



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:43 pm BST

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](mailto: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>.

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

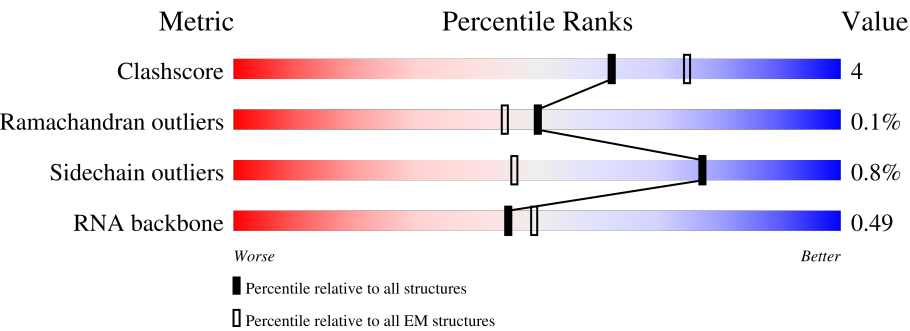
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 3.90 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	<div><div>8%</div><div>93%</div><div>.</div><div>.</div></div>
2	I	312	<div><div>5%</div><div>54%</div><div>.</div><div>44%</div></div>
3	A	2335	<div><div>10%</div><div>68%</div><div>.</div><div>29%</div></div>
4	r	972	<div><div>8%</div><div>87%</div><div>13%</div></div>
5	N	199	<div><div>.</div><div>28%</div><div>.</div><div>72%</div></div>
6	q	73	<div><div>7%</div><div>100%</div></div>
7	R	229	<div><div>.</div><div>96%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
8	5	116	
9	6	106	
10	X	641	
11	v	536	
12	G	514	
13	Z	230	
14	K	439	
15	A4	1077	

## 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		

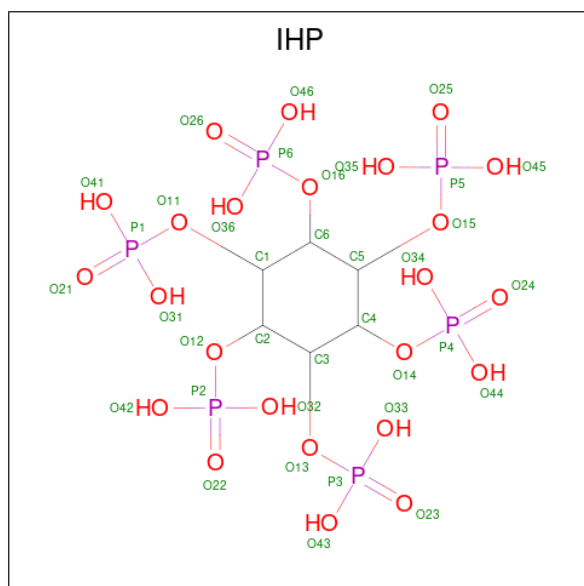
- Molecule 14 is a protein called Microfibrillar-associated protein 1.

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.

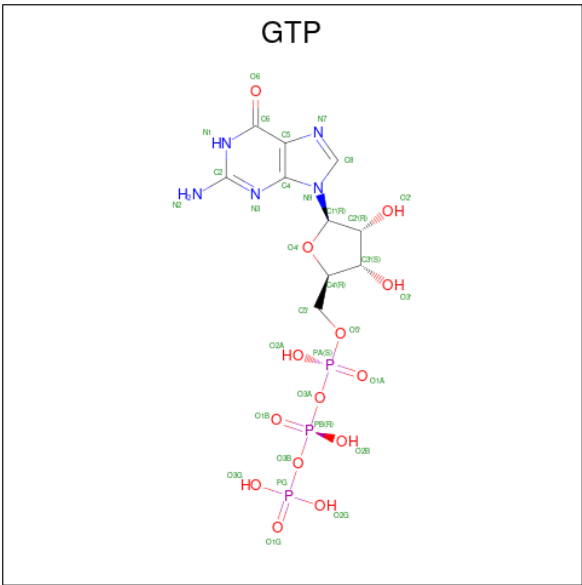
Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	246	Total	C	N	O		0	0
			1235	743	246	246			

- 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:  $C_{10}H_{16}N_5O_{14}P_3$ ).



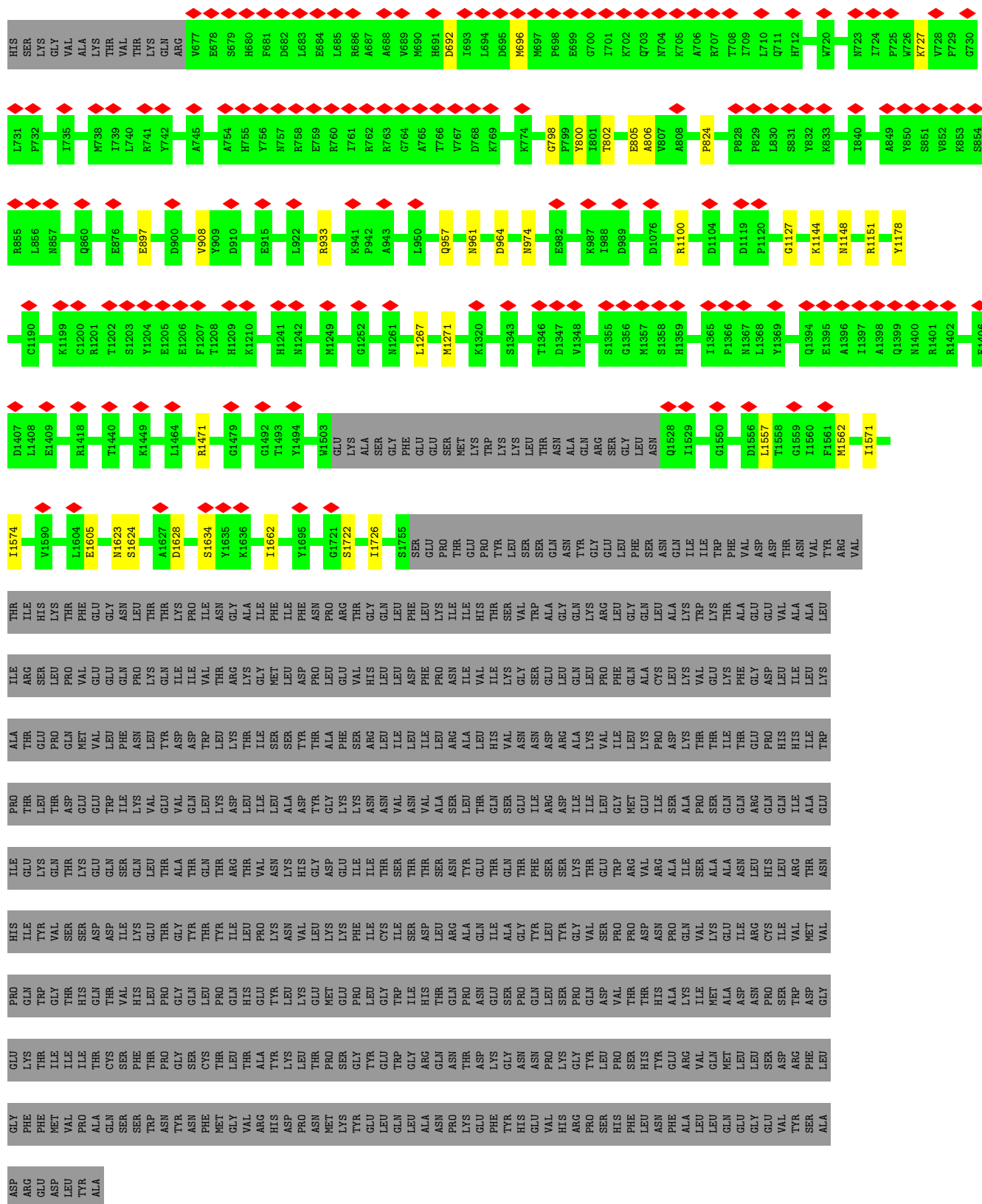
Mol	Chain	Residues	Atoms					AltConf
17	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

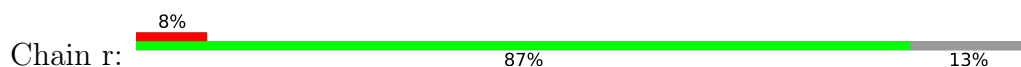
Mol	Chain	Residues	Atoms		AltConf
18	r	1	Total	Mg	0
			1	1	



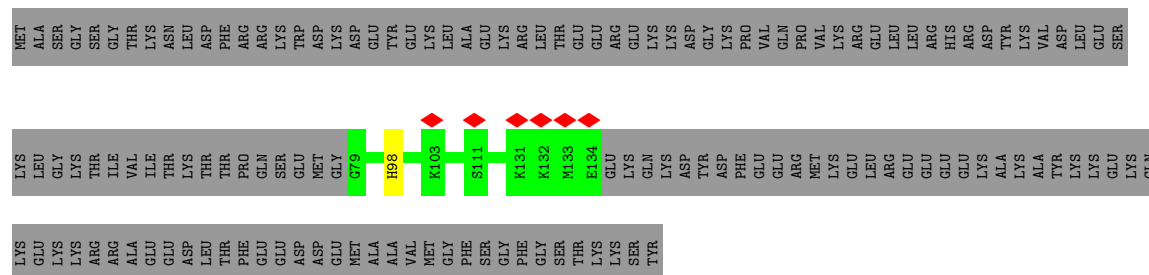




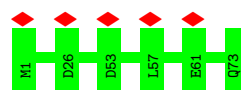
• Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component



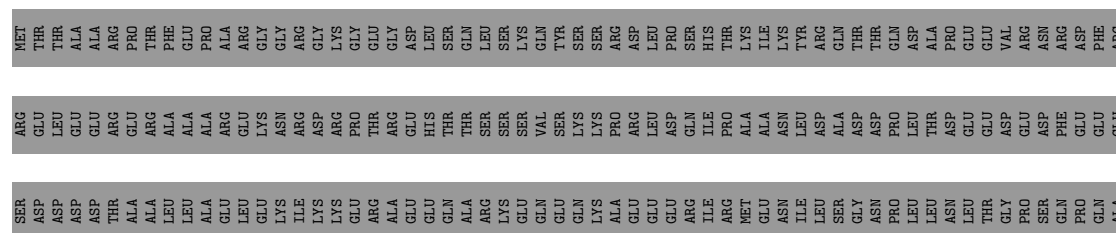
- Molecule 5: Zinc finger matrin-type protein 2

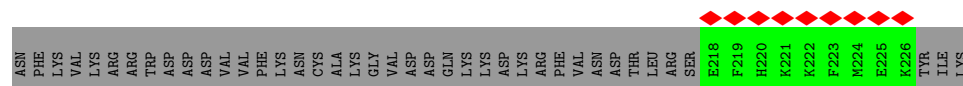


- Molecule 6: Ubiquitin-like protein 5

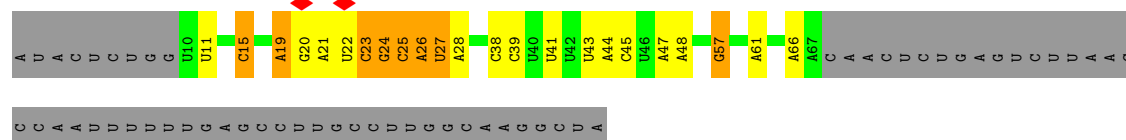
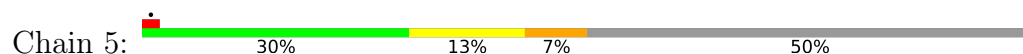


- Molecule 7: Spliceosome-associated protein CWC15 homolog

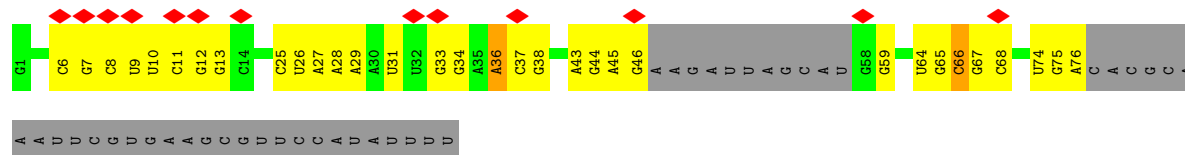
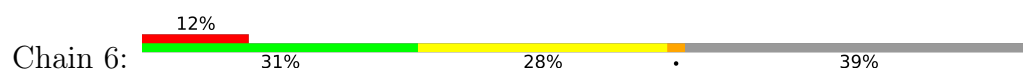




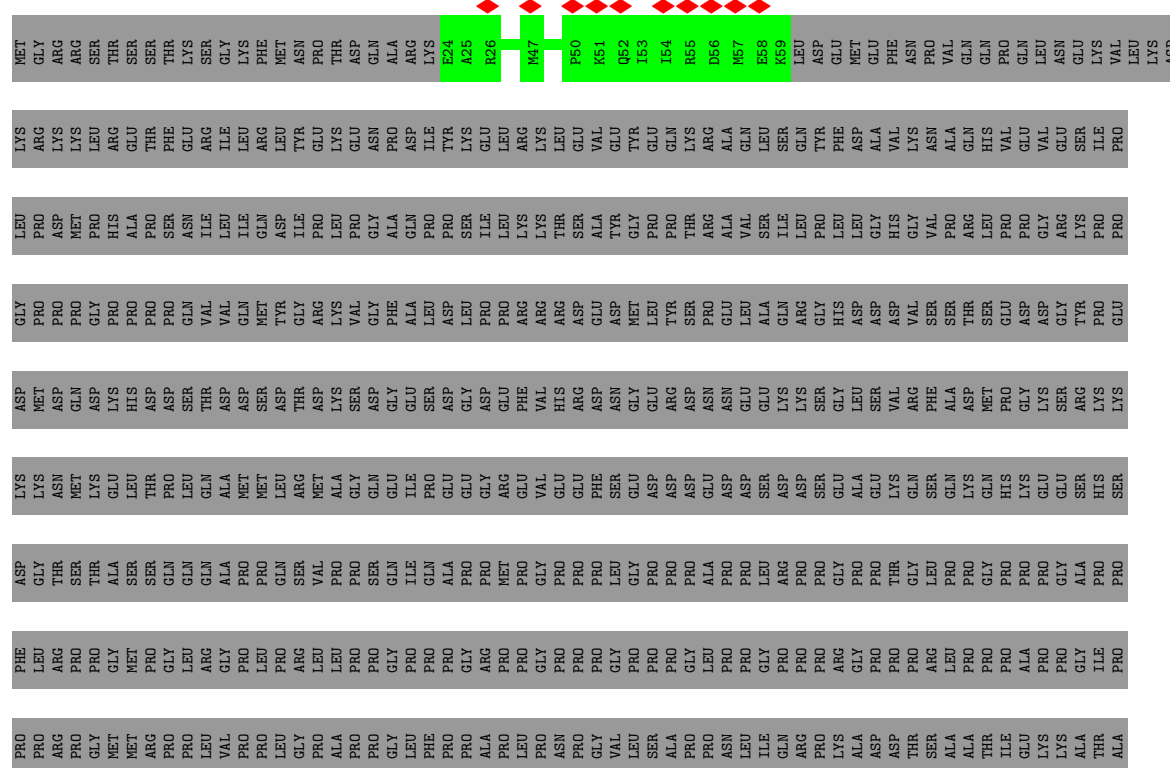
• Molecule 8: U5 small nuclear RNA



• Molecule 9: U6 small nuclear RNA



• Molecule 10: WW domain-binding protein 11



THR	ILE	SER	ALA	LYS	PRO	GLN	THR	THR	ASN	PRO	PRO	LYS	LYS	ALA	ALA	GLU	THR	THR	ARG	PHE	VAL	PRO	THR	THR	ALA	ALA	LEU	ARG	VAL	ARG	GLU	LYS	GLY	THR	THR	ALA	ALA	ALA	PRO	GLN	ARG	LYS	LYS	SER	SER	ASP	ASP	GLY	LEU	PRO	LYS	SER	GLY	PRO	SER	SER	PRO	VAL	PRO
VAL	SER	VAL	GLN	THR	LYS	ASP	VAL	TYR	GLU	ALA	ALA	PHE	MET	LYS	GLU	MET	GLY	GLY	LEU	LEU																																							

- Molecule 11: SNW domain-containing protein 1



NET	ALA	LEU	THR	SER	PHE	LEU	PRO	ALA	THR	GLN	LEU	SER	GLN	ASP	GLN	LEU	GLU	ALA	ALA	ARG	SER	GLN	ARG	SER	GLN	ARG	GLN	THR	SER	LEU	VAL	SER	SER	ARG	ARG	GLU	PRO	PRO	PRO	ASP	LEU	LEU	GLU	ASP	PHE	GLY	GLY	ASP
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GLY	GLY	GLY	PRO	PHO	GLU	ILE	HIS	VAL	ALA	ALA	GLN	TYR	PRO	LEU	ASP	MET	GLY	ARG	LYS	LYS	MET	MET	SER	ASN	ALA	LEU	ALA	ILE	GLN	VAL	ASP	SER	SER	GLY	GLY	LYS	LYS	TYR	ASP	ASP	ILE	ALA	ALA	ARG	GLN	GLY	GLN	GLY	SER	SER	LYS	ASP	VAL	VAL	ILE	ILE	TYR	SER	TYR	THR	ASP	LEU	VAL
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PRO	LYS	GLY	VAL	MET	ASN	ALA	ASP	ASP	PRO	PRO	LEU	GLN	ARG	PRO	ASP	EL37	EL38	AI39	I140	I141	E142	I143	I144	K146	I147	R148	V149	A150	L151	E152	K153	S154	V155	S156	Q157	K158	V159	ALA	ALA	ALA	ALA	PRO	PRO	VAL	ARG	ALA	ALA	ASP	LYS	LEU	ALA	ALA	PRO	ALA	GLN	TYR	ILE	ILE	ARG	ARG	TYR	TYR
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PRO	SER	GLN	GLN	GLY	VAL	ALA	PHE	ASN	SER	GLY	ALA	LYS	GLN	ARG	ILE	ARG	MET	VAL	GLU	MET	GLN	LYS	ASP	PRO	MET	LYS	GLY	ILE	ASN	LYS	ILE	PRO	ARG	PHE	LYS	ILE	ILE	ASN	LYS	LYS	ILE	PRO	PRO	ARG	GLY	PRO	PRO	SER	PRO	PRO	ALA	ALA	PRO	VAL	MET	HIS	LYS	THR	THR	VAL	LYS
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GLU	GLN	GLN	GLU	TRP	LYS	ILE	PRO	PRO	CYS	CYS	ILE	SER	ASN	LYS	ASN	ALA	ALA	ASP	ASP	ARG	LEU	LEU	GLN	THR	VAL	HIS	ILE	ASN	E282	E283	E284	E285	E312	E313	GLN	GLN	LYS	GLU	GLU	LYS	GLY	GLU	GLU	GLU	LYS	LEU	LEU
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GLU	MET	ALA	GLN	LYS	ALA	ARG	GLU	ARG	ARG	ARG	ALA	GLY	ILE	LYS	LYS	HIS	VAL	GLU	LYS	GLU	GLY	GLY	GLU	ALA	ALA	ARG	ARG	GLU	GLU	ASP	ASP	ILE	ARG	HIS	ASP	ASP	ARG	ARG	ARG	LYS	GLU	GLU	ARG	GLN	HIS	ASP	ASP	ASN	ALA	ALA	PRO	LYS	ASP	LYS	ARG	ARG	ARG	LYS	LYS	LEU	GLN	ARG	ASN	ASN	GLU	ASN
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ARG ASP  
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GLU  
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ASP  
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GLU  
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VAL  
TYR  
ASP  
GLN  
ALA  
TRP  
ARG  
GLY  
LYS  
ASP  
MET  
ALA

SER	ILE	TYR	ARG	PRO	SER	LYS	ASN	LEU	ASP	LYS	ASP	MET	TYR	GLY	ASP	ASP	LEU	GLU	ALA	ILE	ARG	LYS	THR	ASN	ARG	PHE	VAL	PRO	PRO	ASP	LYS	LYS	GLU	GLU	PHE	SER	GLY	SER	ASP	ARG	ARG	GLN	ARG	GLY	ARG	GLU	GLY	PRO	PRO	VAL	Gln	PHE	GLU	ASP	PRO	PHE	GLY	ASP	LYS	PHE	LEU	ASP
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GLU  
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ASP  
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HIS  
GLU  
GLY  
LYS  
LYS  
ARG  
LYS  
GLU

- Molecule 12: Pleiotropic regulator 1



MET	VAL	GLU	GLU	GLN	LYS	HIS	SER	VAL	HIS	THR	LEU	VAL	PHE	ARG	SER	LEU	LYS	ARG	THR	HIS	ASP	MET	PHE	VAL	ALA	ASN	ASP	GLY	LYS	PRO	VAL	PRO	LEU	ASP	GLU	GLU	SER	LYS	HIS	LYS	ARG	LYS	MET	ALA	ILE	TYR	GLY	PRO	VAL	LEU	HIS	MET	PRO	THR
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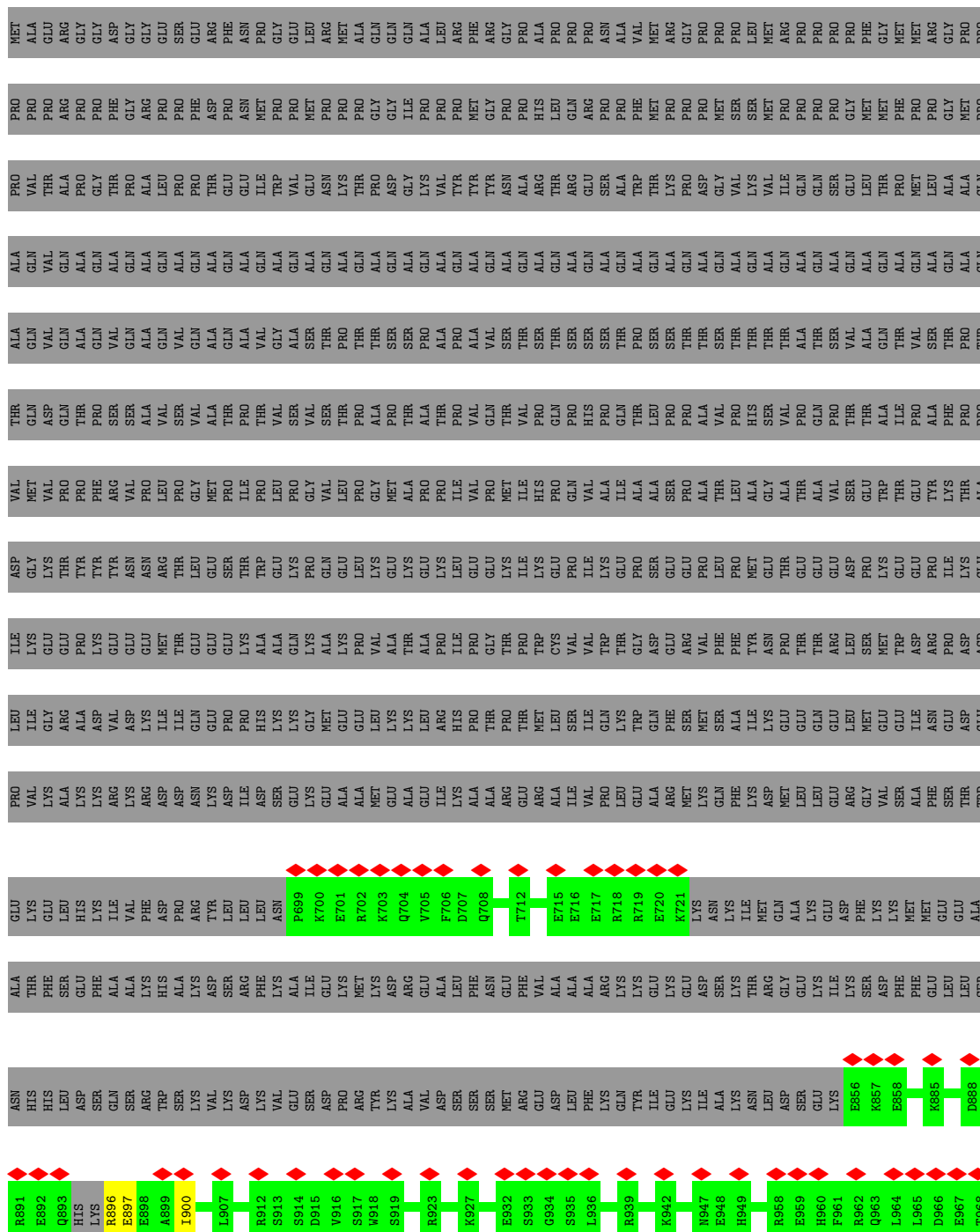
SER	LYS	GLU	ASN	LEU	GLY	LYS	GLY	PRO	PRO	ASN	ALA	THR	SER	TYR	VAL	HIS	LYS	GLN	TYR	PRO	ALA	ASN	GLN	GLY	PHE	VAL	VAL	GLY	THR	HIS	PRO	PRO	TYR	PRO	PRO	GLY	GLY	VAL	ALA	LEU	THR	ALA	ASP	THR	LYS	ILE	GLN	ARG	MET	PRO	SER	GLU
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SER	ALA	ALA	GLN	SER	LEU	ALA	VAL	ALA	ALA	LEU	PRO	PRO	GLN	THR	LYS	ALA	ASP	ALA	ALA	ASN	ARG	ARG	THR	ALA	ALA	PRO	PRO	GLY	SER	SER	GLY	SER	GLU	TYR	ARG	HIS	PRO	GLY	ALA	ALA	SER	SER	ASP	ARG	PRO	GLN	PRO	THR	THR	ALA	MET	ASN	SER	SER	ILE	VAL	LEU	MET	MET	GLU	THR	THR	ASN	LYS	ASN	ALA	ALA	LEU	MET	LEU	ALA	ALA	VAL
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K181	A182	P183	T184	M185	P186	K187	P188	Q189	W190	H191	P192	P193	W194	K195	L196	Y197	R198	S201	G202	H203	L204	G205	W206	V207	R208	C209	I210	E213	P214	G215	M216	Q217	W218	F219	V220	T221	G222	S223	A224	D225	R226	T227	T228	K229	I230	W231	D232	L233	A234	S235	G236	K237	L238	K239	L240	S241	I242
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- 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 (Å)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, IHP, MG

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	0.25	0/870	0.46	0/1208
2	I	0.28	0/1174	0.50	0/1616
3	A	0.27	0/10821	0.49	1/14985 (0.0%)
4	r	0.28	0/5232	0.51	2/7255 (0.0%)
5	N	0.22	0/296	0.35	0/410
6	q	0.27	0/533	0.51	0/727
7	R	0.21	0/44	0.28	0/60
8	5	0.30	0/1360	0.85	0/2113
9	6	0.24	0/1557	0.80	1/2423 (0.0%)
10	X	0.23	0/182	0.31	0/254
11	v	0.23	0/273	0.29	0/379
12	G	0.27	0/1616	0.50	0/2258
13	Z	0.20	0/696	0.71	0/1083
14	K	0.31	0/813	0.49	0/1106
15	A4	0.22	0/1235	0.33	0/1725
All	All	0.27	0/26702	0.55	4/37602 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	141	GLY	C-N-CA	-7.18	103.76	121.70
4	r	141	GLY	CA-C-O	-6.42	109.05	120.60
9	6	66	C	C6-N1-C2	-5.16	118.24	120.30
3	A	257	LEU	CA-CB-CG	5.07	126.95	115.30

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	3	0
3	A	10522	0	7599	48	0
4	r	5120	0	3785	0	0
5	N	295	0	149	2	0
6	q	523	0	472	0	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	27	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	0	0
18	r	1	0	0	0	0
All	All	25904	0	17331	133	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 (133) 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)
8:5:24:G:N1	8:5:57:G:N3	1.75	1.33
3:A:599:MET:HE3	13:Z:52:C:C2	1.74	1.22
8:5:24:G:C6	8:5:57:G:N3	2.05	1.22
3:A:599:MET:HE3	13:Z:52:C:N3	1.55	1.21
12:G:381:HIS:CB	12:G:382:PRO:HD3	1.73	1.17
8:5:24:G:C6	8:5:57:G:C2	2.35	1.15
8:5:24:G:N2	8:5:57:G:O2'	1.86	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:24:G:H22	8:5:57:G:H1'	1.25	1.00
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
3:A:599:MET:HE3	13:Z:52:C:O2	1.65	0.96
3:A:599:MET:CE	13:Z:52:C:C2	2.53	0.90
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
8:5:24:G:C2	8:5:57:G:N3	2.46	0.83
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
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
3:A:584:HIS:O	3:A:588:LEU:N	2.26	0.69
3:A:663:ARG:NH2	9:6:65:G:O6	2.26	0.69
8:5:19:A:N3	8:5:23:C:C5	2.61	0.69
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:A:599:MET:HE2	13:Z:52:C:O2	2.07	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
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:1557:LEU:HD11	9:6:44:G:C4	2.50	0.46
14:K:380:VAL:O	14:K:385:ARG:HD3	2.15	0.46
8:5:24:G:C8	8:5:26:A:N6	2.83	0.46
12:G:382:PRO:HB2	12:G:383:ARG:H	1.58	0.46
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
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:798:GLY:O	3:A:800:TYR:N	2.50	0.44
9:6:36:A:HO2'	9:6:38:G:H8	1.66	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
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
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
3:A:1722:SER:O	3:A:1726:ILE:HD12	2.19	0.41
12:G:379:VAL:CB	12:G:419:LEU:C	2.89	0.41
3:A:1571:ILE:HA	3:A:1574:ILE:HG22	2.02	0.41
3:A:974:ASN:O	3:A:1178:TYR:N	2.54	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)
14:K:390:LYS:CG	14:K:390:LYS:O	2.70	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%)	22	57
14	K	121/439 (28%)	100 (83%)	20 (16%)	1 (1%)	16	51
15	A4	240/1077 (22%)	233 (97%)	7 (3%)	0	100	100
All	All	3698/7471 (50%)	3258 (88%)	437 (12%)	3 (0%)	50	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%)	539 (99%)	5 (1%)	75	83
4	r	269/866 (31%)	267 (99%)	2 (1%)	81	86
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%)	45	64
15	A4	3/938 (0%)	3 (100%)	0	100	100
All	All	1034/5972 (17%)	1026 (99%)	8 (1%)	77	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	86	ARG
3	A	240	ARG
3	A	727	LYS
3	A	1471	ARG
3	A	1562	MET
4	r	140	HIS
4	r	194	LYS
14	K	370	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1241	HIS
5	N	98	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
9	6	27	A
9	6	28	A
9	6	29	A
9	6	31	U
9	6	33	G

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Mol	Chain	Res	Type
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
16	IHP	A	3001	-	36,36,36	1.44	6 (16%)	54,60,60	0.71	1 (1%)
17	GTP	r	1500	18,4	26,34,34	0.99	2 (7%)	32,54,54	0.84	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	IHP	A	3001	-	-	10/30/54/54	0/1/1/1
17	GTP	r	1500	18,4	-	5/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	3001	IHP	P2-O12	3.30	1.65	1.59
16	A	3001	IHP	P3-O13	3.06	1.65	1.59
16	A	3001	IHP	P4-O14	3.03	1.65	1.59
16	A	3001	IHP	P5-O15	3.03	1.65	1.59
16	A	3001	IHP	P1-O11	3.02	1.65	1.59
16	A	3001	IHP	P6-O16	2.86	1.64	1.59
17	r	1500	GTP	C5-C6	-2.50	1.42	1.47
17	r	1500	GTP	C8-N7	-2.06	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	3001	IHP	C5-C6-C1	2.33	115.51	110.41
17	r	1500	GTP	PA-O3A-PB	2.23	140.49	132.83

There are no chirality outliers.

All (15) 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
16	A	3001	IHP	C1-O11-P1-O31
16	A	3001	IHP	C4-O14-P4-O24
17	r	1500	GTP	C5'-O5'-PA-O1A
16	A	3001	IHP	C1-O11-P1-O21

*Continued on next page...*

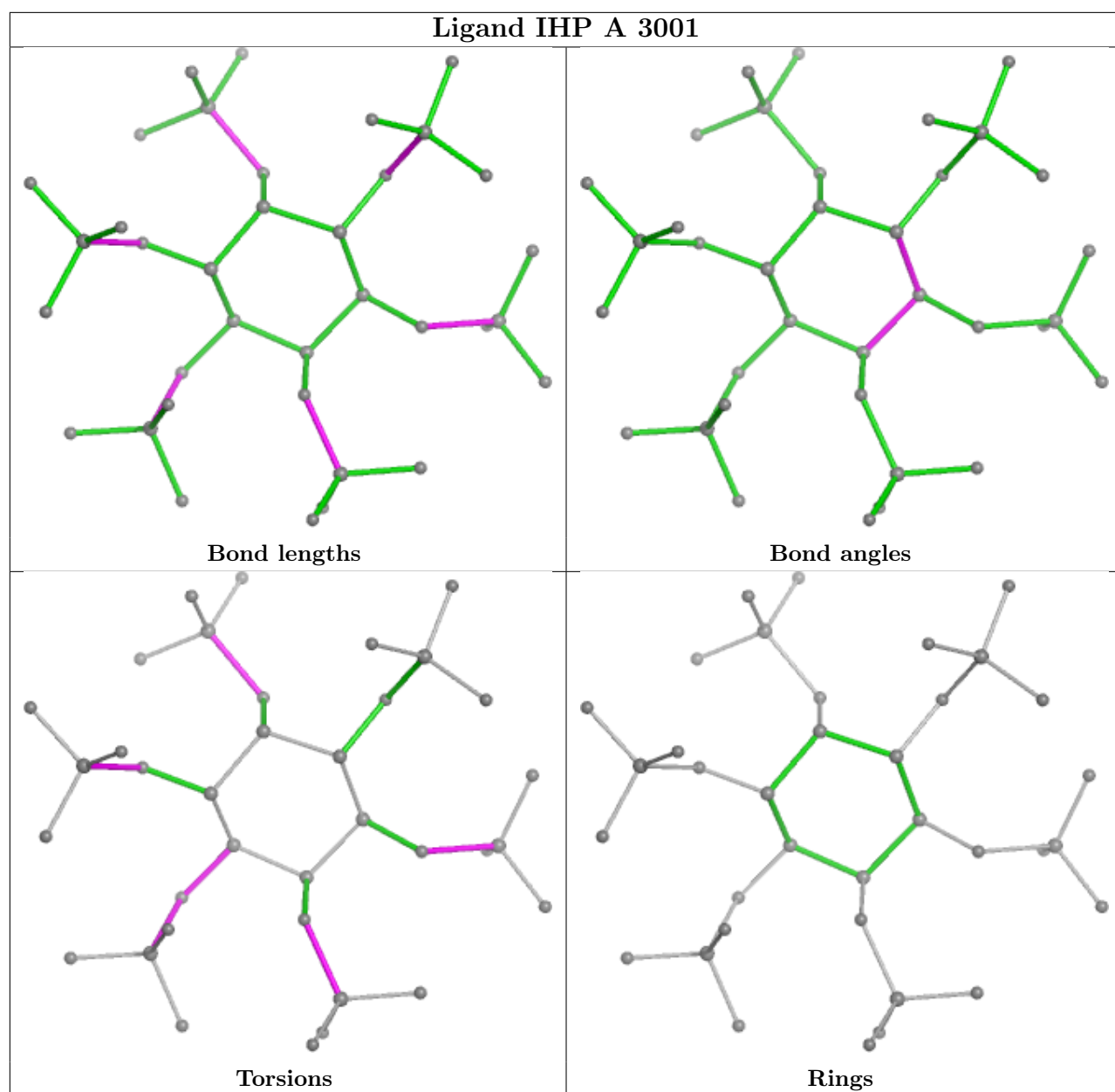
*Continued from previous page...*

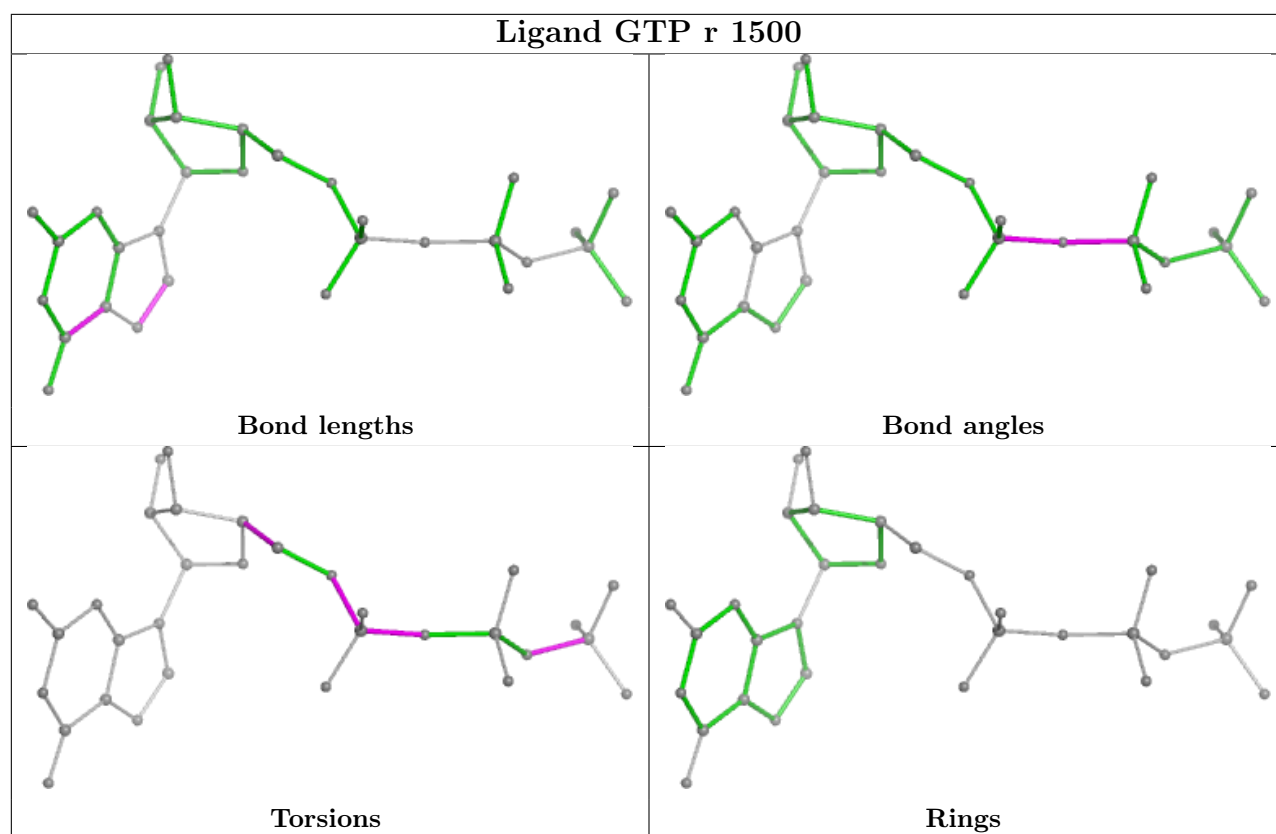
Mol	Chain	Res	Type	Atoms
17	r	1500	GTP	PB-O3B-PG-O2G
16	A	3001	IHP	C6-O16-P6-O36
16	A	3001	IHP	C6-O16-P6-O46
17	r	1500	GTP	C3'-C4'-C5'-O5'
17	r	1500	GTP	PB-O3A-PA-O2A
16	A	3001	IHP	C2-O12-P2-O22
16	A	3001	IHP	C3-O13-P3-O43
16	A	3001	IHP	C4-O14-P4-O34
17	r	1500	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

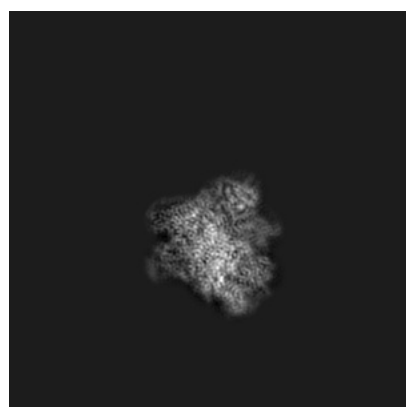
## 6 Map visualisation [i](#)

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

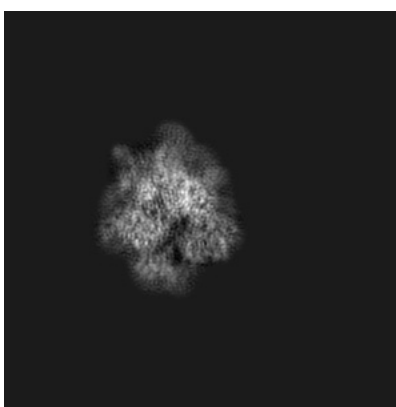
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

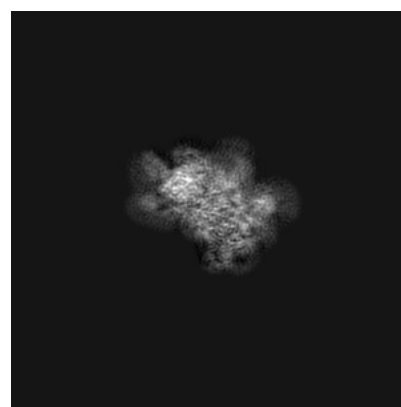
#### 6.1.1 Primary map



X



Y

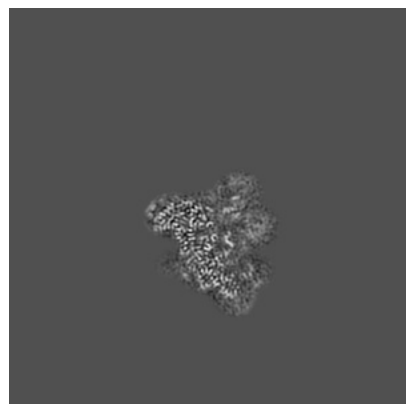


Z

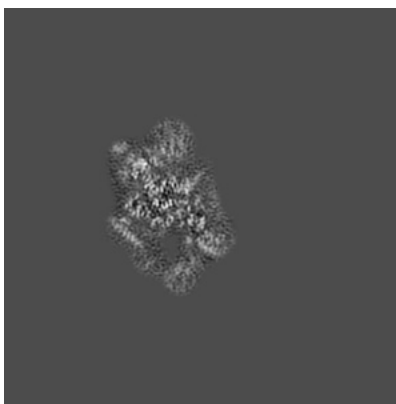
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

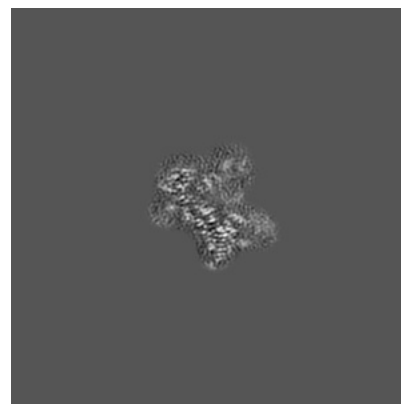
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

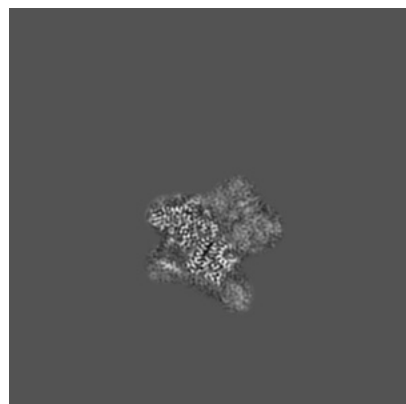


Z Index: 192

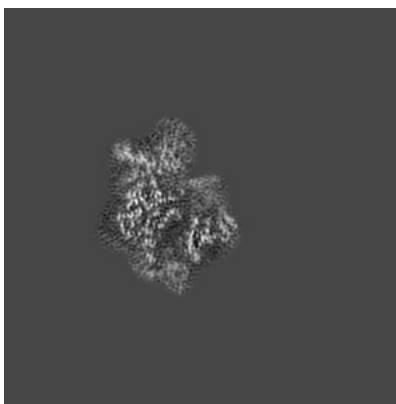
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

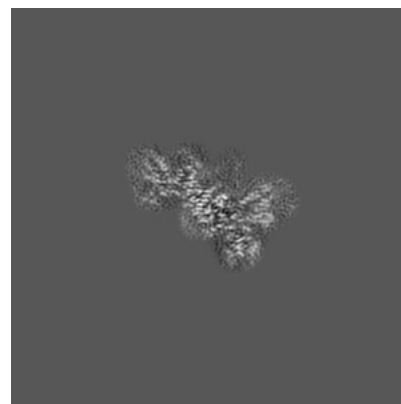
### 6.3.1 Primary map



X Index: 203



Y Index: 201

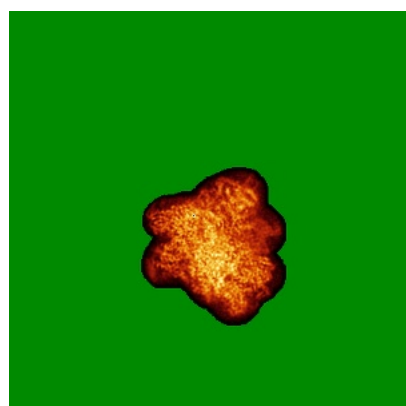


Z Index: 149

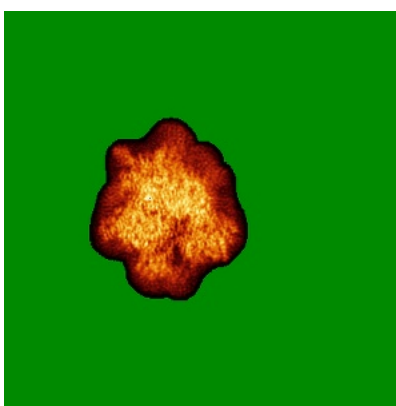
The images above show the largest variance slices of the map in three orthogonal directions.

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

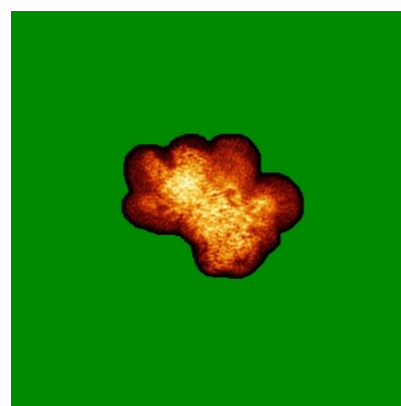
### 6.4.1 Primary map



X



Y

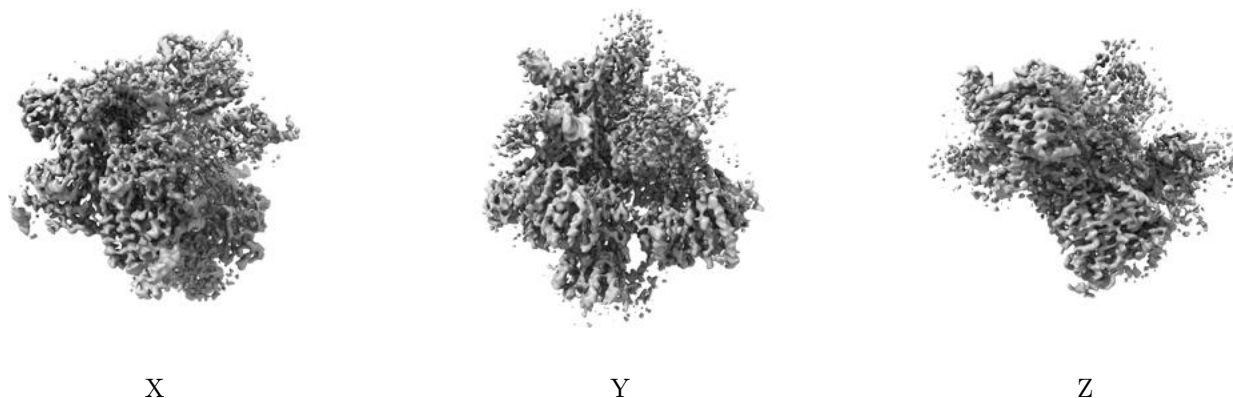


Z

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](#)

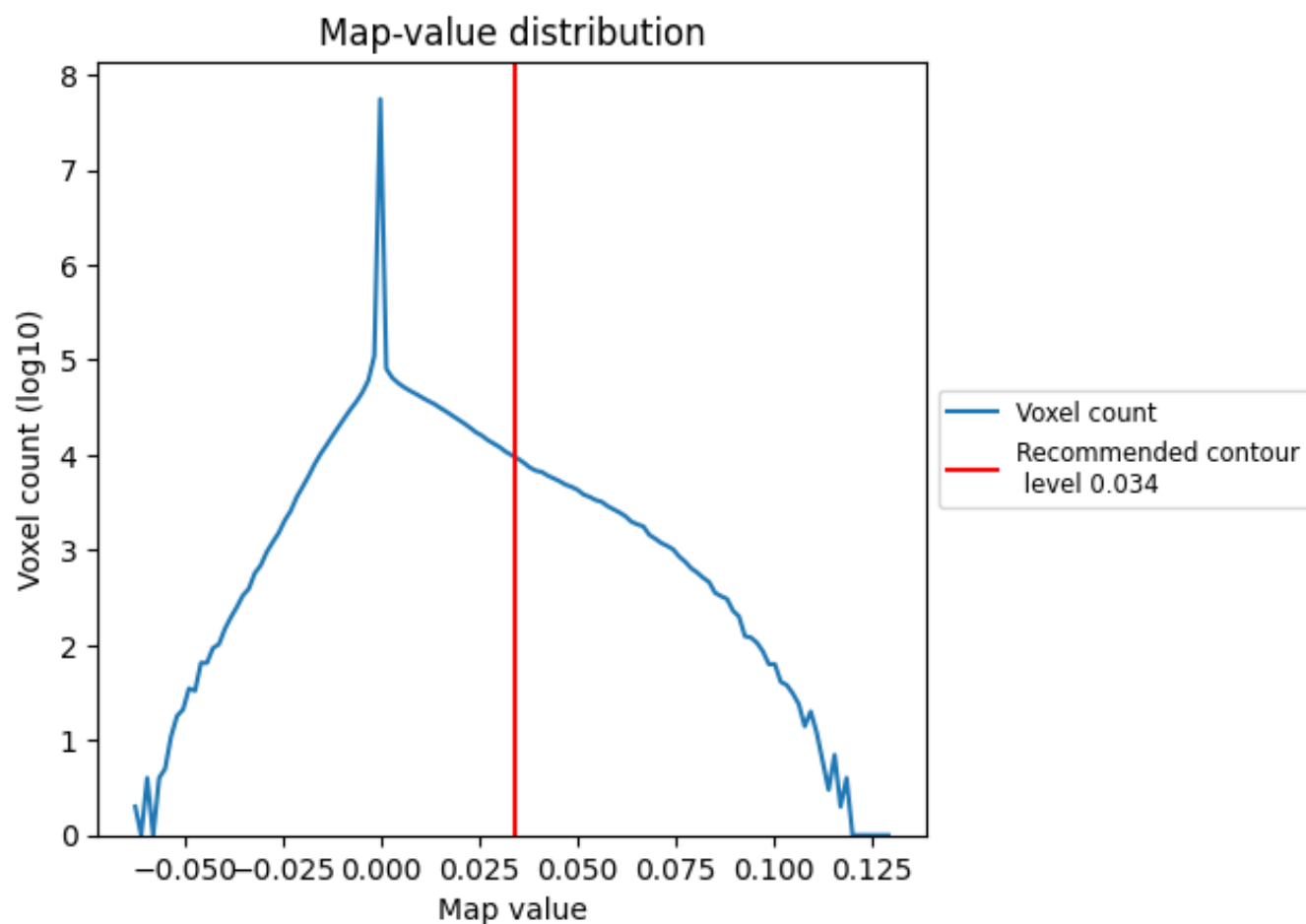
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

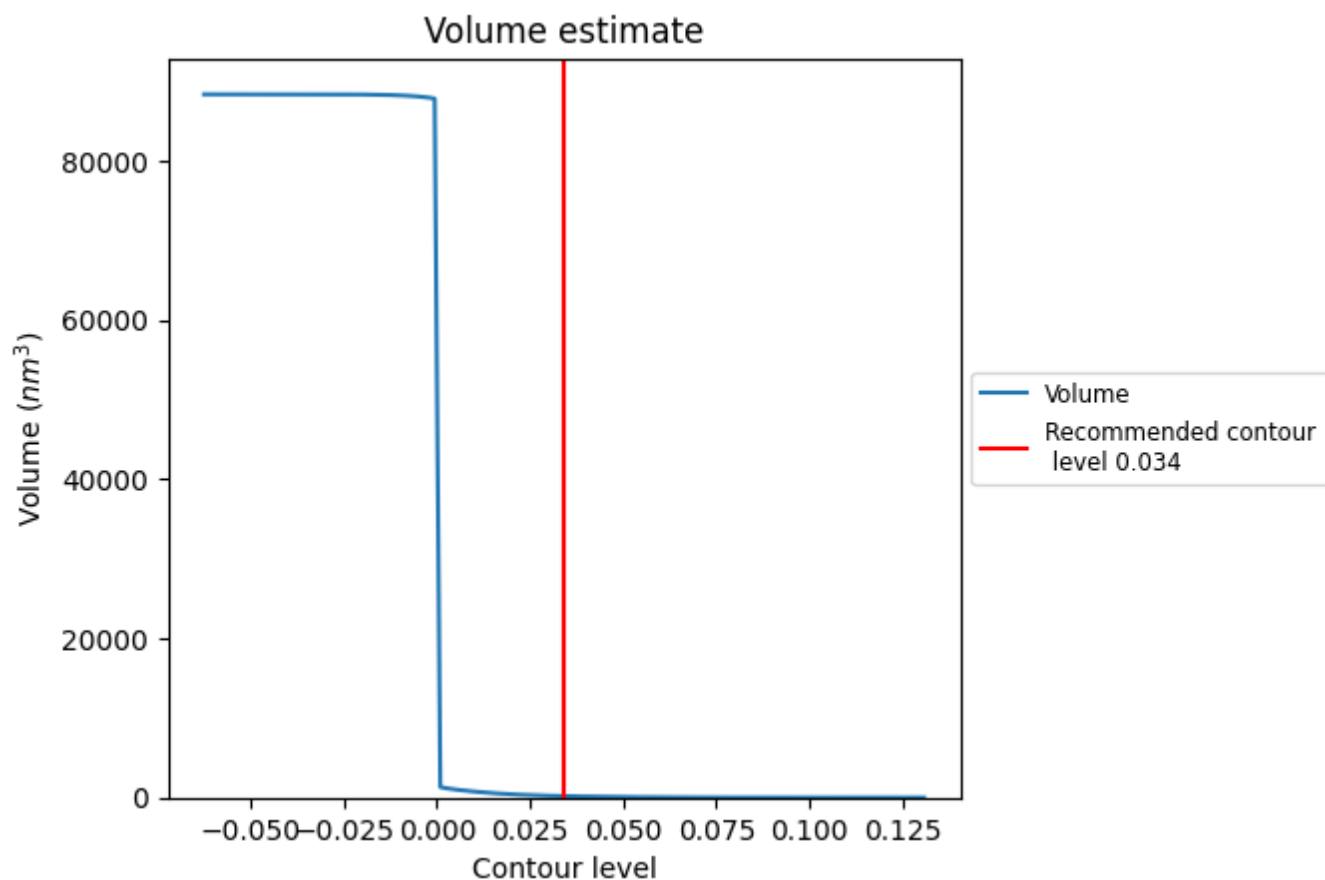
This section contains the results of statistical analysis of the map.

### 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.

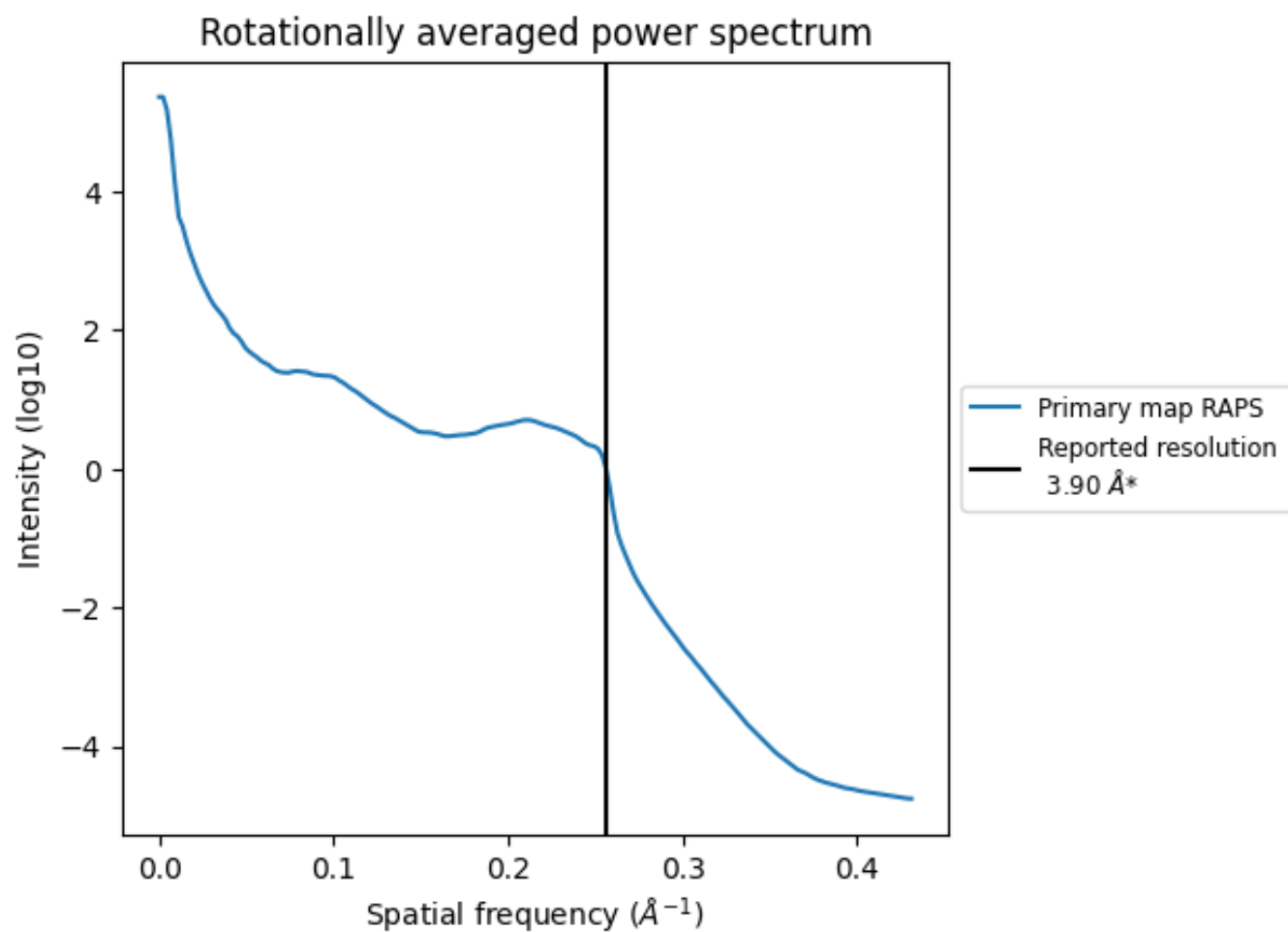
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183  $\text{nm}^3$ ; 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<sup>-1</sup>

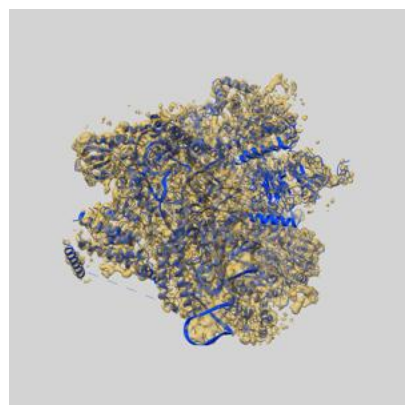
## 8 Fourier-Shell correlation

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

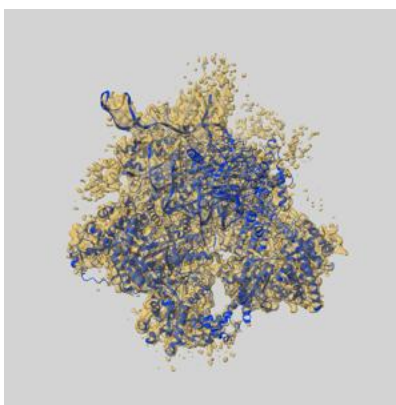
## 9 Map-model fit [i](#)

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.

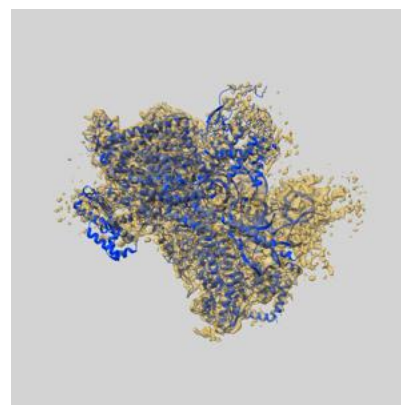
### 9.1 Map-model overlay [i](#)



X



Y



Z

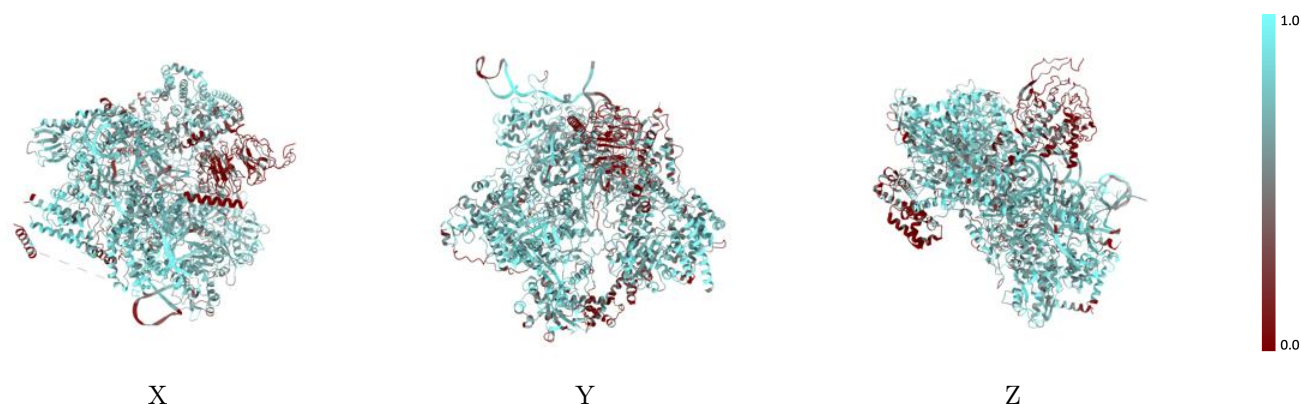
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



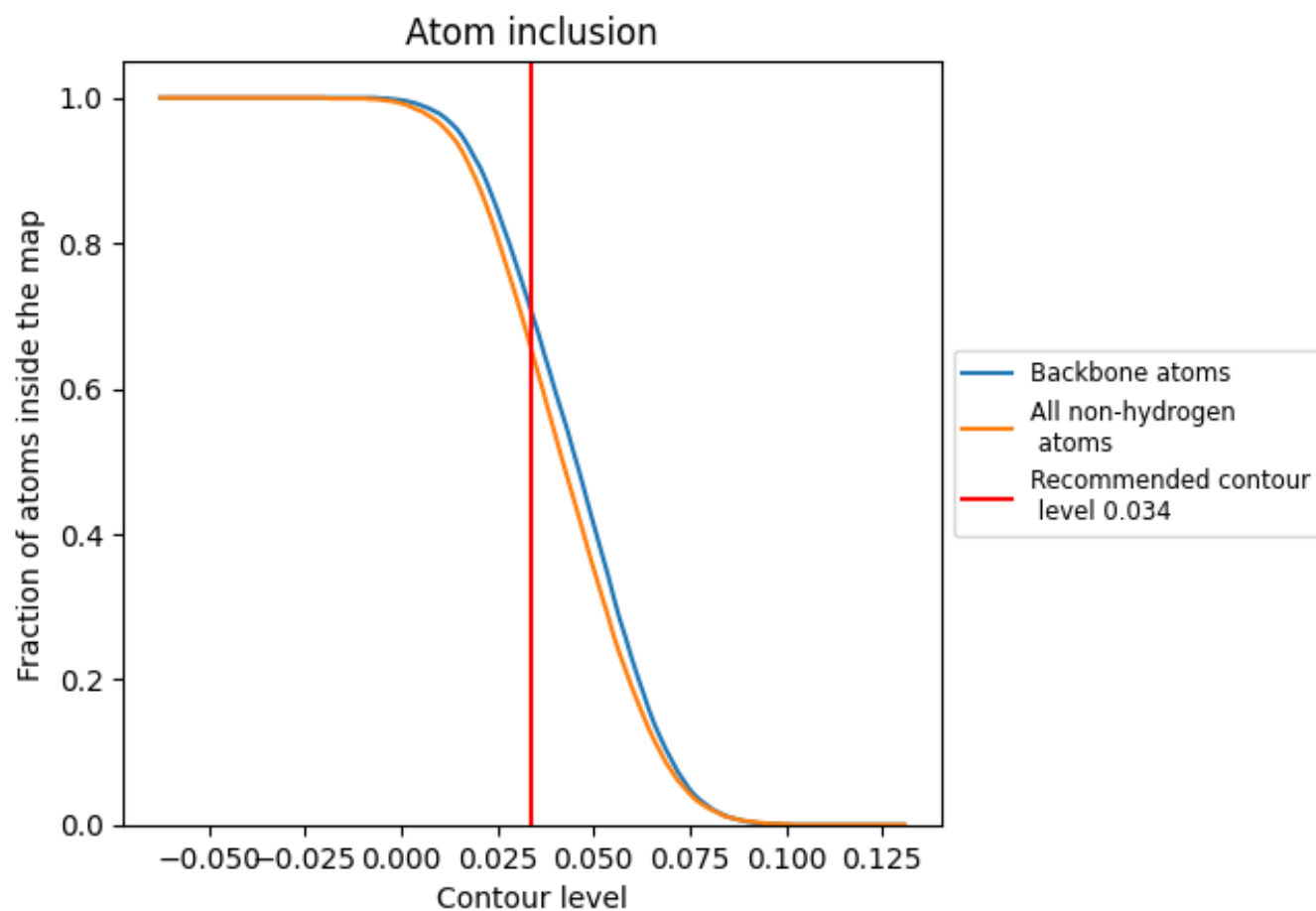
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

