wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 08:17 pm GMT

PDB ID	:	6RBD
EMDB ID	:	EMD-4792
Title	:	State 1 of yeast Tsr1-TAP Rps20-Deltaloop pre-40S particles
Authors	:	Shayan, R.; Mitterer, V.; Ferreira-Cerca, S.; Murat, G.; Enne, T.; Rinaldi, D.; Weigl, S.; Omanic, H.; Gleizes, P.E.; Kressler, D.; Pertschy, B.; Plisson-Chastang, C.
Deposited on	:	2019-04-10
Resolution	:	3.47 Å(reported)
Based on initial models	:	6FAI, ?, 6EML

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

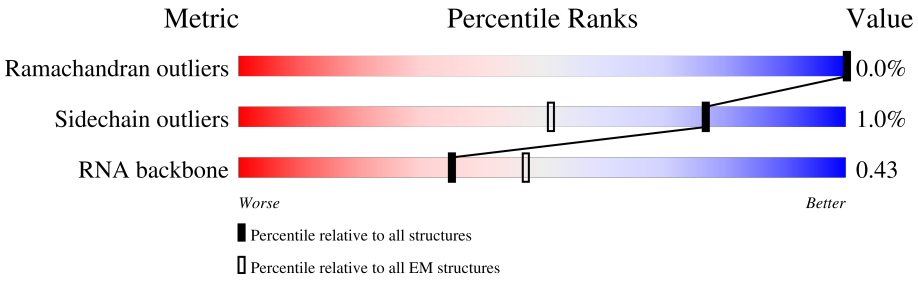
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.47 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)
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	b	82	98%
2	e	63	8%, 75%, 24%
3	2	1801	6%, 60%, 34%
4	A	252	81%, 18%
5	B	255	84%, 16%
6	C	254	84%, 15%
7	E	261	98%
8	G	236	98%

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Mol	Chain	Length	Quality of chain
9	H	190	97%
10	I	200	94% 6%
11	J	197	93% 6%
12	L	156	88% 10%
13	N	151	99%
14	V	87	100%
15	W	130	96%
16	X	145	6% 98%
17	Y	135	99%
18	c	67	15% 94% 6%
19	d	56	27% 62% 34%
20	h	274	66% 34%
21	i	483	7% 29% 71%
22	k	788	75% 23%
23	l	425	13% 63% 36%
24	y	318	14% 47% 52%
25	F	225	6% 91% 8%
26	M	143	35% 86% 13%
27	O	137	93% 7%
28	P	142	11% 80% 20%
29	Q	143	5% 89% 11%
30	R	136	38% 91% 8%
31	S	146	10% 71% 29%
32	T	144	5% 98%
33	Z	108	57% 42%

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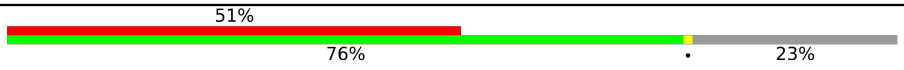
Mol	Chain	Length	Quality of chain
34	D	240	
35	U	121	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 81048 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 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	81	610	382	110	113	5	0	0

- Molecule 2 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	e	48	384	242	81	59	2	0	0

- Molecule 3 is a RNA chain called 20S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	1777	37868	16929	6704	12458	1777	0	0

- Molecule 4 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	206	1611	1036	285	288	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP P32905

- Molecule 5 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	214	1709	1084	310	311	4	0	0

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 7 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1873	1172	366	332	3		

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	H	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 14 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 15 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 18 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 19 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	37	Total	C	N	O	S	0	0
			302	186	62	50	4		

- Molecule 20 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 21 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	139	Total	C	N	O	S	0	0
			1116	731	181	202	2		

- Molecule 22 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	605	Total	C	N	O	S	0	0
			4860	3112	849	885	14		

- Molecule 23 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	271	Total	C	N	O	S	0	0
			2199	1390	385	407	17		

- Molecule 24 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	154	Total	C	N	O	S	0	0
			1245	788	223	225	9		

- Molecule 25 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	125	Total	C	N	O	S	0	0
			941	591	166	182	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	127	Total	C	N	O	S	0	0
			926	569	185	169	3		

- Molecule 28 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	114	Total	C	N	O	S	0	0
			902	574	166	155	7		

- Molecule 29 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Q	127	Total	C	N	O	0	0
			993	640	177	176		

- Molecule 30 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 31 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	104	Total	C	N	O	S	0	0
			840	528	154	156	2		

- Molecule 32 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 33 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	63	Total	C	N	O	0	0
			512	328	94	90		

- Molecule 34 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	185	Total	C	N	O	S	0	0
			1442	911	266	259	6		

- Molecule 35 is a protein called 40S ribosomal protein S20.

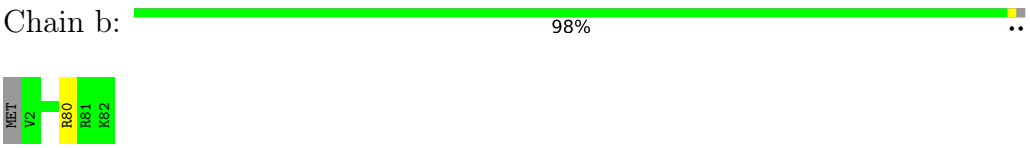
Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	82	Total	C	N	O	S	0	0
			674	431	123	119	1		

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.

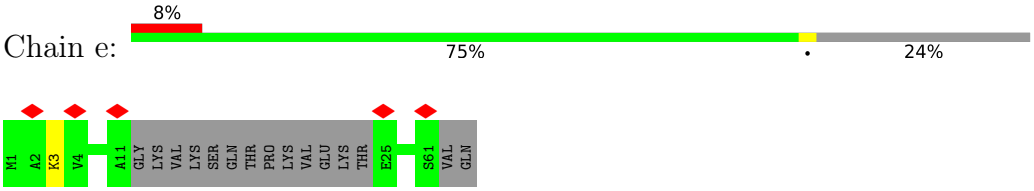
• Molecule 1: 40S ribosomal protein S27-A

Chain b:



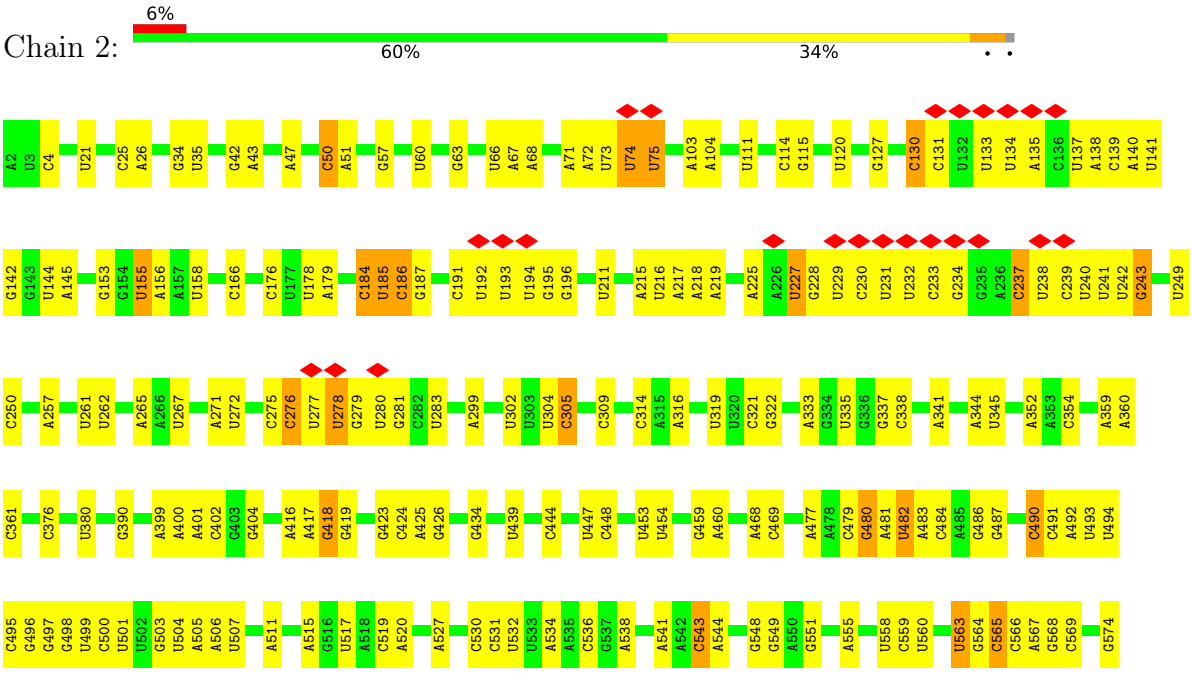
• Molecule 2: 40S ribosomal protein S30-A

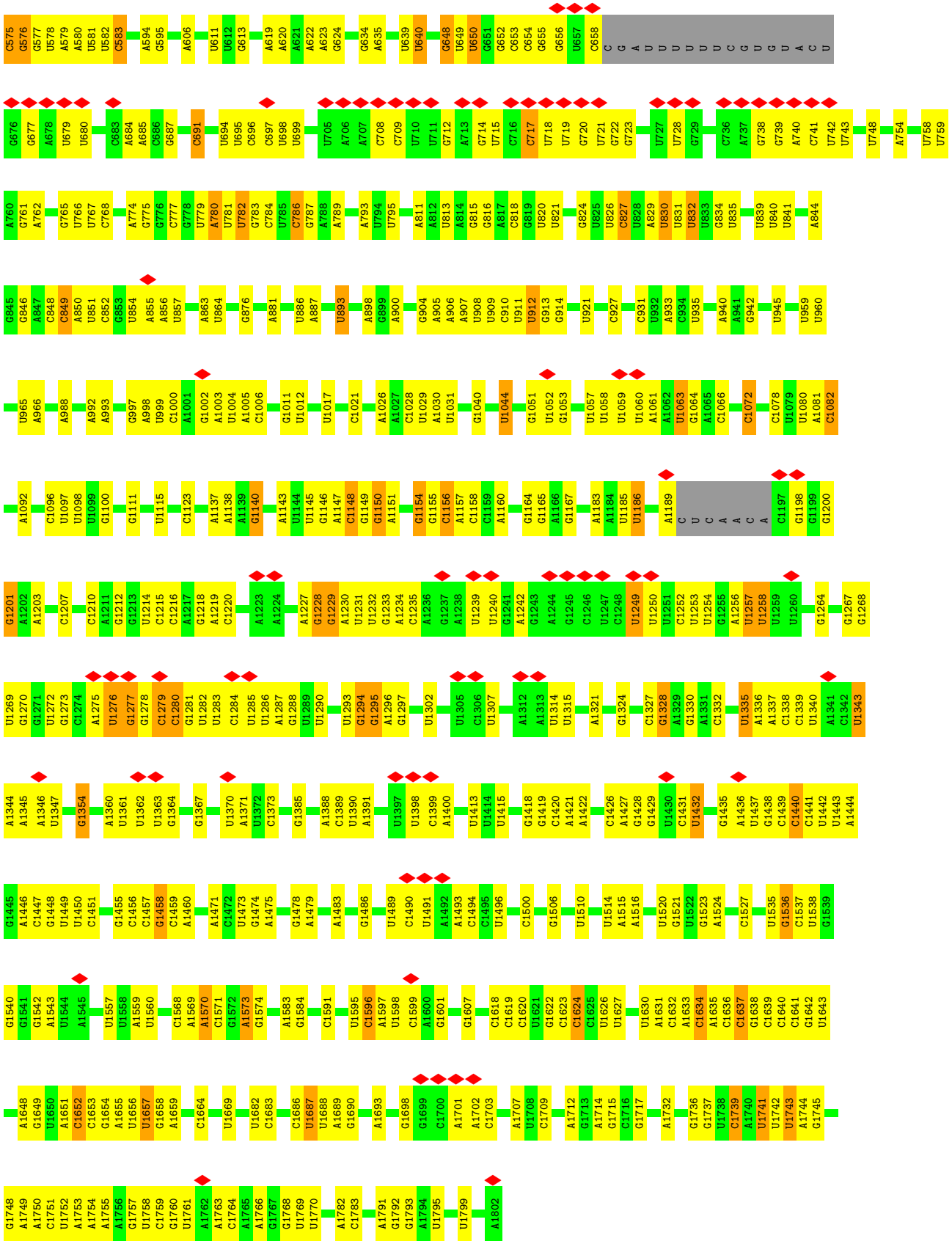
Chain e:



• Molecule 3: 20S ribosomal RNA

Chain 2:



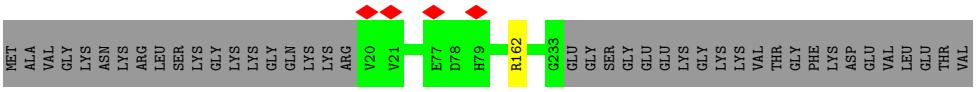


• Molecule 4: 40S ribosomal protein S0-A

Chain A:

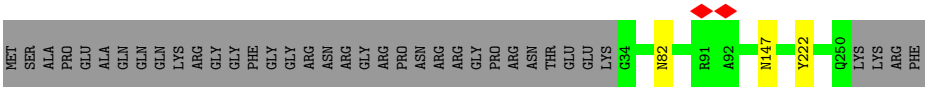
• Molecule 5: 40S ribosomal protein S1-A

Chain B:



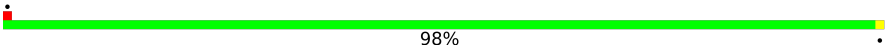
• Molecule 6: 40S ribosomal protein S2

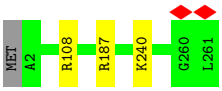
Chain C:



• Molecule 7: 40S ribosomal protein S4-A

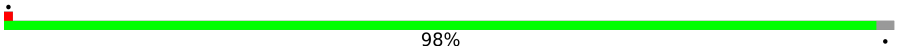
Chain E:

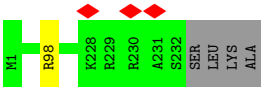




• Molecule 8: 40S ribosomal protein S6-A

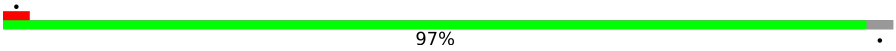
Chain G:

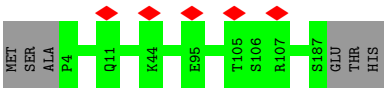




• Molecule 9: 40S ribosomal protein S7-A

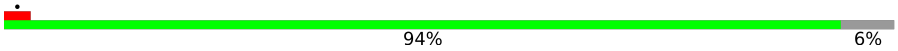
Chain H:

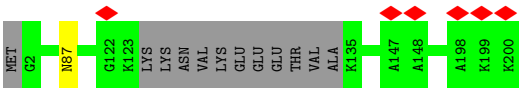




• Molecule 10: 40S ribosomal protein S8-A

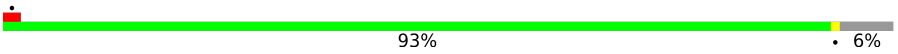
Chain I:

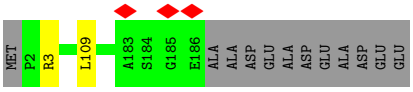




• Molecule 11: 40S ribosomal protein S9-A

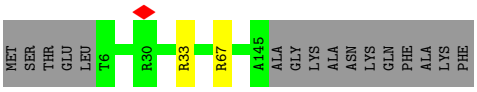
Chain J:





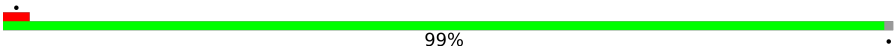
• Molecule 12: 40S ribosomal protein S11-A

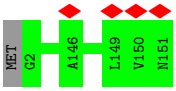
Chain L:



• Molecule 13: 40S ribosomal protein S13

Chain N:





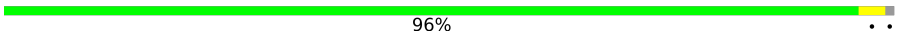
• Molecule 14: 40S ribosomal protein S21-A

Chain V:

There are no outlier residues recorded for this chain.

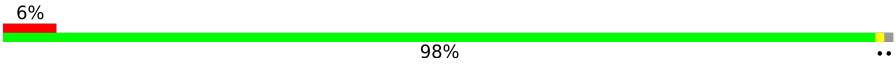
• Molecule 15: 40S ribosomal protein S22-A

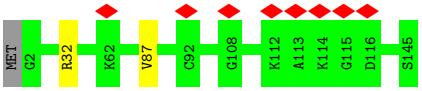
Chain W:



• Molecule 16: 40S ribosomal protein S23-A

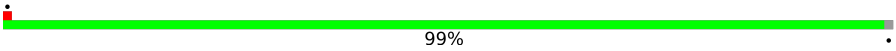
Chain X:





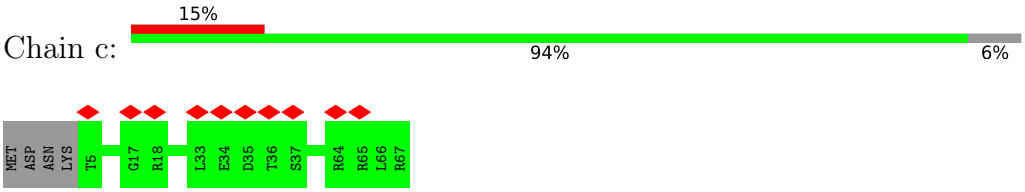
• Molecule 17: 40S ribosomal protein S24-A

Chain Y:



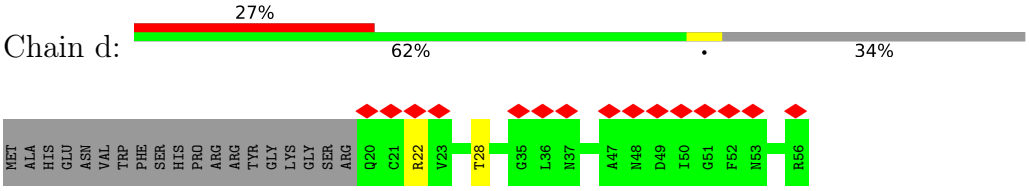
• Molecule 18: 40S ribosomal protein S28-A

Chain c:



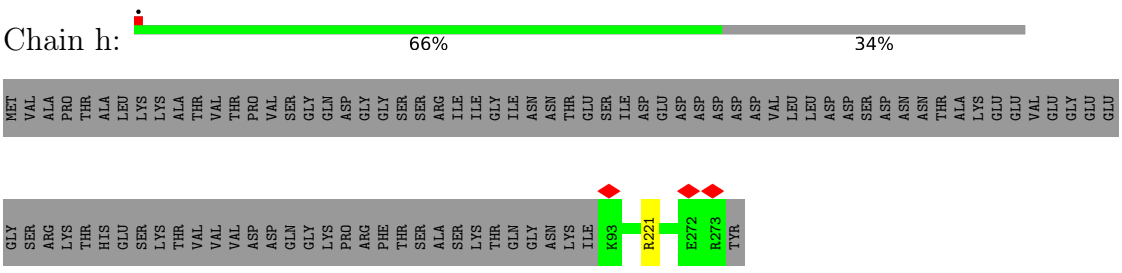
• Molecule 19: 40S ribosomal protein S29-A

Chain d:



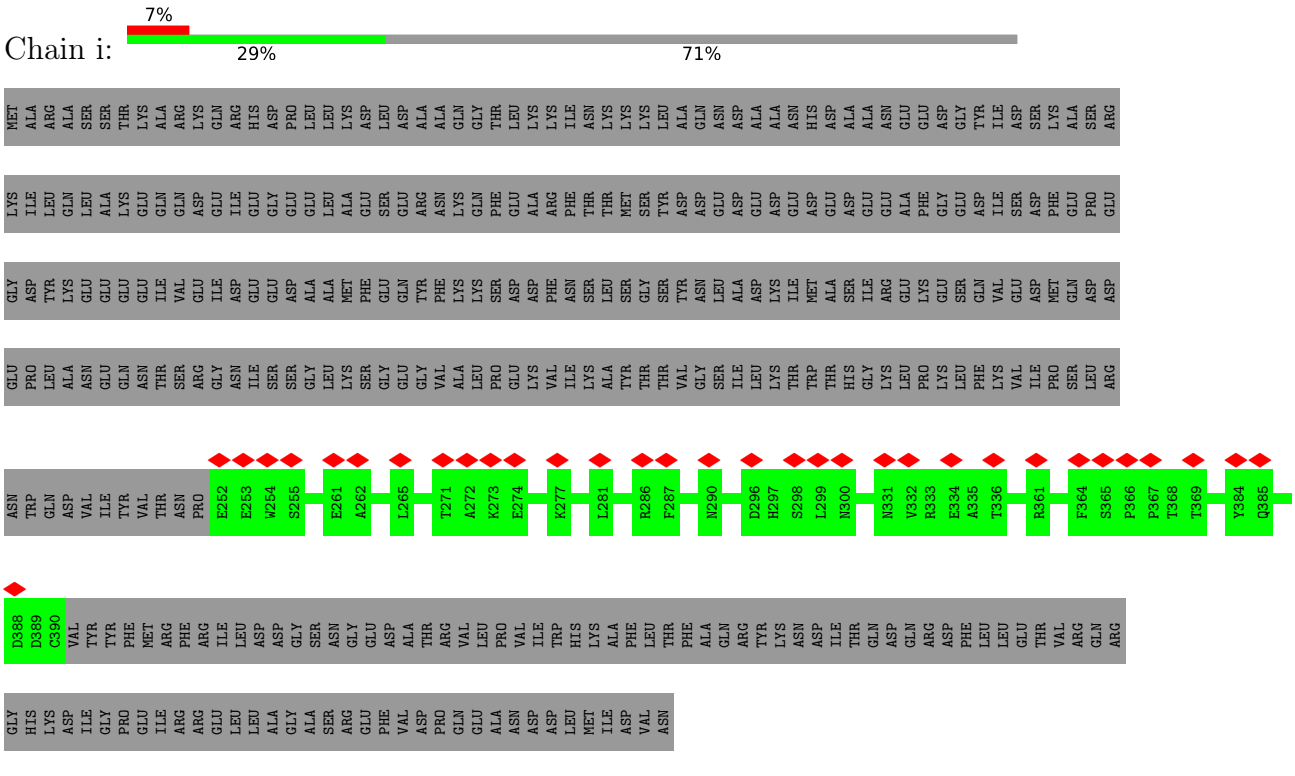
• Molecule 20: Pre-rRNA-processing protein PNO1

Chain h:



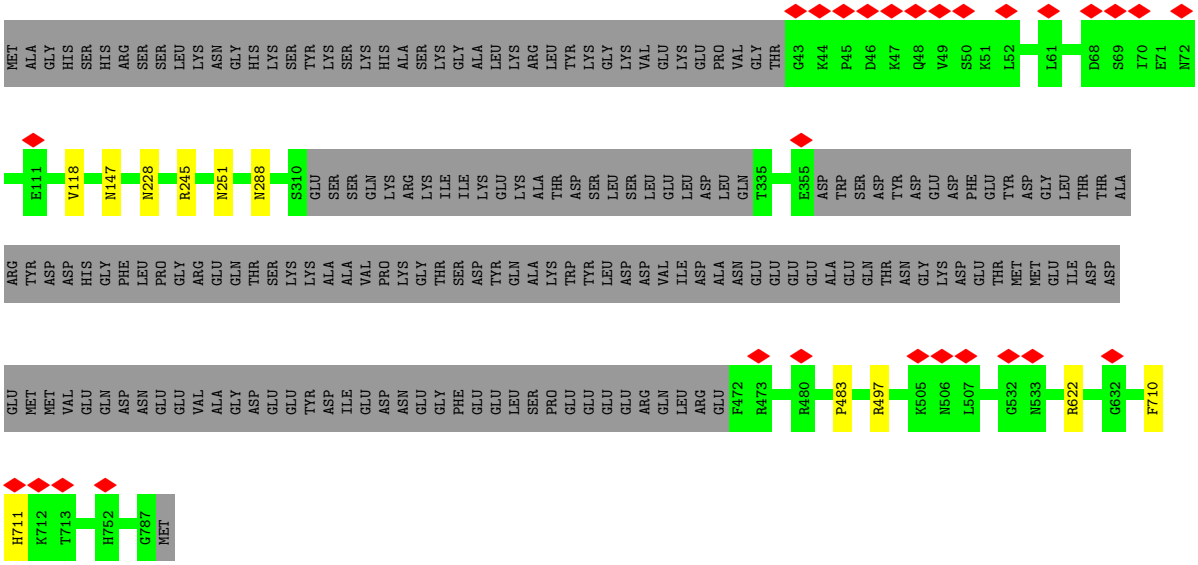
• Molecule 21: Essential nuclear protein 1

Chain i:



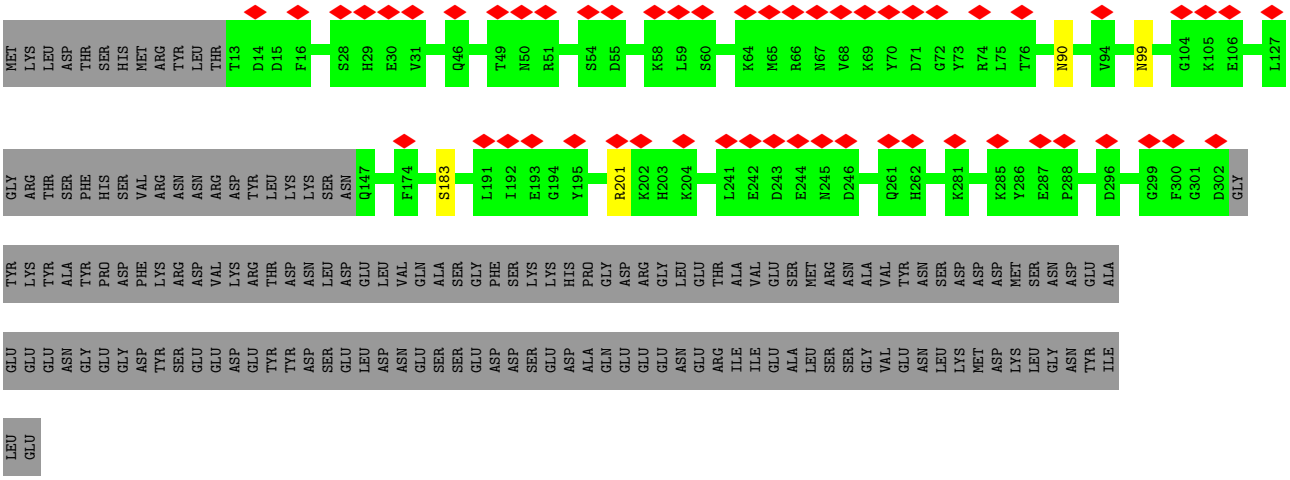
• Molecule 22: Ribosome biogenesis protein TSR1

Chain k:



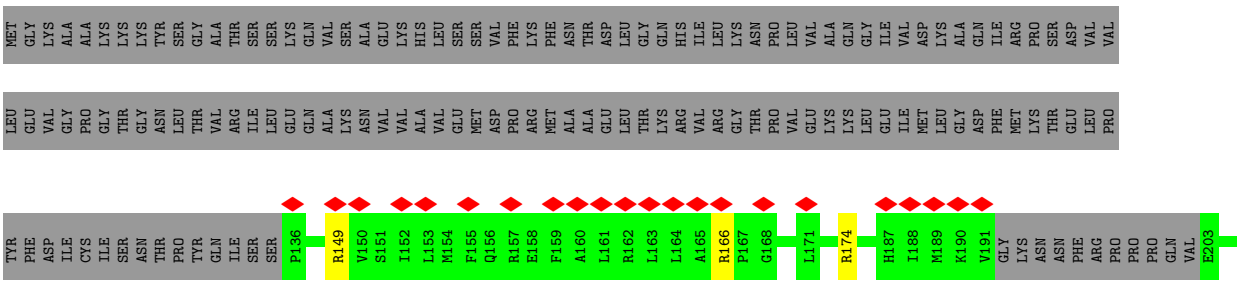
• Molecule 23: Serine/threonine-protein kinase RIO2

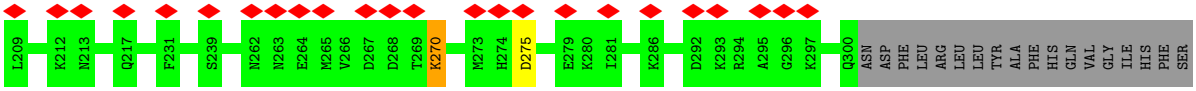
Chain l:



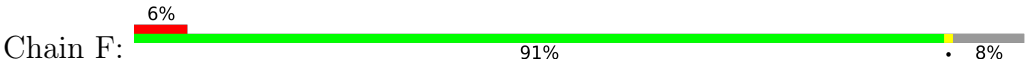
• Molecule 24: Dimethyladenosine transferase

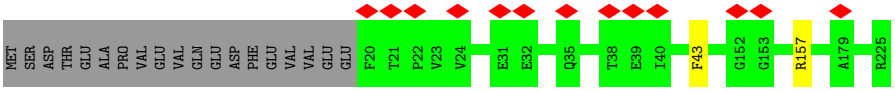
Chain y:



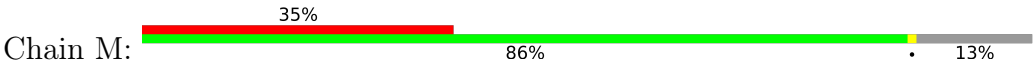


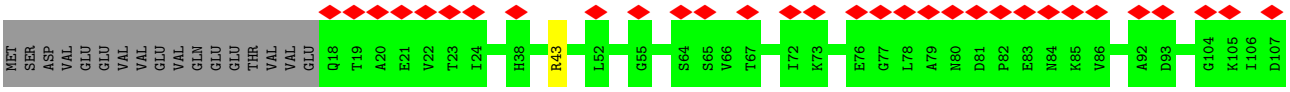
• Molecule 25: 40S ribosomal protein S5

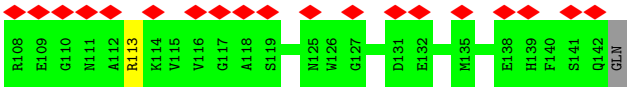




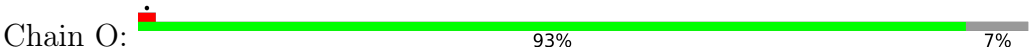
• Molecule 26: 40S ribosomal protein S12

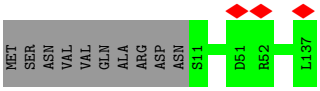




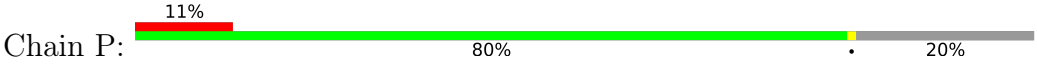


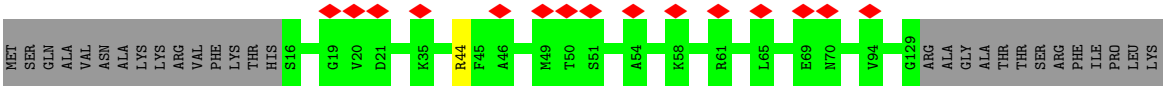
• Molecule 27: 40S ribosomal protein S14-A



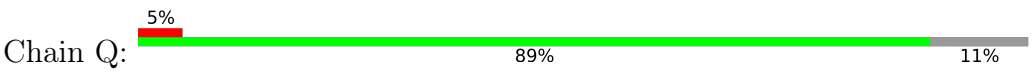


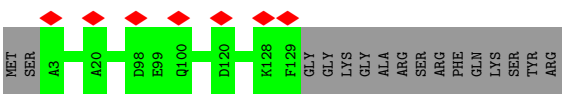
• Molecule 28: 40S ribosomal protein S15



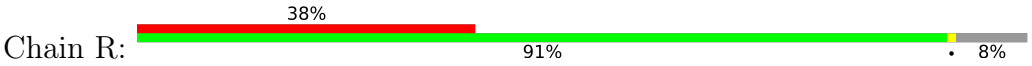


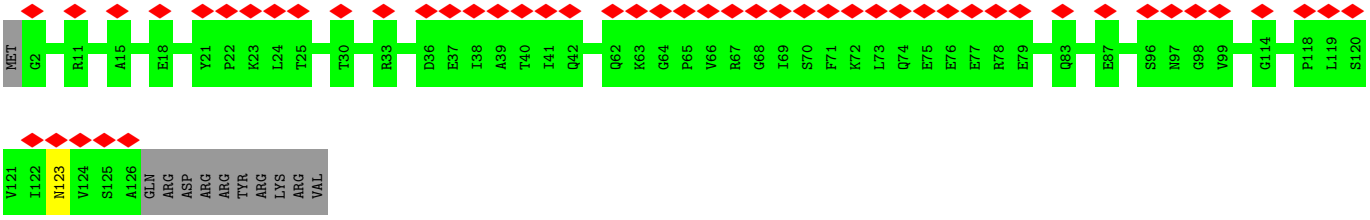
• Molecule 29: 40S ribosomal protein S16-A



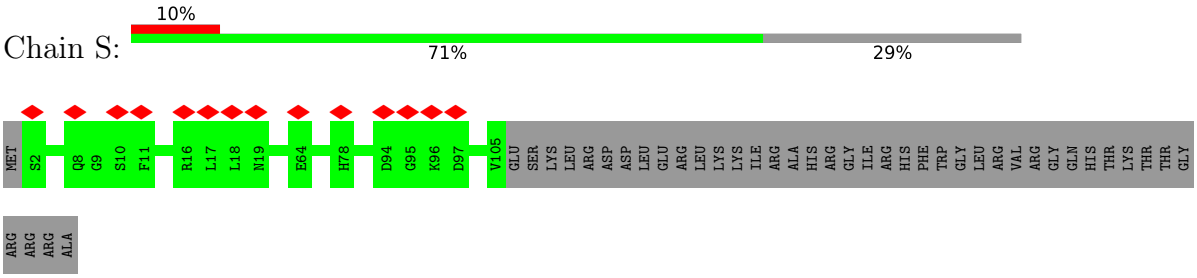


• Molecule 30: 40S ribosomal protein S17-A

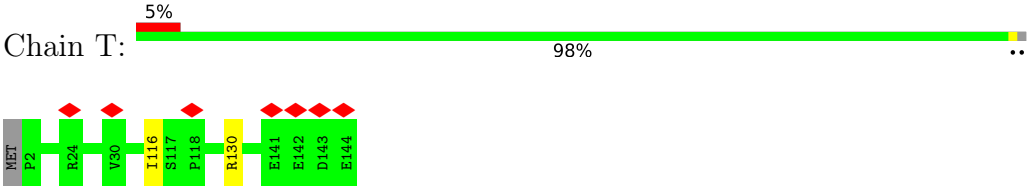




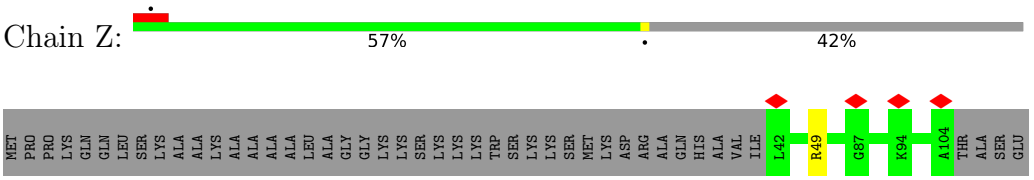
• Molecule 31: 40S ribosomal protein S18-A



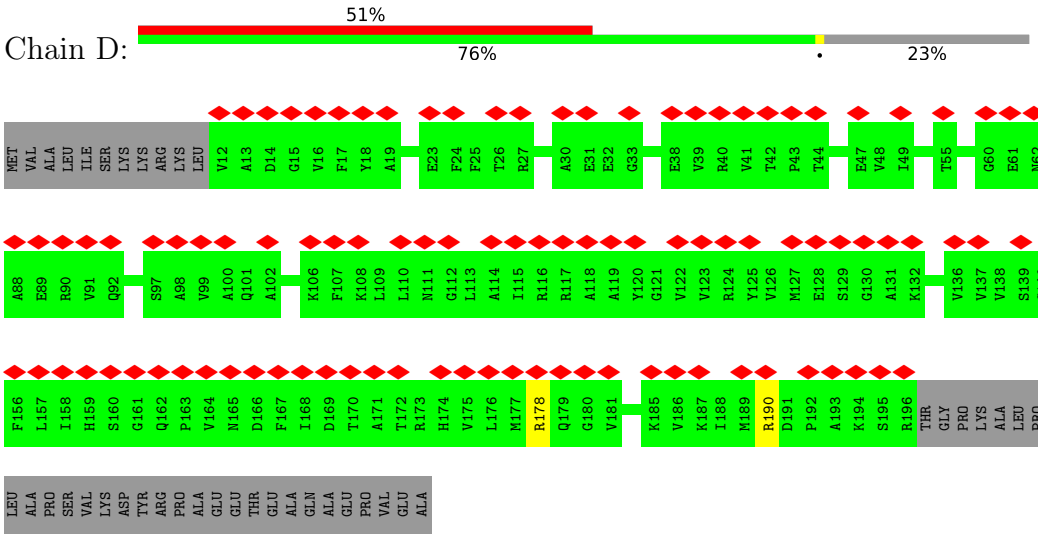
• Molecule 32: 40S ribosomal protein S19-A



• Molecule 33: 40S ribosomal protein S25-A

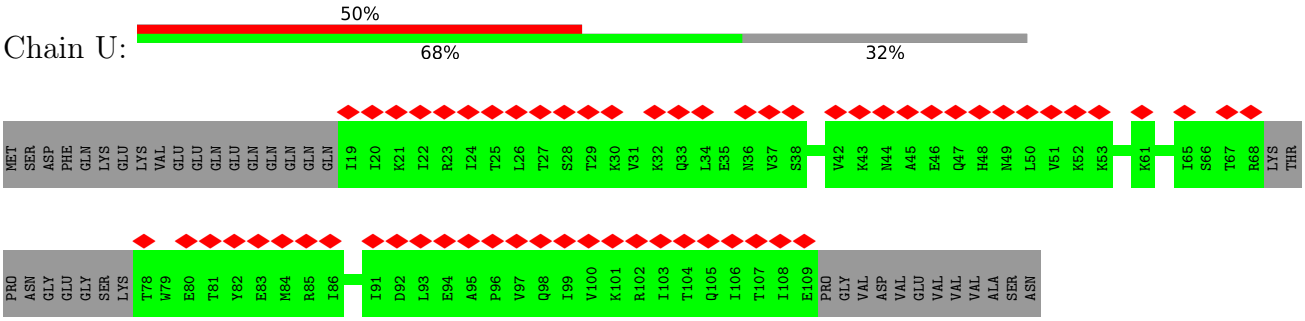


• Molecule 34: 40S ribosomal protein S3



• Molecule 35: 40S ribosomal protein S20

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54130	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 ($e^-/Å^2$)	32.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	b	0.32	0/620	0.55	0/838
2	e	0.37	0/390	0.62	0/517
3	2	0.58	0/42353	1.19	375/65990 (0.6%)
4	A	0.36	0/1653	0.56	1/2261 (0.0%)
5	B	0.33	0/1735	0.59	0/2335
6	C	0.36	0/1665	0.57	0/2263
7	E	0.40	0/2109	0.59	0/2839
8	G	0.35	0/1897	0.52	0/2532
9	H	0.31	0/1506	0.53	0/2028
10	I	0.40	0/1514	0.56	0/2021
11	J	0.37	0/1519	0.57	1/2035 (0.0%)
12	L	0.43	0/1155	0.56	0/1557
13	N	0.33	0/1215	0.55	0/1638
14	V	0.39	0/693	0.53	0/935
15	W	0.43	0/1038	0.63	0/1395
16	X	0.40	0/1139	0.59	0/1518
17	Y	0.39	0/1087	0.54	0/1449
18	c	0.27	0/499	0.57	0/670
19	d	0.27	0/305	0.51	0/401
20	h	0.30	0/1462	0.53	0/1969
21	i	0.29	0/1145	0.54	0/1556
22	k	0.31	0/4970	0.53	0/6718
23	l	0.29	0/2243	0.56	0/3014
24	y	0.28	0/1265	0.58	0/1702
25	F	0.28	0/1629	0.55	0/2202
26	M	0.28	0/949	0.55	0/1284
27	O	0.31	0/937	0.53	0/1261
28	P	0.28	0/921	0.51	0/1237
29	Q	0.30	0/1011	0.58	0/1362
30	R	0.27	0/1010	0.55	0/1355
31	S	0.28	0/853	0.55	0/1154
32	T	0.30	0/1130	0.52	1/1517 (0.1%)
33	Z	0.45	0/519	0.77	0/696
34	D	0.30	0/1459	0.56	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
35	U	0.26	0/681	0.49	0/917
All	All	0.47	0/86276	0.95	378/125123 (0.3%)

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
22	k	0	3
24	y	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2	1634	C	N1-C2-O2	13.79	127.17	118.90
3	2	1634	C	C2-N1-C1'	12.73	132.81	118.80
3	2	1148	C	N1-C2-O2	12.30	126.28	118.90
3	2	695	U	N1-C2-O2	12.00	131.20	122.80
3	2	1279	C	N1-C2-O2	11.69	125.91	118.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	k	118	VAL	Peptide
22	k	710	PHE	Peptide
22	k	711	HIS	Peptide
24	y	270	LYS	Peptide
24	y	275	ASP	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	b	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
2	e	44/63 (70%)	40 (91%)	4 (9%)	0	100	100
4	A	204/252 (81%)	189 (93%)	15 (7%)	0	100	100
5	B	212/255 (83%)	197 (93%)	15 (7%)	0	100	100
6	C	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
7	E	258/261 (99%)	249 (96%)	9 (4%)	0	100	100
8	G	230/236 (98%)	224 (97%)	6 (3%)	0	100	100
9	H	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
10	I	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
11	J	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
12	L	138/156 (88%)	136 (99%)	2 (1%)	0	100	100
13	N	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
14	V	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
15	W	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
16	X	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
17	Y	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
18	c	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
19	d	33/56 (59%)	29 (88%)	4 (12%)	0	100	100
20	h	179/274 (65%)	174 (97%)	5 (3%)	0	100	100
21	i	137/483 (28%)	133 (97%)	4 (3%)	0	100	100
22	k	597/788 (76%)	562 (94%)	34 (6%)	1 (0%)	47	80
23	l	267/425 (63%)	233 (87%)	33 (12%)	1 (0%)	34	70
24	y	150/318 (47%)	128 (85%)	22 (15%)	0	100	100
25	F	204/225 (91%)	195 (96%)	9 (4%)	0	100	100
26	M	123/143 (86%)	117 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	O	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
28	P	112/142 (79%)	108 (96%)	4 (4%)	0	100	100
29	Q	125/143 (87%)	120 (96%)	5 (4%)	0	100	100
30	R	123/136 (90%)	120 (98%)	3 (2%)	0	100	100
31	S	102/146 (70%)	92 (90%)	10 (10%)	0	100	100
32	T	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
33	Z	61/108 (56%)	60 (98%)	1 (2%)	0	100	100
34	D	179/240 (75%)	173 (97%)	6 (3%)	0	100	100
35	U	78/121 (64%)	76 (97%)	2 (3%)	0	100	100
All	All	5360/6890 (78%)	5072 (95%)	286 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	l	183	SER
22	k	483	PRO

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	b	70/71 (99%)	69 (99%)	1 (1%)	67	85
2	e	40/54 (74%)	39 (98%)	1 (2%)	47	74
4	A	171/210 (81%)	170 (99%)	1 (1%)	86	94
5	B	191/224 (85%)	190 (100%)	1 (0%)	88	95
6	C	176/205 (86%)	173 (98%)	3 (2%)	60	82
7	E	221/222 (100%)	218 (99%)	3 (1%)	67	85
8	G	198/201 (98%)	197 (100%)	1 (0%)	88	95
9	H	165/170 (97%)	165 (100%)	0	100	100
10	I	150/161 (93%)	149 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	J	158/166 (95%)	157 (99%)	1 (1%)	86 94
12	L	125/137 (91%)	123 (98%)	2 (2%)	62 82
13	N	127/128 (99%)	127 (100%)	0	100 100
14	V	74/74 (100%)	74 (100%)	0	100 100
15	W	110/111 (99%)	106 (96%)	4 (4%)	35 65
16	X	119/120 (99%)	117 (98%)	2 (2%)	60 82
17	Y	112/113 (99%)	112 (100%)	0	100 100
18	c	56/60 (93%)	56 (100%)	0	100 100
19	d	33/49 (67%)	31 (94%)	2 (6%)	18 50
20	h	158/238 (66%)	157 (99%)	1 (1%)	86 94
21	i	125/424 (30%)	125 (100%)	0	100 100
22	k	523/703 (74%)	516 (99%)	7 (1%)	69 86
23	l	246/384 (64%)	243 (99%)	3 (1%)	71 87
24	y	141/283 (50%)	137 (97%)	4 (3%)	43 72
25	F	173/191 (91%)	171 (99%)	2 (1%)	71 87
26	M	101/119 (85%)	99 (98%)	2 (2%)	55 79
27	O	91/105 (87%)	91 (100%)	0	100 100
28	P	95/118 (80%)	94 (99%)	1 (1%)	73 88
29	Q	107/119 (90%)	107 (100%)	0	100 100
30	R	113/124 (91%)	112 (99%)	1 (1%)	78 91
31	S	93/129 (72%)	93 (100%)	0	100 100
32	T	115/116 (99%)	114 (99%)	1 (1%)	78 91
33	Z	56/89 (63%)	55 (98%)	1 (2%)	59 81
34	D	149/195 (76%)	147 (99%)	2 (1%)	69 86
35	U	79/114 (69%)	79 (100%)	0	100 100
All	All	4661/5927 (79%)	4613 (99%)	48 (1%)	77 89

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	k	288	ASN
24	y	166	ARG
22	k	497	ARG

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Mol	Chain	Res	Type
23	l	99	ASN
24	y	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
16	X	48	HIS
25	F	104	ASN
20	h	131	ASN
25	F	103	ASN
31	S	87	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	1772/1801 (98%)	617 (34%)	17 (0%)

5 of 617 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	4	C
3	2	25	C
3	2	26	A
3	2	34	G
3	2	42	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	1570	A
3	2	1652	C
3	2	1150	G
3	2	1156	C
3	2	1229	G

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	D	2
3	2	2
22	k	1
19	d	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	52:ALA	C	53:THR	N	3.81
1	2	1377:U	O3'	1378:U	P	3.34
1	2	1219:A	O3'	1220:C	P	3.23
1	k	80:ASN	C	81:GLY	N	3.23
1	d	31:ILE	C	32:ARG	N	3.21

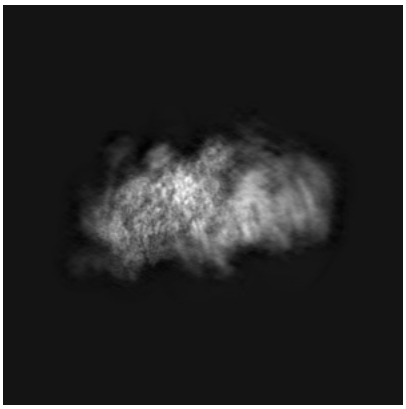
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4792. These allow visual inspection of the internal detail of the map and identification of artifacts.

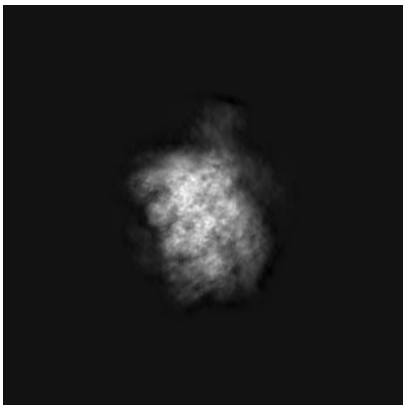
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

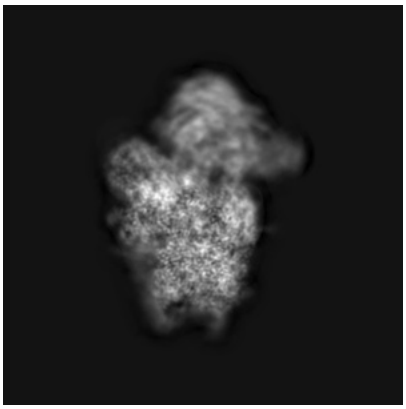
6.1.1 Primary map



X

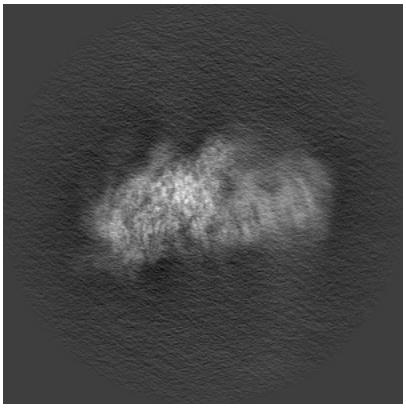


Y

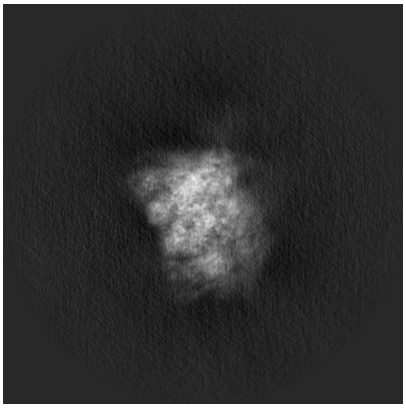


Z

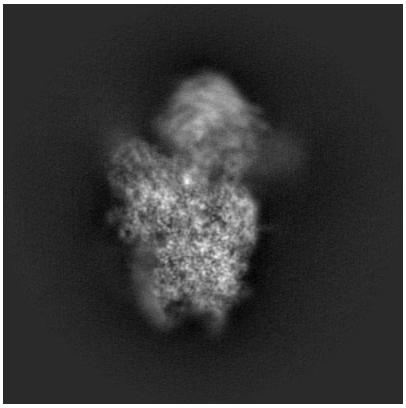
6.1.2 Raw map



X



Y

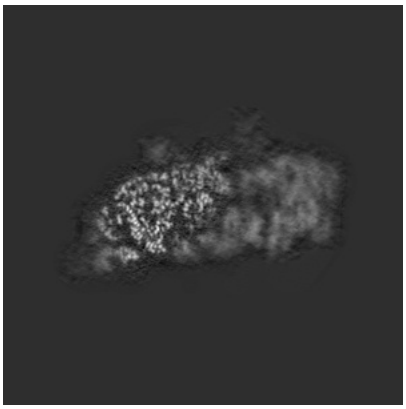


Z

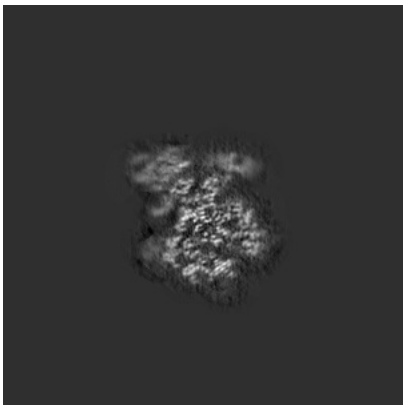
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

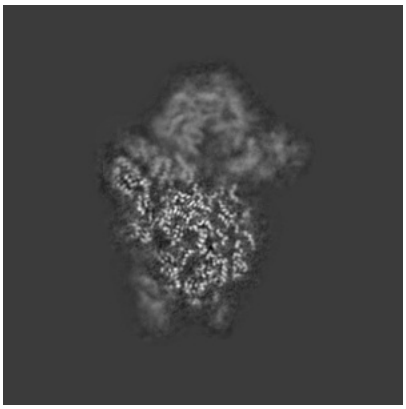
6.2.1 Primary map



X Index: 192

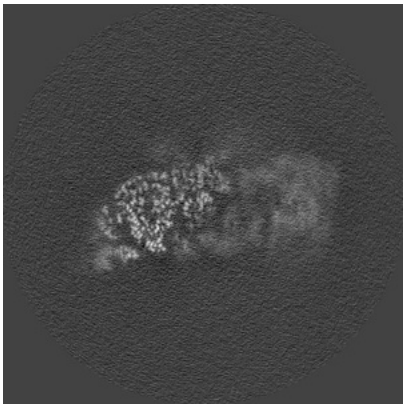


Y Index: 192

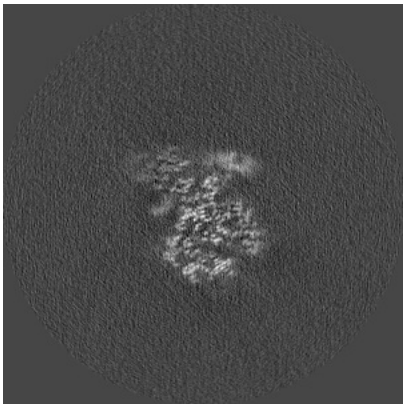


Z Index: 192

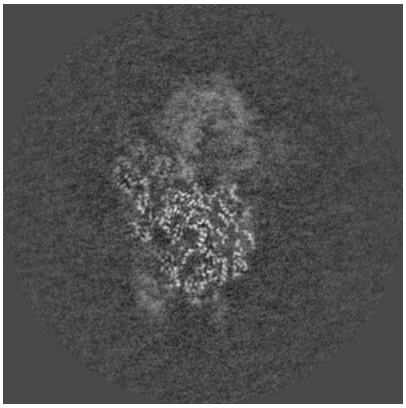
6.2.2 Raw map



X Index: 192



Y Index: 192

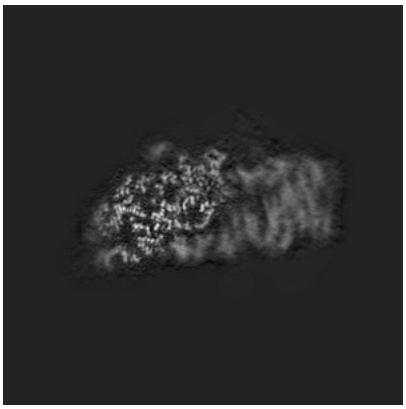


Z Index: 192

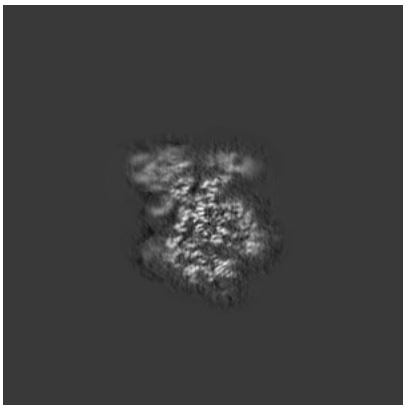
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

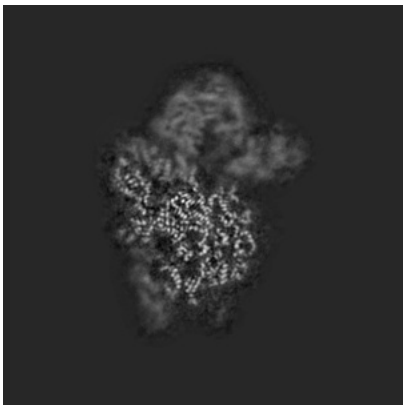
6.3.1 Primary map



X Index: 188

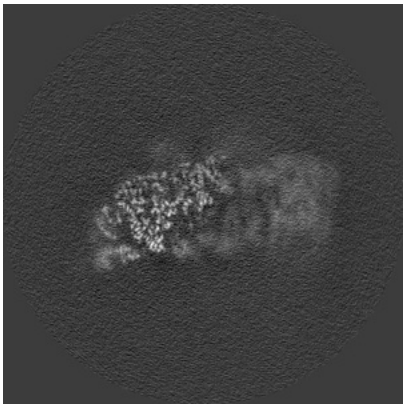


Y Index: 191

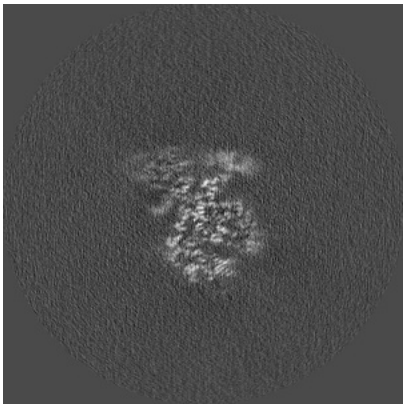


Z Index: 194

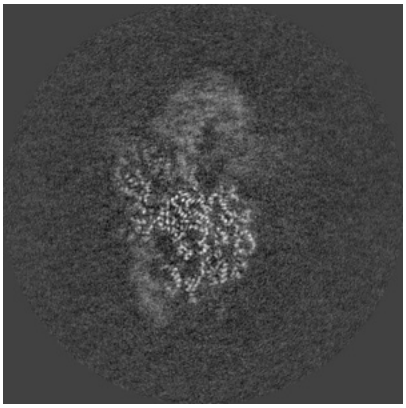
6.3.2 Raw map



X Index: 191



Y Index: 191

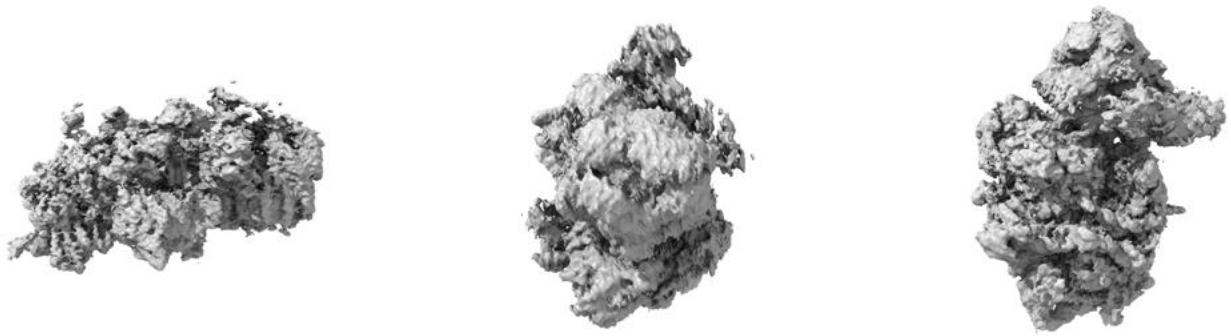


Z Index: 194

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

6.4 Orthogonal surface views (i)

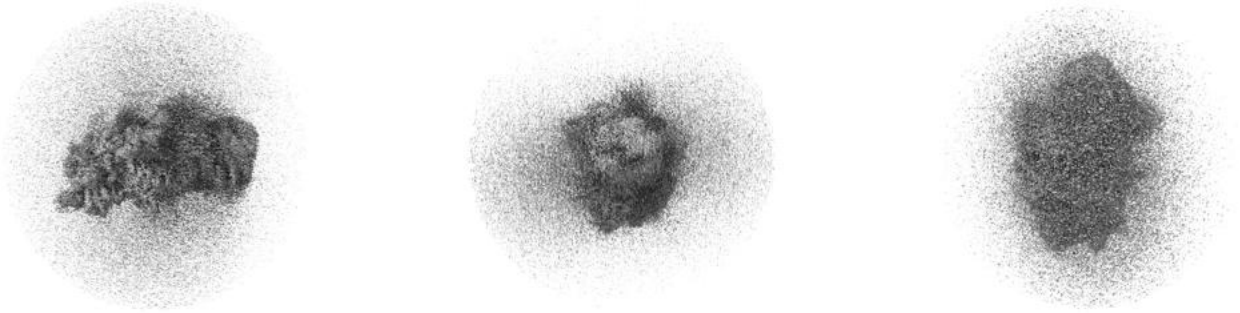
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

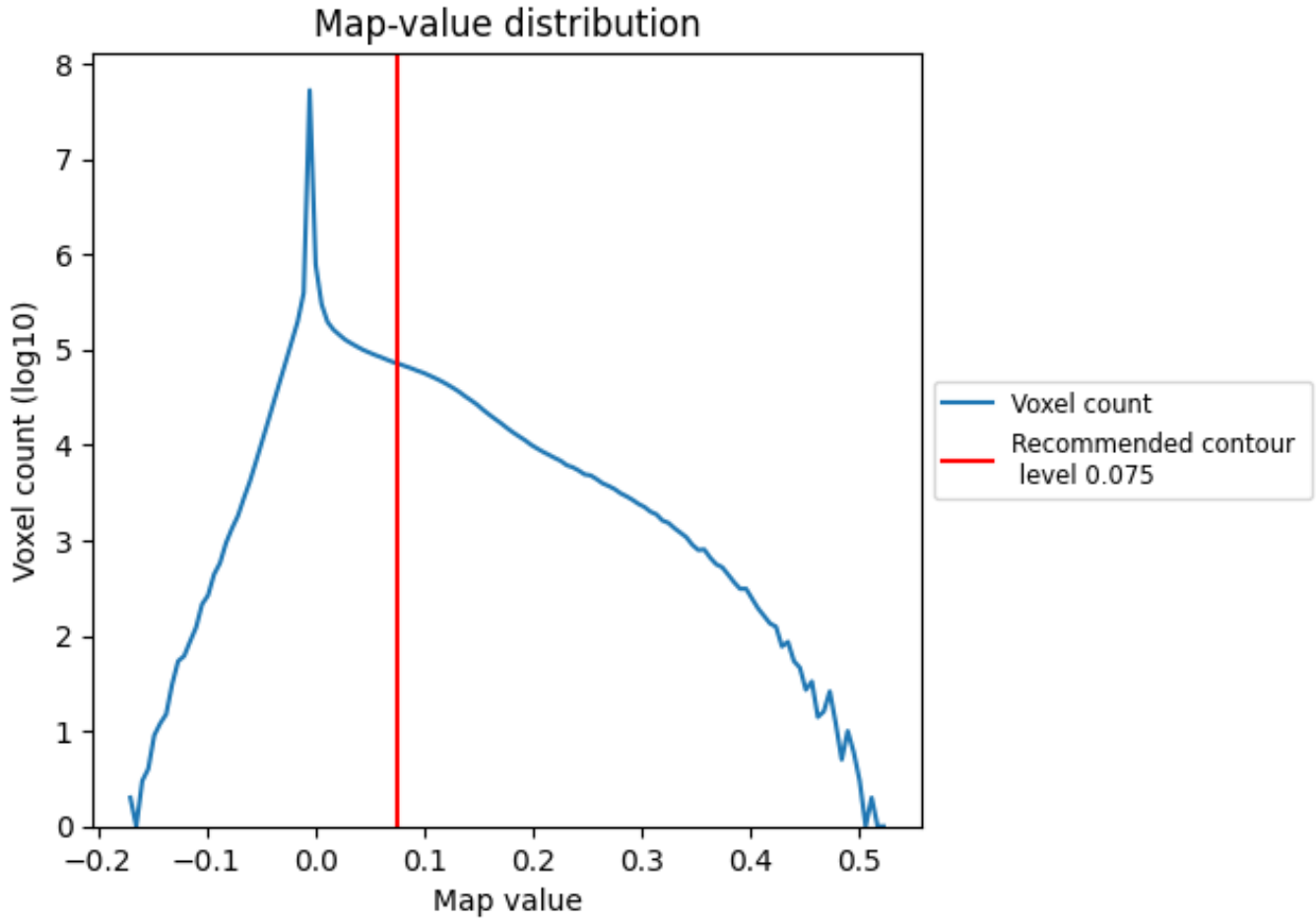
6.5 Mask visualisation (i)

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

7 Map analysis

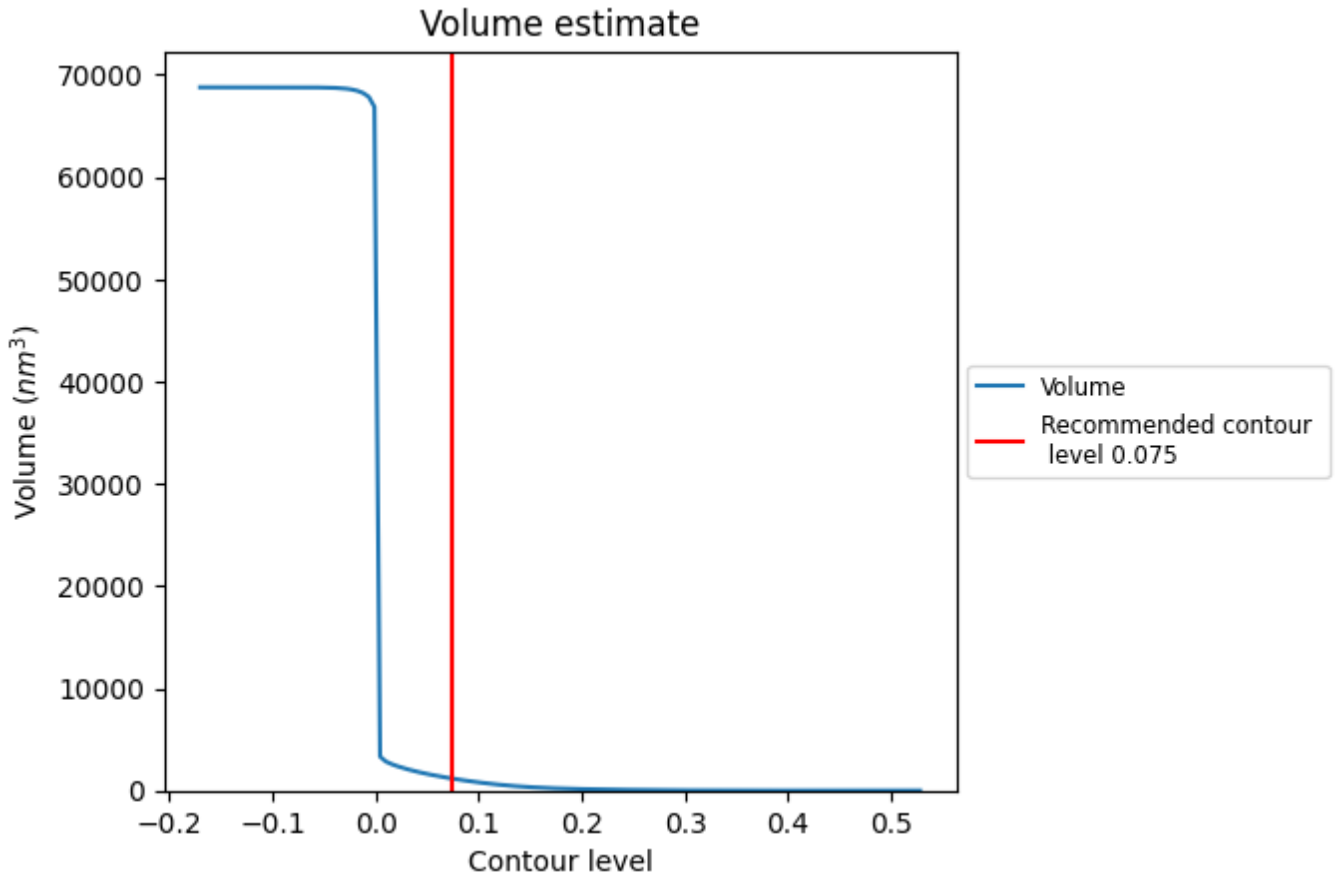
This section contains the results of statistical analysis of the map.

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.

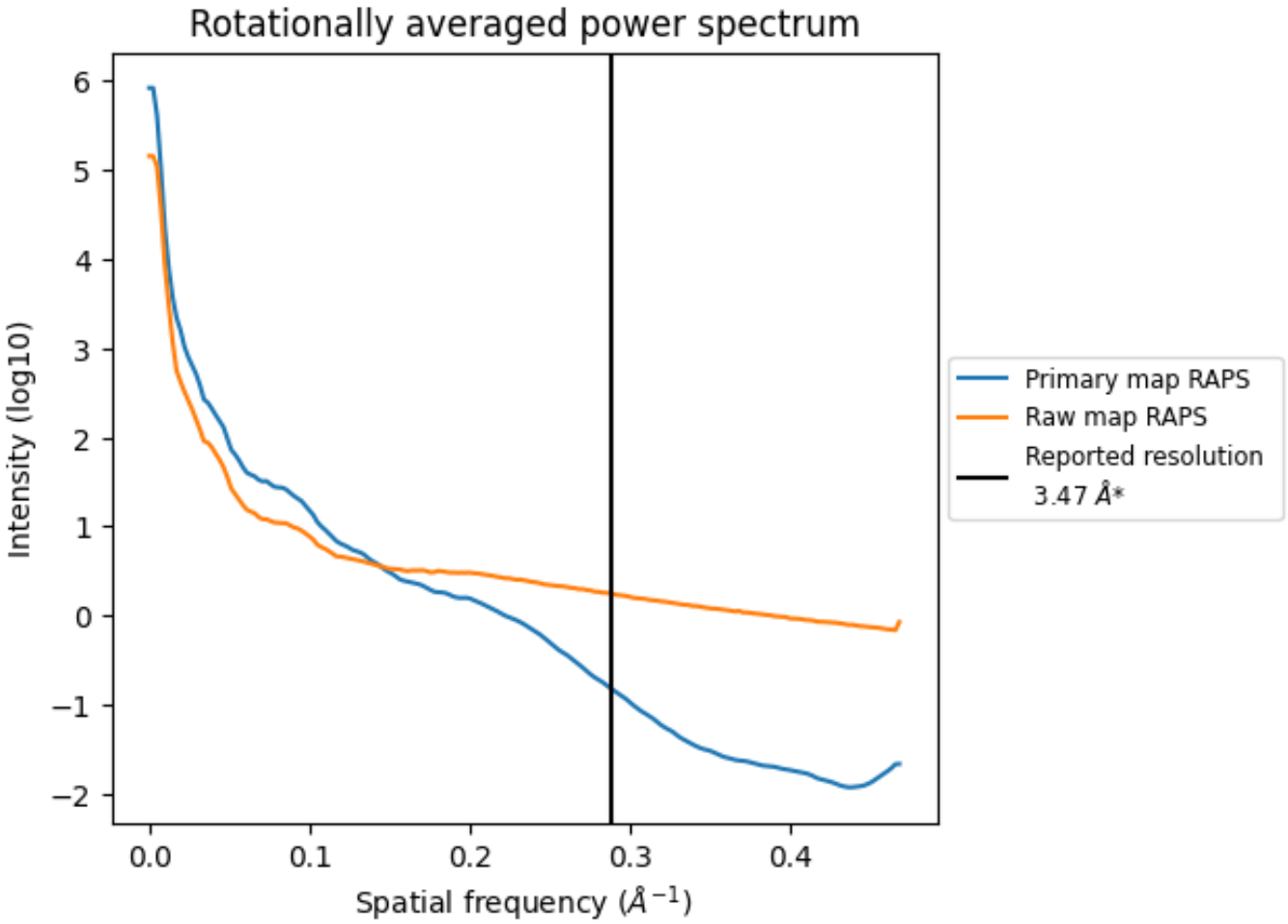
7.2 Volume estimate (i)



The volume at the recommended contour level is 1165 nm^3; this corresponds to an approximate mass of 1053 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)

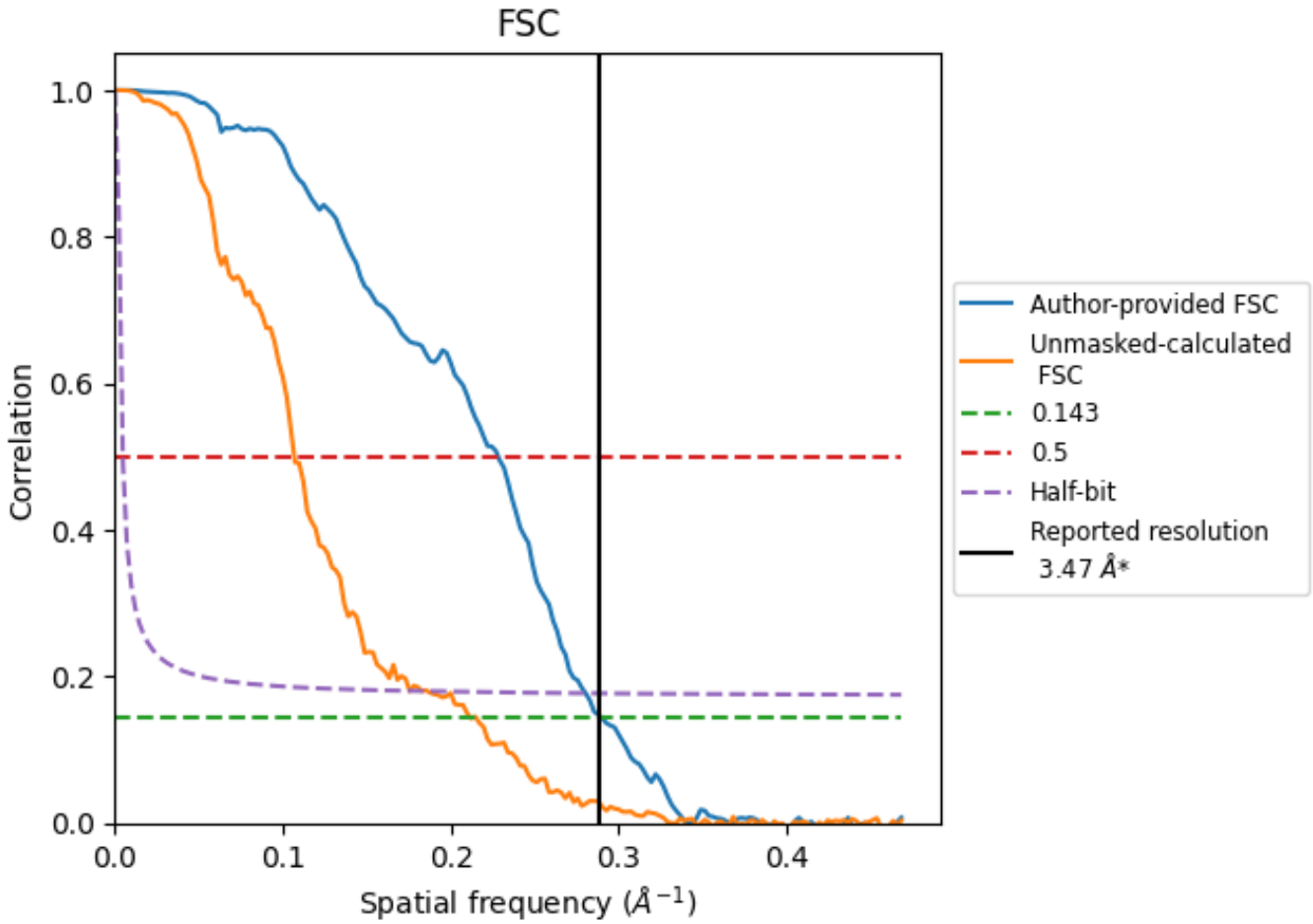


*Reported resolution corresponds to spatial frequency of 0.288 Å^{-1}

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 0.288 Å^{-1}

8.2 Resolution estimates (i)

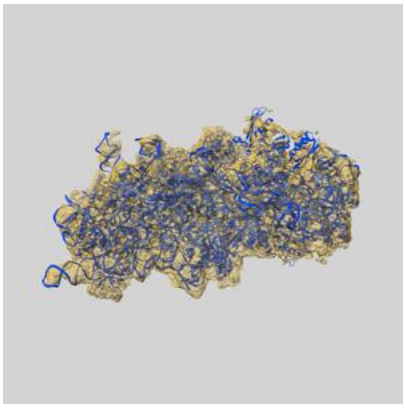
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.45	4.38	3.57
Unmasked-calculated*	4.71	9.35	5.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.71 differs from the reported value 3.47 by more than 10 %

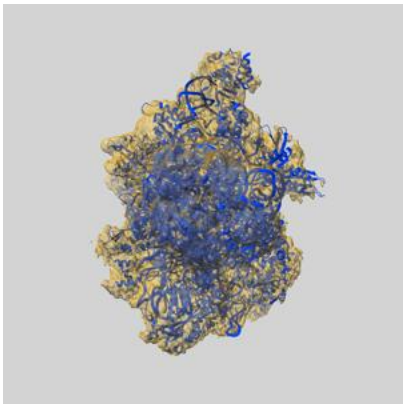
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4792 and PDB model 6RBD. Per-residue inclusion information can be found in section 3 on page 11.

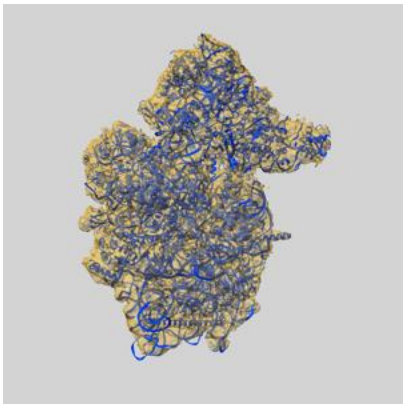
9.1 Map-model overlay



X



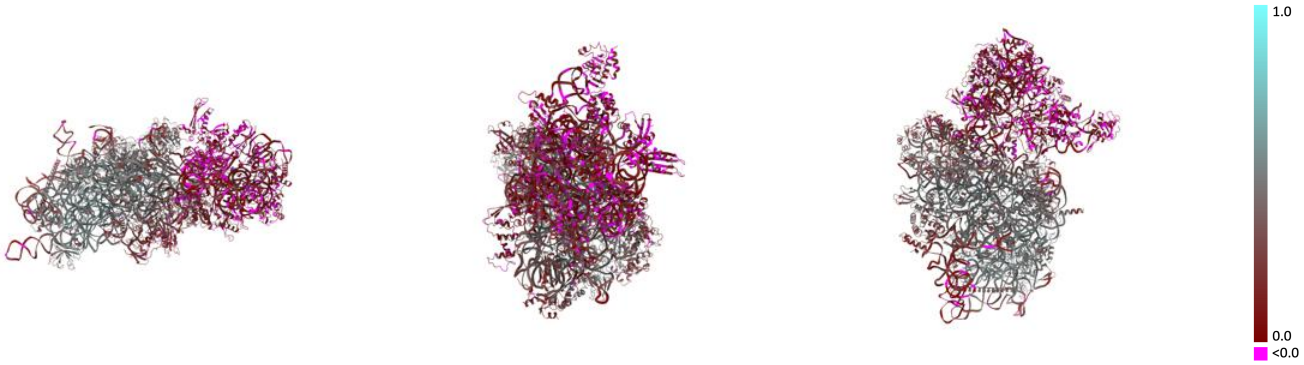
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 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.

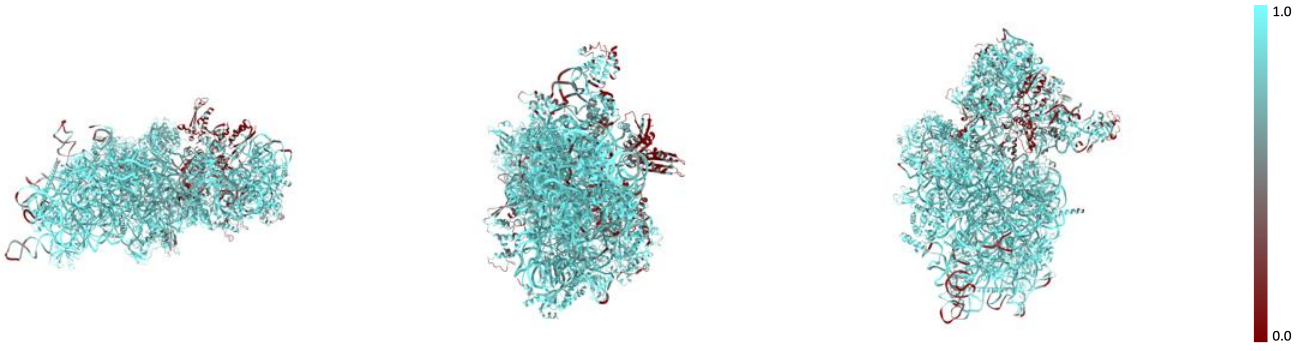
9.2 Q-score mapped to coordinate model



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.

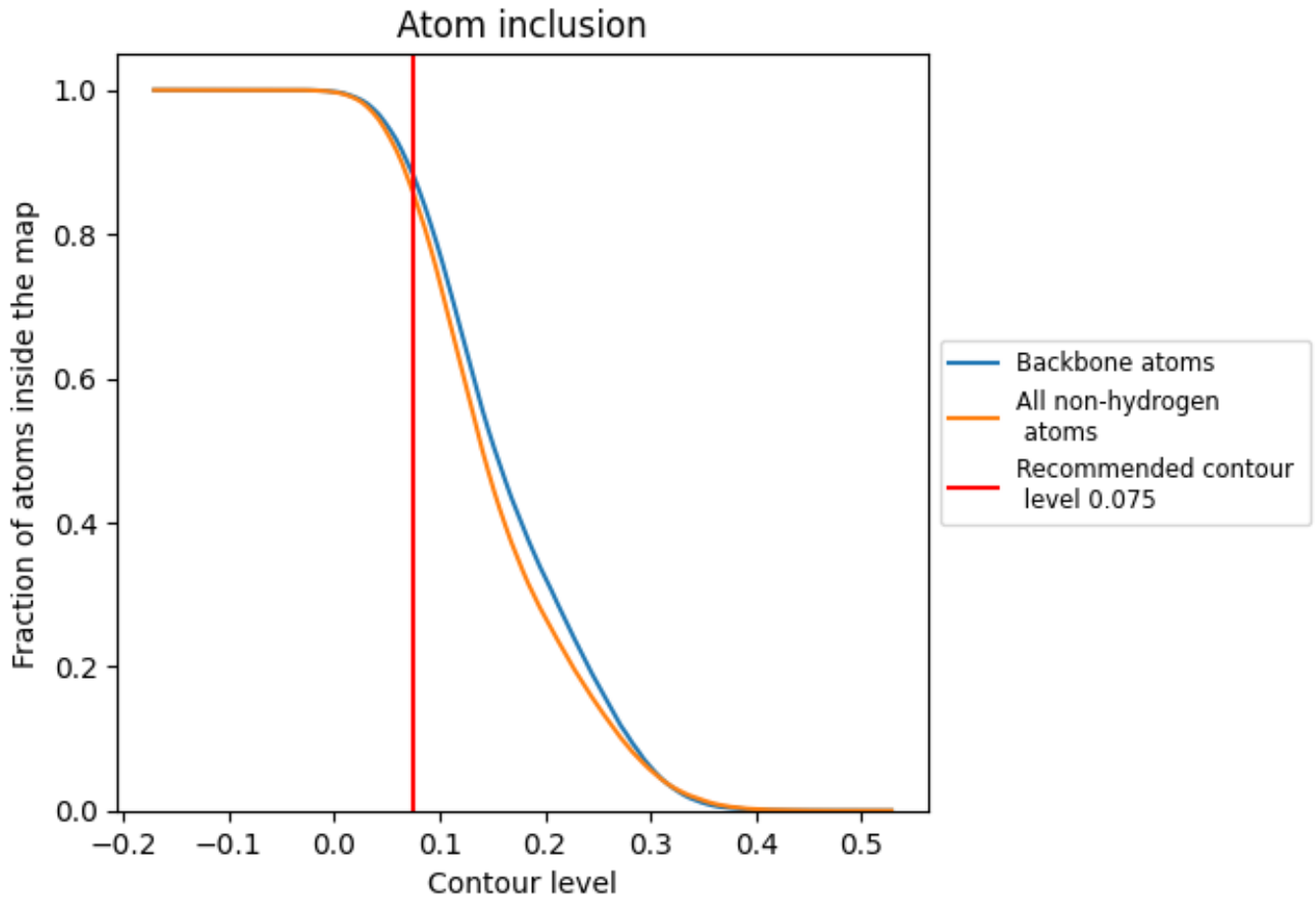
9.3 Atom inclusion mapped to coordinate model



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 (0.075).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8584	0.3010
2	0.8913	0.3250
A	0.9618	0.3880
B	0.8833	0.3430
C	0.9372	0.4320
D	0.3214	0.0700
E	0.9583	0.4940
F	0.8765	0.1080
G	0.9111	0.4150
H	0.8774	0.2990
I	0.9234	0.4640
J	0.9327	0.4440
L	0.9536	0.5010
M	0.5685	0.0680
N	0.9212	0.4260
O	0.8817	0.3060
P	0.7979	0.0860
Q	0.8901	0.1090
R	0.5432	0.1460
S	0.7704	0.0940
T	0.9038	0.0940
U	0.2473	0.0500
V	0.9578	0.4180
W	0.9569	0.4660
X	0.9068	0.4370
Y	0.9356	0.4610
Z	0.8508	0.1010
b	0.9218	0.4210
c	0.7715	0.1320
d	0.5155	0.0700
e	0.7989	0.3590
h	0.8680	0.2590
i	0.6858	0.0500
k	0.8767	0.2590
l	0.7076	0.1000
y	0.6086	0.1220