Full wwPDB EM Validation Report ⓘ

Mar 23, 2022 – 07:46 pm GMT

PDB ID	:	7Q4O
EMDB ID	:	EMD-13811
Title	:	Substrate-bound A-like U2 snRNP
Authors	:	Tholen, J.; Galej, W.P.
Deposited on	:	2021-11-01
Resolution	:	2.20 Å(reported)
Based on initial models	:	7Q3L, 7ABH, 3LQV

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

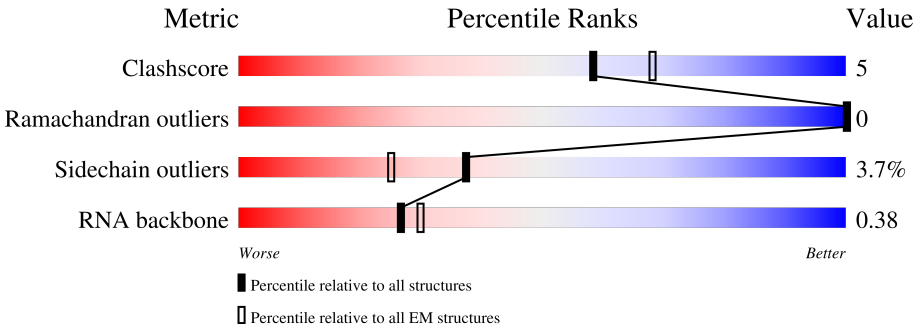
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=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	1	464	5% · 91%
2	2	188	8% 7% · · 81%
3	9	501	17% · · 80%
4	A	1304	30% 56% 7% · 36%
5	B	895	13% · 86%
6	C	1217	18% 89% 7% · ·
7	E	86	62% 13% · 24%

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Mol	Chain	Length	Quality of chain
8	F	125	69% 57% 12% 28%
9	G	110	58% 15% 26%
10	h	17	41% 35% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ZN	G	203	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21212 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 Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	41	Total	C	N	O	S	0	0
			321	200	57	61	3		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	35	Total	C	N	O	P	0	0
			739	333	119	252	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	98	Total	C	N	O	S	0	0
			782	496	135	147	4		

- Molecule 4 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	836	Total	C	N	O	S	0	0
			6639	4258	1149	1193	39		

- Molecule 5 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	124	Total	C	N	O	S	0	0
			1043	674	185	181	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	1181	Total	C	N	O	S	1	0
			9255	5877	1575	1757	46		

- Molecule 7 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	65	Total	C	N	O	S	0	0
			531	338	92	96	5		

- Molecule 8 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	90	Total	C	N	O	S	0	0
			745	479	130	132	4		

- Molecule 9 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	81	Total	C	N	O	S	0	0
			592	362	105	112	13		

- Molecule 10 is a RNA chain called BPS oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	13	Total	C	N	O	P	0	0
			275	124	51	87	13		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	1	1	Total	Zn	0
			1	1	
11	9	1	Total	Zn	0
			1	1	
11	G	3	Total	Zn	0
			3	3	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	2	2	Total	O	0
			2	2	
12	A	53	Total	O	0
			53	53	
12	B	15	Total	O	0
			15	15	

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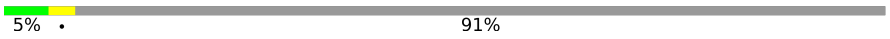
Mol	Chain	Residues	Atoms	AltConf
12	C	175	Total O 175 175	0
12	E	28	Total O 28 28	0
12	G	9	Total O 9 9	0
12	h	3	Total O 3 3	0

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.

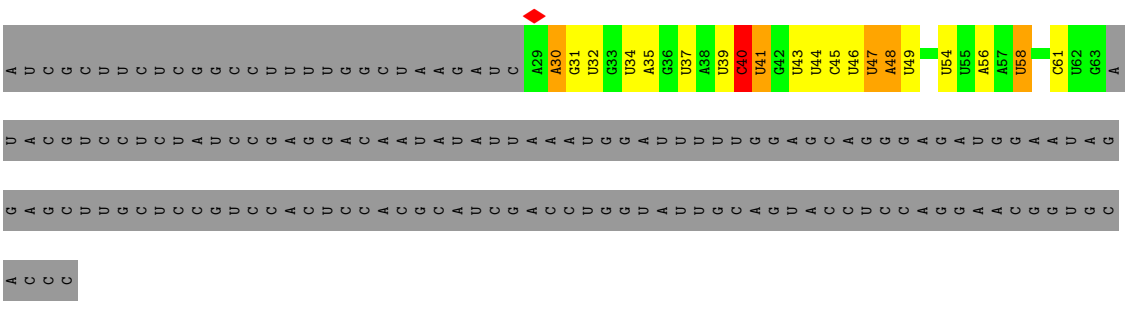
• Molecule 1: Splicing factor 3A subunit 2

Chain 1:



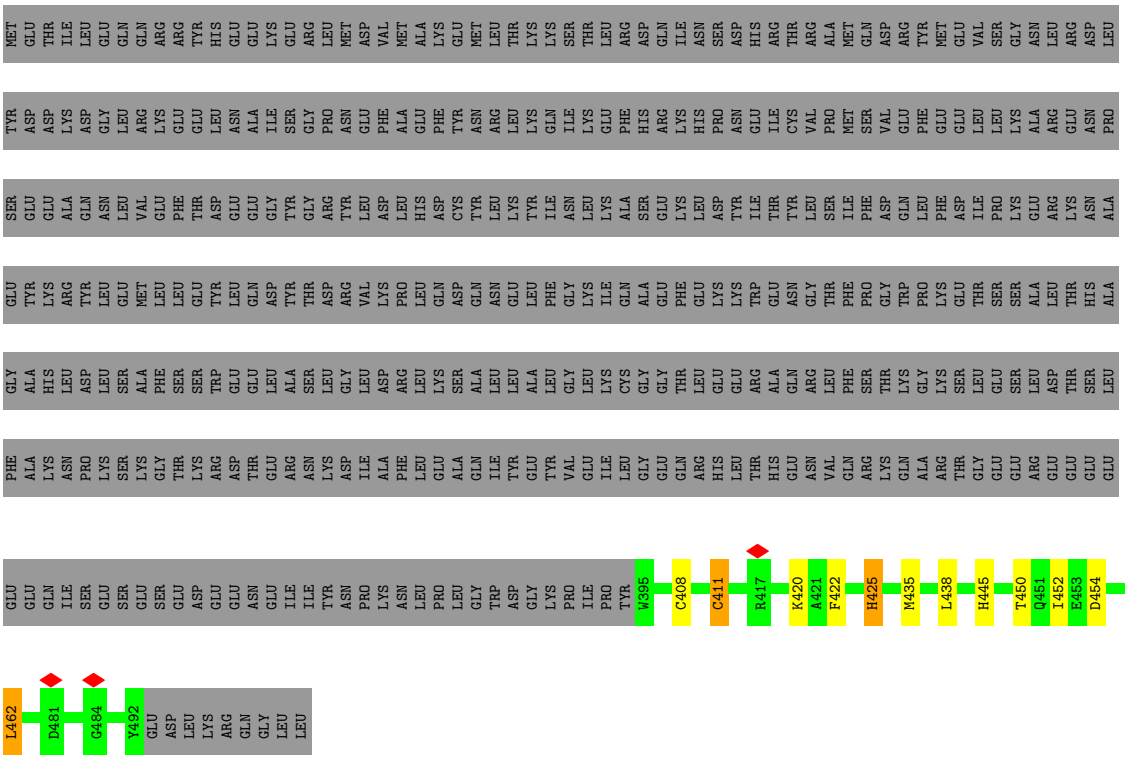
• Molecule 2: U2 snRNA

Chain 2:



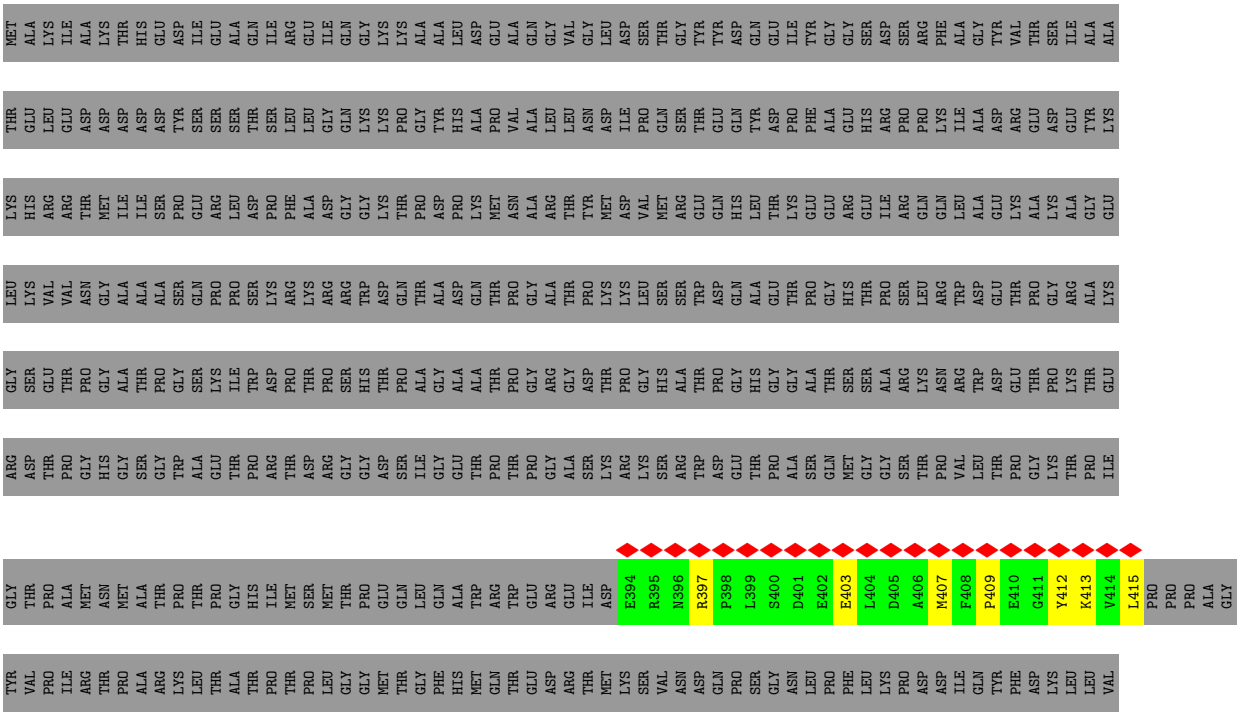
• Molecule 3: Splicing factor 3A subunit 3

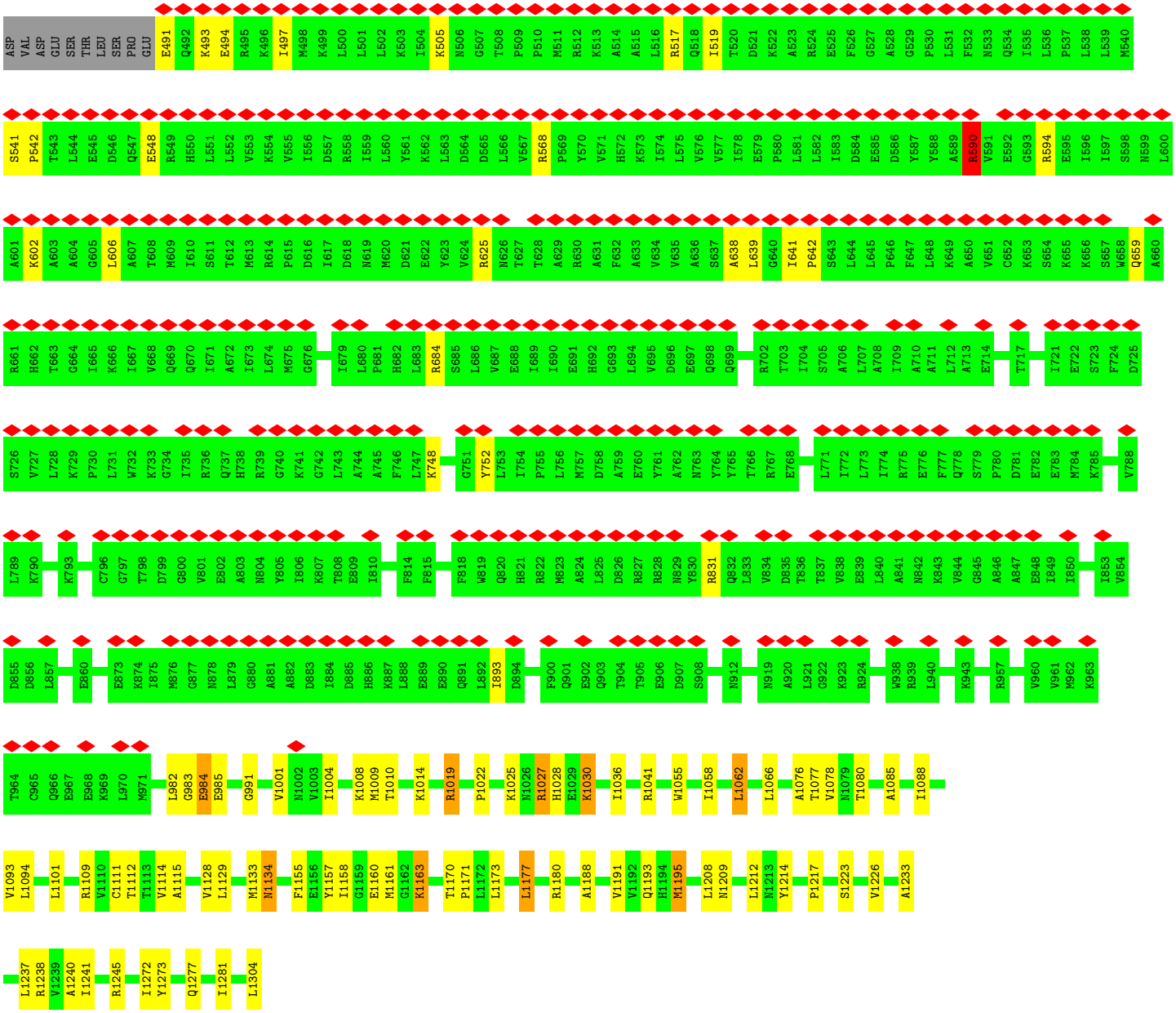
Chain 9:



• Molecule 4: Splicing factor 3B subunit 1

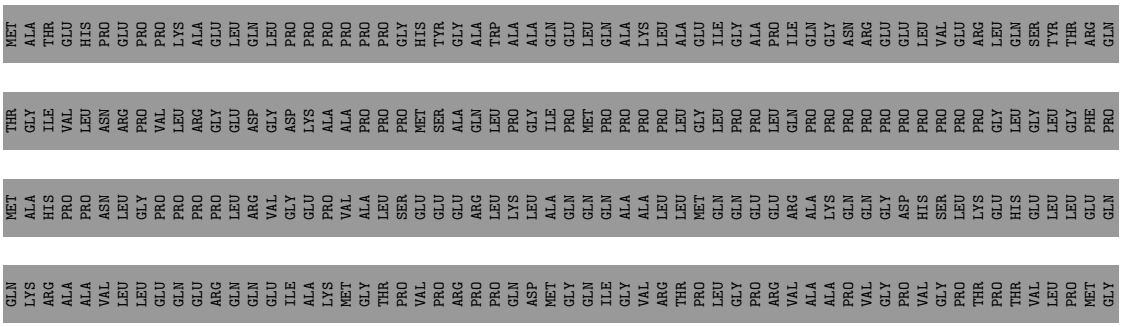
Chain A:

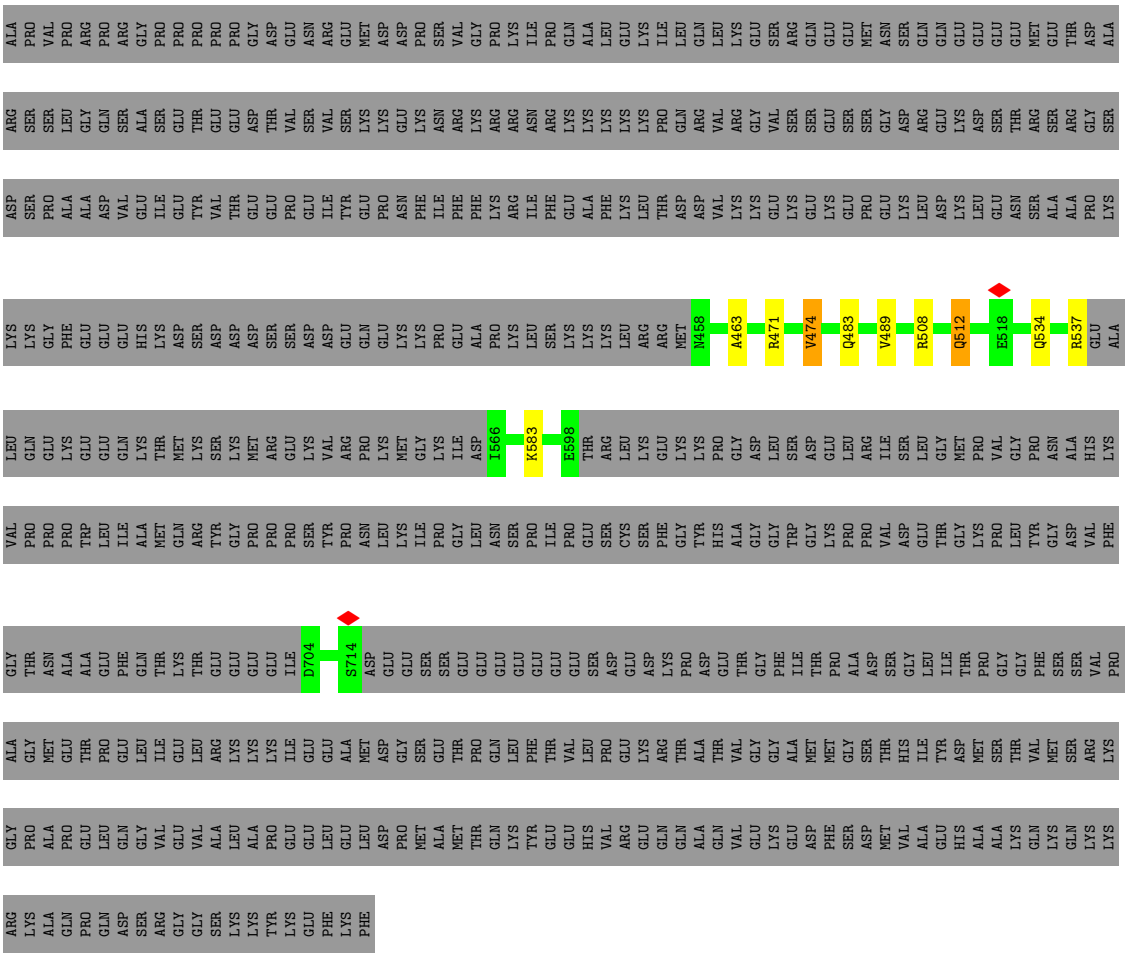




• Molecule 5: Splicing factor 3B subunit 2

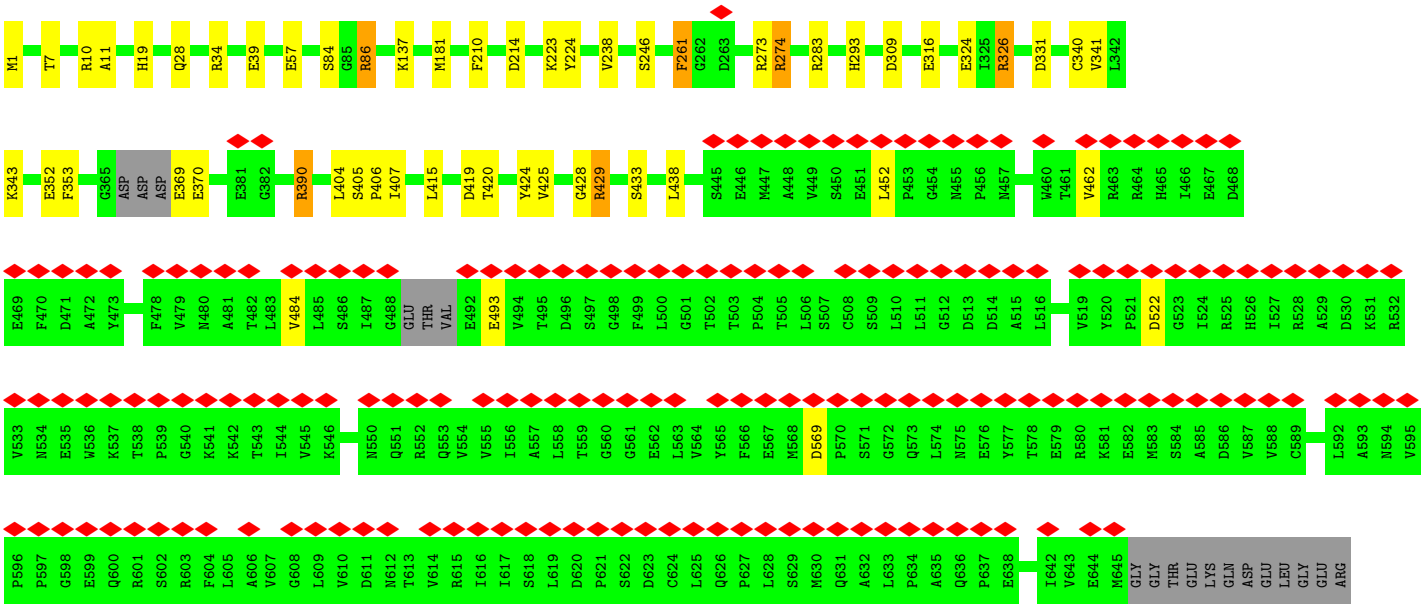
Chain B: 13% 86%

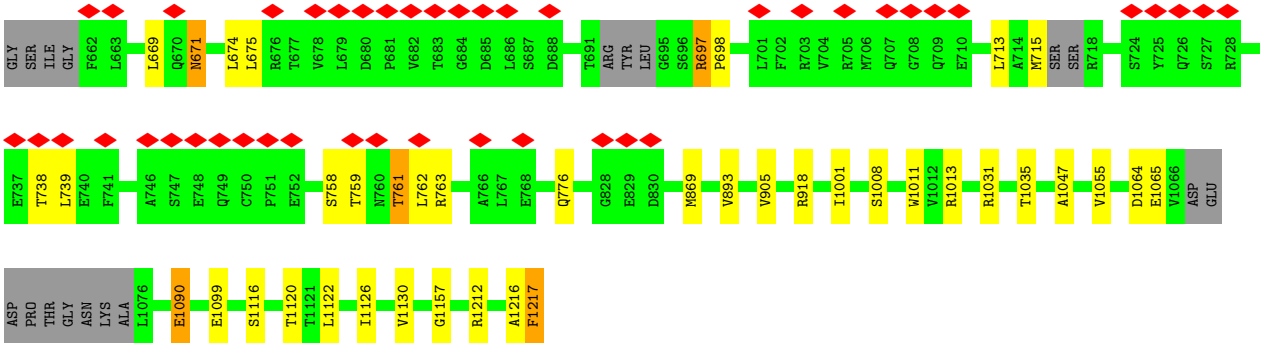




• Molecule 6: Splicing factor 3B subunit 3

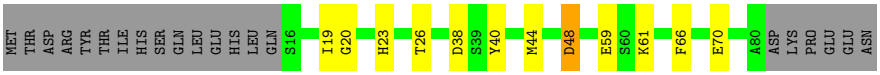
Chain C:





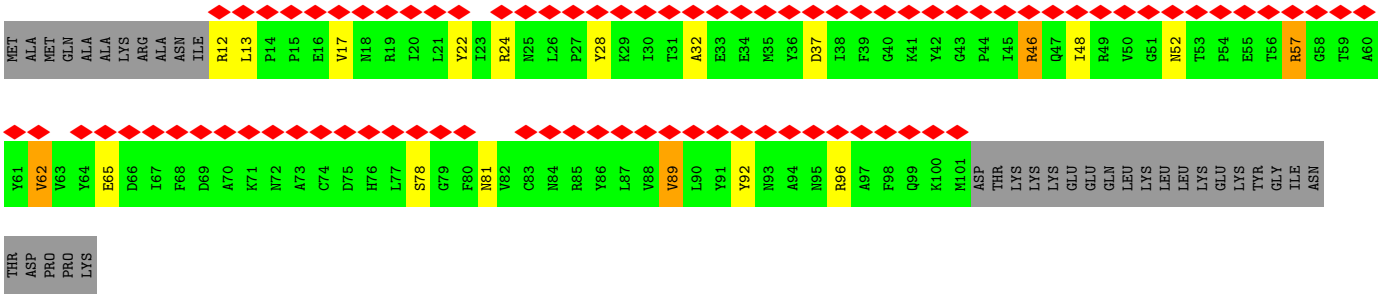
• Molecule 7: Splicing factor 3B subunit 5

Chain E:



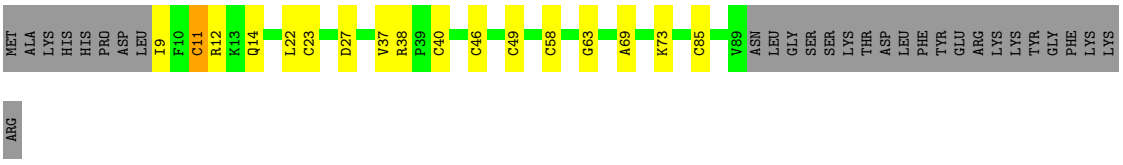
• Molecule 8: Splicing factor 3B subunit 6

Chain F:



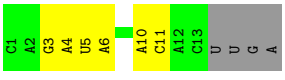
• Molecule 9: PHD finger-like domain-containing protein 5A

Chain G:



• Molecule 10: BPS oligo

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	158286	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 ($e^-/Å^2$)	52.03	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00561	Depositor
Map size (Å)	409.60022, 409.60022, 409.60022	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.64000034, 0.64000034, 0.64000034	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: PSU, OMU, ZN, OMC

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	1	0.42	0/329	0.91	2/445 (0.4%)
2	2	0.69	0/578	1.19	12/899 (1.3%)
3	9	0.31	0/805	0.63	0/1097
4	A	0.34	0/6764	0.74	7/9156 (0.1%)
5	B	0.35	0/1072	0.65	0/1445
6	C	0.34	0/9442	0.68	1/12807 (0.0%)
7	E	0.35	0/547	0.71	0/739
8	F	0.31	0/763	0.73	0/1034
9	G	0.35	0/599	0.70	0/806
10	h	0.69	0/307	1.10	4/475 (0.8%)
All	All	0.36	0/21206	0.73	26/28903 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	590	ARG	NE-CZ-NH1	8.35	124.48	120.30
4	A	684	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	2	32	U	P-O3'-C3'	-7.26	110.99	119.70
2	2	34	PSU	P-O3'-C3'	-6.97	111.34	119.70
4	A	684	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	2	54	PSU	P-O3'-C3'	-6.43	111.99	119.70
1	1	78	HIS	O-C-N	-6.26	112.69	122.70
4	A	568	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	2	31	G	P-O3'-C3'	-5.98	112.52	119.70
10	h	4	A	P-O3'-C3'	-5.88	112.65	119.70
2	2	35	A	P-O3'-C3'	-5.80	112.73	119.70
2	2	37	PSU	P-O3'-C3'	-5.78	112.77	119.70
2	2	48	A	P-O3'-C3'	-5.76	112.79	119.70
10	h	5	U	P-O3'-C3'	-5.73	112.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	61	OMC	P-O3'-C3'	-5.69	112.87	119.70
2	2	56	A	P-O3'-C3'	-5.58	113.00	119.70
2	2	58	PSU	P-O3'-C3'	-5.54	113.05	119.70
4	A	684	ARG	CD-NE-CZ	5.48	131.27	123.60
10	h	6	A	P-O3'-C3'	-5.37	113.26	119.70
4	A	625	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	1	77	LYS	CA-C-N	-5.21	105.73	117.20
2	2	30	A	P-O3'-C3'	-5.16	113.50	119.70
10	h	3	G	P-O3'-C3'	-5.10	113.58	119.70
6	C	1217	PHE	CB-CA-C	-5.09	100.22	110.40
4	A	594	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	2	44	PSU	P-O3'-C3'	-5.04	113.66	119.70

There are no chirality outliers.

There are no planarity outliers.

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	1	321	0	289	17	0
2	2	739	0	376	2	0
3	9	782	0	705	8	0
4	A	6639	0	6827	68	0
5	B	1043	0	1042	6	0
6	C	9255	0	9175	82	0
7	E	531	0	501	13	0
8	F	745	0	736	13	0
9	G	592	0	563	12	0
10	h	275	0	142	0	0
11	1	1	0	0	0	0
11	9	1	0	0	0	0
11	G	3	0	0	3	0
12	2	2	0	0	0	0
12	A	53	0	0	0	0
12	B	15	0	0	0	0
12	C	175	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	E	28	0	0	0	0
12	G	9	0	0	0	0
12	h	3	0	0	0	0
All	All	21212	0	20356	198	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 5.

All (198) 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)
6:C:181:MET:HE1	6:C:261:PHE:CE1	1.61	1.32
6:C:181:MET:HE1	6:C:261:PHE:CZ	1.69	1.28
6:C:1013:ARG:NH1	6:C:1065:GLU:HG2	1.63	1.13
1:1:73:THR:HA	1:1:78:HIS:CD2	1.87	1.07
6:C:1013:ARG:HH12	6:C:1065:GLU:CG	1.71	1.03
3:9:445:HIS:CD2	3:9:462:LEU:HD11	1.96	1.00
6:C:181:MET:CE	6:C:261:PHE:CZ	2.47	0.97
6:C:1013:ARG:HH12	6:C:1065:GLU:HG2	1.21	0.95
6:C:181:MET:CE	6:C:261:PHE:CE1	2.50	0.95
6:C:316:GLU:HG3	6:C:326:ARG:NH1	1.80	0.94
9:G:46:CYS:SG	11:G:202:ZN:ZN	1.54	0.94
6:C:316:GLU:HG3	6:C:326:ARG:HH11	1.38	0.87
6:C:1013:ARG:HH12	6:C:1065:GLU:CD	1.78	0.86
6:C:210:PHE:CD1	6:C:261:PHE:HE1	1.92	0.85
9:G:23:CYS:HG	11:G:203:ZN:ZN	0.92	0.83
4:A:1160:GLU:O	4:A:1163:LYS:HG2	1.78	0.82
6:C:369:GLU:N	6:C:369:GLU:OE1	2.12	0.81
1:1:79:GLN:NE2	1:1:79:GLN:HA	1.97	0.78
1:1:61:THR:HG21	1:1:72:HIS:CE1	2.20	0.77
4:A:1223:SER:HB3	4:A:1226:VAL:HG12	1.68	0.76
3:9:438:LEU:HD11	3:9:452:ILE:HG23	1.68	0.74
6:C:1035:THR:HG22	6:C:1047:ALA:HB3	1.68	0.74
6:C:210:PHE:CD1	6:C:261:PHE:CE1	2.76	0.73
4:A:407:MET:CE	8:F:92:TYR:CE1	2.72	0.73
1:1:58:LEU:HG	1:1:81:ASN:OD1	1.89	0.72
1:1:73:THR:HA	1:1:78:HIS:HD2	1.54	0.72
9:G:23:CYS:SG	11:G:203:ZN:ZN	1.77	0.72
9:G:11:CYS:SG	9:G:85:CYS:HB3	2.30	0.71
4:A:407:MET:HE1	8:F:92:TYR:CE1	2.25	0.71
1:1:58:LEU:CD2	1:1:81:ASN:HB3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:748:LYS:HE2	4:A:752:TYR:CE2	2.30	0.67
6:C:697:ARG:HG2	6:C:698:PRO:HD2	1.77	0.67
6:C:352:GLU:HG3	7:E:61:LYS:HE3	1.76	0.66
1:1:58:LEU:HD23	1:1:81:ASN:HB3	1.77	0.66
6:C:758:SER:H	6:C:761:THR:HG22	1.63	0.64
6:C:1013:ARG:HH11	6:C:1065:GLU:HG2	1.61	0.64
1:1:72:HIS:CE1	1:1:78:HIS:HB2	2.33	0.64
6:C:210:PHE:CE1	6:C:261:PHE:HE1	2.16	0.64
6:C:1013:ARG:NH1	6:C:1065:GLU:CG	2.38	0.64
4:A:1058:ILE:HG22	4:A:1062:LEU:CD2	2.29	0.63
4:A:1101:LEU:O	4:A:1109:ARG:HD3	1.98	0.63
4:A:1193:GLN:HB2	4:A:1233:ALA:HA	1.81	0.63
4:A:1001:VAL:HG23	4:A:1041:ARG:HD2	1.80	0.62
6:C:210:PHE:CE1	6:C:261:PHE:CE1	2.88	0.62
6:C:86:ARG:HD2	6:C:1157:GLY:O	2.00	0.61
6:C:352:GLU:OE1	6:C:429:ARG:NH2	2.33	0.61
4:A:1055:TRP:HD1	4:A:1088:ILE:HD11	1.66	0.61
6:C:429:ARG:NH2	7:E:59:GLU:O	2.34	0.60
6:C:324:GLU:CD	6:C:326:ARG:NH1	2.55	0.59
6:C:293:HIS:CD2	6:C:341:VAL:HG11	2.37	0.59
1:1:46:PHE:HB2	1:1:69:TYR:CZ	2.37	0.59
6:C:761:THR:HG23	6:C:763:ARG:HG3	1.85	0.58
4:A:982:LEU:HB3	4:A:1019:ARG:HH11	1.69	0.58
4:A:1022:PRO:HA	4:A:1025:LYS:HE2	1.84	0.58
1:1:71:ALA:HB3	2:2:40:OMC:HM21	1.85	0.58
6:C:739:LEU:HD23	6:C:758:SER:HB2	1.86	0.58
4:A:985:GLU:HA	8:F:81:ASN:HB3	1.86	0.58
4:A:1134:ASN:HD21	5:B:534:GLN:HA	1.69	0.57
6:C:352:GLU:CG	7:E:61:LYS:HE3	2.34	0.57
6:C:1008:SER:HB3	6:C:1031:ARG:HB2	1.85	0.57
4:A:1058:ILE:O	4:A:1062:LEU:HD22	2.04	0.57
6:C:1212:ARG:O	6:C:1212:ARG:HG2	2.05	0.57
4:A:1177:LEU:HD13	4:A:1188:ALA:HB3	1.86	0.57
4:A:1281:ILE:HD11	7:E:38:ASP:HB3	1.86	0.56
1:1:72:HIS:O	1:1:78:HIS:HB3	2.05	0.56
6:C:1013:ARG:HD3	6:C:1064:ASP:O	2.06	0.56
4:A:1129:LEU:O	4:A:1133:MET:HG2	2.05	0.56
6:C:669:LEU:HB3	6:C:671:ASN:OD1	2.06	0.56
6:C:331:ASP:OD1	6:C:390:ARG:NH2	2.38	0.55
9:G:38:ARG:HB3	9:G:73:LYS:HG3	1.89	0.55
6:C:353:PHE:HB3	6:C:406:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1116:SER:HB2	6:C:1130:VAL:HG12	1.87	0.55
4:A:1058:ILE:HG22	4:A:1062:LEU:HD22	1.89	0.55
4:A:1078:VAL:HG11	4:A:1114:VAL:HG12	1.89	0.55
8:F:28:TYR:CE1	8:F:57:ARG:HD3	2.42	0.55
4:A:1273:TYR:CE2	7:E:20:GLY:HA3	2.42	0.54
6:C:293:HIS:CD2	6:C:341:VAL:CG1	2.91	0.54
1:1:69:TYR:O	1:1:73:THR:HG23	2.07	0.54
8:F:46:ARG:HG2	8:F:65:GLU:CD	2.29	0.53
4:A:407:MET:HE1	8:F:92:TYR:HE1	1.73	0.52
5:B:474:VAL:CG1	5:B:489:VAL:HG13	2.39	0.52
5:B:474:VAL:HG12	5:B:489:VAL:HG13	1.91	0.52
6:C:1116:SER:CB	6:C:1130:VAL:HG12	2.38	0.52
4:A:1212:LEU:HD22	4:A:1241:ILE:HD11	1.91	0.52
4:A:1036:ILE:CD1	4:A:1062:LEU:HD11	2.39	0.52
4:A:1237:LEU:O	4:A:1241:ILE:HG12	2.09	0.52
6:C:181:MET:HE3	6:C:210:PHE:HD1	1.75	0.52
4:A:1155:PHE:CZ	4:A:1195:MET:CE	2.93	0.52
6:C:918:ARG:HH11	6:C:918:ARG:HG2	1.75	0.52
4:A:1085:ALA:HB2	4:A:1093:VAL:HG11	1.92	0.51
6:C:429:ARG:O	6:C:429:ARG:HG3	2.10	0.51
4:A:409:PRO:HG2	4:A:412:TYR:HE1	1.74	0.51
4:A:1155:PHE:CZ	4:A:1195:MET:HE3	2.46	0.51
6:C:84:SER:OG	6:C:86:ARG:HG3	2.10	0.51
6:C:407:ILE:HG23	6:C:425:VAL:CG1	2.40	0.51
4:A:415:LEU:HD13	8:F:32:ALA:HA	1.92	0.50
4:A:590:ARG:CB	4:A:590:ARG:HH11	2.24	0.50
6:C:19:HIS:CE1	6:C:340:CYS:HB3	2.48	0.49
4:A:1273:TYR:CZ	7:E:20:GLY:HA3	2.48	0.49
1:1:61:THR:HG23	1:1:63:HIS:NE2	2.27	0.49
6:C:316:GLU:HG2	6:C:326:ARG:HD2	1.93	0.49
4:A:748:LYS:HE2	4:A:752:TYR:CD2	2.48	0.49
6:C:34:ARG:HH11	6:C:39:GLU:CD	2.16	0.49
6:C:223:LYS:HE3	6:C:224:TYR:CE2	2.48	0.49
4:A:1157:TYR:CD1	9:G:37:VAL:HG21	2.48	0.48
6:C:415:LEU:HB2	6:C:424:TYR:OH	2.12	0.48
9:G:9:ILE:O	9:G:9:ILE:HG23	2.13	0.48
3:9:408:CYS:SG	3:9:411:CYS:HB2	2.53	0.48
6:C:316:GLU:CG	6:C:326:ARG:HD2	2.44	0.48
4:A:1223:SER:HB3	4:A:1226:VAL:CG1	2.42	0.47
3:9:422:PHE:HZ	3:9:450:THR:CG2	2.27	0.47
6:C:738:THR:O	6:C:758:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:58:CYS:HB3	9:G:63:GLY:H	1.78	0.47
3:9:454:ASP:OD2	5:B:463:ALA:HB1	2.14	0.47
4:A:1062:LEU:HD12	4:A:1077:THR:HG23	1.97	0.47
6:C:283:ARG:NH1	7:E:59:GLU:OE2	2.45	0.47
6:C:10:ARG:HD3	6:C:57:GLU:OE2	2.14	0.47
4:A:409:PRO:HG2	4:A:412:TYR:CE1	2.48	0.47
6:C:407:ILE:HG23	6:C:425:VAL:HG13	1.97	0.47
4:A:407:MET:HE3	8:F:92:TYR:CE1	2.50	0.46
3:9:422:PHE:HZ	3:9:450:THR:HG21	1.81	0.46
1:1:72:HIS:O	1:1:78:HIS:CB	2.63	0.46
8:F:48:ILE:HG12	8:F:62:VAL:HB	1.96	0.46
6:C:1001:ILE:HD12	6:C:1011:TRP:CD1	2.49	0.46
6:C:1122:LEU:HD12	6:C:1122:LEU:HA	1.81	0.46
6:C:34:ARG:NH1	6:C:39:GLU:CD	2.69	0.46
6:C:34:ARG:NH1	6:C:39:GLU:OE1	2.42	0.46
9:G:46:CYS:SG	9:G:49:CYS:SG	3.14	0.46
4:A:1170:THR:N	4:A:1171:PRO:HD2	2.31	0.45
6:C:428:GLY:HA3	6:C:433:SER:HA	1.97	0.45
4:A:641:ILE:N	4:A:642:PRO:HD2	2.32	0.45
4:A:602:LYS:HD3	4:A:638:ALA:HB1	1.97	0.45
6:C:713:LEU:HG	6:C:715:MET:SD	2.56	0.45
7:E:40:TYR:O	7:E:44:MET:HG2	2.17	0.45
8:F:22:TYR:CE2	8:F:24:ARG:HG2	2.52	0.45
6:C:1090:GLU:H	6:C:1090:GLU:HG3	1.68	0.45
6:C:893:VAL:HG22	6:C:905:VAL:HG22	2.00	0.44
4:A:991:GLY:HA3	4:A:1030:LYS:HG3	1.99	0.44
4:A:1158:ILE:HB	4:A:1161:MET:HB2	1.98	0.44
4:A:983:GLY:O	4:A:984:GLU:C	2.56	0.44
6:C:28:GLN:NE2	6:C:343:LYS:HB2	2.33	0.44
9:G:22:LEU:HG	9:G:69:ALA:HB2	2.00	0.44
4:A:1157:TYR:CE1	9:G:37:VAL:HG21	2.53	0.44
7:E:66:PHE:O	7:E:70:GLU:HG2	2.18	0.44
4:A:1177:LEU:HB3	4:A:1214:TYR:HB3	2.00	0.44
6:C:1[A]:MET:HE1	6:C:1055:VAL:HG21	2.00	0.44
4:A:1055:TRP:CD1	4:A:1088:ILE:HD11	2.50	0.43
4:A:1076:ALA:O	4:A:1080:THR:HG23	2.18	0.43
8:F:78:SER:HA	8:F:89:VAL:HG13	2.01	0.43
6:C:11:ALA:O	6:C:34:ARG:HD3	2.17	0.43
6:C:671:ASN:OD1	6:C:671:ASN:N	2.48	0.43
4:A:1027:ARG:CG	4:A:1027:ARG:HH11	2.31	0.43
6:C:407:ILE:HG12	6:C:425:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:452:LEU:HD21	6:C:762:LEU:HD22	1.99	0.43
4:A:1066:LEU:CD1	4:A:1112:THR:HG22	2.48	0.43
6:C:404:LEU:HD11	6:C:438:LEU:HD21	1.99	0.43
9:G:40:CYS:HB2	9:G:73:LYS:HG2	2.01	0.43
6:C:1099:GLU:HB3	7:E:48:ASP:OD2	2.19	0.43
6:C:405:SER:HA	6:C:406:PRO:HA	1.75	0.43
6:C:674:LEU:HG	6:C:675:LEU:N	2.34	0.43
4:A:1173:LEU:O	4:A:1177:LEU:HD22	2.19	0.43
4:A:1214:TYR:O	4:A:1217:PRO:HD2	2.18	0.43
4:A:1238:ARG:HD3	4:A:1272:ILE:HA	2.01	0.42
6:C:1120:THR:HG22	6:C:1126:ILE:HG12	2.01	0.42
6:C:181:MET:CE	6:C:261:PHE:HZ	2.21	0.42
4:A:590:ARG:HH11	4:A:590:ARG:HB2	1.83	0.42
4:A:1114:VAL:HG13	4:A:1157:TYR:OH	2.19	0.42
6:C:273:ARG:NH2	6:C:283:ARG:O	2.51	0.42
6:C:283:ARG:NH2	7:E:59:GLU:OE2	2.51	0.42
4:A:1078:VAL:HG13	4:A:1115:ALA:HA	2.02	0.42
4:A:1177:LEU:HD13	4:A:1188:ALA:CB	2.50	0.42
6:C:7:THR:HG21	6:C:10:ARG:HG2	2.02	0.42
1:1:58:LEU:HD21	1:1:81:ASN:HB3	2.00	0.42
4:A:1066:LEU:HD22	4:A:1111:CYS:HB3	2.01	0.42
4:A:1208:LEU:HD13	4:A:1240:ALA:HB1	2.02	0.42
4:A:1304:LEU:HD12	4:A:1304:LEU:HA	1.89	0.42
6:C:238:VAL:HB	6:C:246:SER:O	2.20	0.42
4:A:541:SER:HA	4:A:542:PRO:HD3	1.97	0.41
4:A:1028:HIS:HB2	8:F:78:SER:O	2.20	0.41
1:1:59:CYS:HB2	1:1:61:THR:HG22	2.02	0.41
7:E:23:HIS:H	7:E:26:THR:HG1	1.68	0.41
8:F:46:ARG:HG2	8:F:65:GLU:OE2	2.20	0.41
1:1:56:CYS:HB3	1:1:61:THR:HG22	2.03	0.41
3:9:438:LEU:HD23	3:9:438:LEU:HA	1.81	0.41
4:A:1180:ARG:HG2	5:B:512:GLN:HE21	1.86	0.41
6:C:274:ARG:NH1	6:C:309:ASP:OD1	2.53	0.41
6:C:1216:ALA:O	6:C:1217:PHE:O	2.38	0.41
4:A:1028:HIS:HD2	4:A:1030:LYS:HB3	1.86	0.41
6:C:484:VAL:O	6:C:493:GLU:HA	2.21	0.41
6:C:1008:SER:CB	6:C:1031:ARG:HB2	2.51	0.41
5:B:483:GLN:H	5:B:483:GLN:HG2	1.66	0.40
6:C:137:LYS:HD2	7:E:19:ILE:HD13	2.03	0.40
3:9:411:CYS:SG	3:9:425:HIS:CD2	3.14	0.40
4:A:1094:LEU:HD22	4:A:1128:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1173:LEU:HD21	4:A:1191:VAL:HG11	2.02	0.40
4:A:505:LYS:HZ3	4:A:548:GLU:CD	2.24	0.40
4:A:606:LEU:HB2	4:A:639:LEU:HD13	2.02	0.40
2:2:40:OMC:H1'	2:2:40:OMC:HM23	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	39/464 (8%)	38 (97%)	1 (3%)	0	100	100
3	9	96/501 (19%)	91 (95%)	5 (5%)	0	100	100
4	A	832/1304 (64%)	822 (99%)	10 (1%)	0	100	100
5	B	118/895 (13%)	117 (99%)	1 (1%)	0	100	100
6	C	1167/1217 (96%)	1127 (97%)	40 (3%)	0	100	100
7	E	63/86 (73%)	61 (97%)	2 (3%)	0	100	100
8	F	88/125 (70%)	87 (99%)	1 (1%)	0	100	100
9	G	79/110 (72%)	70 (89%)	9 (11%)	0	100	100
All	All	2482/4702 (53%)	2413 (97%)	69 (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	
1	1	34/382 (9%)	31 (91%)	3 (9%)	10	10
3	9	78/446 (18%)	73 (94%)	5 (6%)	17	20
4	A	714/1104 (65%)	684 (96%)	30 (4%)	30	38
5	B	113/776 (15%)	107 (95%)	6 (5%)	22	27
6	C	1018/1051 (97%)	998 (98%)	20 (2%)	55	69
7	E	56/77 (73%)	55 (98%)	1 (2%)	59	72
8	F	79/109 (72%)	69 (87%)	10 (13%)	4	3
9	G	65/95 (68%)	61 (94%)	4 (6%)	18	21
All	All	2157/4040 (53%)	2078 (96%)	79 (4%)	37	43

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	53	SER
1	1	55	GLU
1	1	81	ASN
3	9	411	CYS
3	9	420	LYS
3	9	425	HIS
3	9	435	MET
3	9	462	LEU
4	A	397	ARG
4	A	403	GLU
4	A	413	LYS
4	A	491	GLU
4	A	493	LYS
4	A	494	GLU
4	A	497	ILE
4	A	517	ARG
4	A	519	ILE
4	A	590	ARG
4	A	659	GLN
4	A	831	ARG
4	A	893	ILE
4	A	984	GLU
4	A	1004	ILE
4	A	1008	LYS
4	A	1009	MET

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Mol	Chain	Res	Type
4	A	1010	THR
4	A	1014	LYS
4	A	1019	ARG
4	A	1027	ARG
4	A	1030	LYS
4	A	1062	LEU
4	A	1134	ASN
4	A	1163	LYS
4	A	1177	LEU
4	A	1195	MET
4	A	1209	ASN
4	A	1245	ARG
4	A	1277	GLN
5	B	471	ARG
5	B	474	VAL
5	B	508	ARG
5	B	512	GLN
5	B	537	ARG
5	B	583	LYS
6	C	86	ARG
6	C	214	ASP
6	C	261	PHE
6	C	274	ARG
6	C	326	ARG
6	C	370	GLU
6	C	390	ARG
6	C	419	ASP
6	C	420	THR
6	C	429	ARG
6	C	462	VAL
6	C	522	ASP
6	C	569	ASP
6	C	671	ASN
6	C	697	ARG
6	C	759	THR
6	C	761	THR
6	C	776	GLN
6	C	869	MET
6	C	1090	GLU
7	E	48	ASP
8	F	12	ARG
8	F	13	LEU

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Mol	Chain	Res	Type
8	F	17	VAL
8	F	37	ASP
8	F	46	ARG
8	F	52	ASN
8	F	57	ARG
8	F	62	VAL
8	F	89	VAL
8	F	96	ARG
9	G	11	CYS
9	G	12	ARG
9	G	14	GLN
9	G	27	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	79	GLN
3	9	413	ASN
4	A	659	GLN
4	A	1028	HIS
5	B	496	ASN
5	B	512	GLN
6	C	293	HIS
6	C	670	GLN
8	F	25	ASN
8	F	52	ASN
9	G	14	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	h	12/17 (70%)	2 (16%)	0
2	2	34/188 (18%)	9 (26%)	2 (5%)
All	All	46/205 (22%)	11 (23%)	2 (4%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	30	A
2	2	40	OMC

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Mol	Chain	Res	Type
2	2	41	PSU
2	2	45	C
2	2	46	U
2	2	47	OMU
2	2	48	A
2	2	49	U
2	2	58	PSU
10	h	10	A
10	h	11	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	45	C
2	2	48	A

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	$\#\|Z\| > 2$
2	PSU	2	34	2,10	17,21,22	1.44	2 (11%)	20,30,33	3.18	6 (30%)
2	PSU	2	39	2,10	17,21,22	1.44	2 (11%)	20,30,33	3.24	8 (40%)
2	PSU	2	58	2	17,21,22	1.42	2 (11%)	20,30,33	3.24	8 (40%)
2	OMC	2	40	2,10	15,22,23	0.76	1 (6%)	17,31,34	1.89	4 (23%)
2	PSU	2	41	2,10	17,21,22	1.44	2 (11%)	20,30,33	3.24	8 (40%)
2	PSU	2	37	2,10	17,21,22	1.42	2 (11%)	20,30,33	3.26	8 (40%)
2	OMU	2	47	2	14,22,23	1.13	1 (7%)	14,31,34	1.24	1 (7%)
2	OMC	2	61	2	15,22,23	0.76	1 (6%)	17,31,34	1.43	2 (11%)
2	PSU	2	44	2	17,21,22	1.51	2 (11%)	20,30,33	3.29	8 (40%)
2	PSU	2	43	2	17,21,22	1.48	2 (11%)	20,30,33	3.28	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PSU	2	54	2	17,21,22	1.42	2 (11%)	20,30,33	3.20	7 (35%)

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
2	PSU	2	34	2,10	-	0/7/25/26	0/2/2/2
2	PSU	2	39	2,10	-	0/7/25/26	0/2/2/2
2	PSU	2	58	2	-	2/7/25/26	0/2/2/2
2	OMC	2	40	2,10	-	3/7/27/28	0/2/2/2
2	PSU	2	41	2,10	-	0/7/25/26	0/2/2/2
2	PSU	2	37	2,10	-	2/7/25/26	0/2/2/2
2	OMU	2	47	2	-	2/7/27/28	0/2/2/2
2	OMC	2	61	2	-	1/7/27/28	0/2/2/2
2	PSU	2	44	2	-	2/7/25/26	0/2/2/2
2	PSU	2	43	2	-	2/7/25/26	0/2/2/2
2	PSU	2	54	2	-	1/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	37	PSU	C5-C4	4.22	1.50	1.41
2	2	44	PSU	C5-C4	4.21	1.50	1.41
2	2	34	PSU	C5-C4	4.20	1.50	1.41
2	2	43	PSU	C5-C4	4.20	1.50	1.41
2	2	58	PSU	C5-C4	4.16	1.50	1.41
2	2	54	PSU	C5-C4	4.06	1.50	1.41
2	2	39	PSU	C5-C4	4.06	1.50	1.41
2	2	41	PSU	C5-C4	4.02	1.50	1.41
2	2	44	PSU	C5-C1'	-3.46	1.49	1.52
2	2	47	OMU	C4-N3	3.28	1.38	1.33
2	2	43	PSU	C5-C1'	-3.21	1.49	1.52
2	2	41	PSU	C5-C1'	-3.02	1.49	1.52
2	2	39	PSU	C5-C1'	-3.01	1.49	1.52
2	2	34	PSU	C5-C1'	-2.94	1.49	1.52
2	2	54	PSU	C5-C1'	-2.86	1.49	1.52
2	2	58	PSU	C5-C1'	-2.61	1.50	1.52
2	2	37	PSU	C5-C1'	-2.53	1.50	1.52
2	2	40	OMC	O4'-C1'	2.37	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	61	OMC	O4'-C1'	2.36	1.44	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	37	PSU	N3-C2-N1	-8.71	121.50	128.43
2	2	58	PSU	N3-C2-N1	-8.69	121.52	128.43
2	2	34	PSU	N3-C2-N1	-8.67	121.54	128.43
2	2	39	PSU	N3-C2-N1	-8.66	121.54	128.43
2	2	43	PSU	N3-C2-N1	-8.63	121.57	128.43
2	2	44	PSU	N3-C2-N1	-8.60	121.59	128.43
2	2	41	PSU	N3-C2-N1	-8.59	121.60	128.43
2	2	54	PSU	N3-C2-N1	-8.58	121.61	128.43
2	2	37	PSU	C2-N3-C4	7.41	121.39	115.14
2	2	43	PSU	C2-N3-C4	7.17	121.19	115.14
2	2	39	PSU	C2-N3-C4	7.12	121.15	115.14
2	2	44	PSU	C2-N3-C4	7.09	121.13	115.14
2	2	34	PSU	C2-N3-C4	7.02	121.07	115.14
2	2	54	PSU	C2-N3-C4	6.94	121.00	115.14
2	2	58	PSU	C2-N3-C4	6.86	120.93	115.14
2	2	41	PSU	C2-N3-C4	6.84	120.92	115.14
2	2	44	PSU	C5-C4-N3	-5.46	118.33	125.36
2	2	43	PSU	C5-C4-N3	-5.43	118.37	125.36
2	2	37	PSU	C5-C4-N3	-5.25	118.59	125.36
2	2	39	PSU	C5-C4-N3	-5.22	118.64	125.36
2	2	54	PSU	C5-C4-N3	-5.15	118.73	125.36
2	2	40	OMC	C4-N3-C2	5.14	121.55	116.34
2	2	34	PSU	C5-C4-N3	-5.13	118.76	125.36
2	2	41	PSU	C5-C4-N3	-5.11	118.77	125.36
2	2	58	PSU	C5-C4-N3	-5.08	118.81	125.36
2	2	61	OMC	C4-N3-C2	4.58	120.99	116.34
2	2	58	PSU	C6-N1-C2	4.25	122.37	115.36
2	2	44	PSU	C6-N1-C2	4.13	122.18	115.36
2	2	41	PSU	C6-N1-C2	4.12	122.16	115.36
2	2	43	PSU	C6-N1-C2	4.12	122.15	115.36
2	2	34	PSU	C6-N1-C2	4.11	122.14	115.36
2	2	39	PSU	C6-N1-C2	4.08	122.08	115.36
2	2	54	PSU	C6-N1-C2	4.07	122.08	115.36
2	2	37	PSU	C6-N1-C2	3.99	121.94	115.36
2	2	47	OMU	C5-C4-N3	-3.89	114.74	123.31
2	2	44	PSU	C5-C6-N1	-3.79	119.78	124.44
2	2	43	PSU	C5-C6-N1	-3.72	119.86	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	41	PSU	C5-C6-N1	-3.72	119.86	124.44
2	2	58	PSU	C5-C6-N1	-3.65	119.95	124.44
2	2	54	PSU	C5-C6-N1	-3.61	120.01	124.44
2	2	39	PSU	C5-C6-N1	-3.60	120.02	124.44
2	2	34	PSU	C5-C6-N1	-3.57	120.05	124.44
2	2	58	PSU	C5-C1'-C2'	-3.47	109.13	115.32
2	2	39	PSU	C5-C1'-C2'	-3.39	109.28	115.32
2	2	37	PSU	C5-C6-N1	-3.29	120.39	124.44
2	2	44	PSU	C3'-C2'-C1'	3.20	105.62	101.93
2	2	41	PSU	C5-C1'-C2'	-3.18	109.65	115.32
2	2	41	PSU	C3'-C2'-C1'	3.09	105.49	101.93
2	2	34	PSU	C5-C1'-C2'	-3.01	109.95	115.32
2	2	43	PSU	C5-C1'-C2'	-3.00	109.97	115.32
2	2	40	OMC	C6-N1-C2	-2.94	116.52	121.20
2	2	54	PSU	C5-C1'-C2'	-2.94	110.07	115.32
2	2	37	PSU	C3'-C2'-C1'	2.75	105.10	101.93
2	2	37	PSU	C5-C1'-C2'	-2.56	110.76	115.32
2	2	54	PSU	C3'-C2'-C1'	2.45	104.75	101.93
2	2	58	PSU	C3'-C2'-C1'	2.41	104.71	101.93
2	2	39	PSU	C3'-C2'-C1'	2.38	104.68	101.93
2	2	40	OMC	N4-C4-N3	2.36	120.22	116.49
2	2	44	PSU	C5-C1'-C2'	-2.35	111.13	115.32
2	2	43	PSU	C3'-C2'-C1'	2.28	104.56	101.93
2	2	61	OMC	N4-C4-N3	2.22	120.00	116.49
2	2	39	PSU	O4'-C1'-C5	2.20	113.33	109.93
2	2	58	PSU	O4'-C1'-C5	2.18	113.31	109.93
2	2	40	OMC	O4'-C1'-C2'	-2.16	102.84	106.59
2	2	37	PSU	C4'-O4'-C1'	2.05	111.95	109.42
2	2	41	PSU	O4'-C1'-C5	2.04	113.09	109.93
2	2	44	PSU	O4'-C1'-C2'	2.01	107.92	104.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	40	OMC	C1'-C2'-O2'-CM2
2	2	43	PSU	O4'-C1'-C5-C4
2	2	43	PSU	O4'-C1'-C5-C6
2	2	44	PSU	O4'-C1'-C5-C4
2	2	44	PSU	O4'-C1'-C5-C6
2	2	37	PSU	C3'-C4'-C5'-O5'
2	2	37	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	58	PSU	O4'-C4'-C5'-O5'
2	2	58	PSU	C3'-C4'-C5'-O5'
2	2	40	OMC	C3'-C4'-C5'-O5'
2	2	54	PSU	C3'-C4'-C5'-O5'
2	2	40	OMC	O4'-C4'-C5'-O5'
2	2	47	OMU	C3'-C2'-O2'-CM2
2	2	61	OMC	O4'-C4'-C5'-O5'
2	2	47	OMU	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	40	OMC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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.

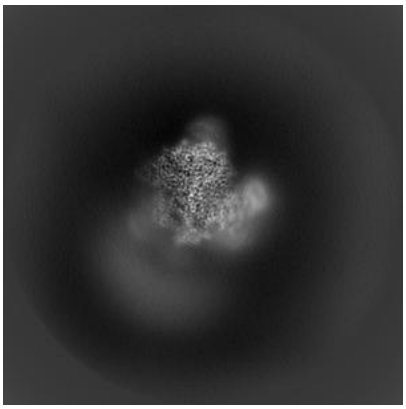
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13811. These allow visual inspection of the internal detail of the map and identification of artifacts.

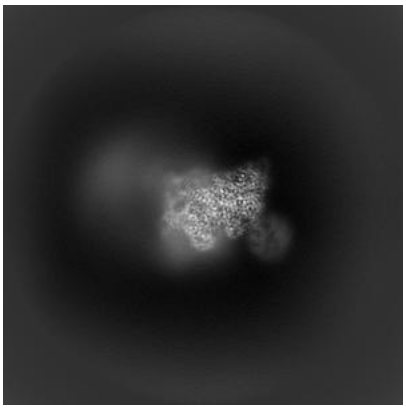
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

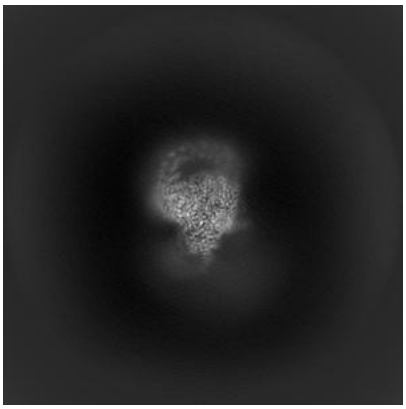
6.1.1 Primary map



X

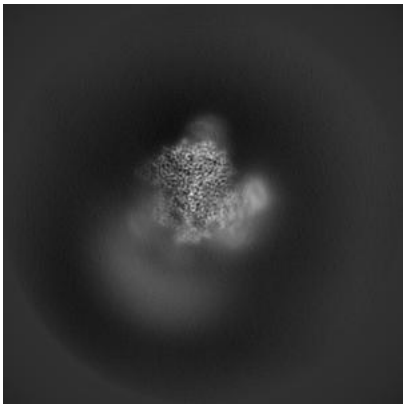


Y

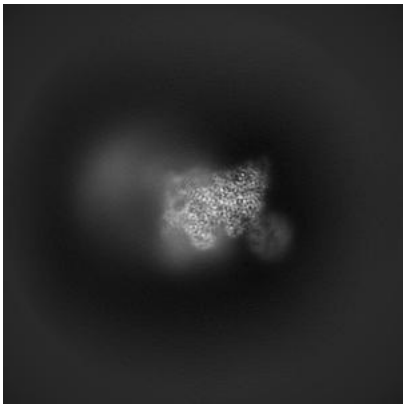


Z

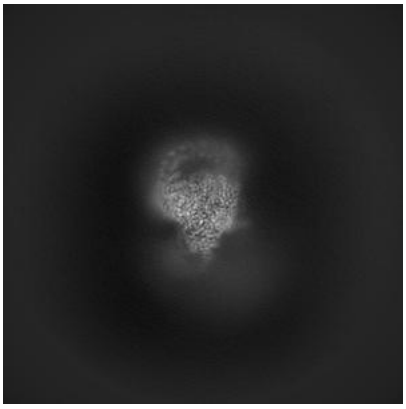
6.1.2 Raw map



X



Y

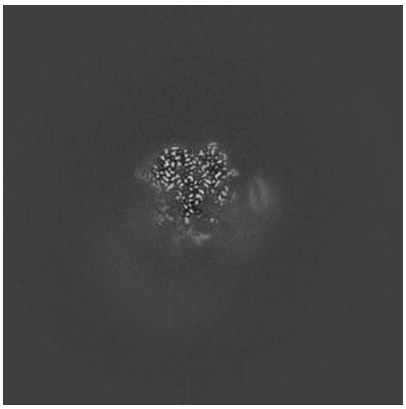


Z

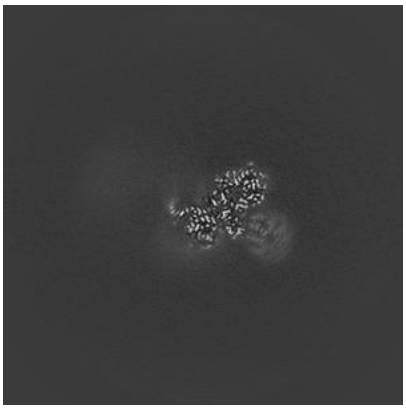
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

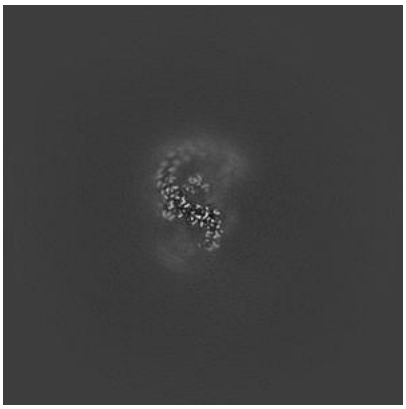
6.2.1 Primary map



X Index: 320

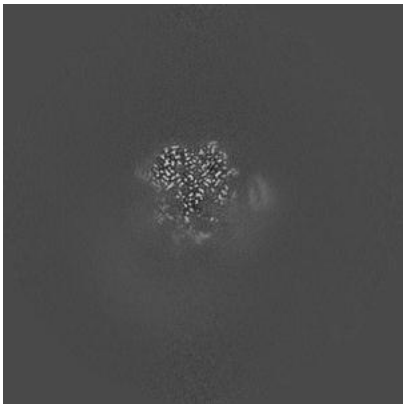


Y Index: 320

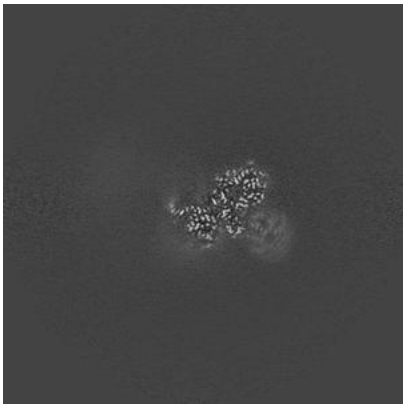


Z Index: 320

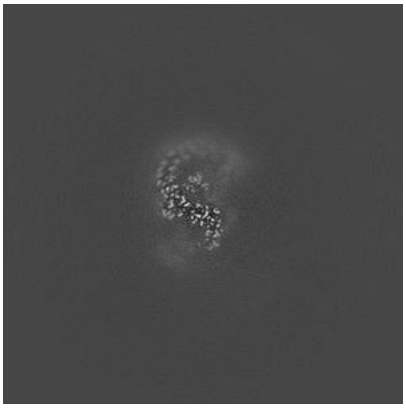
6.2.2 Raw map



X Index: 320



Y Index: 320

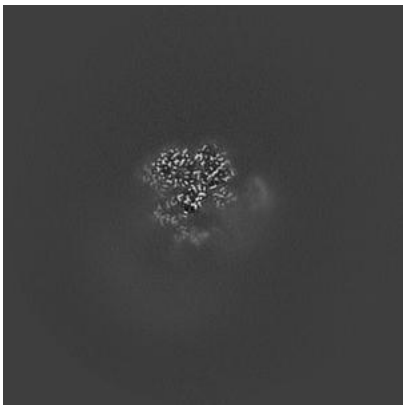


Z Index: 320

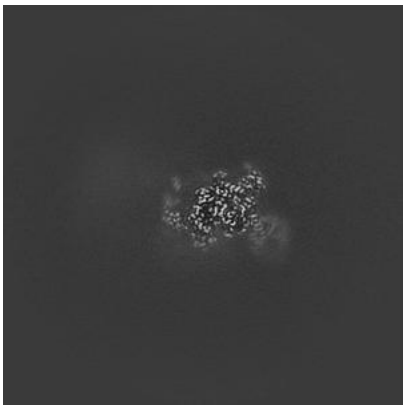
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

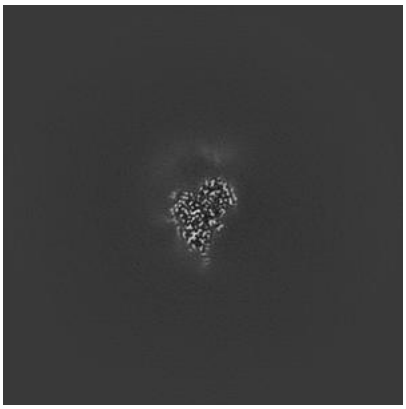
6.3.1 Primary map



X Index: 325

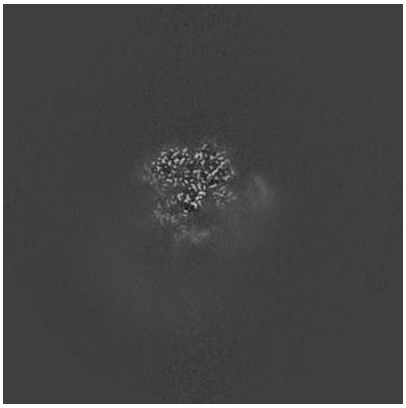


Y Index: 307

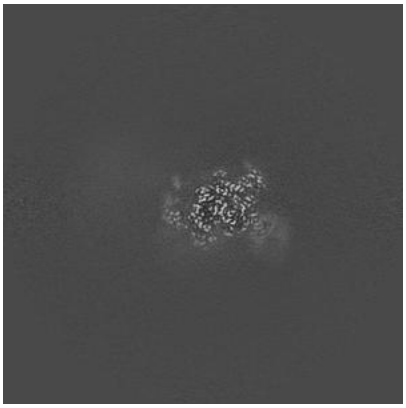


Z Index: 361

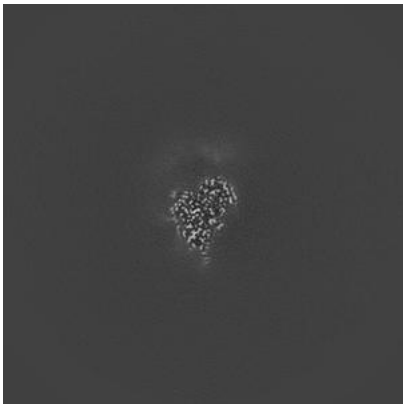
6.3.2 Raw map



X Index: 325



Y Index: 307

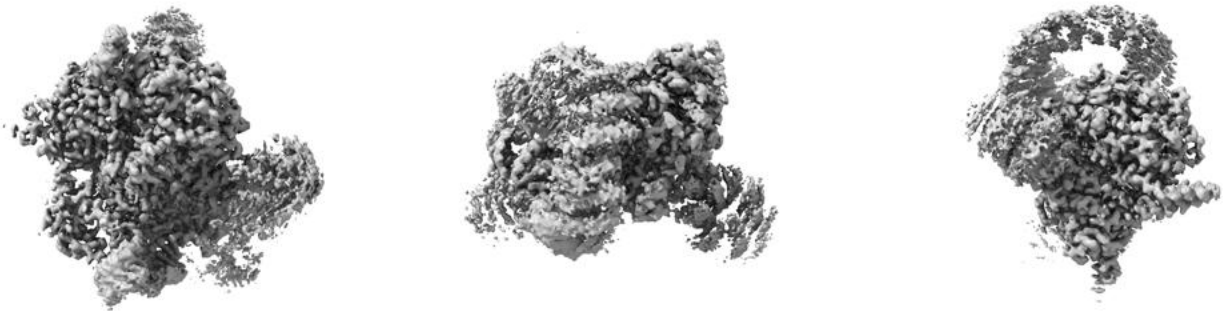


Z Index: 361

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00561. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

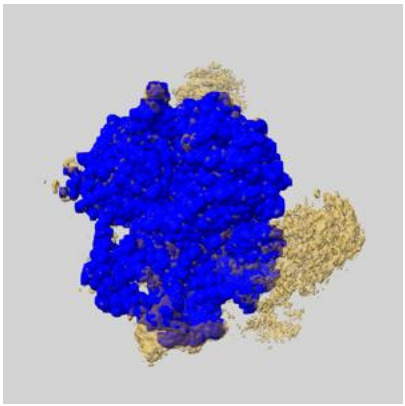
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

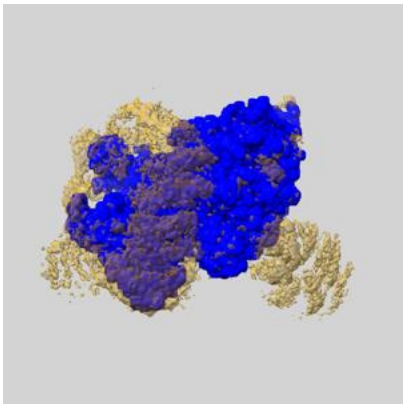
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

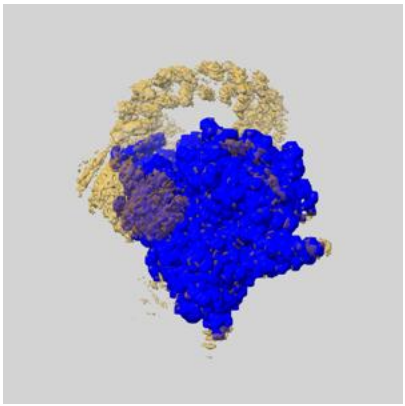
6.5.1 emd_13811_msk_1.map (i)



X



Y

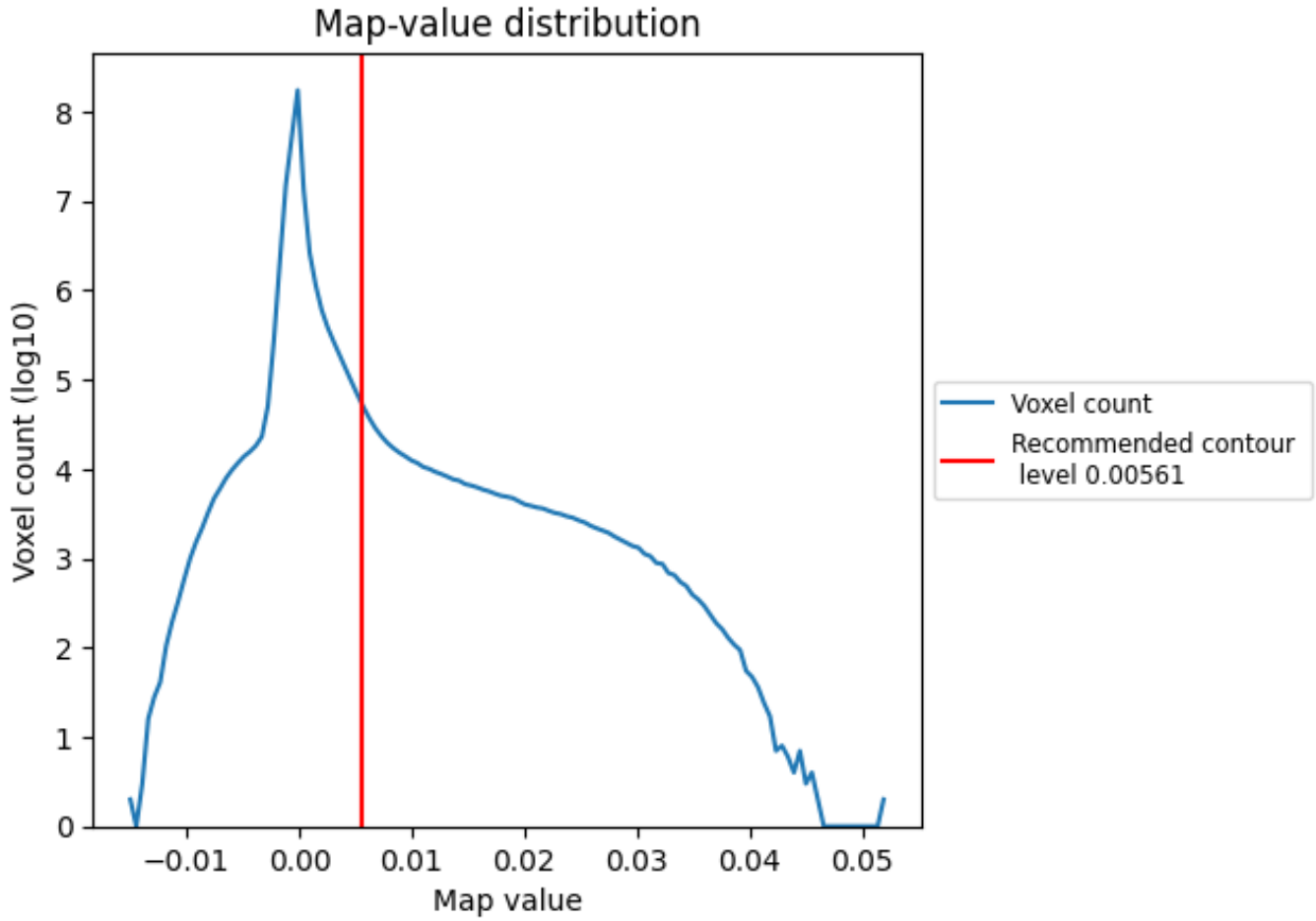


Z

7 Map analysis

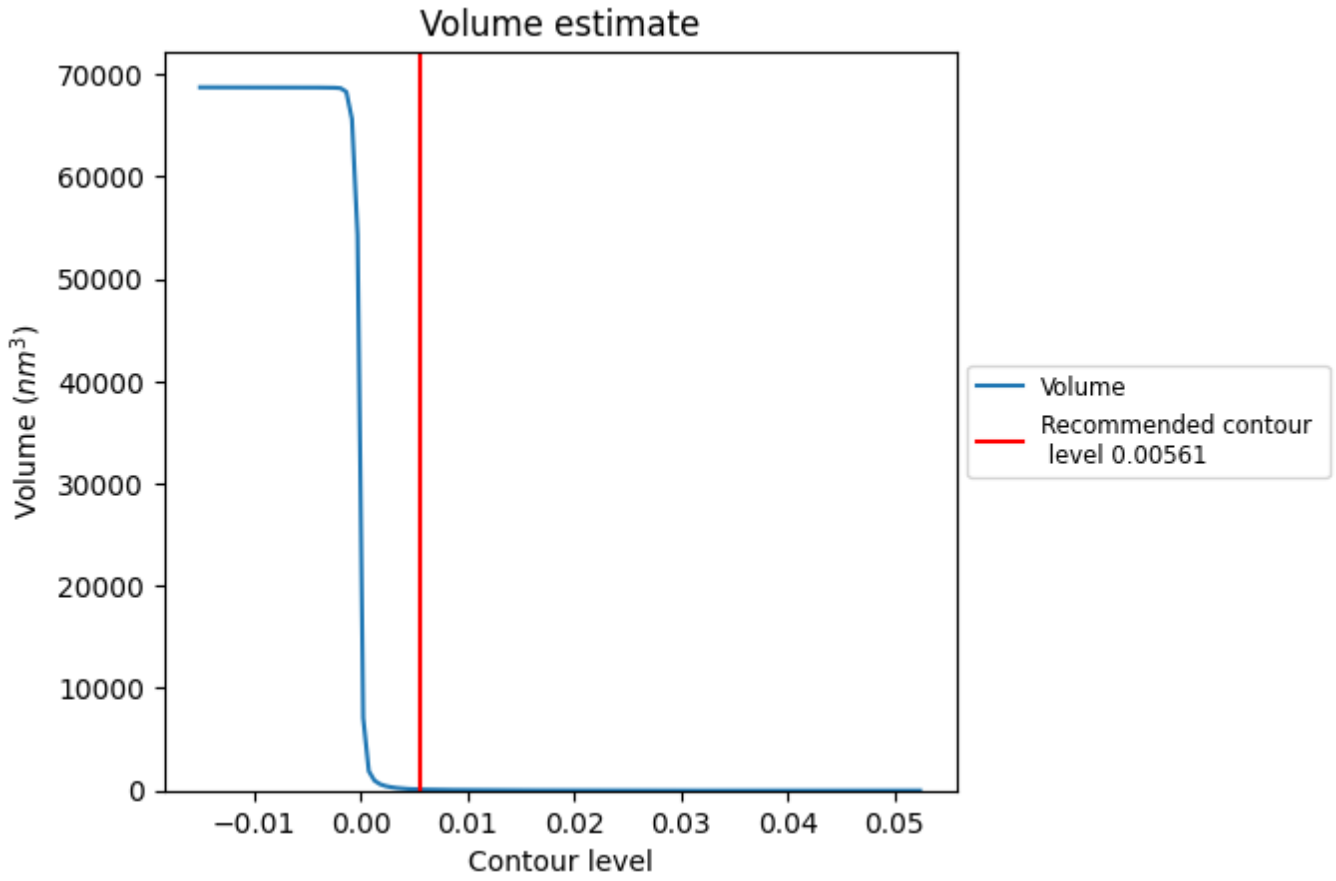
This section contains the results of statistical analysis of the map.

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.

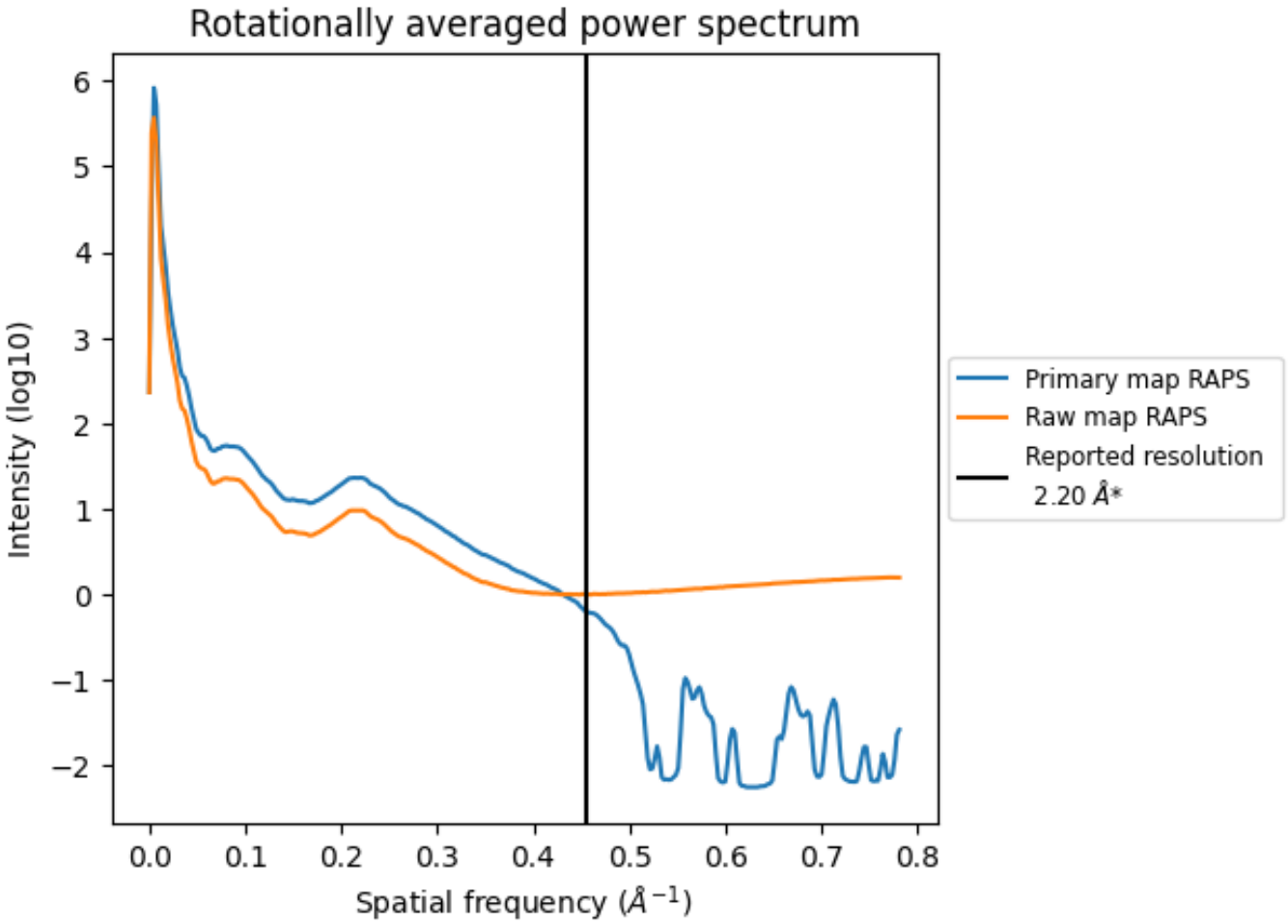
7.2 Volume estimate



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 99 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)

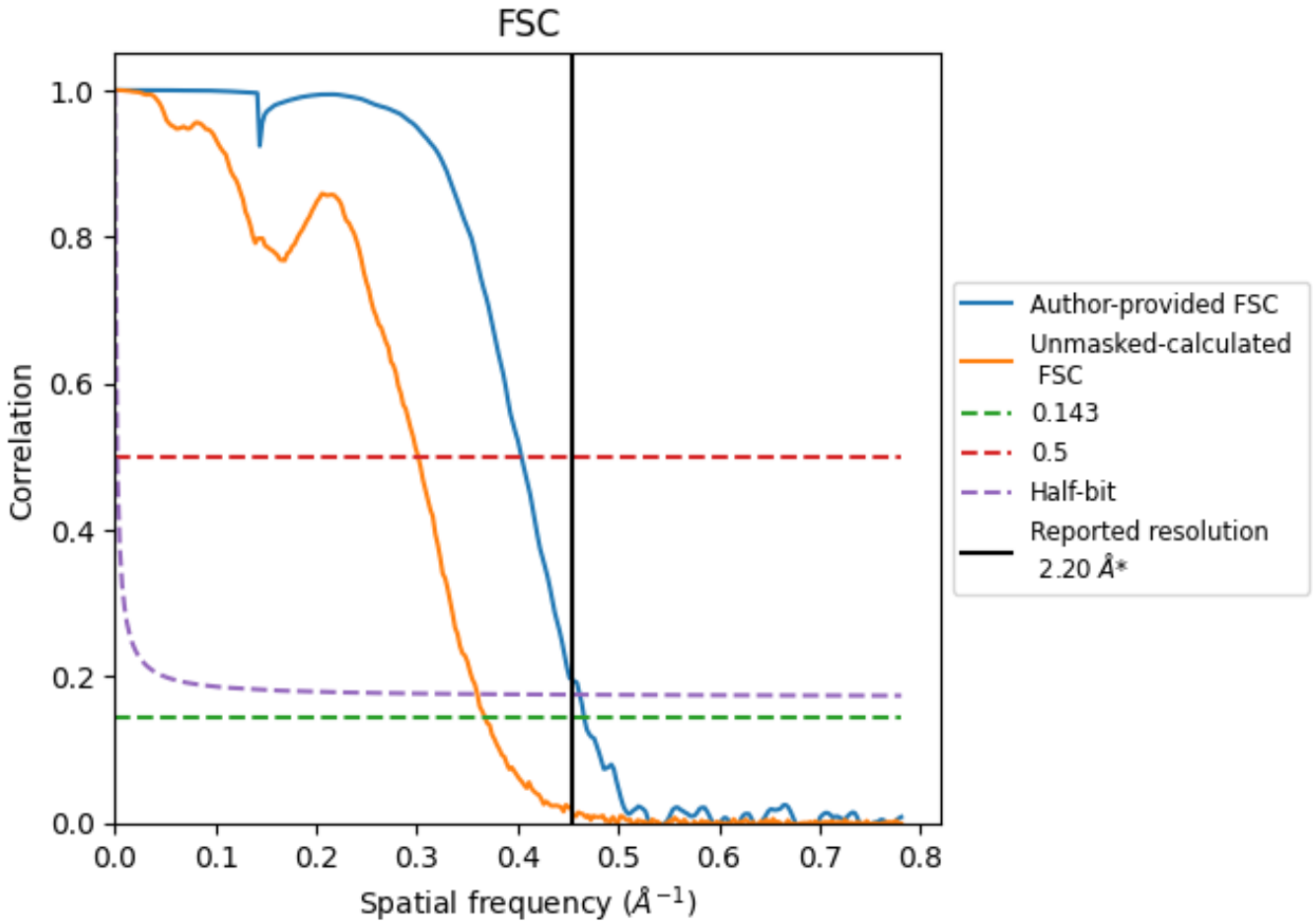


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

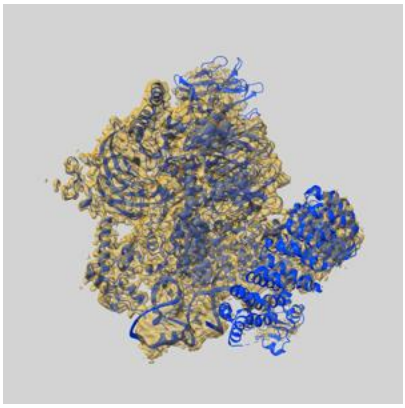
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.48	2.16
Unmasked-calculated*	2.72	3.32	2.78

*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 2.72 differs from the reported value 2.2 by more than 10 %

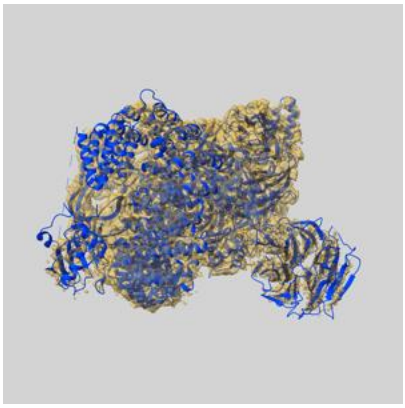
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13811 and PDB model 7Q4O. Per-residue inclusion information can be found in section 3 on page 7.

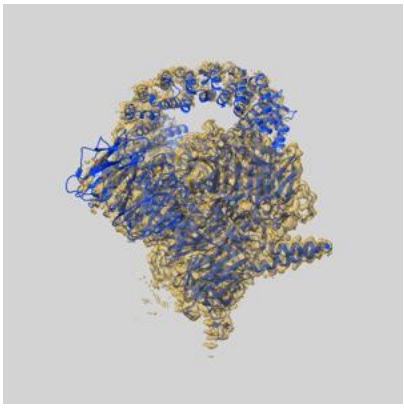
9.1 Map-model overlay



X



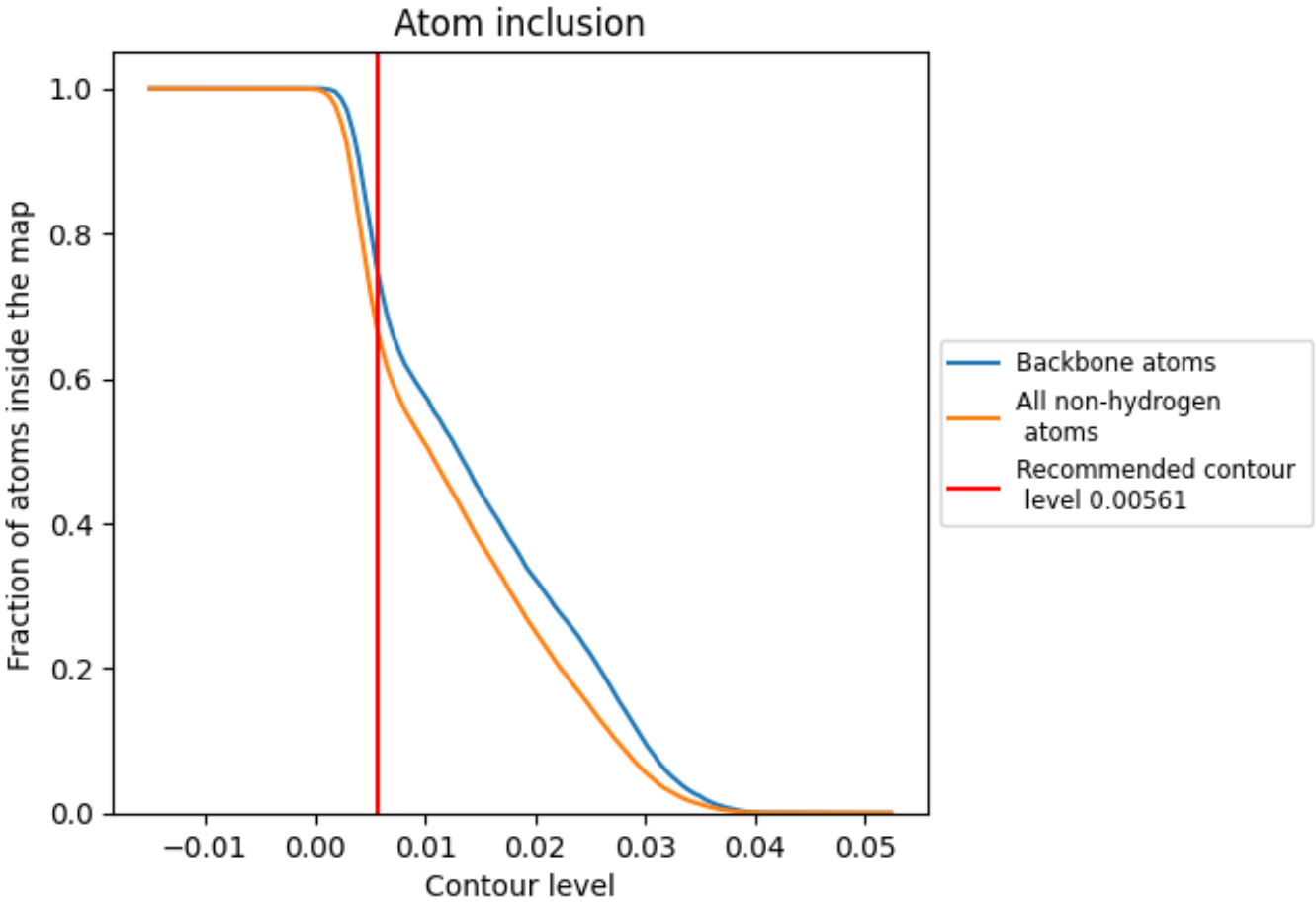
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00561 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 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.