



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:01 pm BST

PDB ID : 7AAV / pdb_00007aav
EMDB ID : EMD-11693
Title : Human pre-Bact-2 spliceosome core structure
Authors : Townsend, C.; Kastner, B.; Leelaram, M.N.; Bertram, K.; Stark, H.;
Luehrmann, R.
Deposited on : 2020-09-04
Resolution : 4.20 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.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

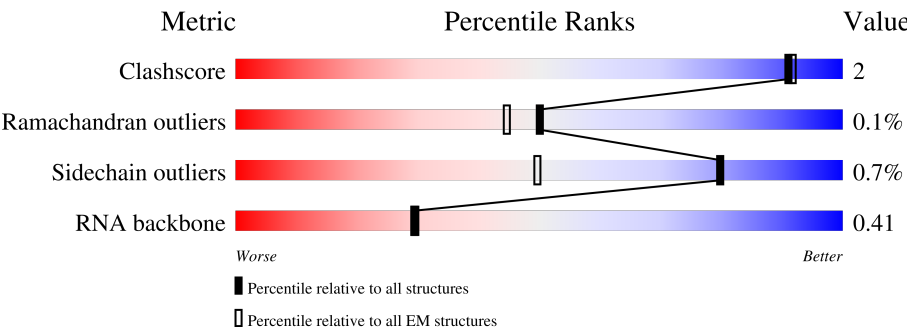
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



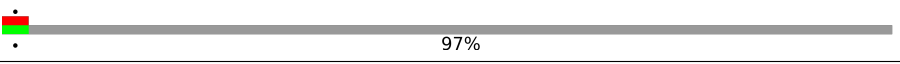





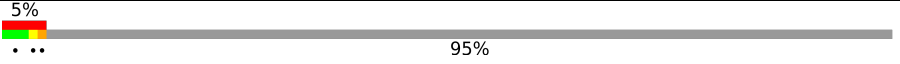

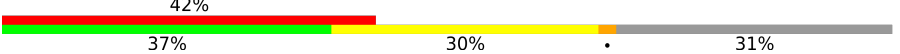
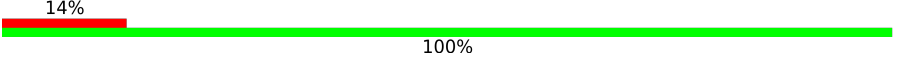
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	r	972	<div> <div>35%</div> <div>92%</div> <div>8%</div> </div>
2	Q	144	<div> <div>22%</div> <div>96%</div> <div>.</div> </div>
3	L	802	<div> <div>9%</div> <div>13%</div> <div>87%</div> </div>
4	R	229	<div> <div>17%</div> <div>19%</div> <div>81%</div> </div>
5	K	439	<div> <div>17%</div> <div>26%</div> <div>72%</div> </div>
6	G	514	<div> <div>45%</div> <div>60%</div> <div>38%</div> </div>
7	Z	230	<div> <div>7%</div> <div>5%</div> <div>5%</div> <div>87%</div> </div>

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Mol	Chain	Length	Quality of chain
8	8	579	
9	I	312	
10	A	2335	
11	P	420	
12	v	536	
13	N	199	
14	2	188	
15	5	116	
16	6	106	
17	q	73	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 25867 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 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	r	895	Total	C	N	O	0	0
			4834	3011	921	902		

- Molecule 2 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	138	Total	C	N	O	0	0
			758	471	147	140		

- Molecule 3 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	103	Total	C	N	O	0	0
			517	311	103	103		

- Molecule 4 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	R	44	Total	C	N	O	0	0
			219	131	44	44		

- Molecule 5 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	123	Total	C	N	O	S	0	0
			779	489	152	136	2		

- Molecule 6 is a protein called Pleiotropic regulator 1.

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

- Molecule 7 is a RNA chain called MINX M3 pre-mRNA.

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

- Molecule 8 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	8	18	Total	C	N	O	0	0
			92	56	18	18		

- Molecule 9 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 10 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1656	Total	C	N	O	S	0	0
			9649	6144	1793	1707	5		

- Molecule 11 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	162	Total	C	N	O	0	0
			825	501	162	162		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	v	206	Total	C	N	O	0	0
			1053	641	206	206		

- Molecule 13 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 14 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	10	Total	C	N	O	P	0	0
			215	96	40	69	10		

- Molecule 15 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	69	Total	C	N	O	P	0	0
			1453	651	243	490	69		

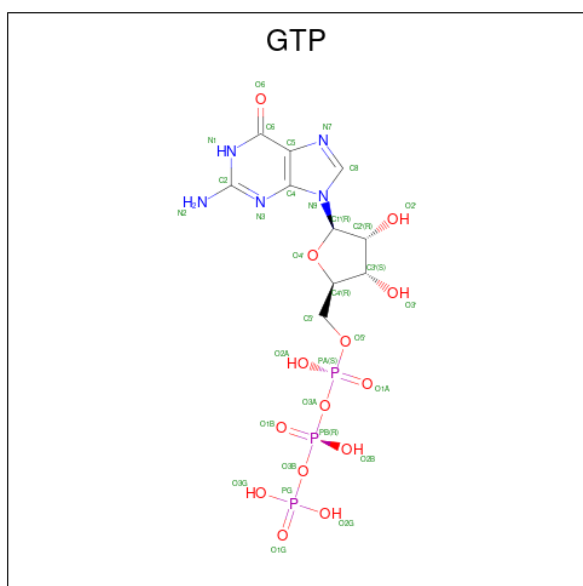
- Molecule 16 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	73	Total	C	N	O	P	0	0
			1560	698	286	503	73		

- Molecule 17 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	q	73	Total	C	N	O	0	0
			458	300	80	78		

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

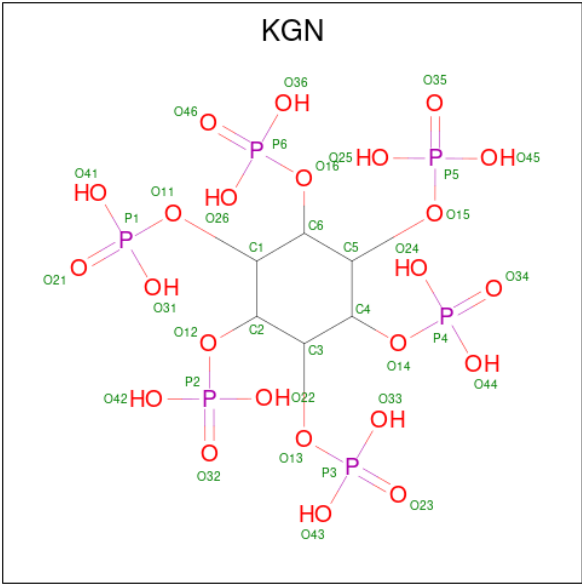


Mol	Chain	Residues	Atoms					AltConf
18	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 20 is D-chiro inositol hexakisphosphate (CCD ID: KGN) (formula: C₆H₁₈O₂₄P₆).

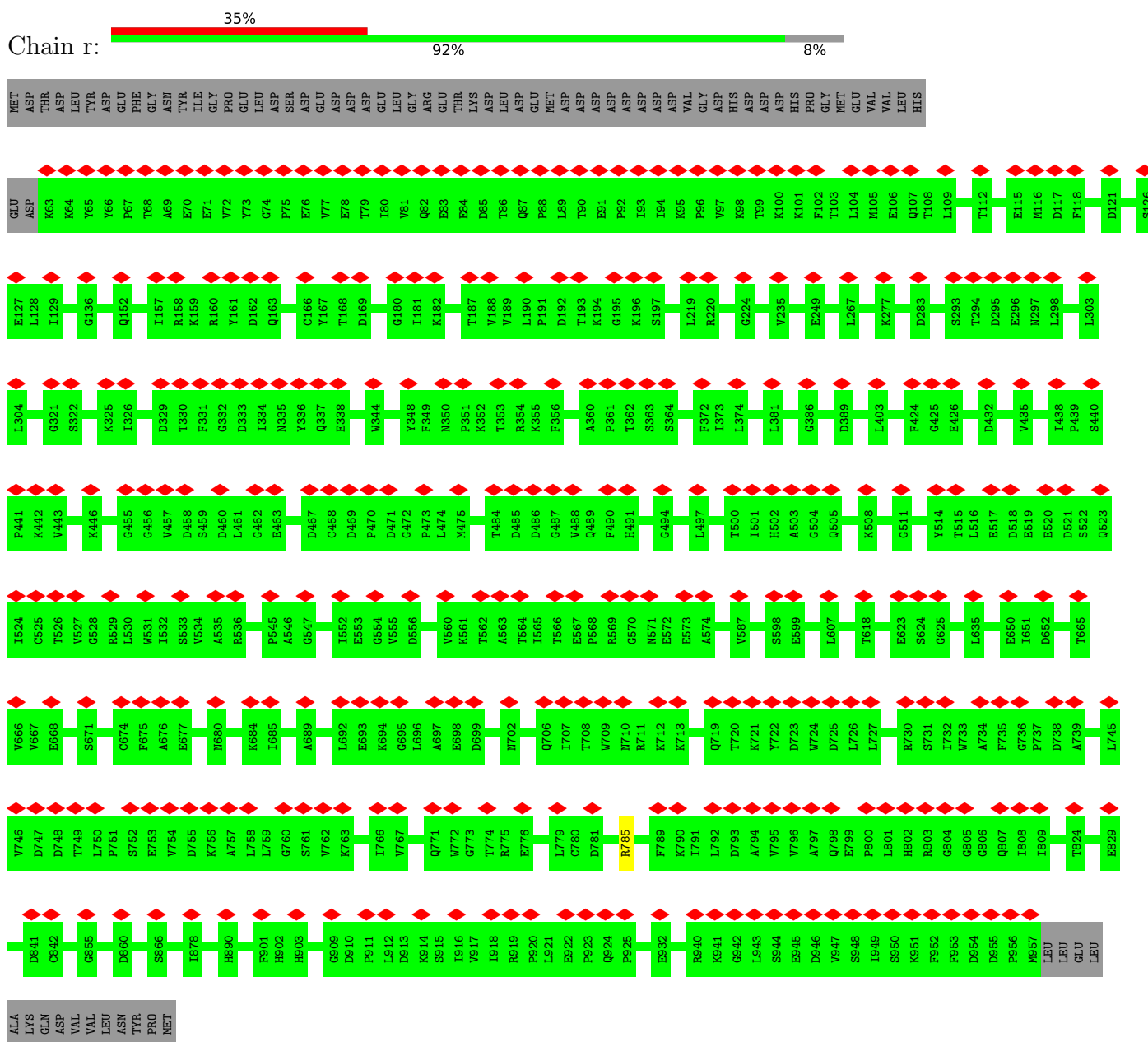


Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			36	6	24	6	

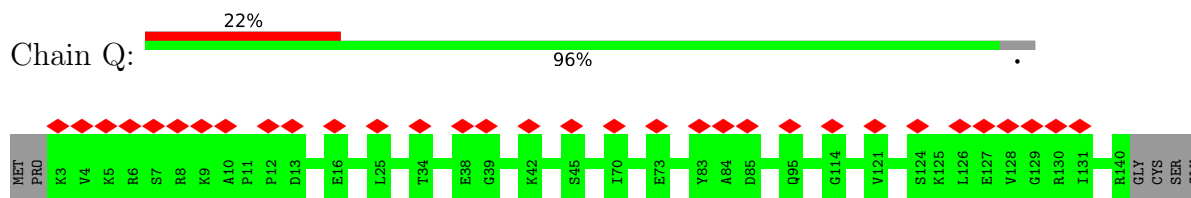
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

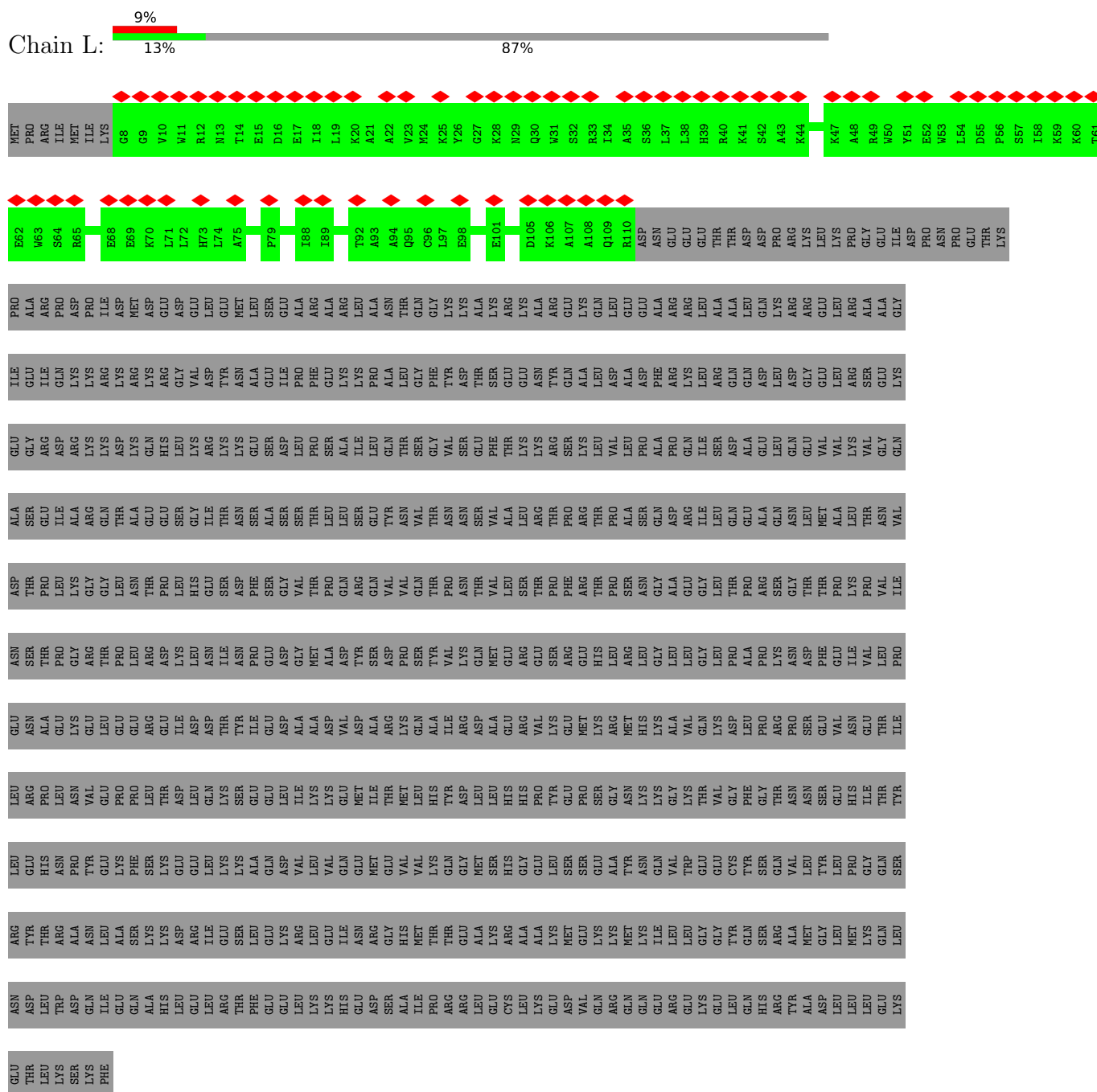
- Molecule 1: 116 kDa U5 small nuclear ribonucleoprotein component



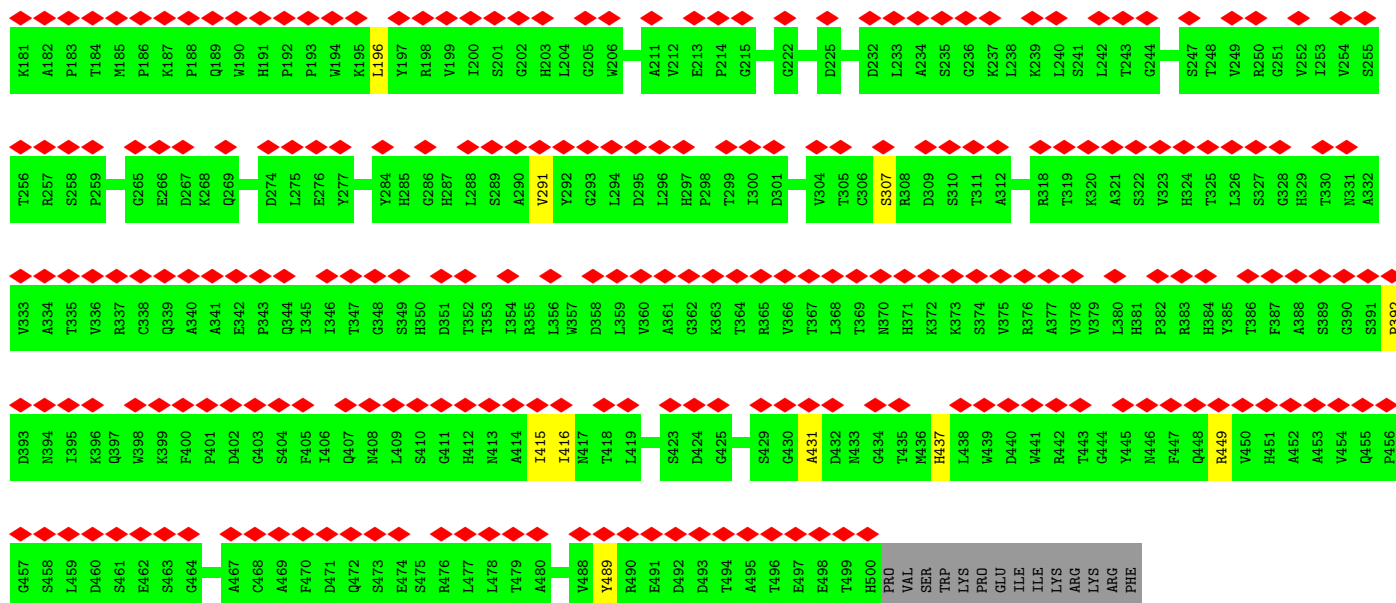
- Molecule 2: Protein BUD31 homolog



- Molecule 3: Cell division cycle 5-like protein



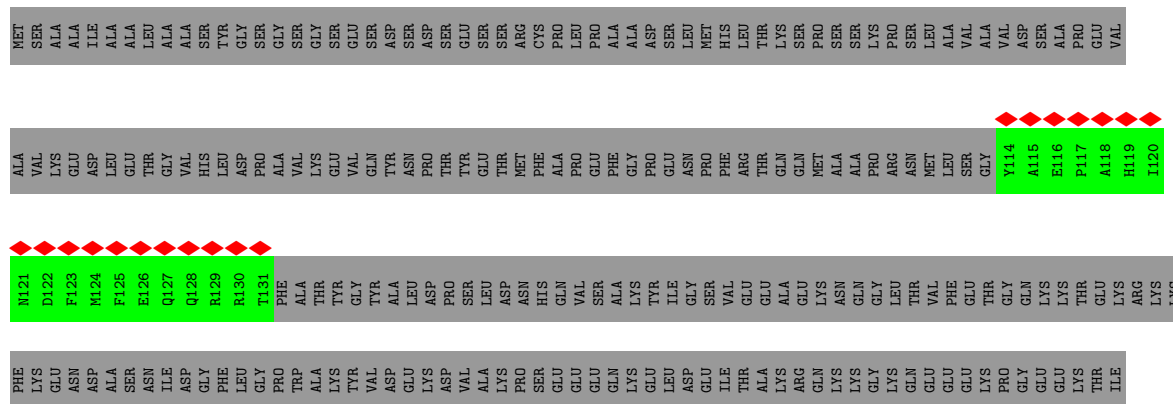
- Molecule 4: Spliceosome-associated protein CWC15 homolog



• Molecule 7: MINX M3 pre-mRNA



• Molecule 8: Pre-mRNA-processing factor 17

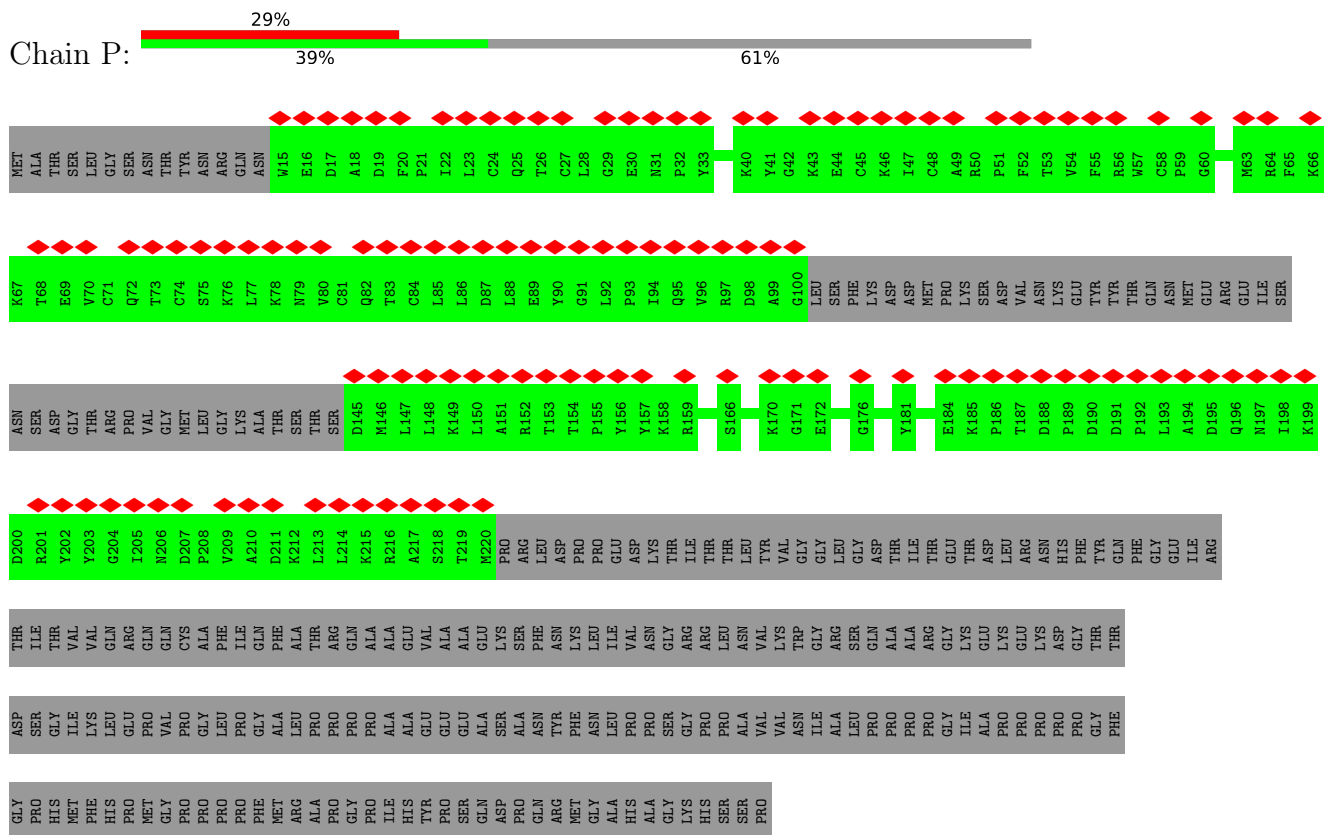




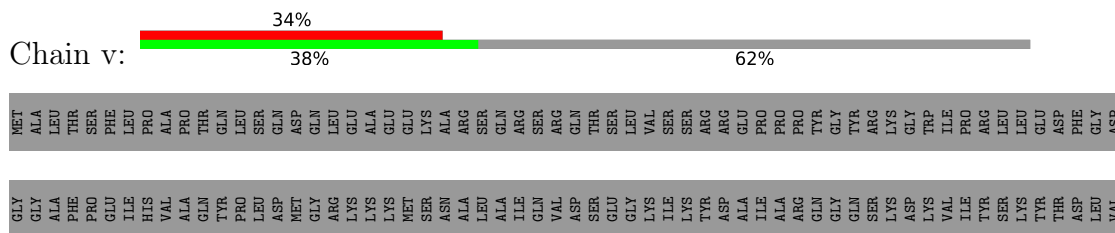


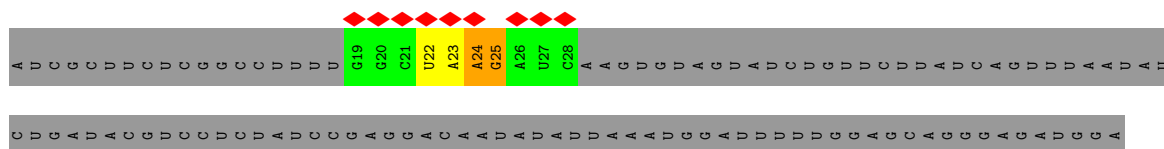
[illegible]

- Molecule 11: Pre-mRNA-splicing factor RBM22



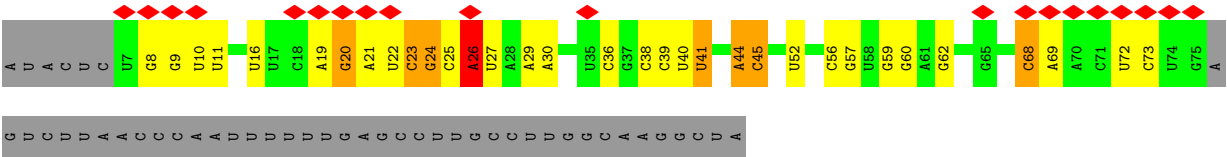
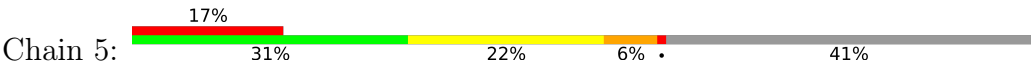
- Molecule 12: SNW domain-containing protein 1



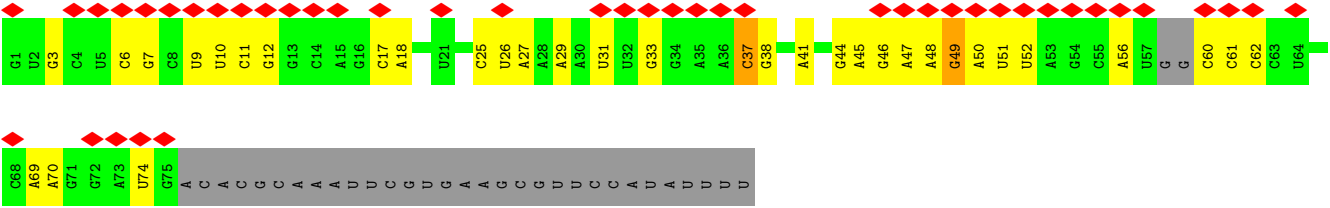




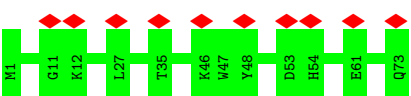
• Molecule 15: U5 snRNA



• Molecule 16: U6 snRNA



• Molecule 17: Ubiquitin-like protein 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39336	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	0.134	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.051	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KGN, GTP, 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	r	0.26	0/4931	0.46	0/6891
2	Q	0.25	0/773	0.41	0/1078
3	L	0.25	0/519	0.45	0/725
4	R	0.24	0/218	0.49	0/303
5	K	0.28	0/791	0.49	0/1079
6	G	0.26	0/1616	0.49	0/2258
7	Z	0.28	0/696	1.01	7/1083 (0.6%)
8	8	0.23	0/92	0.37	0/128
9	I	0.23	0/888	0.41	0/1241
10	A	0.26	0/9886	0.46	0/13772
11	P	0.24	0/835	0.47	0/1170
12	v	0.26	0/1064	0.44	0/1491
13	N	0.23	0/276	0.39	0/383
14	2	0.42	0/240	1.25	4/372 (1.1%)
15	5	0.34	0/1620	1.17	17/2518 (0.7%)
16	6	0.25	0/1745	0.94	4/2715 (0.1%)
17	q	0.24	0/467	0.47	0/643
All	All	0.26	0/26657	0.61	32/37850 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	23	C	C2-N1-C1'	11.87	131.85	118.80
15	5	45	C	C2-N1-C1'	10.61	130.47	118.80
15	5	23	C	N1-C2-O2	9.22	124.43	118.90
7	Z	71	C	N1-C2-O2	8.74	124.14	118.90
15	5	23	C	C6-N1-C2	-8.67	116.83	120.30
15	5	23	C	C6-N1-C1'	-7.92	111.30	120.80
15	5	23	C	N3-C2-O2	-7.66	116.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	45	C	C6-N1-C1'	-7.35	111.98	120.80
15	5	45	C	C6-N1-C2	-7.19	117.42	120.30
14	2	25	G	N3-C4-N9	-7.12	121.73	126.00
15	5	45	C	N1-C2-O2	7.08	123.15	118.90
7	Z	71	C	N3-C2-O2	-6.75	117.17	121.90
14	2	25	G	C8-N9-C1'	6.62	135.61	127.00
14	2	25	G	C4-N9-C1'	-6.61	117.91	126.50
15	5	23	C	C5-C6-N1	6.54	124.27	121.00
15	5	26	A	P-O3'-C3'	6.54	127.55	119.70
16	6	49	G	P-O3'-C3'	6.28	127.24	119.70
7	Z	71	C	C2-N1-C1'	6.18	125.60	118.80
16	6	60	C	C2-N1-C1'	6.01	125.41	118.80
16	6	60	C	N1-C2-O2	6.00	122.50	118.90
15	5	45	C	C5-C6-N1	5.91	123.95	121.00
7	Z	74	G	P-O3'-C3'	5.82	126.68	119.70
15	5	68	C	C2-N1-C1'	5.76	125.13	118.80
7	Z	71	C	C6-N1-C2	-5.69	118.03	120.30
15	5	68	C	N1-C2-O2	5.59	122.26	118.90
15	5	73	C	N1-C2-O2	5.58	122.25	118.90
15	5	45	C	N3-C2-O2	-5.35	118.16	121.90
16	6	37	C	N1-C2-O2	5.29	122.08	118.90
15	5	24	G	O4'-C1'-N9	-5.25	104.00	108.20
7	Z	70	G	P-O3'-C3'	5.24	125.99	119.70
7	Z	71	C	C5-C6-N1	5.18	123.59	121.00
14	2	25	G	N3-C2-N2	-5.06	116.36	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	r	4834	0	2682	0	0
2	Q	758	0	401	0	0
3	L	517	0	257	0	0
4	R	219	0	91	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	779	0	575	5	0
6	G	1604	0	795	5	0
7	Z	622	0	315	6	0
8	8	92	0	46	0	0
9	I	883	0	414	1	0
10	A	9649	0	6011	31	0
11	P	825	0	410	0	0
12	v	1053	0	550	0	0
13	N	277	0	114	0	0
14	2	215	0	109	1	0
15	5	1453	0	736	11	0
16	6	1560	0	790	3	0
17	q	458	0	337	0	0
18	r	32	0	12	0	0
19	r	1	0	0	0	0
20	A	36	0	0	0	0
All	All	25867	0	14645	51	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 2.

All (51) 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)
10:A:1416:ILE:CB	10:A:1417:PRO:HD3	2.13	0.79
7:Z:54:G:N1	15:5:44:A:C8	2.60	0.68
10:A:466:ALA:HB2	15:5:20:G:H1	1.59	0.67
10:A:520:TYR:O	10:A:555:LYS:NZ	2.35	0.59
6:G:437:HIS:HA	6:G:449:ARG:HA	1.85	0.57
10:A:424:ILE:O	10:A:635:ARG:NH1	2.38	0.57
10:A:1416:ILE:CB	10:A:1417:PRO:CD	2.82	0.56
10:A:1127:GLY:O	10:A:1151:ARG:NH2	2.40	0.54
7:Z:57:C:N3	15:5:41:U:O4	2.40	0.54
10:A:1580:HIS:NE2	16:6:44:G:OP2	2.42	0.53
10:A:419:ARG:NH2	15:5:26:A:OP1	2.42	0.51
5:K:341:TYR:H	7:Z:53:C:H5'	1.77	0.50
6:G:196:LEU:HA	6:G:489:TYR:HA	1.94	0.50
6:G:416:ILE:HA	6:G:431:ALA:HA	1.95	0.49
10:A:1615:HIS:NE2	16:6:41:A:OP1	2.40	0.49
10:A:420:ARG:NH2	15:5:56:C:O2'	2.42	0.49
10:A:586:GLY:O	10:A:592:TYR:OH	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:291:VAL:HA	6:G:307:SER:HA	1.95	0.48
5:K:380:VAL:O	5:K:385:ARG:NH2	2.44	0.48
9:I:29:ILE:HA	9:I:67:PRO:HG3	1.96	0.47
10:A:980:ARG:HA	10:A:1094:ARG:HA	1.96	0.47
7:Z:54:G:C6	15:5:44:A:N7	2.83	0.46
15:5:59:G:N1	15:5:60:G:O6	2.48	0.46
10:A:594:TYR:O	15:5:44:A:O2'	2.34	0.46
10:A:949:PRO:O	10:A:953:TYR:N	2.41	0.46
10:A:584:HIS:O	10:A:589:THR:N	2.49	0.45
7:Z:54:G:O6	15:5:44:A:N7	2.50	0.45
10:A:648:LEU:HA	10:A:651:TRP:HB2	1.99	0.45
16:6:17:C:H2'	16:6:18:A:H8	1.82	0.45
5:K:320:ARG:NH1	5:K:322:ASN:O	2.50	0.44
10:A:144:TRP:HZ3	10:A:629:PHE:HB2	1.82	0.44
10:A:228:TRP:O	10:A:416:GLY:N	2.52	0.43
10:A:781:ARG:NH1	14:2:24:A:OP1	2.42	0.43
10:A:828:PRO:HA	10:A:829:PRO:HD3	1.90	0.43
10:A:1630:LEU:HA	10:A:1661:TRP:HA	2.00	0.43
10:A:496:VAL:O	10:A:500:GLY:N	2.45	0.43
15:5:29:A:H2'	15:5:30:A:H8	1.84	0.43
10:A:155:LYS:NZ	10:A:624:GLY:O	2.39	0.43
7:Z:55:A:H2'	7:Z:56:A:H8	1.84	0.42
5:K:371:LYS:HA	5:K:374:LEU:HD23	2.01	0.42
10:A:63:PRO:HB2	10:A:64:GLU:H	1.63	0.42
10:A:1589:ILE:HG22	10:A:1664:ILE:HD13	2.02	0.42
6:G:392:PRO:HB3	6:G:415:ILE:HA	2.02	0.42
10:A:1382:SER:HA	10:A:1415:GLY:HA2	2.02	0.41
5:K:358:ARG:HD2	5:K:360:PHE:HE1	1.85	0.41
10:A:136:ILE:O	10:A:140:TYR:N	2.53	0.41
10:A:1386:TRP:HE1	10:A:1416:ILE:H	1.69	0.41
15:5:29:A:H2'	15:5:30:A:C8	2.56	0.41
10:A:540:PHE:HB2	10:A:545:HIS:CE1	2.56	0.41
10:A:136:ILE:HG22	10:A:138:PRO:HD2	2.03	0.40
10:A:1386:TRP:CZ2	10:A:1417:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	r	893/972 (92%)	808 (90%)	85 (10%)	0	100	100
2	Q	136/144 (94%)	126 (93%)	10 (7%)	0	100	100
3	L	101/802 (13%)	94 (93%)	7 (7%)	0	100	100
4	R	42/229 (18%)	40 (95%)	2 (5%)	0	100	100
5	K	121/439 (28%)	108 (89%)	13 (11%)	0	100	100
6	G	318/514 (62%)	296 (93%)	22 (7%)	0	100	100
8	8	16/579 (3%)	16 (100%)	0	0	100	100
9	I	174/312 (56%)	161 (92%)	13 (8%)	0	100	100
10	A	1650/2335 (71%)	1479 (90%)	169 (10%)	2 (0%)	48	82
11	P	158/420 (38%)	152 (96%)	6 (4%)	0	100	100
12	v	198/536 (37%)	180 (91%)	18 (9%)	0	100	100
13	N	54/199 (27%)	52 (96%)	2 (4%)	0	100	100
17	q	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
All	All	3932/7554 (52%)	3581 (91%)	349 (9%)	2 (0%)	50	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	A	1413	ASP
10	A	1414	ARG

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	r	112/866 (13%)	111 (99%)	1 (1%)	75	83
2	Q	16/130 (12%)	16 (100%)	0	100	100
3	L	3/709 (0%)	3 (100%)	0	100	100
5	K	40/395 (10%)	38 (95%)	2 (5%)	20	44
6	G	13/441 (3%)	13 (100%)	0	100	100
8	8	1/502 (0%)	1 (100%)	0	100	100
9	I	6/293 (2%)	6 (100%)	0	100	100
10	A	331/2108 (16%)	330 (100%)	1 (0%)	91	92
11	P	12/361 (3%)	12 (100%)	0	100	100
12	v	15/459 (3%)	15 (100%)	0	100	100
17	q	22/66 (33%)	22 (100%)	0	100	100
All	All	571/6330 (9%)	567 (99%)	4 (1%)	80	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	r	785	ARG
5	K	370	ASN
5	K	376	LYS
10	A	1026	ASN

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

Mol	Chain	Res	Type
5	K	370	ASN
10	A	545	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	2	9/188 (4%)	4 (44%)	1 (11%)
15	5	68/116 (58%)	27 (39%)	1 (1%)
16	6	71/106 (66%)	29 (40%)	1 (1%)
7	Z	28/230 (12%)	13 (46%)	2 (7%)
All	All	176/640 (27%)	73 (41%)	5 (2%)

All (73) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	Z	51	U
7	Z	52	C
7	Z	53	C
7	Z	54	G
7	Z	55	A
7	Z	60	U
7	Z	61	A
7	Z	62	A
7	Z	63	G
7	Z	71	C
7	Z	72	A
7	Z	75	U
7	Z	78	A
14	2	22	U
14	2	23	A
14	2	24	A
14	2	25	G
15	5	8	G
15	5	9	G
15	5	10	U
15	5	11	U
15	5	16	U
15	5	19	A
15	5	20	G
15	5	21	A
15	5	22	U
15	5	23	C
15	5	24	G
15	5	25	C
15	5	26	A
15	5	27	U
15	5	36	C
15	5	38	C
15	5	39	C
15	5	40	U
15	5	41	U
15	5	44	A
15	5	45	C
15	5	52	U
15	5	57	G
15	5	62	G
15	5	68	C
15	5	69	A

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Mol	Chain	Res	Type
15	5	72	U
16	6	3	G
16	6	6	C
16	6	7	G
16	6	9	U
16	6	10	U
16	6	11	C
16	6	12	G
16	6	25	C
16	6	26	U
16	6	27	A
16	6	29	A
16	6	31	U
16	6	33	G
16	6	37	C
16	6	38	G
16	6	45	A
16	6	46	G
16	6	47	A
16	6	48	A
16	6	49	G
16	6	50	A
16	6	51	U
16	6	52	U
16	6	56	A
16	6	61	C
16	6	62	C
16	6	69	A
16	6	70	A
16	6	74	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	Z	70	G
7	Z	74	G
14	2	22	U
15	5	26	A
16	6	49	G

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	$\# Z > 2$
20	KGN	A	3001	-	36,36,36	1.48	6 (16%)	54,60,60	0.76	1 (1%)
18	GTP	r	1500	1,19	26,34,34	1.14	2 (7%)	32,54,54	1.49	7 (21%)

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
20	KGN	A	3001	-	-	6/30/54/54	0/1/1/1
18	GTP	r	1500	1,19	-	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)
18	r	1500	GTP	C5-C6	-4.06	1.39	1.47
20	A	3001	KGN	P2-O12	3.44	1.65	1.59
20	A	3001	KGN	P3-O13	3.10	1.65	1.59
20	A	3001	KGN	P6-O16	3.09	1.65	1.59
20	A	3001	KGN	P1-O11	3.03	1.65	1.59
20	A	3001	KGN	P4-O14	3.02	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	3001	KGN	P5-O15	3.00	1.65	1.59
18	r	1500	GTP	C2-N3	2.20	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	r	1500	GTP	PB-O3B-PG	-3.40	121.14	132.83
18	r	1500	GTP	C5-C6-N1	3.17	119.55	113.95
18	r	1500	GTP	C8-N7-C5	3.03	108.76	102.99
18	r	1500	GTP	C3'-C2'-C1'	2.95	105.42	100.98
20	A	3001	KGN	O12-C2-C1	2.94	115.63	108.69
18	r	1500	GTP	C2-N1-C6	-2.86	119.83	125.10
18	r	1500	GTP	PA-O3A-PB	-2.63	123.80	132.83
18	r	1500	GTP	O6-C6-C5	-2.14	120.18	124.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

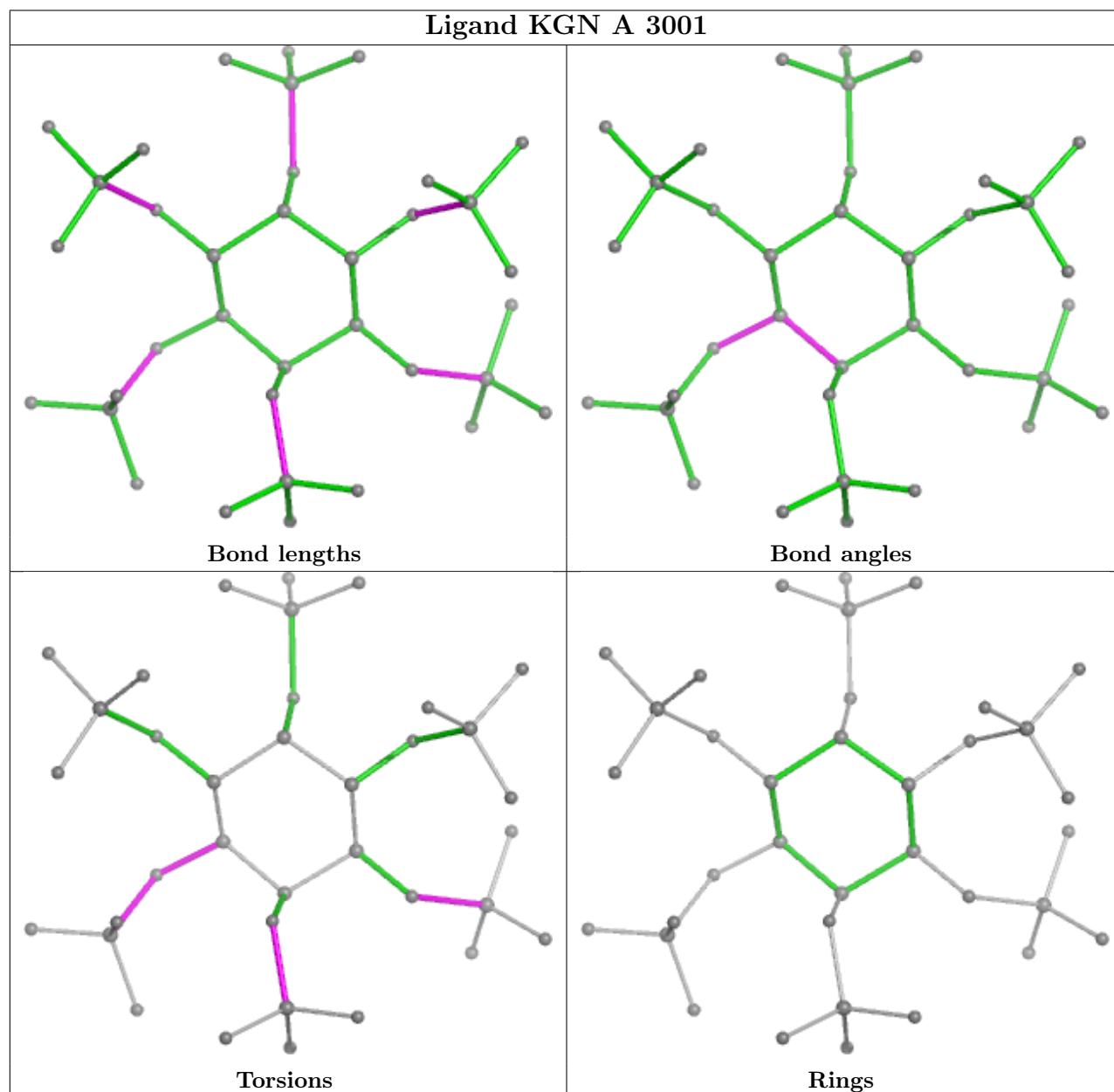
Mol	Chain	Res	Type	Atoms
18	r	1500	GTP	C5'-O5'-PA-O2A
20	A	3001	KGN	C1-O11-P1-O21
20	A	3001	KGN	C2-O12-P2-O32
20	A	3001	KGN	C1-C2-O12-P2
18	r	1500	GTP	O4'-C4'-C5'-O5'
18	r	1500	GTP	C3'-C4'-C5'-O5'
18	r	1500	GTP	C5'-O5'-PA-O3A
20	A	3001	KGN	C6-O16-P6-O26
18	r	1500	GTP	C5'-O5'-PA-O1A
20	A	3001	KGN	C3-C2-O12-P2
20	A	3001	KGN	C1-O11-P1-O41

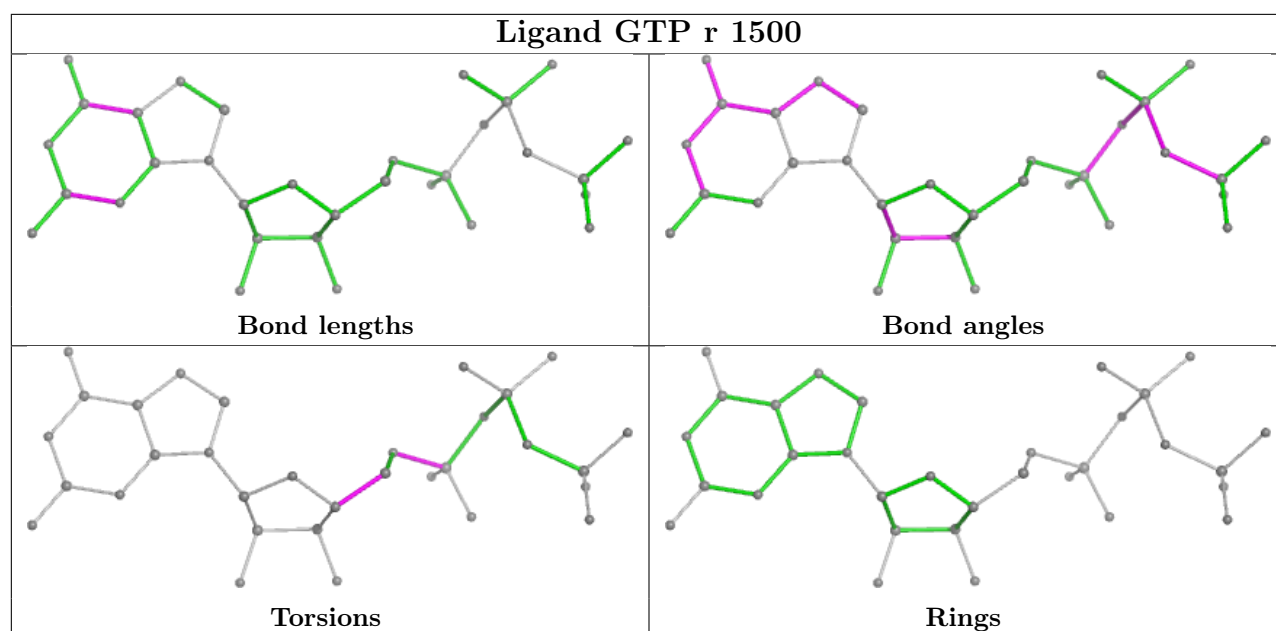
There are no ring outliers.

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.

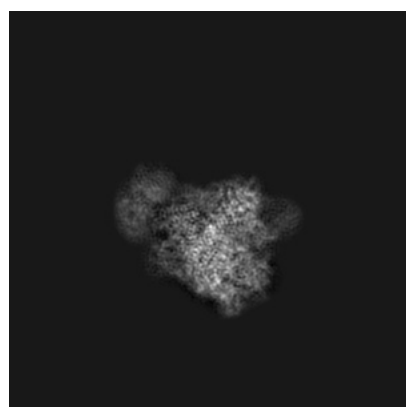
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11693. These allow visual inspection of the internal detail of the map and identification of artifacts.

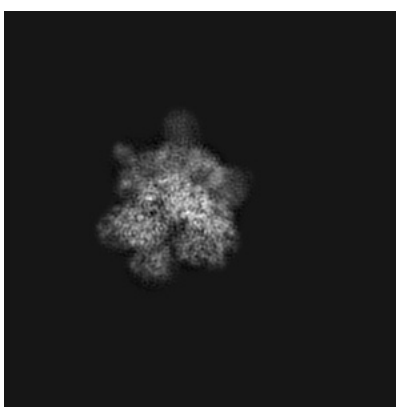
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

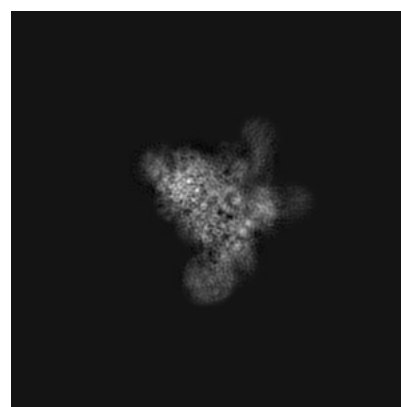
6.1.1 Primary map



X



Y

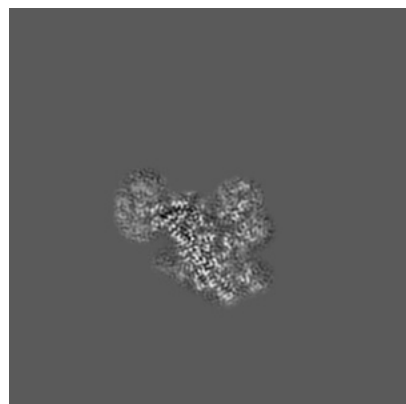


Z

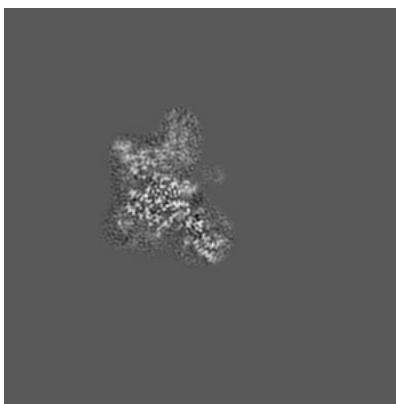
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

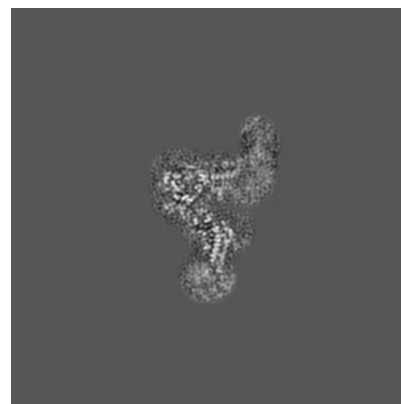
6.2.1 Primary map



X Index: 192



Y Index: 192

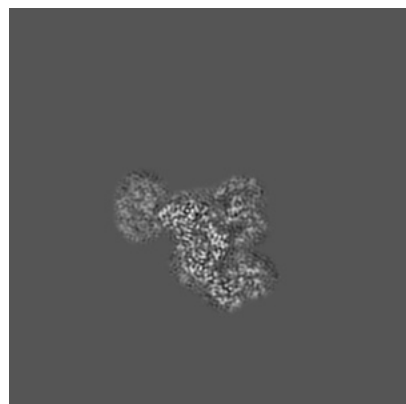


Z Index: 192

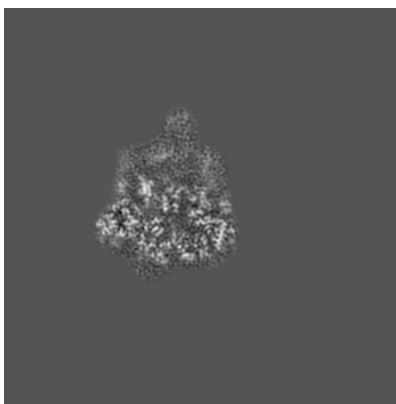
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

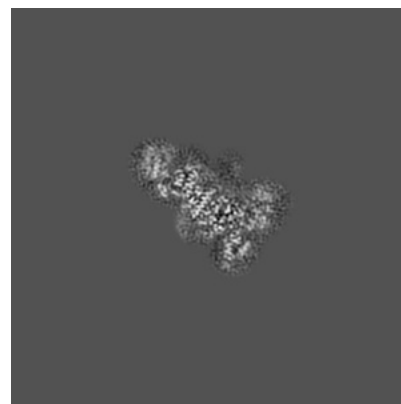
6.3.1 Primary map



X Index: 186



Y Index: 211

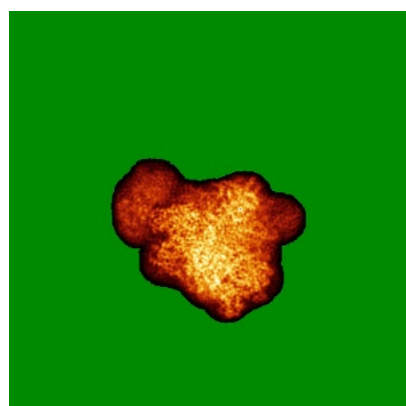


Z Index: 147

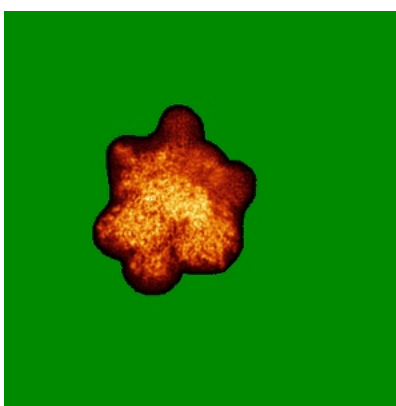
The images above show the largest variance slices of the map in three orthogonal directions.

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

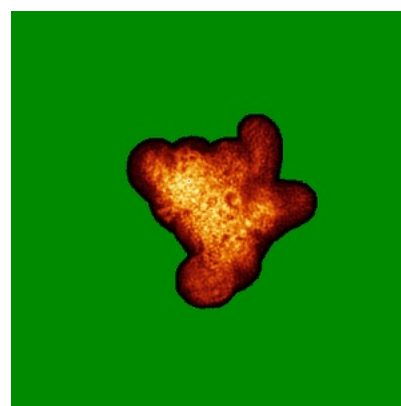
6.4.1 Primary map



X



Y

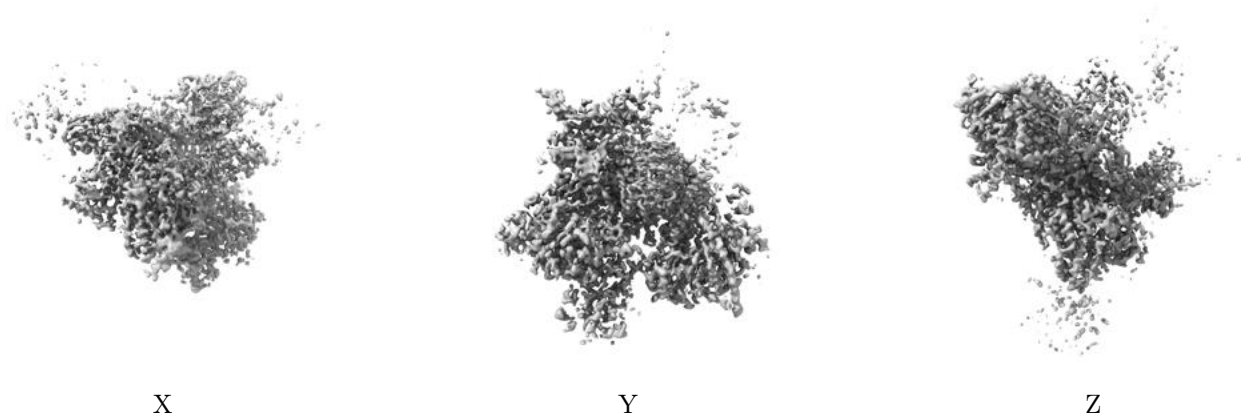


Z

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

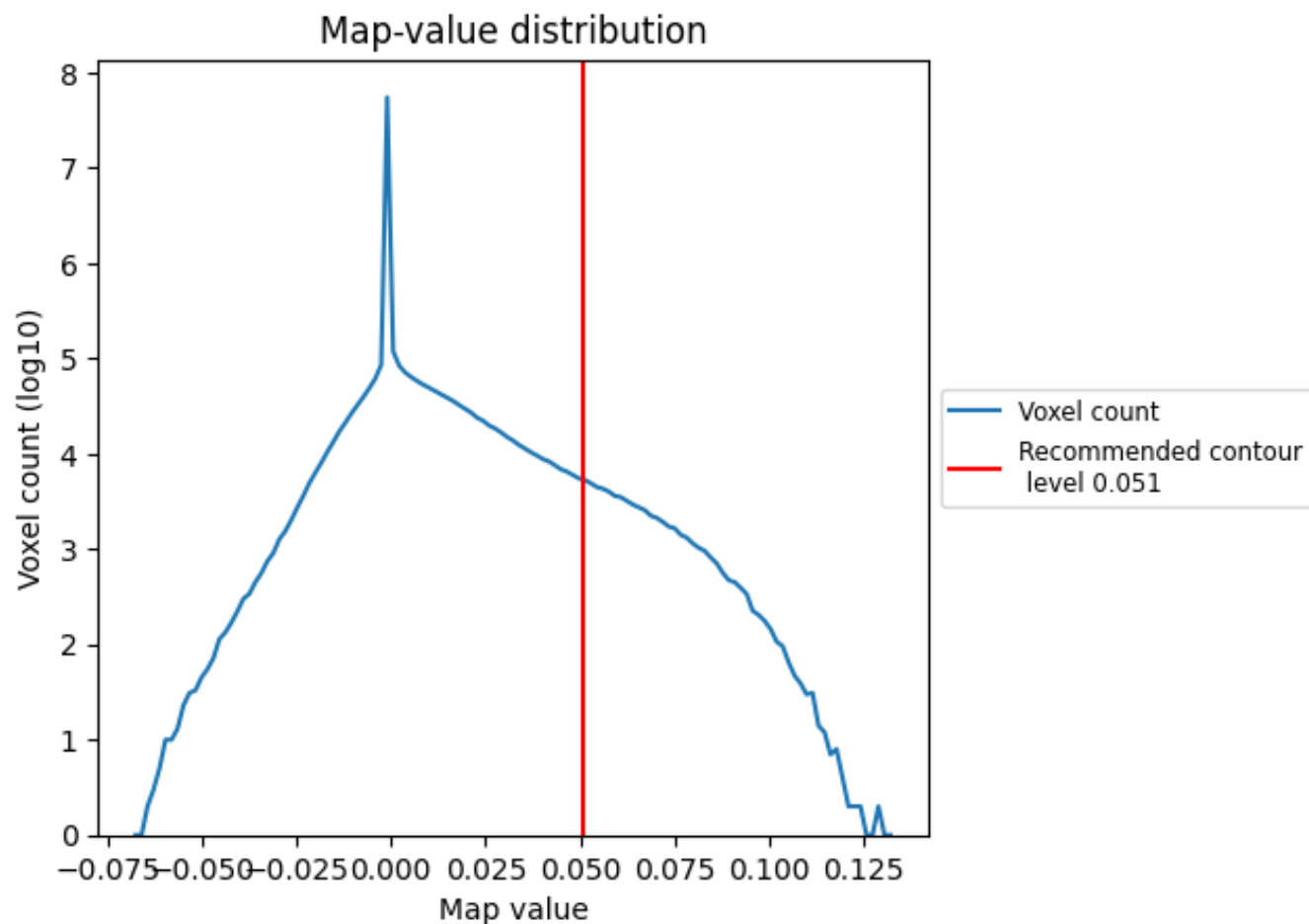
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

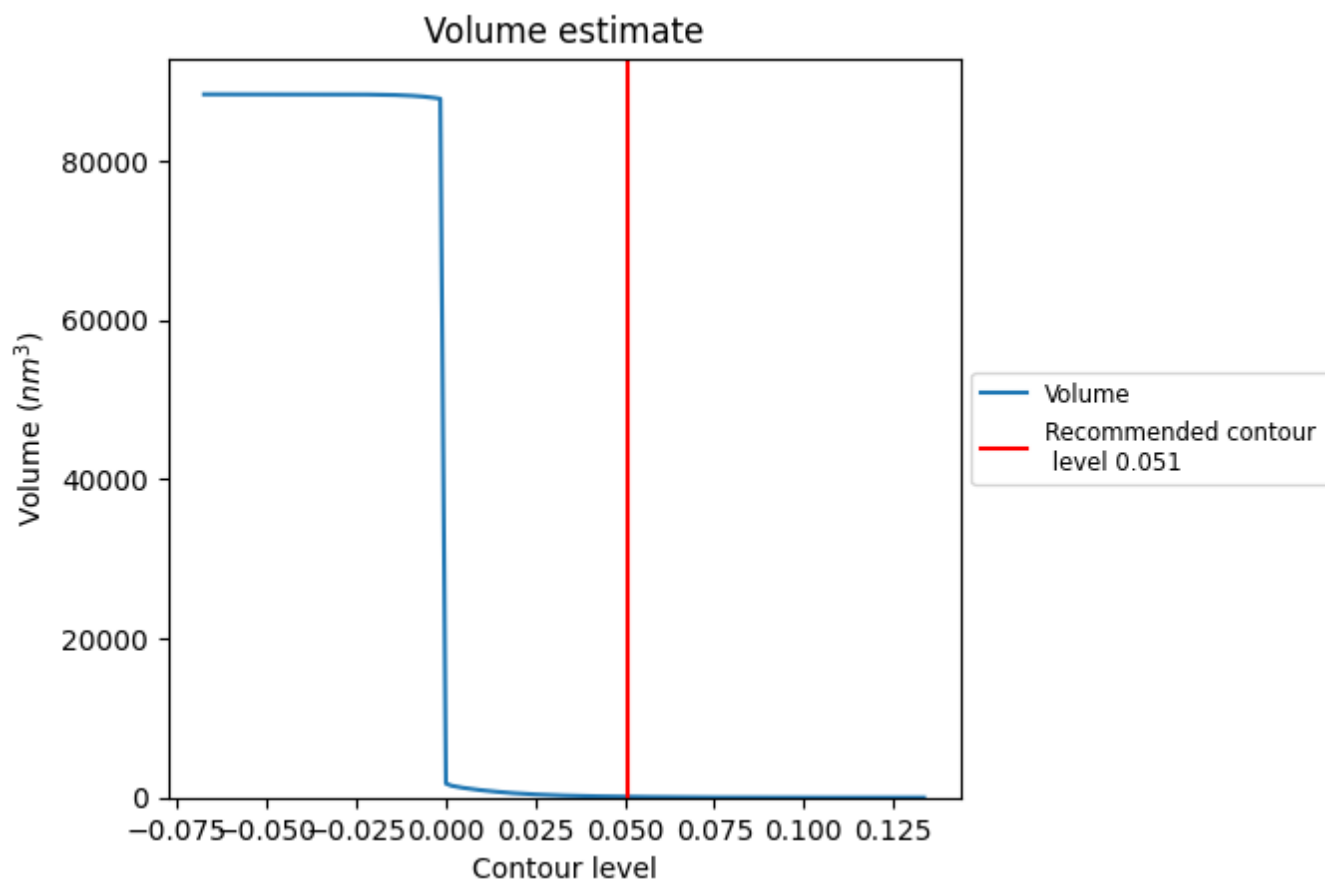
This section contains the results of statistical analysis of the map.

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.

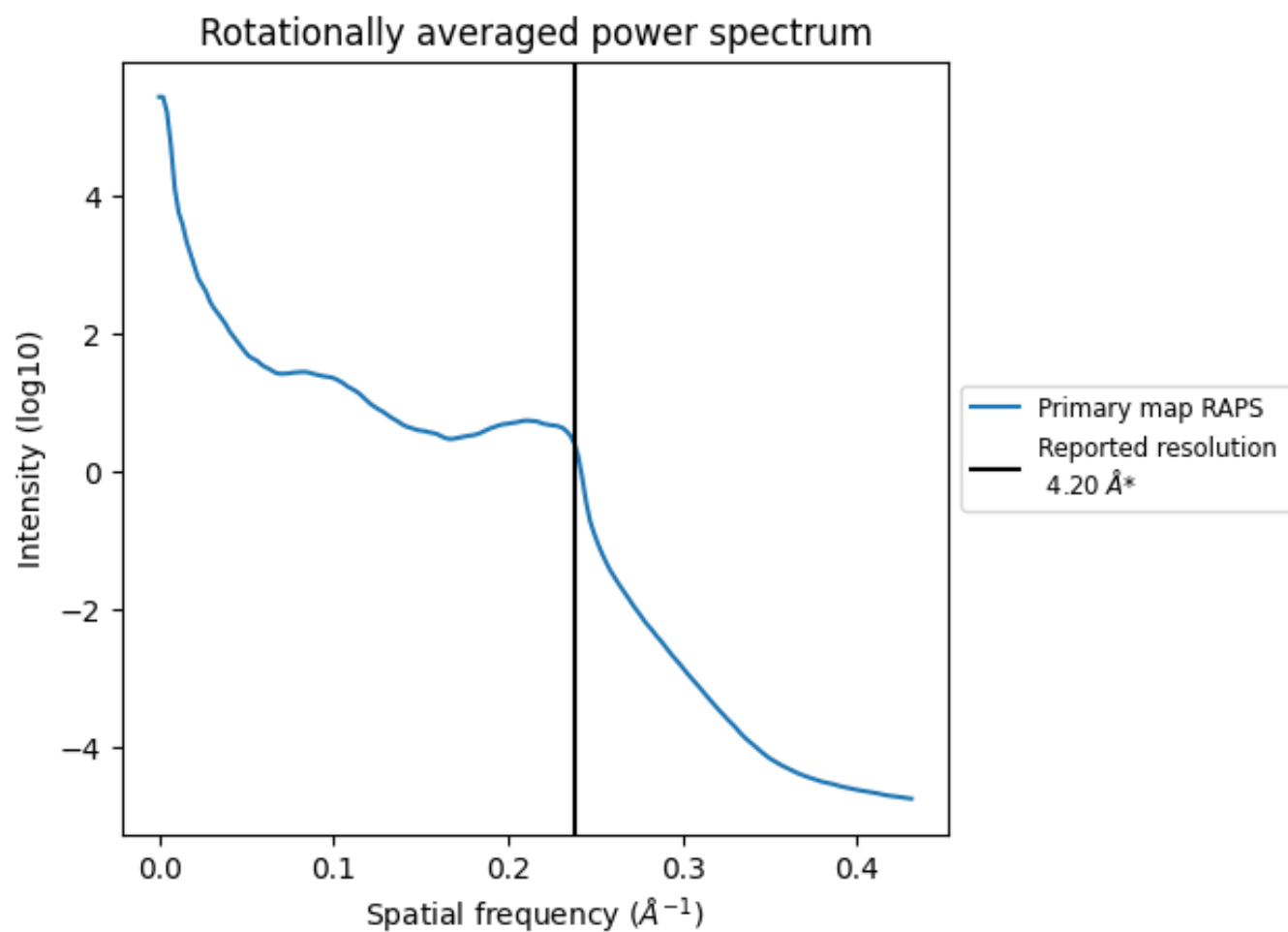
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm^3 ; this corresponds to an approximate mass of 89 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 0.238 Å⁻¹

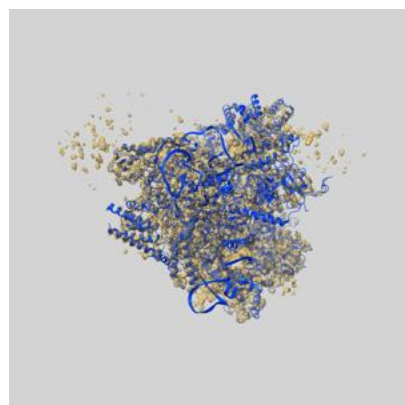
8 Fourier-Shell correlation

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

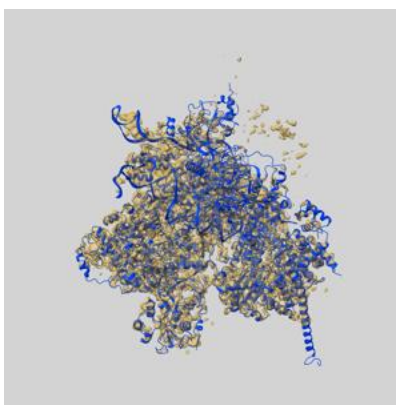
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11693 and PDB model 7AAV. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

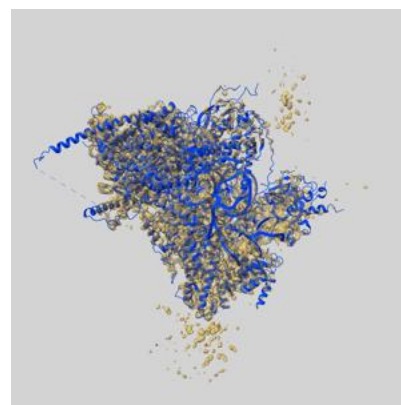
9.1 Map-model overlay [i](#)



X



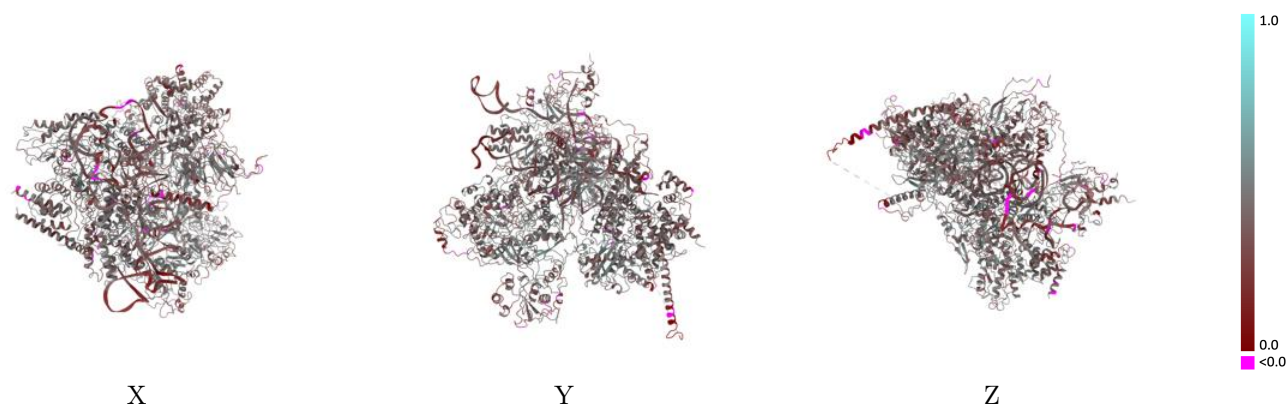
Y



Z

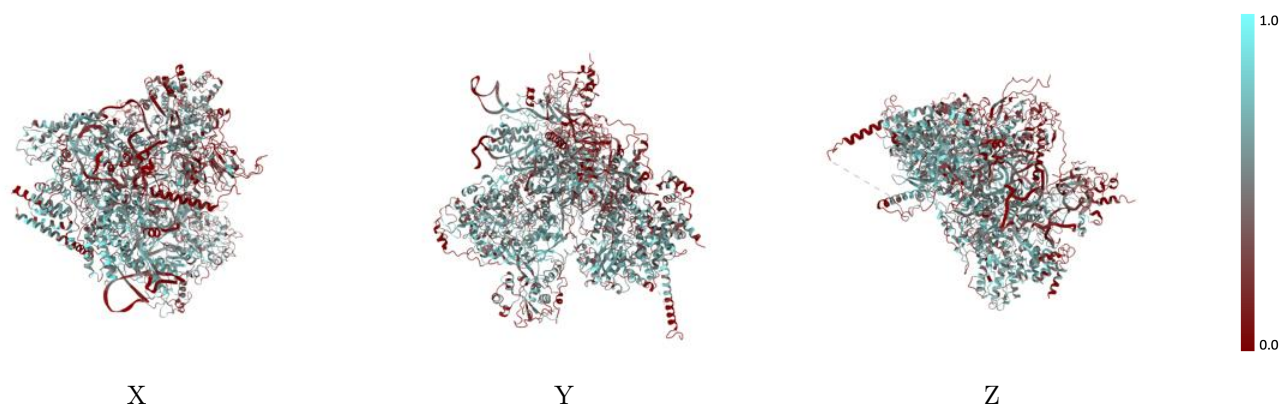
The images above show the 3D surface view of the map at the recommended contour level 0.051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



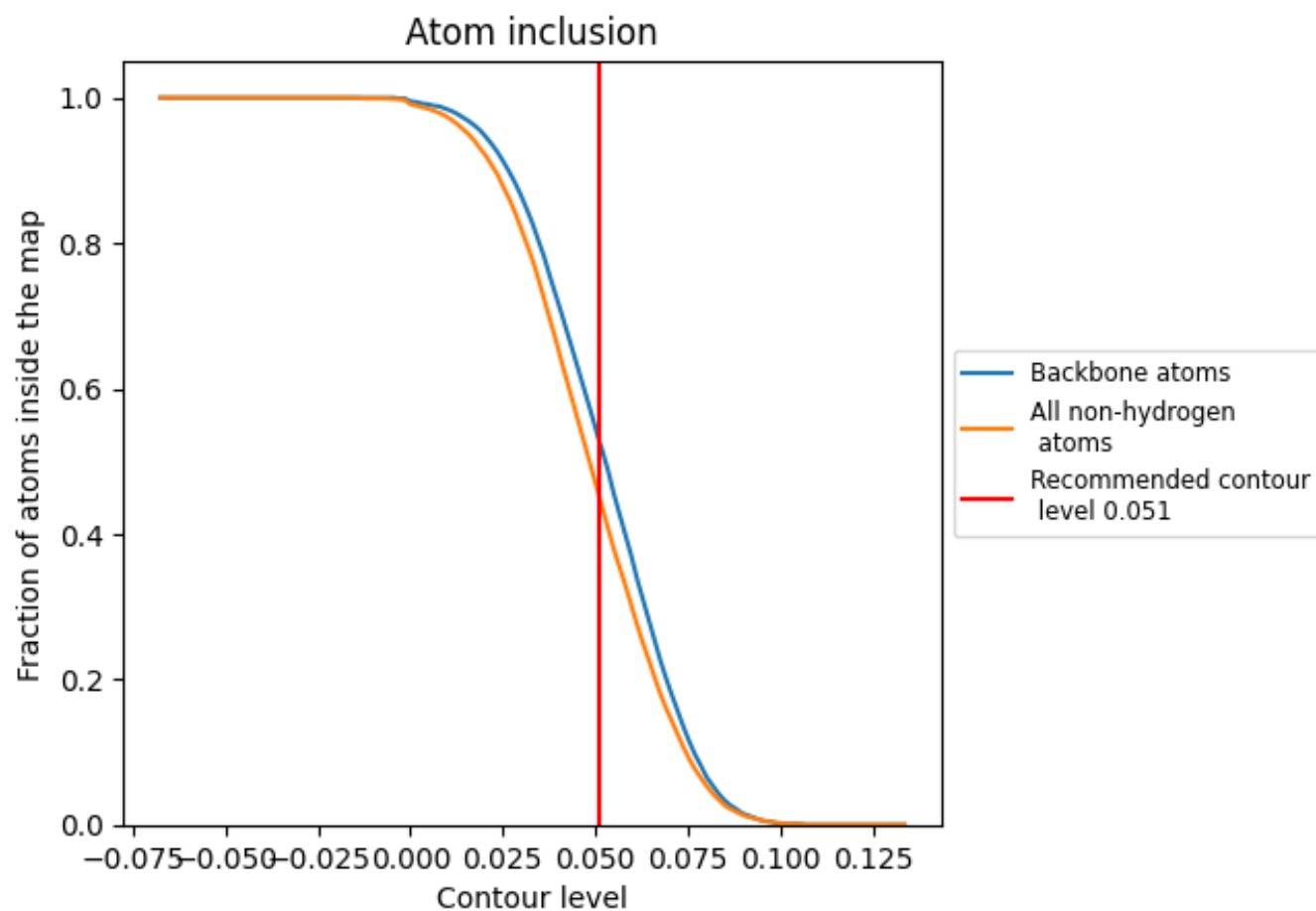
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.051).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 45% 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 (0.051) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4530	 0.3930
2	 0.1860	 0.3280
5	 0.4970	 0.3280
6	 0.3260	 0.2800
8	 0.0110	 0.2700
A	 0.5370	 0.4200
G	 0.2910	 0.4130
I	 0.5780	 0.4240
K	 0.3490	 0.3950
L	 0.3060	 0.3380
N	 0.1370	 0.3080
P	 0.2580	 0.3730
Q	 0.6010	 0.4330
R	 0.1730	 0.3470
Z	 0.3750	 0.3140
q	 0.5890	 0.4790
r	 0.4990	 0.4170
v	 0.1550	 0.3000

