	1.91	0.52
6:B2:661:CYS:HB3	6:B2:670:TRP:HE1	1.75	0.52
1:2:41:PSU:H2'	1:2:42:G:H8	1.75	0.52
5:B1:811:LEU:HG	5:B1:812:PRO:HD3	1.92	0.51
7:B3:546:LYS:HD2	7:B3:589:CYS:HA	1.93	0.51
4:A:704:ARG:HH21	5:B1:977:VAL:HG23	1.75	0.50
7:B3:1073:ASN:HA	7:B3:1076:LEU:HD12	1.92	0.50
7:B3:358:LEU:HD21	7:B3:399:ASP:HB3	1.92	0.50
7:B3:520:TYR:HB2	7:B3:521:PRO:HD2	1.93	0.50
5:B1:397:ARG:HH21	5:B1:399:LEU:HD13	1.76	0.50
1:2:31:G:N2	3:R:3:U:O2	2.45	0.50
1:2:58:PSU:H2'	1:2:59:A:O4'	2.12	0.49
10:B6:20:ILE:HG23	10:B6:63:VAL:HG22	1.94	0.49
4:A:802:ALA:HB3	5:B1:623:TYR:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A3:383:LEU:HD12	12:A3:383:LEU:H	1.78	0.49
6:B2:586:ILE:HG13	6:B2:587:HIS:H	1.76	0.49
2:H:23:CYS:HB3	2:H:58:CYS:HB2	1.94	0.49
7:B3:449:VAL:HG22	7:B3:763:ARG:HG3	1.95	0.49
5:B1:793:LYS:HG3	5:B1:839:GLU:HG2	1.95	0.49
10:B6:22:TYR:HE1	10:B6:59:THR:HB	1.79	0.48
7:B3:800:ILE:HD13	7:B3:891:VAL:HB	1.95	0.48
3:R:-11:U:H2'	3:R:-10:U:C6	2.49	0.48
5:B1:387:ARG:HH22	5:B1:469:PRO:HG2	1.79	0.48
5:B1:477:LYS:NZ	5:B1:494:GLU:HG3	2.29	0.48
7:B3:544:ILE:HA	7:B3:558:LEU:HA	1.94	0.48
1:2:44:PSU:H4'	1:2:45:C:OP1	2.13	0.48
7:B3:316:GLU:HG3	7:B3:326:ARG:HE	1.79	0.48
8:B4:45:PRO:HG2	8:B4:56:TYR:CE2	2.49	0.48
5:B1:477:LYS:HZ3	5:B1:494:GLU:HG3	1.79	0.48
5:B1:622:GLU:HG3	5:B1:625:ARG:HH21	1.78	0.48
7:B3:520:TYR:CE1	7:B3:525:ARG:HG3	2.48	0.48
1:2:44:PSU:H3'	1:2:44:PSU:OP2	2.14	0.48
7:B3:617:ILE:HG12	7:B3:627:PRO:HA	1.95	0.48
7:B3:675:LEU:HD23	7:B3:686:LEU:HD12	1.95	0.48
7:B3:533:VAL:HG12	7:B3:535:GLU:HB2	1.96	0.48
4:A:706:ALA:HA	4:A:709:ARG:HE	1.78	0.47
7:B3:745:PHE:HB2	7:B3:755:VAL:HG13	1.95	0.47
3:R:-14:U:H1'	12:A3:400:HIS:NE2	2.30	0.47
5:B1:509:PRO:HA	5:B1:512:ARG:HB3	1.97	0.47
10:B6:24:ARG:HG3	10:B6:88:VAL:HB	1.96	0.47
7:B3:328:LYS:HG2	7:B3:372:GLU:HB3	1.97	0.47
7:B3:43:PRO:HB3	7:B3:50:VAL:HG12	1.96	0.46
7:B3:599:GLU:HG2	7:B3:603:ARG:HH21	1.80	0.46
5:B1:811:LEU:HA	5:B1:814:PHE:HB3	1.98	0.46
7:B3:899:THR:HG21	7:B3:904:TYR:HE2	1.79	0.46
7:B3:360:GLN:HB3	7:B3:396:VAL:HG23	1.98	0.46
7:B3:1053:ILE:HG23	7:B3:1093:MET:HE1	1.96	0.46
7:B3:114:ARG:HG3	9:B5:41:CYS:SG	2.55	0.46
7:B3:1003:SER:HB2	7:B3:1033:VAL:HG21	1.96	0.46
5:B1:1026:ASN:HD22	5:B1:1031:VAL:HG11	1.81	0.46
7:B3:519:VAL:HG22	7:B3:524:ILE:HD12	1.96	0.46
7:B3:1207:LYS:HE2	7:B3:1207:LYS:HB2	1.83	0.46
3:R:2:U:H2'	3:R:3:U:O4'	2.16	0.46
5:B1:728:LEU:HD22	5:B1:732:TRP:HZ3	1.81	0.46
1:2:47:OMC:C5	12:A3:383:LEU:HD11	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B2:604:LYS:NZ	8:B4:27:PRO:HB3	2.31	0.45
5:B1:1245:ARG:HA	5:B1:1245:ARG:HD3	1.82	0.45
4:A:803:VAL:HG21	5:B1:583:ILE:HD11	1.97	0.45
7:B3:1049:LYS:HA	7:B3:1100:THR:HG23	1.98	0.45
10:B6:28:TYR:HB3	10:B6:57:ARG:HE	1.82	0.45
7:B3:1008:SER:OG	7:B3:1031:ARG:HG3	2.16	0.45
7:B3:665:LEU:HD11	7:B3:679:LEU:HD13	1.99	0.45
7:B3:1165:SER:HB2	7:B3:1169:PRO:HA	1.99	0.45
7:B3:645:MET:HE2	7:B3:645:MET:HB2	1.91	0.44
7:B3:152:LEU:HA	7:B3:152:LEU:HD23	1.86	0.44
7:B3:312:LYS:O	7:B3:327:LEU:HA	2.18	0.44
6:B2:661:CYS:HB3	6:B2:670:TRP:NE1	2.31	0.44
7:B3:757:ILE:HG22	7:B3:762:LEU:HD22	1.97	0.44
5:B1:921:LEU:HD23	5:B1:921:LEU:HA	1.85	0.44
5:B1:1292:LYS:HA	5:B1:1292:LYS:HD2	1.83	0.44
7:B3:635:ALA:HB3	7:B3:669:LEU:HD23	1.98	0.44
5:B1:1006:MET:HG2	5:B1:1046:GLY:HA3	1.99	0.44
7:B3:164:ASN:HD22	7:B3:190:GLU:HB3	1.83	0.44
7:B3:596:PRO:HD2	7:B3:599:GLU:HB3	2.00	0.44
7:B3:644:GLU:O	7:B3:645:MET:HG3	2.18	0.44
4:A:802:ALA:HB3	5:B1:623:TYR:CE2	2.52	0.44
5:B1:387:ARG:HH12	5:B1:469:PRO:HD2	1.82	0.44
1:2:44:PSU:HN3	3:R:-10:U:H3	1.64	0.43
10:B6:64:TYR:HB2	10:B6:70:ALA:HB2	1.99	0.43
12:A3:443:THR:HG23	12:A3:445:HIS:H	1.82	0.43
5:B1:1183:VAL:HA	5:B1:1186:GLN:HG2	2.00	0.43
7:B3:88:VAL:HG12	7:B3:104:GLN:HG3	2.00	0.43
7:B3:896:PHE:HB2	7:B3:899:THR:HG22	2.00	0.43
5:B1:653:LYS:HB2	5:B1:653:LYS:HE2	1.76	0.43
7:B3:930:LEU:HD12	7:B3:930:LEU:HA	1.83	0.43
7:B3:965:LYS:HG3	7:B3:986:ILE:O	2.19	0.43
5:B1:560:LEU:HD23	5:B1:560:LEU:HA	1.84	0.43
9:B5:63:ARG:HA	9:B5:63:ARG:HD3	1.89	0.43
7:B3:288:VAL:HG12	9:B5:62:ALA:HB3	2.01	0.43
7:B3:552:ARG:HD3	7:B3:600:GLN:O	2.19	0.43
7:B3:617:ILE:HG23	7:B3:626:GLN:H	1.84	0.43
5:B1:717:THR:HA	5:B1:718:PRO:HA	1.89	0.43
1:2:43:PSU:C2	1:2:44:PSU:C2	3.06	0.42
11:A2:47:MET:SD	11:A2:57:LYS:HE2	2.59	0.42
5:B1:539:LEU:HA	5:B1:539:LEU:HD23	1.80	0.42
4:A:704:ARG:HG2	5:B1:981:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:508:THR:HG22	5:B1:511:MET:SD	2.60	0.42
5:B1:754:ILE:HG22	5:B1:798:THR:HG21	2.01	0.42
1:2:31:G:H2'	1:2:32:U:C6	2.53	0.42
5:B1:544:LEU:HD12	5:B1:544:LEU:HA	1.95	0.42
5:B1:1106:ARG:HG3	5:B1:1107:GLN:N	2.34	0.42
5:B1:1245:ARG:HD2	6:B2:587:HIS:CE1	2.54	0.42
9:B5:44:MET:HG2	9:B5:65:ARG:HG2	2.01	0.42
5:B1:468:LYS:HD2	5:B1:470:ASP:OD1	2.20	0.42
6:B2:616:SER:HA	8:B4:80:TYR:CE1	2.54	0.42
7:B3:4:TYR:HB3	7:B3:1130:VAL:HG23	2.00	0.42
7:B3:117:PRO:HA	7:B3:134:ALA:HB2	2.02	0.42
7:B3:426:ALA:HB1	7:B3:785:PRO:HG2	2.01	0.42
7:B3:546:LYS:HD3	7:B3:546:LYS:HA	1.74	0.42
8:B4:70:ALA:O	8:B4:74:MET:HB2	2.19	0.42
5:B1:802:GLU:HB2	5:B1:805:TYR:CE2	2.55	0.42
12:A3:381:LYS:HB3	12:A3:383:LEU:HG	2.02	0.42
4:A:799:TYR:O	4:A:803:VAL:HG23	2.20	0.42
5:B1:747:LEU:O	5:B1:750:ILE:HG22	2.20	0.42
5:B1:856:ASP:HB3	5:B1:864:TYR:CE2	2.54	0.42
12:A3:466:LYS:HD3	12:A3:466:LYS:HA	1.91	0.42
5:B1:718:PRO:HA	5:B1:756:LEU:HD22	2.00	0.42
5:B1:1021:THR:HB	5:B1:1022:PRO:HD3	2.02	0.42
5:B1:494:GLU:HA	5:B1:497:ILE:HG12	2.02	0.41
7:B3:117:PRO:HD3	7:B3:138:GLN:NE2	2.35	0.41
10:B6:33:GLU:H	10:B6:33:GLU:HG3	1.73	0.41
5:B1:939:ARG:HE	5:B1:947:VAL:HG13	1.85	0.41
7:B3:546:LYS:HB2	7:B3:557:ALA:HB3	2.02	0.41
7:B3:722:SER:HB2	7:B3:731:LEU:HD13	2.02	0.41
6:B2:571:LEU:HD23	6:B2:571:LEU:HA	1.92	0.41
7:B3:463:ARG:O	7:B3:510:LEU:HD11	2.21	0.41
1:2:54:PSU:H2'	1:2:55:U:C6	2.55	0.41
5:B1:732:TRP:CZ2	5:B1:750:ILE:HD11	2.56	0.41
8:B4:20:LEU:HD11	8:B4:24:VAL:HG11	2.02	0.41
8:B4:79:LEU:HD12	8:B4:79:LEU:HA	1.95	0.41
1:2:40:OMC:H2'	1:2:41:PSU:H6	1.85	0.41
2:H:5:HIS:HA	2:H:6:PRO:HD3	1.93	0.41
5:B1:943:LYS:HA	5:B1:943:LYS:HD2	1.82	0.41
5:B1:1245:ARG:HD2	6:B2:587:HIS:ND1	2.35	0.41
7:B3:412:ILE:HG23	7:B3:1107:THR:HG21	2.03	0.41
7:B3:610:VAL:HG23	7:B3:636:GLN:HE22	1.86	0.41
7:B3:1020:GLN:H	7:B3:1020:GLN:HG3	1.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B4:77:ILE:O	8:B4:84:ILE:HG12	2.21	0.41
5:B1:641:ILE:N	5:B1:642:PRO:HD2	2.36	0.41
7:B3:802:THR:HG22	7:B3:864:SER:HB2	2.02	0.41
7:B3:475:ILE:HG21	7:B3:508:CYS:SG	2.61	0.40
12:A3:461:LYS:HE3	12:A3:461:LYS:HB2	1.84	0.40
5:B1:676:GLY:O	5:B1:715:ALA:HB1	2.21	0.40
5:B1:806:ILE:HG22	5:B1:811:LEU:HD23	2.04	0.40
10:B6:14:PRO:HA	10:B6:15:PRO:HD3	1.96	0.40
5:B1:776:GLU:OE1	5:B1:784:MET:HE2	2.21	0.40
7:B3:328:LYS:HB3	7:B3:328:LYS:HE3	1.81	0.40
3:R:-1:C:H5	5:B1:1106:ARG:HH12	1.69	0.40
7:B3:528:ARG:HG3	7:B3:529:ALA:N	2.36	0.40
7:B3:1009:PHE:HZ	7:B3:1046:GLY:HA3	1.86	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	
2	H	101/110 (92%)	95 (94%)	6 (6%)	0	100	100
4	A	25/824 (3%)	25 (100%)	0	0	100	100
5	B1	891/1304 (68%)	866 (97%)	25 (3%)	0	100	100
6	B2	246/895 (28%)	233 (95%)	13 (5%)	0	100	100
7	B3	1192/1217 (98%)	1140 (96%)	52 (4%)	0	100	100
8	B4	87/424 (20%)	83 (95%)	4 (5%)	0	100	100
9	B5	73/86 (85%)	70 (96%)	3 (4%)	0	100	100
10	B6	96/125 (77%)	93 (97%)	3 (3%)	0	100	100
11	A2	49/464 (11%)	48 (98%)	1 (2%)	0	100	100
12	A3	121/501 (24%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2881/5950 (48%)	2771 (96%)	110 (4%)	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	
2	H	89/95 (94%)	89 (100%)	0	100	100
4	A	24/704 (3%)	24 (100%)	0	100	100
5	B1	775/1104 (70%)	774 (100%)	1 (0%)	88	89
6	B2	201/776 (26%)	200 (100%)	1 (0%)	81	82
7	B3	1037/1051 (99%)	1036 (100%)	1 (0%)	88	89
8	B4	74/336 (22%)	74 (100%)	0	100	100
9	B5	66/77 (86%)	66 (100%)	0	100	100
10	B6	84/109 (77%)	84 (100%)	0	100	100
11	A2	42/382 (11%)	42 (100%)	0	100	100
12	A3	106/446 (24%)	106 (100%)	0	100	100
All	All	2498/5080 (49%)	2495 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B1	817	HIS
6	B2	609	LEU
7	B3	667	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
5	B1	463	ASN

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Mol	Chain	Res	Type
5	B1	506	ASN
5	B1	572	HIS
5	B1	662	HIS
5	B1	698	GLN
5	B1	794	GLN
5	B1	842	ASN
5	B1	1100	ASN
5	B1	1186	GLN
5	B1	1218	ASN
6	B2	467	GLN
6	B2	496	ASN
6	B2	503	HIS
6	B2	587	HIS
7	B3	104	GLN
7	B3	138	GLN
7	B3	164	ASN
7	B3	206	GLN
7	B3	422	GLN
7	B3	636	GLN
7	B3	932	ASN
7	B3	941	HIS
10	B6	99	GLN
12	A3	379	ASN
12	A3	448	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/37 (97%)	7 (19%)	1 (2%)
3	R	31/42 (73%)	14 (45%)	0
All	All	67/79 (84%)	21 (31%)	1 (1%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	30	A
1	2	31	G
1	2	44	PSU
1	2	45	C
1	2	46	U
1	2	47	OMC

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Mol	Chain	Res	Type
1	2	48	A
3	R	-17	U
3	R	-16	U
3	R	-15	U
3	R	-14	U
3	R	-13	U
3	R	-8	U
3	R	0	A
3	R	3	U
3	R	4	U
3	R	5	U
3	R	6	U
3	R	9	U
3	R	12	U
3	R	13	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	44	PSU

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	2	43	1,3	18,21,22	0.99	1 (5%)	21,30,33	1.13	2 (9%)
1	PSU	2	34	1,3	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
1	OMC	2	47	1	19,22,23	0.52	0	25,31,34	1.03	2 (8%)
1	PSU	2	58	1	18,21,22	1.12	1 (5%)	21,30,33	1.74	4 (19%)
1	PSU	2	39	1	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
1	OMC	2	40	1,3	19,22,23	0.48	0	25,31,34	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2	44	1,3	18,21,22	0.88	1 (5%)	21,30,33	0.96	1 (4%)
1	PSU	2	41	1	18,21,22	1.13	1 (5%)	21,30,33	1.84	4 (19%)
1	PSU	2	37	1	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
1	PSU	2	54	1	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
1	OMC	2	61	1	19,22,23	0.49	0	25,31,34	0.73	0

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
1	PSU	2	43	1,3	-	1/7/25/26	0/2/2/2
1	PSU	2	34	1,3	-	0/7/25/26	0/2/2/2
1	OMC	2	47	1	-	6/9/27/28	0/2/2/2
1	PSU	2	58	1	-	2/7/25/26	0/2/2/2
1	PSU	2	39	1	-	0/7/25/26	0/2/2/2
1	OMC	2	40	1,3	-	0/9/27/28	0/2/2/2
1	PSU	2	44	1,3	-	3/7/25/26	0/2/2/2
1	PSU	2	41	1	-	0/7/25/26	0/2/2/2
1	PSU	2	37	1	-	0/7/25/26	0/2/2/2
1	PSU	2	54	1	-	0/7/25/26	0/2/2/2
1	OMC	2	61	1	-	0/9/27/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	58	PSU	C6-C5	3.86	1.39	1.35
1	2	34	PSU	C6-C5	3.85	1.39	1.35
1	2	39	PSU	C6-C5	3.79	1.39	1.35
1	2	41	PSU	C6-C5	3.77	1.39	1.35
1	2	37	PSU	C6-C5	3.76	1.39	1.35
1	2	54	PSU	C6-C5	3.76	1.39	1.35
1	2	43	PSU	C6-C5	3.59	1.39	1.35
1	2	44	PSU	C6-C5	3.23	1.38	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	54	PSU	C4-N3-C2	-4.84	119.70	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	37	PSU	C4-N3-C2	-4.81	119.74	126.37
1	2	54	PSU	N1-C2-N3	4.74	120.17	115.17
1	2	39	PSU	N1-C2-N3	4.74	120.16	115.17
1	2	39	PSU	C4-N3-C2	-4.71	119.89	126.37
1	2	34	PSU	C4-N3-C2	-4.71	119.89	126.37
1	2	37	PSU	N1-C2-N3	4.70	120.12	115.17
1	2	41	PSU	C4-N3-C2	-4.67	119.94	126.37
1	2	34	PSU	N1-C2-N3	4.66	120.09	115.17
1	2	41	PSU	N1-C2-N3	4.62	120.04	115.17
1	2	58	PSU	N1-C2-N3	4.43	119.84	115.17
1	2	58	PSU	C4-N3-C2	-4.33	120.40	126.37
1	2	47	OMC	C1'-N1-C2	3.06	125.21	118.44
1	2	44	PSU	C3'-C2'-C1'	2.97	105.19	101.69
1	2	39	PSU	O2-C2-N1	-2.80	119.90	122.79
1	2	34	PSU	O2-C2-N1	-2.77	119.93	122.79
1	2	54	PSU	O2-C2-N1	-2.70	120.00	122.79
1	2	41	PSU	O2-C2-N1	-2.70	120.00	122.79
1	2	58	PSU	C6-N1-C2	-2.63	120.25	122.69
1	2	47	OMC	C1'-N1-C6	-2.54	115.36	120.78
1	2	39	PSU	C6-N1-C2	-2.49	120.38	122.69
1	2	58	PSU	O2-C2-N1	-2.46	120.25	122.79
1	2	37	PSU	O2-C2-N1	-2.43	120.28	122.79
1	2	43	PSU	O4'-C1'-C2'	-2.43	101.79	105.15
1	2	41	PSU	C6-N1-C2	-2.35	120.51	122.69
1	2	54	PSU	C6-N1-C2	-2.31	120.55	122.69
1	2	34	PSU	C6-N1-C2	-2.31	120.55	122.69
1	2	37	PSU	C6-N1-C2	-2.20	120.65	122.69
1	2	37	PSU	C6-C5-C4	2.18	119.65	118.17
1	2	54	PSU	O4'-C1'-C2'	2.16	108.14	105.15
1	2	39	PSU	C6-C5-C4	2.13	119.61	118.17
1	2	43	PSU	C3'-C2'-C1'	-2.10	99.21	101.69

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	58	PSU	O4'-C1'-C5-C4
1	2	58	PSU	O4'-C1'-C5-C6
1	2	44	PSU	O4'-C4'-C5'-O5'
1	2	47	OMC	C4'-C5'-O5'-P
1	2	47	OMC	O4'-C1'-N1-C6
1	2	44	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	2	47	OMC	O4'-C4'-C5'-O5'
1	2	43	PSU	O4'-C1'-C5-C6
1	2	47	OMC	C2'-C1'-N1-C6
1	2	44	PSU	C2'-C1'-C5-C6
1	2	47	OMC	O4'-C1'-N1-C2
1	2	47	OMC	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	43	PSU	1	0
1	2	47	OMC	2	0
1	2	58	PSU	1	0
1	2	40	OMC	1	0
1	2	44	PSU	4	0
1	2	41	PSU	3	0
1	2	54	PSU	1	0

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 ⓘ

There are no chain breaks in this entry.

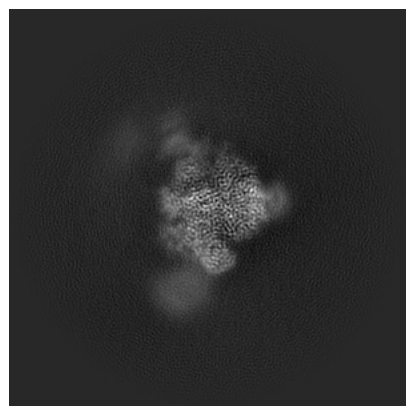
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74089. These allow visual inspection of the internal detail of the map and identification of artifacts.

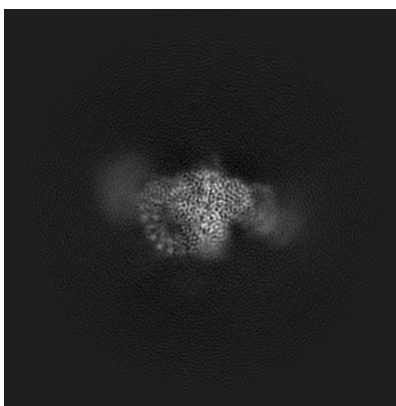
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

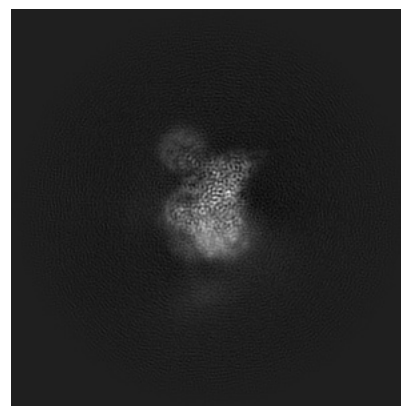
6.1.1 Primary map



X

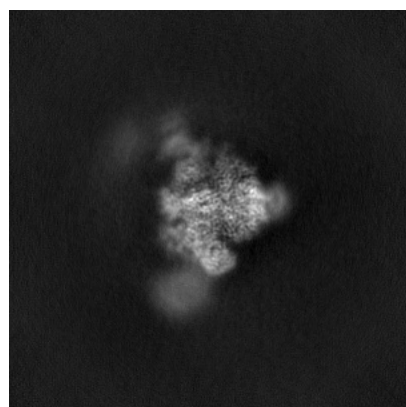


Y

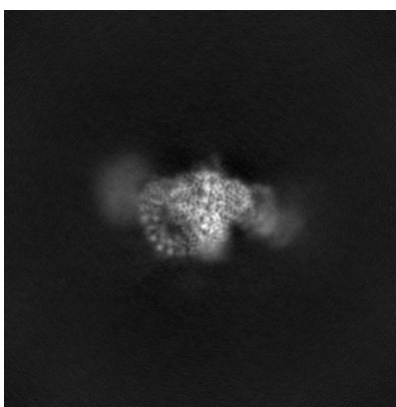


Z

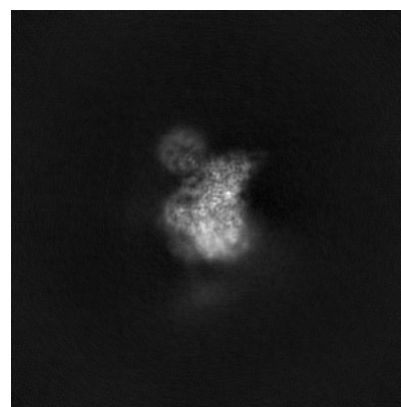
6.1.2 Raw map



X



Y

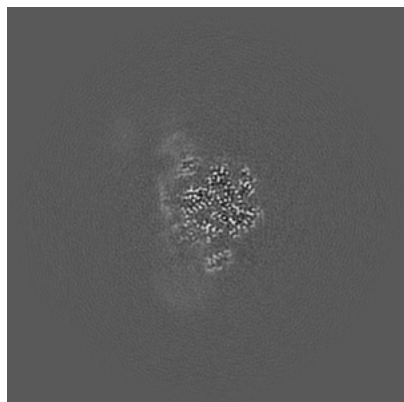


Z

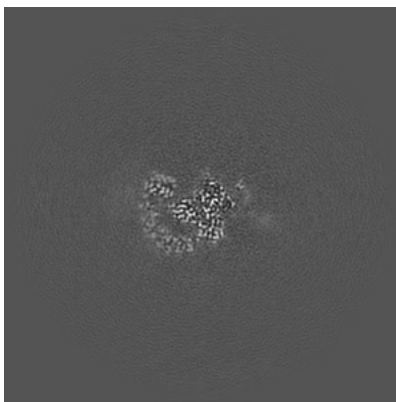
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

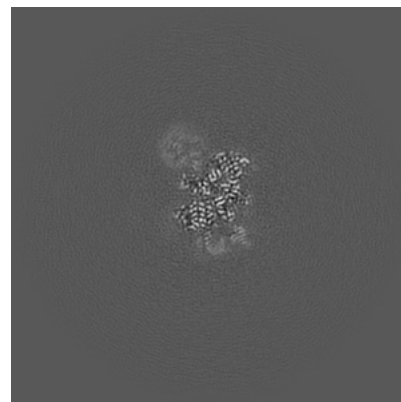
6.2.1 Primary map



X Index: 192

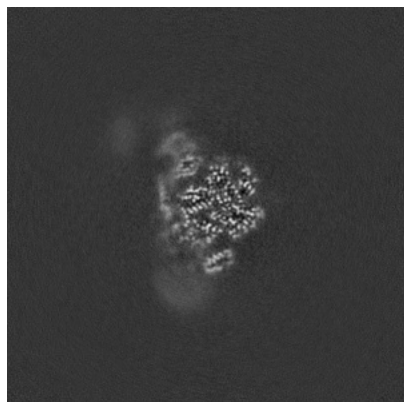


Y Index: 192

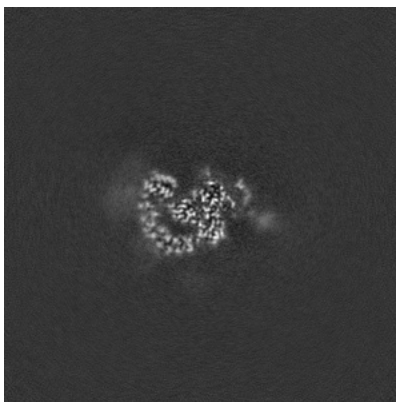


Z Index: 192

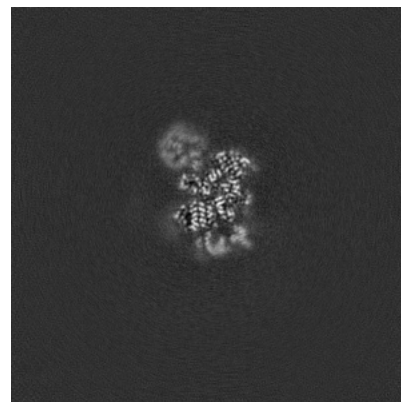
6.2.2 Raw map



X Index: 192



Y Index: 192

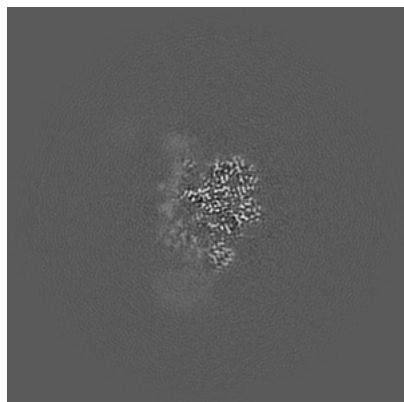


Z Index: 192

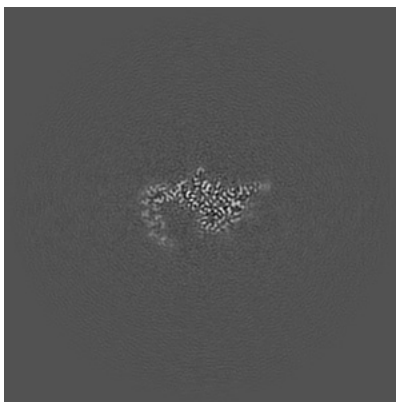
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

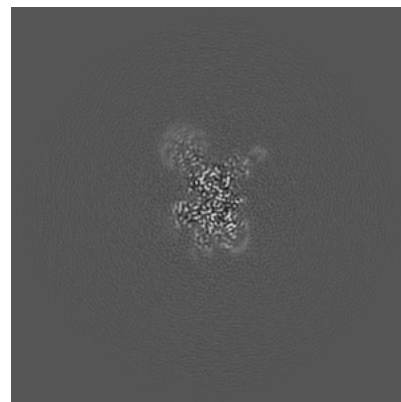
6.3.1 Primary map



X Index: 199

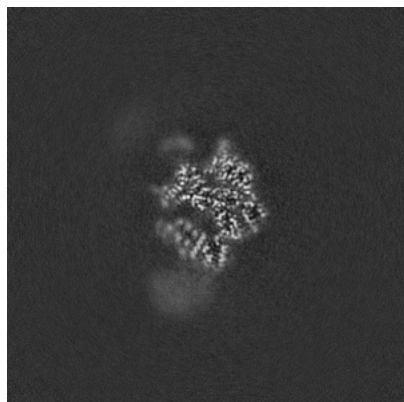


Y Index: 207

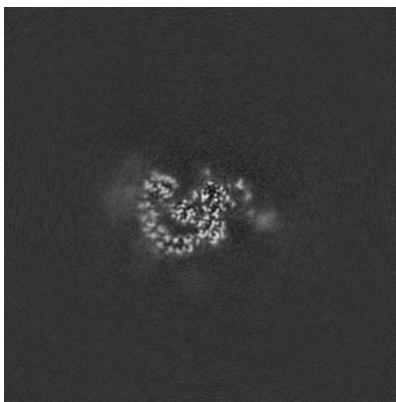


Z Index: 201

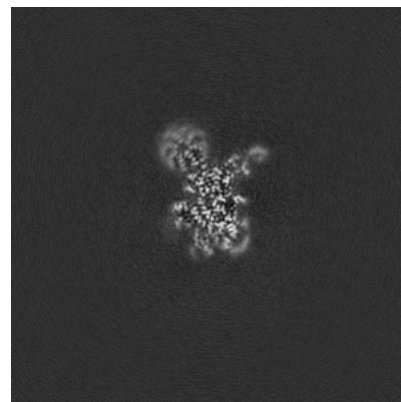
6.3.2 Raw map



X Index: 209



Y Index: 191

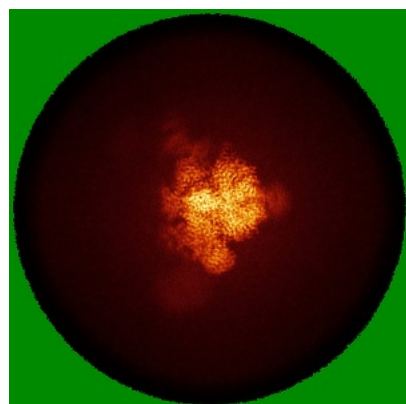


Z Index: 202

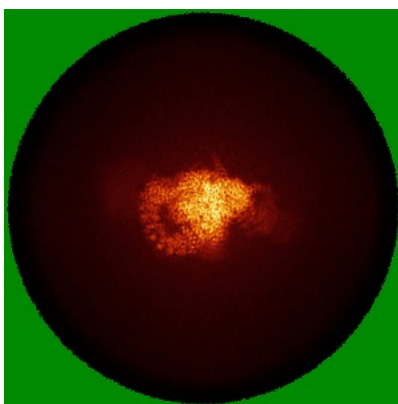
The images above show the largest variance slices of the map in three orthogonal directions.

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

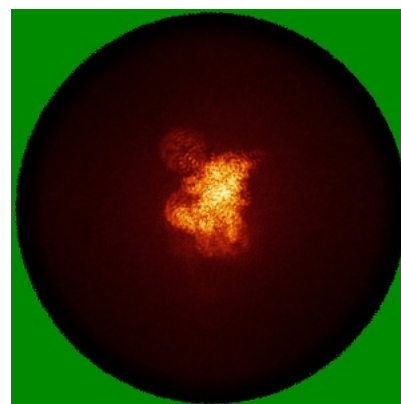
6.4.1 Primary map



X

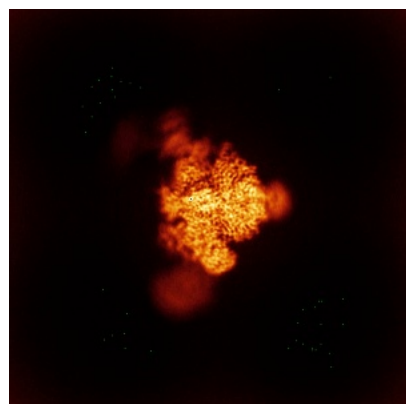


Y

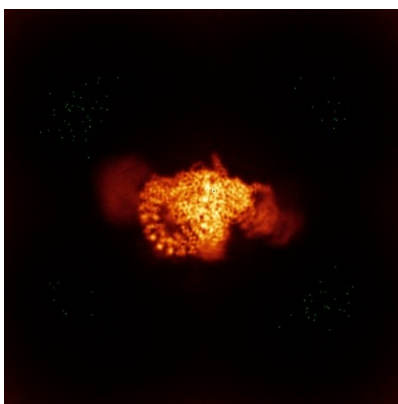


Z

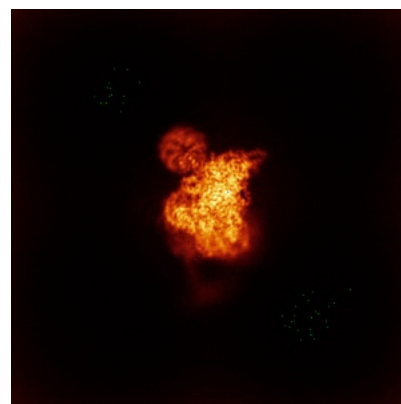
6.4.2 Raw map



X



Y

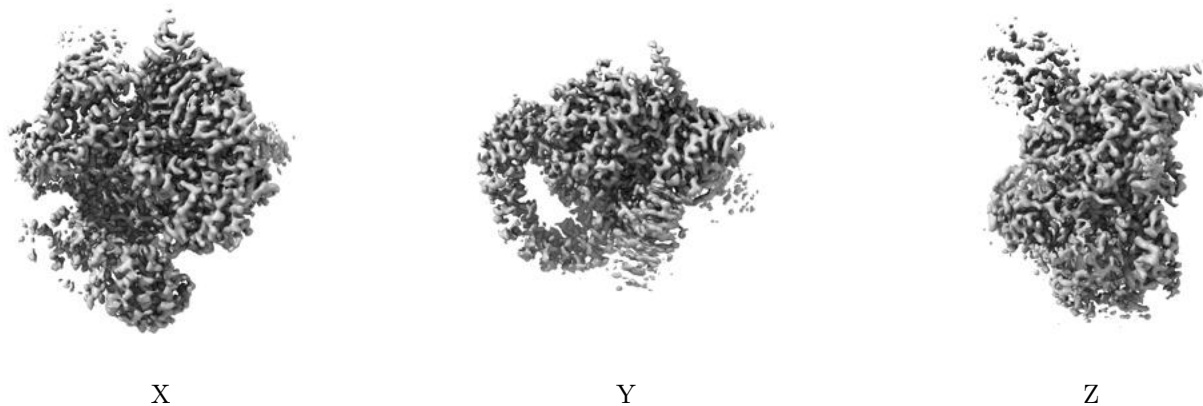


Z

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 0.72. 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.

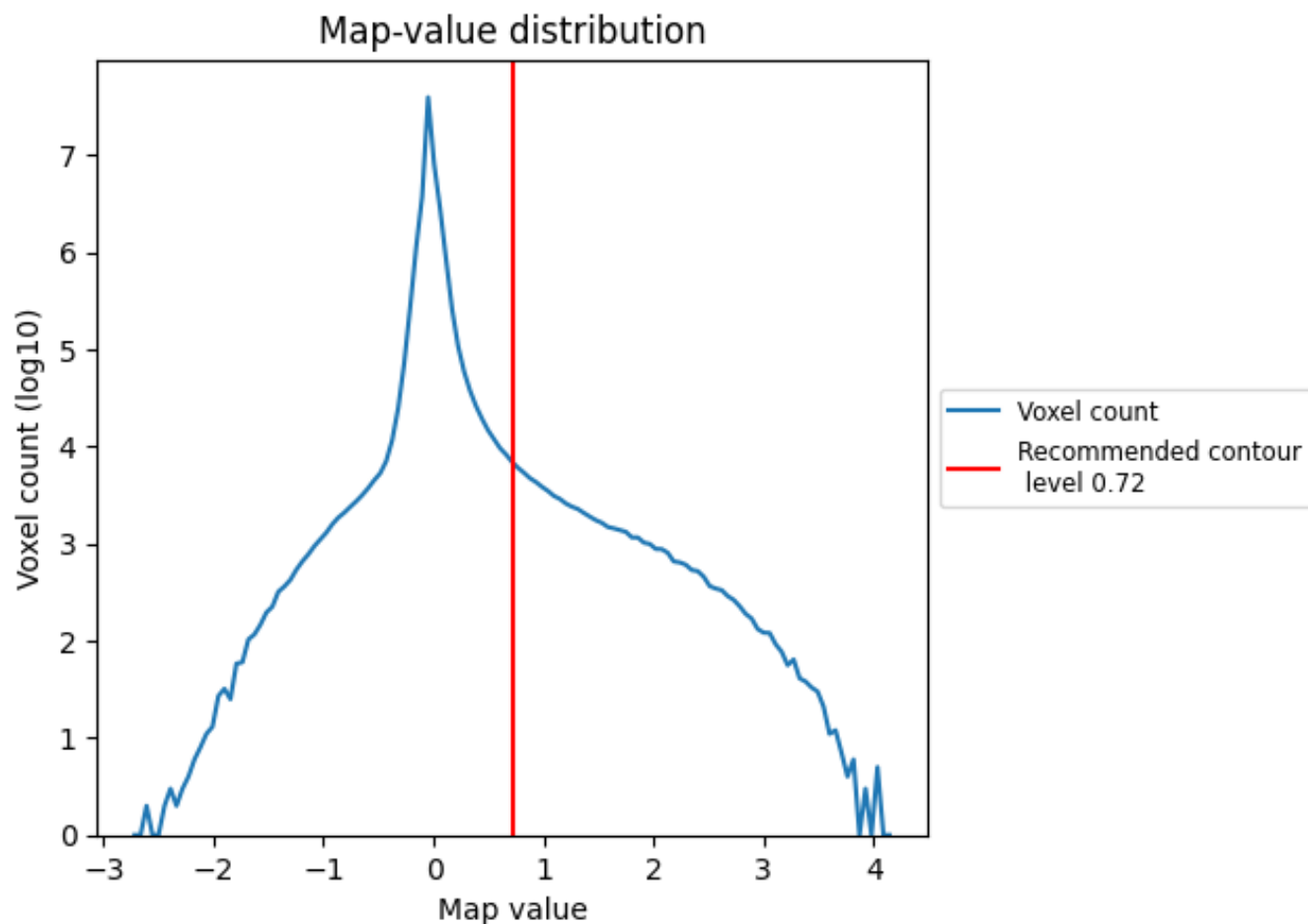
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

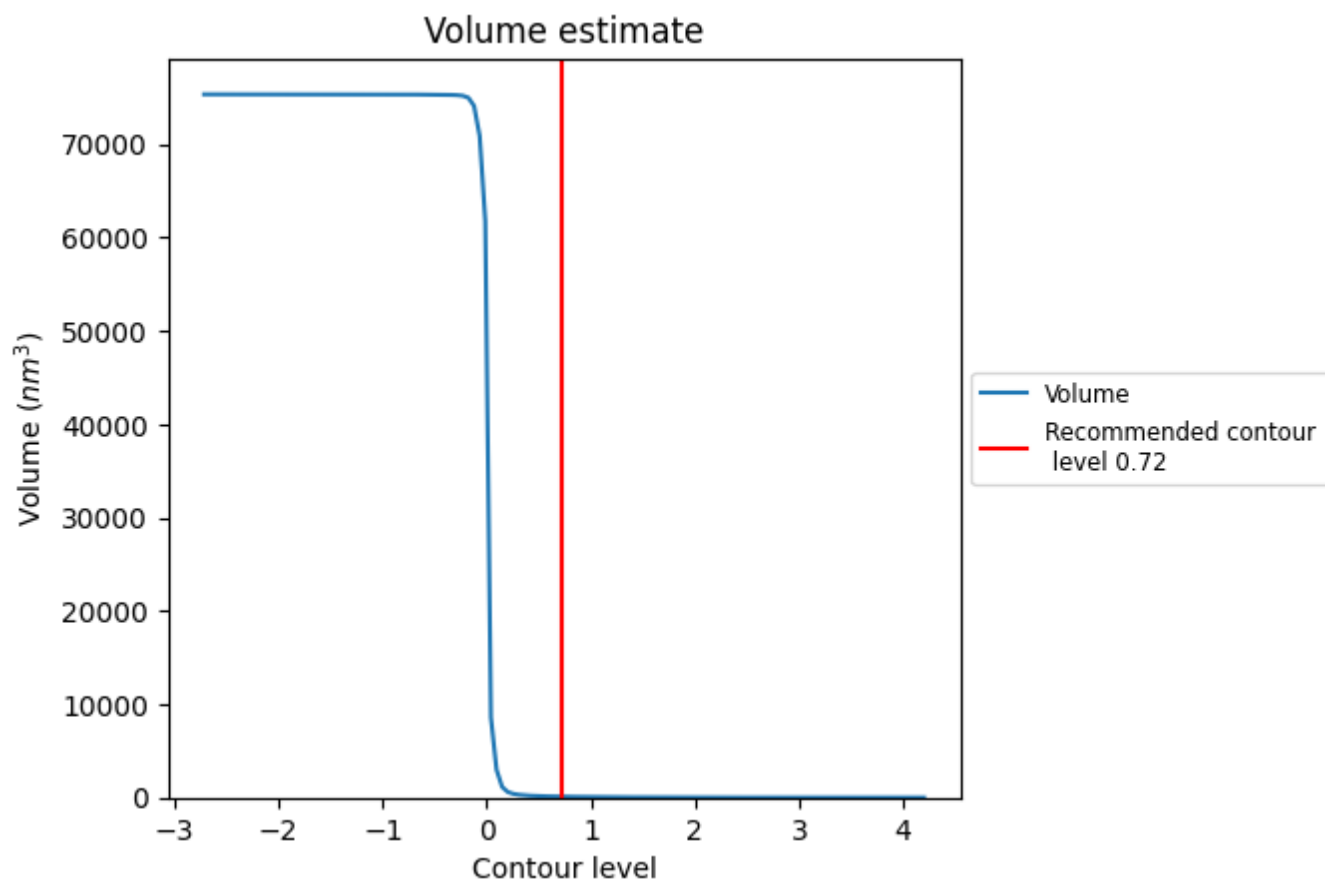
This section contains the results of statistical analysis of the map.

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.

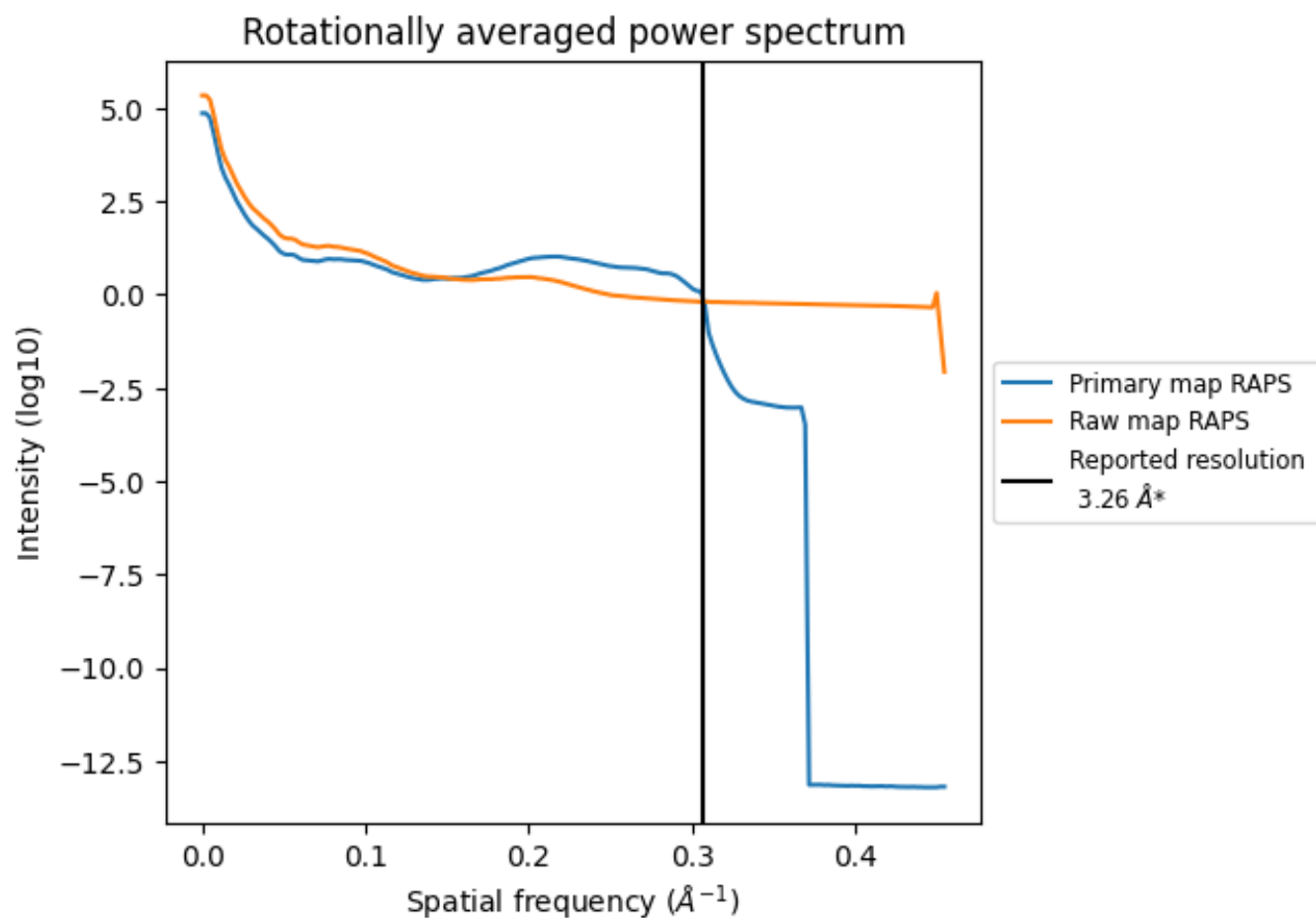
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

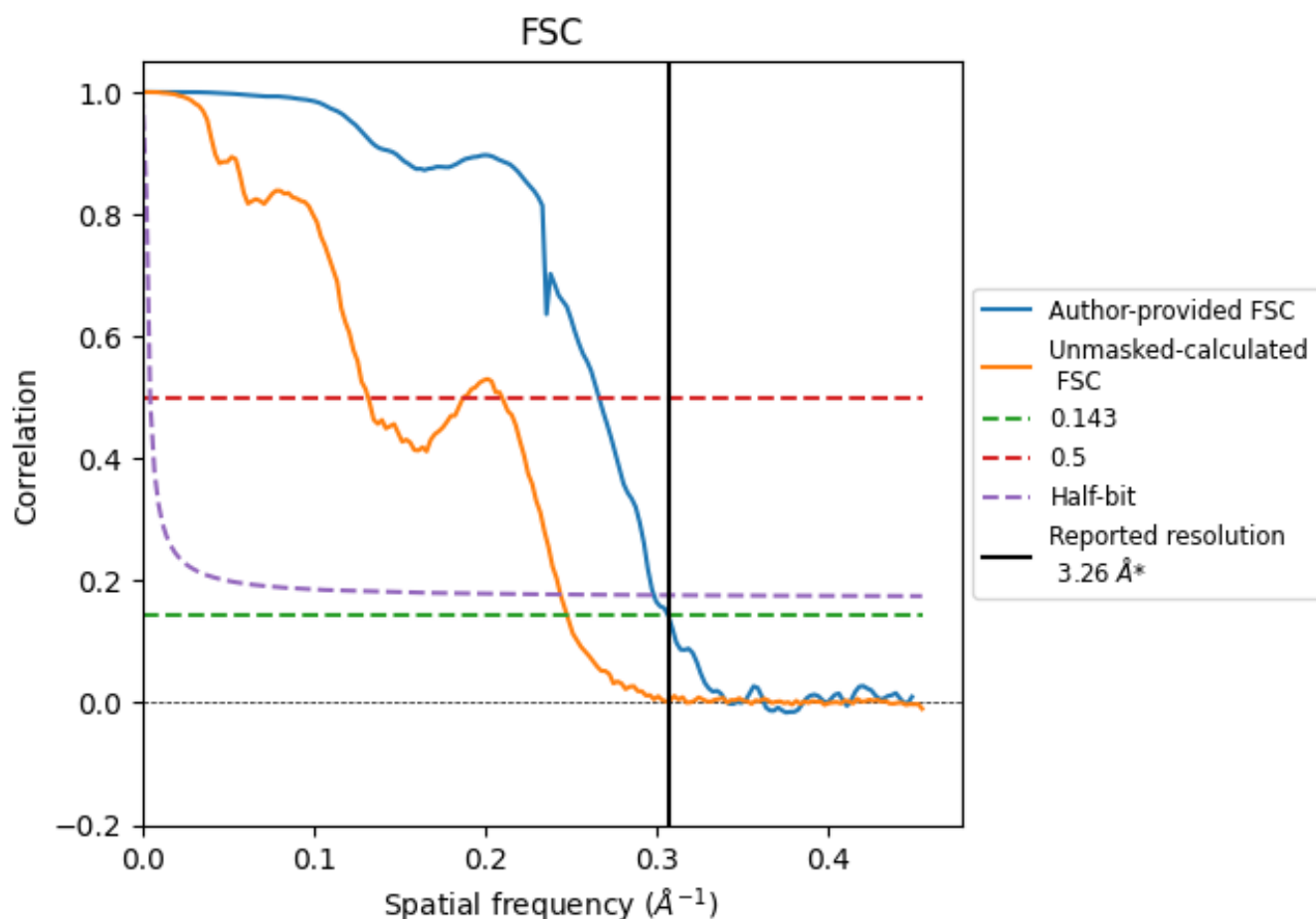


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

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 0.307 \AA^{-1}

8.2 Resolution estimates [i](#)

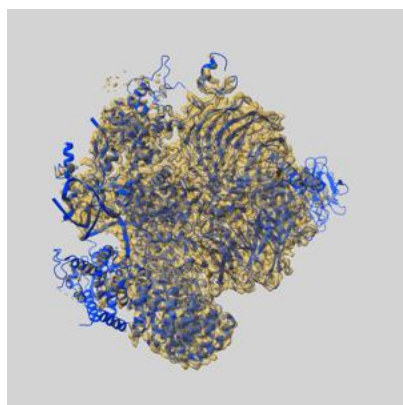
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.76	3.35
Unmasked-calculated*	4.04	7.60	4.10

*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 4.04 differs from the reported value 3.26 by more than 10 %

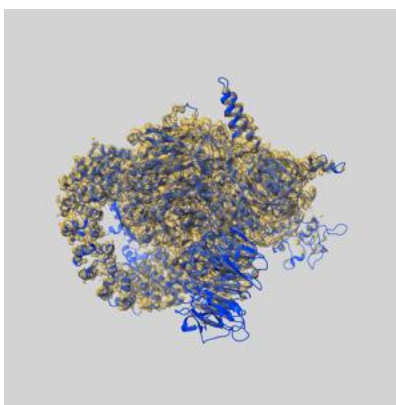
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74089 and PDB model 9ZE2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

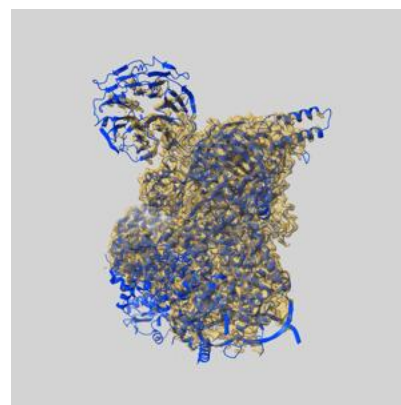
9.1 Map-model overlay [i](#)



X



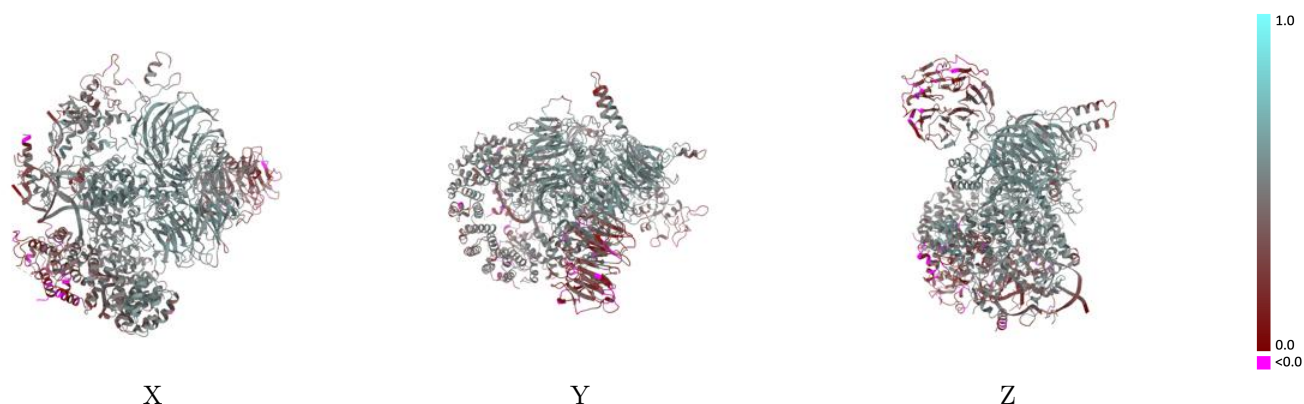
Y



Z

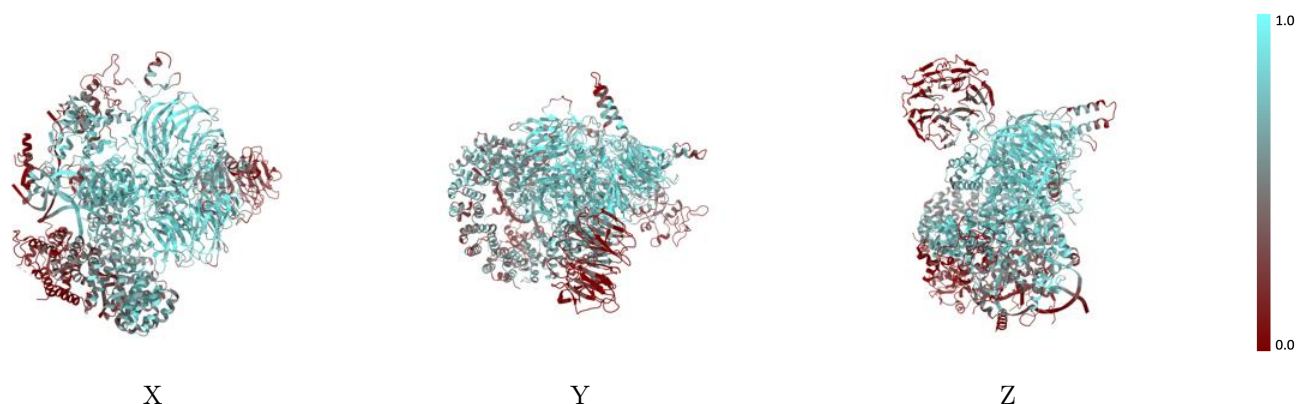
The images above show the 3D surface view of the map at the recommended contour level 0.72 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



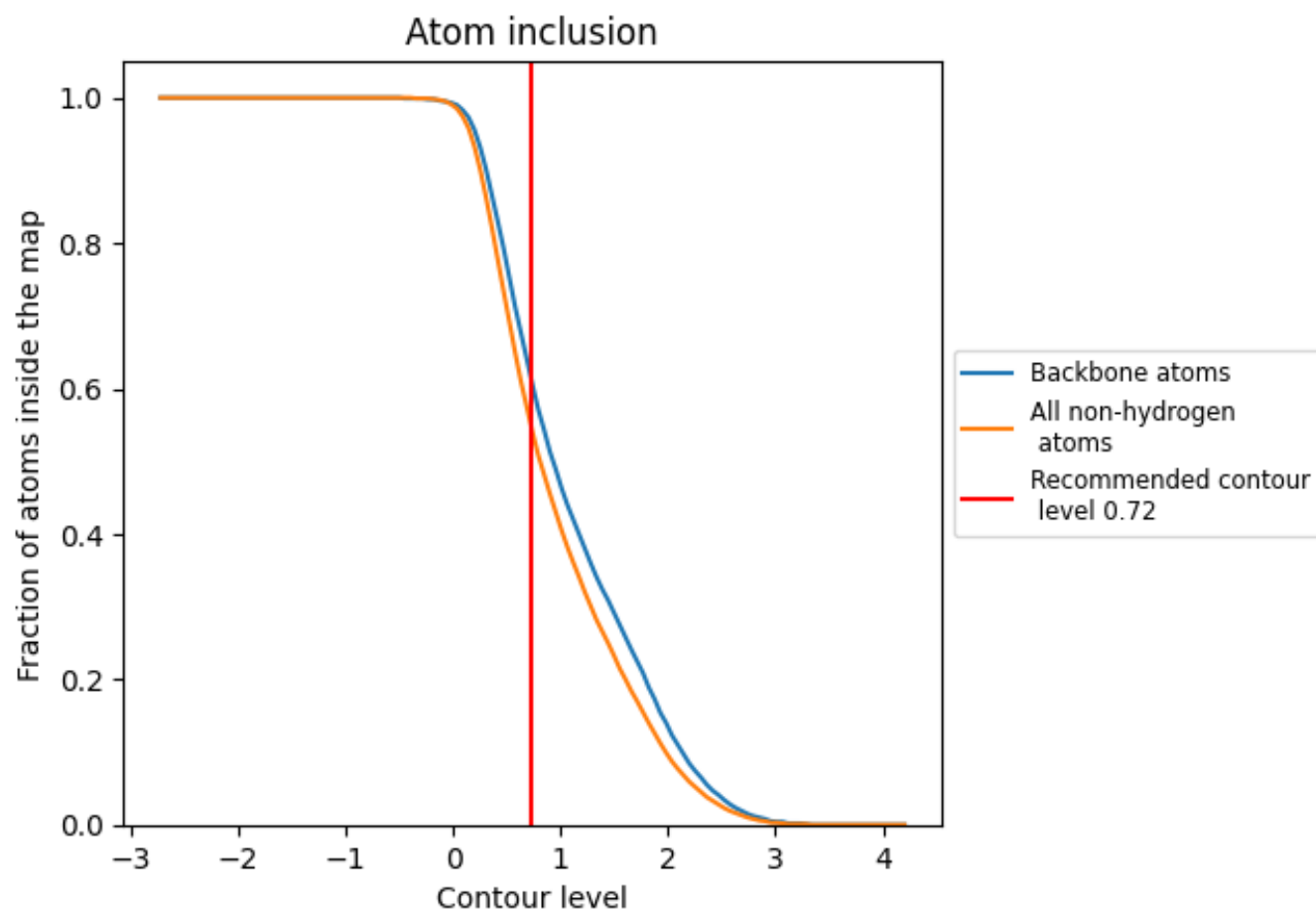
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.72).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 55% 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 (0.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5530	<div></div> 0.4360
2	<div></div> 0.5220	<div></div> 0.4110
A	<div></div> 0.0000	<div></div> 0.1220
A2	<div></div> 0.3880	<div></div> 0.4180
A3	<div></div> 0.6090	<div></div> 0.4740
B1	<div></div> 0.5600	<div></div> 0.4410
B2	<div></div> 0.4490	<div></div> 0.4020
B3	<div></div> 0.6190	<div></div> 0.4610
B4	<div></div> 0.4130	<div></div> 0.4020
B5	<div></div> 0.8110	<div></div> 0.5500
B6	<div></div> 0.0100	<div></div> 0.1870
H	<div></div> 0.7910	<div></div> 0.5300
R	<div></div> 0.3630	<div></div> 0.3600

1.0

0.0

<0.0