



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:30 AM UTC

PDB ID : 7ABF / pdb_00007abf
EMDB ID : EMD-11694
Title : Human pre-Bact-1 spliceosome core structure
Authors : Townsend, C.; Kastner, B.; Leelaram, M.N.; Bertram, K.; Stark, H.;
Luehrmann, R.
Deposited on : 2020-09-07
Resolution : 3.90 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:

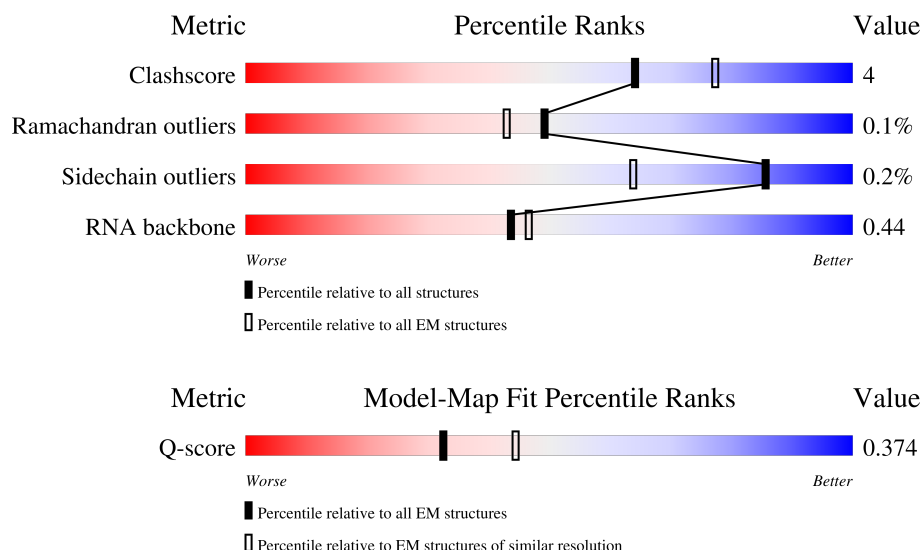
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	Q	144	8% 93% . .
2	I	312	5% 54% . 44%
3	A	2335	10% 68% . 29%

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Mol	Chain	Length	Quality of chain
4	r	972	
5	N	199	
6	q	73	
7	R	229	
8	5	116	
9	6	106	
10	X	641	
11	v	536	
12	G	514	
13	Z	230	
14	K	439	
15	A4	1077	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	GTP	r	1500	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 25904 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 Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	138	Total	C	N	O	S	0	0
			850	542	151	155	2		

- Molecule 2 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	176	Total	C	N	O	S	0	0
			1151	752	201	195	3		

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1656	Total	C	N	O	S	0	0
			10522	6814	1920	1763	25		

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	r	844	Total	C	N	O	S	0	0
			5120	3284	935	894	7		

- Molecule 5 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	56	Total	C	N	O	0	0
			295	181	58	56		

- Molecule 6 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	q	73	Total	C	N	O	S	0	0
			523	343	88	91	1		

- Molecule 7 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 8 is a RNA chain called U5 small nuclear RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	5	58	Total	C	N	O	P	0	0
			1220	547	203	412	58		

- Molecule 9 is a RNA chain called U6 small nuclear RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	65	Total	C	N	O	P	0	0
			1392	622	257	448	65		

- Molecule 10 is a protein called WW domain-binding protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	36	Total	C	N	O	0	0
			182	110	36	36		

- Molecule 11 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	v	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 12 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	320	Total	C	N	O	0	0
			1604	964	320	320		

- Molecule 13 is a RNA chain called MINX M3 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	29	Total	C	N	O	P	0	0
			622	278	116	199	29		

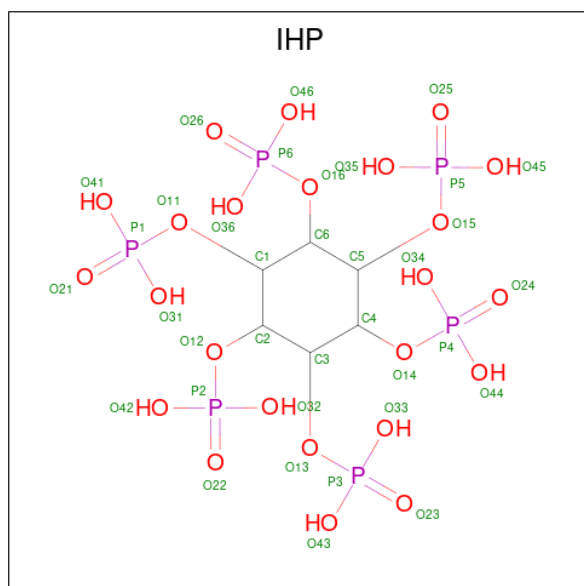
- Molecule 14 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	123	Total	C	N	O	S	0	0
			799	504	156	137	2		

- Molecule 15 is a protein called Transcription elongation regulator 1.

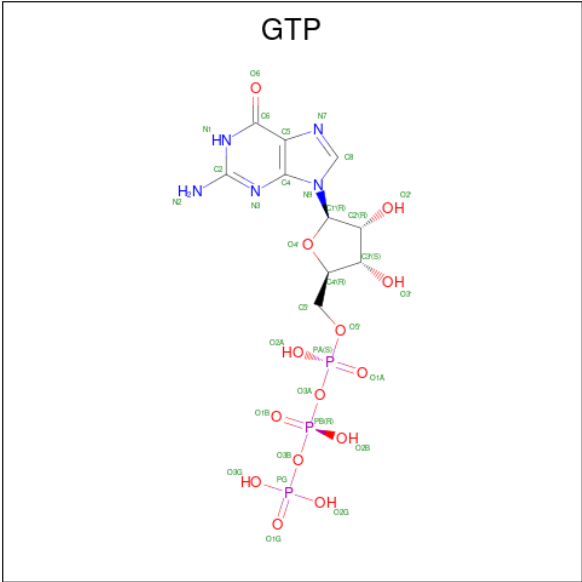
Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	246	Total	C	N	O		0	0
			1235	743	246	246			

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 17 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

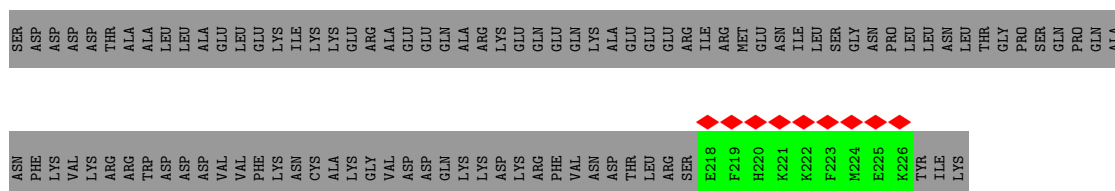


Mol	Chain	Residues	Atoms					AltConf
17	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

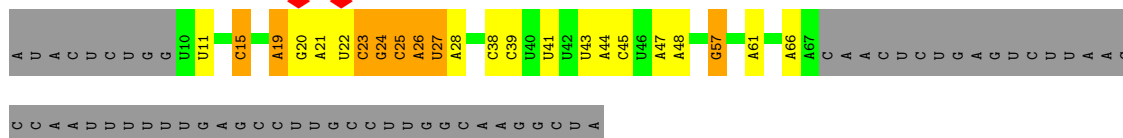
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	r	1	Total	Mg	0
			1	1	

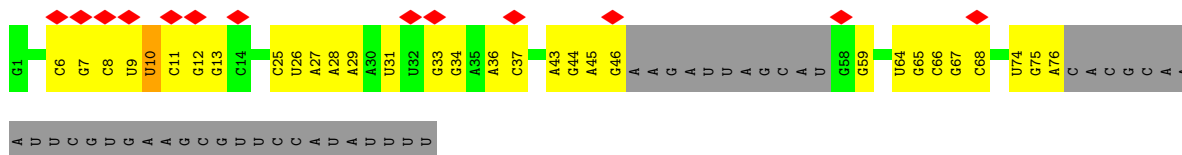
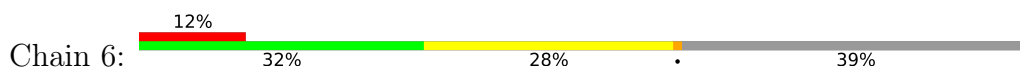




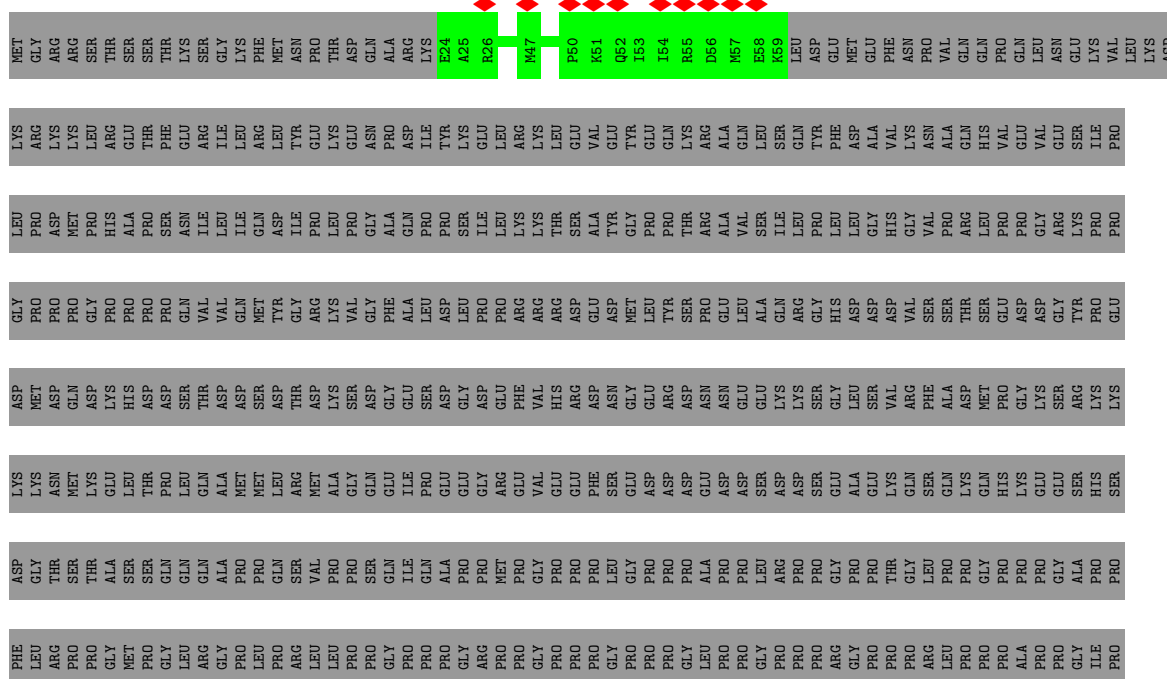
- Molecule 8: U5 small nuclear RNA

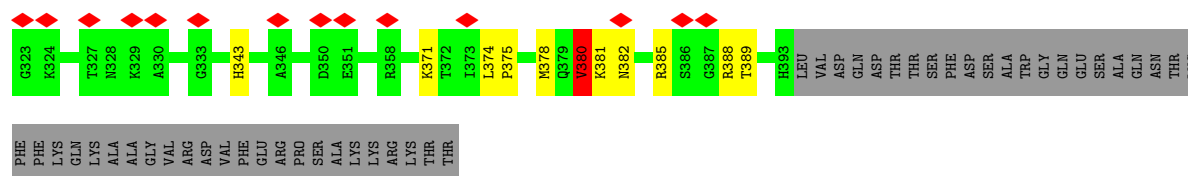


- Molecule 9: U6 small nuclear RNA

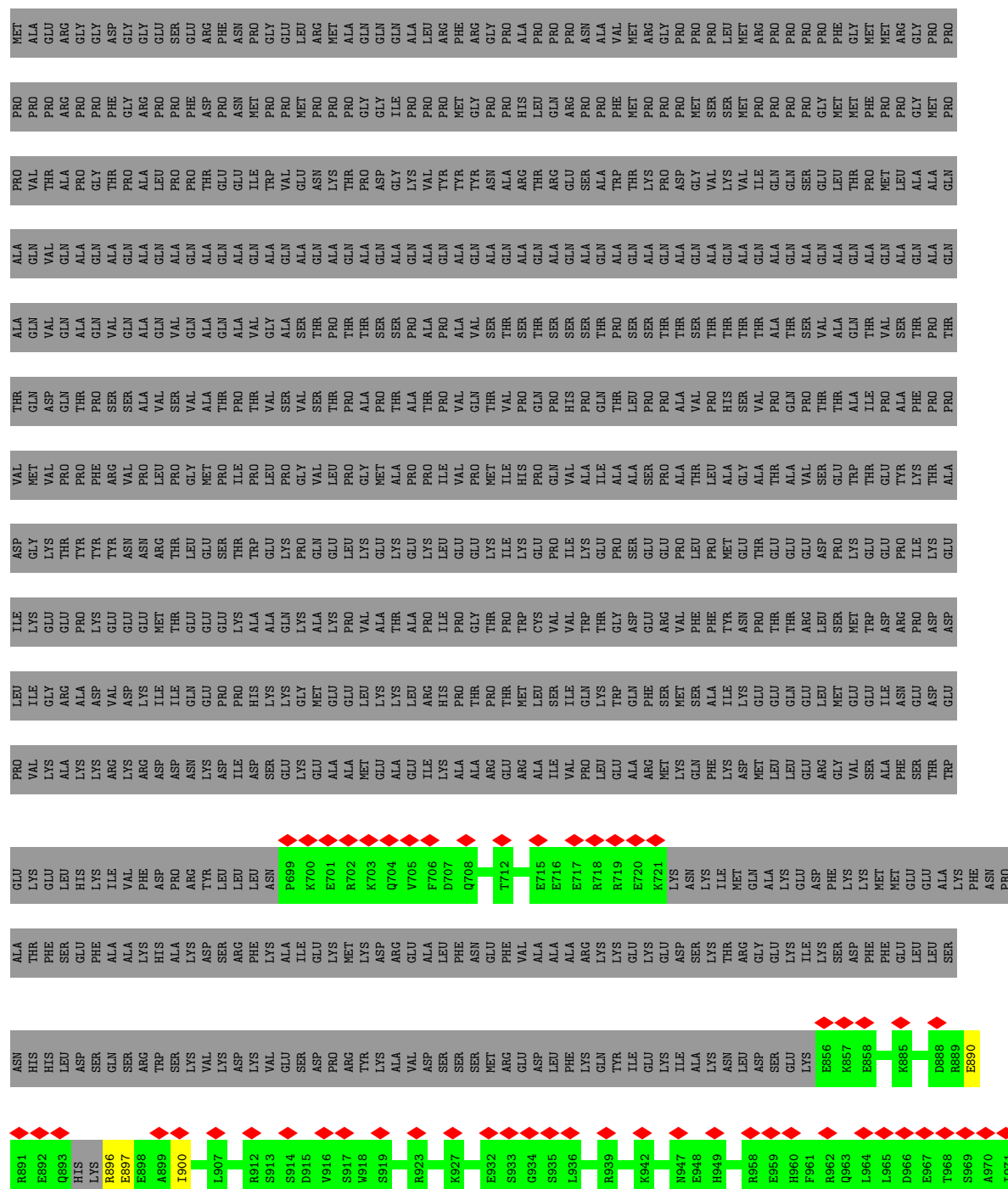


- Molecule 10: WW domain-binding protein 11





• Molecule 15: Transcription elongation regulator 1



K978	E979	Y980	K981	K982	I983	I984	K985	E986	D987	P988	R989	C990	I991	K992	F993	S994	S995	S996	D997	R998	K999	K1000	Q1001	R1002	E1003	E1006	Y1007	I1008	K1011	Y1012	I1013	T1014	A1015	K1016	A1017	D1018	F1019	R1020	T1021	L1022	L1023	K1024	E1025	T1026	K1027	F1028	I1029	T1030	Y1031	R1032	S1033	K1034	K1035	L1036	I1037	Q1038	E1039
S1040	D1041	Q1042	H1043	L1044	K1045	D1046	V1047	E1048	K1049	I1050	L1051	Q1052	N1053	D1054	K1055	R1056	Y1057	L1058	V1059	L1060	D1061	C1062	V1063	P1064	E1065	E1066	R1067	R1068	K1069	L1070	I1071	V1072	A1073	Y1074	V1075	D1076	D1077	L1078	D1079	R1080	ARG	GLY	PRO	PRO	PRO	PRO	THR	ALA	SER	GLU	PRO	THR	ARG	ARG	SER	THR	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	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: MG, IHP, GTP

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	Q	0.14	0/870	0.34	0/1208
2	I	0.16	0/1174	0.34	0/1616
3	A	0.17	0/10821	0.38	0/14985
4	r	0.19	1/5232 (0.0%)	0.41	3/7255 (0.0%)
5	N	0.09	0/296	0.22	0/410
6	q	0.17	0/533	0.32	0/727
7	R	0.04	0/44	0.12	0/60
8	5	0.16	0/1360	0.33	0/2113
9	6	0.12	0/1557	0.27	0/2423
10	X	0.08	0/182	0.20	0/254
11	v	0.09	0/273	0.17	0/379
12	G	0.23	0/1616	0.34	0/2258
13	Z	0.10	0/696	0.16	0/1083
14	K	0.30	0/813	0.46	0/1106
15	A4	0.09	0/1235	0.20	0/1725
All	All	0.17	1/26702 (0.0%)	0.36	3/37602 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	r	141	GLY	C-N	5.45	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	141	GLY	CA-C-N	-11.96	103.76	122.17
4	r	141	GLY	C-N-CA	-11.96	103.76	122.17
4	r	141	GLY	CA-C-O	-6.62	109.05	120.57

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	Q	850	0	574	2	0
2	I	1151	0	915	4	0
3	A	10522	0	7599	48	0
4	r	5120	0	3785	32	0
5	N	295	0	149	2	0
6	q	523	0	472	3	0
7	R	45	0	17	0	0
8	5	1220	0	618	36	0
9	6	1392	0	705	11	0
10	X	182	0	85	0	0
11	v	275	0	138	0	0
12	G	1604	0	795	13	0
13	Z	622	0	315	26	0
14	K	799	0	609	11	0
15	A4	1235	0	539	2	0
16	A	36	0	6	0	0
17	r	32	0	10	12	0
18	r	1	0	0	0	0
All	All	25904	0	17331	171	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 (171) 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)
4:r:140:HIS:CE1	4:r:230:ASP:CB	2.07	1.38
8:5:24:G:N1	8:5:57:G:N3	1.75	1.33
3:A:599:MET:HE3	13:Z:52:C:O2	1.31	1.29
8:5:24:G:C6	8:5:57:G:N3	2.05	1.22
4:r:141:GLY:O	4:r:228:PHE:CD2	1.97	1.18
12:G:381:HIS:CB	12:G:382:PRO:HD3	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:24:G:C6	8:5:57:G:C2	2.35	1.15
3:A:599:MET:HE1	13:Z:52:C:N3	1.68	1.09
8:5:24:G:N2	8:5:57:G:O2'	1.86	1.07
3:A:599:MET:HE3	13:Z:52:C:C2	1.93	1.02
8:5:24:G:N1	8:5:57:G:C4	2.26	1.02
8:5:24:G:H22	8:5:57:G:C1'	1.74	1.00
8:5:24:G:H22	8:5:57:G:H1'	1.25	1.00
4:r:259:LYS:CB	17:r:1500:GTP:N7	2.25	0.99
12:G:381:HIS:CB	12:G:382:PRO:CD	2.40	0.99
8:5:24:G:H22	8:5:57:G:C2'	1.76	0.98
8:5:19:A:C2	8:5:23:C:C5	2.51	0.98
4:r:142:LYS:HB2	17:r:1500:GTP:O1B	1.69	0.91
3:A:599:MET:CE	13:Z:52:C:C2	2.53	0.90
4:r:141:GLY:O	4:r:228:PHE:HD2	1.51	0.88
8:5:24:G:N2	8:5:57:G:H1'	1.88	0.88
8:5:24:G:C6	8:5:57:G:C4	2.60	0.88
3:A:599:MET:CE	13:Z:52:C:N3	2.36	0.87
8:5:24:G:H1	8:5:57:G:H1'	1.40	0.87
3:A:599:MET:CE	13:Z:52:C:O2	2.23	0.85
8:5:24:G:H1	8:5:57:G:C1'	1.91	0.83
4:r:140:HIS:ND1	4:r:230:ASP:CB	2.39	0.83
8:5:24:G:C2	8:5:57:G:N3	2.46	0.83
4:r:140:HIS:ND1	4:r:230:ASP:N	2.28	0.82
13:Z:52:C:C5	14:K:389:THR:CB	2.65	0.79
8:5:24:G:N2	8:5:57:G:C2'	2.42	0.79
8:5:24:G:N1	8:5:57:G:H1'	1.99	0.77
9:6:43:A:H61	13:Z:62:A:H61	1.33	0.76
15:A4:890:GLU:O	15:A4:897:GLU:N	2.21	0.74
3:A:663:ARG:NH1	9:6:64:U:OP2	2.21	0.74
8:5:24:G:C5	8:5:57:G:C2	2.76	0.74
12:G:381:HIS:CB	12:G:388:ALA:H	2.00	0.73
9:6:59:G:O6	9:6:76:A:N1	2.22	0.73
8:5:24:G:C5	8:5:57:G:N2	2.57	0.73
4:r:142:LYS:NZ	17:r:1500:GTP:O3G	2.20	0.73
3:A:824:PRO:O	3:A:933:ARG:NH1	2.22	0.72
9:6:34:G:OP2	9:6:34:G:N2	2.23	0.72
14:K:378:MET:HG2	14:K:381:LYS:HE3	1.72	0.70
3:A:964:ASP:O	3:A:1100:ARG:NH2	2.24	0.70
8:5:24:G:C2	8:5:57:G:H1'	2.26	0.70
4:r:259:LYS:CB	17:r:1500:GTP:C5	2.68	0.69
3:A:584:HIS:O	3:A:588:LEU:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:663:ARG:NH2	9:6:65:G:O6	2.26	0.69
4:r:311:SER:O	4:r:315:SER:N	2.26	0.69
8:5:19:A:N3	8:5:23:C:C5	2.61	0.69
17:r:1500:GTP:H3'	17:r:1500:GTP:N3	2.09	0.67
8:5:43:U:O2'	9:6:67:G:O6	2.09	0.67
3:A:658:ARG:NH2	9:6:66:C:OP2	2.27	0.67
12:G:195:LYS:N	12:G:490:ARG:O	2.27	0.67
4:r:208:HIS:O	4:r:212:SER:N	2.27	0.66
3:A:419:ARG:NH1	8:5:25:C:OP1	2.27	0.66
3:A:474:ARG:NH1	8:5:15:C:OP2	2.28	0.66
13:Z:75:U:H2'	13:Z:76:A:H8	1.59	0.66
4:r:140:HIS:HE1	4:r:230:ASP:CB	1.98	0.66
8:5:19:A:C2	8:5:23:C:H5	2.14	0.65
3:A:1127:GLY:O	3:A:1151:ARG:NH2	2.30	0.65
3:A:546:LEU:HD12	3:A:648:LEU:HD21	1.79	0.64
3:A:635:ARG:NH1	8:5:27:U:OP2	2.30	0.64
3:A:1628:ASP:N	3:A:1662:ILE:O	2.30	0.64
3:A:119:LEU:N	3:A:128:PHE:O	2.32	0.62
3:A:119:LEU:O	3:A:128:PHE:N	2.32	0.62
13:Z:77:G:H2'	13:Z:78:A:H8	1.64	0.62
4:r:718:PHE:O	4:r:723:ASP:N	2.33	0.62
8:5:19:A:N3	8:5:23:C:H5	1.96	0.61
8:5:24:G:O6	8:5:57:G:C4	2.52	0.61
12:G:195:LYS:O	12:G:490:ARG:N	2.34	0.61
4:r:142:LYS:NZ	17:r:1500:GTP:O3B	2.34	0.60
13:Z:67:C:H2'	13:Z:68:U:C6	2.37	0.59
5:N:98:HIS:CD2	13:Z:67:C:H4'	2.38	0.59
13:Z:74:G:H3'	13:Z:75:U:H5'	1.83	0.59
12:G:380:LEU:O	12:G:421:VAL:CB	2.52	0.57
3:A:152:ARG:NH1	3:A:616:PHE:O	2.37	0.57
4:r:686:THR:N	4:r:793:ASP:O	2.38	0.57
13:Z:55:A:H2'	13:Z:56:A:H8	1.68	0.57
13:Z:54:G:O2'	13:Z:55:A:H5''	2.03	0.56
13:Z:75:U:H2'	13:Z:76:A:C8	2.39	0.56
3:A:612:ILE:O	3:A:616:PHE:N	2.38	0.55
8:5:24:G:N2	8:5:57:G:C1'	2.51	0.55
8:5:47:A:O4'	14:K:388:ARG:NH1	2.39	0.55
3:A:1605:GLU:O	3:A:1634:SER:N	2.38	0.55
13:Z:66:C:O2'	13:Z:67:C:H5'	2.07	0.54
12:G:438:LEU:O	12:G:447:PHE:N	2.39	0.54
4:r:207:GLY:O	4:r:238:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:77:G:H2'	13:Z:78:A:C8	2.43	0.54
14:K:380:VAL:HG13	14:K:382:ASN:H	1.72	0.53
4:r:141:GLY:O	4:r:228:PHE:CE2	2.59	0.53
3:A:1623:ASN:OD1	3:A:1624:SER:N	2.42	0.53
3:A:613:TYR:O	3:A:617:ASN:N	2.40	0.53
2:I:29:ILE:HD11	2:I:71:LEU:CD1	2.38	0.52
4:r:350:ASN:O	4:r:354:ARG:N	2.41	0.52
14:K:371:LYS:HA	14:K:374:LEU:HD23	1.92	0.51
12:G:219:PHE:N	12:G:231:TRP:O	2.43	0.51
4:r:141:GLY:HA3	4:r:258:ASN:CB	2.40	0.51
3:A:191:ILE:O	3:A:191:ILE:HG22	2.11	0.50
3:A:957:GLN:O	3:A:961:ASN:N	2.43	0.50
8:5:44:A:OP1	9:6:67:G:N1	2.44	0.50
13:Z:61:A:H2'	13:Z:62:A:O4'	2.11	0.50
12:G:379:VAL:CB	12:G:419:LEU:CB	2.90	0.50
3:A:193:LEU:N	3:A:208:TYR:OH	2.45	0.49
4:r:142:LYS:NZ	17:r:1500:GTP:PG	2.85	0.49
3:A:267:LYS:HE2	3:A:459:LEU:HD11	1.95	0.49
13:Z:56:A:O2'	13:Z:57:C:H5'	2.12	0.49
8:5:19:A:C2	8:5:23:C:C6	2.98	0.49
13:Z:53:C:O2'	13:Z:54:G:H5'	2.12	0.49
4:r:311:SER:N	4:r:316:ILE:O	2.45	0.48
14:K:374:LEU:HB3	14:K:375:PRO:HD2	1.95	0.48
8:5:24:G:N1	8:5:57:G:C1'	2.64	0.48
13:Z:65:G:O2'	13:Z:66:C:H5'	2.14	0.48
3:A:382:GLU:O	3:A:384:VAL:N	2.46	0.47
3:A:692:ASP:O	3:A:696:MET:N	2.47	0.47
4:r:555:VAL:HG12	4:r:555:VAL:O	2.14	0.47
15:A4:896:ARG:O	15:A4:900:ILE:N	2.46	0.47
13:Z:70:G:C6	13:Z:71:C:H1'	2.50	0.47
3:A:897:GLU:O	3:A:908:VAL:N	2.45	0.47
3:A:1144:LYS:O	3:A:1148:ASN:ND2	2.47	0.47
4:r:589:LYS:N	4:r:659:VAL:O	2.45	0.47
3:A:1557:LEU:HD11	9:6:44:G:C4	2.50	0.46
4:r:140:HIS:ND1	4:r:230:ASP:CA	2.79	0.46
4:r:144:CYS:N	17:r:1500:GTP:O2A	2.35	0.46
14:K:380:VAL:O	14:K:385:ARG:HD3	2.15	0.46
17:r:1500:GTP:N3	17:r:1500:GTP:C3'	2.77	0.46
8:5:24:G:C8	8:5:26:A:N6	2.83	0.46
12:G:379:VAL:CB	12:G:419:LEU:C	2.89	0.46
12:G:382:PRO:HB2	12:G:383:ARG:H	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:58:ARG:NH2	1:Q:62:ASP:OD1	2.47	0.46
3:A:802:THR:O	3:A:805:GLU:N	2.49	0.45
3:A:1267:LEU:O	3:A:1271:MET:N	2.46	0.45
6:q:8:ASP:OD1	6:q:9:ARG:N	2.50	0.45
2:I:106:TYR:O	2:I:110:THR:N	2.49	0.44
8:5:24:G:O6	8:5:57:G:C2	2.64	0.44
3:A:147:MET:HE1	3:A:191:ILE:HD12	1.99	0.44
3:A:798:GLY:O	3:A:800:TYR:N	2.50	0.44
4:r:142:LYS:HZ3	17:r:1500:GTP:PG	2.36	0.44
4:r:838:ALA:O	4:r:869:TYR:N	2.50	0.43
4:r:275:TYR:HH	4:r:344:TRP:CD1	2.36	0.43
4:r:938:ARG:NH2	4:r:944:SER:O	2.52	0.43
6:q:34:GLN:NE2	14:K:343:HIS:O	2.51	0.43
12:G:381:HIS:CB	12:G:388:ALA:HB3	2.49	0.43
13:Z:61:A:H2'	13:Z:62:A:C8	2.54	0.43
3:A:802:THR:O	3:A:806:ALA:N	2.46	0.43
13:Z:52:C:H5	14:K:389:THR:CB	2.26	0.43
3:A:652:LEU:O	3:A:656:LEU:HD23	2.19	0.42
9:6:8:C:N4	9:6:9:U:O2	2.53	0.42
3:A:249:LEU:HD23	3:A:249:LEU:O	2.20	0.42
4:r:396:LEU:O	4:r:400:GLY:N	2.47	0.42
14:K:374:LEU:HD12	14:K:378:MET:SD	2.59	0.42
2:I:64:ASN:OD1	2:I:65:ILE:N	2.52	0.42
3:A:105:ASN:ND2	3:A:129:VAL:HG11	2.34	0.42
3:A:101:LYS:O	3:A:105:ASN:N	2.53	0.42
6:q:26:ASP:OD1	6:q:27:LEU:N	2.53	0.42
3:A:446:SER:O	3:A:450:LEU:HD23	2.20	0.42
8:5:19:A:C4	8:5:23:C:H5	2.37	0.42
14:K:304:ILE:O	14:K:308:ARG:N	2.52	0.42
5:N:98:HIS:HD2	13:Z:67:C:H4'	1.85	0.42
1:Q:3:LYS:N	1:Q:26:ASP:OD1	2.53	0.41
12:G:379:VAL:CB	12:G:419:LEU:O	2.68	0.41
2:I:29:ILE:O	2:I:32:SER:OG	2.35	0.41
3:A:1722:SER:O	3:A:1726:ILE:HD12	2.19	0.41
4:r:142:LYS:NZ	17:r:1500:GTP:O1B	2.53	0.41
3:A:1571:ILE:HA	3:A:1574:ILE:HG22	2.02	0.41
9:6:9:U:O2'	9:6:10:U:O4'	2.37	0.41
3:A:974:ASN:O	3:A:1178:TYR:N	2.54	0.40
17:r:1500:GTP:N3	17:r:1500:GTP:C2'	2.83	0.40
8:5:24:G:C4	8:5:57:G:N2	2.89	0.40
3:A:136:ILE:HG22	3:A:138:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:245:HIS:NE2	4:r:249:GLU:OE2	2.54	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	Q	136/144 (94%)	110 (81%)	26 (19%)	0	100	100
2	I	174/312 (56%)	152 (87%)	22 (13%)	0	100	100
3	A	1650/2335 (71%)	1408 (85%)	242 (15%)	0	100	100
4	r	842/972 (87%)	769 (91%)	73 (9%)	0	100	100
5	N	54/199 (27%)	53 (98%)	1 (2%)	0	100	100
6	q	71/73 (97%)	62 (87%)	9 (13%)	0	100	100
7	R	7/229 (3%)	7 (100%)	0	0	100	100
10	X	34/641 (5%)	33 (97%)	1 (3%)	0	100	100
11	v	51/536 (10%)	51 (100%)	0	0	100	100
12	G	318/514 (62%)	280 (88%)	36 (11%)	2 (1%)	21	55
14	K	121/439 (28%)	100 (83%)	20 (16%)	1 (1%)	16	50
15	A4	240/1077 (22%)	233 (97%)	7 (3%)	0	100	100
All	All	3698/7471 (50%)	3258 (88%)	437 (12%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	G	381	HIS
12	G	382	PRO
14	K	380	VAL

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	Q	42/130 (32%)	42 (100%)	0	100	100
2	I	70/293 (24%)	70 (100%)	0	100	100
3	A	544/2108 (26%)	544 (100%)	0	100	100
4	r	269/866 (31%)	268 (100%)	1 (0%)	84	83
5	N	5/181 (3%)	5 (100%)	0	100	100
6	q	43/66 (65%)	43 (100%)	0	100	100
10	X	1/554 (0%)	1 (100%)	0	100	100
12	G	13/441 (3%)	13 (100%)	0	100	100
14	K	44/395 (11%)	43 (98%)	1 (2%)	44	63
15	A4	3/938 (0%)	3 (100%)	0	100	100
All	All	1034/5972 (17%)	1032 (100%)	2 (0%)	85	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	r	140	HIS
14	K	380	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	326	HIS
3	A	439	GLN
3	A	495	GLN
3	A	815	HIS
3	A	884	HIS
3	A	1148	ASN
3	A	1546	ASN
4	r	175	GLN
6	q	34	GLN

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Mol	Chain	Res	Type
6	q	54	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	Z	28/230 (12%)	9 (32%)	0
8	5	57/116 (49%)	20 (35%)	1 (1%)
9	6	63/106 (59%)	20 (31%)	0
All	All	148/452 (32%)	49 (33%)	1 (0%)

All (49) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	5	11	U
8	5	15	C
8	5	19	A
8	5	20	G
8	5	21	A
8	5	22	U
8	5	23	C
8	5	24	G
8	5	25	C
8	5	26	A
8	5	27	U
8	5	28	A
8	5	38	C
8	5	39	C
8	5	41	U
8	5	45	C
8	5	48	A
8	5	57	G
8	5	61	A
8	5	66	A
9	6	6	C
9	6	7	G
9	6	10	U
9	6	11	C
9	6	12	G
9	6	13	G
9	6	25	C
9	6	26	U

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Mol	Chain	Res	Type
9	6	27	A
9	6	28	A
9	6	29	A
9	6	31	U
9	6	33	G
9	6	36	A
9	6	37	C
9	6	45	A
9	6	46	G
9	6	68	C
9	6	74	U
9	6	75	G
13	Z	51	U
13	Z	52	C
13	Z	53	C
13	Z	54	G
13	Z	55	A
13	Z	61	A
13	Z	63	G
13	Z	71	C
13	Z	75	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	5	26	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, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	GTP	r	1500	18	33,34,34	0.82	1 (3%)	50,54,54	0.75	1 (2%)
16	IHP	A	3001	-	36,36,36	1.49	6 (16%)	60,60,60	0.93	3 (5%)

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
17	GTP	r	1500	18	-	6/22/38/38	0/3/3/3
16	IHP	A	3001	-	-	8/30/54/54	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	3001	IHP	P2-O12	3.43	1.65	1.59
16	A	3001	IHP	P3-O13	3.17	1.65	1.59
16	A	3001	IHP	P4-O14	3.14	1.65	1.59
16	A	3001	IHP	P5-O15	3.14	1.65	1.59
16	A	3001	IHP	P1-O11	3.13	1.65	1.59
16	A	3001	IHP	P6-O16	2.96	1.64	1.59
17	r	1500	GTP	PA-O3A	2.74	1.62	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	r	1500	GTP	O2A-PA-O3A	3.36	116.36	107.27
16	A	3001	IHP	C5-C6-C1	2.32	115.51	110.43
16	A	3001	IHP	P6-O16-C6	-2.31	117.26	123.43
16	A	3001	IHP	P1-O11-C1	-2.30	117.30	123.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

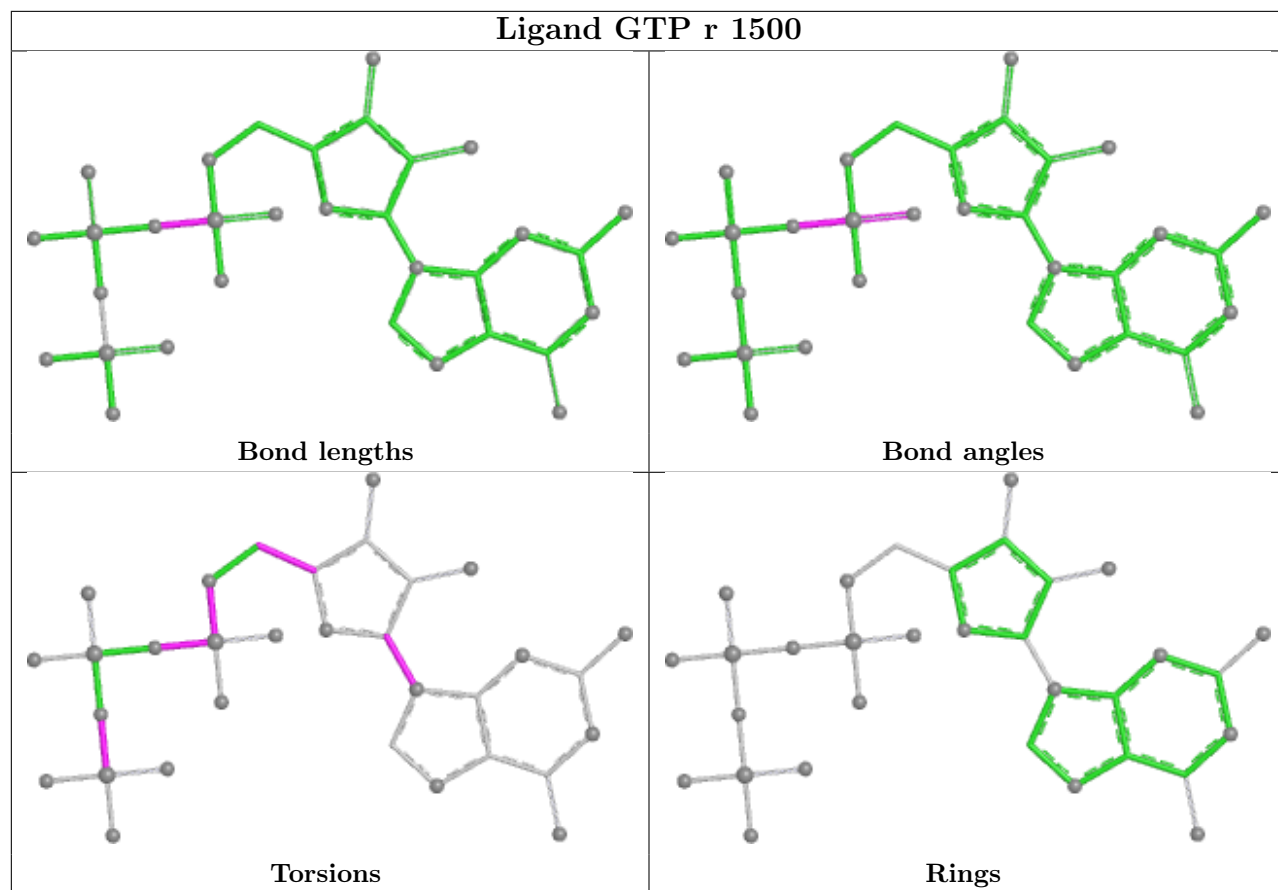
Mol	Chain	Res	Type	Atoms
16	A	3001	IHP	C1-C2-O12-P2
16	A	3001	IHP	C3-C2-O12-P2
17	r	1500	GTP	C5'-O5'-PA-O1A
17	r	1500	GTP	PB-O3B-PG-O2G
17	r	1500	GTP	C3'-C4'-C5'-O5'
17	r	1500	GTP	PB-O3A-PA-O2A
16	A	3001	IHP	C1-O11-P1-O31
16	A	3001	IHP	C1-O11-P1-O21
16	A	3001	IHP	C4-O14-P4-O24
17	r	1500	GTP	O4'-C4'-C5'-O5'
16	A	3001	IHP	C4-O14-P4-O34
16	A	3001	IHP	C6-O16-P6-O36
16	A	3001	IHP	C6-O16-P6-O46
17	r	1500	GTP	C2'-C1'-N9-C8

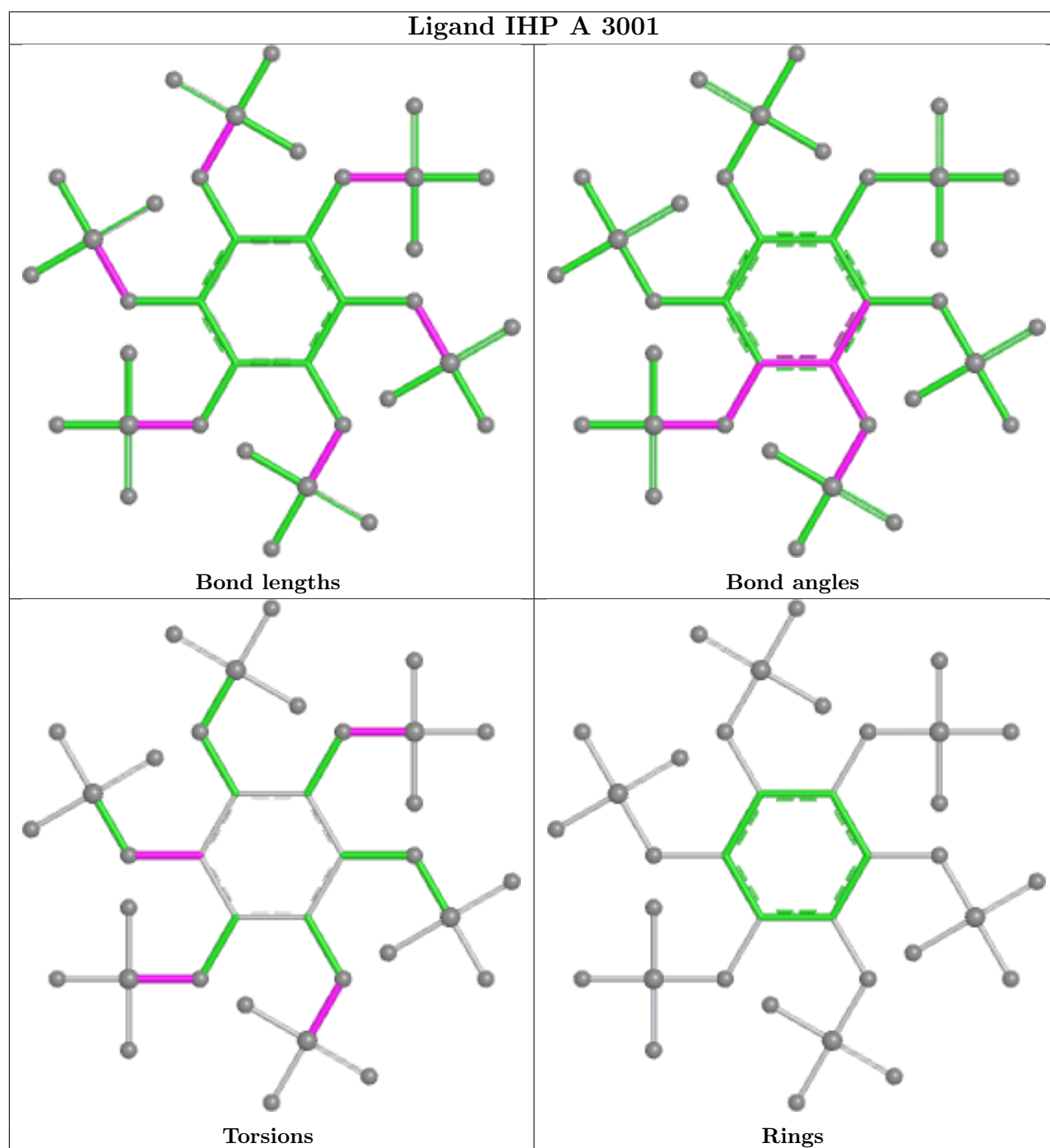
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	r	1500	GTP	12	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

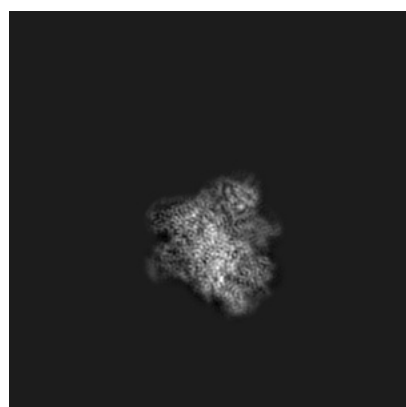
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11694. These allow visual inspection of the internal detail of the map and identification of artifacts.

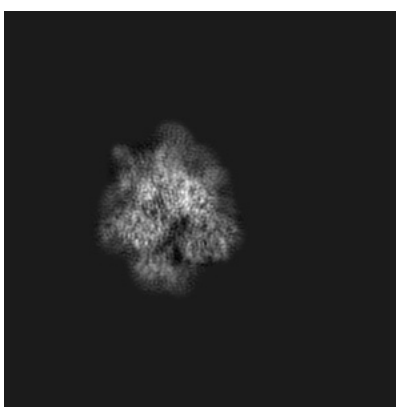
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

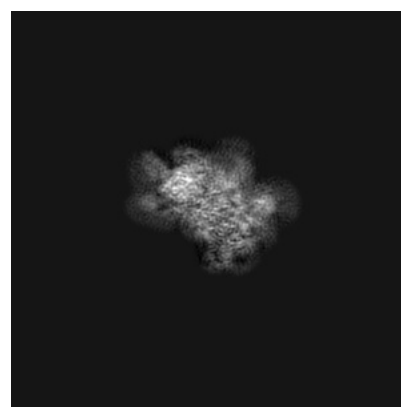
6.1.1 Primary map



X



Y

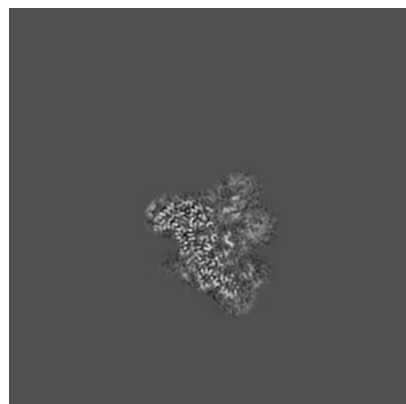


Z

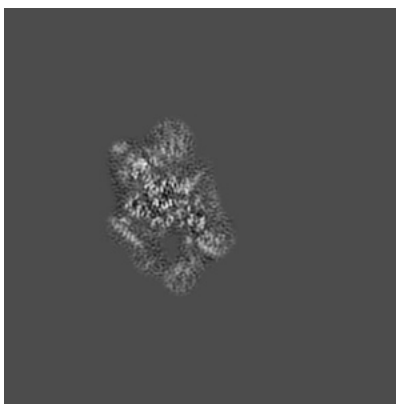
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

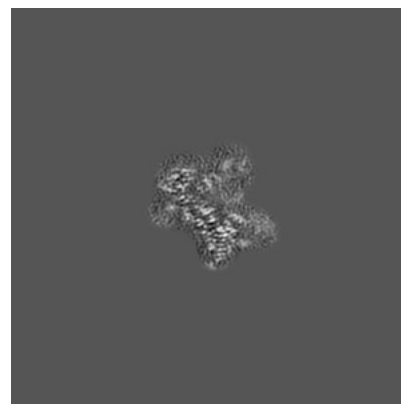
6.2.1 Primary map



X Index: 192



Y Index: 192

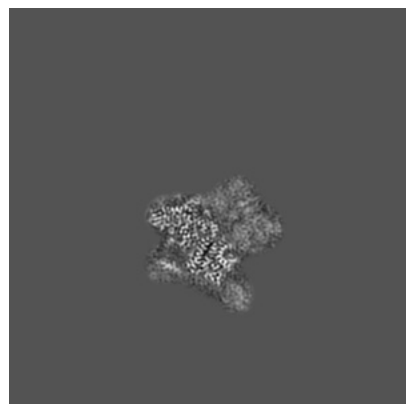


Z Index: 192

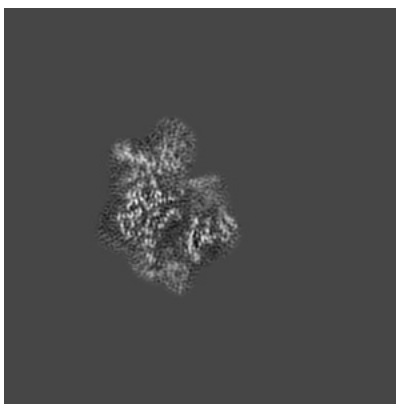
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

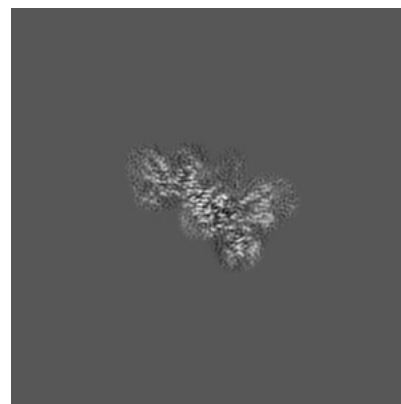
6.3.1 Primary map



X Index: 203



Y Index: 201

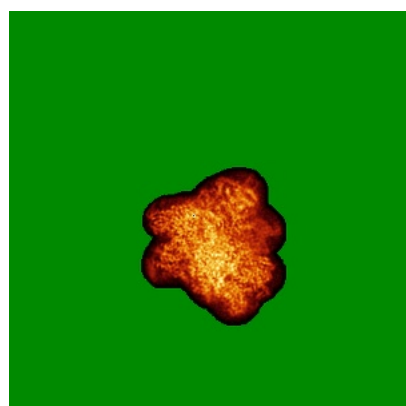


Z Index: 149

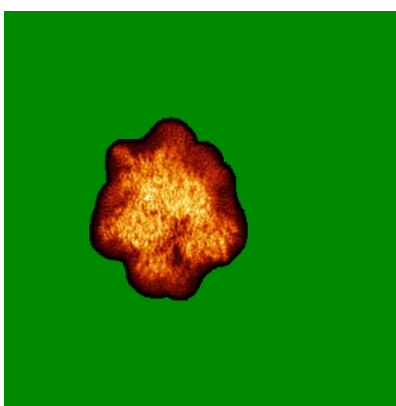
The images above show the largest variance slices of the map in three orthogonal directions.

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

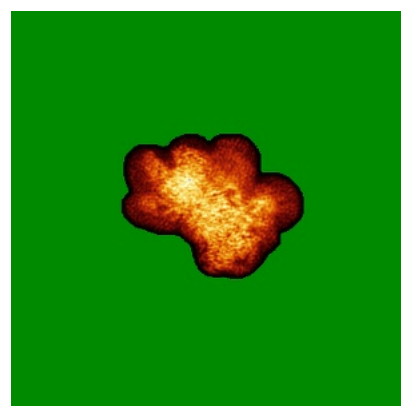
6.4.1 Primary map



X



Y

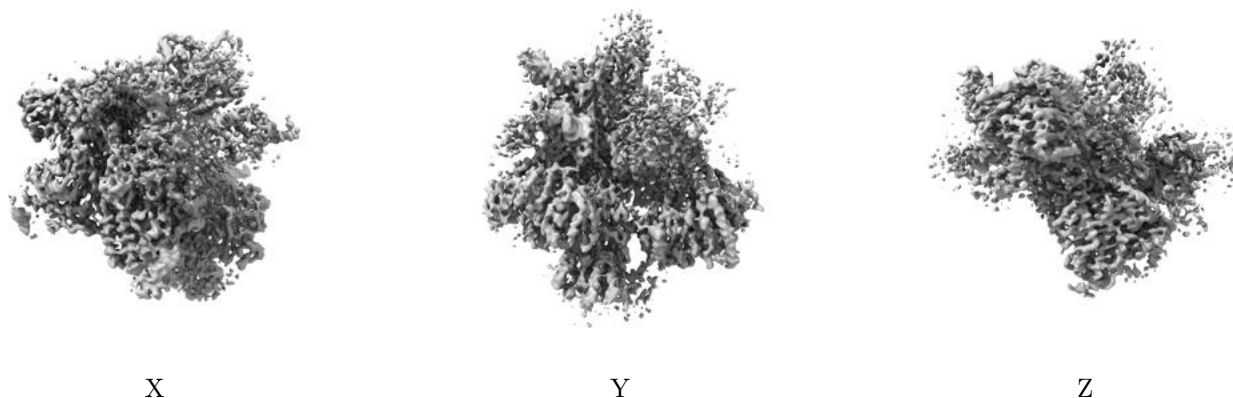


Z

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 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

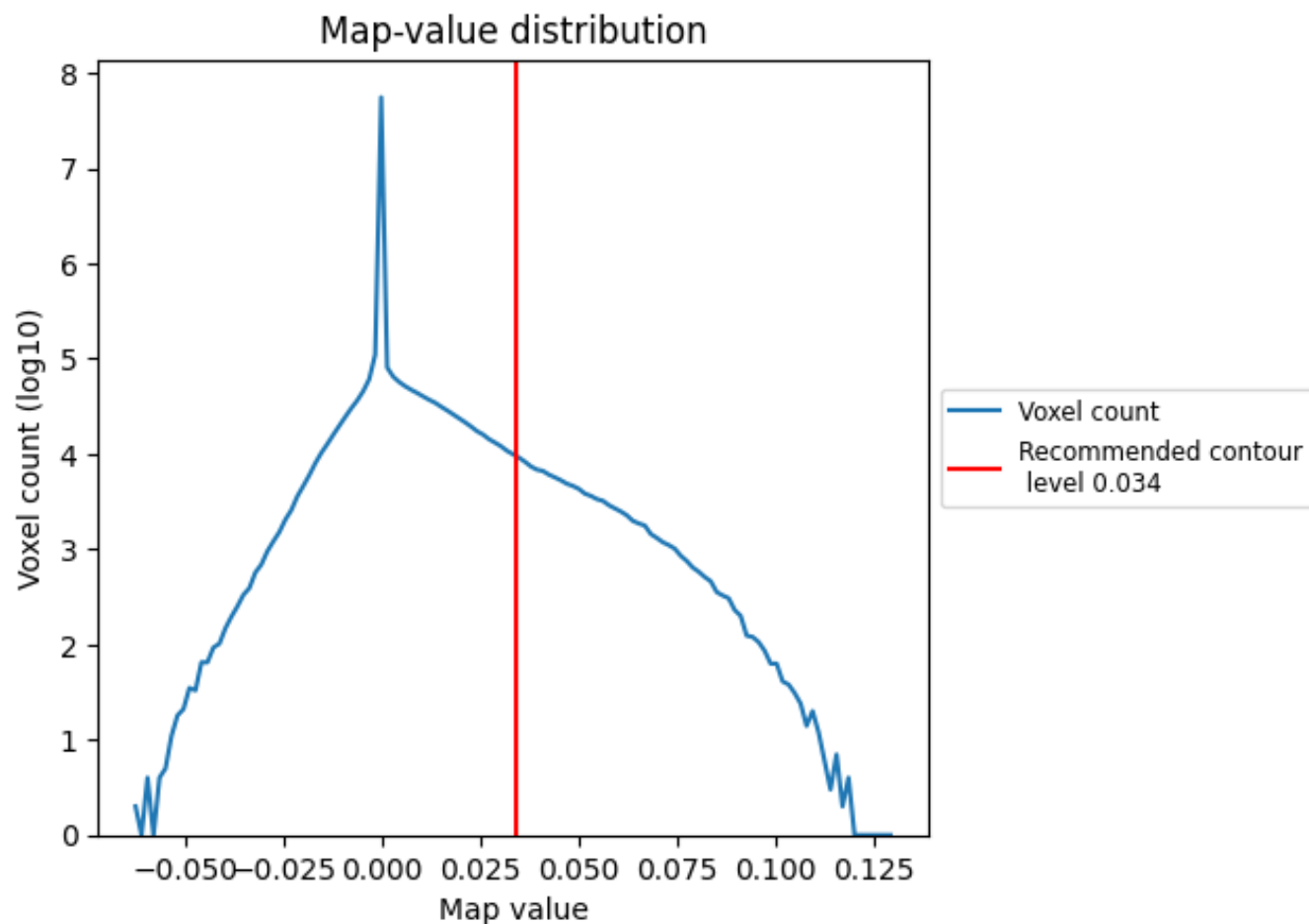
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

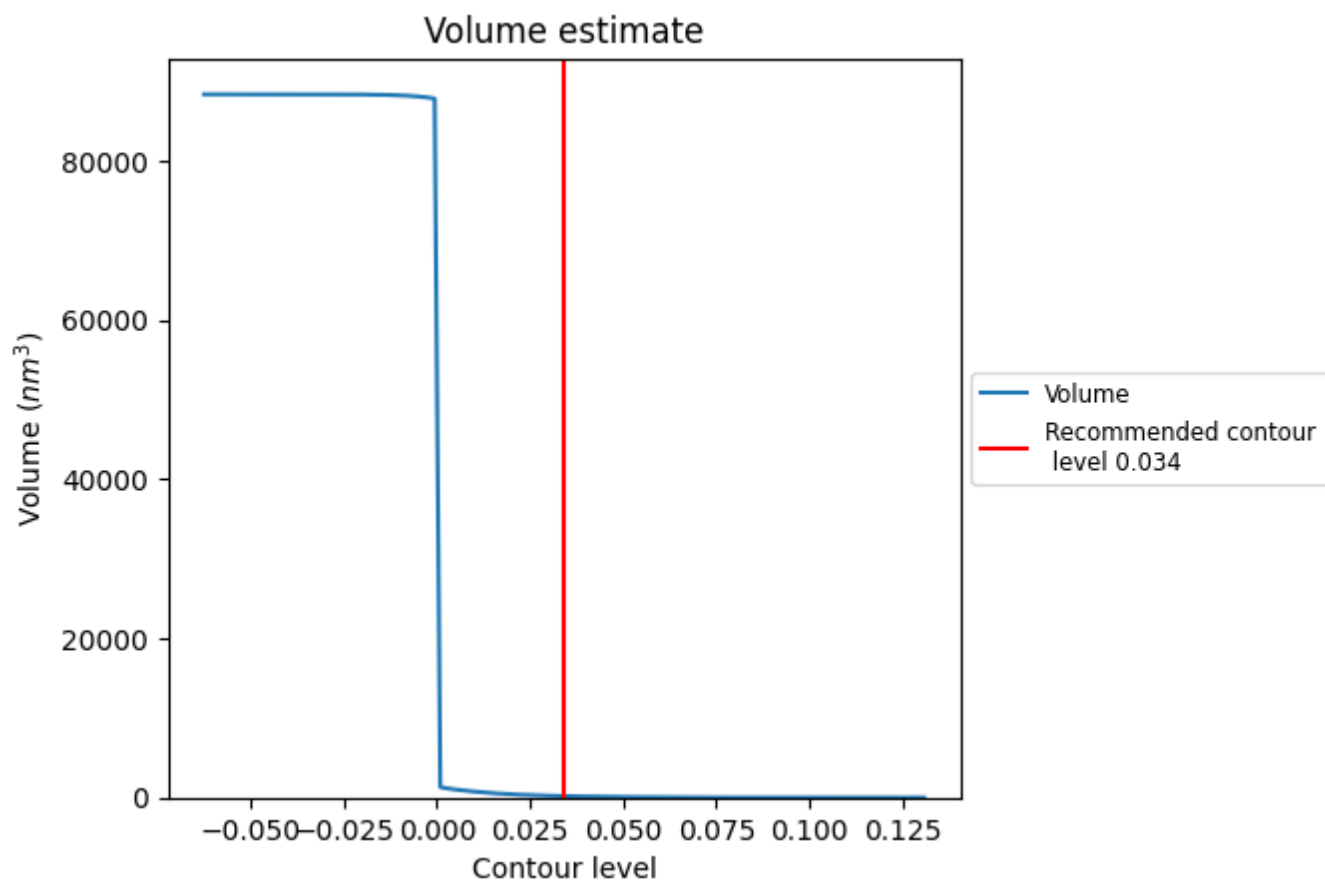
This section contains the results of statistical analysis of the map.

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.

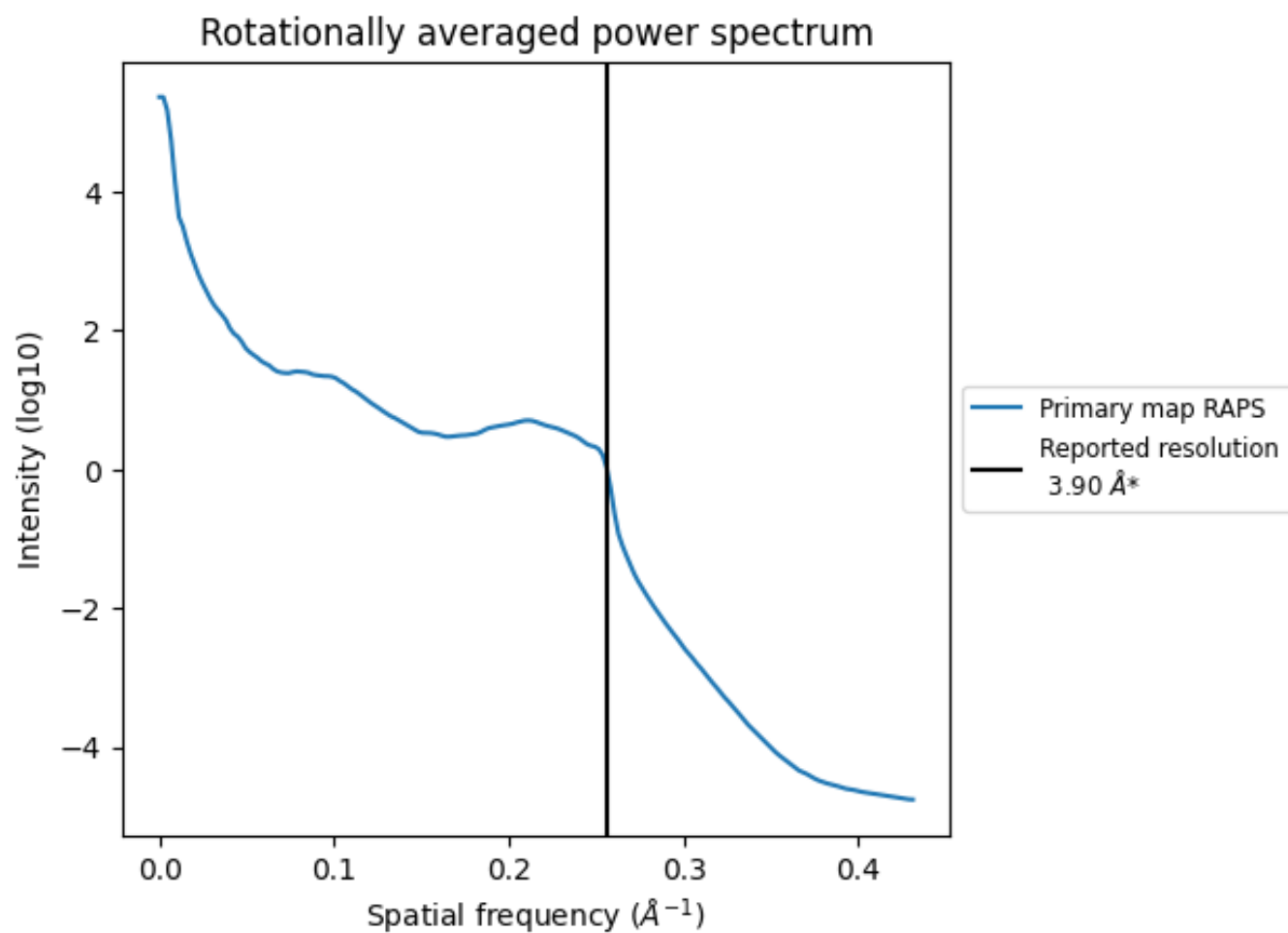
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm³; this corresponds to an approximate mass of 165 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 0.256 Å⁻¹

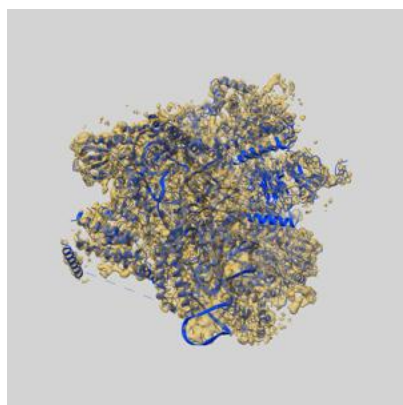
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

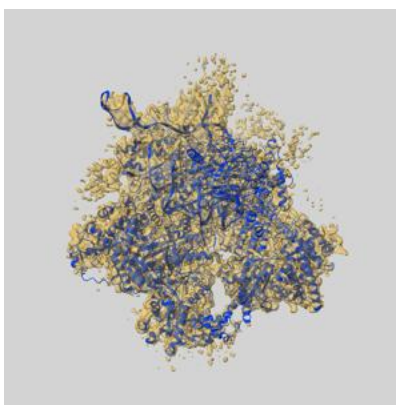
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11694 and PDB model 7ABF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

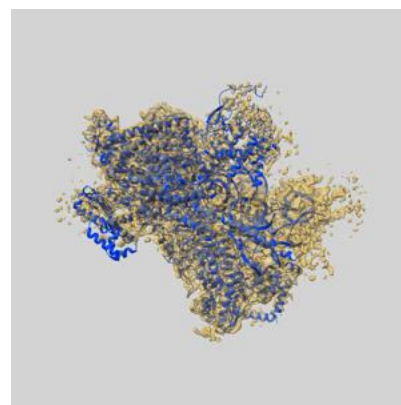
9.1 Map-model overlay [i](#)



X



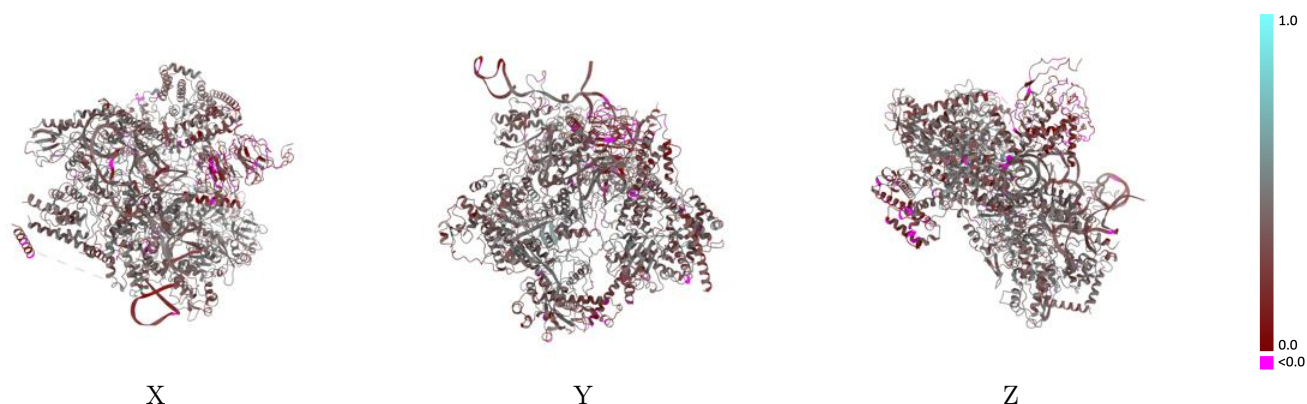
Y



Z

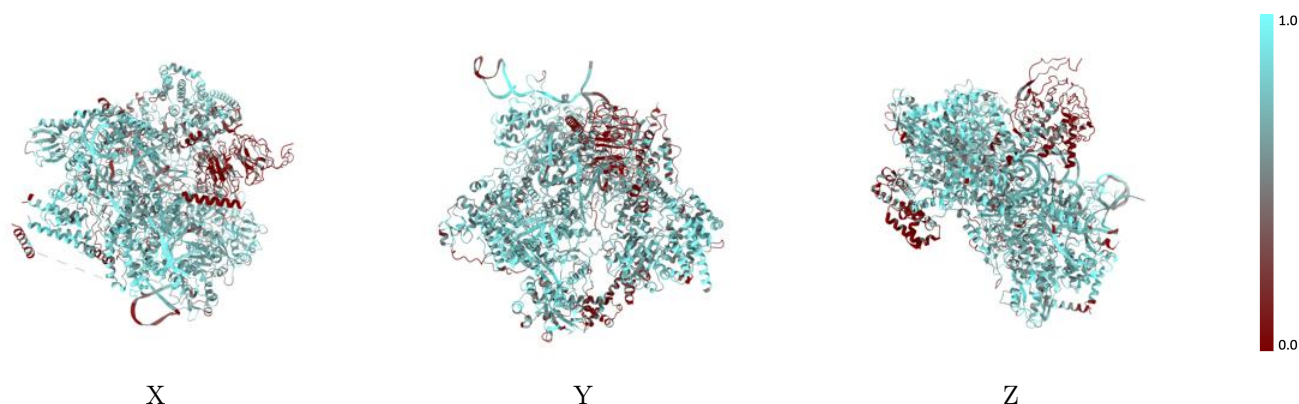
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



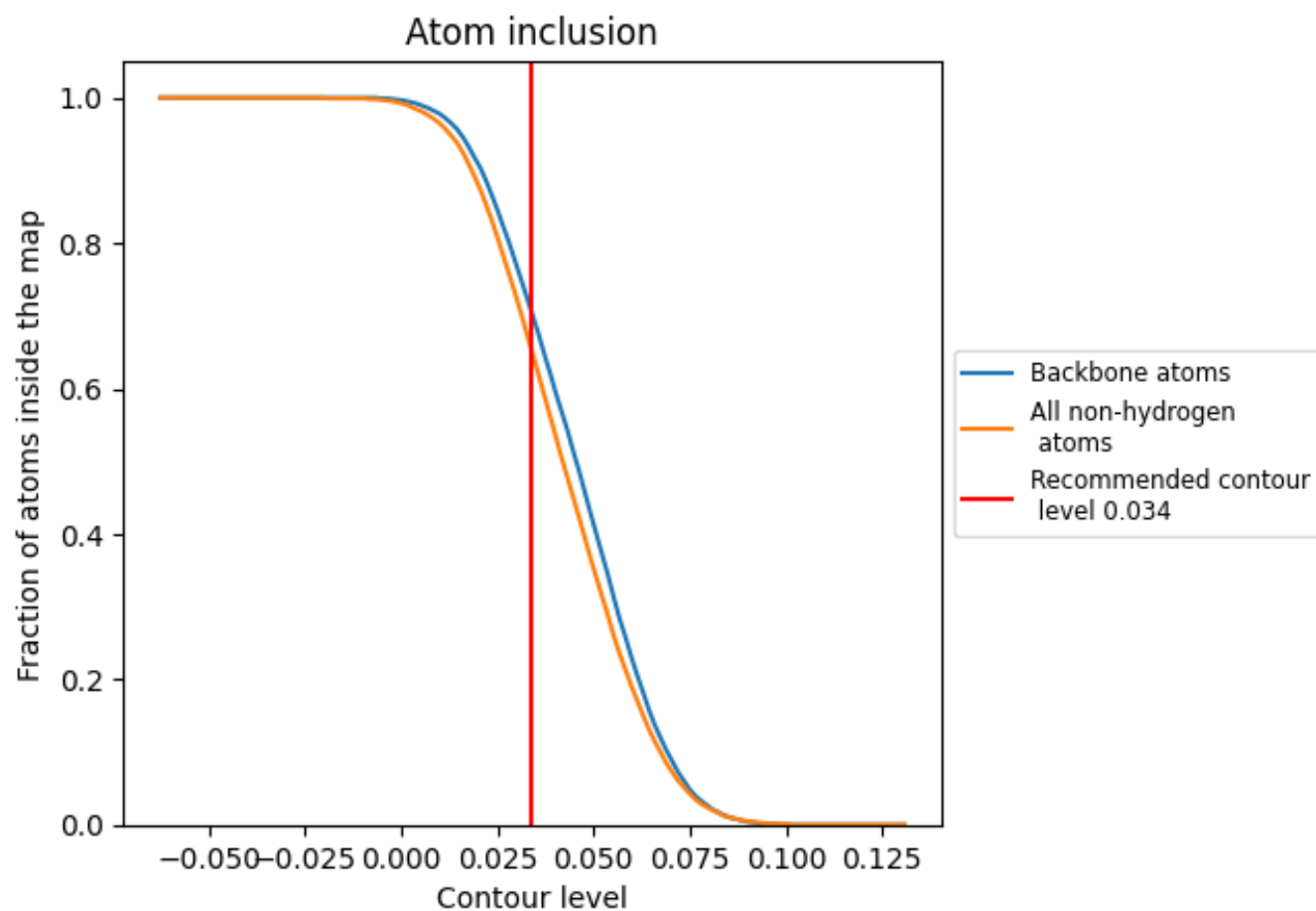
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.3740
5	 0.8010	 0.3930
6	 0.6690	 0.3050
A	 0.6870	 0.3950
A4	 0.3850	 0.2490
G	 0.1800	 0.2200
I	 0.7230	 0.3990
K	 0.5910	 0.3740
N	 0.7520	 0.4090
Q	 0.7550	 0.3810
R	 0.1560	 0.3850
X	 0.6100	 0.3690
Z	 0.7520	 0.3830
q	 0.6720	 0.4560
r	 0.7190	 0.4120
v	 0.4660	 0.2590

