Full wwPDB EM Validation Report ⓘ

Apr 8, 2024 – 10:27 am BST

PDB ID	:	8Q7V
EMDB ID	:	EMD-18234
Title	:	Structure of the recycling U5 snRNP bound to chaperones CD2BP2 and TSSC4 (State 1)
Authors	:	Riabov Bassat, D.; Plaschka, C.; Vorlaender, M.K.
Deposited on	:	2023-08-17
Resolution	:	3.80 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:

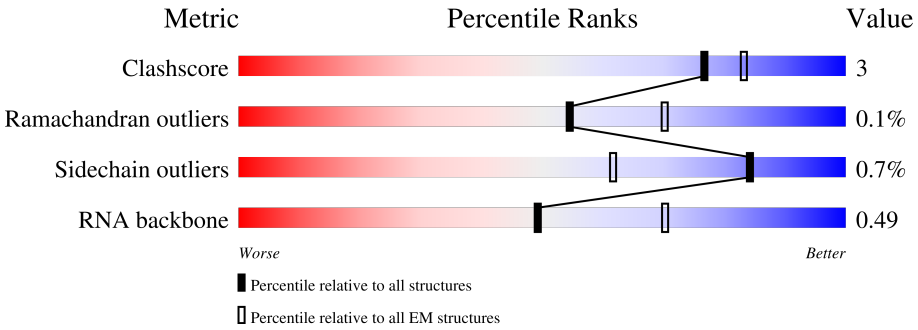
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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	5	117	46% 35% 8% 11%
2	A	2335	7% 63% 7% 30%
3	B	2136	99%
4	C	972	80% 7% 13%
5	D	357	78% 84% 14%
6	F	941	98%
7	G	343	15% 83%

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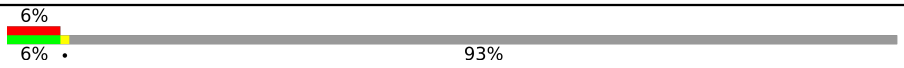
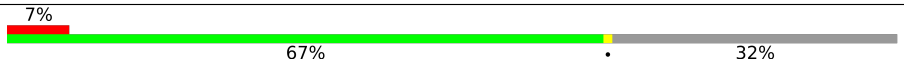
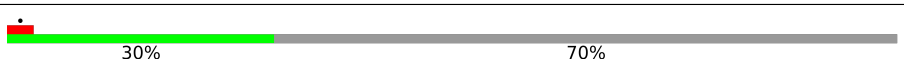
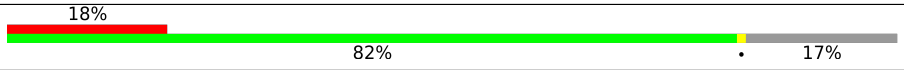
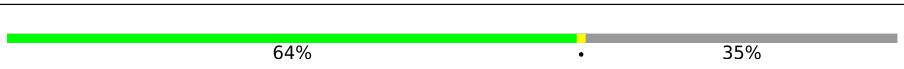
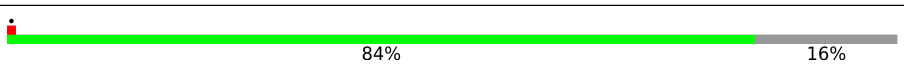
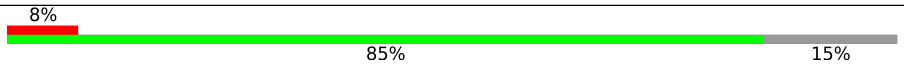
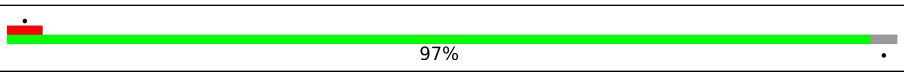
Mol	Chain	Length	Quality of chain
8	H	329	
9	a	119	
10	b	240	
11	c	118	
12	d	126	
13	e	92	
14	f	86	
15	g	76	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52625 atoms, of which 24571 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 U5 snRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	5	104	3301	983	1109	372	734	103	0	0

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	1645	27194	8822	13524	2388	2397	63	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	B	28	432	128	223	39	40	2	0	0

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	C	846	13374	4268	6698	1121	1254	33	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	D	306	2193	894	686	306	307	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	F	23	173	69	58	23	23	0	0

- Molecule 7 is a protein called CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	60	Total	C	H	N	O	S	0	0
			899	291	425	79	103	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP O95400
G	0	PRO	-	expression tag	UNP O95400

- Molecule 8 is a protein called Protein TSSC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	22	Total	C	H	N	O	S	0	0
			357	114	174	35	33	1		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	81	Total	C	H	N	O	0	0
			567	239	166	81	81		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	73	Total	C	H	N	O	0	0
			511	214	151	73	73		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	98	Total	C	H	N	O	0	0
			688	291	201	98	98		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	82	Total	C	H	N	O	S	0	0
			1312	406	666	114	120	6		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	77	Total	C	H	N	O	0	0
			541	227	160	77	77		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	73	Total	C	H	N	O	0	0
			513	210	157	73	73		

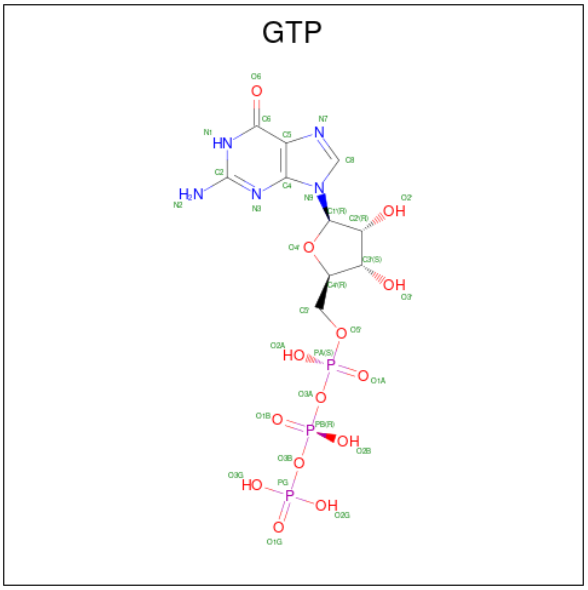
- Molecule 15 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	74	Total	C	H	N	O	0	0
			525	215	161	74	75		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	Mg	0
			1	1	

- Molecule 17 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

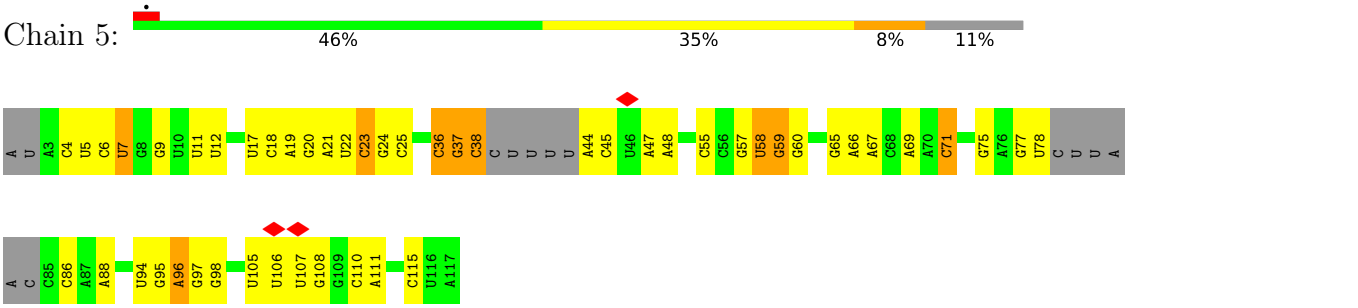


Mol	Chain	Residues	Atoms						AltConf
17	C	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

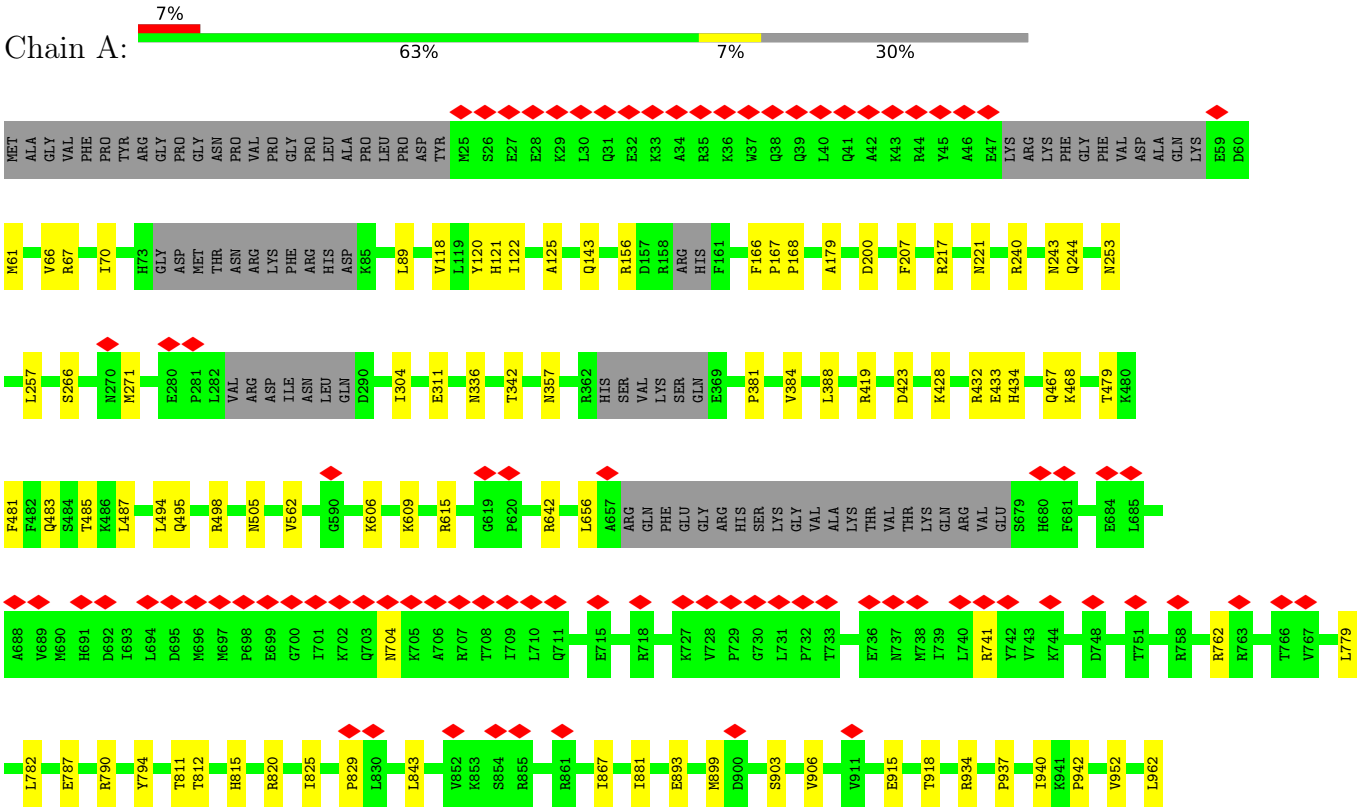
3 Residue-property plots (i)

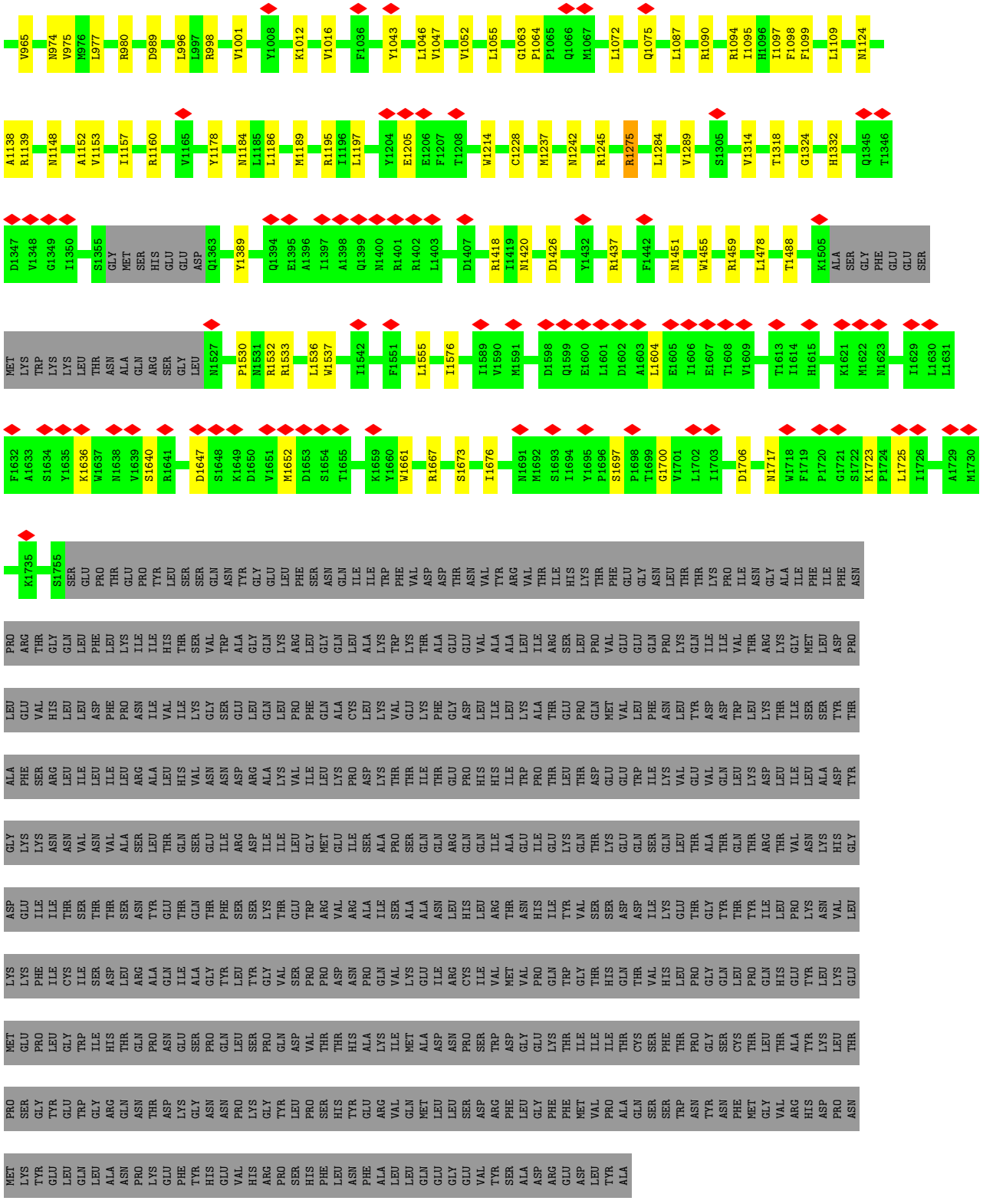
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U5 snRNA



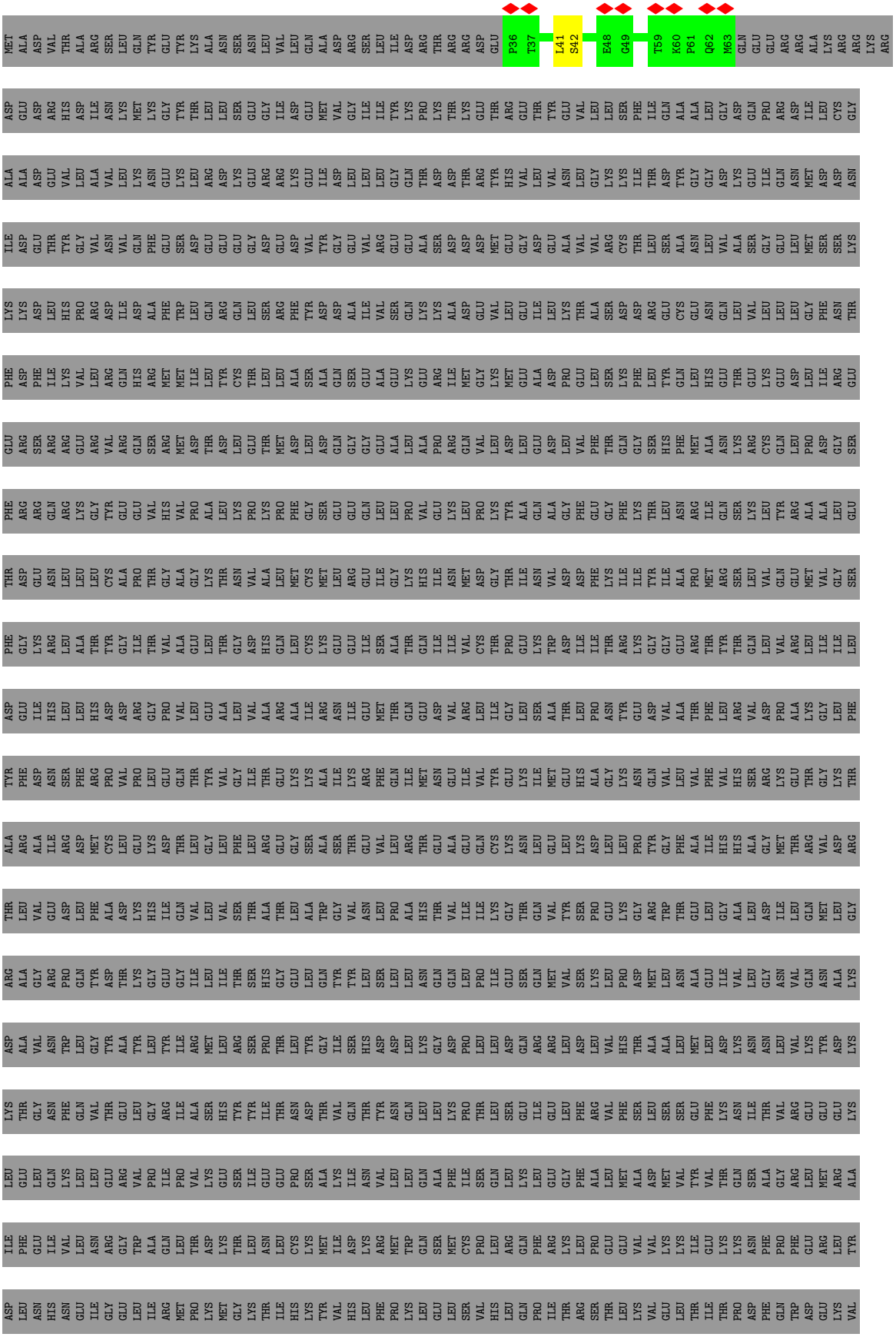
• Molecule 2: Pre-mRNA-processing-splicing factor 8

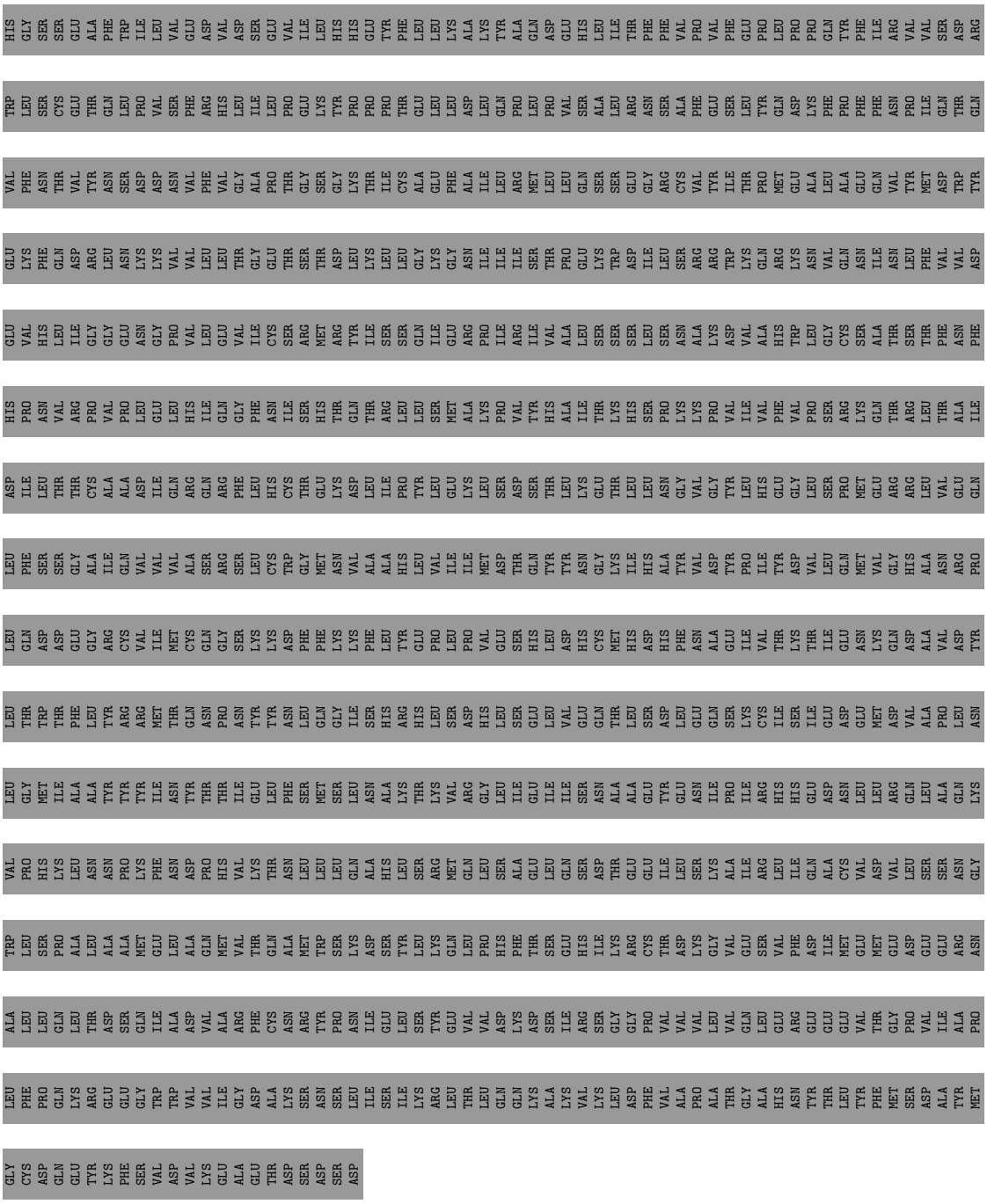




• Molecule 3: U5 small nuclear ribonucleoprotein 200 kDa helicase

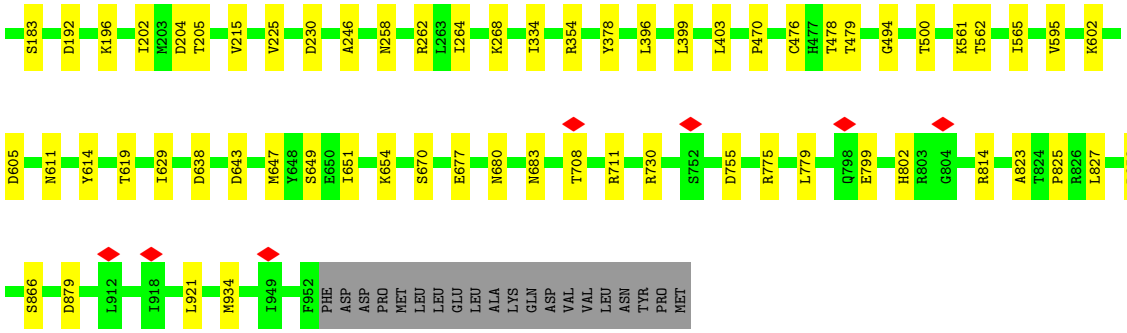
Chain B: 99%


P36
T37
L41
S42
E48
G49
T59
K60
P61
Q62
M63



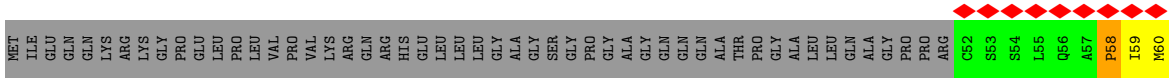
• Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component

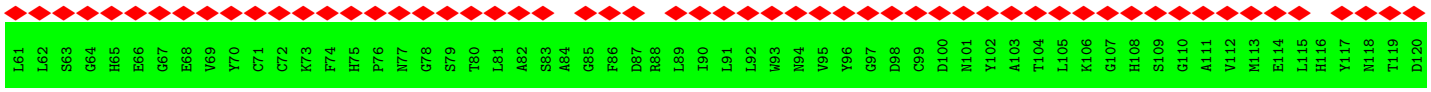
Chain C:

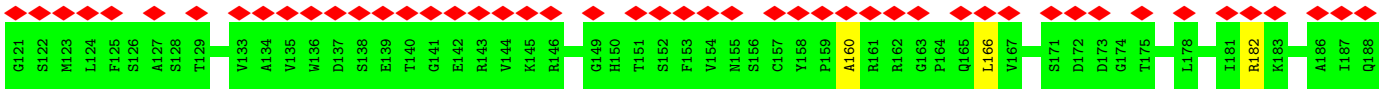


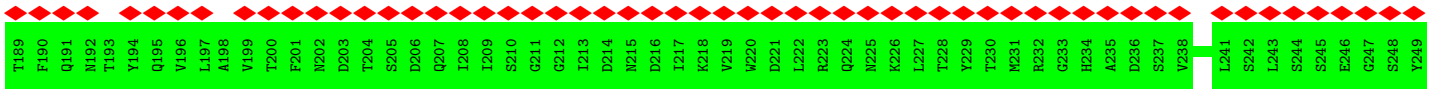
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

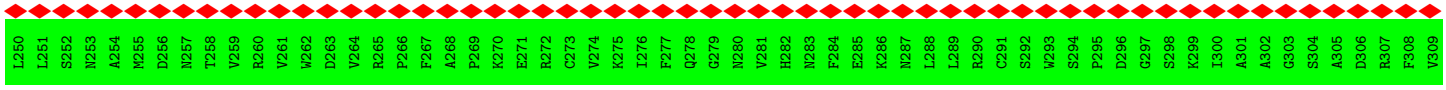
Chain D:

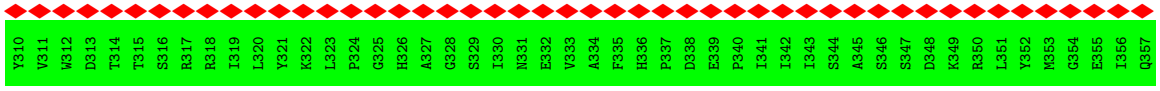






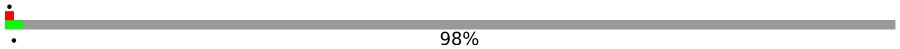


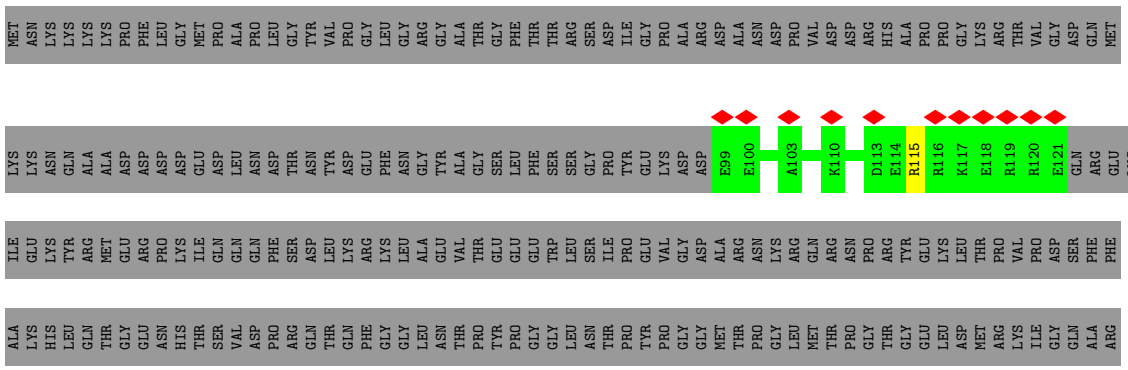


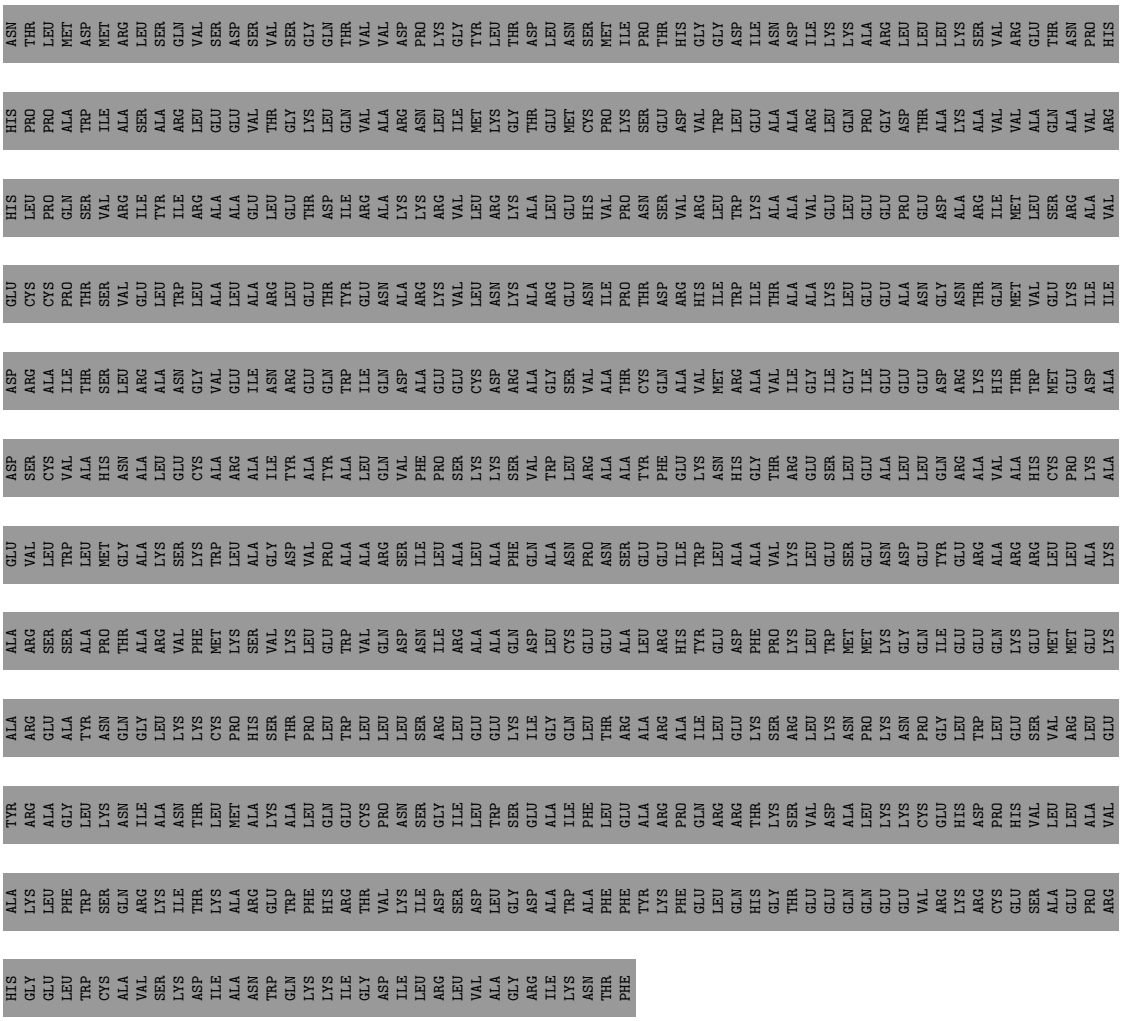


• Molecule 6: Pre-mRNA-processing factor 6

Chain F:

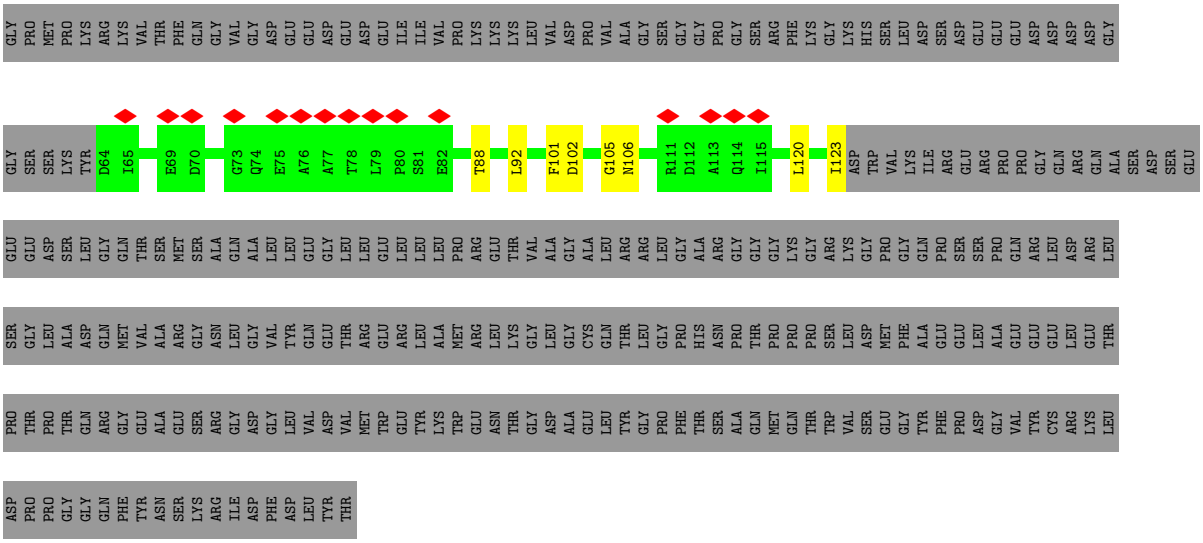






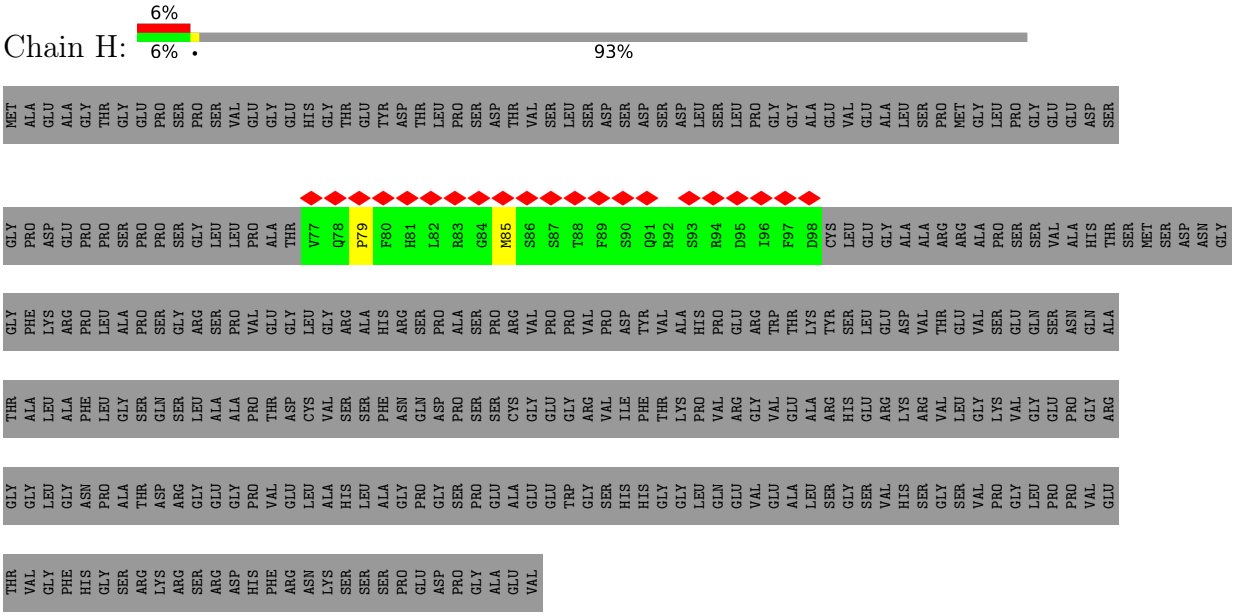
• Molecule 7: CD2 antigen cytoplasmic tail-binding protein 2

Chain G:



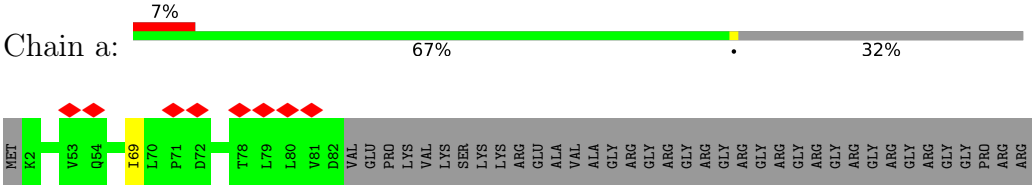
• Molecule 8: Protein TSSC4

Chain H:



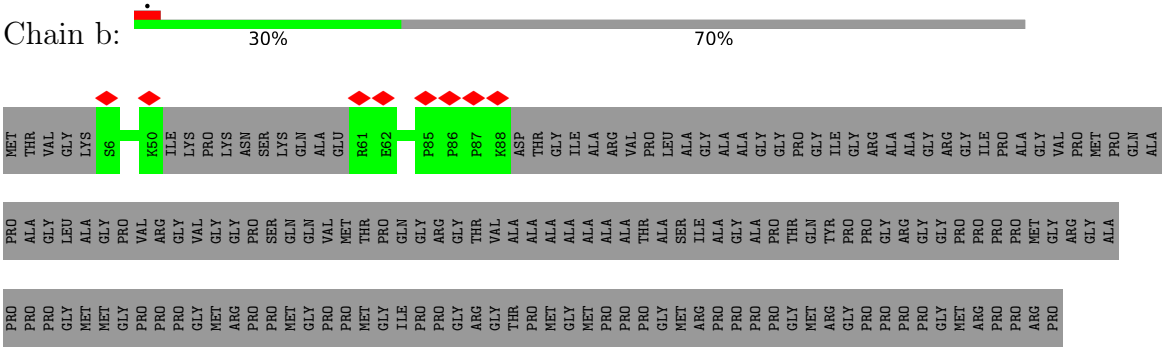
• Molecule 9: Small nuclear ribonucleoprotein Sm D1

Chain a:



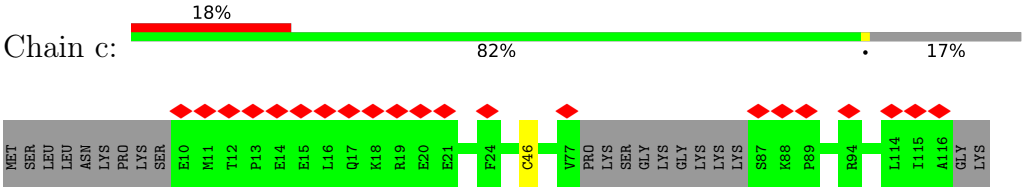
• Molecule 10: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



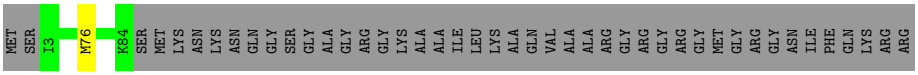
• Molecule 11: Small nuclear ribonucleoprotein Sm D2

Chain c:

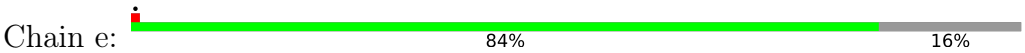


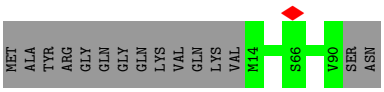
• Molecule 12: Small nuclear ribonucleoprotein Sm D3

Chain d:

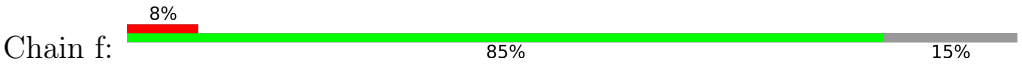


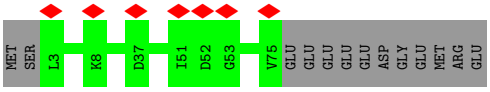
• Molecule 13: Small nuclear ribonucleoprotein E



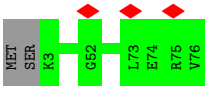


• Molecule 14: Small nuclear ribonucleoprotein F





• Molecule 15: Small nuclear ribonucleoprotein G



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.226	Depositor
Minimum map value	-0.408	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	5	0.33	1/2444 (0.0%)	1.18	21/3798 (0.6%)
2	A	0.29	0/14051	0.50	2/19064 (0.0%)
3	B	0.33	0/210	0.68	0/278
4	C	0.32	0/6826	0.58	2/9272 (0.0%)
5	D	0.28	0/1506	0.58	0/2091
6	F	0.22	0/114	0.38	0/158
7	G	0.27	0/482	0.59	0/653
8	H	0.32	0/187	0.74	0/249
9	a	0.24	0/400	0.58	1/556 (0.2%)
10	b	0.24	0/358	0.53	0/495
11	c	0.25	0/485	0.56	0/674
12	d	0.30	0/654	0.51	0/881
13	e	0.30	0/380	0.58	0/528
14	f	0.27	0/355	0.62	0/490
15	g	0.25	0/363	0.54	0/501
All	All	0.30	1/28815 (0.0%)	0.63	26/39688 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3
11	c	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	96	A	N9-C4	5.25	1.41	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	23	C	C2-N1-C1'	11.66	131.63	118.80
1	5	57	G	O4'-C1'-N9	10.42	116.53	108.20
1	5	23	C	N1-C2-O2	9.88	124.83	118.90
1	5	23	C	C6-N1-C1'	-8.01	111.19	120.80
1	5	23	C	N3-C2-O2	-8.01	116.29	121.90
1	5	23	C	C6-N1-C2	-7.79	117.19	120.30
1	5	36	C	N1-C2-O2	7.78	123.57	118.90
4	C	775	ARG	NE-CZ-NH2	7.65	124.13	120.30
4	C	730	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	5	36	C	C6-N1-C2	-6.53	117.69	120.30
1	5	96	A	C2-N3-C4	6.49	113.84	110.60
1	5	23	C	C5-C6-N1	6.48	124.24	121.00
1	5	36	C	N3-C2-O2	-6.22	117.55	121.90
1	5	115	C	C2-N1-C1'	6.12	125.54	118.80
1	5	55	C	N1-C2-O2	5.75	122.35	118.90
1	5	7	U	N1-C2-O2	5.66	126.76	122.80
2	A	1418	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	5	71	C	C2-N1-C1'	5.58	124.94	118.80
9	a	69	ILE	C-N-CA	5.37	135.14	121.70
1	5	7	U	N3-C2-O2	-5.21	118.56	122.20
1	5	36	C	C2-N1-C1'	5.19	124.51	118.80
1	5	38	C	N1-C2-O2	5.16	122.00	118.90
2	A	1275	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	5	36	C	C5-C6-N1	5.08	123.54	121.00
1	5	115	C	N1-C2-O2	5.02	121.91	118.90
1	5	96	A	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1205	GLU	Peptide
2	A	1275	ARG	Sidechain
2	A	166	PHE	Peptide
11	c	46	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	2192	1109	1111	10	0
2	A	13670	13524	13515	92	0
3	B	209	223	223	2	0
4	C	6676	6698	6697	36	0
5	D	1507	686	685	4	0
6	F	115	58	57	1	0
7	G	474	425	424	5	0
8	H	183	174	173	1	0
9	a	401	166	165	0	0
10	b	360	151	149	0	0
11	c	487	201	199	0	0
12	d	646	666	665	0	0
13	e	381	160	159	0	0
14	f	356	157	156	0	0
15	g	364	161	160	0	0
16	C	1	0	0	0	0
17	C	32	12	12	1	0
All	All	28054	24571	24550	135	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 3.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:143:THR:HG22	17:C:1101:GTP:O2B	1.69	0.91
1:5:77:G:O2'	5:D:182:ARG:O	1.88	0.91
2:A:1087:LEU:HB2	2:A:1098:PHE:HB3	1.74	0.68
2:A:974:ASN:HB2	2:A:1178:TYR:HB3	1.80	0.63
4:C:476:CYS:HB2	4:C:565:ILE:HB	1.80	0.62
2:A:998:ARG:HH12	8:H:79:PRO:HA	1.63	0.61
2:A:1214:TRP:HB2	2:A:1228:CYS:HB3	1.84	0.60
2:A:606:LYS:O	2:A:609:LYS:HB3	2.03	0.59
2:A:915:GLU:OE1	2:A:1012:LYS:NZ	2.36	0.59
2:A:975:VAL:HB	2:A:1099:PHE:HB2	1.83	0.59
2:A:820:ARG:NH2	2:A:1063:GLY:O	2.37	0.57
2:A:1289:VAL:HG21	3:B:42:SER:HA	1.85	0.57
2:A:1072:LEU:HD22	2:A:1087:LEU:HD22	1.87	0.57
2:A:1661:TRP:HD1	2:A:1697:SER:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:17:U:H3	1:5:60:G:H1	1.52	0.56
2:A:419:ARG:NH1	2:A:423:ASP:O	2.40	0.55
2:A:762:ARG:NH2	2:A:903:SER:O	2.40	0.55
7:G:120:LEU:HD12	7:G:123:ILE:HD11	1.88	0.55
4:C:853:ARG:NH2	4:C:879:ASP:O	2.38	0.55
2:A:980:ARG:HH11	2:A:1094:ARG:HD2	1.72	0.55
2:A:843:LEU:HD22	2:A:867:ILE:HG23	1.88	0.54
2:A:253:ASN:ND2	2:A:336:ASN:OD1	2.41	0.54
2:A:70:ILE:HG21	2:A:495:GLN:HG2	1.90	0.54
4:C:159:LYS:HE2	4:C:164:ASP:HA	1.89	0.53
2:A:1532:ARG:HD2	7:G:105:GLY:HA3	1.90	0.53
2:A:200:ASP:OD1	2:A:240:ARG:NH1	2.42	0.53
2:A:217:ARG:NH2	2:A:221:ASN:O	2.42	0.53
2:A:1667:ARG:NH1	2:A:1673:SER:OG	2.42	0.53
2:A:1124:ASN:ND2	2:A:1148:ASN:OD1	2.40	0.53
2:A:1237:MET:HG2	2:A:1284:LEU:HD13	1.91	0.53
2:A:1138:ALA:O	2:A:1184:ASN:ND2	2.42	0.52
2:A:1043:TYR:O	2:A:1046:LEU:HB3	2.09	0.52
5:D:160:ALA:HB3	5:D:166:LEU:H	1.74	0.52
4:C:799:GLU:HB2	4:C:802:HIS:HD2	1.75	0.52
2:A:479:THR:HG22	2:A:481:PHE:H	1.74	0.52
2:A:1530:PRO:HD2	2:A:1533:ARG:HH21	1.75	0.52
4:C:779:LEU:HD11	4:C:825:PRO:HB2	1.91	0.52
2:A:122:ILE:HG22	2:A:483:GLN:HE22	1.75	0.51
2:A:1242:ASN:OD1	2:A:1245:ARG:NH1	2.43	0.51
4:C:177:ARG:NH1	4:C:638:ASP:OD2	2.43	0.51
2:A:304:ILE:HD13	4:C:921:LEU:HA	1.93	0.51
2:A:1090:ARG:HG3	2:A:1095:ILE:HG22	1.93	0.51
2:A:1604:LEU:HD11	2:A:1725:LEU:HD13	1.92	0.50
4:C:396:LEU:HD13	4:C:403:LEU:HD13	1.94	0.50
2:A:61:MET:SD	2:A:120:TYR:OH	2.70	0.50
2:A:812:THR:HG23	2:A:1055:LEU:HD11	1.93	0.50
2:A:433:GLU:O	2:A:434:HIS:ND1	2.44	0.50
2:A:1555:LEU:HA	7:G:88:THR:HB	1.93	0.50
2:A:1184:ASN:HD22	2:A:1195:ARG:HH21	1.59	0.50
2:A:1332:HIS:HB3	3:B:41:LEU:HB2	1.94	0.50
2:A:257:LEU:HD13	2:A:311:GLU:HB2	1.94	0.49
2:A:977:LEU:HD23	2:A:1097:ILE:HD12	1.93	0.49
2:A:899:MET:HB3	2:A:906:VAL:HG13	1.94	0.49
7:G:102:ASP:OD1	7:G:106:ASN:N	2.45	0.49
2:A:1437:ARG:NH2	2:A:1455:TRP:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:827:LEU:HD11	4:C:934:MET:HB2	1.95	0.48
1:5:12:U:H3	1:5:65:G:H1	1.60	0.48
4:C:134:LEU:HD13	4:C:202:ILE:HG23	1.95	0.48
2:A:962:LEU:HB2	2:A:965:VAL:HB	1.96	0.48
2:A:89:LEU:HD11	2:A:656:LEU:HD22	1.96	0.48
2:A:118:VAL:HG21	2:A:487:LEU:HD12	1.97	0.47
4:C:683:ASN:OD1	4:C:683:ASN:N	2.45	0.47
2:A:1426:ASP:OD2	2:A:1459:ARG:NH1	2.43	0.47
2:A:1530:PRO:HD2	2:A:1533:ARG:HD3	1.96	0.47
4:C:614:TYR:OH	4:C:643:ASP:OD2	2.29	0.47
5:D:58:PRO:O	5:D:60:MET:N	2.45	0.47
7:G:92:LEU:HD13	7:G:101:PHE:HE2	1.79	0.47
4:C:619:THR:HG22	4:C:629:ILE:HG12	1.97	0.47
2:A:881:ILE:HG12	2:A:918:THR:HG22	1.96	0.47
2:A:143:GLN:NE2	2:A:207:PHE:O	2.43	0.46
2:A:893:GLU:HG2	2:A:1016:VAL:HB	1.97	0.46
2:A:952:VAL:HG22	2:A:1189:MET:HE3	1.97	0.46
4:C:479:THR:HA	4:C:562:THR:HG22	1.98	0.46
2:A:811:THR:O	2:A:815:HIS:ND1	2.36	0.46
4:C:183:SER:HA	4:C:204:ASP:O	2.16	0.46
2:A:1109:LEU:HG	2:A:1152:ALA:HB1	1.98	0.46
4:C:755:ASP:OD1	4:C:755:ASP:N	2.49	0.46
4:C:677:GLU:O	4:C:814:ARG:NH1	2.49	0.46
2:A:787:GLU:HA	2:A:790:ARG:HG2	1.98	0.45
2:A:937:PRO:HD2	2:A:940:ILE:HD12	1.99	0.45
4:C:643:ASP:O	4:C:647:MET:HB2	2.16	0.45
1:5:11:U:H5'	2:A:217:ARG:HH12	1.81	0.45
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.98	0.45
2:A:1640:SER:O	2:A:1717:ASN:ND2	2.44	0.45
4:C:225:VAL:HG21	4:C:246:ALA:HB1	1.99	0.44
4:C:478:THR:HA	4:C:494:GLY:HA3	1.99	0.44
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.99	0.44
2:A:1064:PRO:HD3	2:A:1075:GLN:HE21	1.81	0.44
2:A:779:LEU:HD23	2:A:782:LEU:HD12	1.99	0.44
2:A:1139:ARG:HA	2:A:1186:LEU:HD11	1.98	0.44
1:5:58:U:H2'	1:5:59:G:C8	2.53	0.43
2:A:266:SER:OG	2:A:271:MET:O	2.36	0.43
1:5:18:C:H2'	1:5:19:A:H8	1.82	0.43
2:A:1647:ASP:O	2:A:1723:LYS:NZ	2.41	0.43
2:A:428:LYS:O	2:A:432:ARG:HB2	2.18	0.43
2:A:825:ILE:HB	2:A:1001:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1640:SER:HA	2:A:1652:MET:HA	2.00	0.43
4:C:602:LYS:O	4:C:605:ASP:HB2	2.19	0.42
4:C:649:SER:HB3	4:C:651:ILE:HG12	1.99	0.42
4:C:264:ILE:HG12	4:C:378:TYR:CE1	2.54	0.42
2:A:342:THR:OG1	4:C:268:LYS:NZ	2.52	0.42
2:A:1488:THR:HB	2:A:1537:TRP:CE2	2.55	0.42
4:C:205:THR:HB	4:C:215:VAL:HG22	2.01	0.42
1:5:19:A:N6	2:A:467:GLN:O	2.44	0.42
2:A:388:LEU:HD11	4:C:399:LEU:HD11	2.01	0.42
2:A:428:LYS:HE2	2:A:432:ARG:HH21	1.84	0.42
1:5:77:G:O3'	5:D:182:ARG:O	2.37	0.42
2:A:942:PRO:HB2	2:A:1437:ARG:HD2	2.01	0.42
1:5:37:G:N2	1:5:44:A:N3	2.67	0.41
2:A:384:VAL:HG21	4:C:334:ILE:HD11	2.02	0.41
2:A:1184:ASN:HB3	2:A:1197:LEU:HD13	2.01	0.41
4:C:192:ASP:OD1	4:C:196:LYS:N	2.51	0.41
4:C:670:SER:HB3	4:C:823:ALA:HB2	2.01	0.41
2:A:167:PRO:HA	2:A:168:PRO:HD3	1.88	0.41
2:A:468:LYS:HE2	6:F:115:ARG:HA	2.01	0.41
2:A:494:LEU:HD21	2:A:562:VAL:HG21	2.01	0.41
2:A:1314:VAL:HG23	2:A:1478:LEU:HD13	2.02	0.41
1:5:110:C:H2'	1:5:111:A:H8	1.84	0.41
2:A:1052:VAL:O	2:A:1160:ARG:NH2	2.47	0.41
4:C:470:PRO:O	4:C:500:THR:OG1	2.28	0.41
2:A:794:TYR:OH	2:A:989:ASP:OD1	2.34	0.41
2:A:1099:PHE:HZ	2:A:1157:ILE:HD11	1.85	0.41
4:C:595:VAL:HG22	4:C:654:LYS:HG3	2.02	0.41
2:A:1318:THR:HB	2:A:1324:GLY:HA3	2.02	0.41
2:A:996:LEU:HD23	2:A:1047:VAL:HG21	2.01	0.41
2:A:244:GLN:O	2:A:615:ARG:NH1	2.53	0.41
2:A:357:ASN:ND2	4:C:866:SER:O	2.54	0.41
2:A:66:VAL:HG11	2:A:485:THR:HG21	2.02	0.40
4:C:561:LYS:NZ	4:C:614:TYR:O	2.53	0.40
2:A:121:HIS:HB3	2:A:125:ALA:H	1.86	0.40
2:A:975:VAL:HG11	2:A:1153:VAL:HG21	2.02	0.40
2:A:1536:LEU:HD21	2:A:1576:ILE:HD11	2.03	0.40
2:A:1700:GLY:O	2:A:1717:ASN:N	2.49	0.40
2:A:381:PRO:O	4:C:354:ARG:NH1	2.54	0.40
4:C:230:ASP:OD2	4:C:262:ARG:NH2	2.55	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	1627/2335 (70%)	1577 (97%)	49 (3%)	1 (0%)	51 83
3	B	26/2136 (1%)	25 (96%)	1 (4%)	0	100 100
4	C	844/972 (87%)	813 (96%)	30 (4%)	1 (0%)	51 83
5	D	304/357 (85%)	283 (93%)	19 (6%)	2 (1%)	22 60
6	F	21/941 (2%)	21 (100%)	0	0	100 100
7	G	58/343 (17%)	48 (83%)	10 (17%)	0	100 100
8	H	20/329 (6%)	14 (70%)	5 (25%)	1 (5%)	2 23
9	a	79/119 (66%)	74 (94%)	5 (6%)	0	100 100
10	b	69/240 (29%)	68 (99%)	1 (1%)	0	100 100
11	c	94/118 (80%)	88 (94%)	6 (6%)	0	100 100
12	d	80/126 (64%)	75 (94%)	5 (6%)	0	100 100
13	e	75/92 (82%)	73 (97%)	2 (3%)	0	100 100
14	f	71/86 (83%)	65 (92%)	6 (8%)	0	100 100
15	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
All	All	3440/8270 (42%)	3294 (96%)	141 (4%)	5 (0%)	54 83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	59	ILE
4	C	711	ARG
5	D	58	PRO
2	A	829	PRO
8	H	85	MET

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	1471/2108 (70%)	1459 (99%)	12 (1%)	81 89
3	B	23/1908 (1%)	23 (100%)	0	100 100
4	C	748/866 (86%)	744 (100%)	4 (0%)	88 94
7	G	50/282 (18%)	50 (100%)	0	100 100
8	H	21/264 (8%)	21 (100%)	0	100 100
12	d	72/101 (71%)	71 (99%)	1 (1%)	67 81
All	All	2385/5529 (43%)	2368 (99%)	17 (1%)	84 91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	156	ARG
2	A	243	ASN
2	A	498	ARG
2	A	505	ASN
2	A	642	ARG
2	A	704	ASN
2	A	741	ARG
2	A	934	ARG
2	A	1389	TYR
2	A	1420	ASN
2	A	1451	ASN
2	A	1636	LYS
4	C	258	ASN
4	C	611	ASN
4	C	680	ASN
4	C	708	THR
12	d	76	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	210	HIS
2	A	243	ASN
2	A	253	ASN
2	A	397	ASN
2	A	483	GLN
2	A	505	ASN
2	A	509	HIS
2	A	704	ASN
2	A	793	ASN
2	A	1075	GLN
2	A	1129	ASN
2	A	1293	ASN
2	A	1332	HIS
2	A	1451	ASN
2	A	1460	HIS
2	A	1531	ASN
4	C	154	HIS
4	C	201	ASN
4	C	210	ASN
4	C	258	ASN
4	C	611	ASN
4	C	642	HIS
7	G	74	GLN
12	d	16	HIS
12	d	60	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	101/117 (86%)	35 (34%)	3 (2%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	4	C
1	5	5	U
1	5	6	C
1	5	7	U
1	5	9	G
1	5	20	G
1	5	21	A
1	5	22	U

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Mol	Chain	Res	Type
1	5	23	C
1	5	24	G
1	5	25	C
1	5	36	C
1	5	37	G
1	5	38	C
1	5	45	C
1	5	47	A
1	5	48	A
1	5	58	U
1	5	59	G
1	5	66	A
1	5	67	A
1	5	69	A
1	5	71	C
1	5	75	G
1	5	78	U
1	5	86	C
1	5	88	A
1	5	94	U
1	5	95	G
1	5	97	G
1	5	98	G
1	5	105	U
1	5	106	U
1	5	107	U
1	5	108	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	58	U
1	5	96	A
1	5	105	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	GTP	C	1101	16	26,34,34	1.24	4 (15%)	32,54,54	1.61	5 (15%)

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
17	GTP	C	1101	16	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	1101	GTP	C8-N7	-2.55	1.30	1.35
17	C	1101	GTP	C5-C4	-2.33	1.37	1.43
17	C	1101	GTP	PG-O3G	-2.24	1.46	1.54
17	C	1101	GTP	PG-O2G	-2.09	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	1101	GTP	PA-O3A-PB	-5.00	115.68	132.83
17	C	1101	GTP	PB-O3B-PG	-4.59	117.09	132.83
17	C	1101	GTP	O3G-PG-O2G	3.02	119.19	107.64
17	C	1101	GTP	O6-C6-N1	-2.41	117.80	120.65
17	C	1101	GTP	O6-C6-C5	2.12	128.52	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	1101	GTP	PB-O3B-PG-O2G
17	C	1101	GTP	PA-O3A-PB-O2B

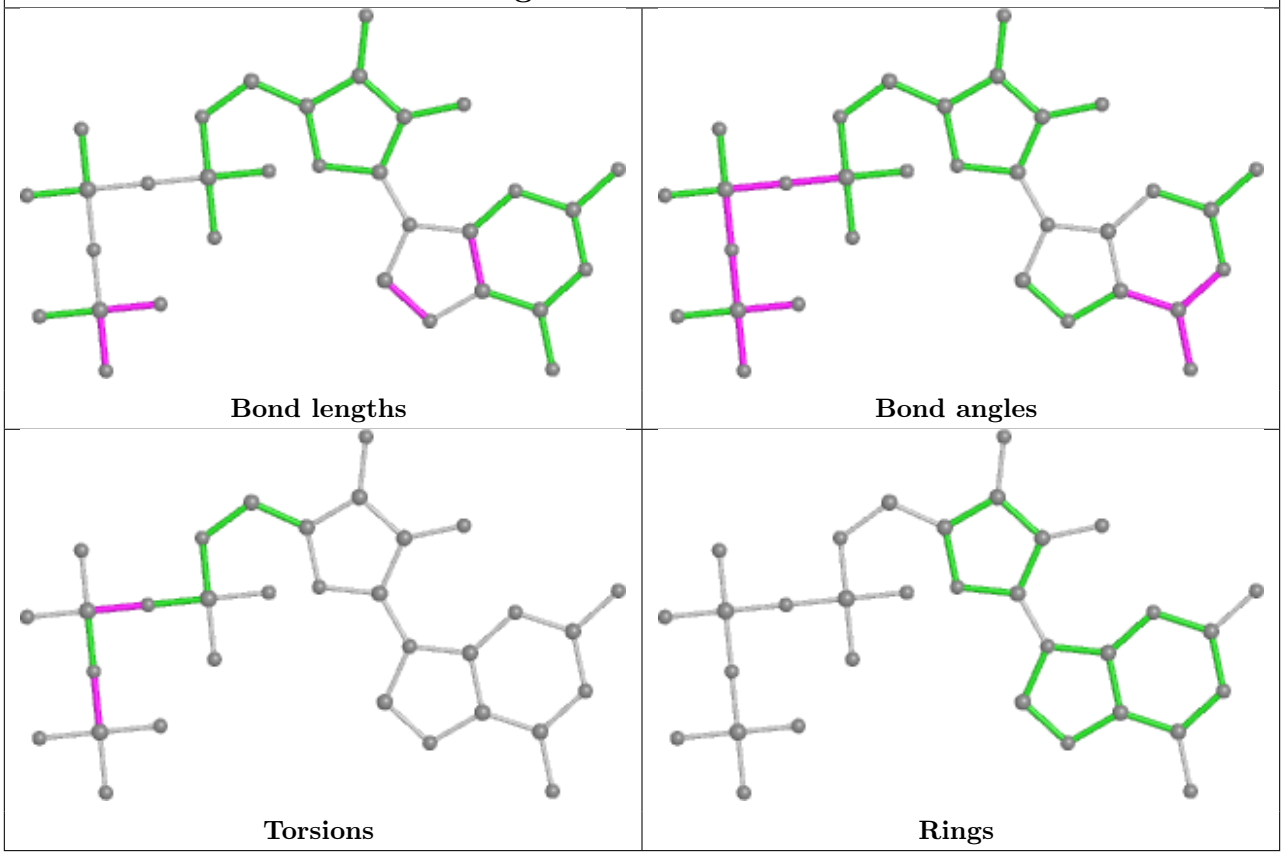
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	1101	GTP	1	0

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

Ligand GTP C 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

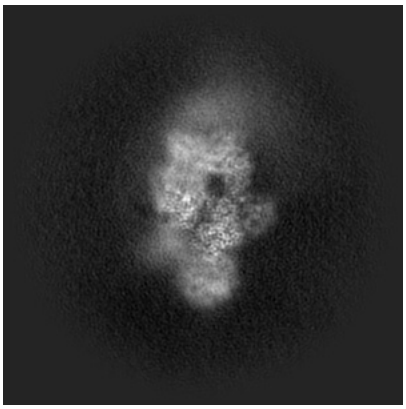
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18234. These allow visual inspection of the internal detail of the map and identification of artifacts.

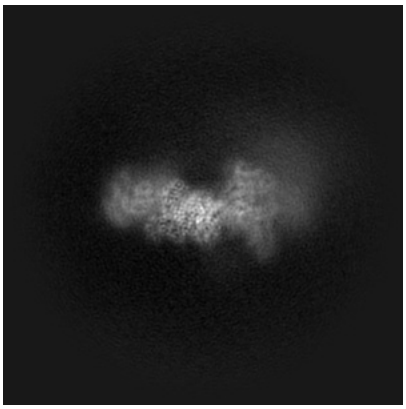
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

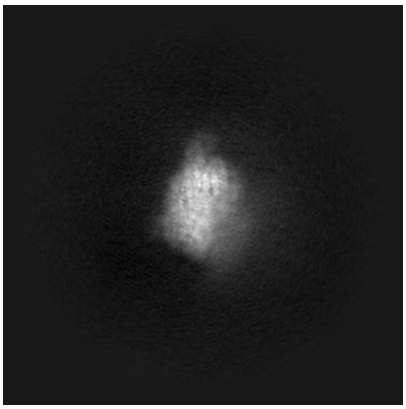
6.1.1 Primary map



X

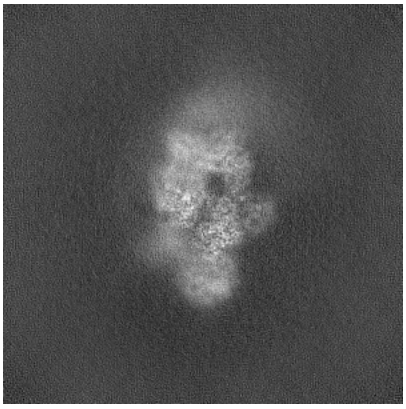


Y

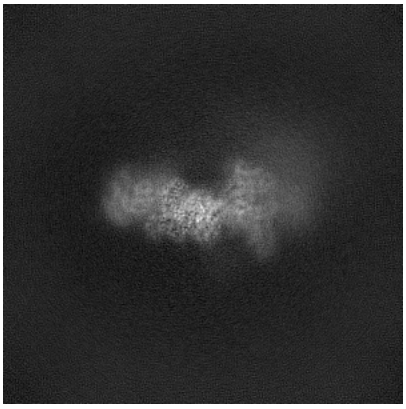


Z

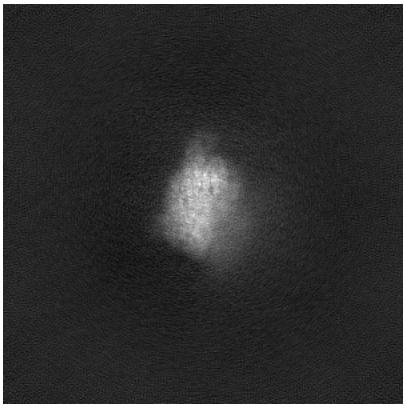
6.1.2 Raw map



X



Y

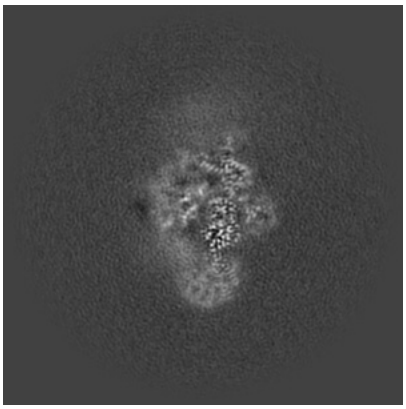


Z

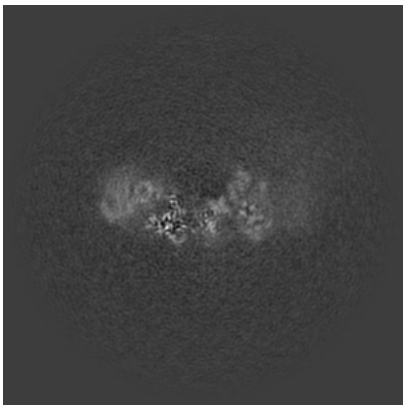
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

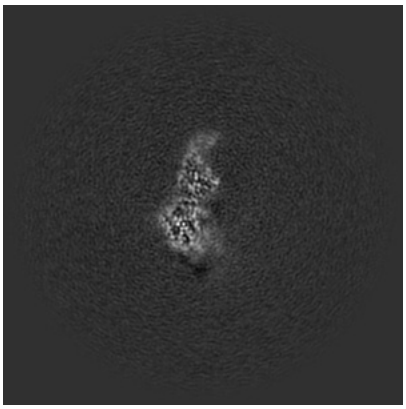
6.2.1 Primary map



X Index: 180

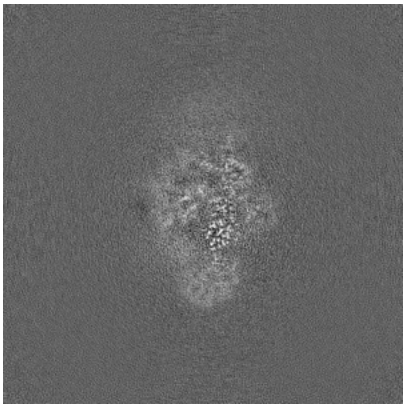


Y Index: 180

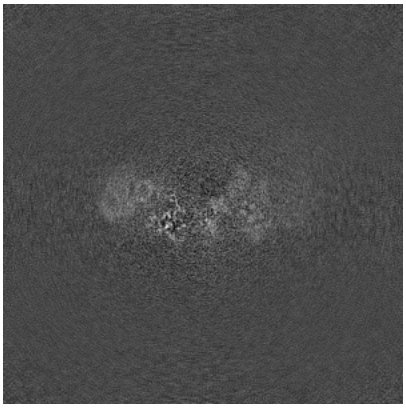


Z Index: 180

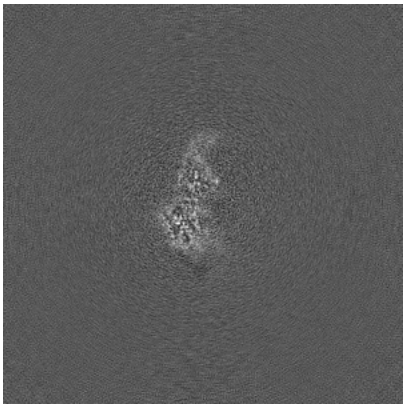
6.2.2 Raw map



X Index: 180



Y Index: 180

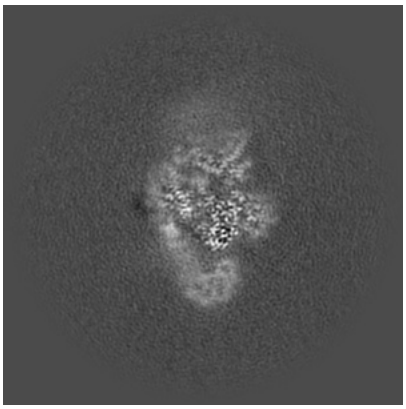


Z Index: 180

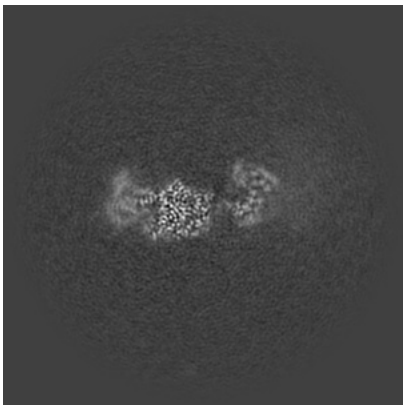
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

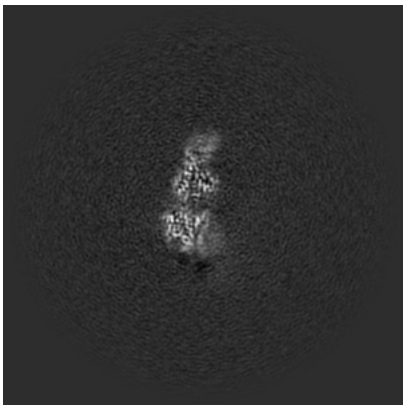
6.3.1 Primary map



X Index: 174

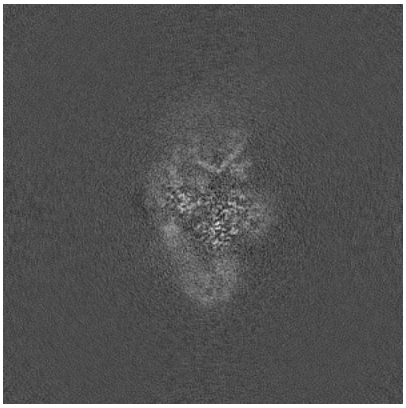


Y Index: 197

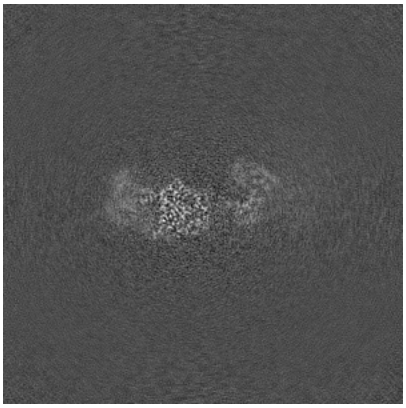


Z Index: 175

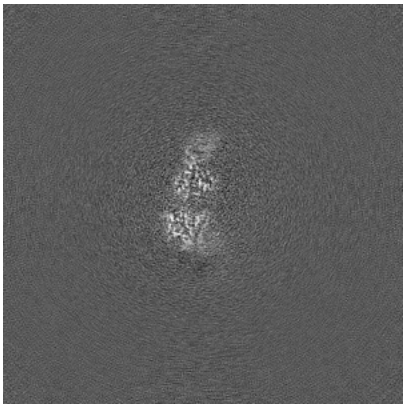
6.3.2 Raw map



X Index: 173



Y Index: 197

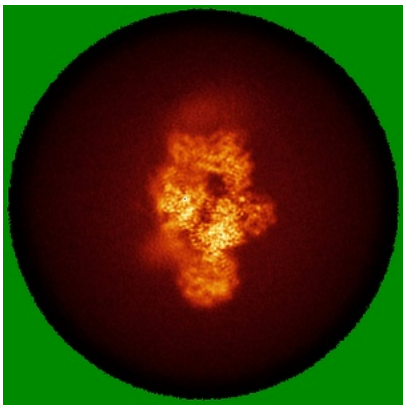


Z Index: 175

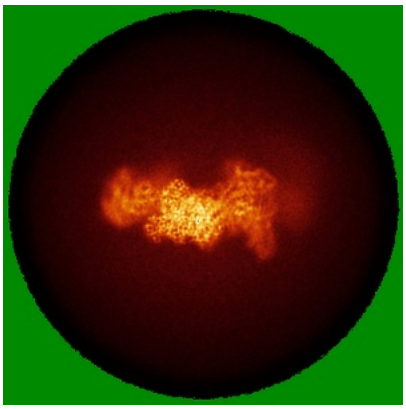
The images above show the largest variance slices of the map in three orthogonal directions.

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

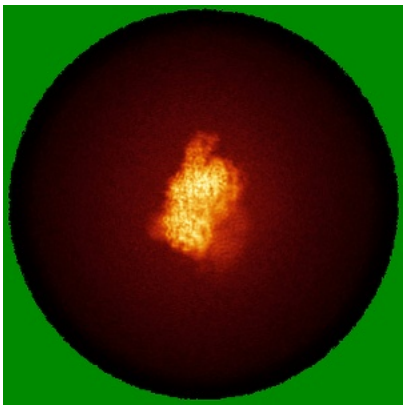
6.4.1 Primary map



X

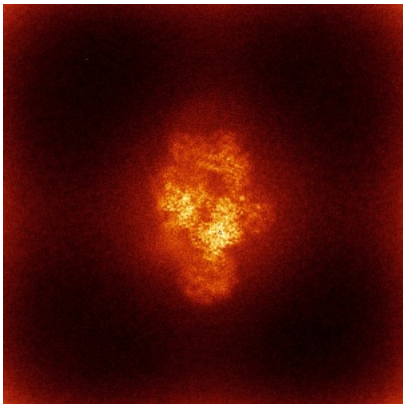


Y

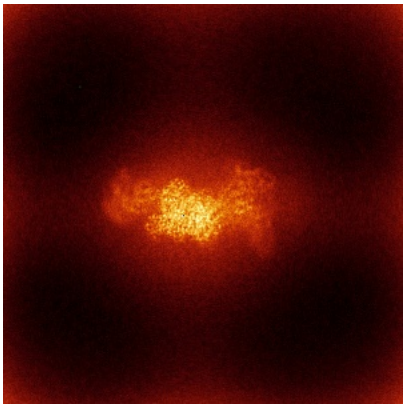


Z

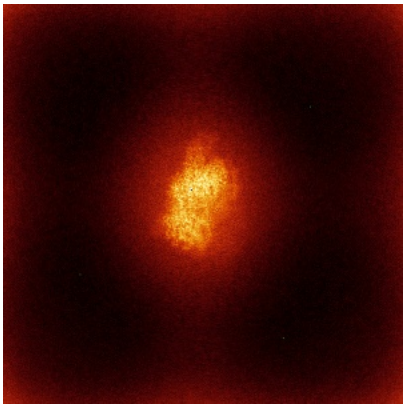
6.4.2 Raw map



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.

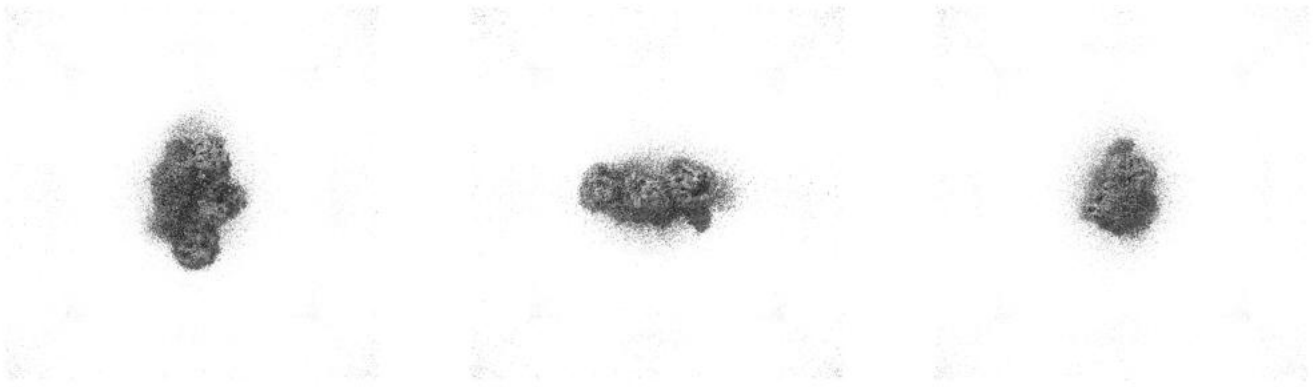
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

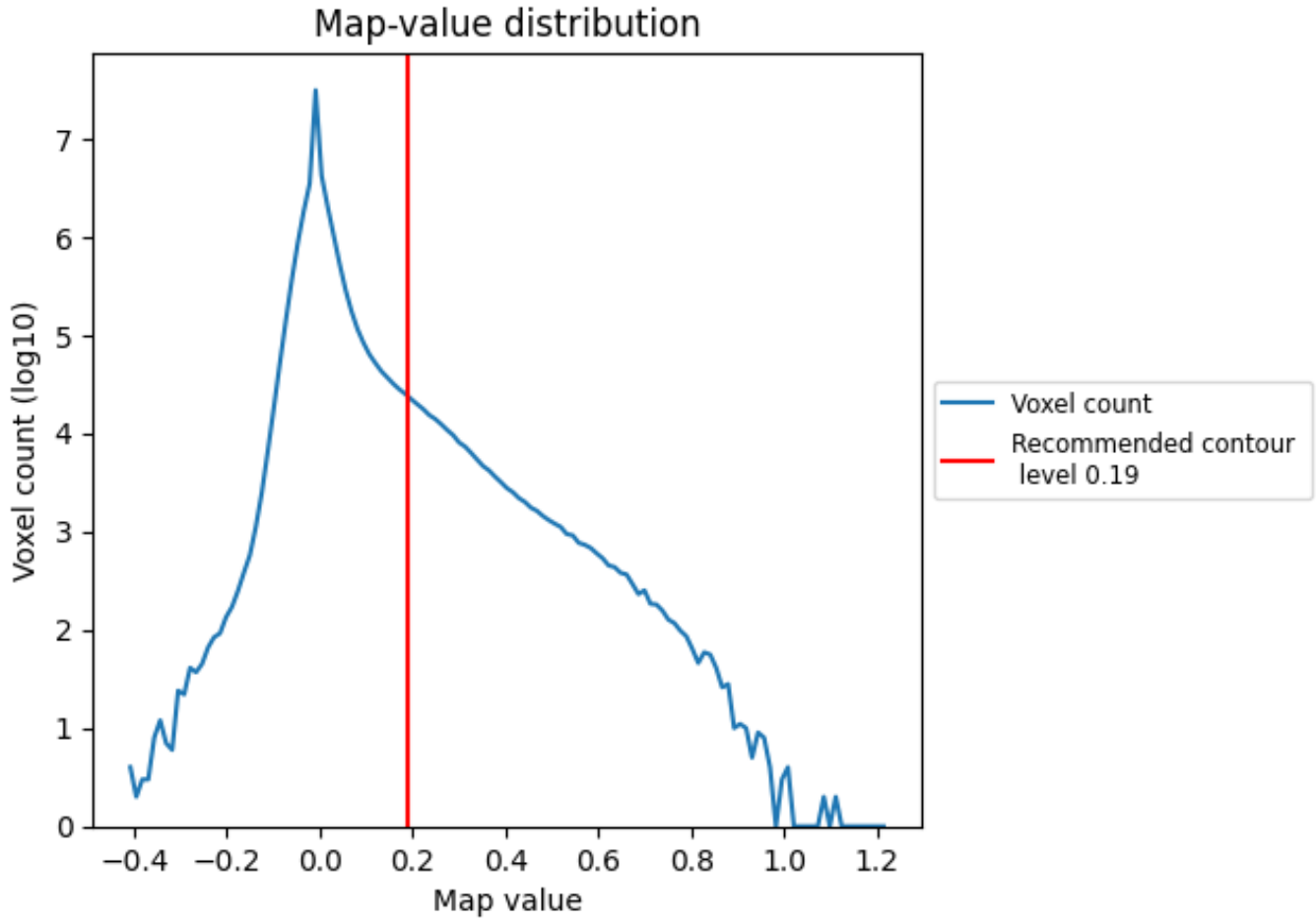
6.6 Mask visualisation (i)

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

7 Map analysis

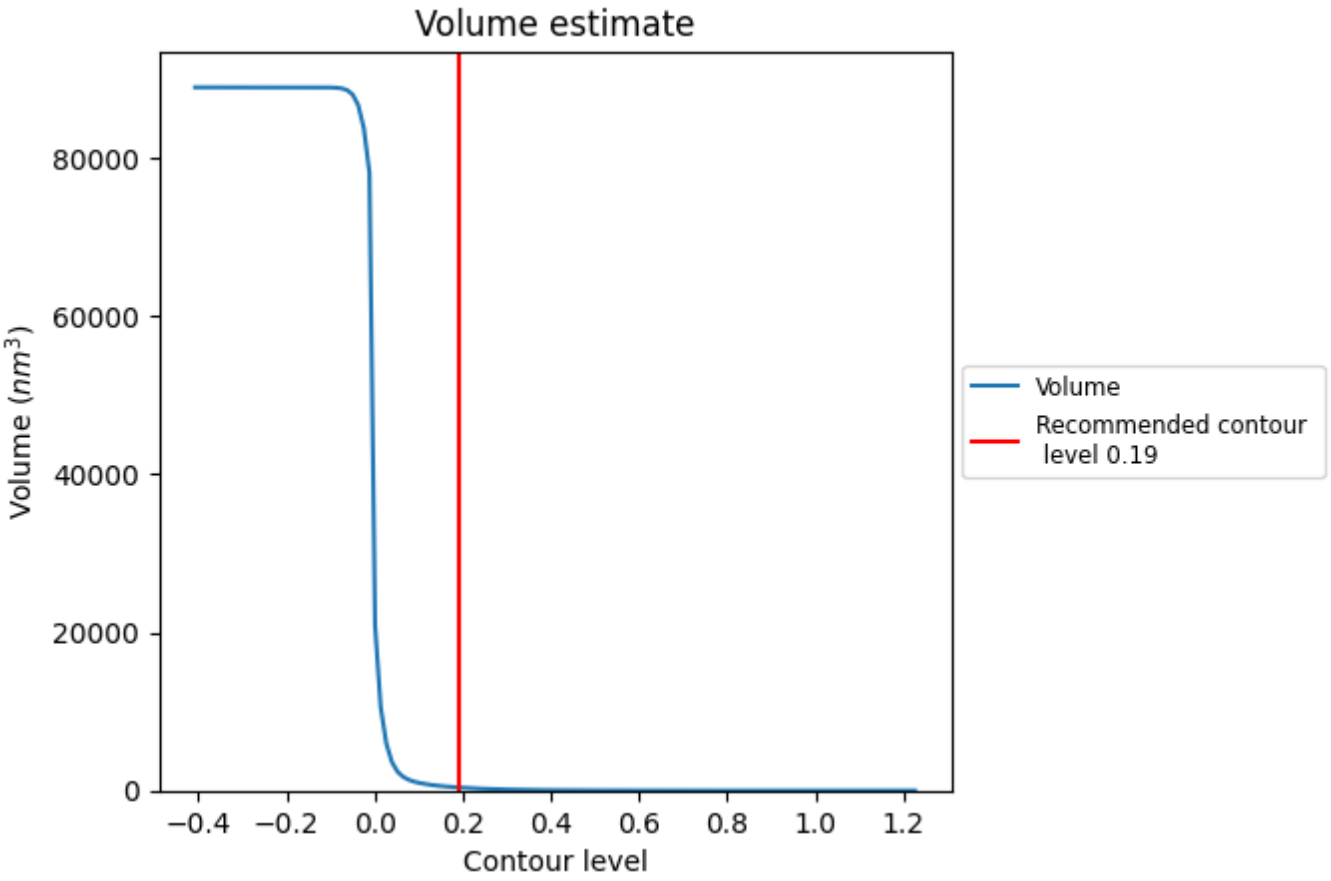
This section contains the results of statistical analysis of the map.

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.

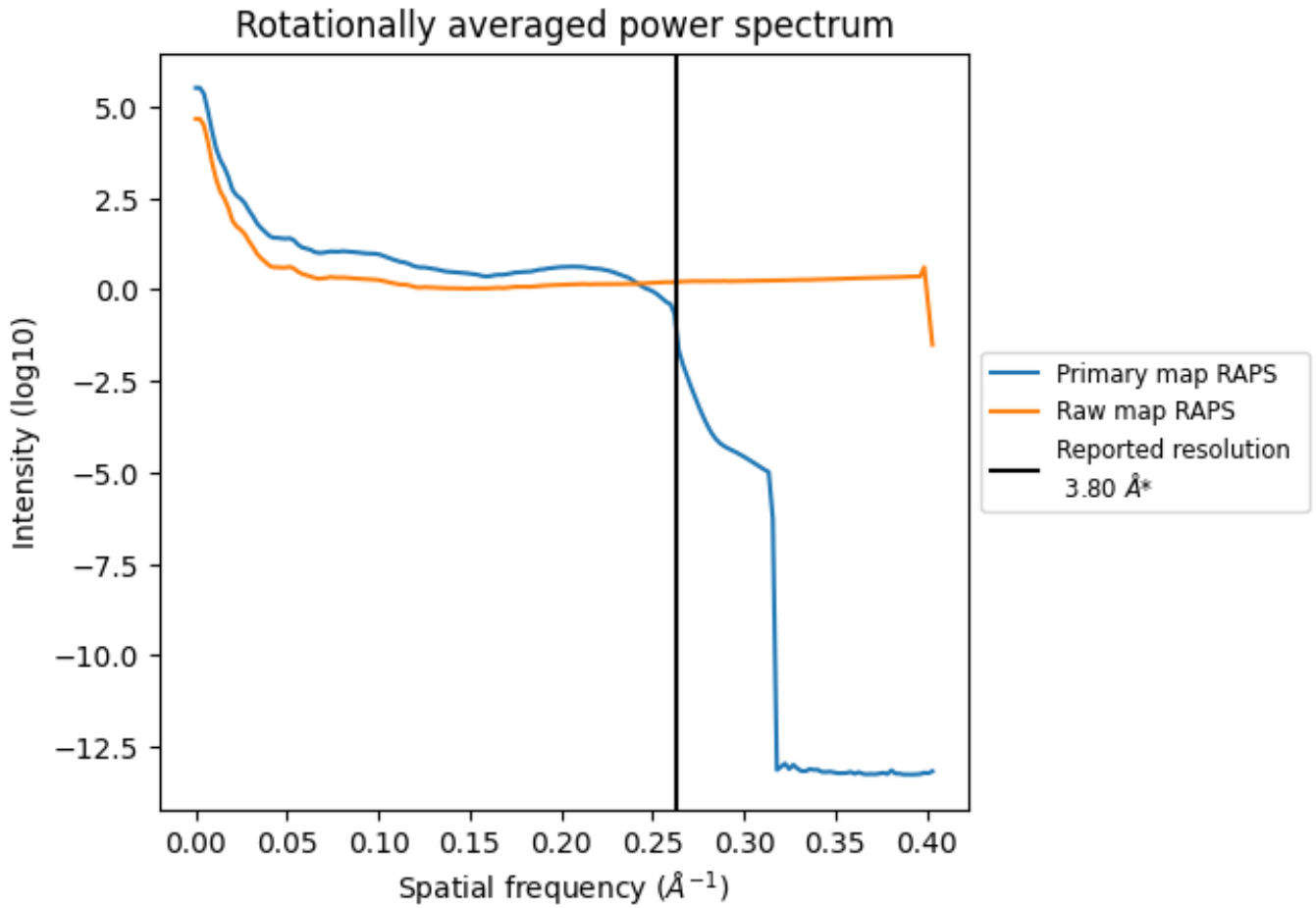
7.2 Volume estimate (i)



The volume at the recommended contour level is 390 nm^3; this corresponds to an approximate mass of 353 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)

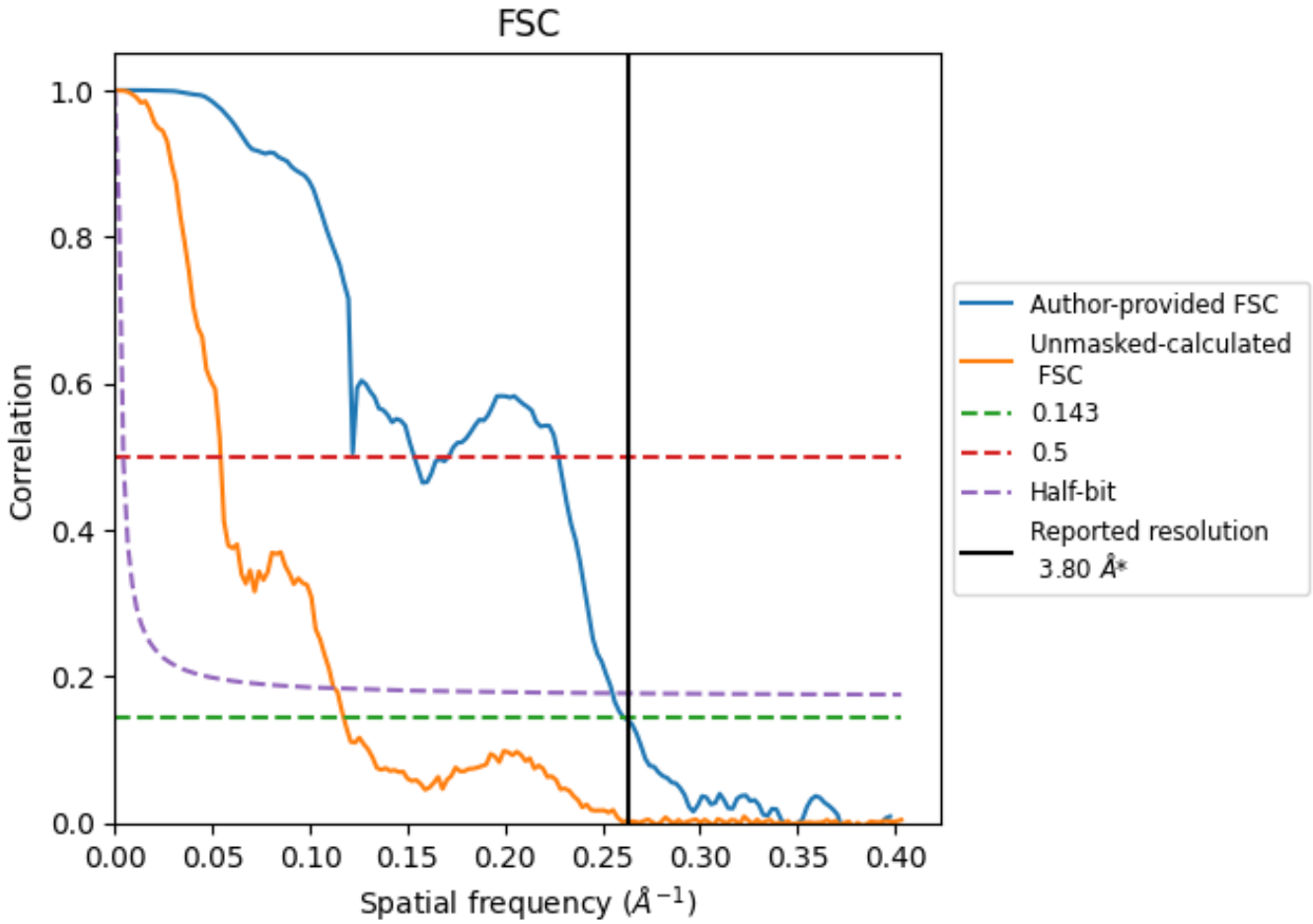


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

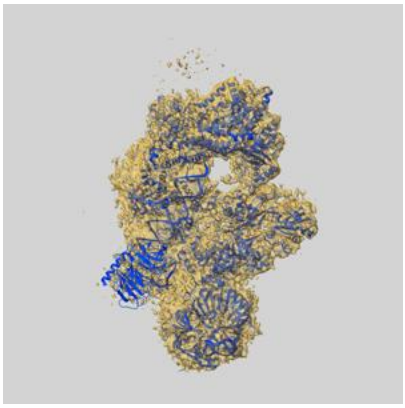
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	6.51	3.92
Unmasked-calculated*	8.52	18.42	8.87

*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 8.52 differs from the reported value 3.8 by more than 10 %

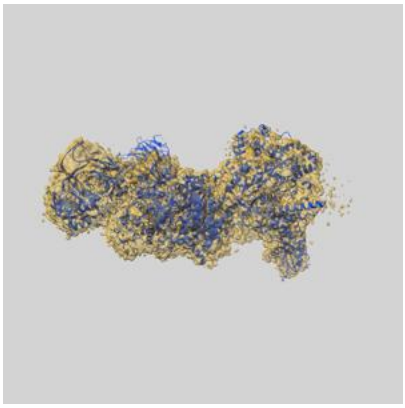
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18234 and PDB model 8Q7V. Per-residue inclusion information can be found in section 3 on page 8.

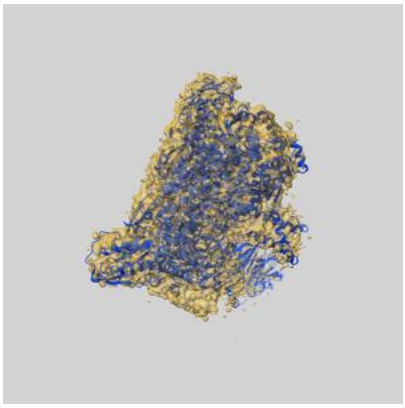
9.1 Map-model overlay



X



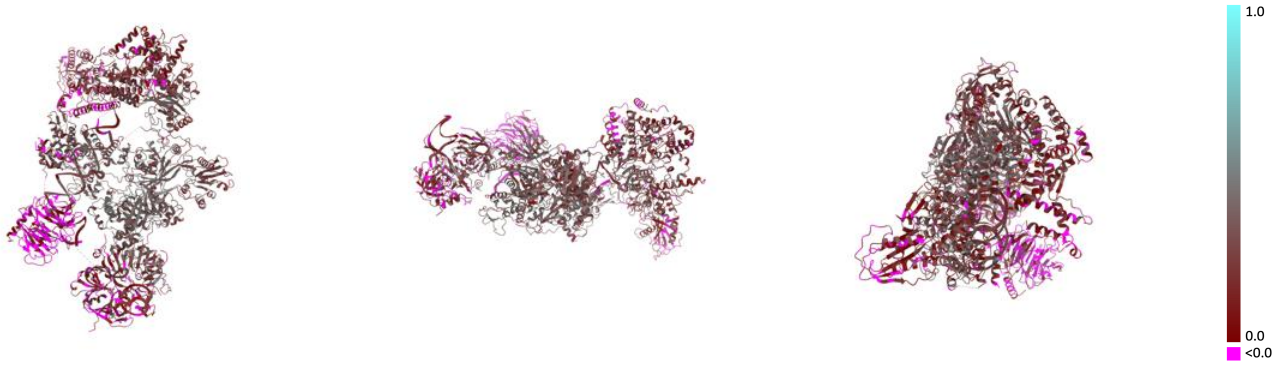
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

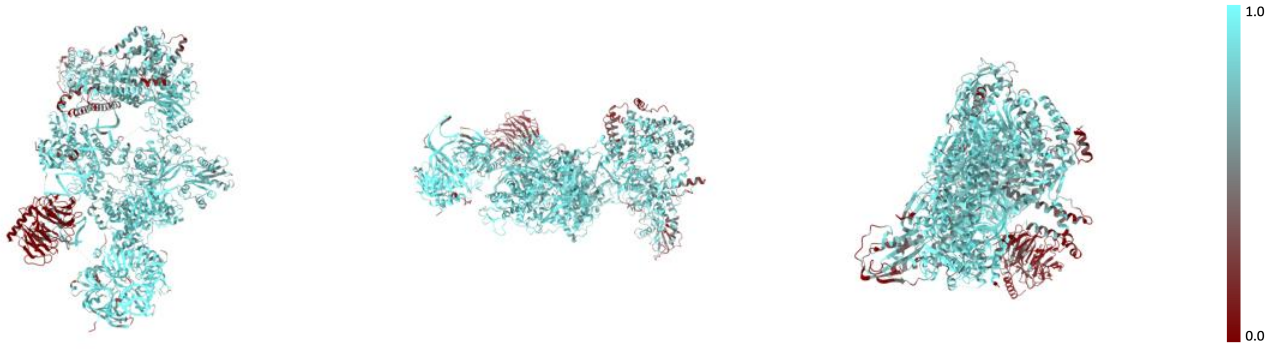
9.2 Q-score mapped to coordinate model (i)



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.

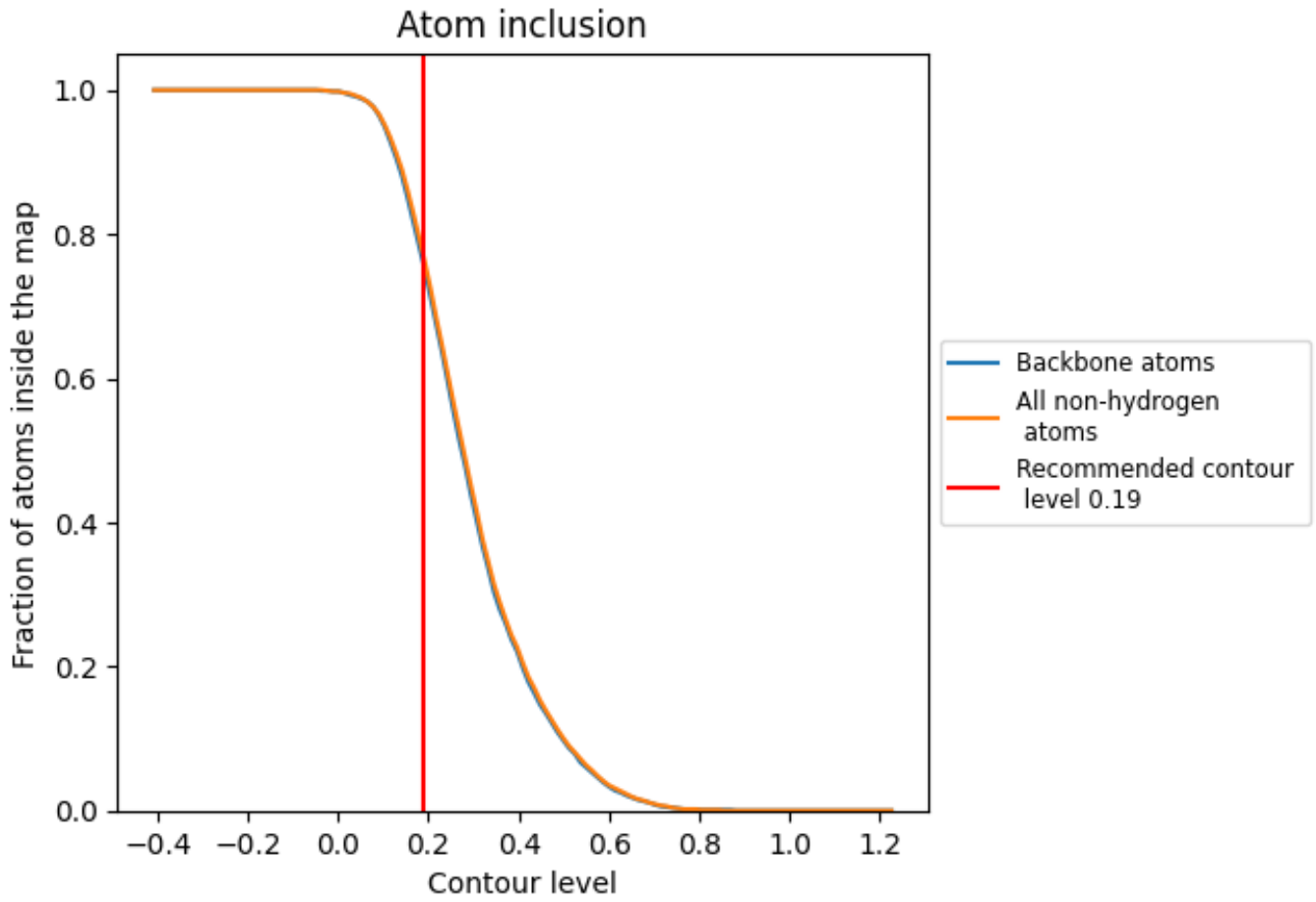
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 77% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.2520
5	0.9090	0.2160
A	0.7620	0.2550
B	0.5460	0.2160
C	0.8570	0.3580
D	0.1070	-0.0250
F	0.5560	0.1250
G	0.6670	0.1790
H	0.1360	0.0850
a	0.8730	0.1390
b	0.8780	0.2400
c	0.7600	0.0970
d	0.8550	0.3190
e	0.9320	0.1190
f	0.8740	0.1110
g	0.9310	0.2850