



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2024 – 07:59 AM EST

PDB ID : 6N7P
EMDB ID : EMD-0360
Title : *S. cerevisiae* spliceosomal E complex (UBC4)
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2018-11-27
Resolution : 3.60 Å (reported)

This is a wwPDB EM Validation Summary 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:

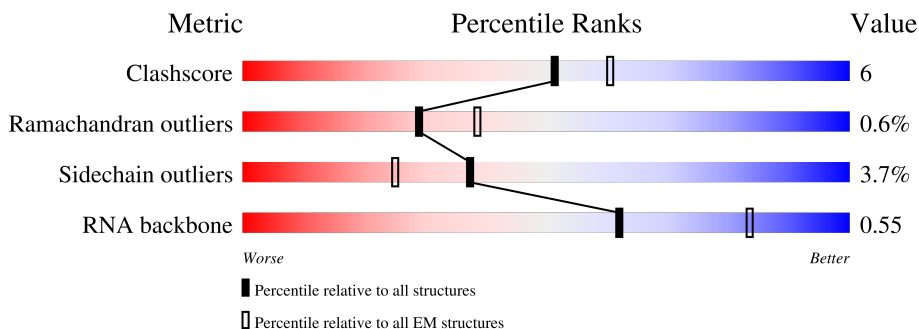
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	300	
2	B	231	
3	C	350	
4	D	544	
5	E	629	
6	F	523	
7	G	492	

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Mol	Chain	Length	Quality of chain
8	H	105	 21% 94% 6%
9	I	261	 22% 63% 9% 26%
10	J	583	 34% 33% 66%
11	K	196	 58% 5% 37%
12	L	146	 70% 12% 18%
13	M	110	 7% 79% 18% 8%
14	N	101	 79% 12% 8%
15	O	94	 70% 9% 21%
16	P	86	 67% 16% 14%
17	Q	77	 77% 14% 8%
18	R	568	 51% 52% 38% 8%
19	r	253	 6% 91% 8%
20	X	861	 96% 89% 5% 8%
21	Y	208	 66% 65% 34%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 41488 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 U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	186	1207	745	228	233	1	0	0

- Molecule 2 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1570	976	301	288	5	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	132	1058	674	193	187	4	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLY	-	expression tag	UNP P32605
C	300	ARG	-	expression tag	UNP P32605
C	301	ARG	-	expression tag	UNP P32605
C	302	ILE	-	expression tag	UNP P32605
C	303	PRO	-	expression tag	UNP P32605
C	304	GLY	-	expression tag	UNP P32605
C	305	LEU	-	expression tag	UNP P32605
C	306	ILE	-	expression tag	UNP P32605
C	307	ASN	-	expression tag	UNP P32605
C	308	PRO	-	expression tag	UNP P32605
C	309	TRP	-	expression tag	UNP P32605
C	310	LYS	-	expression tag	UNP P32605
C	311	ARG	-	expression tag	UNP P32605
C	312	ARG	-	expression tag	UNP P32605
C	313	TRP	-	expression tag	UNP P32605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
C	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
C	320	VAL	-	expression tag	UNP P32605
C	321	SER	-	expression tag	UNP P32605
C	322	ALA	-	expression tag	UNP P32605
C	323	ALA	-	expression tag	UNP P32605
C	324	ASN	-	expression tag	UNP P32605
C	325	ARG	-	expression tag	UNP P32605
C	326	PHE	-	expression tag	UNP P32605
C	327	LYS	-	expression tag	UNP P32605
C	328	LYS	-	expression tag	UNP P32605
C	329	ILE	-	expression tag	UNP P32605
C	330	SER	-	expression tag	UNP P32605
C	331	SER	-	expression tag	UNP P32605
C	332	SER	-	expression tag	UNP P32605
C	333	GLY	-	expression tag	UNP P32605
C	334	ALA	-	expression tag	UNP P32605
C	335	LEU	-	expression tag	UNP P32605
C	336	ASP	-	expression tag	UNP P32605
C	337	TYR	-	expression tag	UNP P32605
C	338	ASP	-	expression tag	UNP P32605
C	339	ILE	-	expression tag	UNP P32605
C	340	PRO	-	expression tag	UNP P32605
C	341	THR	-	expression tag	UNP P32605
C	342	THR	-	expression tag	UNP P32605
C	343	ALA	-	expression tag	UNP P32605
C	344	SER	-	expression tag	UNP P32605
C	345	GLU	-	expression tag	UNP P32605
C	346	ASN	-	expression tag	UNP P32605
C	347	LEU	-	expression tag	UNP P32605
C	348	TYR	-	expression tag	UNP P32605
C	349	PHE	-	expression tag	UNP P32605
C	350	GLN	-	expression tag	UNP P32605

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	544	4561	2990	723	828	20	0	0

- Molecule 5 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	576	3981	2527	693	752	9	0	0

- Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	267	1818	1128	326	353	11	0	0

- Molecule 7 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	239	1954	1267	321	354	12	0	0

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	105	685	425	127	132	1	0	0

- Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	192	1409	878	262	258	11	0	0

- Molecule 10 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	198	984	588	198	198	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	123	1008	636	191	178	3	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	119	Total	C	N	O	S	0	0
			921	578	164	176	3		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	107	Total	C	N	O	S	0	0
			858	545	159	150	4		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	93	Total	C	N	O	S	0	0
			710	450	122	134	4		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	74	Total	C	N	O	S	0	0
			563	375	90	95	3		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	74	Total	C	N	O	S	0	0
			584	377	103	103	1		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	71	Total	C	N	O	S	0	0
			543	344	95	103	1		

- Molecule 18 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	558	Total	C	N	O	P	0	0
			11822	5287	2003	3974	558		

- Molecule 19 is a RNA chain called UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	22	Total	C	N	O	P	0	0
			471	211	85	153	22		

- Molecule 20 is a protein called Nuclear cap-binding protein complex subunit 1.

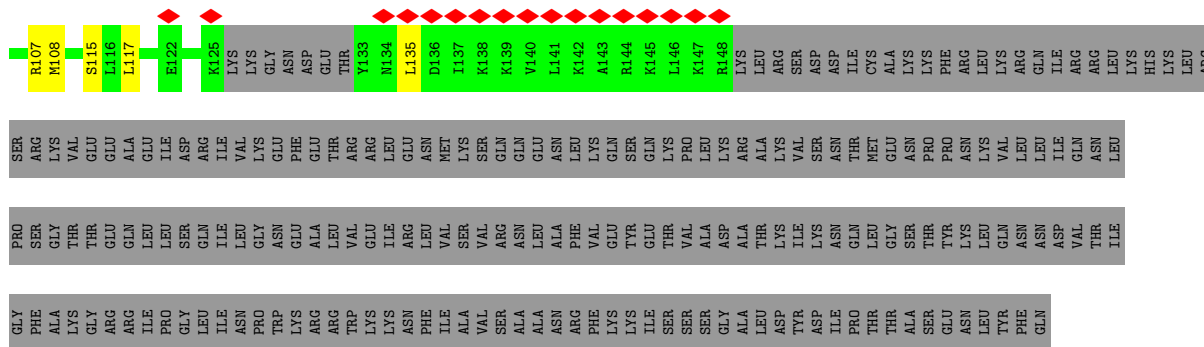
Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	826	Total	C	N	O	0	0
			4101	2449	826	826		

- Molecule 21 is a protein called Nuclear cap-binding protein subunit 2.

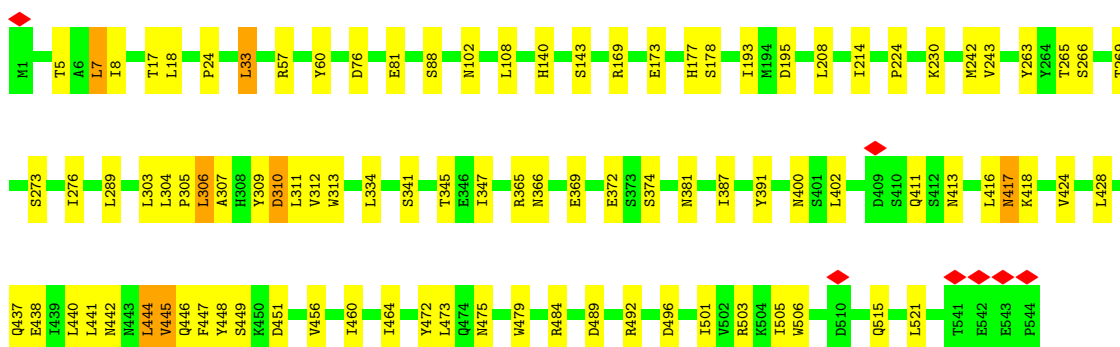
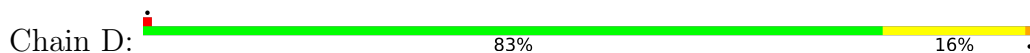
Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	138	Total	C	N	O	0	0
			677	401	138	138		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

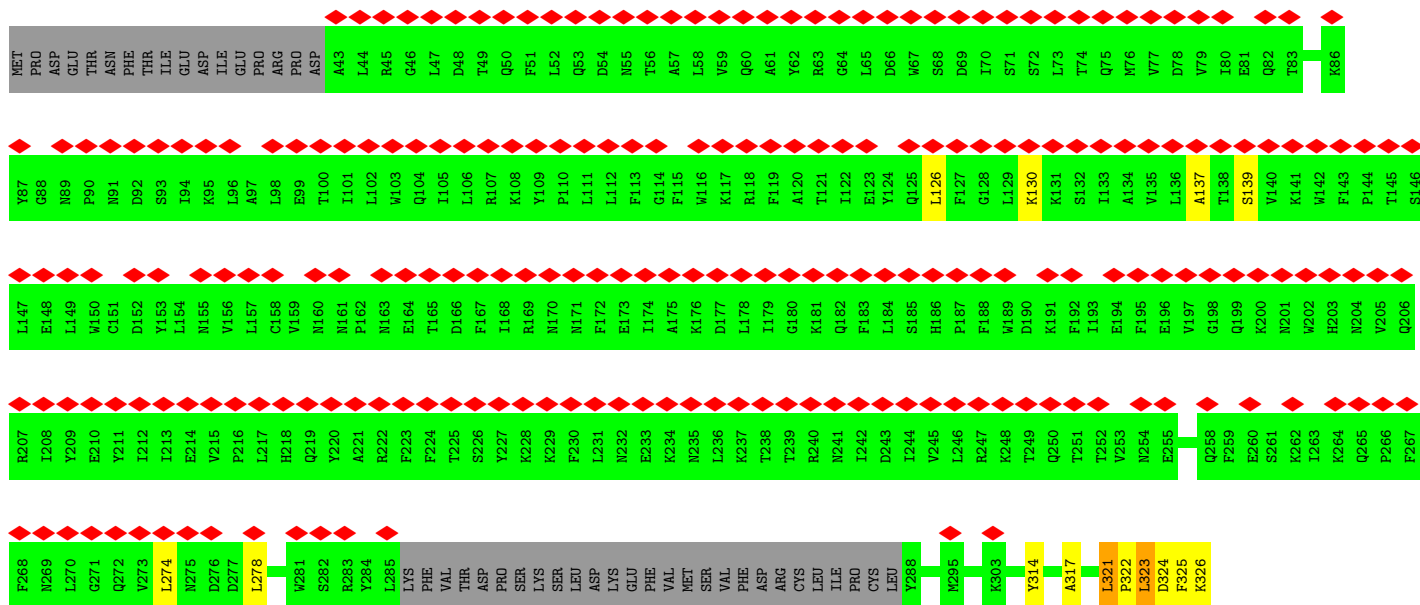
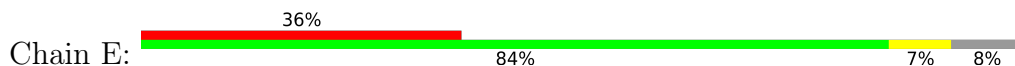
Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	

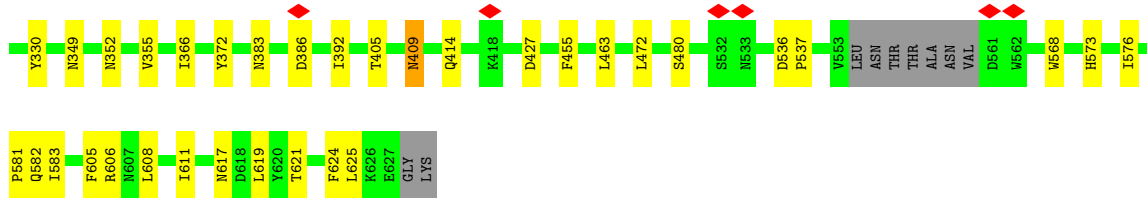


• Molecule 4: U1 small nuclear ribonucleoprotein component PRP42

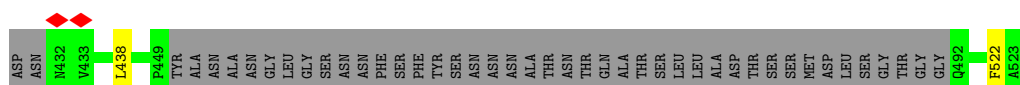
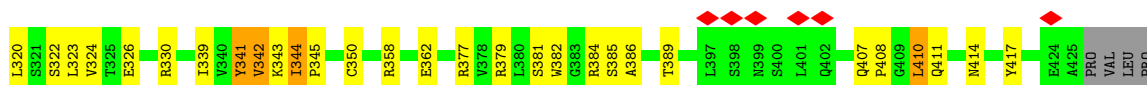
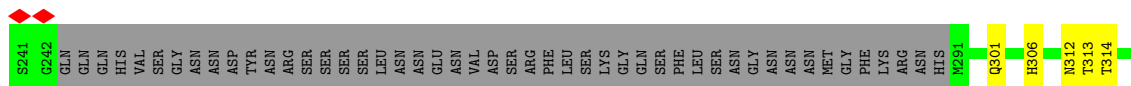
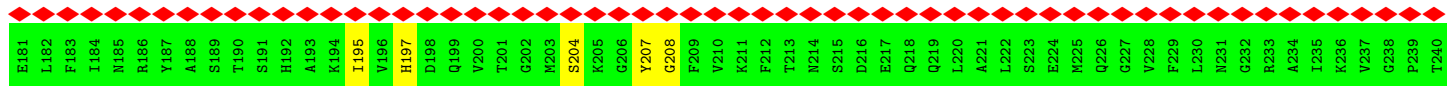
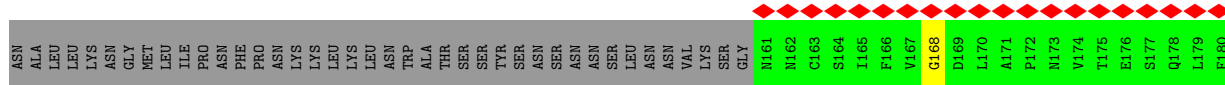
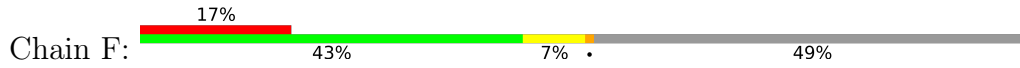


• Molecule 5: Pre-mRNA-processing factor 39

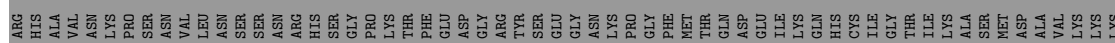
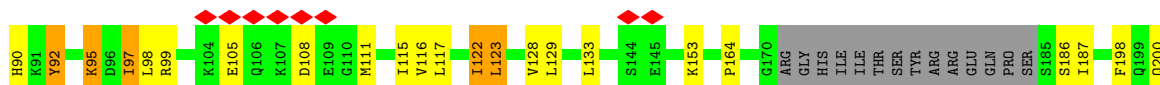
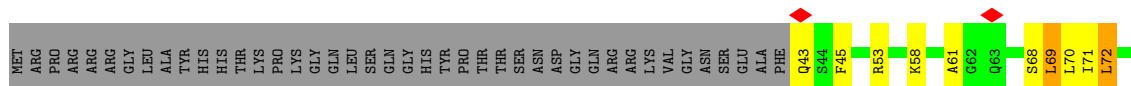
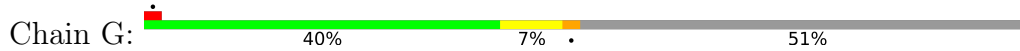


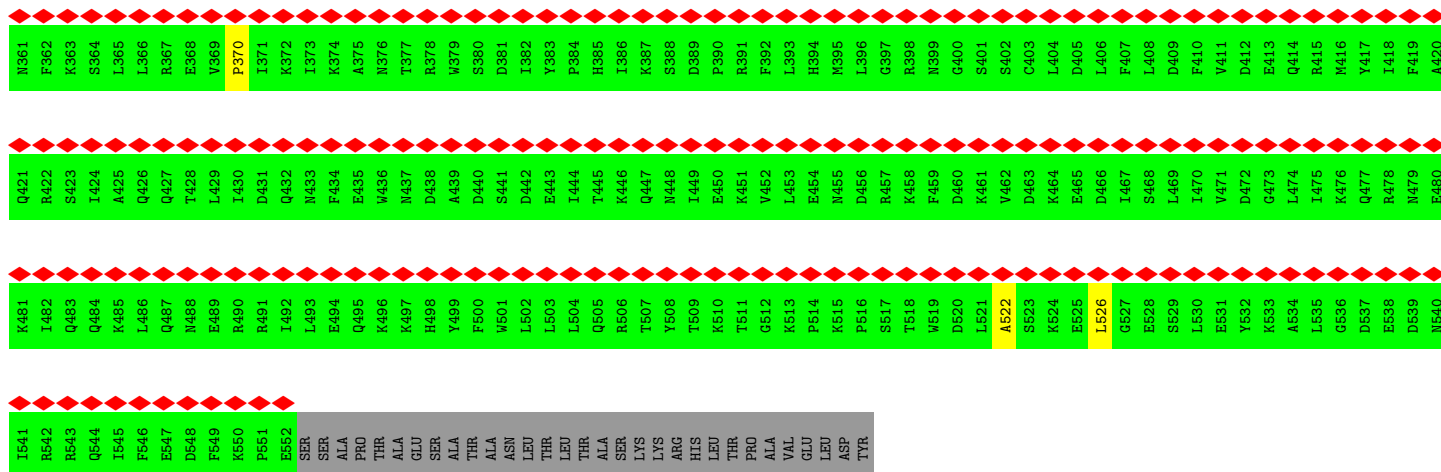


• Molecule 6: Protein NAM8

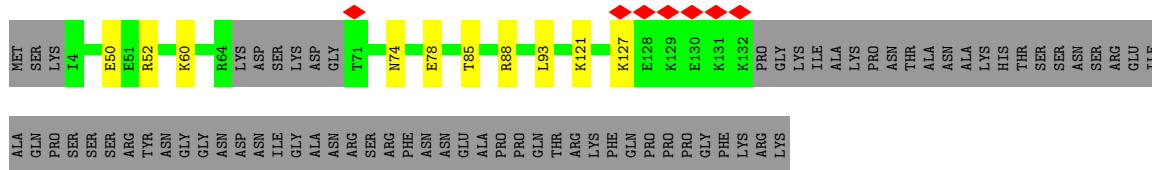


• Molecule 7: 56 kDa U1 small nuclear ribonucleoprotein component

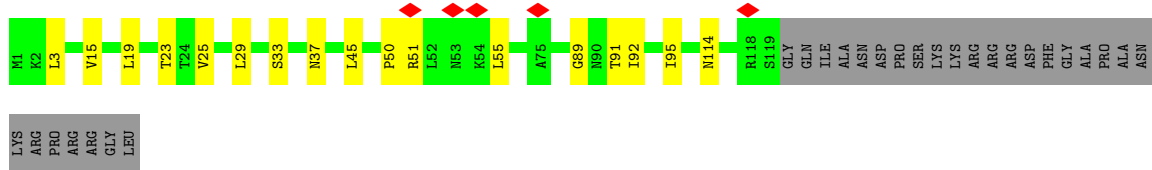




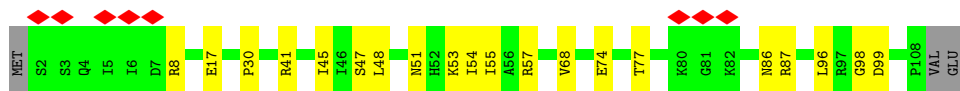
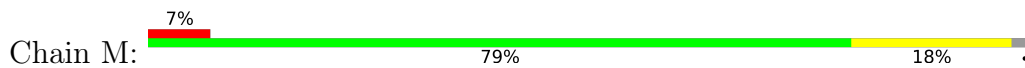
• Molecule 11: Small nuclear ribonucleoprotein-associated protein B



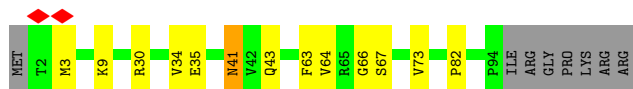
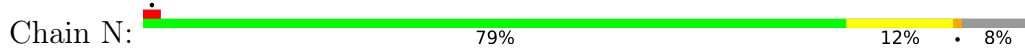
• Molecule 12: Small nuclear ribonucleoprotein Sm D1



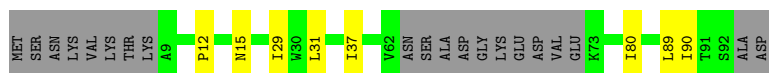
• Molecule 13: Small nuclear ribonucleoprotein Sm D2



• Molecule 14: Small nuclear ribonucleoprotein Sm D3



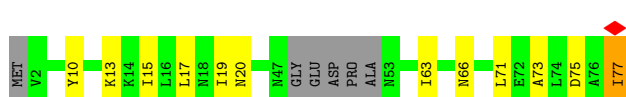
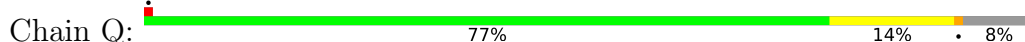
• Molecule 15: Small nuclear ribonucleoprotein E



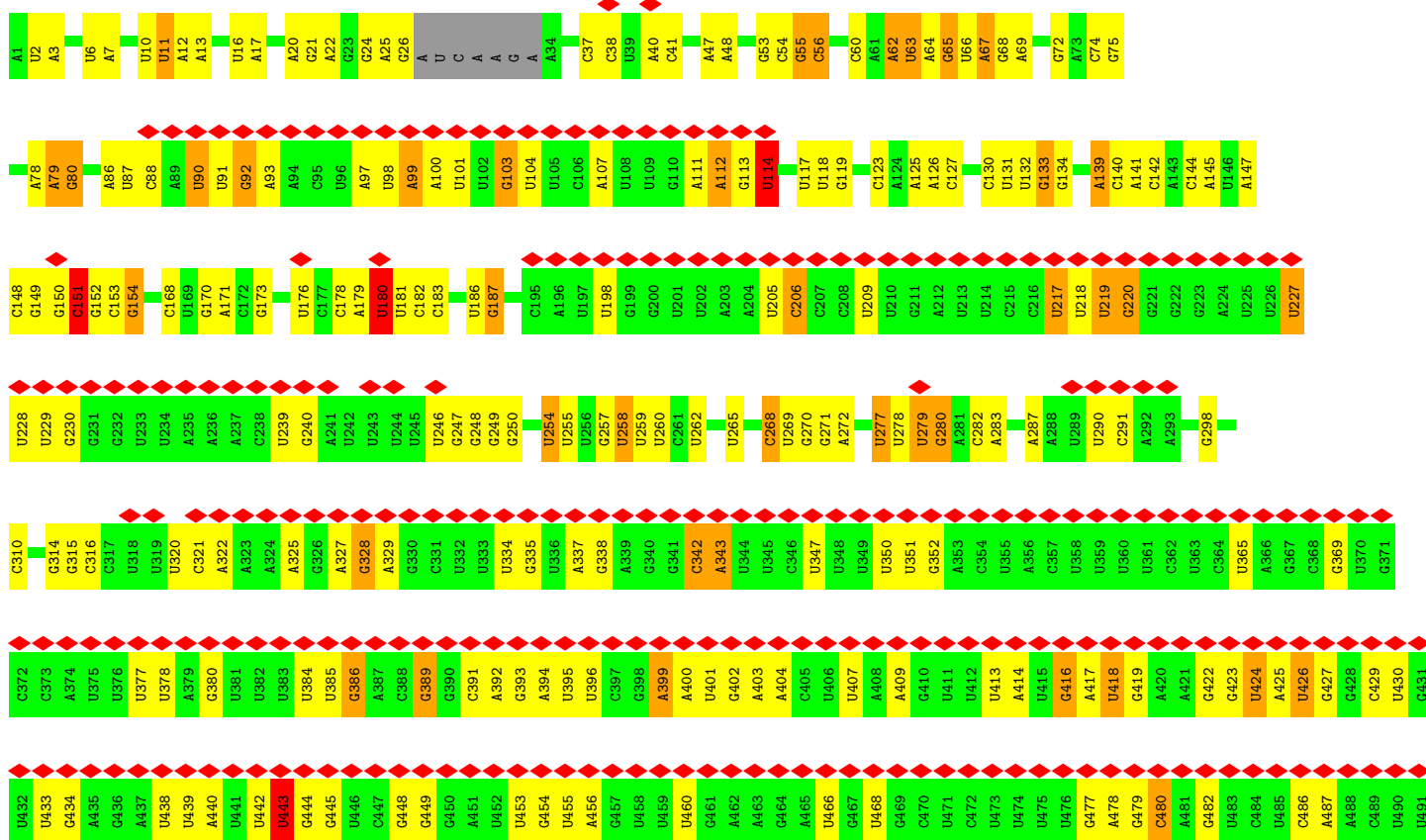
● Molecule 16: Small nuclear ribonucleoprotein F

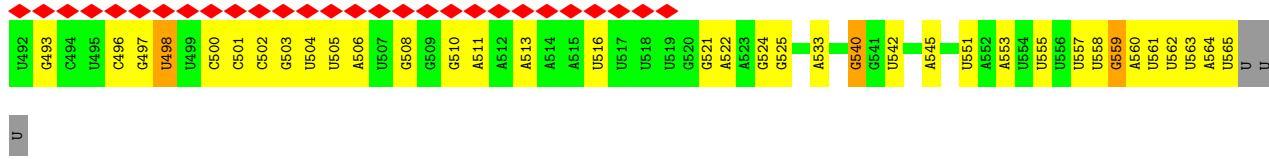


● Molecule 17: Small nuclear ribonucleoprotein G

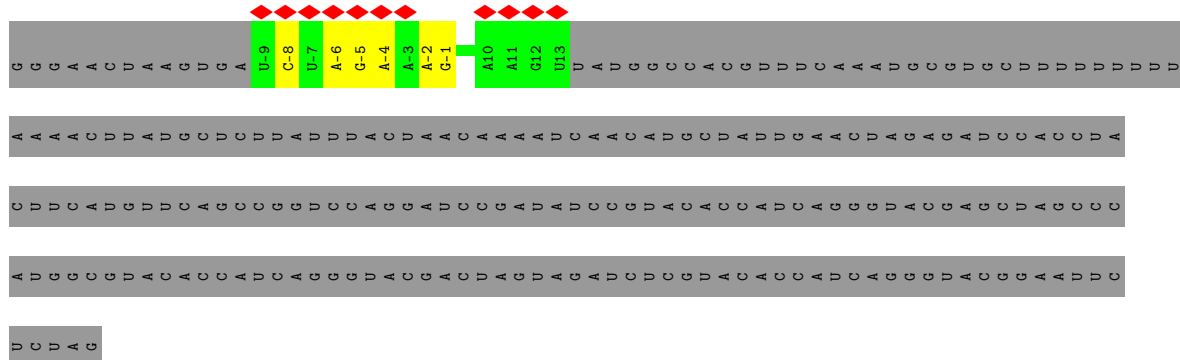


● Molecule 18: U1 snRNA

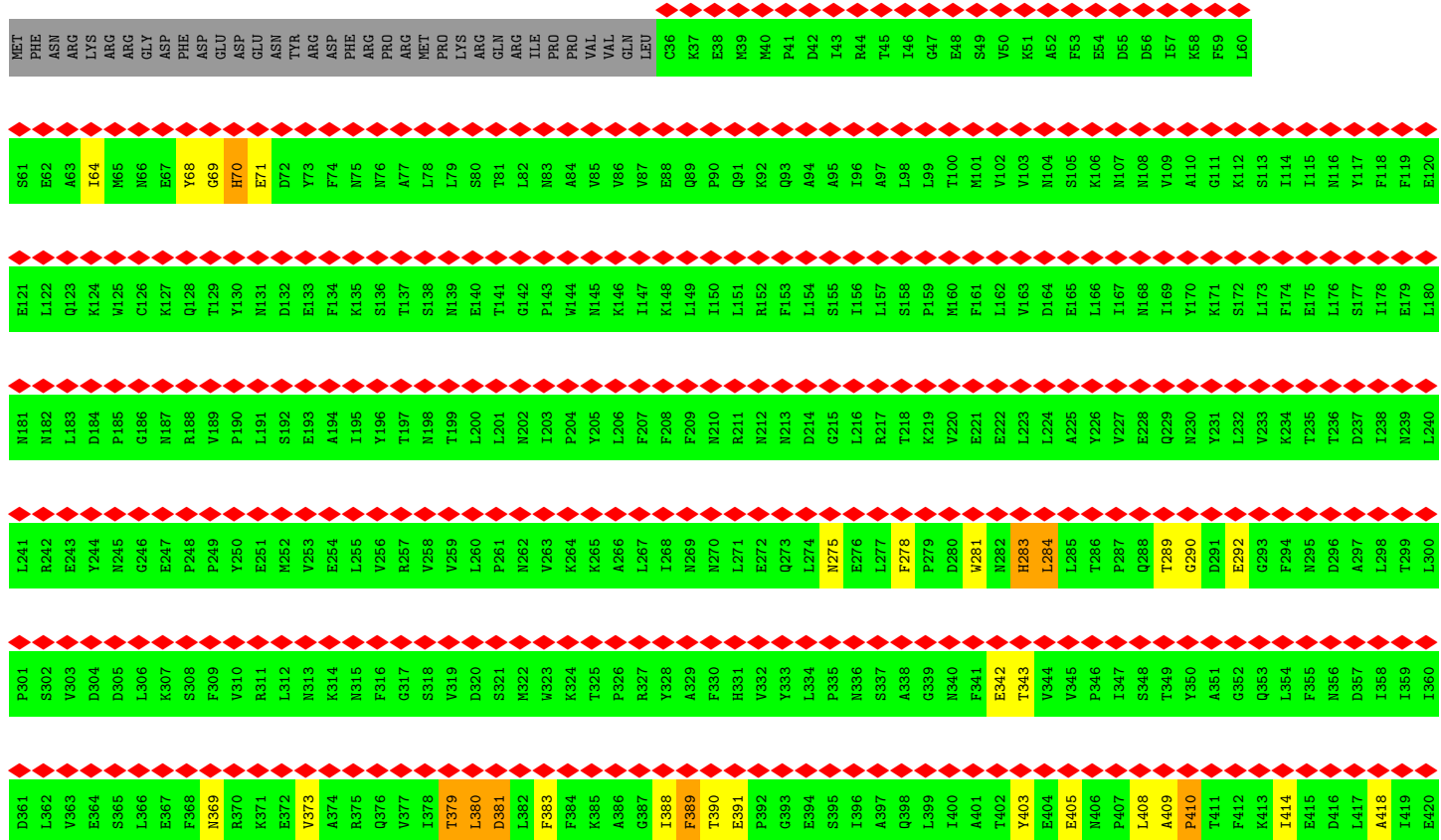
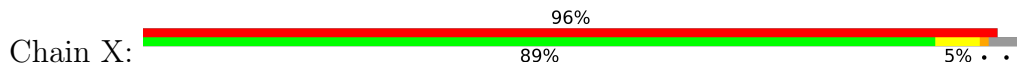




• Molecule 19: UBC4 pre-mRNA



• Molecule 20: Nuclear cap-binding protein complex subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124825	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.206	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	522.24, 522.24, 522.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.46	0/1224	0.59	0/1675
2	B	0.54	0/1601	0.65	0/2154
3	C	0.44	0/1072	0.68	0/1437
4	D	0.76	0/4676	0.72	0/6320
5	E	0.55	0/4046	0.60	0/5539
6	F	0.60	0/1844	0.68	0/2511
7	G	0.61	0/1996	0.68	0/2682
8	H	0.49	0/428	0.55	0/575
9	I	0.38	0/1428	0.60	0/1924
10	J	0.37	0/983	0.49	0/1371
11	K	0.66	0/1014	0.73	0/1350
12	L	0.57	0/930	0.73	0/1261
13	M	0.53	0/872	0.63	0/1174
14	N	0.71	0/722	0.72	0/979
15	O	0.55	0/573	0.68	0/778
16	P	0.65	0/597	0.74	0/809
17	Q	0.64	0/546	0.69	0/735
18	R	0.66	0/13201	1.19	79/20553 (0.4%)
19	r	0.52	0/527	1.05	0/819
20	X	0.26	0/4100	0.59	4/5721 (0.1%)
21	Y	0.26	0/676	0.55	0/937
All	All	0.59	0/43056	0.87	83/61304 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
20	X	0	24

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	26

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	227	U	N1-C2-O2	12.02	131.22	122.80
18	R	227	U	C2-N1-C1'	11.79	131.85	117.70
18	R	227	U	N3-C2-O2	-11.14	114.40	122.20
18	R	442	U	OP2-P-O3'	-10.46	82.18	105.20
18	R	442	U	OP1-P-O3'	-10.46	82.20	105.20

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	12	ARG	Peptide,Sidechain
20	X	281	TRP	Peptide
20	X	284	LEU	Peptide
20	X	69	GLY	Peptide
20	X	70	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1207	0	927	14	0
2	B	1570	0	1553	33	0
3	C	1058	0	1118	26	0
4	D	4561	0	4549	72	0
5	E	3981	0	3282	35	0
6	F	1818	0	1567	29	0
7	G	1954	0	1961	44	0
8	H	685	0	477	4	0
9	I	1409	0	1285	24	0
10	J	984	0	416	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1008	0	1109	9	0
12	L	921	0	972	10	0
13	M	858	0	882	13	0
14	N	710	0	730	16	0
15	O	563	0	594	5	0
16	P	584	0	586	11	0
17	Q	543	0	560	7	0
18	R	11822	0	5939	99	0
19	r	471	0	236	0	0
20	X	4101	0	1779	14	0
21	Y	677	0	298	1	0
22	B	1	0	0	0	0
22	I	2	0	0	0	0
All	All	41488	0	30820	413	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 6.

The worst 5 of 413 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:D:303:LEU:CD1	4:D:312:VAL:HG11	1.70	1.21
2:B:8:TYR:CE1	14:N:82:PRO:HG3	1.80	1.15
3:C:13:PRO:HD2	3:C:19:TYR:CD1	1.82	1.14
2:B:136:LEU:HD23	2:B:137:PRO:HD2	1.11	1.09
2:B:8:TYR:HE1	14:N:82:PRO:CG	1.64	1.09

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	A	182/300 (61%)	162 (89%)	17 (9%)	3 (2%)	9	46
2	B	193/231 (84%)	180 (93%)	10 (5%)	3 (2%)	9	46
3	C	126/350 (36%)	120 (95%)	6 (5%)	0	100	100
4	D	542/544 (100%)	515 (95%)	27 (5%)	0	100	100
5	E	570/629 (91%)	532 (93%)	38 (7%)	0	100	100
6	F	259/523 (50%)	240 (93%)	19 (7%)	0	100	100
7	G	235/492 (48%)	218 (93%)	17 (7%)	0	100	100
8	H	50/105 (48%)	47 (94%)	3 (6%)	0	100	100
9	I	186/261 (71%)	174 (94%)	11 (6%)	1 (0%)	29	68
10	J	196/583 (34%)	185 (94%)	10 (5%)	1 (0%)	29	68
11	K	119/196 (61%)	111 (93%)	8 (7%)	0	100	100
12	L	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
13	M	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
14	N	91/101 (90%)	84 (92%)	7 (8%)	0	100	100
15	O	70/94 (74%)	68 (97%)	2 (3%)	0	100	100
16	P	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
17	Q	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
20	X	824/861 (96%)	727 (88%)	80 (10%)	17 (2%)	7	40
21	Y	136/208 (65%)	120 (88%)	15 (11%)	1 (1%)	22	61
All	All	4140/5897 (70%)	3827 (92%)	287 (7%)	26 (1%)	29	64

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
2	B	139	ARG
10	J	370	PRO
20	X	71	GLU
20	X	284	LEU

5.3.2 Protein sidechains [i](#)

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	A	82/265 (31%)	78 (95%)	4 (5%)	25	59
2	B	171/214 (80%)	161 (94%)	10 (6%)	20	55
3	C	117/317 (37%)	112 (96%)	5 (4%)	29	63
4	D	508/519 (98%)	491 (97%)	17 (3%)	38	69
5	E	316/603 (52%)	307 (97%)	9 (3%)	43	72
6	F	157/451 (35%)	149 (95%)	8 (5%)	24	58
7	G	218/448 (49%)	207 (95%)	11 (5%)	24	59
8	H	48/48 (100%)	46 (96%)	2 (4%)	30	63
9	I	130/234 (56%)	124 (95%)	6 (5%)	27	61
11	K	114/176 (65%)	114 (100%)	0	100	100
12	L	107/129 (83%)	106 (99%)	1 (1%)	78	90
13	M	95/103 (92%)	94 (99%)	1 (1%)	73	88
14	N	81/89 (91%)	78 (96%)	3 (4%)	34	66
15	O	62/83 (75%)	62 (100%)	0	100	100
16	P	64/77 (83%)	59 (92%)	5 (8%)	12	44
17	Q	59/66 (89%)	55 (93%)	4 (7%)	16	50
All	All	2329/3822 (61%)	2243 (96%)	86 (4%)	37	66

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	95	LYS
9	I	118	ASN
7	G	122	ILE
8	H	51	ASN
14	N	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	407	GLN
9	I	40	HIS
6	F	411	GLN
7	G	90	HIS
9	I	118	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	556/568 (97%)	134 (24%)	18 (3%)
19	r	21/253 (8%)	6 (28%)	0
All	All	577/821 (70%)	140 (24%)	18 (3%)

5 of 140 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	10	U
18	R	11	U
18	R	12	A
18	R	13	A
18	R	17	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	277	U
18	R	505	U
18	R	399	A
18	R	133	G
18	R	268	C

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	52:SER	C	1262:UNK	N	64.87

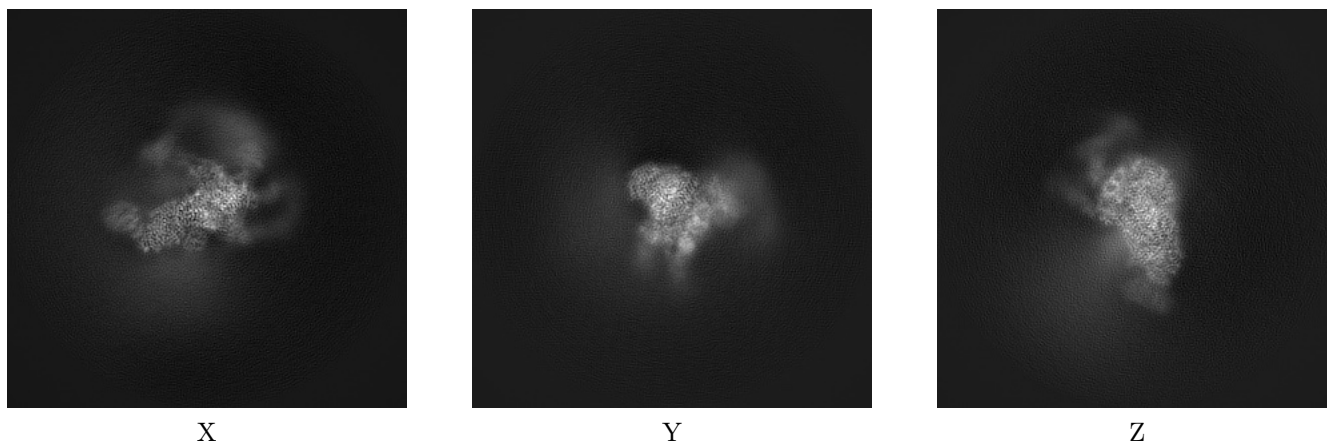
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0360. 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](#)

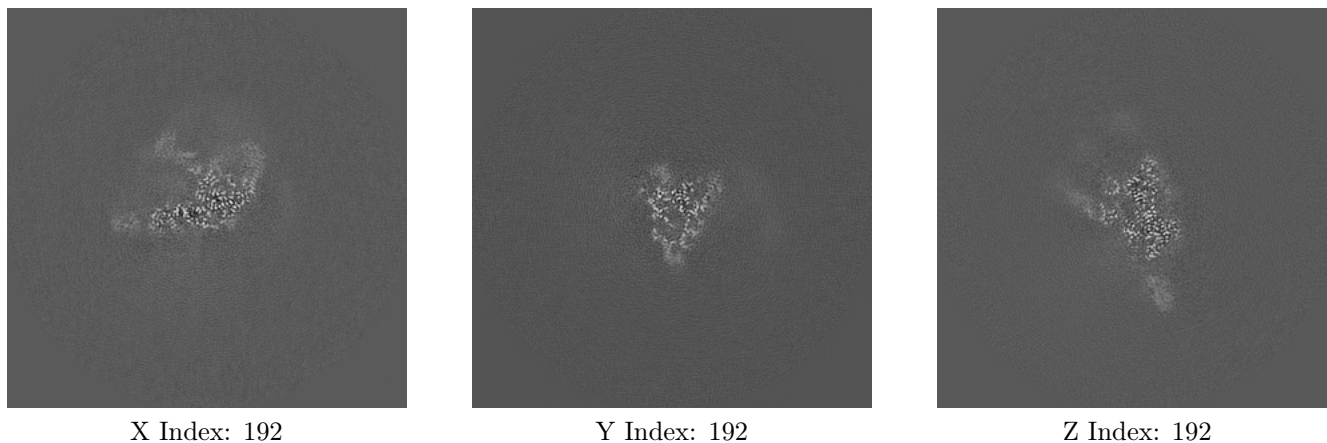
6.1.1 Primary map



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

6.2 Central slices [i](#)

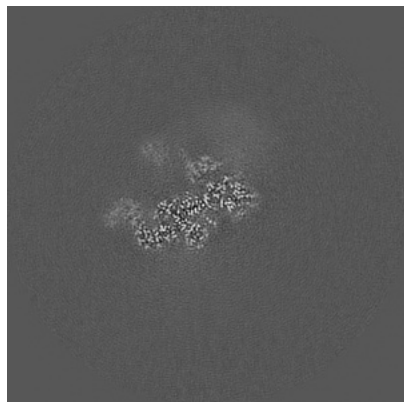
6.2.1 Primary map



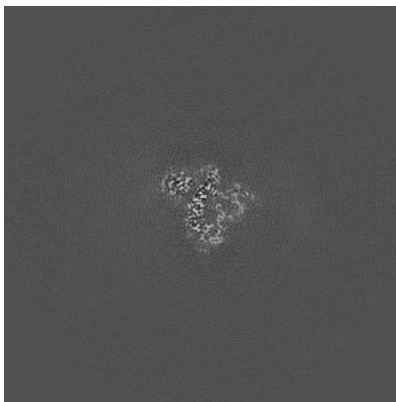
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

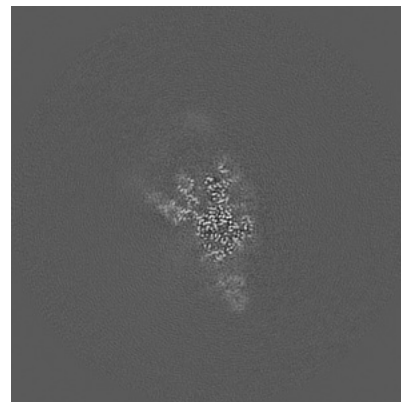
6.3.1 Primary map



X Index: 208



Y Index: 182

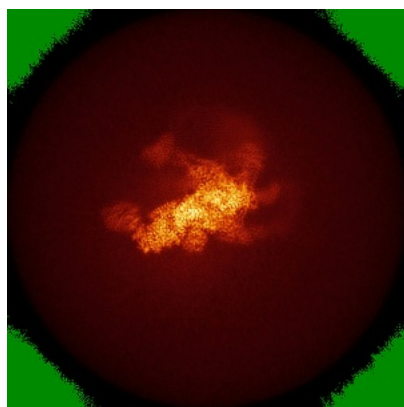


Z Index: 189

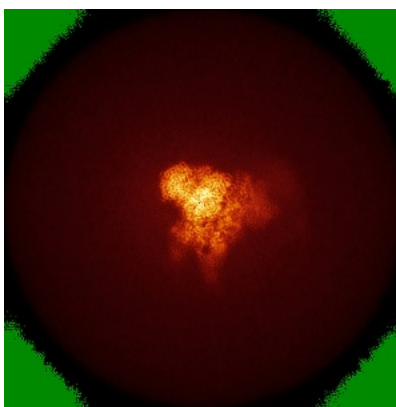
The images above show the largest variance slices of the map in three orthogonal directions.

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

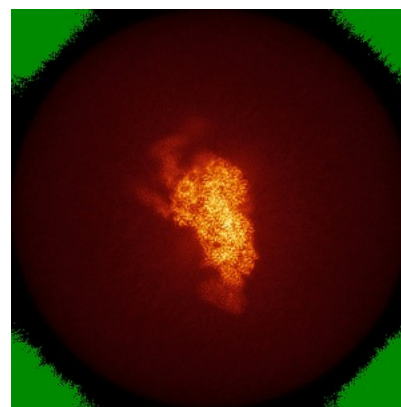
6.4.1 Primary map



X



Y

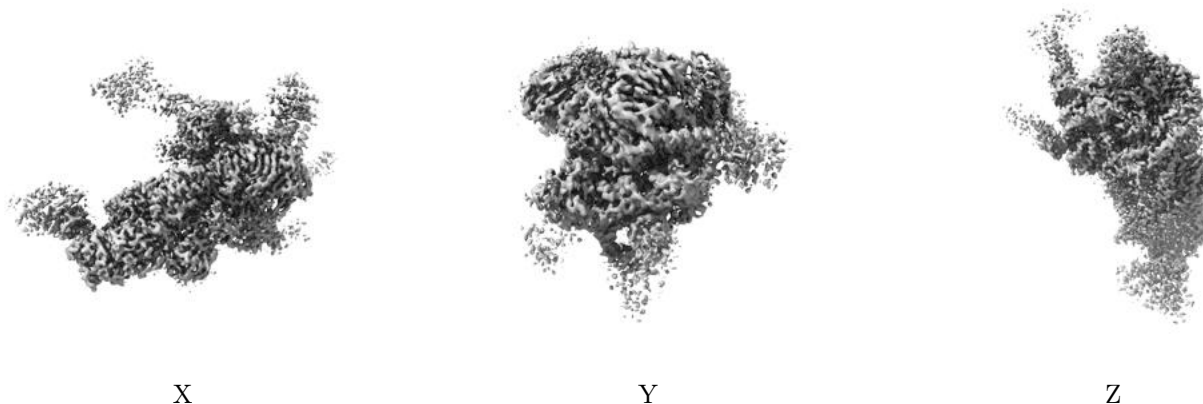


Z

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

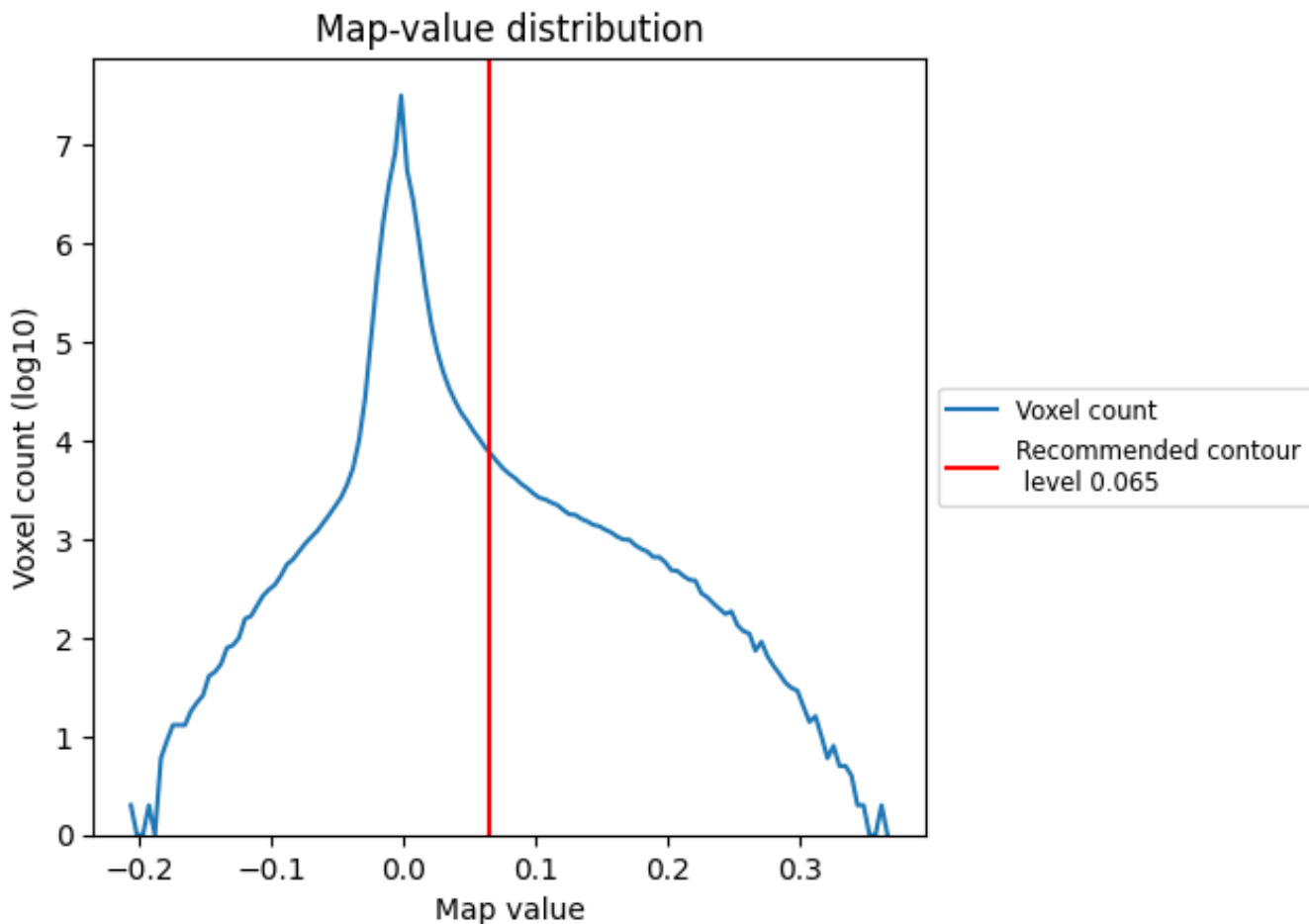
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

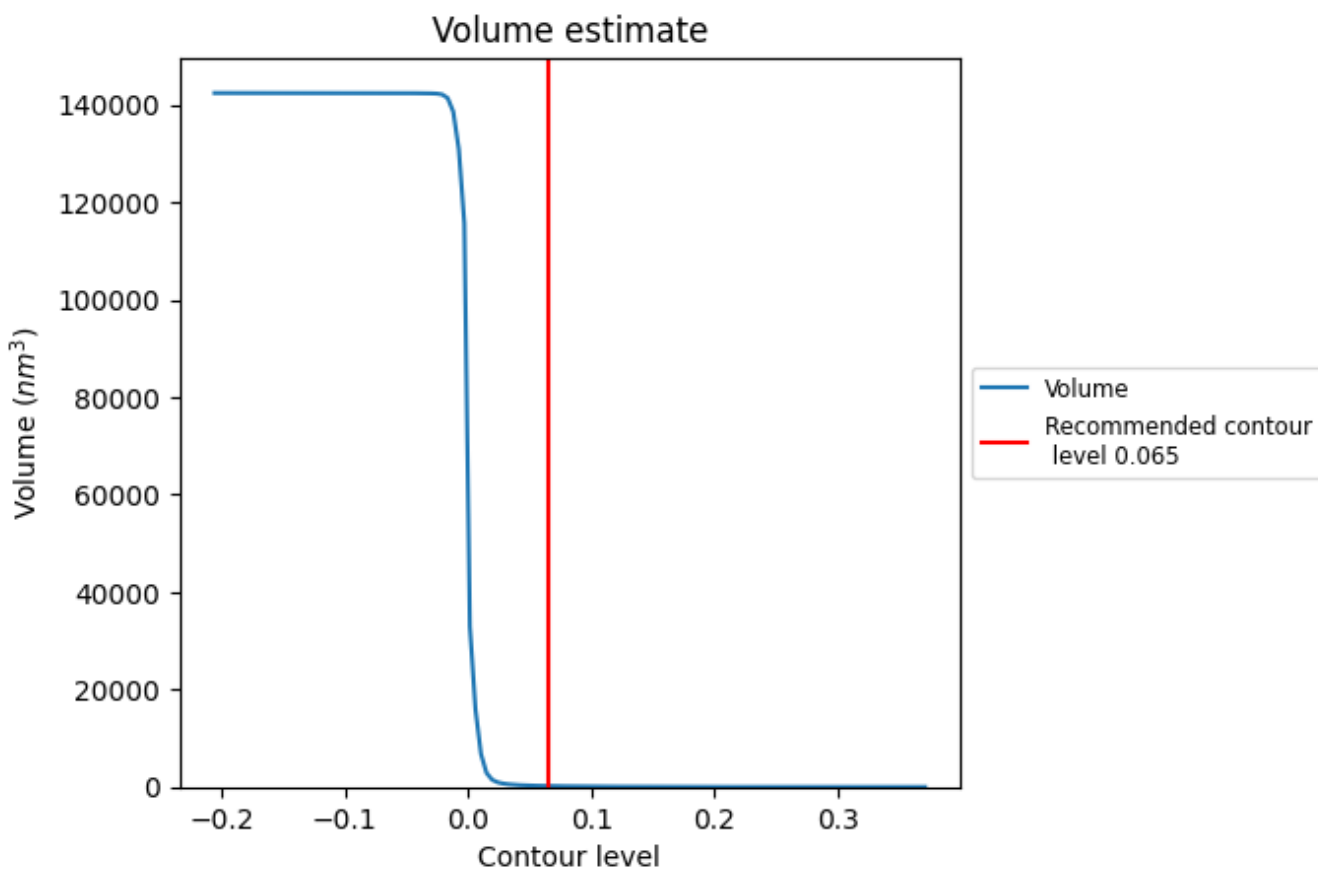
This section contains the results of statistical analysis of the map.

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.

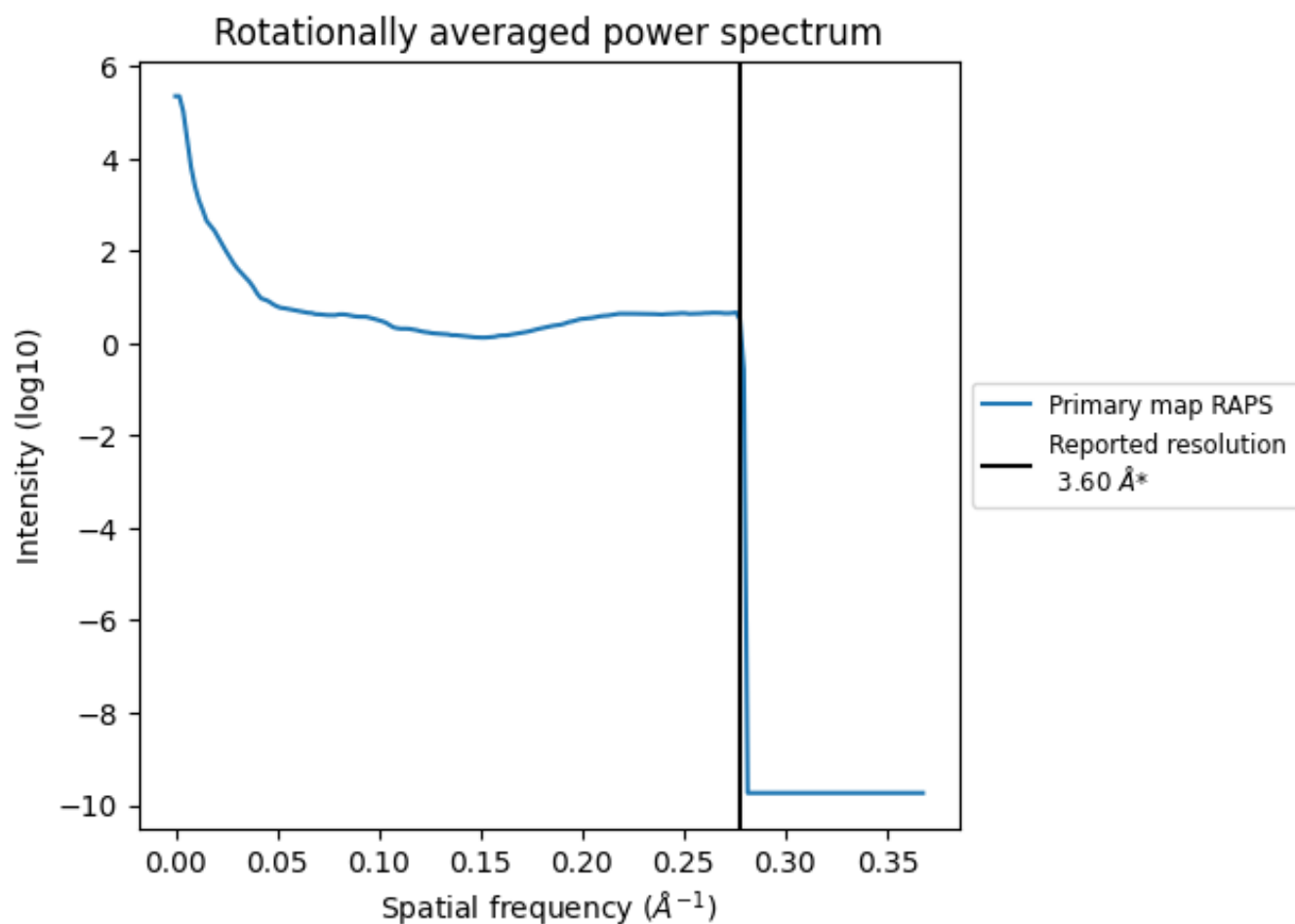
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 171 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 [\(i\)](#)

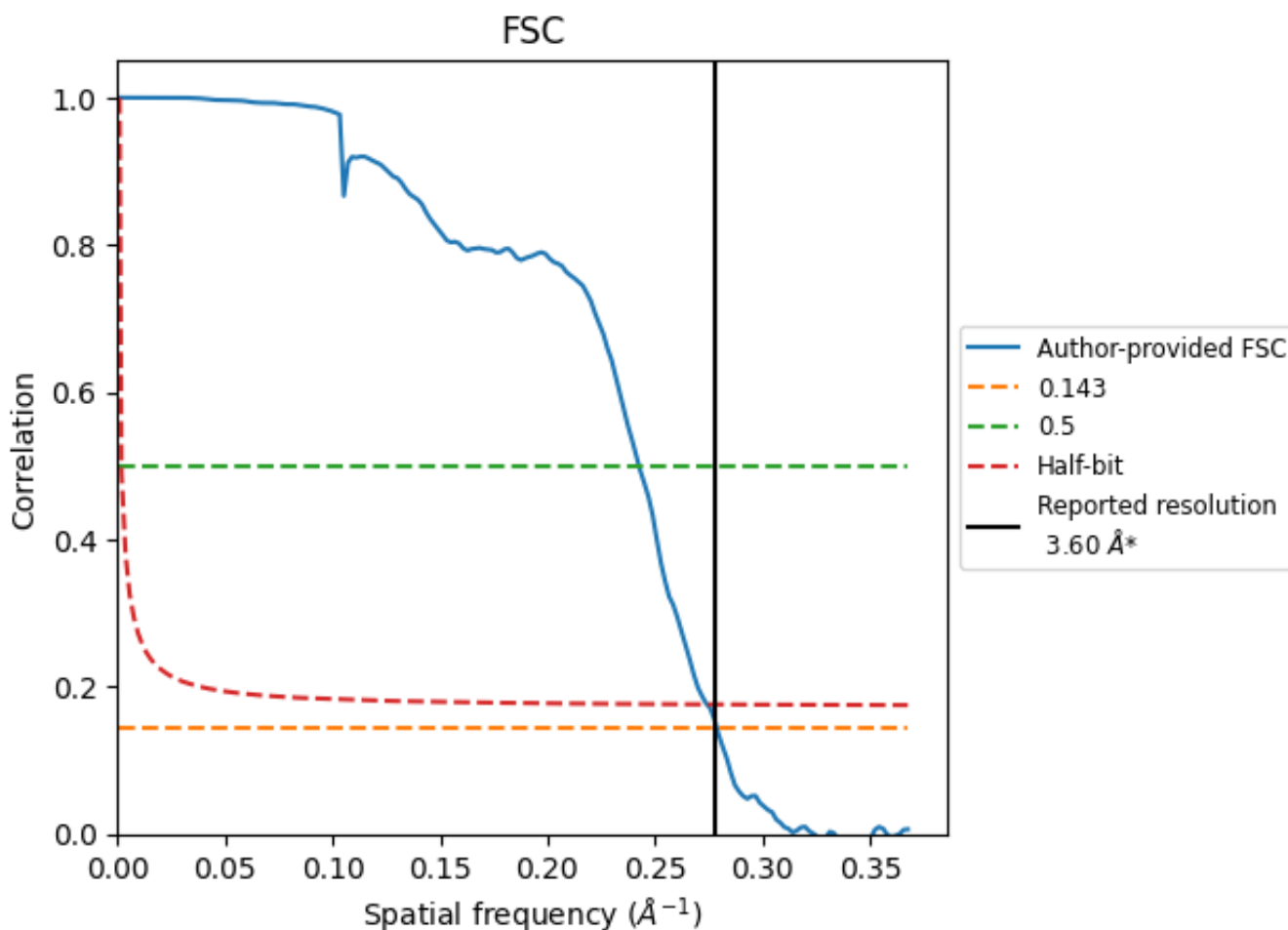


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

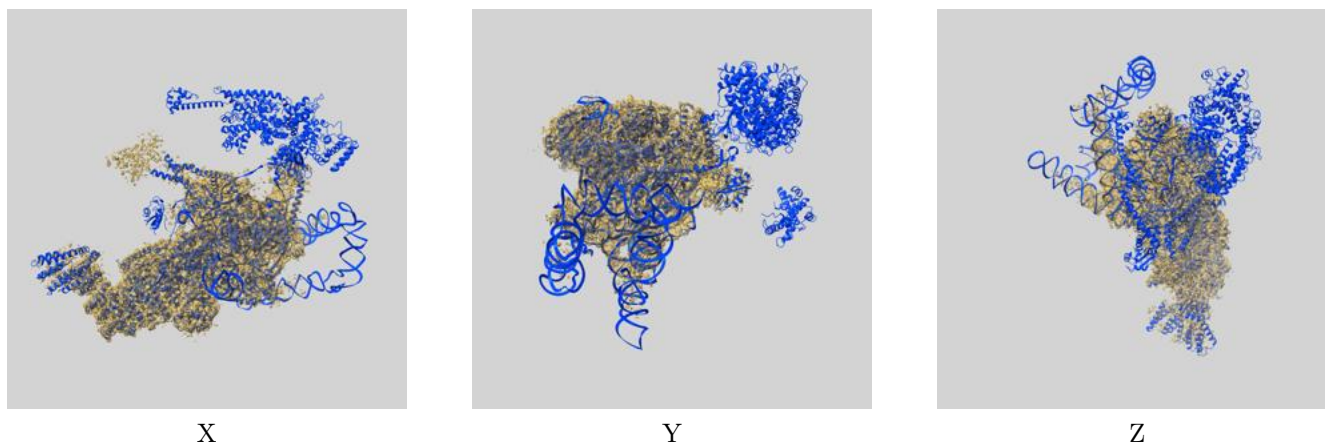
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.12	3.65
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

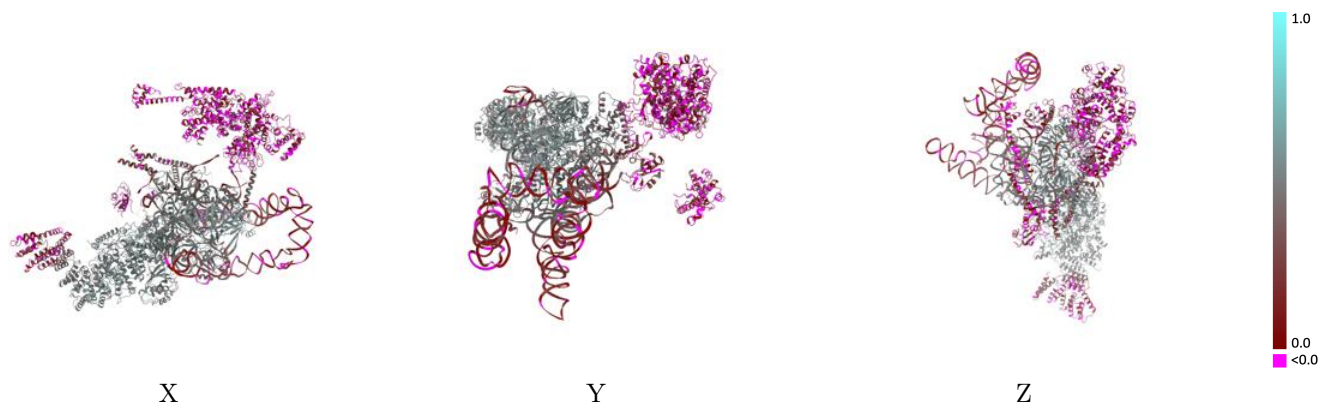
This section contains information regarding the fit between EMDB map EMD-0360 and PDB model 6N7P. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



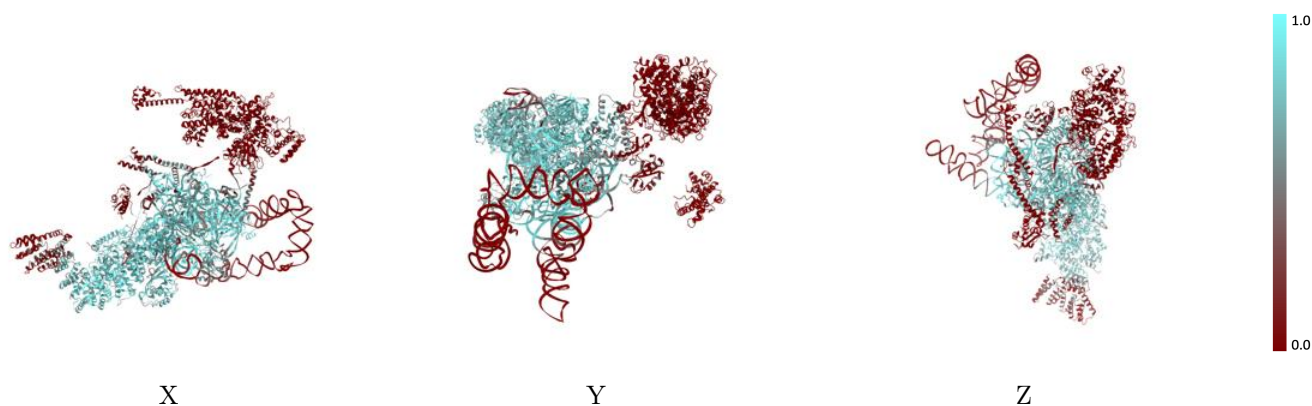
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



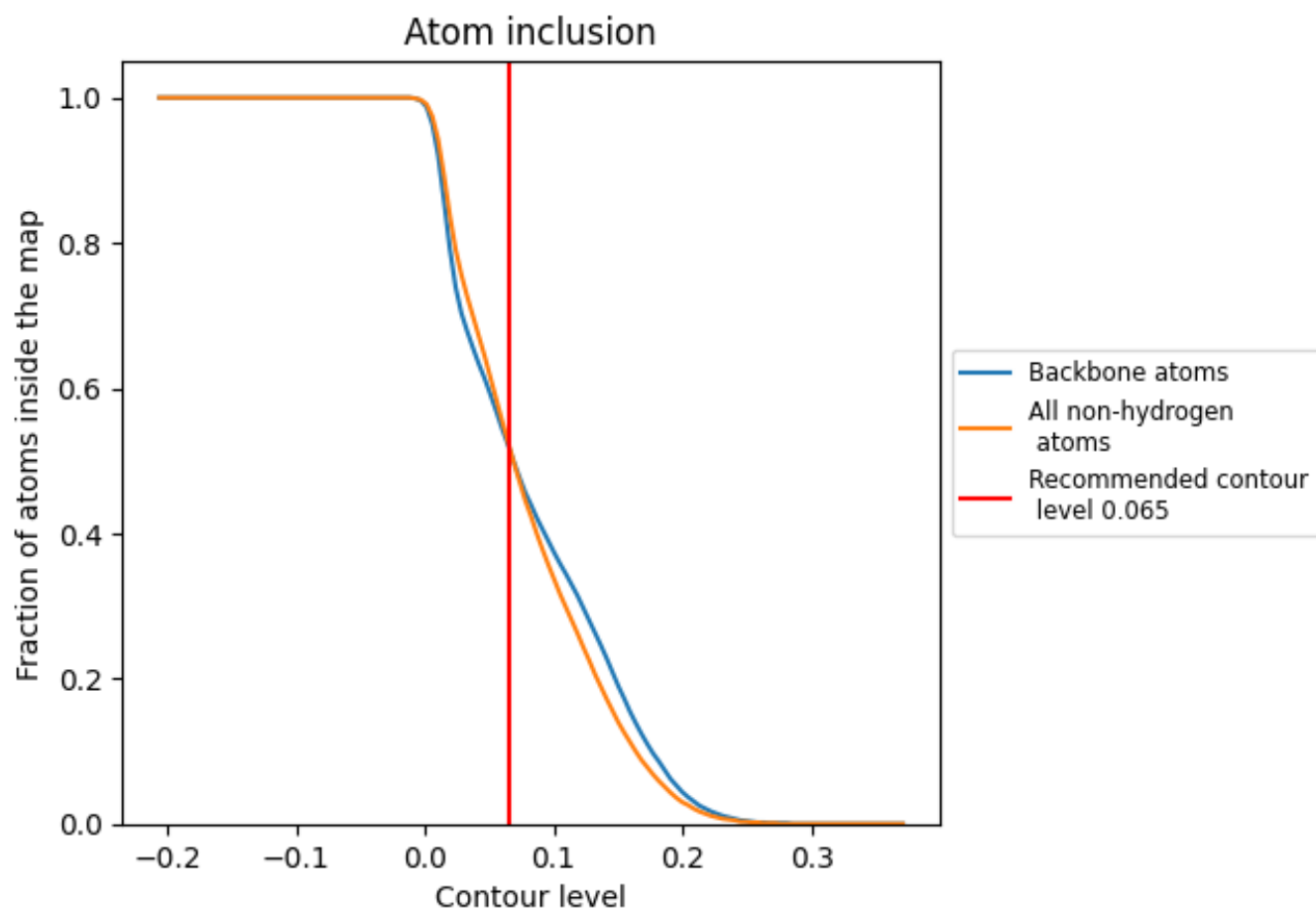
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5230	 0.3520
A	 0.4790	 0.3590
B	 0.7210	 0.4940
C	 0.6150	 0.4190
D	 0.8350	 0.5290
E	 0.5890	 0.3960
F	 0.6130	 0.4260
G	 0.7570	 0.5030
H	 0.6720	 0.4630
I	 0.5690	 0.4080
J	 0.0000	 0.0480
K	 0.7590	 0.5120
L	 0.7970	 0.5130
M	 0.7630	 0.5140
N	 0.7880	 0.5370
O	 0.8070	 0.5180
P	 0.8310	 0.5250
Q	 0.8020	 0.5270
R	 0.4330	 0.2710
X	 0.0000	 0.0480
Y	 0.0000	 0.0440
r	 0.4310	 0.2910

