



wwPDB EM Validation Summary Report ⓘ

May 14, 2024 – 12:21 AM JST

PDB ID : 7EVO
EMDB ID : EMD-31334
Title : The cryo-EM structure of the human 17S U2 snRNP
Authors : Zhang, X.; Zhan, X.; Shi, Y.
Deposited on : 2021-05-21
Resolution : 2.50 Å (reported)

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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:

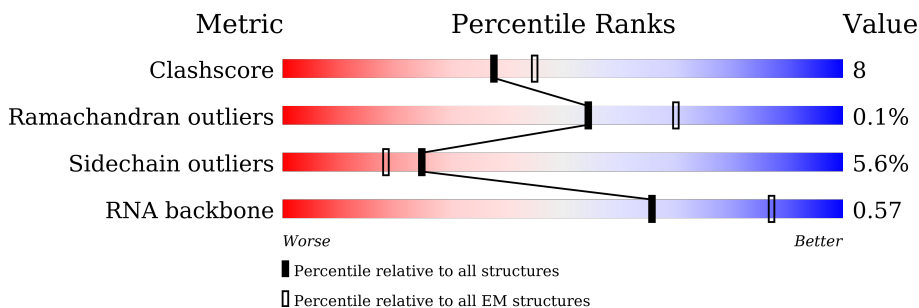
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.50 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.





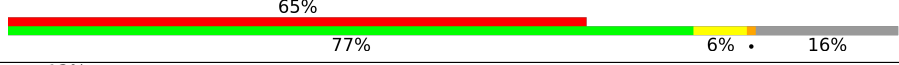

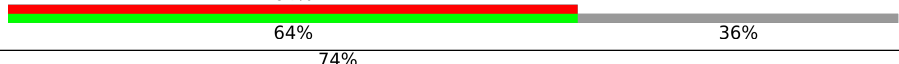



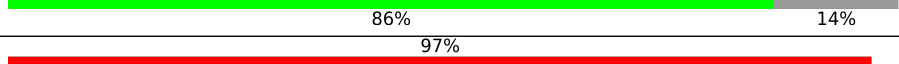
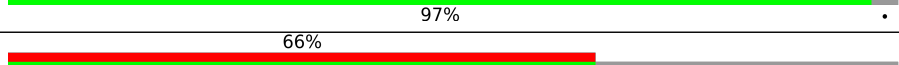



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	H	188	
2	1	1304	
3	2	895	
4	3	1217	
5	4	424	
6	5	86	
7	6	110	

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Mol	Chain	Length	Quality of chain
8	A	793	
9	B	464	
10	C	501	
11	D	755	
12	E	1052	
13	F	255	
14	G	225	
15	a	118	
16	b	86	
17	c	92	
18	d	76	
19	e	126	
20	f	240	
21	g	119	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 32104 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	H	148	3142	1406	551	1039	146	0	0

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	815	6487	4163	1121	1164	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	182	1210	754	229	225	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	1180	9247	5872	1571	1759	45	0	0

- Molecule 5 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	4	160	664	344	160	160	0	0

- Molecule 6 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	539	342	93	99	5	0	0

- Molecule 7 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	85	645	396	114	122	13	0	0

- Molecule 8 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	A	123	504	258	123	123	0	0

- Molecule 9 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	B	100	421	221	100	100	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	422	2103	1174	466	459	4	0	0

- Molecule 11 is a protein called HIV Tat-specific factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	200	1308	788	246	269	5	3	0

- Molecule 12 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	455	2153	1157	487	507	2	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP A0A0C4DG89
E	-18	ALA	-	expression tag	UNP A0A0C4DG89
E	-17	SER	-	expression tag	UNP A0A0C4DG89
E	-16	ASP	-	expression tag	UNP A0A0C4DG89

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	TYR	-	expression tag	UNP A0A0C4DG89
E	-14	LYS	-	expression tag	UNP A0A0C4DG89
E	-13	ASP	-	expression tag	UNP A0A0C4DG89
E	-12	ASP	-	expression tag	UNP A0A0C4DG89
E	-11	ASP	-	expression tag	UNP A0A0C4DG89
E	-10	ASP	-	expression tag	UNP A0A0C4DG89
E	-9	LYS	-	expression tag	UNP A0A0C4DG89
E	-8	ALA	-	expression tag	UNP A0A0C4DG89
E	-7	SER	-	expression tag	UNP A0A0C4DG89
E	-6	ASP	-	expression tag	UNP A0A0C4DG89
E	-5	GLU	-	expression tag	UNP A0A0C4DG89
E	-4	VAL	-	expression tag	UNP A0A0C4DG89
E	-3	ASP	-	expression tag	UNP A0A0C4DG89
E	-2	ALA	-	expression tag	UNP A0A0C4DG89
E	-1	GLY	-	expression tag	UNP A0A0C4DG89
E	0	THR	-	expression tag	UNP A0A0C4DG89

- Molecule 13 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
13	F	162	666	342	162	162	0	0

- Molecule 14 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
14	G	166	685	353	166	166	0	0

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
15	a	90	372	192	90	90	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
16	b	74	308	160	74	74	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	c	79	319	161	79	79	0	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	d	74	305	157	74	74	0	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	e	83	341	175	83	83	0	0

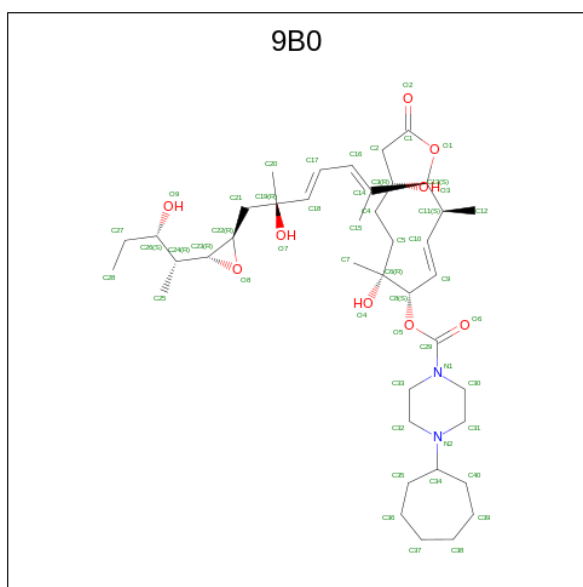
- Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	f	71	293	151	71	71	0	0

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	g	82	337	173	82	82	0	0

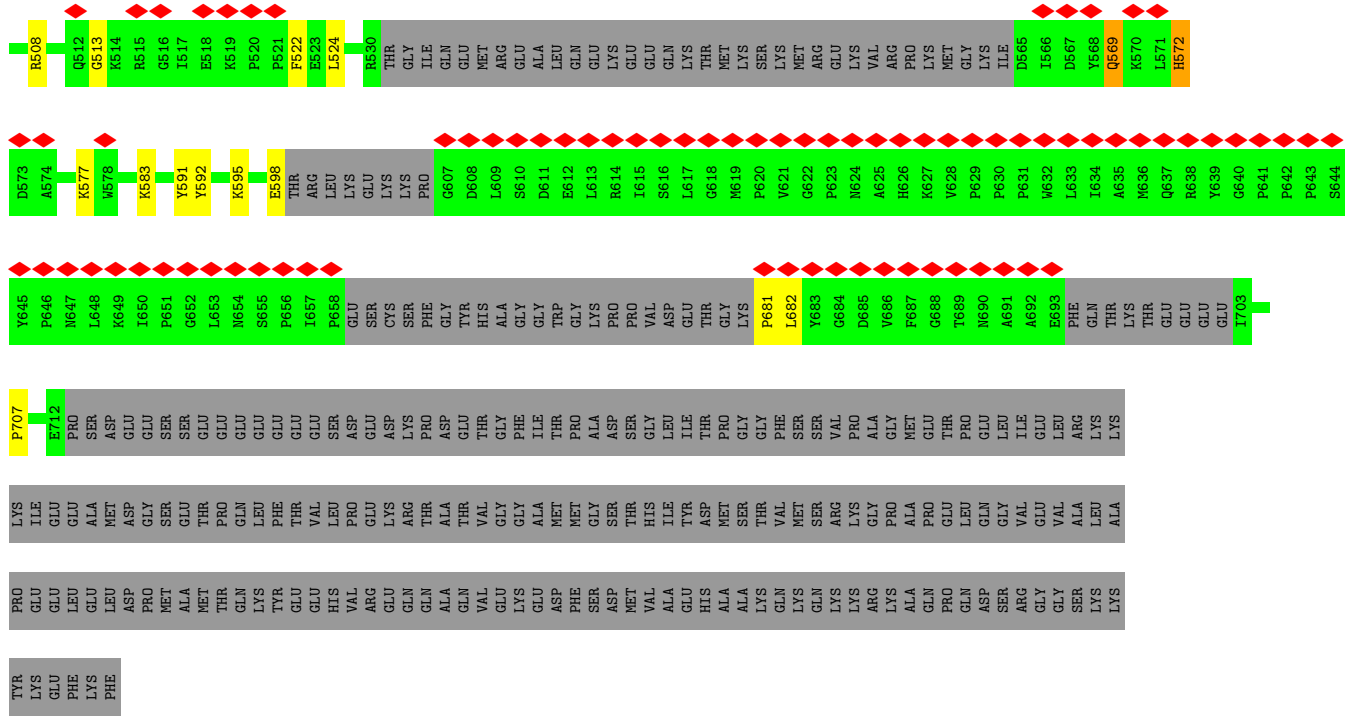
- Molecule 22 is [(2 {S},3 {S},4 {E},6 {S},7 {R},10 {R})-3,7-dimethyl-2-[(2 {E},4 {E},6 {R})-6-methyl-6-oxidanyl-7-[(2 {R},3 {R})-3-[(2 {R},3 {S})-3-oxidanylpentan-2-yl]oxiran-2-yl]hepta-2,4-dien-2-yl]-7,10-bis(oxidanyl)-12-oxidanylidene-1-oxacyclododec-4-en-6-yl] 4-cycloheptylpiperazine-1-carboxylate (three-letter code: 9B0) (formula: C₄₀H₆₆N₂O₉) (labeled as "Ligand of Interest" by depositor).



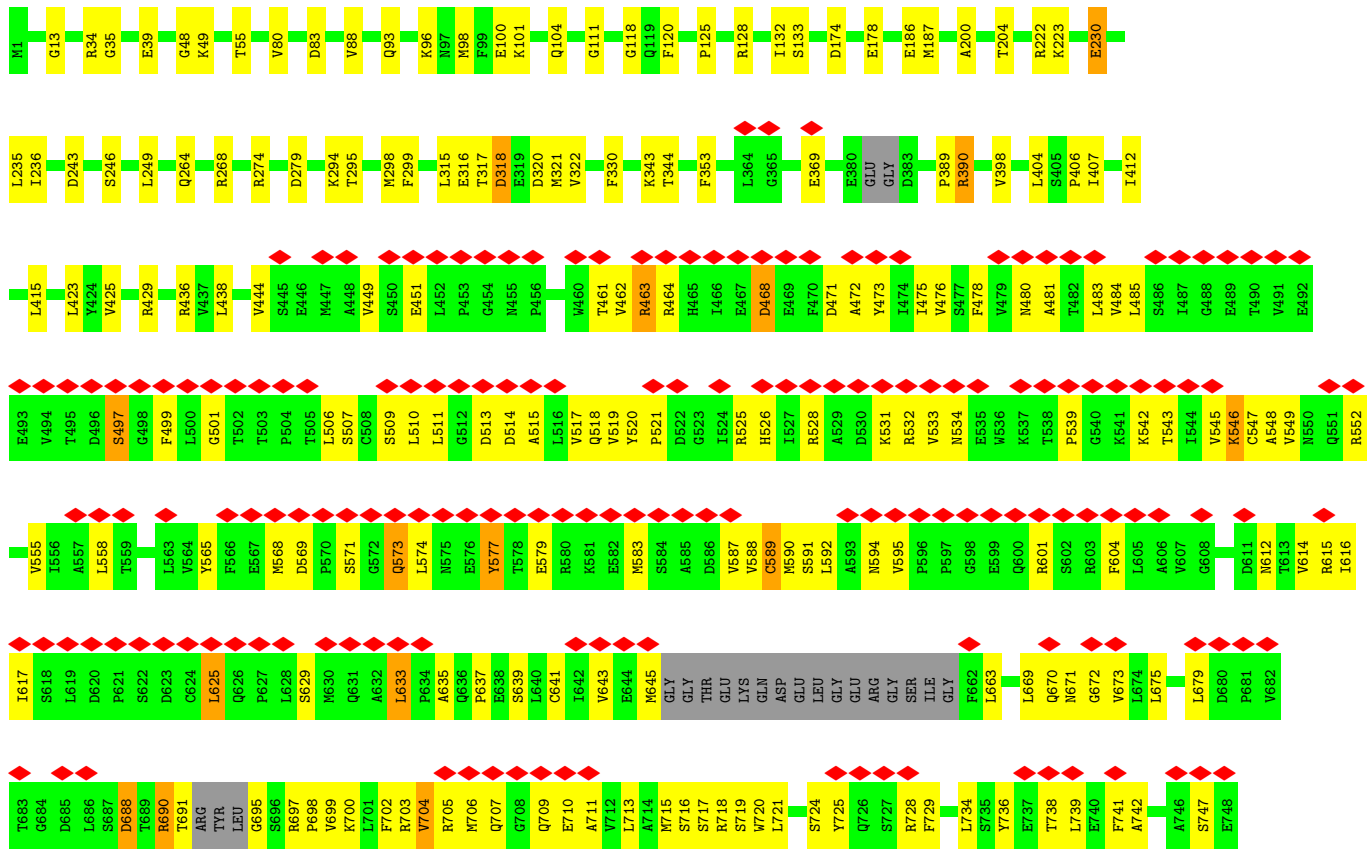
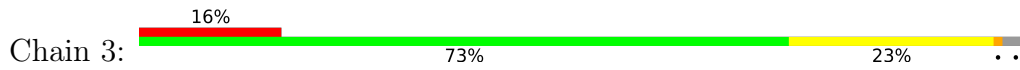
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
22	1	1	51	40	2	9	0

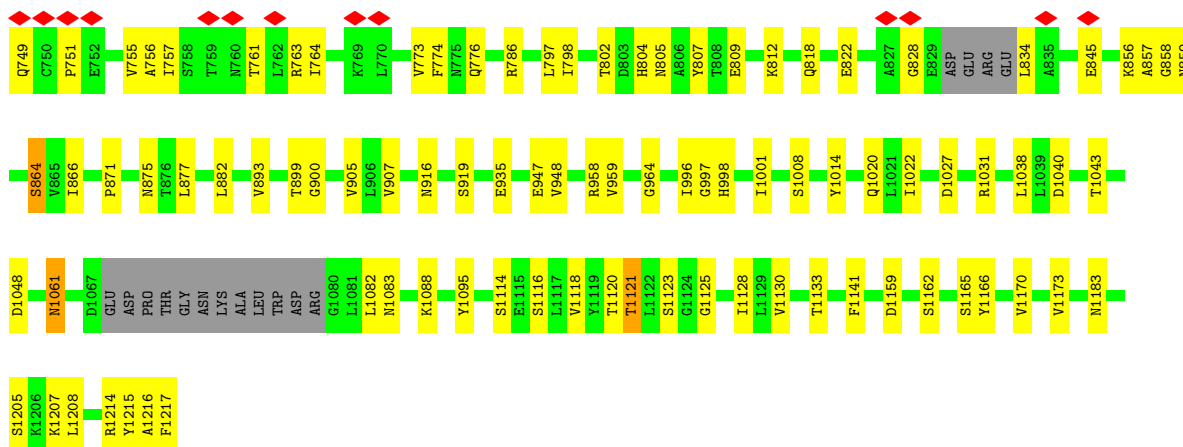
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
23	6	3	3	3	0
23	C	1	1	1	0

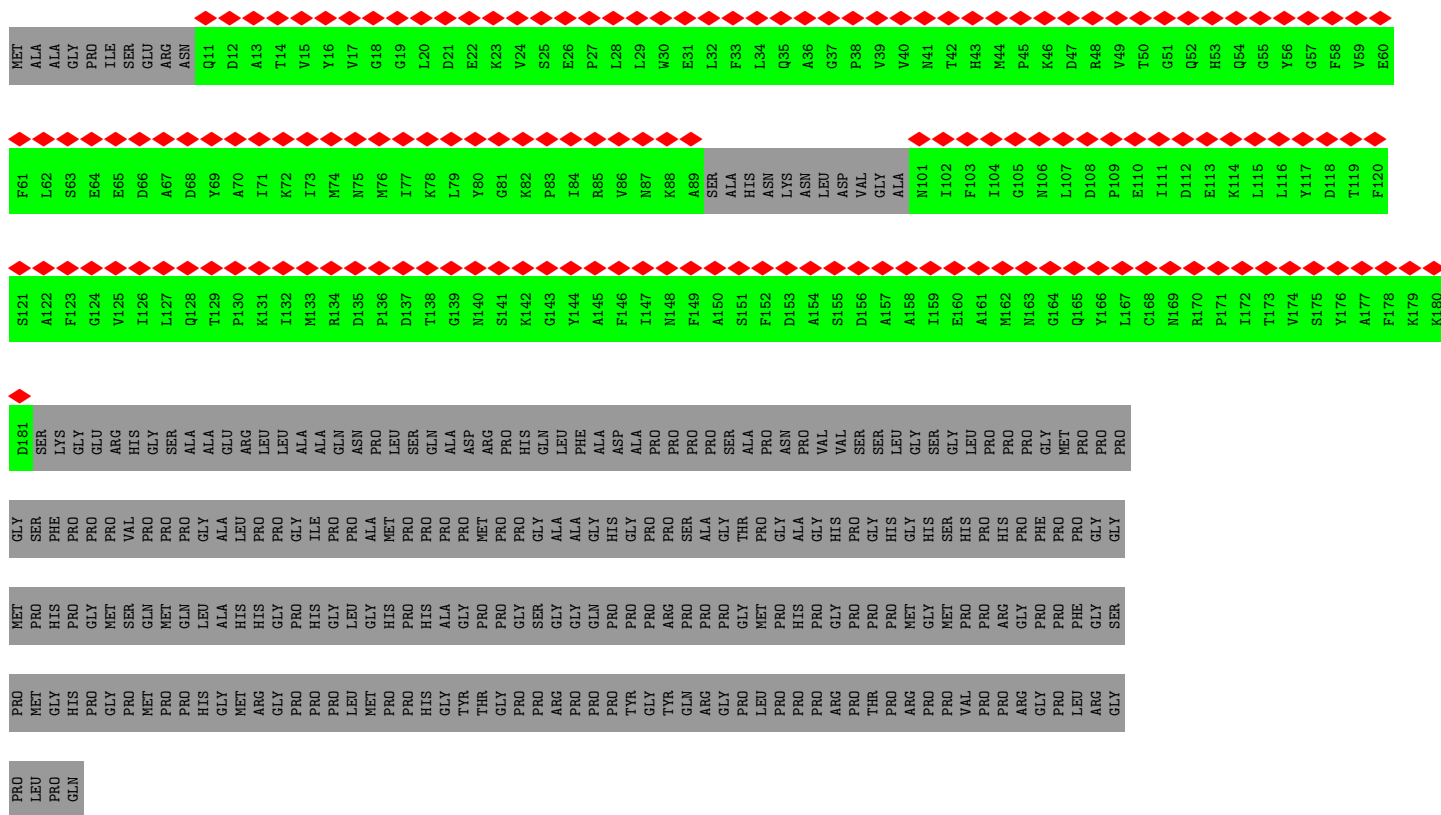


- Molecule 4: Splicing factor 3B subunit 3

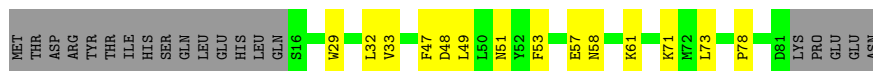




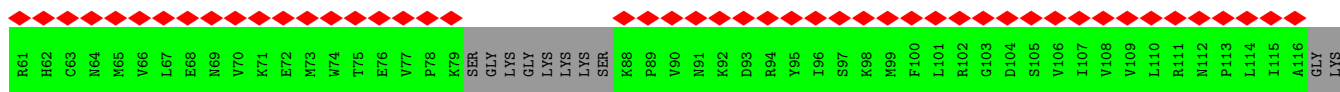
• Molecule 5: Splicing factor 3B subunit 4



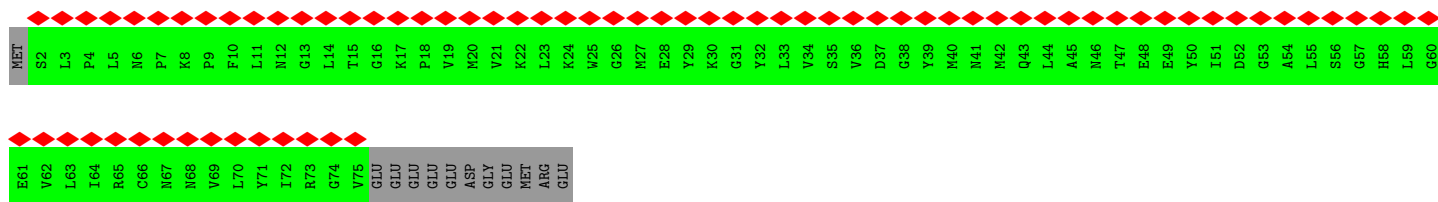
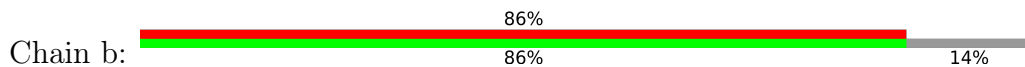
• Molecule 6: Splicing factor 3B subunit 5



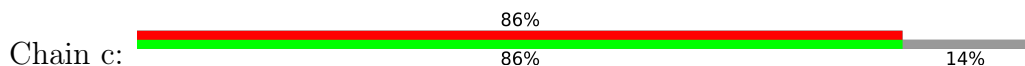
• Molecule 7: PHD finger-like domain-containing protein 5A



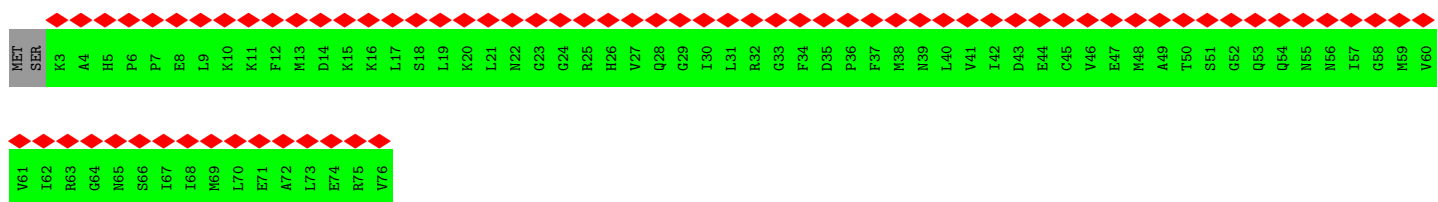
• Molecule 16: Small nuclear ribonucleoprotein F



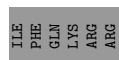
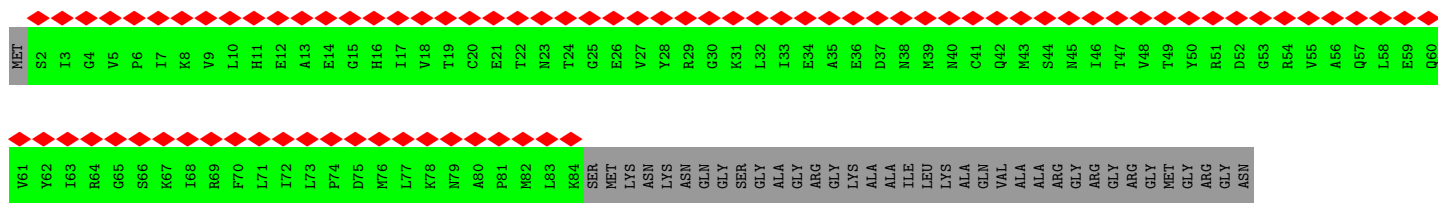
• Molecule 17: Small nuclear ribonucleoprotein E



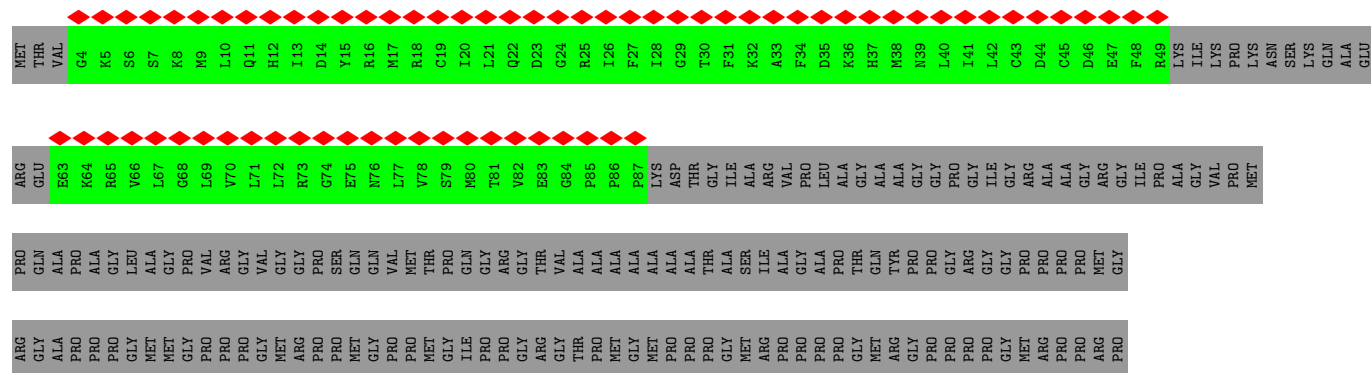
• Molecule 18: Small nuclear ribonucleoprotein G



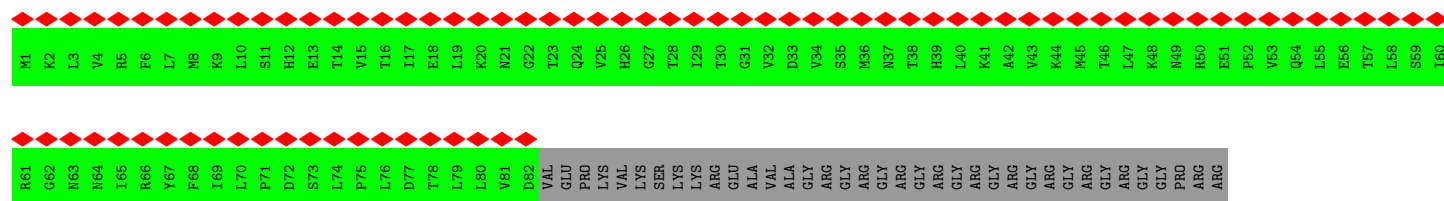
• Molecule 19: Small nuclear ribonucleoprotein Sm D3



• Molecule 20: Small nuclear ribonucleoprotein-associated proteins B and B'



● Molecule 21: Small nuclear ribonucleoprotein Sm D1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	485418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	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, 9B0

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	H	0.41	2/3507 (0.1%)	0.95	17/5454 (0.3%)
2	1	0.27	0/6609	0.45	1/8946 (0.0%)
3	2	0.25	0/1248	0.45	0/1672
4	3	0.27	0/9435	0.49	1/12802 (0.0%)
5	4	0.24	0/670	0.45	0/850
6	5	0.48	1/555 (0.2%)	0.52	0/750
7	6	0.25	0/653	0.45	0/877
8	A	0.24	0/507	0.41	0/640
9	B	0.24	0/426	0.50	0/543
10	C	0.25	0/2133	0.45	0/2773
11	D	0.28	0/1325	0.47	0/1749
12	E	0.41	1/2171 (0.0%)	0.52	0/2779
13	F	0.24	0/671	0.49	0/849
14	G	0.23	0/689	0.46	0/869
15	a	0.24	0/374	0.50	0/472
16	b	0.25	0/311	0.51	0/395
17	c	0.24	0/319	0.49	0/399
18	d	0.25	0/307	0.51	0/388
19	e	0.25	0/343	0.51	0/433
20	f	0.24	0/294	0.49	0/370
21	g	0.23	0/339	0.51	0/428
All	All	0.30	4/32886 (0.0%)	0.56	19/44438 (0.0%)

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
1	H	0	1
10	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	78	PRO	C-N	8.67	1.50	1.34
1	H	45	C	O3'-P	-7.13	1.52	1.61
1	H	55	U	P-OP2	5.57	1.58	1.49
12	E	178	ALA	C-O	5.12	1.33	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	28	C	N1-C1'-C2'	-11.54	98.99	114.00
1	H	120	A	C6-N1-C2	-8.05	113.77	118.60
1	H	42	G	C4'-C3'-O3'	7.34	127.69	113.00
1	H	27	U	C3'-C2'-C1'	7.02	107.11	101.50
1	H	55	U	OP1-P-OP2	6.85	129.88	119.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	C	393	PRO	Mainchain
1	H	43	U	Sidechain

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	H	3142	0	1594	60	0
2	1	6487	0	6700	136	0
3	2	1210	0	1010	27	0
4	3	9247	0	9179	161	0
5	4	664	0	230	0	0
6	5	539	0	505	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	6	645	0	626	9	0
8	A	504	0	150	0	0
9	B	421	0	148	0	0
10	C	2103	0	1108	47	0
11	D	1308	0	1061	25	0
12	E	2153	0	1054	27	0
13	F	666	0	209	0	0
14	G	685	0	226	7	0
15	a	372	0	118	0	0
16	b	308	0	115	0	0
17	c	319	0	92	0	0
18	d	305	0	105	0	0
19	e	341	0	112	0	0
20	f	293	0	99	0	0
21	g	337	0	110	0	0
22	1	51	0	0	9	0
23	6	3	0	0	0	0
23	C	1	0	0	0	0
All	All	32104	0	24551	454	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 8.

The worst 5 of 454 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)
1:H:25:G:H1'	10:C:399:LEU:CD2	1.33	1.55
12:E:226:ASP:OD1	12:E:227:PRO:HD2	1.18	1.31
10:C:396:LEU:HD12	10:C:400:HIS:HD2	0.98	1.13
1:H:25:G:C1'	10:C:399:LEU:CD2	2.25	1.12
10:C:396:LEU:HD12	10:C:400:HIS:CD2	1.88	1.08

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	
2	1	813/1304 (62%)	782 (96%)	31 (4%)	0	100	100
3	2	172/895 (19%)	156 (91%)	15 (9%)	1 (1%)	25	43
4	3	1168/1217 (96%)	1121 (96%)	46 (4%)	1 (0%)	51	73
5	4	156/424 (37%)	153 (98%)	3 (2%)	0	100	100
6	5	64/86 (74%)	63 (98%)	1 (2%)	0	100	100
7	6	83/110 (76%)	79 (95%)	4 (5%)	0	100	100
8	A	121/793 (15%)	121 (100%)	0	0	100	100
9	B	96/464 (21%)	94 (98%)	2 (2%)	0	100	100
10	C	416/501 (83%)	398 (96%)	17 (4%)	1 (0%)	47	68
11	D	198/755 (26%)	182 (92%)	16 (8%)	0	100	100
12	E	447/1052 (42%)	431 (96%)	15 (3%)	1 (0%)	47	68
13	F	160/255 (63%)	160 (100%)	0	0	100	100
14	G	160/225 (71%)	158 (99%)	2 (1%)	0	100	100
15	a	86/118 (73%)	84 (98%)	2 (2%)	0	100	100
16	b	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
17	c	77/92 (84%)	77 (100%)	0	0	100	100
18	d	72/76 (95%)	72 (100%)	0	0	100	100
19	e	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
20	f	67/240 (28%)	67 (100%)	0	0	100	100
21	g	80/119 (67%)	79 (99%)	1 (1%)	0	100	100
All	All	4589/8938 (51%)	4427 (96%)	158 (3%)	4 (0%)	54	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	C	412	GLY
3	2	496	ASN
12	E	585	GLY
4	3	997	GLY

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	
2	1	701/1104 (64%)	666 (95%)	35 (5%)	24	46
3	2	104/776 (13%)	98 (94%)	6 (6%)	20	38
4	3	1022/1051 (97%)	963 (94%)	59 (6%)	20	38
5	4	8/336 (2%)	8 (100%)	0	100	100
6	5	57/77 (74%)	56 (98%)	1 (2%)	59	81
7	6	73/95 (77%)	72 (99%)	1 (1%)	67	86
8	A	4/709 (1%)	4 (100%)	0	100	100
9	B	7/382 (2%)	7 (100%)	0	100	100
10	C	80/446 (18%)	69 (86%)	11 (14%)	3	6
11	D	108/661 (16%)	100 (93%)	8 (7%)	13	27
12	E	73/909 (8%)	66 (90%)	7 (10%)	8	16
13	F	6/218 (3%)	6 (100%)	0	100	100
14	G	7/195 (4%)	7 (100%)	0	100	100
15	a	4/110 (4%)	4 (100%)	0	100	100
16	b	4/74 (5%)	4 (100%)	0	100	100
17	c	1/84 (1%)	1 (100%)	0	100	100
18	d	3/66 (4%)	3 (100%)	0	100	100
19	e	3/101 (3%)	3 (100%)	0	100	100
20	f	3/177 (2%)	3 (100%)	0	100	100
21	g	3/101 (3%)	3 (100%)	0	100	100
All	All	2271/7672 (30%)	2143 (94%)	128 (6%)	25	40

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	D	187	CYS
11	D	237	LYS
4	3	316	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3	298	MET
12	E	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	3	805	ASN
10	C	400	HIS
4	3	870	ASN
4	3	983	ASN
11	D	179	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	H	143/188 (76%)	27 (18%)	0

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	H	22	U
1	H	23	A
1	H	24	A
1	H	43	U
1	H	47	U

There are no RNA pucker outliers to report.

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

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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
22	9B0	1	1500	-	52,54,54	0.73	1 (1%)	61,77,77	0.80	2 (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
22	9B0	1	1500	-	-	25/67/91/91	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	1500	9B0	C17-C16	-3.63	1.32	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	1500	9B0	C17-C16-C14	2.91	131.59	127.32
22	1	1500	9B0	O9-C26-C27	-2.47	104.86	109.35

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

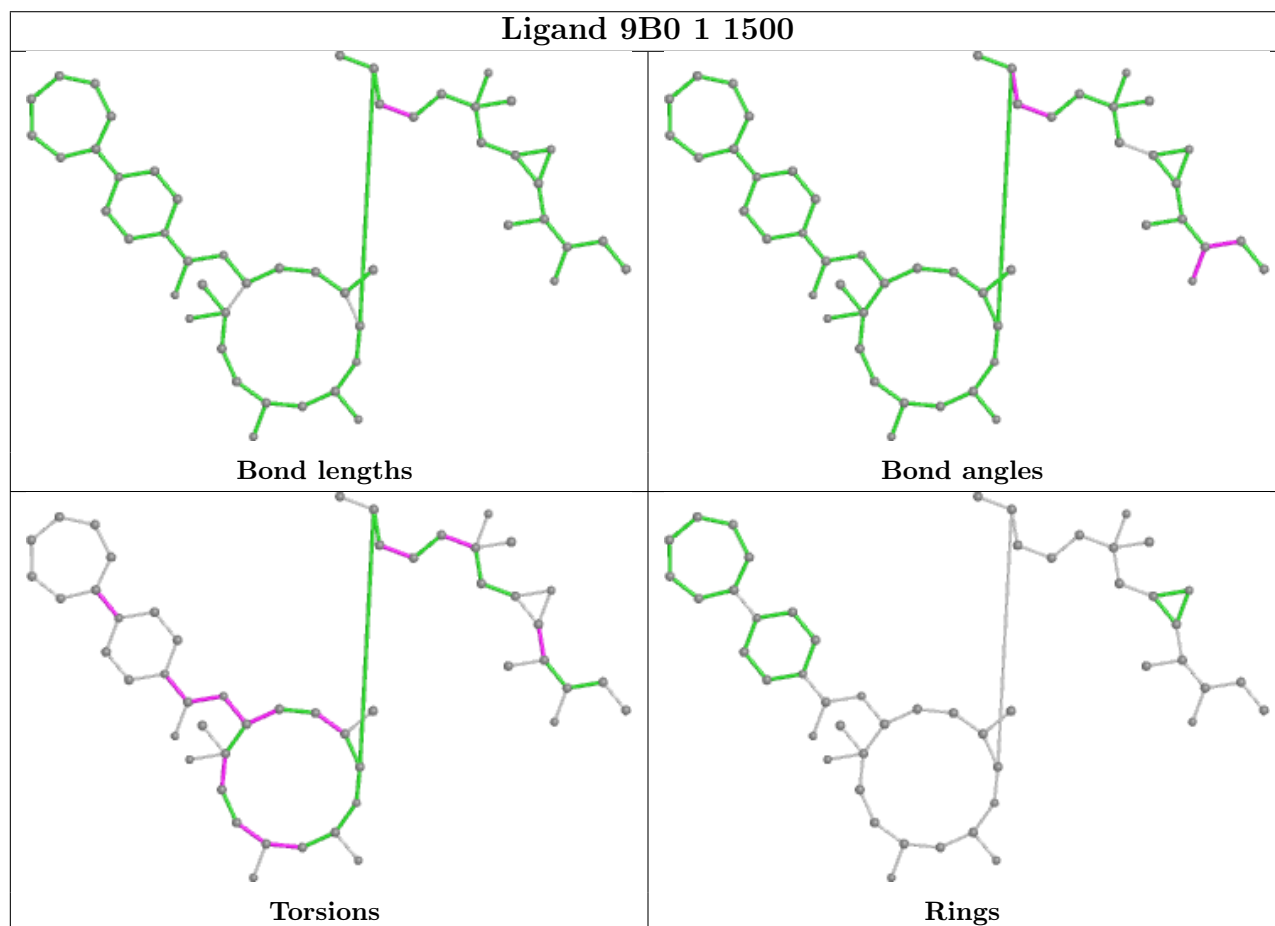
Mol	Chain	Res	Type	Atoms
22	1	1500	9B0	O5-C29-N1-C33
22	1	1500	9B0	O5-C29-N1-C30
22	1	1500	9B0	N1-C29-O5-C8
22	1	1500	9B0	O5-C8-C9-C10
22	1	1500	9B0	C6-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	1500	9B0	9	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

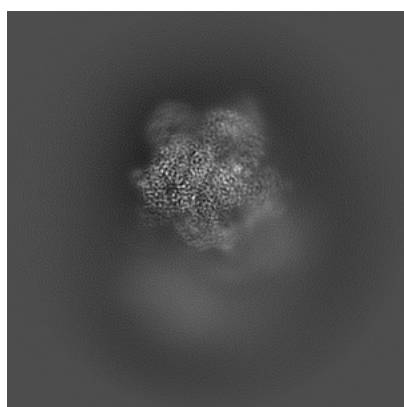
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31334. These allow visual inspection of the internal detail of the map and identification of artifacts.

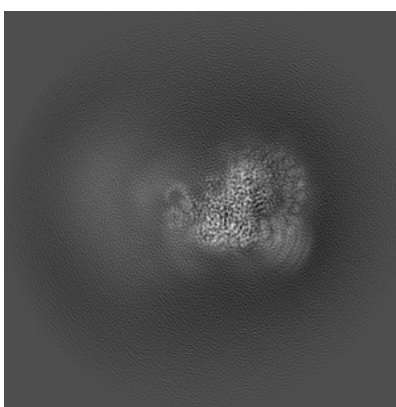
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

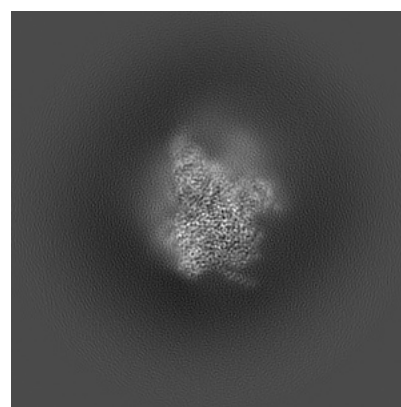
6.1.1 Primary map



X



Y

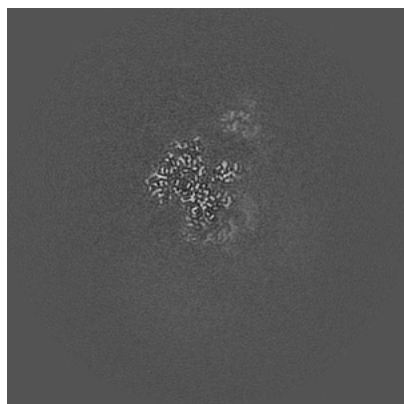


Z

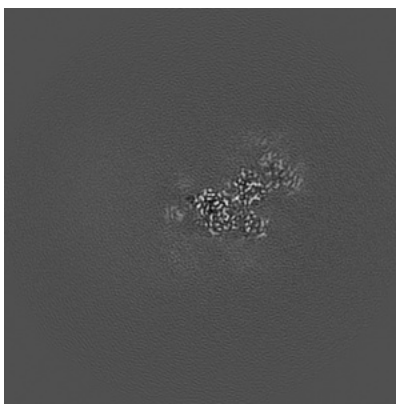
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

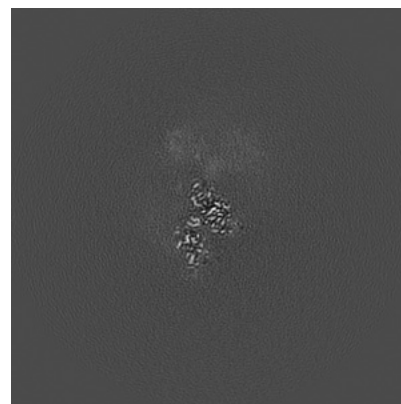
6.2.1 Primary map



X Index: 160



Y Index: 160

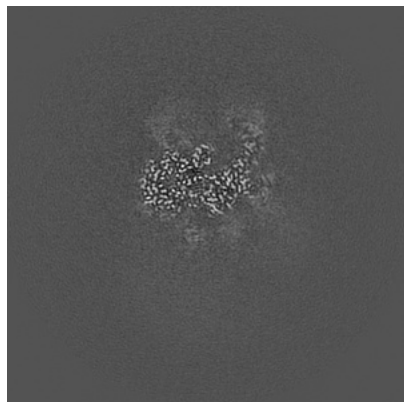


Z Index: 160

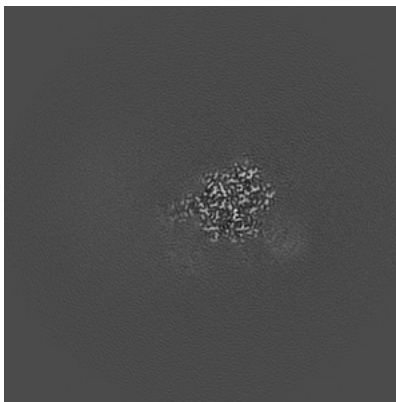
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

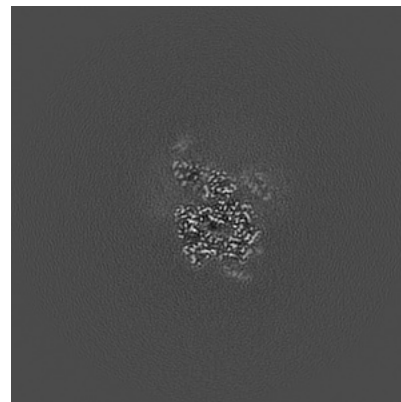
6.3.1 Primary map



X Index: 147



Y Index: 148

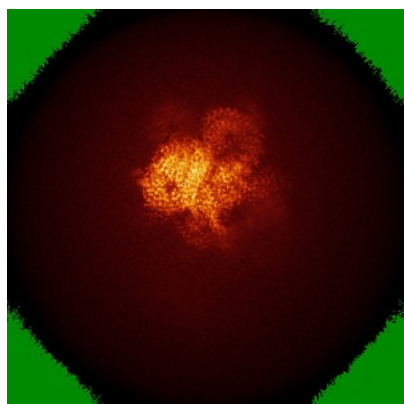


Z Index: 191

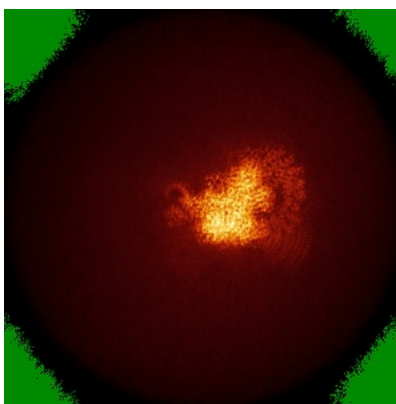
The images above show the largest variance slices of the map in three orthogonal directions.

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

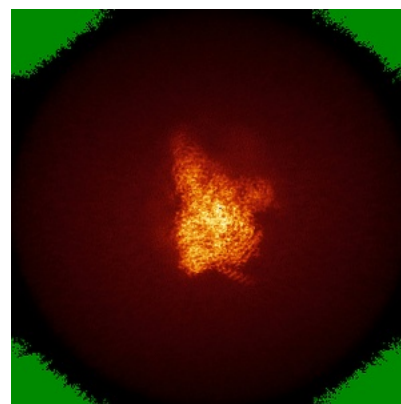
6.4.1 Primary map



X



Y



Z

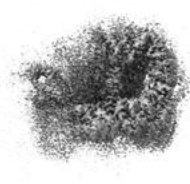
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

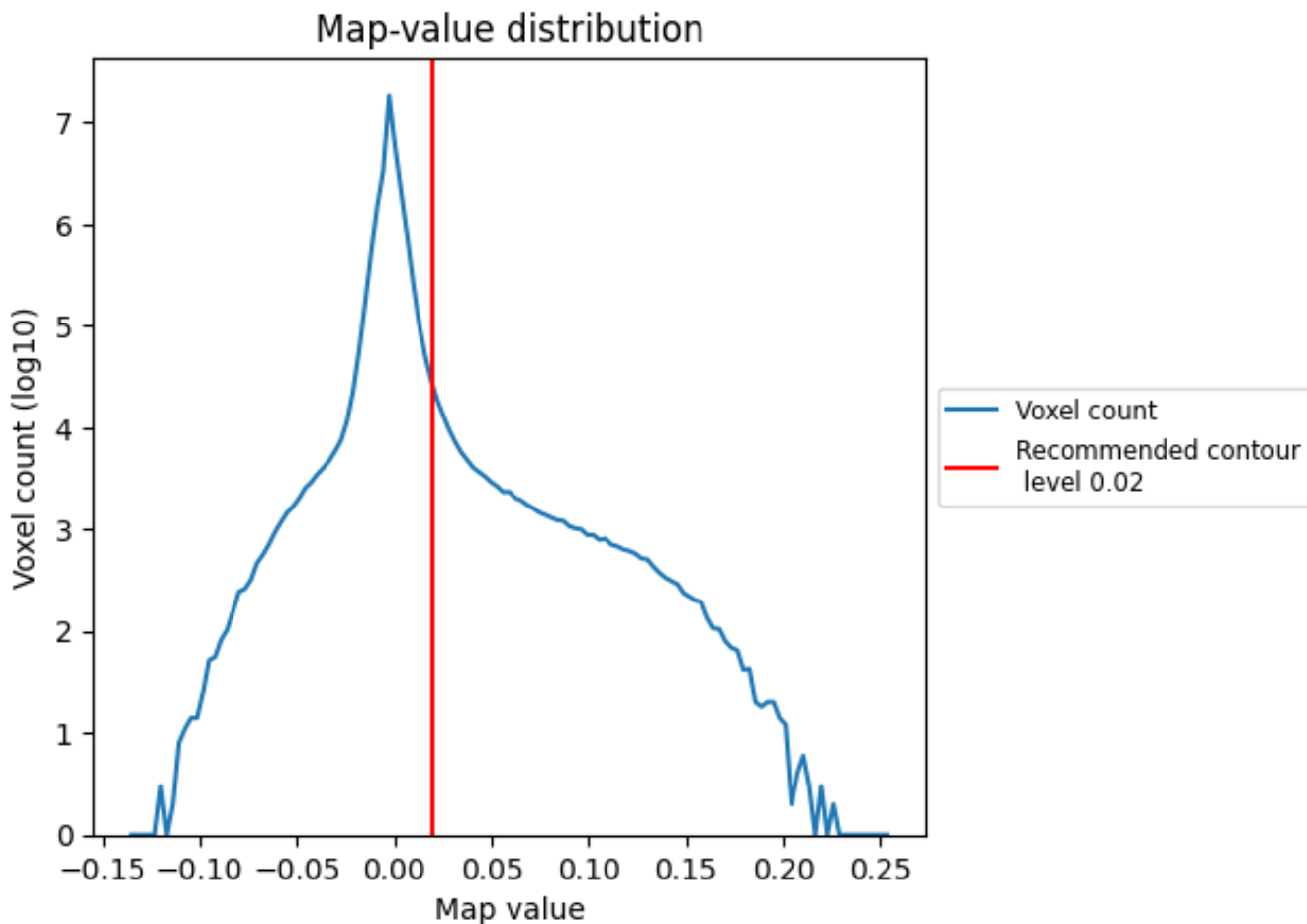
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

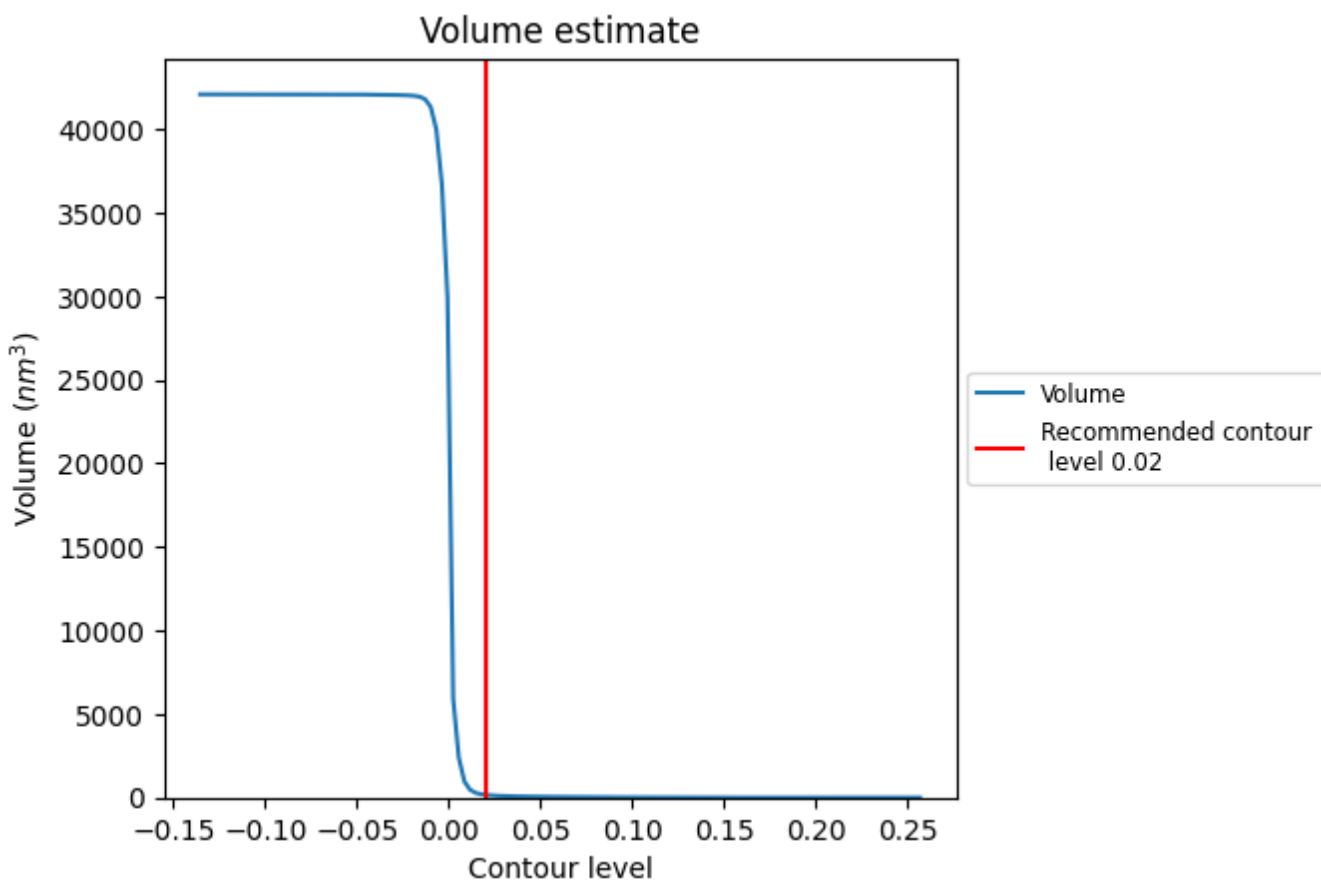
This section contains the results of statistical analysis of the map.

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.

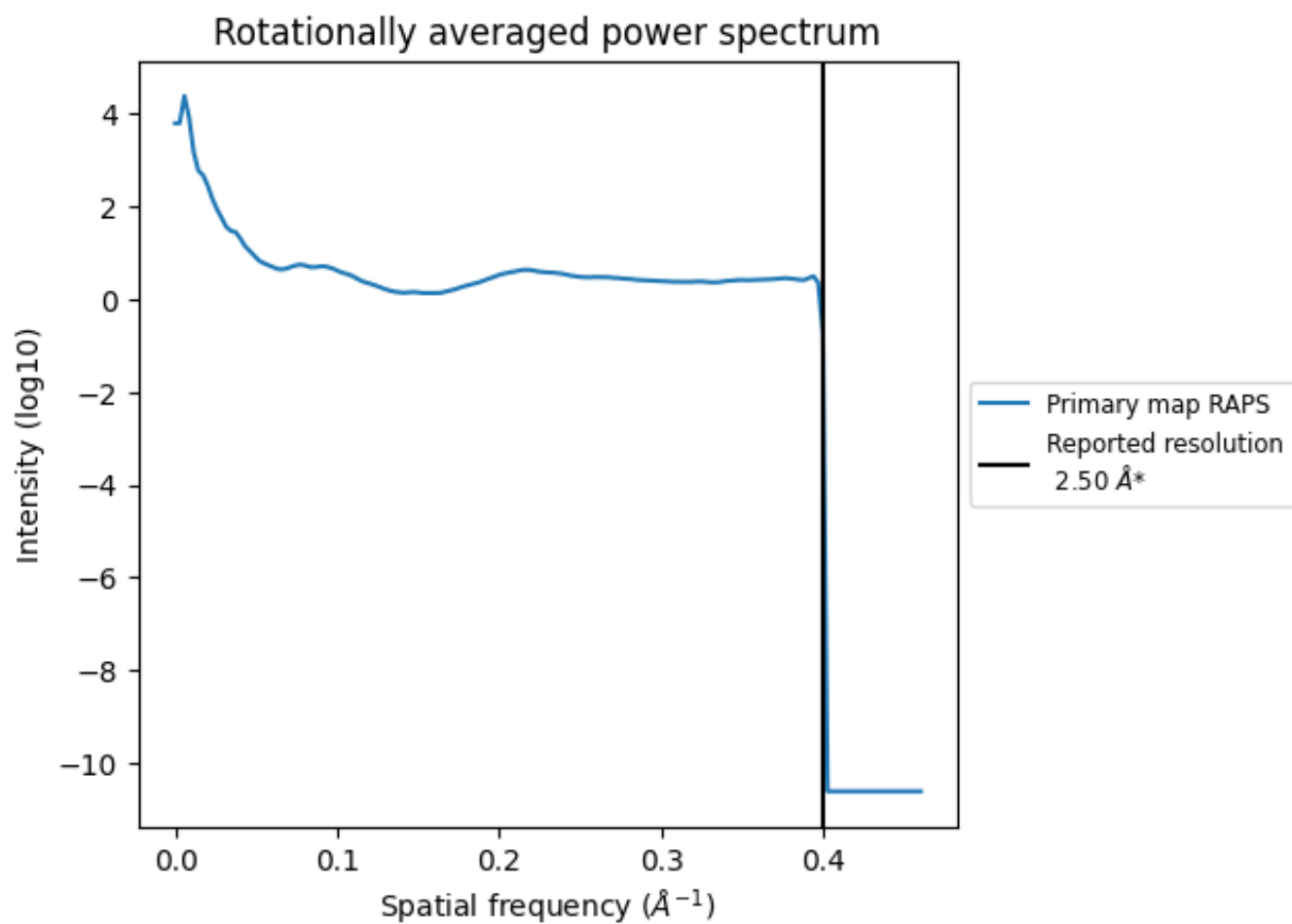
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 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 0.400 Å⁻¹

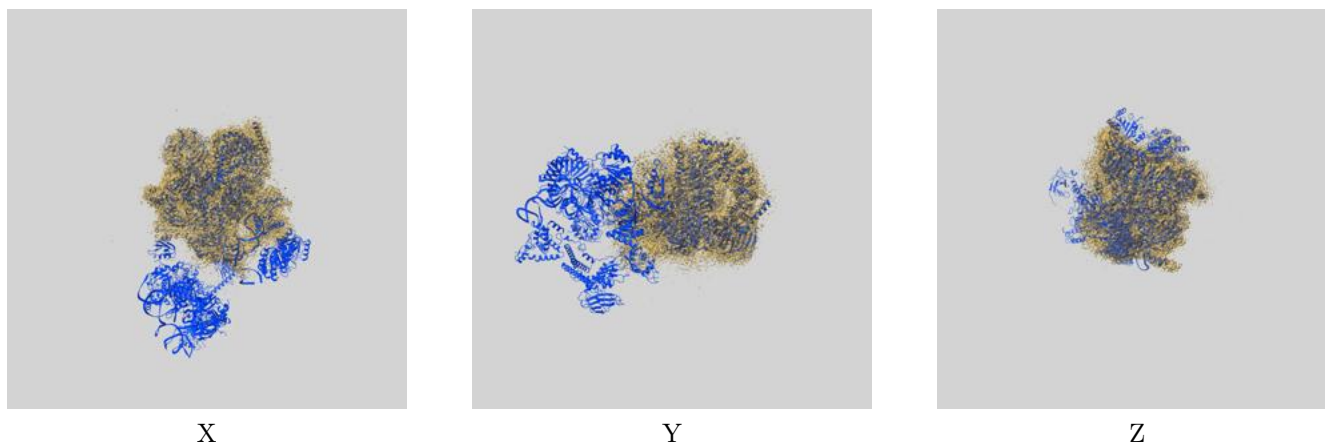
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

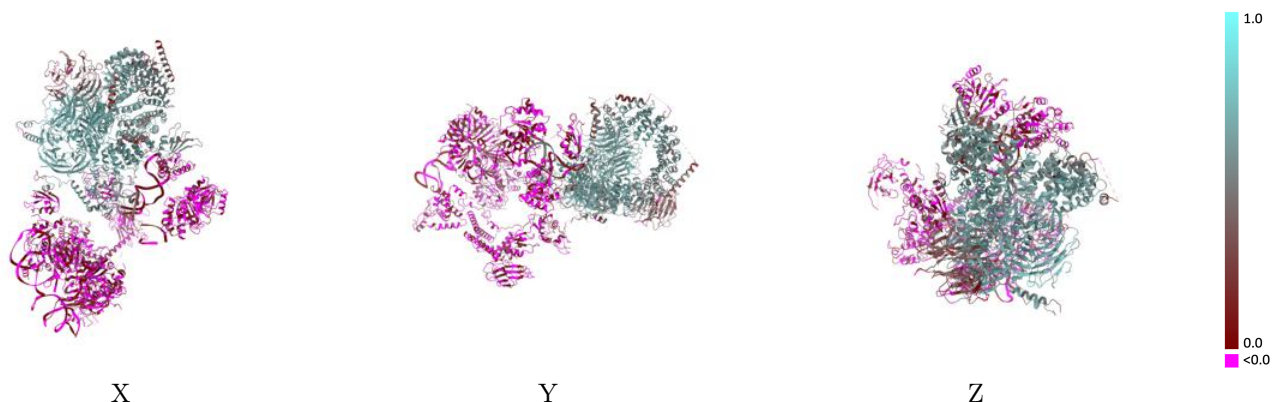
This section contains information regarding the fit between EMDB map EMD-31334 and PDB model 7EVO. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



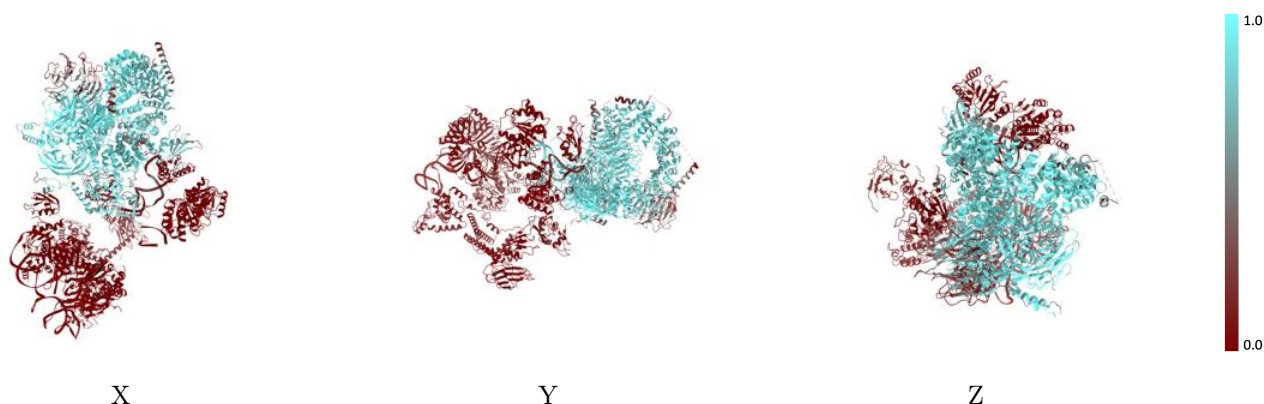
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



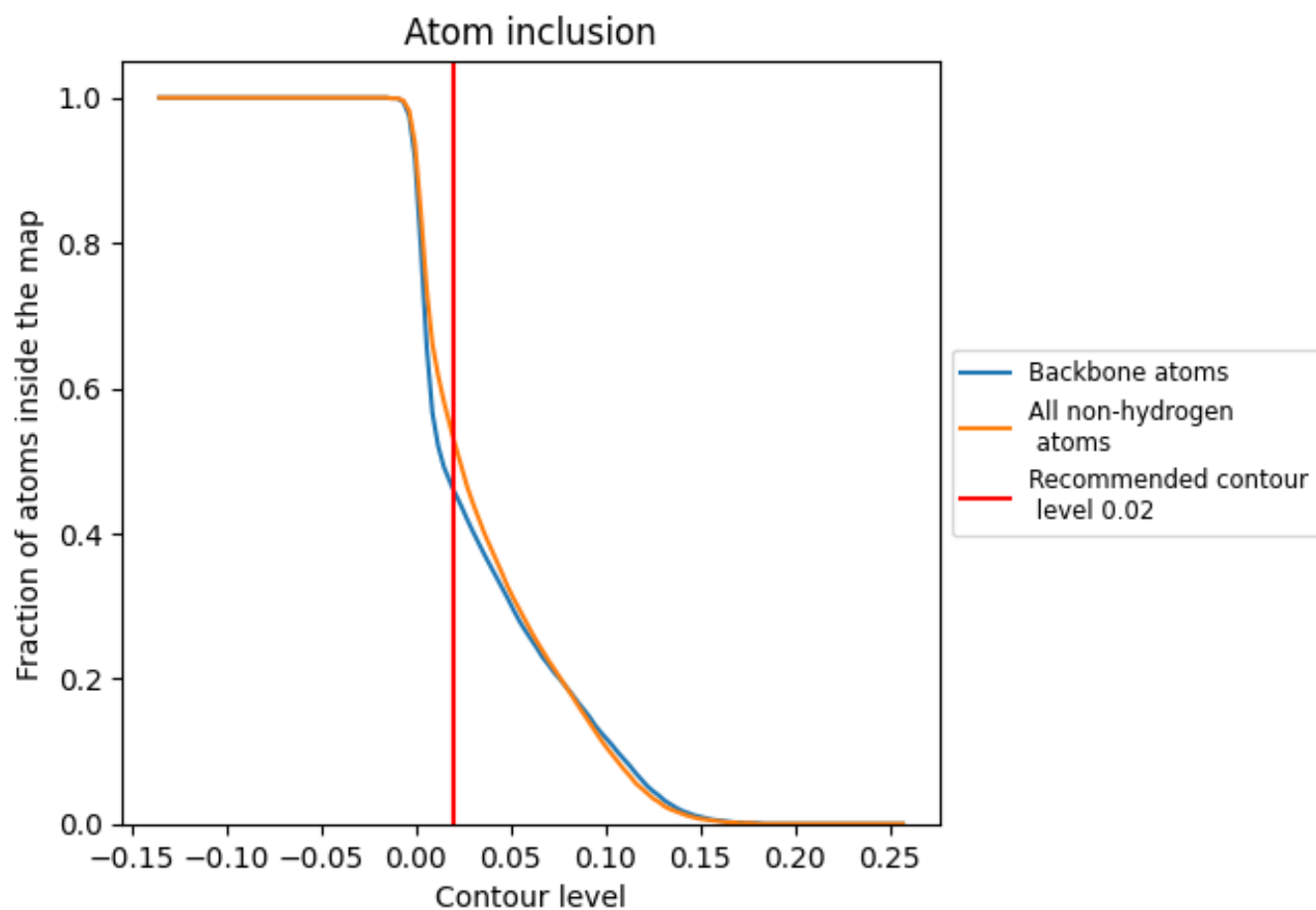
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 53% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5280	 0.3670
1	 0.8730	 0.5840
2	 0.6220	 0.4210
3	 0.8050	 0.5730
4	 0.0040	 0.0160
5	 0.9830	 0.6830
6	 0.9250	 0.6450
A	 0.0000	 0.0030
B	 0.0000	 -0.0050
C	 0.3010	 0.2070
D	 0.5410	 0.3660
E	 0.0920	 0.0680
F	 0.0000	 0.0180
G	 0.0000	 -0.0010
H	 0.1450	 0.0740
a	 0.0000	 0.0310
b	 0.0000	 0.0080
c	 0.0000	 0.0310
d	 0.0000	 -0.0240
e	 0.0000	 0.0410
f	 0.0000	 0.0290
g	 0.0000	 0.0440

