Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 12:37 AM UTC

PDB ID	:	9ZEC / pdb_00009zec
EMDB ID	:	EMD-74099
Title	:	Cryo-EM structure of the endogenous U2/branchpoint spliceosomal complex (SF3A state 1)
Authors	:	Liu, S.; Su, T.; Zhou, Z.H.
Deposited on	:	2025-11-29
Resolution	:	3.61 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

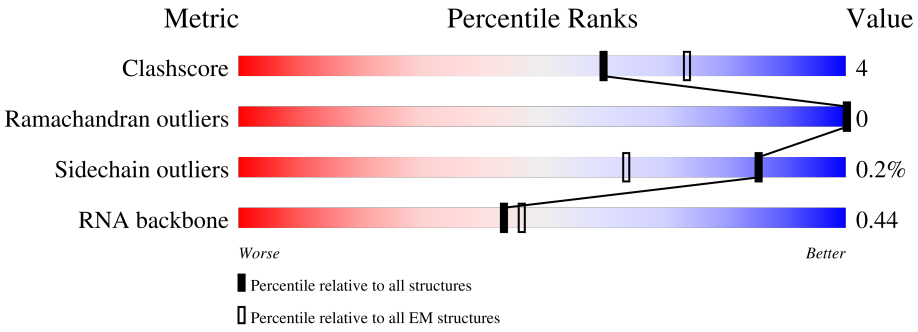
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

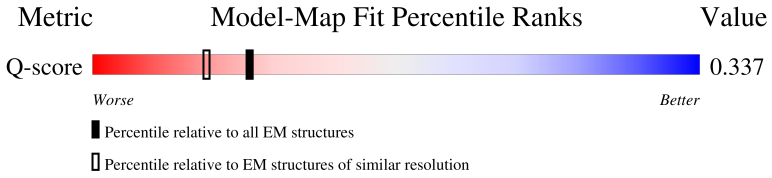
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.61 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11801 (3.11 - 4.10)

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 <=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	2	37	11% 46% 38% 11% 5%
2	A	824	5% . . 94%
3	A1	793	9% 8% . 91%

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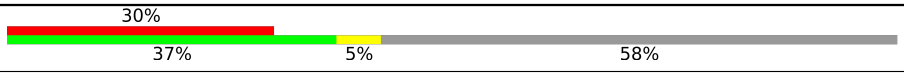
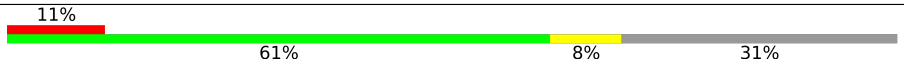
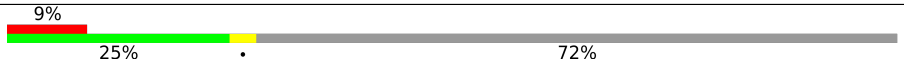
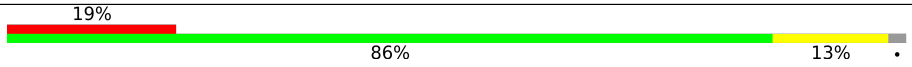
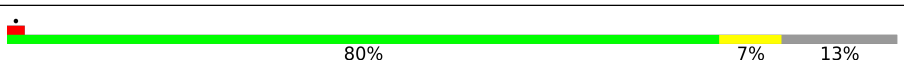
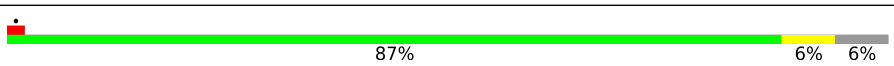
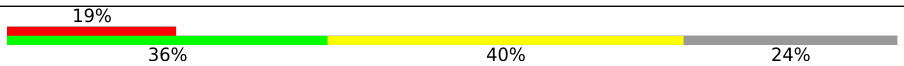
Mol	Chain	Length	Quality of chain
4	A2	464	
5	A3	501	
6	B1	1304	
7	B2	895	
8	B3	1217	
9	B4	424	
10	B5	86	
11	B6	125	
12	H	110	
13	R	42	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 27413 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	2	37	781	352	127	265	37	0	0

- Molecule 2 is a protein called RNA-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	47	408	253	76	76	3	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	MET	-	expression tag	UNP P52756
A	817	ASP	-	expression tag	UNP P52756
A	818	TYR	-	expression tag	UNP P52756
A	819	LYS	-	expression tag	UNP P52756
A	820	ASP	-	expression tag	UNP P52756
A	821	ASP	-	expression tag	UNP P52756
A	822	ASP	-	expression tag	UNP P52756
A	823	ASP	-	expression tag	UNP P52756
A	824	LYS	-	expression tag	UNP P52756

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	A1	72	614	390	104	120	0	0

- Molecule 4 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A2	197	1645	1042	300	295	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A3	123	Total	C	N	O	S	0	0
			1014	646	181	183	4		

- Molecule 6 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B1	895	Total	C	N	O	S	0	0
			7142	4581	1225	1295	41		

- Molecule 7 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B2	250	Total	C	N	O	S	0	0
			1960	1260	348	345	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B3	1198	Total	C	N	O	S	0	0
			9396	5959	1598	1794	45		

- Molecule 9 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B4	205	Total	C	N	O	S	0	0
			1593	1011	270	305	7		

- Molecule 10 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B5	75	Total	C	N	O	S	0	0
			616	390	108	113	5		

- Molecule 11 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B6	98	Total	C	N	O	S	0	0
			805	515	144	142	4		

- Molecule 12 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	103	Total	C	N	O	S	0	0
			794	490	142	148	14		

- Molecule 13 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	32	Total	C	N	O	P	0	0
			642	289	69	252	32		

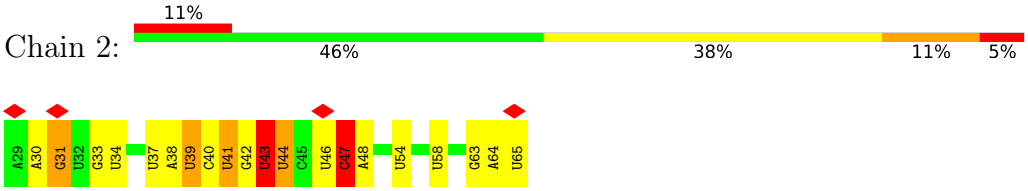
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	H	3	Total	Zn	0
			3	3	

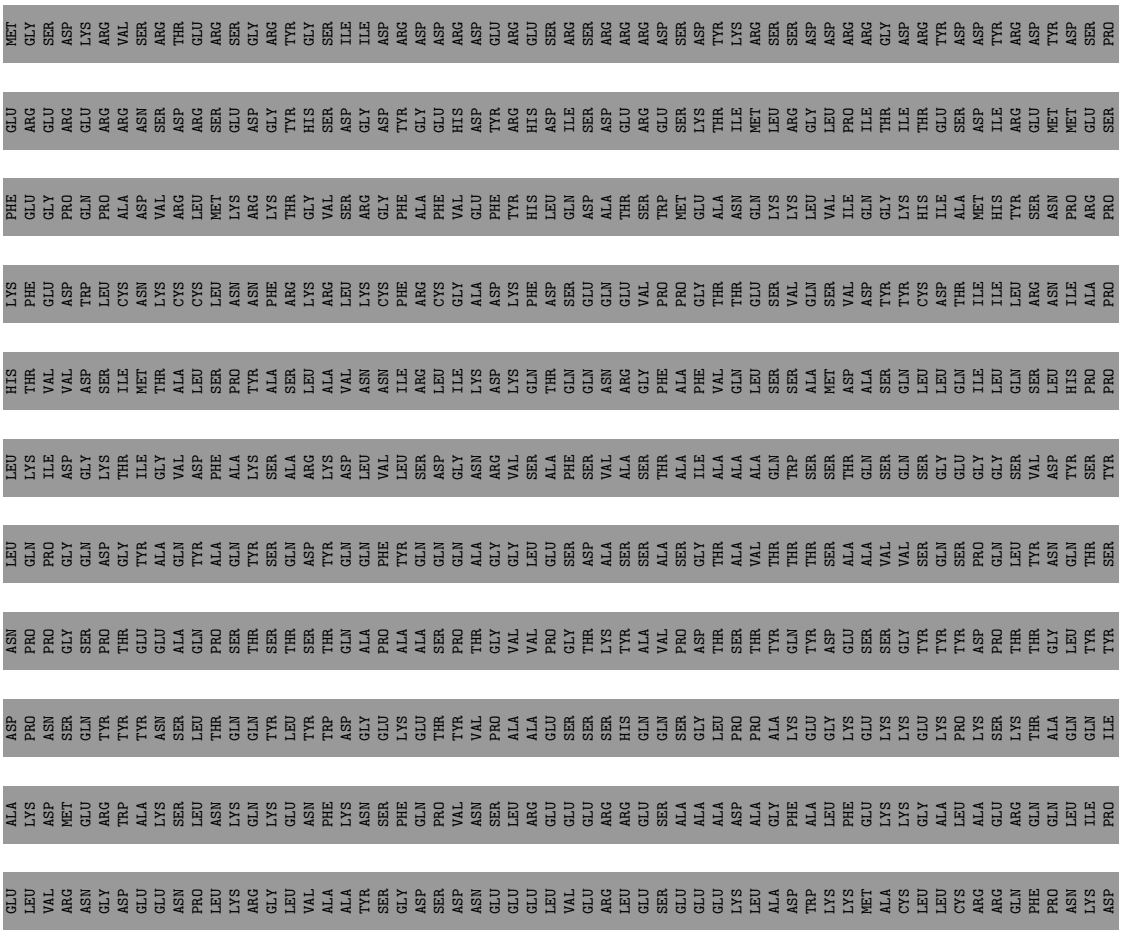
3 Residue-property plots (i)

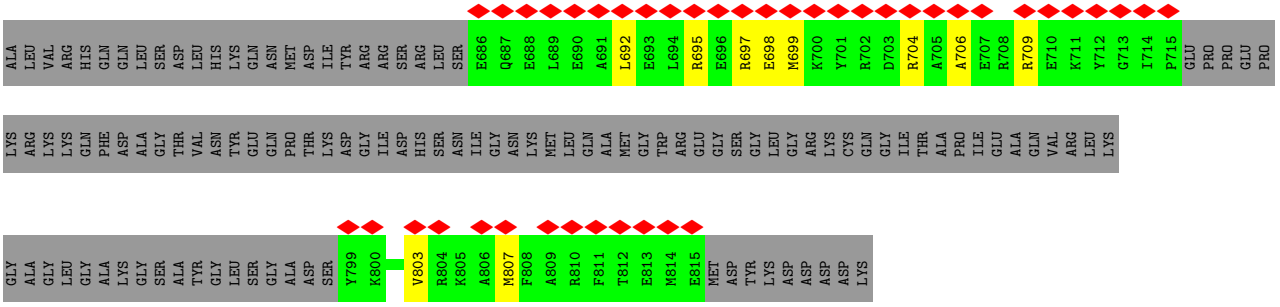
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U2 snRNA



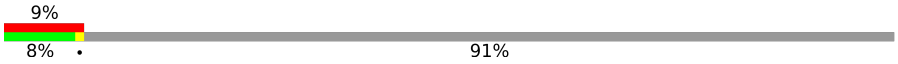
- Molecule 2: RNA-binding protein 5

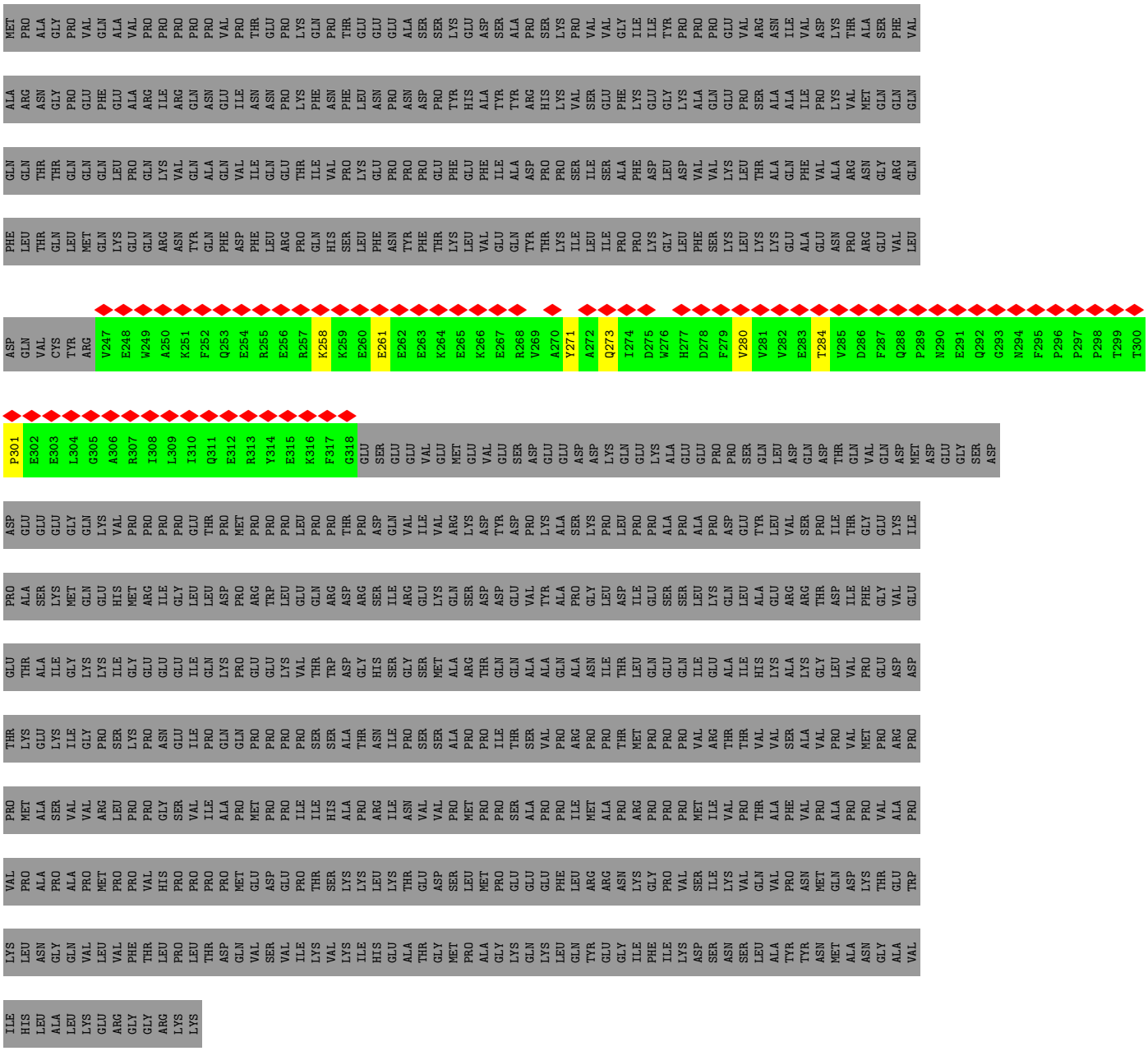




• Molecule 3: Splicing factor 3A subunit 1

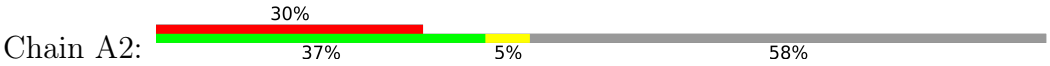
Chain A1:

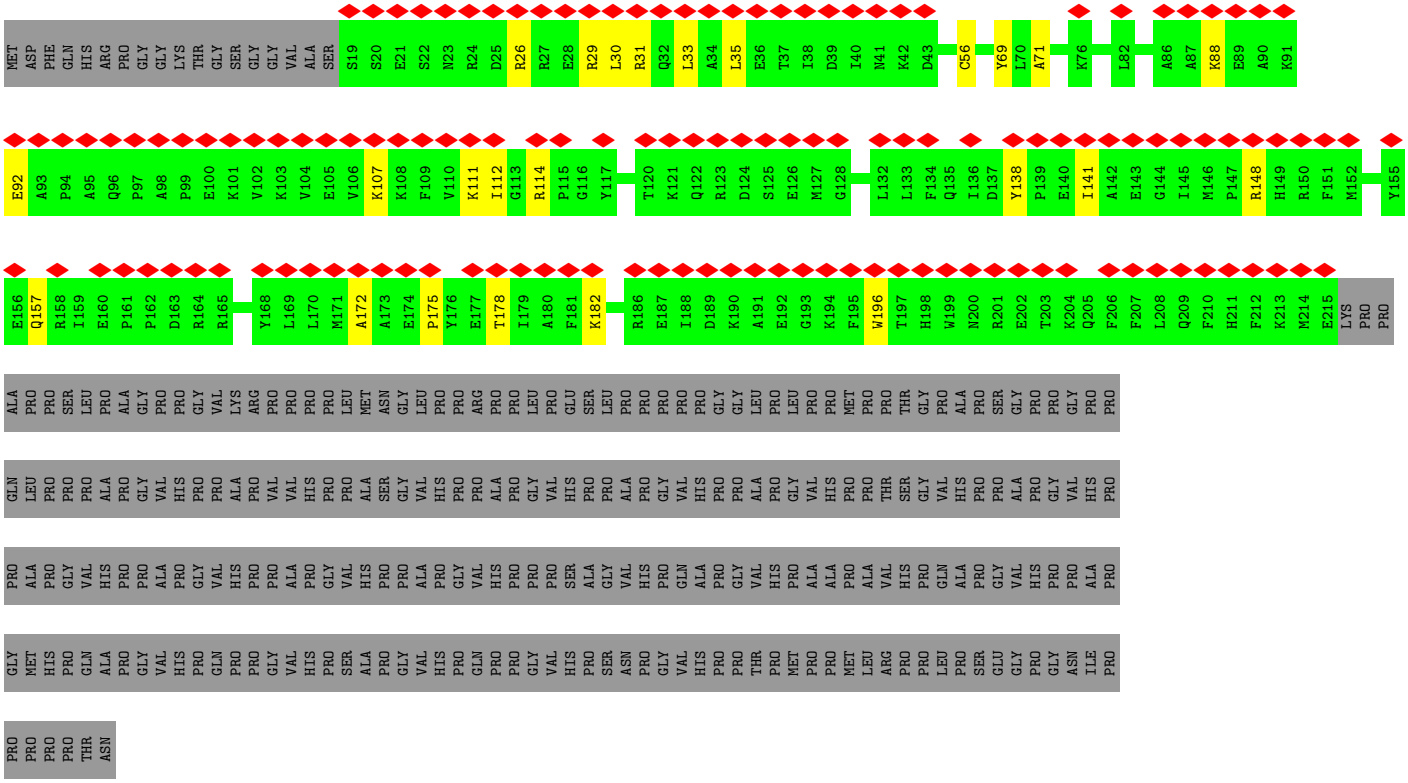




• Molecule 4: Splicing factor 3A subunit 2

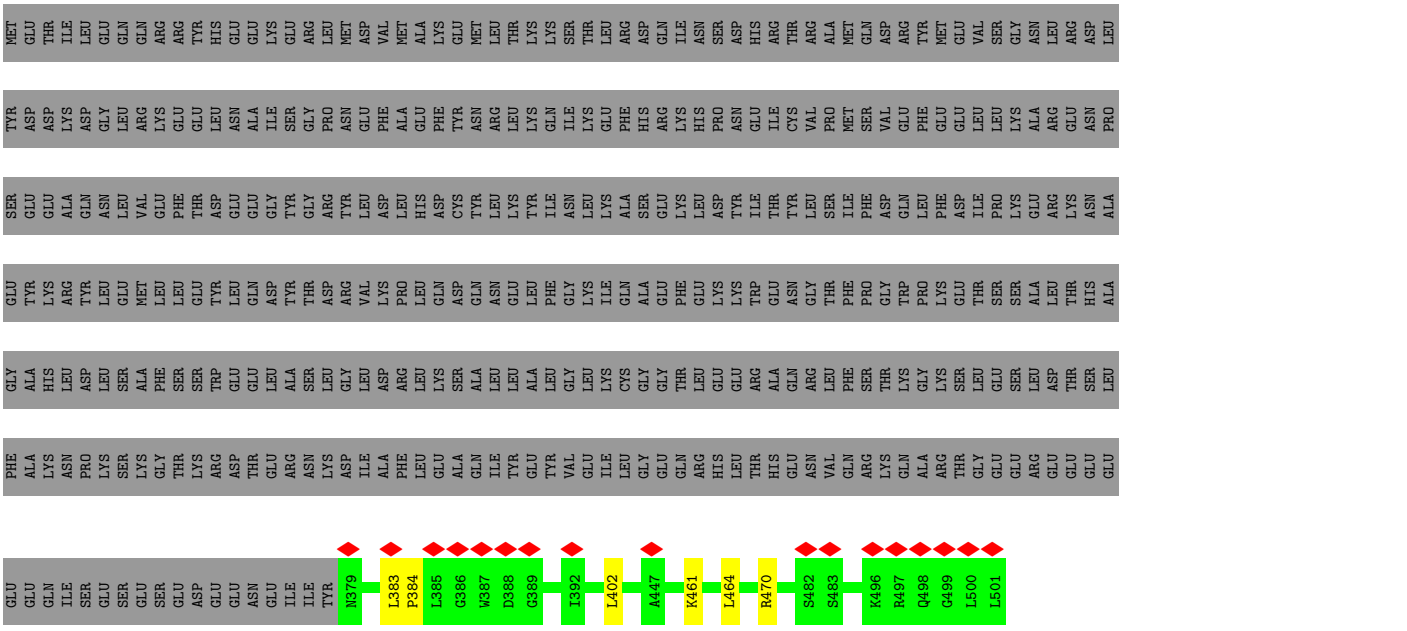
Chain A2:





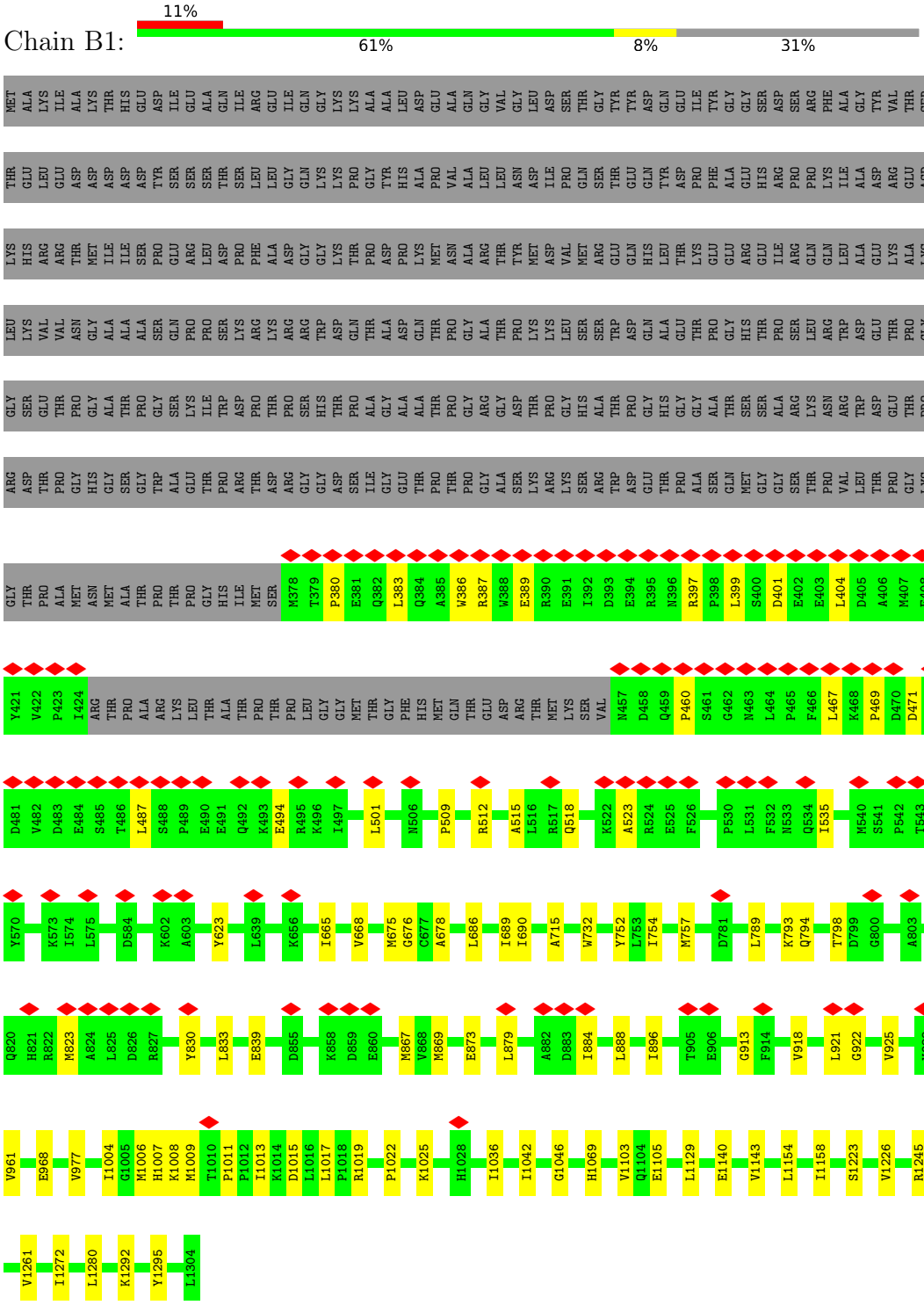
• Molecule 5: Splicing factor 3A subunit 3

Chain A3:



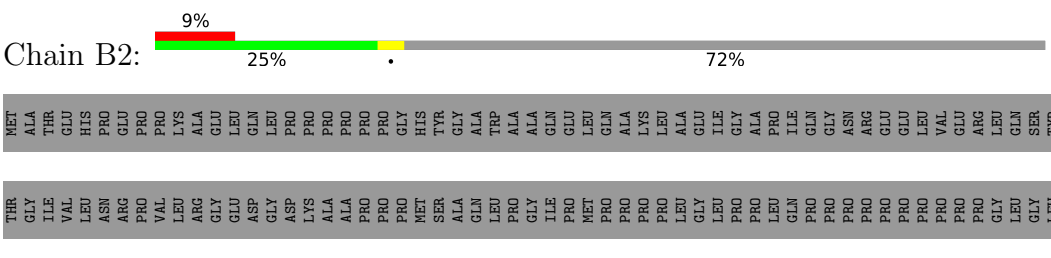
• Molecule 6: Splicing factor 3B subunit 1

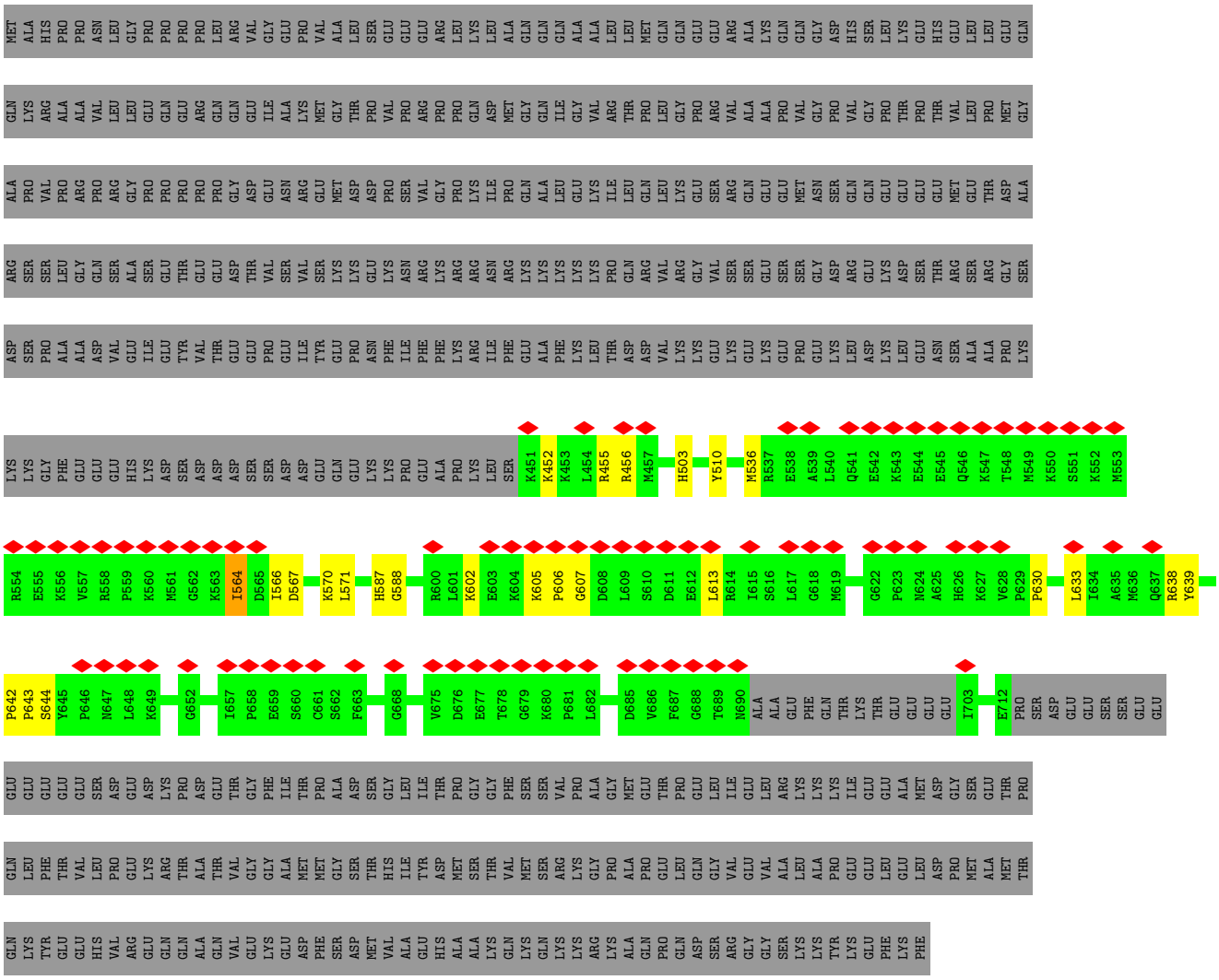
Chain B1:



• Molecule 7: Splicing factor 3B subunit 2

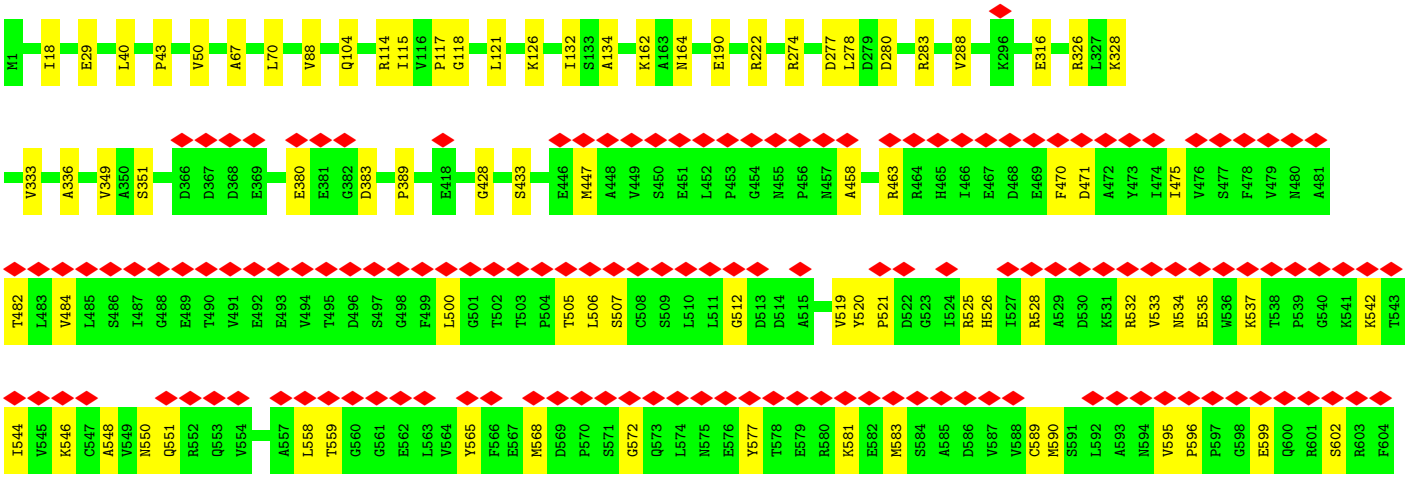
Chain B2:

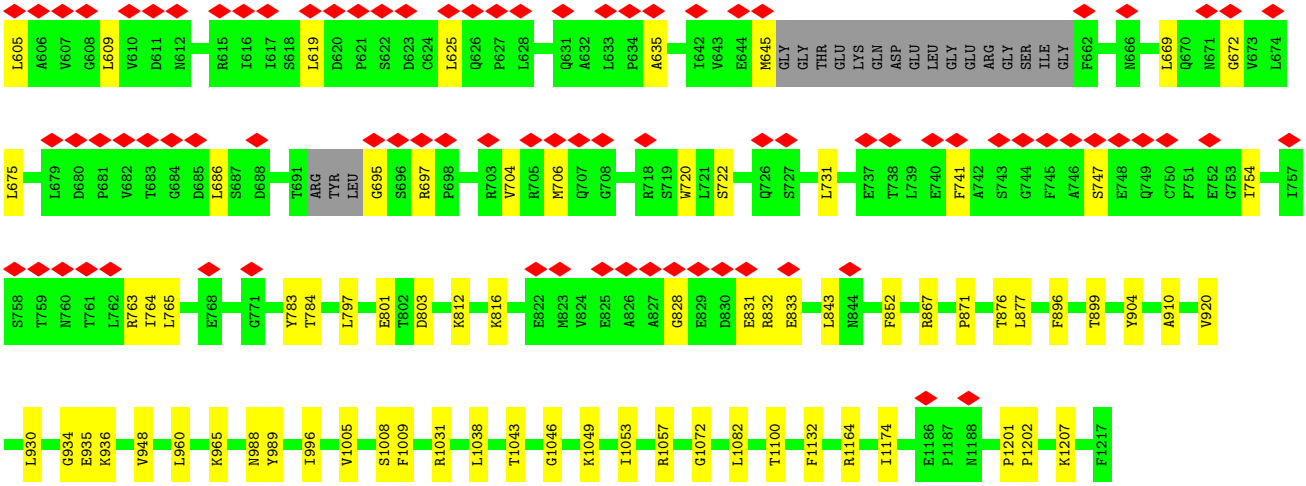




• Molecule 8: Splicing factor 3B subunit 3

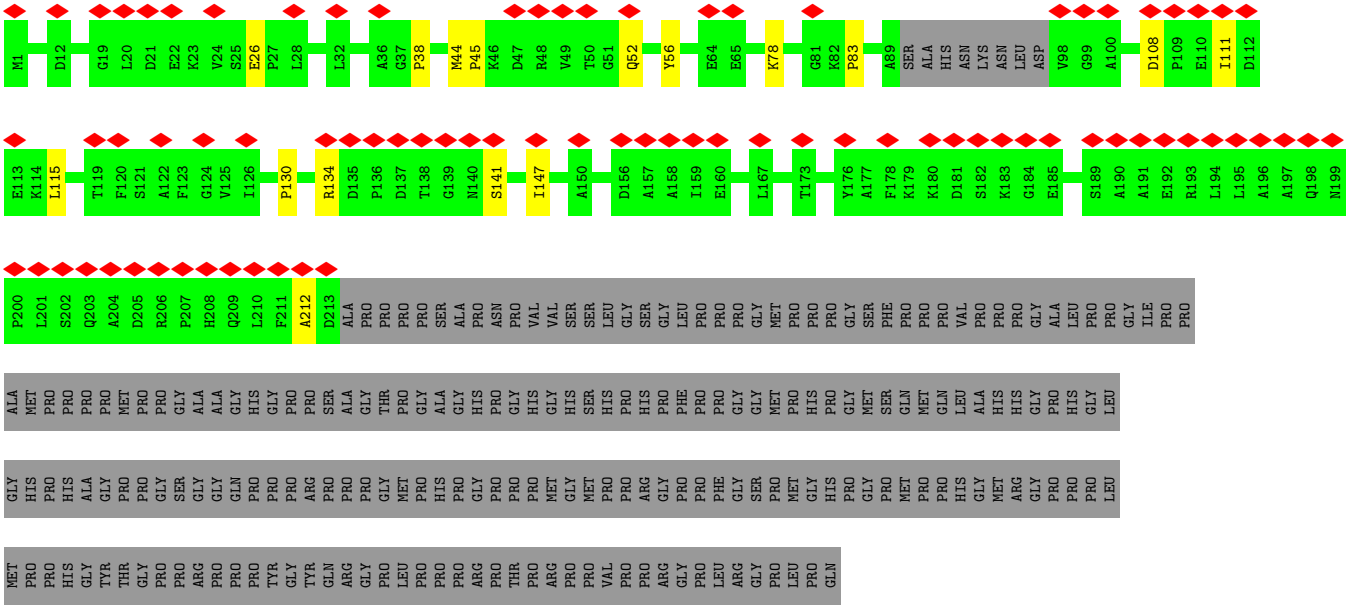
Chain B3:





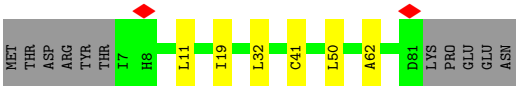
• Molecule 9: Splicing factor 3B subunit 4

Chain B4:



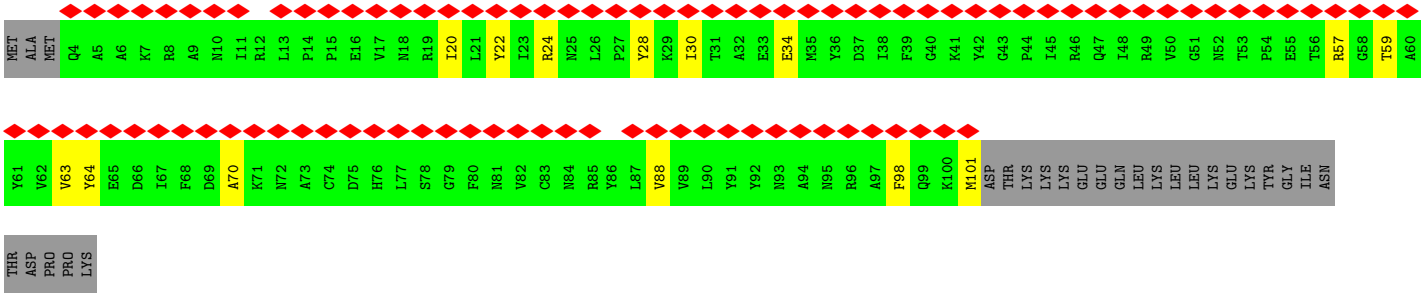
• Molecule 10: Splicing factor 3B subunit 5

Chain B5:

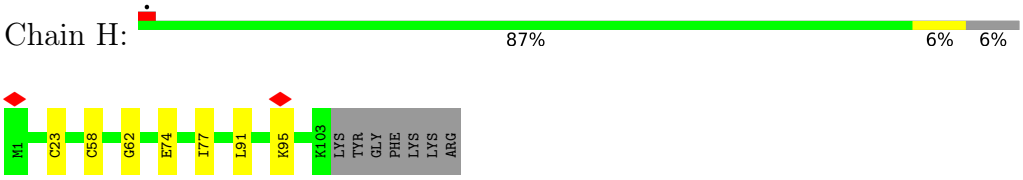


• Molecule 11: Splicing factor 3B subunit 6

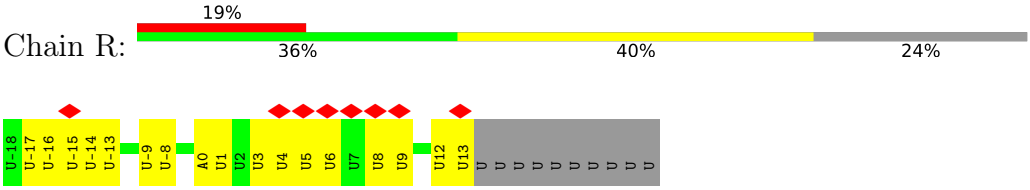
Chain B6:



• Molecule 12: PHD finger-like domain-containing protein 5A



• Molecule 13: Pre-mRNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.809	Depositor
Minimum map value	-1.668	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.08	0/625	0.20	0/972
2	A	0.06	0/412	0.17	0/543
3	A1	0.08	0/630	0.20	0/850
4	A2	0.07	0/1686	0.20	0/2264
5	A3	0.08	0/1045	0.24	0/1416
6	B1	0.10	0/7284	0.26	0/9868
7	B2	0.27	0/2017	0.40	0/2735
8	B3	0.10	0/9590	0.28	0/13015
9	B4	0.08	0/1627	0.25	0/2200
10	B5	0.07	0/634	0.19	0/857
11	B6	0.08	0/823	0.23	0/1114
12	H	0.12	0/807	0.31	0/1082
13	R	0.09	0/706	0.26	0/1089
All	All	0.12	0/27886	0.27	0/38005

There are no bond length outliers.

There are no bond angle outliers.

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	2	781	0	398	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	408	0	402	9	0
3	A1	614	0	573	7	0
4	A2	1645	0	1629	19	0
5	A3	1014	0	974	7	0
6	B1	7142	0	7319	68	0
7	B2	1960	0	1911	17	0
8	B3	9396	0	9309	93	0
9	B4	1593	0	1556	12	0
10	B5	616	0	579	6	0
11	B6	805	0	802	7	0
12	H	794	0	775	6	0
13	R	642	0	324	3	0
14	H	3	0	0	0	0
All	All	27413	0	26551	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B3:920:VAL:HG21	8:B3:948:VAL:HG13	1.62	0.81
6:B1:460:PRO:HD3	6:B1:467:LEU:HD11	1.62	0.81
12:H:58:CYS:HB3	12:H:62:GLY:H	1.49	0.76
8:B3:706:MET:HE1	8:B3:754:ILE:HD11	1.71	0.72
6:B1:1017:LEU:HD21	6:B1:1042:ILE:HG21	1.71	0.72
3:A1:271:TYR:HB2	4:A2:148:ARG:HD2	1.72	0.71
7:B2:605:LYS:HG3	7:B2:607:GLY:H	1.56	0.70
3:A1:273:GLN:HA	4:A2:107:LYS:HG2	1.74	0.69
7:B2:630:PRO:HD2	7:B2:633:LEU:HD22	1.75	0.68
8:B3:447:MET:HB2	8:B3:764:ILE:HG23	1.76	0.66
1:2:42:G:H1	13:R:-9:U:H3	1.45	0.65
9:B4:111:ILE:HG23	9:B4:115:LEU:HD23	1.79	0.65
7:B2:605:LYS:HD2	7:B2:606:PRO:HD2	1.79	0.64
1:2:33:G:H1	13:R:1:U:H3	1.44	0.63
8:B3:507:SER:HB3	8:B3:519:VAL:HB	1.80	0.62
8:B3:877:LEU:HD13	8:B3:935:GLU:HG3	1.82	0.62
6:B1:918:VAL:HG12	6:B1:961:VAL:HG21	1.82	0.62
8:B3:428:GLY:HA3	8:B3:433:SER:HA	1.82	0.62
2:A:803:VAL:HG22	6:B1:623:TYR:HB3	1.83	0.60
6:B1:1140:GLU:HB2	6:B1:1143:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B2:452:LYS:HG3	7:B2:455:ARG:HH21	1.65	0.60
1:2:33:G:N2	13:R:1:U:O2	2.28	0.60
6:B1:811:LEU:HA	6:B1:814:PHE:HB3	1.82	0.60
6:B1:523:ALA:HB1	6:B1:559:ILE:HD13	1.84	0.60
12:H:23:CYS:HB3	12:H:58:CYS:HB2	1.84	0.60
6:B1:968:GLU:HG3	6:B1:1004:ILE:HD11	1.84	0.59
8:B3:115:ILE:HD11	10:B5:19:ILE:HD11	1.84	0.59
4:A2:112:ILE:HD12	4:A2:112:ILE:H	1.68	0.58
6:B1:477:LYS:HZ3	6:B1:494:GLU:HG3	1.68	0.58
4:A2:56:CYS:HB2	4:A2:69:TYR:HE1	1.69	0.58
6:B1:732:TRP:HH2	6:B1:757:MET:HE1	1.69	0.58
8:B3:996:ILE:HD13	8:B3:1038:LEU:HD13	1.85	0.57
5:A3:470:ARG:HH22	8:B3:1072:GLY:HA3	1.69	0.57
4:A2:138:TYR:HB3	4:A2:141:ILE:HB	1.86	0.57
8:B3:316:GLU:HG3	8:B3:326:ARG:HE	1.70	0.57
4:A2:30:LEU:HA	4:A2:33:LEU:HD12	1.87	0.56
6:B1:811:LEU:HG	6:B1:812:PRO:HD3	1.87	0.56
6:B1:1007:HIS:HB3	6:B1:1008:LYS:HD3	1.88	0.56
8:B3:389:PRO:HB2	8:B3:852:PHE:HE2	1.70	0.56
8:B3:635:ALA:HB3	8:B3:669:LEU:HD23	1.87	0.56
4:A2:172:ALA:HB2	4:A2:178:THR:HA	1.87	0.55
11:B6:24:ARG:HG3	11:B6:88:VAL:HB	1.89	0.55
8:B3:1049:LYS:HA	8:B3:1100:THR:HG23	1.89	0.54
6:B1:1103:VAL:HG13	6:B1:1105:GLU:H	1.72	0.54
8:B3:470:PHE:HB3	8:B3:747:SER:HA	1.90	0.54
8:B3:596:PRO:HD2	8:B3:599:GLU:HB3	1.90	0.54
8:B3:18:ILE:HD12	8:B3:67:ALA:HB2	1.90	0.54
8:B3:542:LYS:HD2	8:B3:559:THR:HB	1.89	0.54
6:B1:501:LEU:HD21	6:B1:535:ILE:HG12	1.89	0.53
4:A2:111:LYS:HD2	4:A2:175:PRO:HA	1.90	0.53
8:B3:867:ARG:HH11	8:B3:876:THR:HG21	1.72	0.53
6:B1:1223:SER:HB2	6:B1:1226:VAL:HG12	1.90	0.53
8:B3:548:ALA:HB2	8:B3:590:MET:HB3	1.91	0.52
7:B2:638:ARG:NE	9:B4:212:ALA:HA	2.24	0.52
9:B4:134:ARG:HG2	9:B4:141:SER:HA	1.92	0.52
8:B3:520:TYR:HE1	8:B3:525:ARG:HG3	1.74	0.52
8:B3:675:LEU:HD23	8:B3:686:LEU:HD12	1.92	0.52
6:B1:563:LEU:HD12	6:B1:566:LEU:HD13	1.90	0.52
1:2:47:OMC:H5	5:A3:383:LEU:HD11	1.73	0.52
1:2:41:PSU:H2'	1:2:42:G:C8	2.45	0.52
8:B3:899:THR:HG21	8:B3:904:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B4:26:GLU:HG3	9:B4:44:MET:HG3	1.91	0.51
6:B1:397:ARG:HH21	6:B1:399:LEU:HD13	1.76	0.51
6:B1:665:ILE:HG23	6:B1:690:ILE:HD12	1.92	0.51
12:H:91:LEU:HB2	12:H:95:LYS:HD3	1.92	0.51
6:B1:869:MET:HE1	6:B1:896:ILE:HG22	1.92	0.51
8:B3:550:ASN:ND2	8:B3:602:SER:HB2	2.26	0.51
8:B3:336:ALA:HA	8:B3:351:SER:HA	1.92	0.50
9:B4:130:PRO:HB3	9:B4:147:ILE:HG12	1.93	0.50
6:B1:387:ARG:HH22	6:B1:469:PRO:HG2	1.76	0.50
8:B3:828:GLY:HA2	8:B3:832:ARG:HD3	1.93	0.50
8:B3:278:LEU:HD11	8:B3:812:LYS:HZ3	1.77	0.50
6:B1:1006:MET:HE2	6:B1:1013:ILE:HB	1.93	0.50
7:B2:613:LEU:H	7:B2:613:LEU:HD23	1.76	0.50
9:B4:78:LYS:HA	9:B4:83:PRO:HA	1.93	0.50
6:B1:515:ALA:HA	6:B1:518:GLN:NE2	2.27	0.49
6:B1:686:LEU:HA	6:B1:689:ILE:HD12	1.94	0.49
4:A2:26:ARG:HG2	4:A2:29:ARG:HH21	1.76	0.49
8:B3:29:GLU:HG2	8:B3:40:LEU:HD21	1.95	0.49
8:B3:605:LEU:HB2	8:B3:619:LEU:HD11	1.94	0.49
2:A:706:ALA:HA	2:A:709:ARG:HE	1.77	0.49
8:B3:500:LEU:HB2	8:B3:525:ARG:HH12	1.77	0.49
11:B6:22:TYR:HE1	11:B6:59:THR:HB	1.77	0.49
1:2:63:G:H2'	1:2:64:A:C8	2.48	0.49
8:B3:783:TYR:HB2	8:B3:801:GLU:HB3	1.94	0.49
8:B3:930:LEU:HG	8:B3:934:GLY:HA2	1.93	0.49
6:B1:1272:ILE:HG22	6:B1:1280:LEU:HD11	1.94	0.48
6:B1:830:TYR:HE1	6:B1:867:MET:HG3	1.78	0.48
2:A:692:LEU:O	2:A:695:ARG:HG2	2.14	0.48
8:B3:528:ARG:HG2	8:B3:532:ARG:HH21	1.78	0.48
11:B6:28:TYR:HB3	11:B6:57:ARG:HE	1.78	0.48
11:B6:30:ILE:HG13	11:B6:34:GLU:HB2	1.94	0.48
7:B2:455:ARG:HH22	7:B2:456:ARG:HE	1.62	0.48
8:B3:704:VAL:HG11	8:B3:754:ILE:HG13	1.96	0.48
1:2:41:PSU:H2'	1:2:42:G:H8	1.78	0.47
6:B1:830:TYR:CE1	6:B1:867:MET:HG3	2.49	0.47
8:B3:274:ARG:HB2	8:B3:277:ASP:HB3	1.96	0.47
3:A1:301:PRO:HG3	4:A2:196:TRP:CD2	2.49	0.47
3:A1:273:GLN:HB2	4:A2:107:LYS:HA	1.95	0.47
8:B3:118:GLY:HA2	8:B3:132:ILE:HD11	1.96	0.47
8:B3:528:ARG:HH22	8:B3:572:GLY:HA3	1.80	0.47
2:A:697:ARG:HH11	6:B1:1015:ASP:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B3:565:TYR:HD2	8:B3:577:TYR:HB2	1.78	0.47
8:B3:722:SER:HB2	8:B3:731:LEU:HD13	1.97	0.47
8:B3:288:VAL:HG12	10:B5:62:ALA:HB3	1.97	0.47
7:B2:644:SER:HB3	9:B4:38:PRO:HD3	1.97	0.46
8:B3:551:GLN:HB2	8:B3:595:VAL:HB	1.97	0.46
1:2:40:OMC:H2'	1:2:41:PSU:C6	2.50	0.46
8:B3:520:TYR:CE1	8:B3:525:ARG:HG3	2.50	0.46
8:B3:1132:PHE:HE2	8:B3:1174:ILE:HD12	1.79	0.46
6:B1:675:MET:HB2	6:B1:678:ALA:HB3	1.98	0.46
8:B3:475:ILE:HD13	8:B3:484:VAL:HG13	1.97	0.46
8:B3:831:GLU:HG2	8:B3:833:GLU:H	1.81	0.46
3:A1:284:THR:HG23	4:A2:182:LYS:HB3	1.98	0.46
8:B3:533:VAL:HG12	8:B3:535:GLU:HB2	1.96	0.46
8:B3:512:GLY:HA2	8:B3:568:MET:HE2	1.98	0.46
12:H:95:LYS:HE3	12:H:95:LYS:HB3	1.83	0.46
6:B1:823:MET:HE2	6:B1:833:LEU:HD22	1.98	0.46
8:B3:910:ALA:CB	8:B3:948:VAL:HG12	2.46	0.46
1:2:40:OMC:H2'	1:2:41:PSU:H6	1.81	0.46
8:B3:544:ILE:HA	8:B3:558:LEU:HA	1.98	0.46
4:A2:26:ARG:HA	4:A2:29:ARG:HE	1.82	0.45
6:B1:559:ILE:HD11	6:B1:563:LEU:HD22	1.97	0.45
7:B2:536:MET:H	7:B2:536:MET:HG2	1.59	0.45
7:B2:588:GLY:HA3	8:B3:1082:LEU:HD11	1.98	0.45
8:B3:1008:SER:OG	8:B3:1031:ARG:HG3	2.17	0.45
5:A3:383:LEU:HD12	5:A3:383:LEU:H	1.82	0.45
6:B1:1006:MET:HG2	6:B1:1046:GLY:HA3	1.98	0.45
6:B1:668:VAL:HG21	6:B1:690:ILE:HD11	1.99	0.44
5:A3:464:LEU:HD12	5:A3:464:LEU:HA	1.81	0.44
6:B1:922:GLY:O	6:B1:925:VAL:HG12	2.18	0.44
11:B6:64:TYR:HB2	11:B6:70:ALA:HB2	1.98	0.44
6:B1:793:LYS:HG3	6:B1:839:GLU:HG2	1.99	0.44
8:B3:583:MET:HB3	8:B3:609:LEU:HD21	1.98	0.44
8:B3:114:ARG:HG3	10:B5:41:CYS:SG	2.57	0.44
8:B3:117:PRO:HA	8:B3:134:ALA:HB2	1.99	0.44
6:B1:380:PRO:HA	6:B1:383:LEU:HD12	1.98	0.44
8:B3:164:ASN:HD22	8:B3:190:GLU:HB3	1.82	0.44
2:A:704:ARG:HH21	6:B1:977:VAL:HG23	1.83	0.44
8:B3:797:LEU:HG	8:B3:871:PRO:HG3	1.99	0.44
6:B1:477:LYS:NZ	6:B1:494:GLU:HG3	2.33	0.44
1:2:47:OMC:C5	5:A3:383:LEU:HD11	2.53	0.43
6:B1:509:PRO:HA	6:B1:512:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:31:G:O6	6:B1:1069:HIS:HB3	2.17	0.43
4:A2:111:LYS:HB2	4:A2:175:PRO:HA	2.00	0.43
6:B1:1025:LYS:HA	6:B1:1025:LYS:HD2	1.88	0.43
7:B2:638:ARG:HG3	7:B2:639:TYR:CD1	2.53	0.43
8:B3:482:THR:HG21	8:B3:505:THR:HG22	1.99	0.43
8:B3:463:ARG:HG2	8:B3:471:ASP:HA	2.00	0.43
8:B3:581:LYS:HE3	8:B3:625:LEU:HG	2.00	0.43
8:B3:602:SER:HB3	8:B3:619:LEU:HD13	2.00	0.43
8:B3:162:LYS:HD3	8:B3:222:ARG:NH1	2.33	0.43
8:B3:121:LEU:HD12	8:B3:121:LEU:HA	1.87	0.43
8:B3:126:LYS:HD3	8:B3:126:LYS:HA	1.83	0.43
8:B3:280:ASP:HB3	8:B3:283:ARG:HG3	1.99	0.43
8:B3:506:LEU:HG	8:B3:521:PRO:HD3	2.00	0.43
8:B3:784:THR:HG22	8:B3:803:ASP:OD2	2.17	0.43
8:B3:936:LYS:HB2	8:B3:936:LYS:HE3	1.83	0.43
2:A:692:LEU:HA	2:A:695:ARG:HE	1.84	0.43
2:A:695:ARG:O	2:A:698:GLU:HG2	2.18	0.43
6:B1:819:TRP:CZ3	6:B1:867:MET:HE3	2.53	0.43
6:B1:1036:ILE:HD12	6:B1:1036:ILE:HA	1.89	0.43
1:2:42:G:H2'	1:2:43:PSU:O4	2.19	0.43
2:A:698:GLU:HG3	2:A:699:MET:HE2	2.01	0.43
7:B2:638:ARG:HE	9:B4:212:ALA:HA	1.83	0.43
8:B3:1009:PHE:HZ	8:B3:1046:GLY:HA3	1.83	0.42
8:B3:1043:THR:HG22	8:B3:1057:ARG:HB2	2.01	0.42
9:B4:52:GLN:H	9:B4:52:GLN:HG3	1.63	0.42
10:B5:50:LEU:HD12	10:B5:50:LEU:HA	1.88	0.42
8:B3:520:TYR:HB2	8:B3:521:PRO:HD2	2.00	0.42
8:B3:695:GLY:O	8:B3:697:ARG:HG2	2.19	0.42
6:B1:471:ASP:HB2	6:B1:475:PHE:HD2	1.84	0.42
6:B1:676:GLY:O	6:B1:715:ALA:HB1	2.19	0.42
6:B1:884:ILE:HG23	6:B1:888:LEU:HD23	2.01	0.42
4:A2:31:ARG:HE	4:A2:71:ALA:HA	1.84	0.42
8:B3:960:LEU:HD12	8:B3:960:LEU:HA	1.91	0.42
8:B3:989:TYR:HB3	8:B3:1005:VAL:HB	2.02	0.42
8:B3:43:PRO:HB3	8:B3:50:VAL:HG12	2.02	0.42
8:B3:988:ASN:HB3	8:B3:989:TYR:H	1.53	0.42
2:A:807:MET:HE2	2:A:807:MET:HB3	1.93	0.42
1:2:38:A:H2'	1:2:39:PSU:H6	1.84	0.42
4:A2:88:LYS:O	4:A2:92:GLU:HG2	2.20	0.42
6:B1:460:PRO:HA	6:B1:479:LEU:HA	2.01	0.42
6:B1:563:LEU:HD12	6:B1:563:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B3:328:LYS:HB3	8:B3:328:LYS:HE3	1.79	0.42
6:B1:873:GLU:HG3	6:B1:913:GLY:HA2	2.01	0.42
6:B1:1009:MET:HG3	6:B1:1011:PRO:HD2	2.02	0.42
7:B2:642:PRO:HA	7:B2:643:PRO:HD3	1.98	0.42
8:B3:546:LYS:HD2	8:B3:589:CYS:HA	2.01	0.42
11:B6:20:ILE:HG23	11:B6:63:VAL:HG22	2.01	0.42
6:B1:879:LEU:HD13	6:B1:879:LEU:HA	1.94	0.42
7:B2:564:ILE:H	7:B2:564:ILE:HG13	1.54	0.42
6:B1:752:TYR:HA	6:B1:794:GLN:HE22	1.84	0.42
8:B3:537:LYS:HD3	8:B3:537:LYS:HA	1.81	0.42
9:B4:108:ASP:HB3	9:B4:111:ILE:HG13	2.02	0.42
10:B5:11:LEU:HD12	10:B5:11:LEU:HA	1.90	0.42
8:B3:816:LYS:HG2	8:B3:843:LEU:HD23	2.02	0.41
8:B3:70:LEU:HD12	8:B3:70:LEU:HA	1.90	0.41
8:B3:380:GLU:HB3	8:B3:383:ASP:HB2	2.01	0.41
3:A1:280:VAL:HG11	4:A2:114:ARG:NH2	2.35	0.41
6:B1:401:ASP:HA	6:B1:404:LEU:HD12	2.02	0.41
6:B1:471:ASP:HB2	6:B1:475:PHE:CD2	2.55	0.41
6:B1:921:LEU:HD23	6:B1:921:LEU:HA	1.90	0.41
8:B3:896:PHE:HB2	8:B3:899:THR:HG22	2.03	0.41
6:B1:487:LEU:H	6:B1:487:LEU:HD23	1.86	0.41
6:B1:386:TRP:O	6:B1:389:GLU:HG3	2.21	0.41
6:B1:1245:ARG:HA	6:B1:1245:ARG:HD3	1.89	0.41
6:B1:1292:LYS:HA	6:B1:1292:LYS:HD2	1.85	0.41
8:B3:88:VAL:HG12	8:B3:104:GLN:HG3	2.03	0.41
6:B1:1295:TYR:CD1	10:B5:32:LEU:HD13	2.56	0.41
8:B3:590:MET:HB3	8:B3:590:MET:HE3	1.90	0.41
3:A1:258:LYS:HA	3:A1:261:GLU:HG2	2.03	0.41
6:B1:1247:LEU:HD22	6:B1:1280:LEU:HD22	2.03	0.41
8:B3:672:GLY:HA3	8:B3:695:GLY:N	2.36	0.41
8:B3:1164:ARG:HD3	8:B3:1164:ARG:HA	1.86	0.41
8:B3:1207:LYS:HE2	8:B3:1207:LYS:HB2	1.81	0.41
9:B4:45:PRO:HG2	9:B4:56:TYR:CZ	2.56	0.41
6:B1:1129:LEU:HD23	6:B1:1129:LEU:HA	1.87	0.41
8:B3:645:MET:HE2	8:B3:645:MET:HB2	1.93	0.41
4:A2:35:LEU:HD23	4:A2:35:LEU:HA	1.87	0.41
5:A3:461:LYS:HE3	5:A3:461:LYS:HB2	1.86	0.41
6:B1:754:ILE:HG22	6:B1:798:THR:HG21	2.03	0.41
6:B1:789:LEU:HD12	6:B1:789:LEU:HA	1.85	0.41
6:B1:1019:ARG:O	6:B1:1022:PRO:HD2	2.21	0.41
6:B1:1154:LEU:O	6:B1:1158:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B3:458:ALA:HA	8:B3:741:PHE:CG	2.56	0.41
8:B3:763:ARG:HB3	8:B3:765:LEU:HD21	2.03	0.41
12:H:74:GLU:HA	12:H:77:ILE:HG12	2.02	0.41
12:H:91:LEU:HD23	12:H:91:LEU:H	1.86	0.41
1:2:40:OMC:HM23	1:2:40:OMC:H1'	1.78	0.41
4:A2:157:GLN:H	4:A2:157:GLN:HG3	1.74	0.41
6:B1:1245:ARG:HD2	7:B2:587:HIS:CE1	2.56	0.41
8:B3:526:HIS:HB3	8:B3:534:ASN:HB2	2.03	0.40
9:B4:45:PRO:HG2	9:B4:56:TYR:CE2	2.55	0.40
6:B1:943:LYS:HD2	6:B1:943:LYS:HA	1.83	0.40
8:B3:333:VAL:HG11	8:B3:349:VAL:HG21	2.04	0.40
7:B2:503:HIS:CG	7:B2:510:TYR:HB2	2.55	0.40
6:B1:1258:ALA:HB3	6:B1:1261:VAL:HG12	2.03	0.40
8:B3:720:TRP:HE3	8:B3:731:LEU:HG	1.86	0.40
5:A3:384:PRO:HG2	5:A3:402:LEU:HD13	2.03	0.40
7:B2:602:LYS:HE2	7:B2:602:LYS:HB2	1.85	0.40
8:B3:1201:PRO:N	8:B3:1202:PRO:HD2	2.36	0.40
11:B6:98:PHE:HA	11:B6:101:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	43/824 (5%)	43 (100%)	0	0	100	100
3	A1	70/793 (9%)	69 (99%)	1 (1%)	0	100	100
4	A2	195/464 (42%)	189 (97%)	6 (3%)	0	100	100
5	A3	121/501 (24%)	118 (98%)	3 (2%)	0	100	100
6	B1	891/1304 (68%)	871 (98%)	20 (2%)	0	100	100
7	B2	246/895 (28%)	232 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B3	1192/1217 (98%)	1153 (97%)	39 (3%)	0	100	100
9	B4	201/424 (47%)	196 (98%)	5 (2%)	0	100	100
10	B5	73/86 (85%)	71 (97%)	2 (3%)	0	100	100
11	B6	96/125 (77%)	95 (99%)	1 (1%)	0	100	100
12	H	101/110 (92%)	94 (93%)	7 (7%)	0	100	100
All	All	3229/6743 (48%)	3131 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	40/704 (6%)	40 (100%)	0	100	100
3	A1	64/709 (9%)	64 (100%)	0	100	100
4	A2	174/382 (46%)	174 (100%)	0	100	100
5	A3	106/446 (24%)	106 (100%)	0	100	100
6	B1	775/1104 (70%)	775 (100%)	0	100	100
7	B2	201/776 (26%)	196 (98%)	5 (2%)	42	59
8	B3	1037/1051 (99%)	1035 (100%)	2 (0%)	87	84
9	B4	167/336 (50%)	167 (100%)	0	100	100
10	B5	66/77 (86%)	66 (100%)	0	100	100
11	B6	84/109 (77%)	84 (100%)	0	100	100
12	H	89/95 (94%)	89 (100%)	0	100	100
All	All	2803/5789 (48%)	2796 (100%)	7 (0%)	85	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B2	564	ILE

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Mol	Chain	Res	Type
7	B2	566	ILE
7	B2	567	ASP
7	B2	570	LYS
7	B2	571	LEU
8	B3	965	LYS
8	B3	1053	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
4	A2	23	ASN
4	A2	209	GLN
5	A3	431	HIS
5	A3	448	ASN
6	B1	518	GLN
6	B1	547	GLN
6	B1	662	HIS
6	B1	698	GLN
6	B1	778	GLN
6	B1	1091	HIS
6	B1	1218	ASN
6	B1	1248	GLN
6	B1	1256	HIS
6	B1	1293	ASN
7	B2	496	ASN
7	B2	637	GLN
8	B3	104	GLN
8	B3	138	GLN
8	B3	164	ASN
8	B3	411	GLN
8	B3	861	GLN
8	B3	932	ASN
8	B3	956	GLN
8	B3	988	ASN
8	B3	1096	HIS
8	B3	1105	GLN
8	B3	1147	HIS
9	B4	187	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/37 (97%)	8 (22%)	0
13	R	31/42 (73%)	15 (48%)	1 (3%)
All	All	67/79 (84%)	23 (34%)	1 (1%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	30	A
1	2	31	G
1	2	43	PSU
1	2	44	PSU
1	2	46	U
1	2	47	OMC
1	2	48	A
1	2	65	U
13	R	-17	U
13	R	-16	U
13	R	-15	U
13	R	-14	U
13	R	-13	U
13	R	-8	U
13	R	0	A
13	R	3	U
13	R	4	U
13	R	5	U
13	R	6	U
13	R	8	U
13	R	9	U
13	R	12	U
13	R	13	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	R	8	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	OMC	2	61	1	19,22,23	0.50	0	25,31,34	0.72	0
1	PSU	2	41	1,13	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
1	PSU	2	34	1,13	18,21,22	1.11	1 (5%)	21,30,33	1.89	5 (23%)
1	PSU	2	39	1	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
1	OMC	2	47	1	19,22,23	0.51	0	25,31,34	1.01	2 (8%)
1	PSU	2	54	1	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
1	PSU	2	58	1	18,21,22	1.09	1 (5%)	21,30,33	1.77	4 (19%)
1	PSU	2	37	1	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
1	PSU	2	43	1	18,21,22	1.11	1 (5%)	21,30,33	1.66	4 (19%)
1	OMC	2	40	1,13	19,22,23	0.50	0	25,31,34	0.71	0
1	PSU	2	44	1	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)

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
1	OMC	2	61	1	-	0/9/27/28	0/2/2/2
1	PSU	2	41	1,13	-	0/7/25/26	0/2/2/2
1	PSU	2	34	1,13	-	0/7/25/26	0/2/2/2
1	PSU	2	39	1	-	0/7/25/26	0/2/2/2
1	OMC	2	47	1	-	6/9/27/28	0/2/2/2
1	PSU	2	54	1	-	0/7/25/26	0/2/2/2
1	PSU	2	58	1	-	2/7/25/26	0/2/2/2
1	PSU	2	37	1	-	0/7/25/26	0/2/2/2
1	PSU	2	43	1	-	5/7/25/26	0/2/2/2
1	OMC	2	40	1,13	-	1/9/27/28	0/2/2/2
1	PSU	2	44	1	-	3/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	43	PSU	C6-C5	3.89	1.39	1.35
1	2	44	PSU	C6-C5	3.81	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	58	PSU	C6-C5	3.73	1.39	1.35
1	2	54	PSU	C6-C5	3.73	1.39	1.35
1	2	39	PSU	C6-C5	3.68	1.39	1.35
1	2	34	PSU	C6-C5	3.67	1.39	1.35
1	2	37	PSU	C6-C5	3.66	1.39	1.35
1	2	41	PSU	C6-C5	3.59	1.39	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	37	PSU	C4-N3-C2	-4.85	119.69	126.37
1	2	54	PSU	C4-N3-C2	-4.82	119.73	126.37
1	2	37	PSU	N1-C2-N3	4.77	120.20	115.17
1	2	41	PSU	N1-C2-N3	4.75	120.17	115.17
1	2	44	PSU	N1-C2-N3	4.74	120.17	115.17
1	2	34	PSU	C4-N3-C2	-4.73	119.86	126.37
1	2	41	PSU	C4-N3-C2	-4.72	119.87	126.37
1	2	34	PSU	N1-C2-N3	4.70	120.13	115.17
1	2	54	PSU	N1-C2-N3	4.69	120.11	115.17
1	2	39	PSU	N1-C2-N3	4.68	120.11	115.17
1	2	39	PSU	C4-N3-C2	-4.68	119.92	126.37
1	2	44	PSU	C4-N3-C2	-4.51	120.16	126.37
1	2	58	PSU	N1-C2-N3	4.46	119.88	115.17
1	2	43	PSU	N1-C2-N3	4.33	119.73	115.17
1	2	58	PSU	C4-N3-C2	-4.31	120.44	126.37
1	2	43	PSU	C4-N3-C2	-4.19	120.59	126.37
1	2	41	PSU	O2-C2-N1	-3.10	119.59	122.79
1	2	47	OMC	C1'-N1-C2	2.98	125.03	118.44
1	2	44	PSU	O2-C2-N1	-2.96	119.74	122.79
1	2	39	PSU	O2-C2-N1	-2.76	119.94	122.79
1	2	43	PSU	C6-N1-C2	-2.74	120.15	122.69
1	2	37	PSU	O2-C2-N1	-2.72	119.98	122.79
1	2	58	PSU	C6-N1-C2	-2.71	120.18	122.69
1	2	34	PSU	O2-C2-N1	-2.70	120.00	122.79
1	2	54	PSU	O2-C2-N1	-2.68	120.02	122.79
1	2	44	PSU	C6-N1-C2	-2.65	120.23	122.69
1	2	58	PSU	O2-C2-N1	-2.63	120.07	122.79
1	2	41	PSU	C6-N1-C2	-2.59	120.28	122.69
1	2	43	PSU	O2-C2-N1	-2.52	120.19	122.79
1	2	39	PSU	C6-N1-C2	-2.44	120.42	122.69
1	2	47	OMC	C1'-N1-C6	-2.40	115.65	120.78
1	2	34	PSU	C6-N1-C2	-2.37	120.49	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	37	PSU	C6-N1-C2	-2.31	120.55	122.69
1	2	54	PSU	C6-N1-C2	-2.30	120.56	122.69
1	2	37	PSU	C6-C5-C4	2.25	119.69	118.17
1	2	34	PSU	O4'-C1'-C2'	2.09	108.05	105.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	43	PSU	O4'-C1'-C5-C4
1	2	43	PSU	O4'-C1'-C5-C6
1	2	43	PSU	C3'-C4'-C5'-O5'
1	2	43	PSU	O4'-C4'-C5'-O5'
1	2	44	PSU	O4'-C1'-C5-C4
1	2	44	PSU	O4'-C1'-C5-C6
1	2	58	PSU	O4'-C1'-C5-C4
1	2	58	PSU	O4'-C1'-C5-C6
1	2	47	OMC	O4'-C4'-C5'-O5'
1	2	47	OMC	C3'-C4'-C5'-O5'
1	2	40	OMC	C1'-C2'-O2'-CM2
1	2	47	OMC	C4'-C5'-O5'-P
1	2	47	OMC	O4'-C1'-N1-C6
1	2	47	OMC	C2'-C1'-N1-C6
1	2	43	PSU	C2'-C1'-C5-C6
1	2	47	OMC	O4'-C1'-N1-C2
1	2	44	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	41	PSU	4	0
1	2	39	PSU	1	0
1	2	47	OMC	2	0
1	2	43	PSU	1	0
1	2	40	OMC	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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)

There are no chain breaks in this entry.

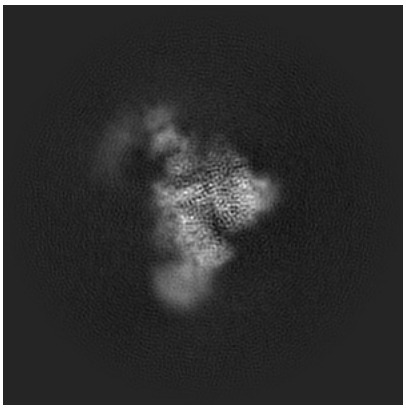
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-74099. These allow visual inspection of the internal detail of the map and identification of artifacts.

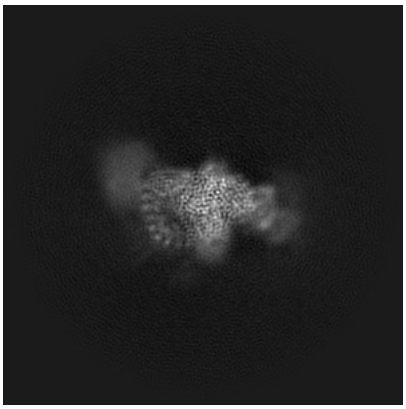
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

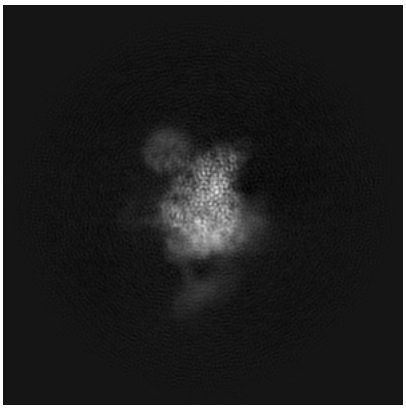
6.1.1 Primary map



X

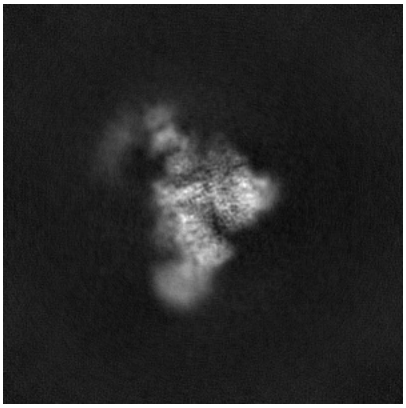


Y

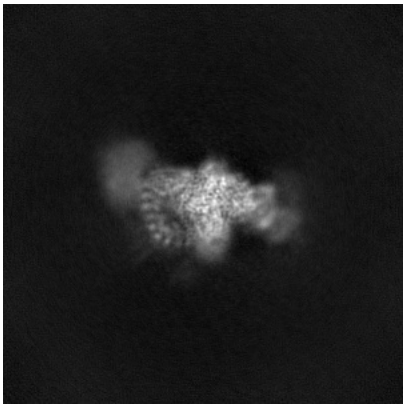


Z

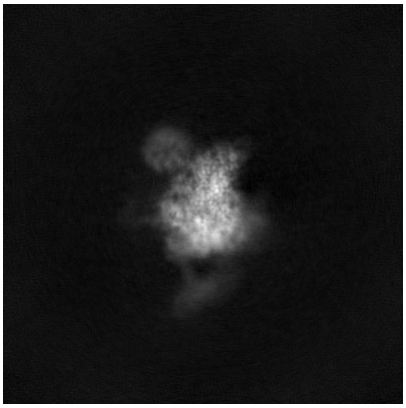
6.1.2 Raw map



X



Y

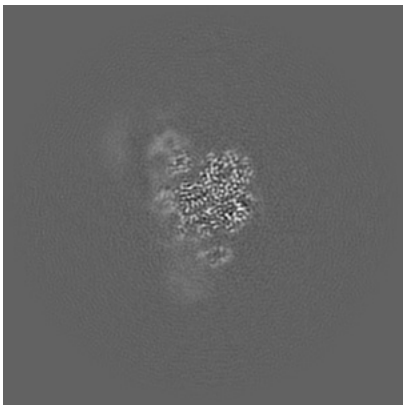


Z

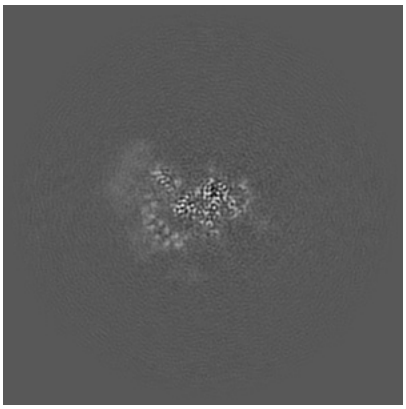
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

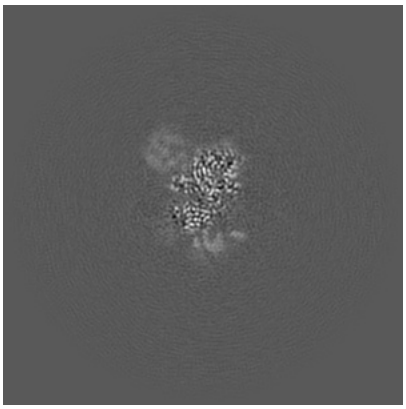
6.2.1 Primary map



X Index: 192

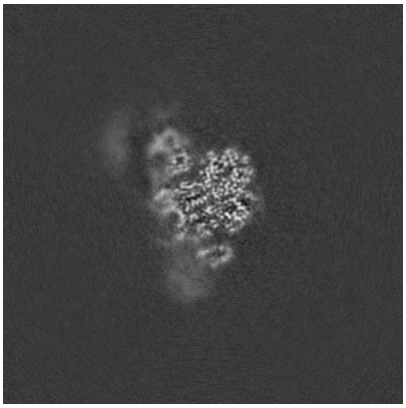


Y Index: 192



Z Index: 192

6.2.2 Raw map



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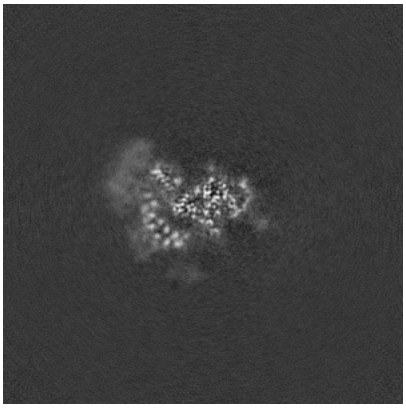
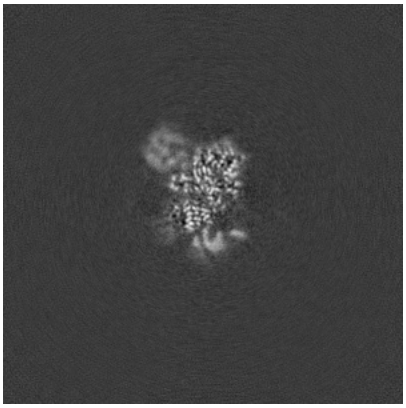


Y Index: 192

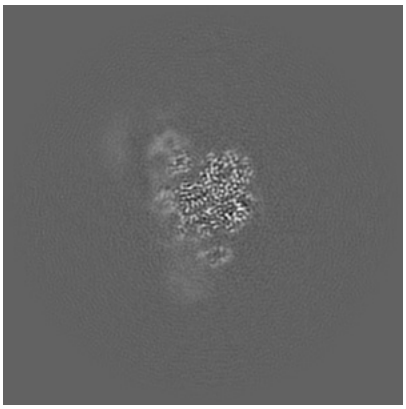


Z Index: 192

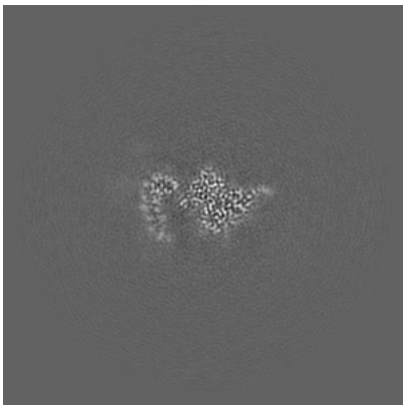
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

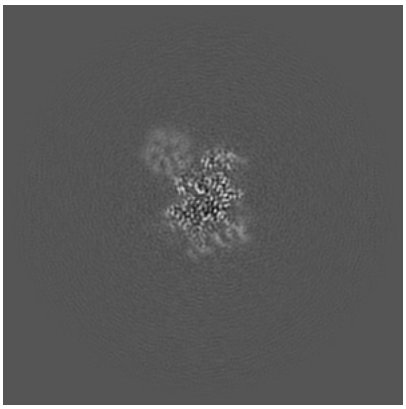
6.3.1 Primary map



X Index: 192

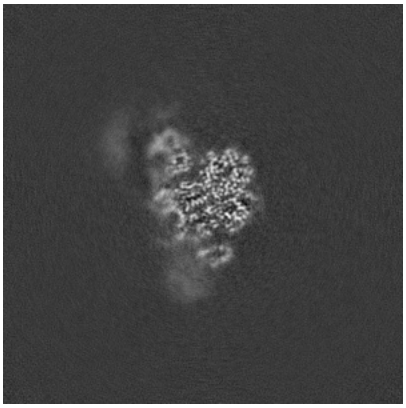


Y Index: 204

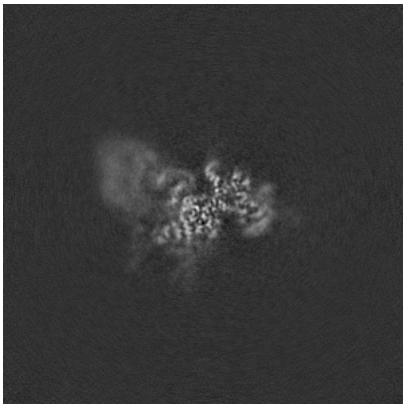


Z Index: 199

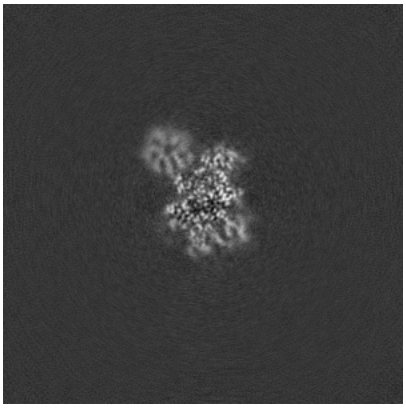
6.3.2 Raw map



X Index: 192



Y Index: 173

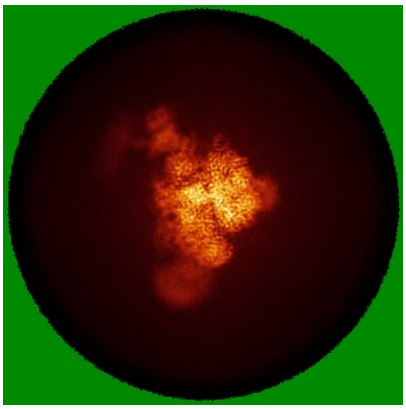


Z Index: 200

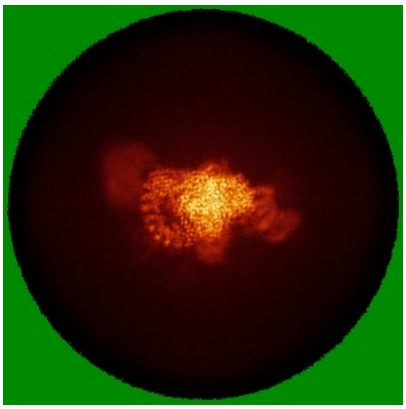
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

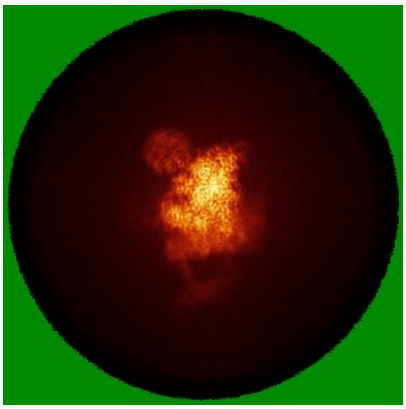
6.4.1 Primary map



X

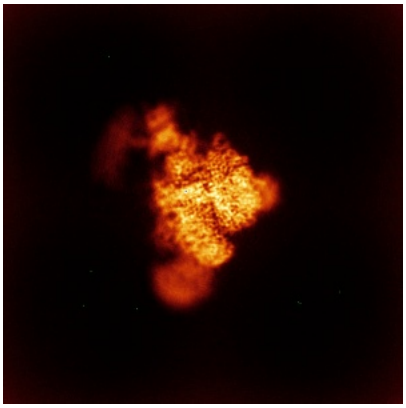


Y

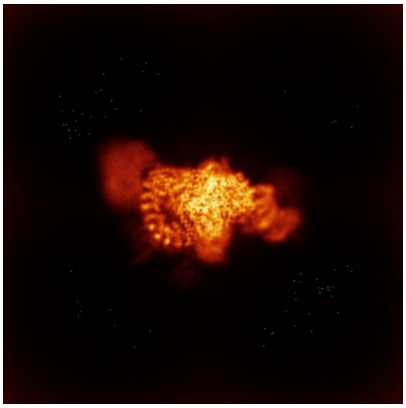


Z

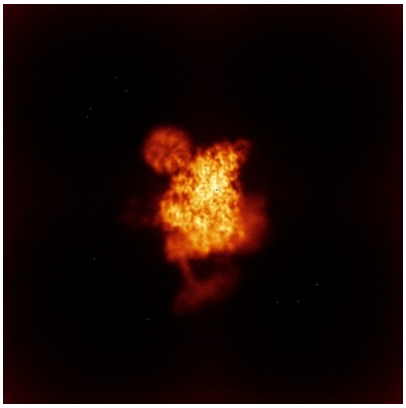
6.4.2 Raw map



X



Y

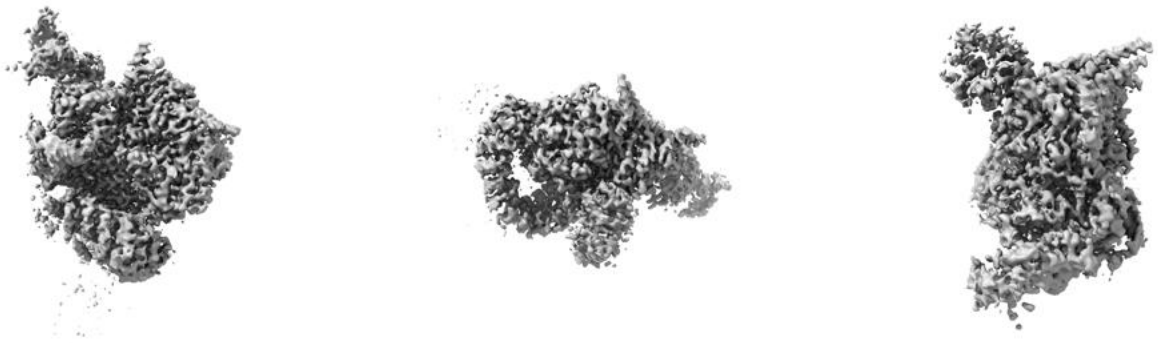


Z

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

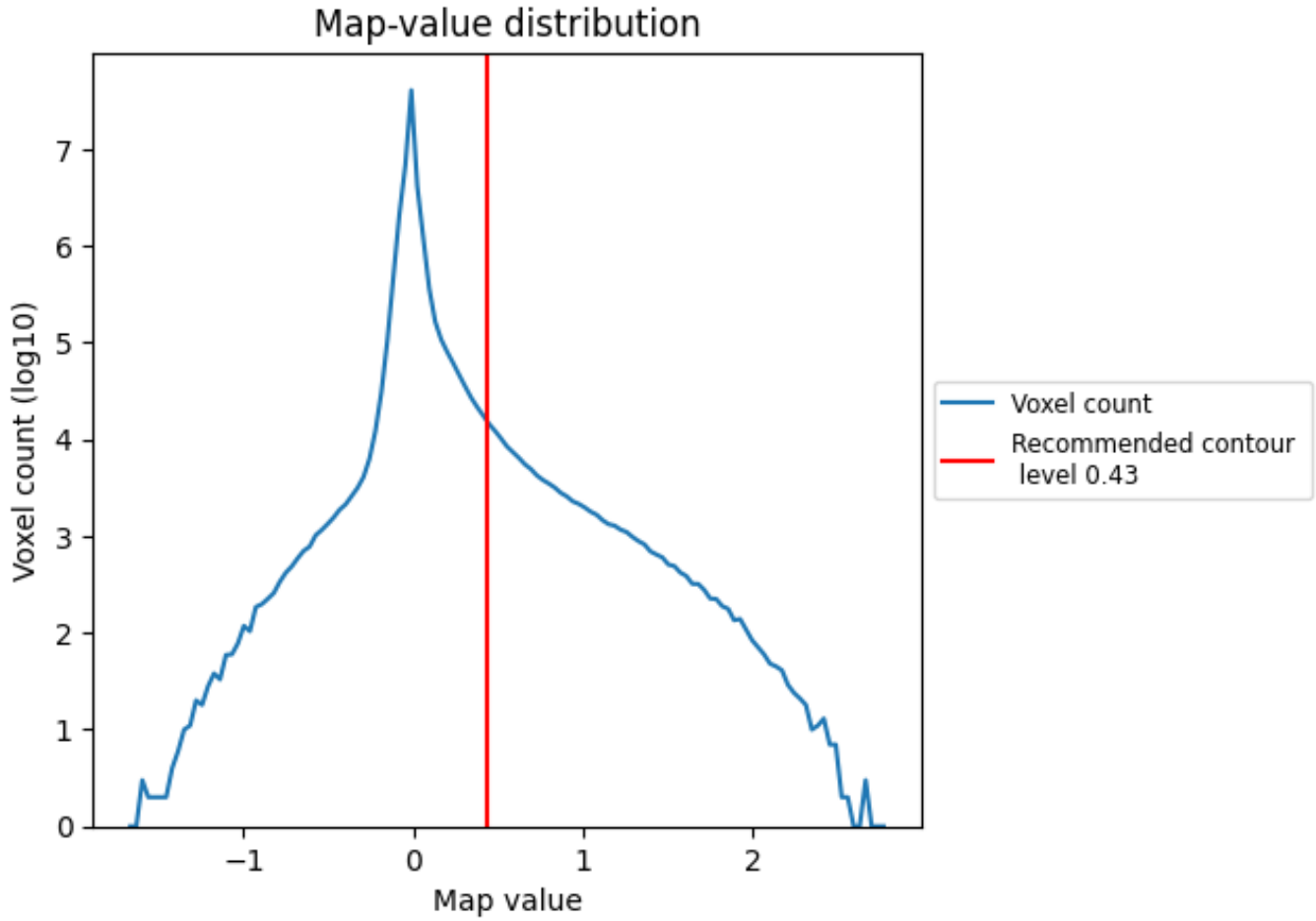
6.6 Mask visualisation (i)

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

7 Map analysis

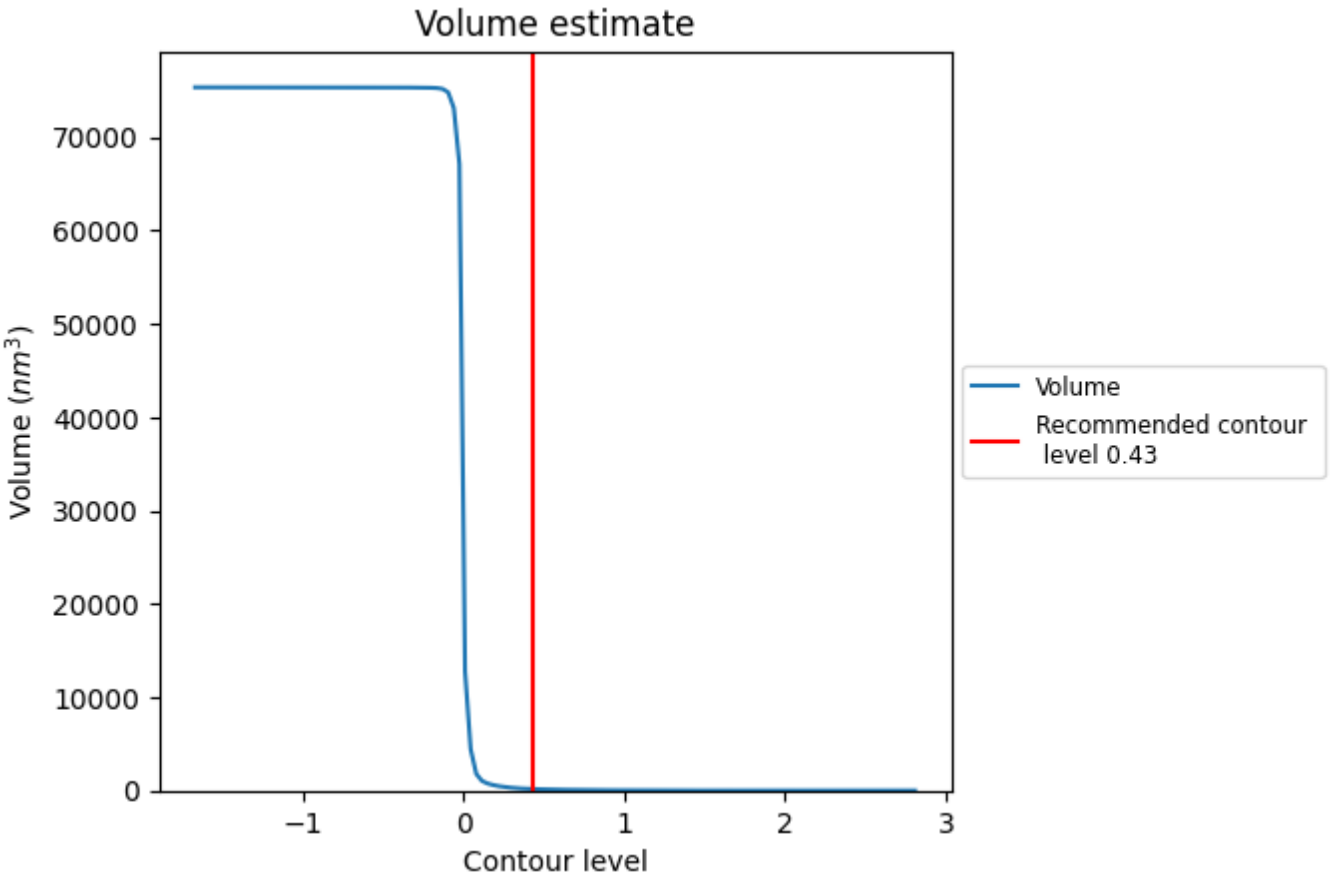
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

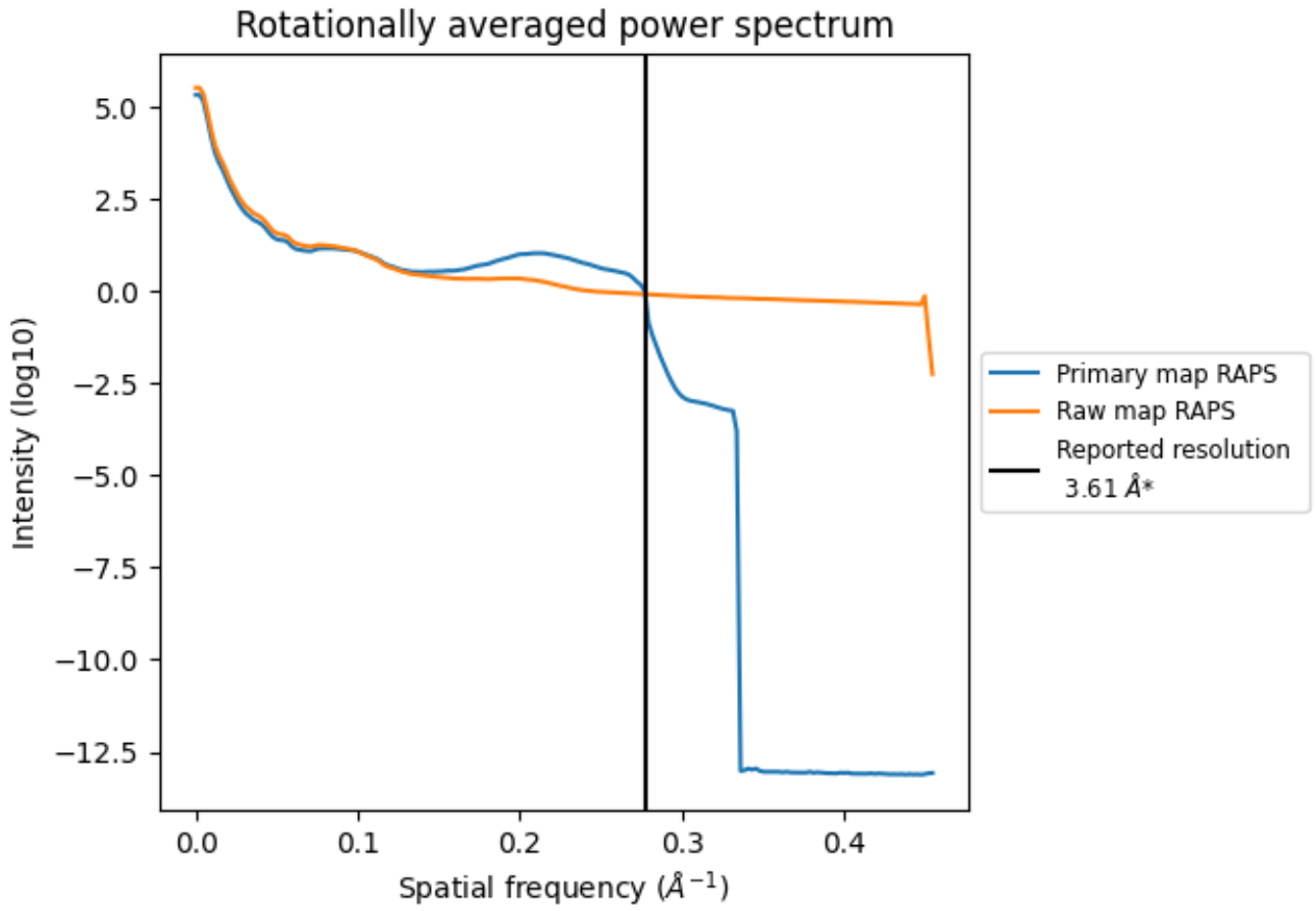
7.2 Volume estimate



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 148 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)

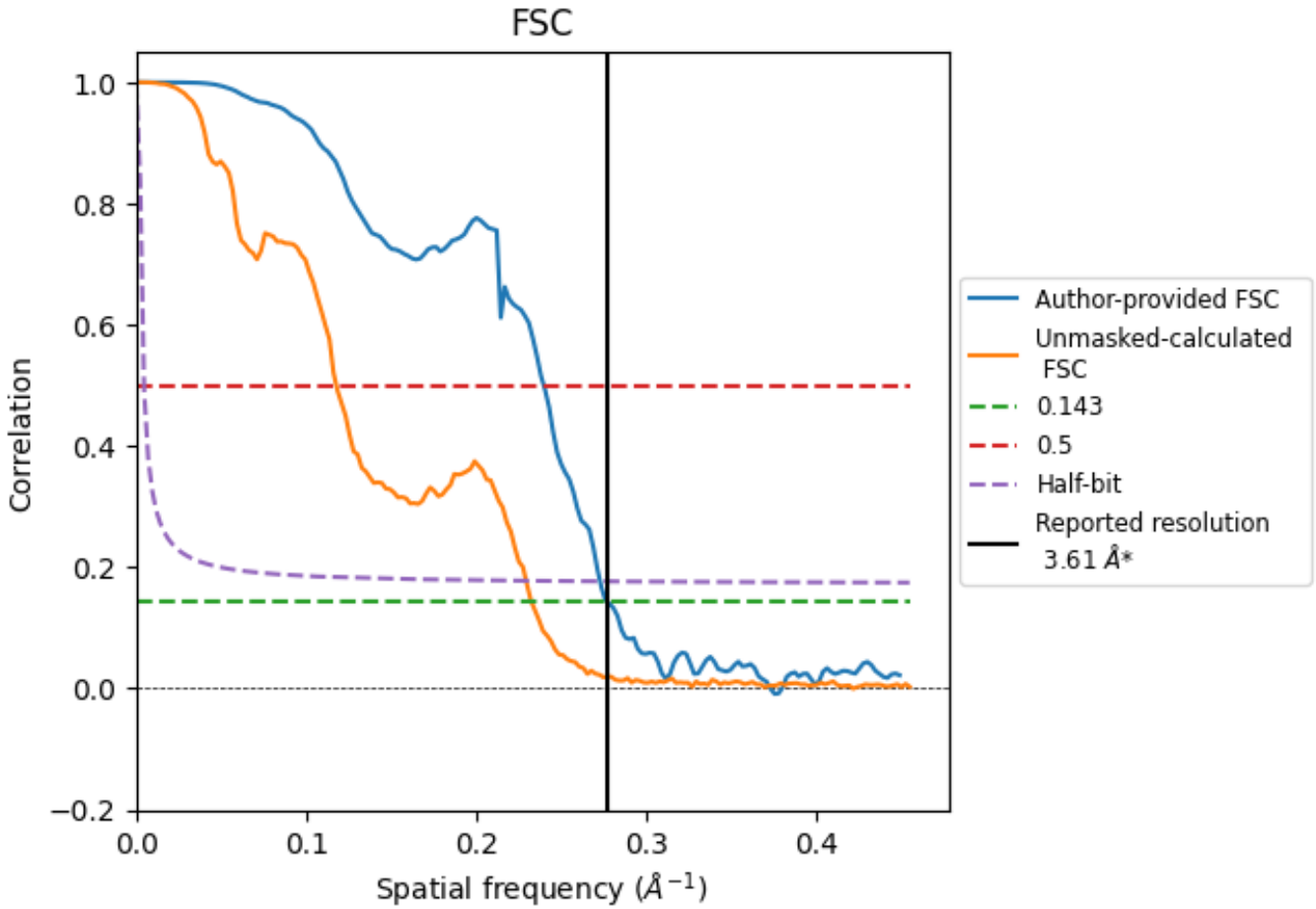


*Reported resolution corresponds to spatial frequency of 0.277 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.277 Å^{-1}

8.2 Resolution estimates (i)

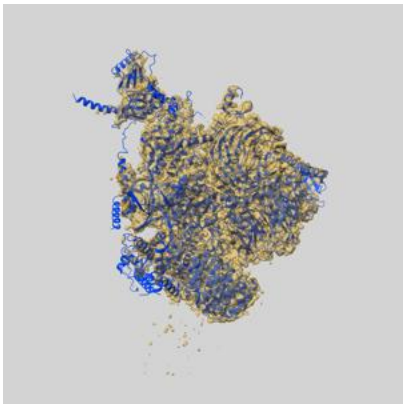
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.61	4.18	3.67
Unmasked-calculated*	4.30	8.50	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.61 by more than 10 %

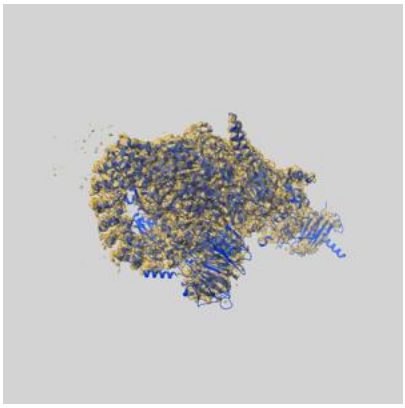
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-74099 and PDB model 9ZEC. Per-residue inclusion information can be found in section 3 on page 7.

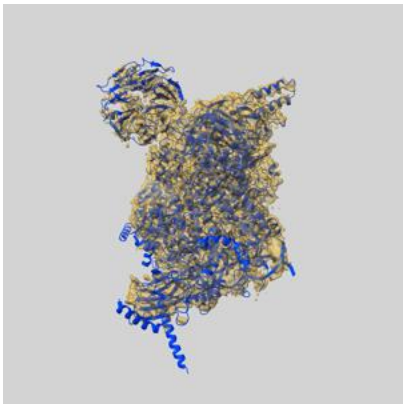
9.1 Map-model overlay



X



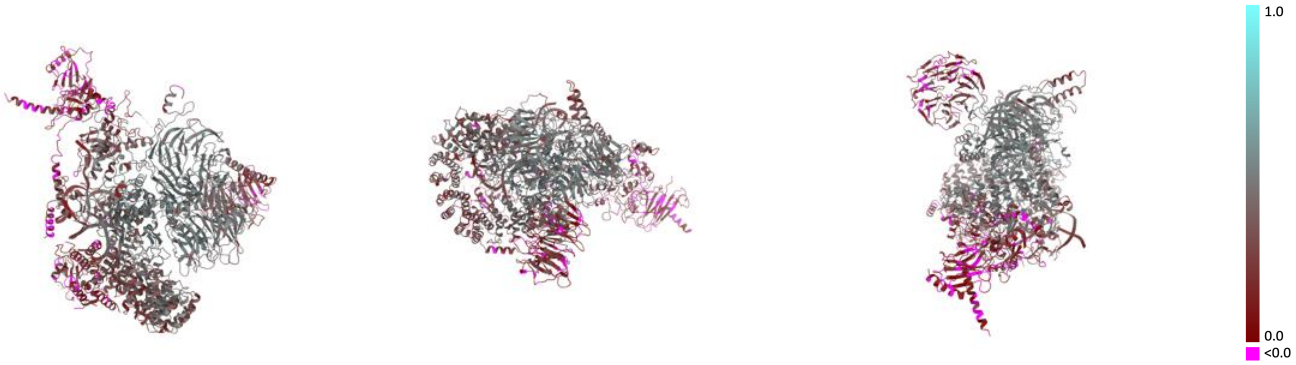
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43 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.

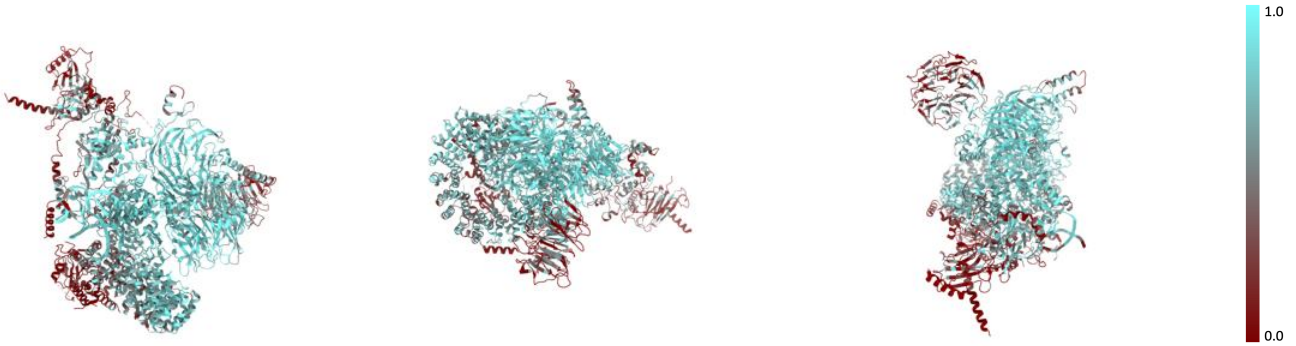
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

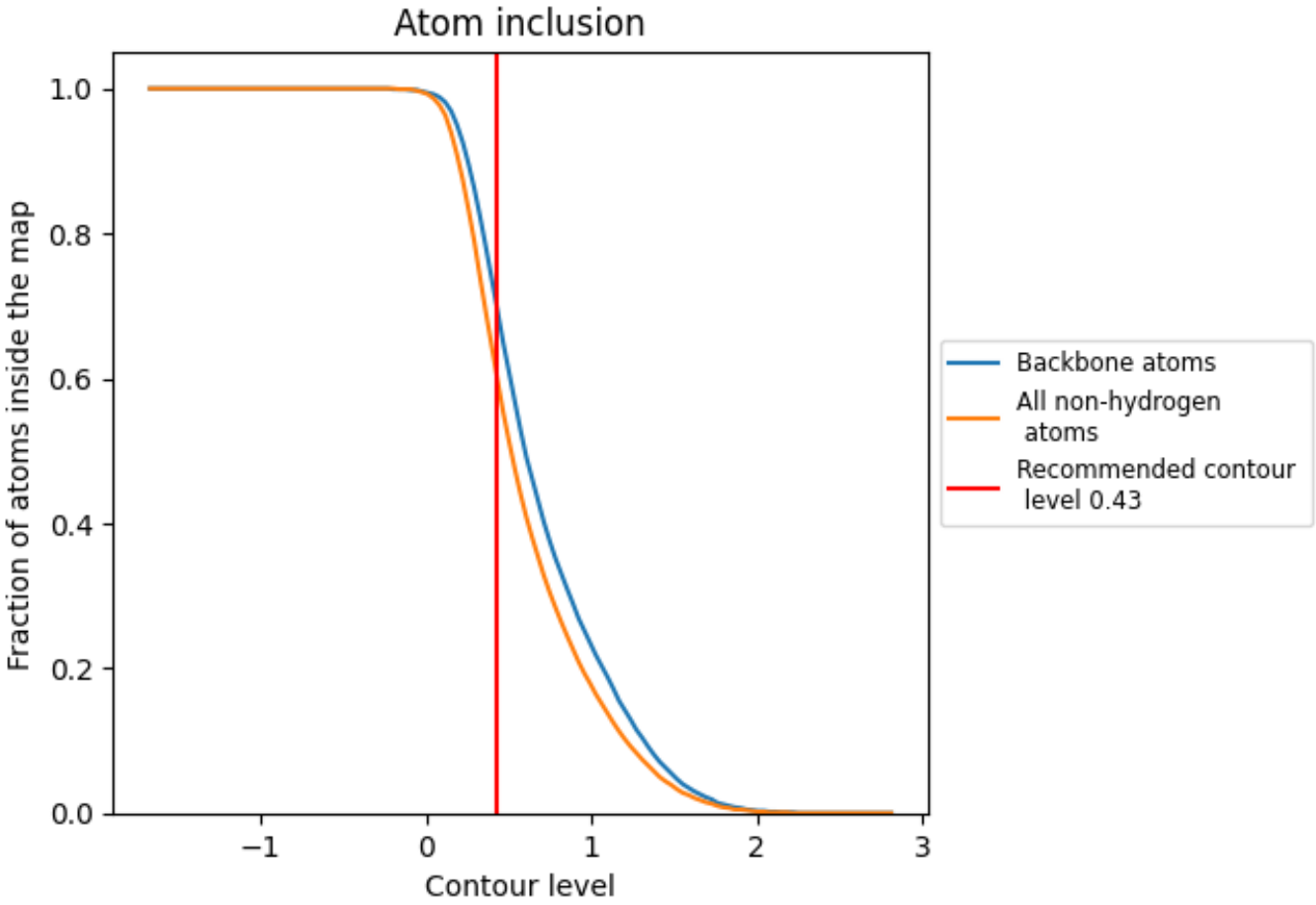
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 60% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.3370
2	0.7530	0.3260
A	0.1410	0.1540
A1	0.0730	0.0780
A2	0.2700	0.1340
A3	0.7030	0.3890
B1	0.6500	0.3590
B2	0.5770	0.3380
B3	0.6810	0.3920
B4	0.4770	0.2210
B5	0.8630	0.4920
B6	0.0270	0.1480
H	0.8250	0.4720
R	0.6450	0.3200