wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 01:18 AM JST

PDB ID	:	7WTX
EMDB ID	:	EMD-32804
Title	:	Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-B1
Authors	:	Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2022-02-05
Resolution	:	3.10 Å(reported)

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:

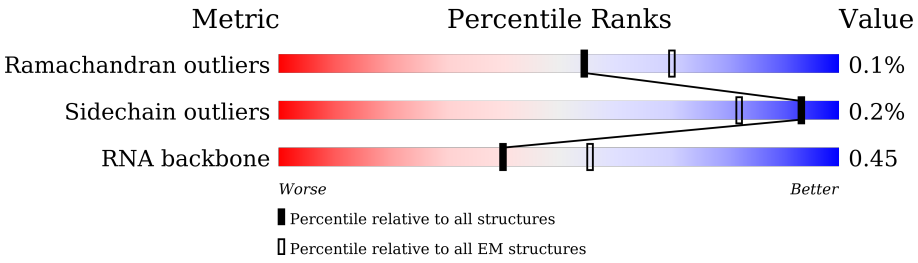
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 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	2	1873	59% 24% 14%
2	F	204	92% 7%
3	M	132	14% 93% 7%
4	P	145	82% 17%
5	Q	146	83% 16%
6	R	135	83% 17%
7	S	152	86% 14%
8	T	145	99%

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Mol	Chain	Length	Quality of chain
9	Z	125	57% 42%
10	c	69	87% 12%
11	f	156	37% 61%
12	A	295	73% 27%
13	B	264	81% 19%
14	C	293	74% 26%
15	E	263	99%
16	G	249	91% 8%
17	H	194	95%
18	I	208	98%
19	J	194	92% 7%
20	L	158	95%
21	N	151	99%
22	O	151	89% 11%
23	V	83	98%
24	W	130	98%
25	X	143	95%
26	Y	133	93% 7%
27	b	84	98%
28	e	59	93% 7%
29	x	252	71% 29%
30	y	412	79% 21%
31	u	804	77% 22%
32	w	437	63% 37%
33	t	475	28% 72%

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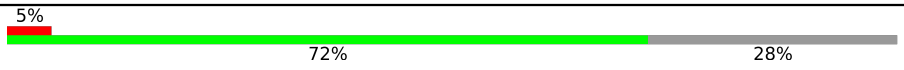
Mol	Chain	Length	Quality of chain
34	K	1297	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 85074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1605	34277	15298	6153	11222	1604	0	0

- Molecule 2 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	189	1495	934	284	270	7	0	0

- Molecule 3 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	123	953	598	169	177	9	0	0

- Molecule 4 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	120	984	625	184	168	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Q	122	969	616	180	170	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	112	911	571	169	168	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	130	Total	C	N	O	S	0	0
			1083	686	214	182	1		

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 9 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 10 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

- Molecule 11 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	61	Total	C	N	O	S	0	0
			498	316	94	81	7		

- Molecule 12 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 14 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 15 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 16 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 19 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 20 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 22 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 28 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 29 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	178	Total	C	N	O	S	0	0
			1391	891	252	244	4		

- Molecule 30 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	325	Total	C	N	O	S	0	0
			2568	1622	473	463	10		

- Molecule 31 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	629	Total	C	N	O	S	0	0
			5062	3249	902	887	24		

- Molecule 32 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	275	Total	C	N	O	S	0	0
			2248	1455	397	387	9		

- Molecule 33 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	132	Total	C	N	O	S	0	0
			1131	701	212	214	4		

- Molecule 34 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	940	Total	C	N	O	S	0	0
			7302	4680	1266	1311	45		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

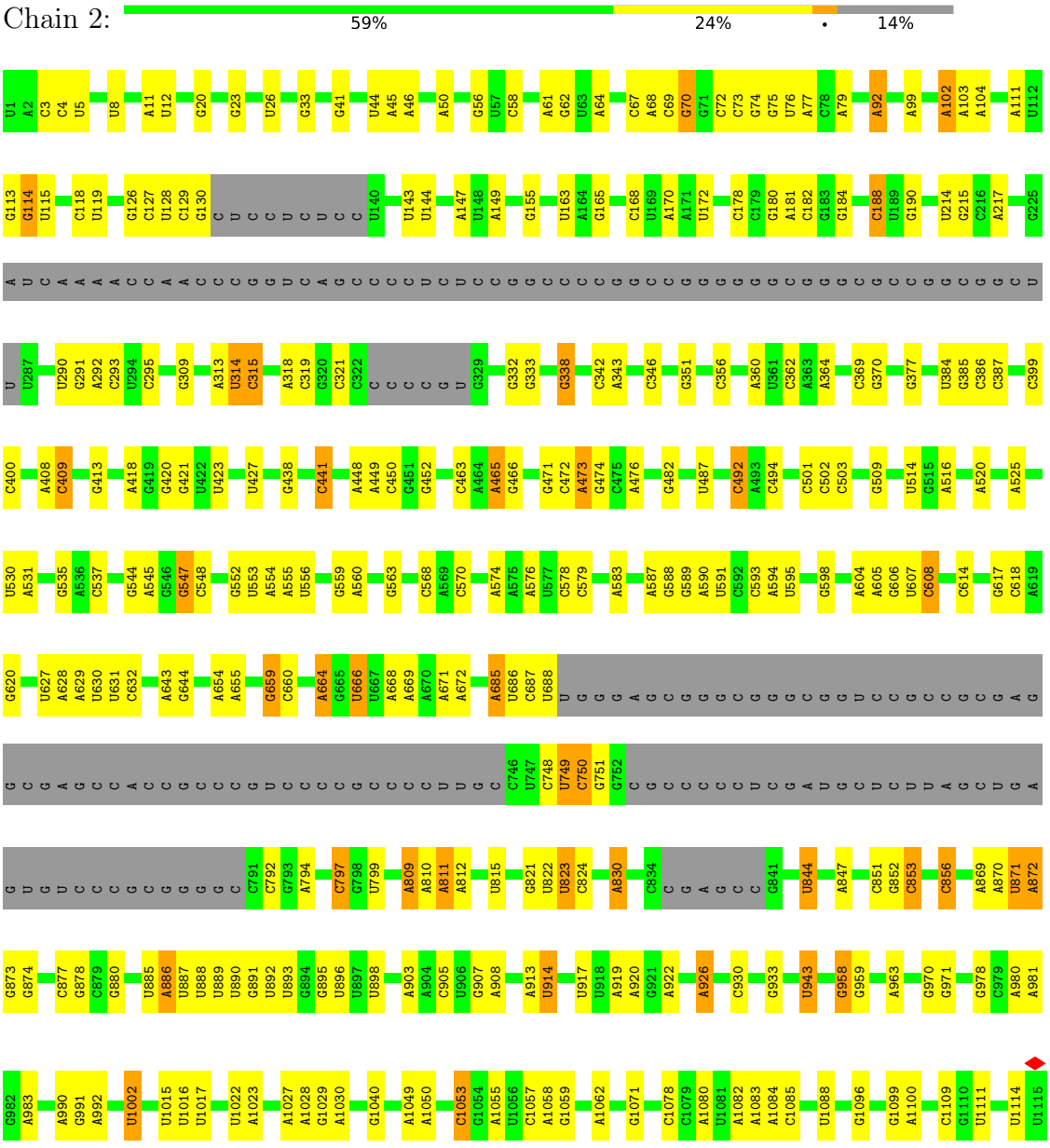
Mol	Chain	Residues	Atoms	AltConf
35	f	1	Total Zn 1 1	0
35	y	1	Total Zn 1 1	0

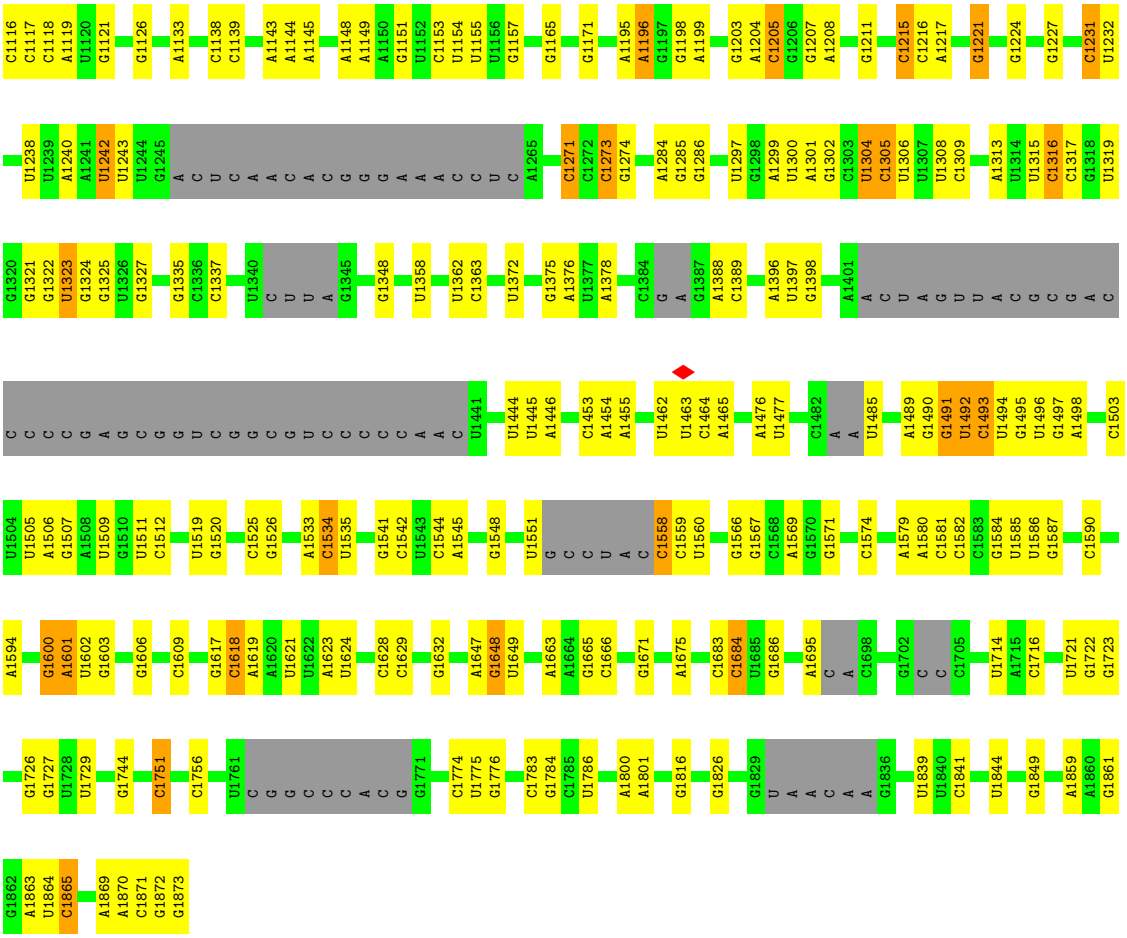
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 18S rRNA

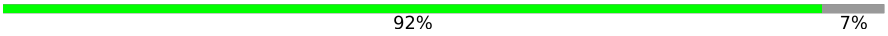
Chain 2:

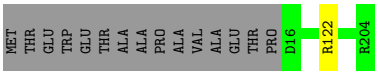




• Molecule 2: 40S ribosomal protein S5

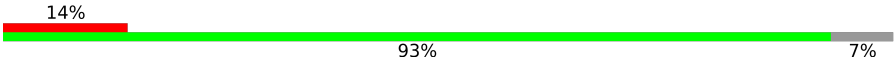
Chain F:

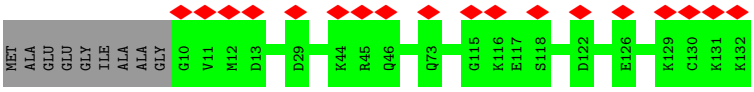




• Molecule 3: 40S ribosomal protein S12

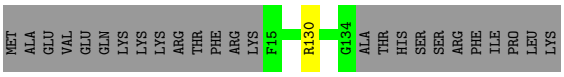
Chain M:





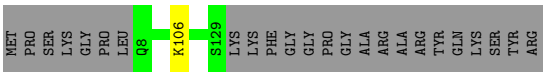
• Molecule 4: 40S ribosomal protein S15

Chain P:



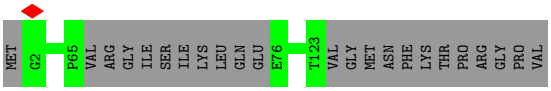
• Molecule 5: 40S ribosomal protein S16

Chain Q:



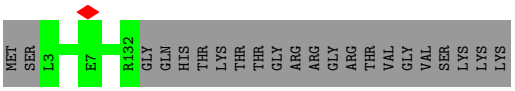
• Molecule 6: 40S ribosomal protein S17

Chain R:



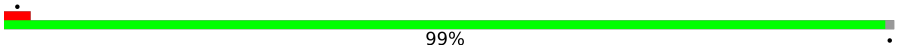
• Molecule 7: 40S ribosomal protein S18

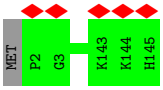
Chain S:



• Molecule 8: 40S ribosomal protein S19

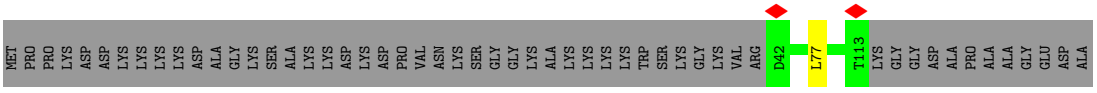
Chain T:





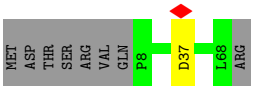
• Molecule 9: 40S ribosomal protein S25

Chain Z:



• Molecule 10: 40S ribosomal protein S28

Chain c:



• Molecule 11: Ubiquitin-40S ribosomal protein S27a

Chain f:

• Molecule 12: 40S ribosomal protein SA

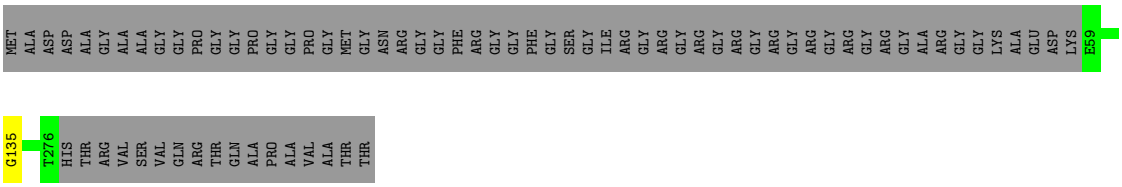
Chain A:

• Molecule 13: 40S ribosomal protein S3a

Chain B:

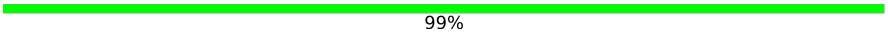
• Molecule 14: 40S ribosomal protein S2

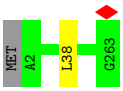
Chain C:



• Molecule 15: 40S ribosomal protein S4, X isoform

Chain E:



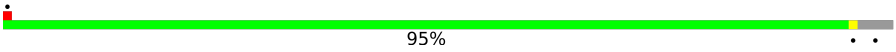


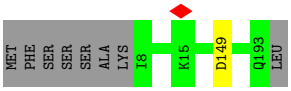
• Molecule 16: 40S ribosomal protein S6

Chain G:

• Molecule 17: 40S ribosomal protein S7

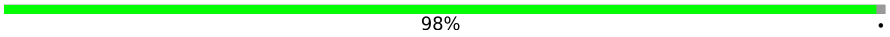
Chain H:

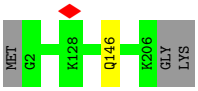




• Molecule 18: 40S ribosomal protein S8

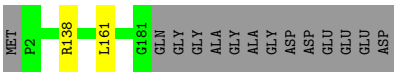
Chain I:





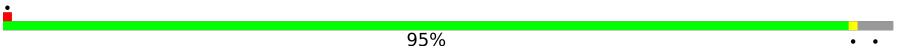
• Molecule 19: 40S ribosomal protein S9

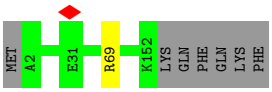
Chain J:



• Molecule 20: 40S ribosomal protein S11

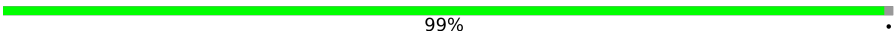
Chain L:





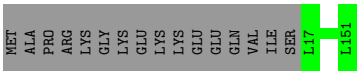
• Molecule 21: 40S ribosomal protein S13

Chain N:



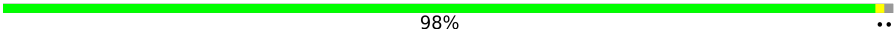
• Molecule 22: 40S ribosomal protein S14

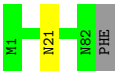
Chain O:



• Molecule 23: 40S ribosomal protein S21

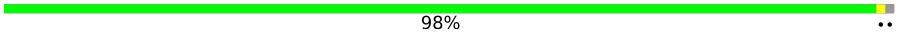
Chain V:

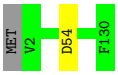




• Molecule 24: 40S ribosomal protein S15a

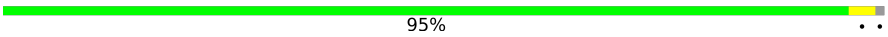
Chain W:





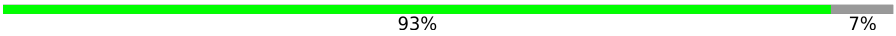
• Molecule 25: 40S ribosomal protein S23

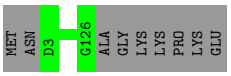
Chain X:



• Molecule 26: 40S ribosomal protein S24

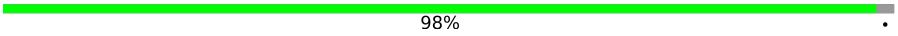
Chain Y:





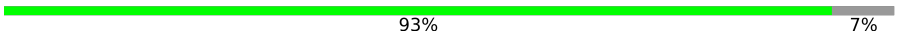
• Molecule 27: 40S ribosomal protein S27

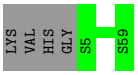
Chain b:



• Molecule 28: 40S ribosomal protein S30

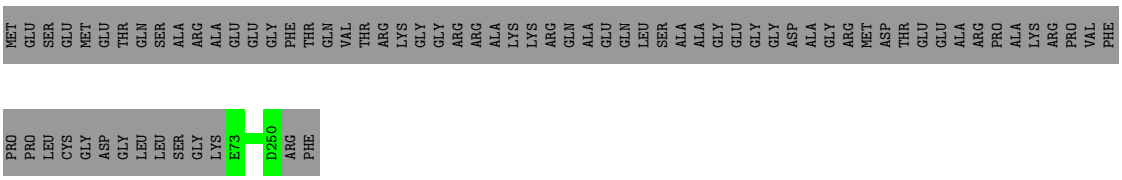
Chain e:





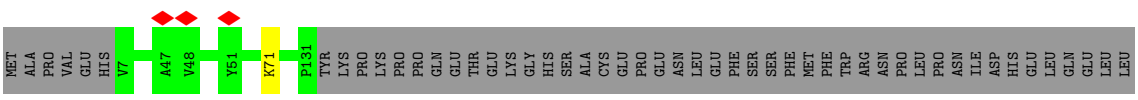
• Molecule 29: RNA-binding protein PNO1

Chain x:



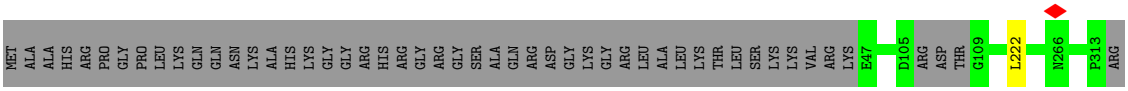
• Molecule 30: RNA-binding protein NOB1

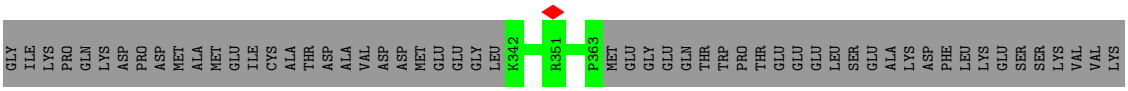
Chain y:

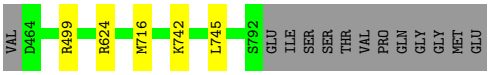


• Molecule 31: Pre-rRNA-processing protein TSR1 homolog

Chain u:





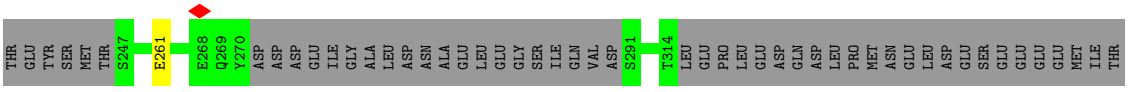


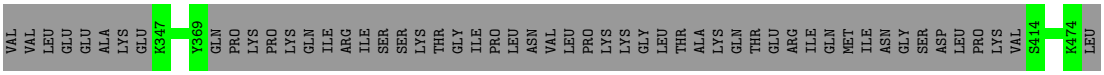
• Molecule 32: Bystin

Chain w:

• Molecule 33: Protein LTV1 homolog

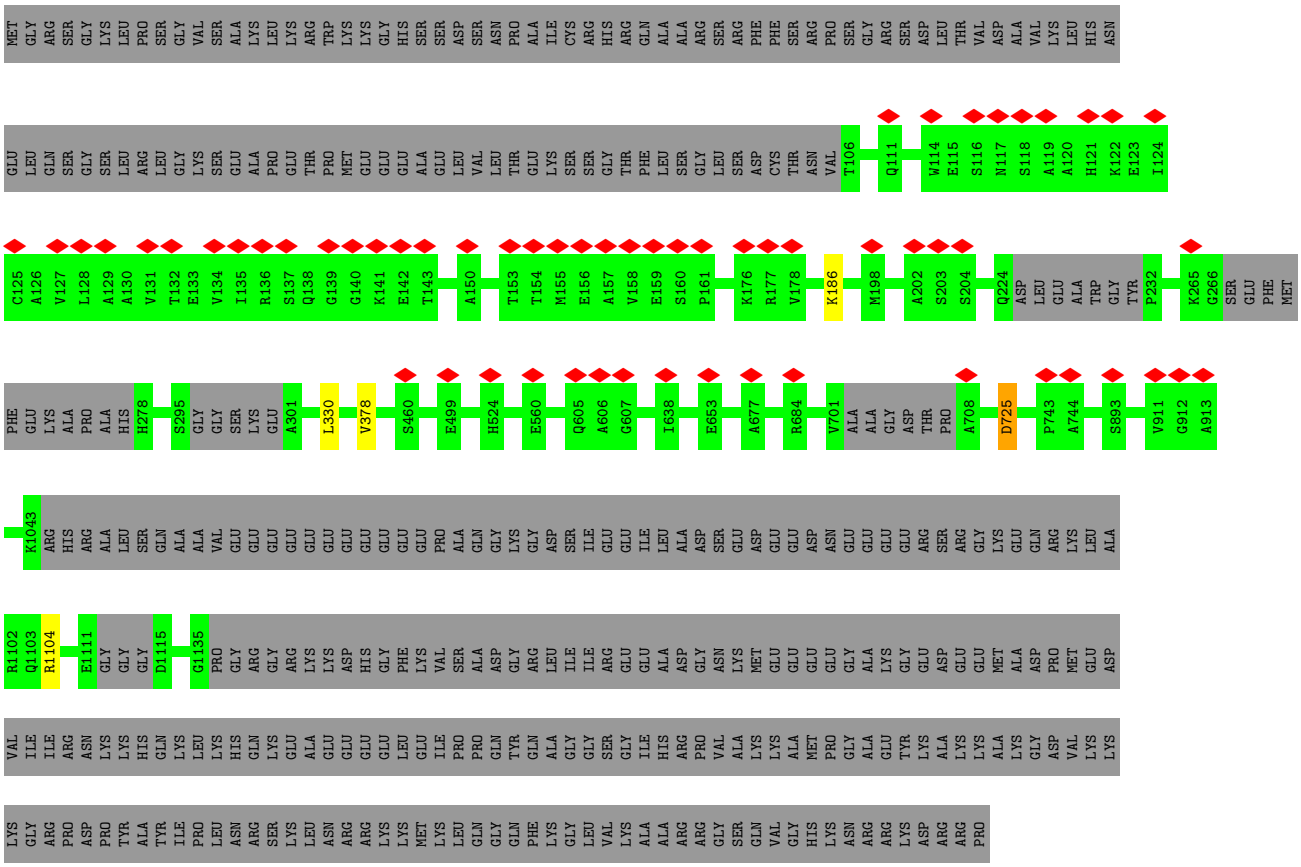
Chain t:





• Molecule 34: RRP12-like protein

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.260	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.85	18/38323 (0.0%)	1.17	252/59711 (0.4%)
2	F	0.30	0/1516	0.61	0/2037
3	M	0.28	0/963	0.55	0/1291
4	P	0.37	0/1003	0.67	0/1341
5	Q	0.33	0/982	0.65	0/1318
6	R	0.29	0/922	0.61	0/1237
7	S	0.31	0/1100	0.65	0/1475
8	T	0.31	0/1142	0.60	0/1530
9	Z	0.29	0/580	0.67	1/780 (0.1%)
10	c	0.33	0/473	0.77	1/633 (0.2%)
11	f	0.35	0/508	0.74	2/670 (0.3%)
12	A	0.45	0/1742	0.66	0/2367
13	B	0.40	0/1756	0.63	0/2350
14	C	0.45	0/1726	0.66	0/2332
15	E	0.48	0/2118	0.70	1/2849 (0.0%)
16	G	0.40	0/1885	0.70	2/2510 (0.1%)
17	H	0.36	0/1524	0.63	1/2042 (0.0%)
18	I	0.48	0/1711	0.70	1/2282 (0.0%)
19	J	0.47	0/1524	0.72	0/2035
20	L	0.48	0/1250	0.65	0/1673
21	N	0.41	0/1226	0.63	0/1649
22	O	0.42	0/1022	0.73	0/1372
23	V	0.44	0/631	0.65	0/844
24	W	0.52	0/1051	0.73	0/1406
25	X	0.52	0/1116	0.71	2/1490 (0.1%)
26	Y	0.43	0/1031	0.68	0/1370
27	b	0.42	0/653	0.63	0/876
28	e	0.42	0/443	0.68	0/582
29	x	0.40	0/1413	0.68	0/1906
30	y	0.37	0/2618	0.67	0/3536
31	u	0.42	0/5187	0.65	4/7011 (0.1%)
32	w	0.30	0/2296	0.60	0/3102

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	t	0.35	0/1143	0.67	0/1515
34	K	0.28	0/7441	0.59	2/10080 (0.0%)
All	All	0.63	18/90019 (0.0%)	0.93	269/129202 (0.2%)

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
11	f	0	2
24	W	0	1
25	X	0	1
34	K	0	1
All	All	0	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1196	A	C6-N1	-9.93	1.28	1.35
1	2	1196	A	N7-C5	-7.05	1.35	1.39
1	2	1221	G	C6-O6	-6.93	1.18	1.24
1	2	685	A	C6-N6	-6.83	1.28	1.33
1	2	492	C	C2-O2	-6.28	1.18	1.24

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	844	U	C5-C4-O4	24.83	140.80	125.90
1	2	1215	C	N3-C4-N4	-24.79	100.65	118.00
1	2	1221	G	N1-C6-O6	-24.26	105.34	119.90
1	2	844	U	N3-C4-O4	-22.20	103.86	119.40
1	2	914	U	C5-C4-O4	20.40	138.14	125.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	K	378	VAL	Peptide
24	W	54	ASP	Peptide
25	X	60	LYS	Peptide

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Mol	Chain	Res	Type	Group
11	f	131	PHE	Peptide
11	f	138	ARG	Sidechain

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	
2	F	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	M	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
4	P	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
5	Q	120/146 (82%)	114 (95%)	6 (5%)	0	100	100
6	R	108/135 (80%)	104 (96%)	4 (4%)	0	100	100
7	S	128/152 (84%)	119 (93%)	9 (7%)	0	100	100
8	T	142/145 (98%)	142 (100%)	0	0	100	100
9	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
10	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
11	f	57/156 (36%)	48 (84%)	9 (16%)	0	100	100
12	A	214/295 (72%)	206 (96%)	8 (4%)	0	100	100
13	B	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
14	C	216/293 (74%)	207 (96%)	8 (4%)	1 (0%)	29	64
15	E	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
16	G	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
17	H	184/194 (95%)	177 (96%)	7 (4%)	0	100	100
18	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	J	178/194 (92%)	173 (97%)	3 (2%)	2 (1%)	14	46
20	L	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
21	N	147/151 (97%)	147 (100%)	0	0	100	100
22	O	133/151 (88%)	126 (95%)	7 (5%)	0	100	100
23	V	80/83 (96%)	80 (100%)	0	0	100	100
24	W	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	X	139/143 (97%)	136 (98%)	2 (1%)	1 (1%)	22	57
26	Y	122/133 (92%)	117 (96%)	5 (4%)	0	100	100
27	b	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
28	e	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
29	x	176/252 (70%)	172 (98%)	4 (2%)	0	100	100
30	y	319/412 (77%)	301 (94%)	18 (6%)	0	100	100
31	u	619/804 (77%)	588 (95%)	31 (5%)	0	100	100
32	w	271/437 (62%)	266 (98%)	5 (2%)	0	100	100
33	t	124/475 (26%)	108 (87%)	15 (12%)	1 (1%)	19	54
34	K	926/1297 (71%)	885 (96%)	40 (4%)	1 (0%)	51	83
All	All	6269/8138 (77%)	6008 (96%)	255 (4%)	6 (0%)	54	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	K	725	ASP
14	C	135	GLY
19	J	138	ARG
25	X	86	PRO
33	t	261	GLU

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	F	159/170 (94%)	158 (99%)	1 (1%)	86 94
3	M	104/108 (96%)	104 (100%)	0	100 100
4	P	107/130 (82%)	106 (99%)	1 (1%)	78 91
5	Q	103/121 (85%)	102 (99%)	1 (1%)	76 90
6	R	101/122 (83%)	101 (100%)	0	100 100
7	S	114/132 (86%)	114 (100%)	0	100 100
8	T	114/115 (99%)	114 (100%)	0	100 100
9	Z	64/103 (62%)	64 (100%)	0	100 100
10	c	52/62 (84%)	52 (100%)	0	100 100
11	f	54/140 (39%)	54 (100%)	0	100 100
12	A	180/243 (74%)	180 (100%)	0	100 100
13	B	194/231 (84%)	194 (100%)	0	100 100
14	C	184/225 (82%)	184 (100%)	0	100 100
15	E	224/225 (100%)	224 (100%)	0	100 100
16	G	200/218 (92%)	199 (100%)	1 (0%)	88 94
17	H	167/174 (96%)	167 (100%)	0	100 100
18	I	178/180 (99%)	178 (100%)	0	100 100
19	J	160/168 (95%)	160 (100%)	0	100 100
20	L	135/142 (95%)	134 (99%)	1 (1%)	84 93
21	N	130/131 (99%)	130 (100%)	0	100 100
22	O	105/119 (88%)	105 (100%)	0	100 100
23	V	66/67 (98%)	65 (98%)	1 (2%)	65 85
24	W	112/113 (99%)	112 (100%)	0	100 100
25	X	113/115 (98%)	112 (99%)	1 (1%)	78 91
26	Y	108/115 (94%)	108 (100%)	0	100 100
27	b	74/76 (97%)	74 (100%)	0	100 100
28	e	45/48 (94%)	45 (100%)	0	100 100
29	x	150/208 (72%)	150 (100%)	0	100 100
30	y	285/367 (78%)	284 (100%)	1 (0%)	91 96
31	u	550/705 (78%)	548 (100%)	2 (0%)	91 96
32	w	240/370 (65%)	239 (100%)	1 (0%)	91 96
33	t	126/434 (29%)	126 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	K	805/1094 (74%)	803 (100%)	2 (0%)	93 97
All	All	5503/6971 (79%)	5490 (100%)	13 (0%)	93 97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	y	71	LYS
31	u	499	ARG
34	K	1104	ARG
32	w	240	ASN
34	K	186	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
32	w	240	ASN
32	w	251	ASN
33	t	308	ASN
9	Z	106	GLN
2	F	95	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1589/1873 (84%)	441 (27%)	29 (1%)

5 of 441 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	5	U
1	2	20	G
1	2	23	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	958	G

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Mol	Chain	Res	Type
1	2	1726	G
1	2	1316	C
1	2	1558	C
1	2	1231	C

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, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

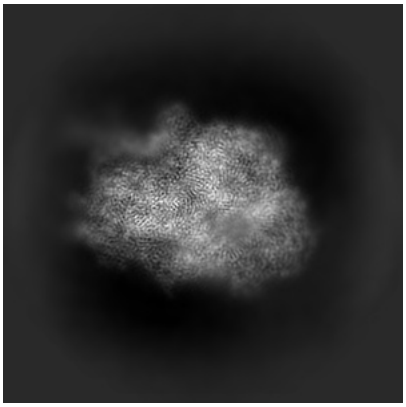
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32804. These allow visual inspection of the internal detail of the map and identification of artifacts.

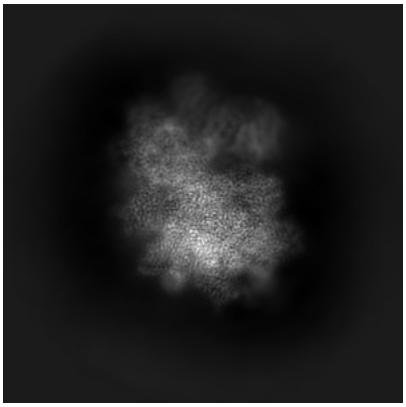
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

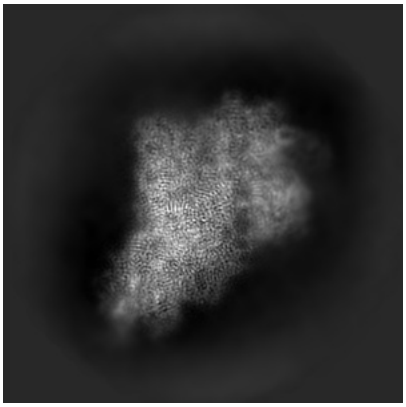
6.1.1 Primary map



X



Y

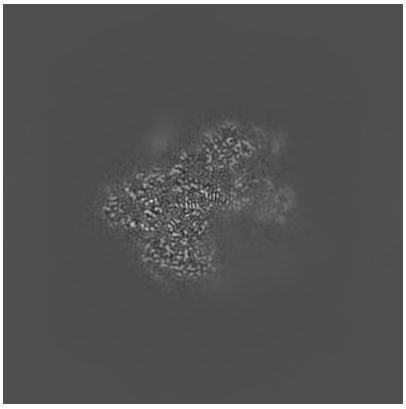


Z

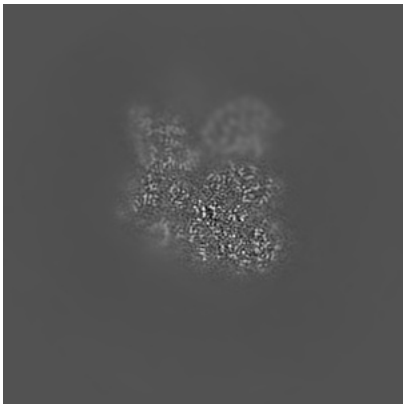
The images above show the map projected in three orthogonal directions.

6.2 Central slices

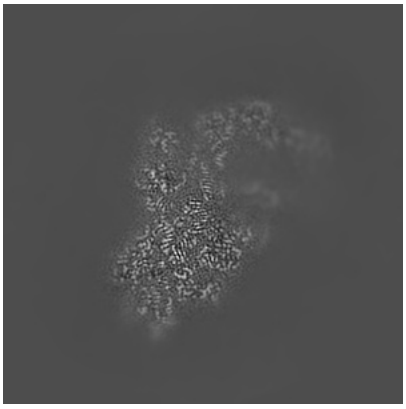
6.2.1 Primary map



X Index: 180



Y Index: 180

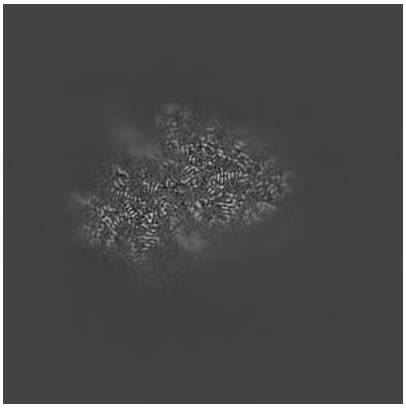


Z Index: 180

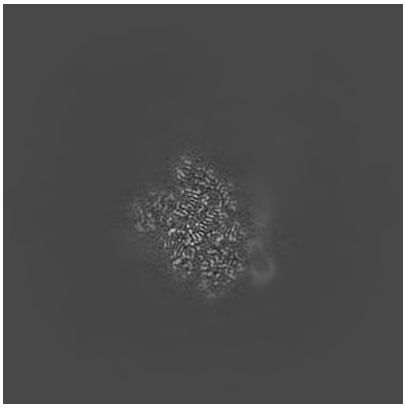
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

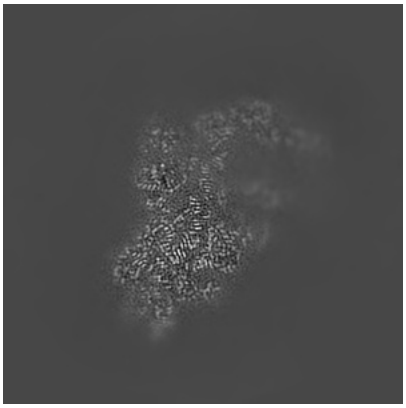
6.3.1 Primary map



X Index: 144



Y Index: 133

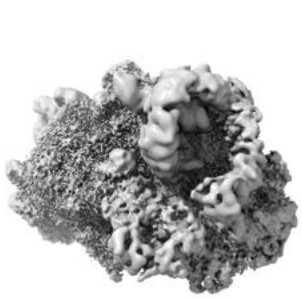


Z Index: 181

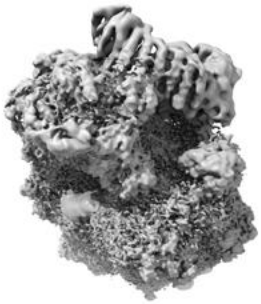
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

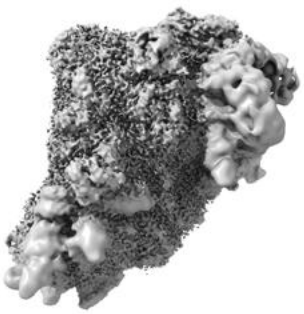
6.4.1 Primary map



X



Y



Z

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

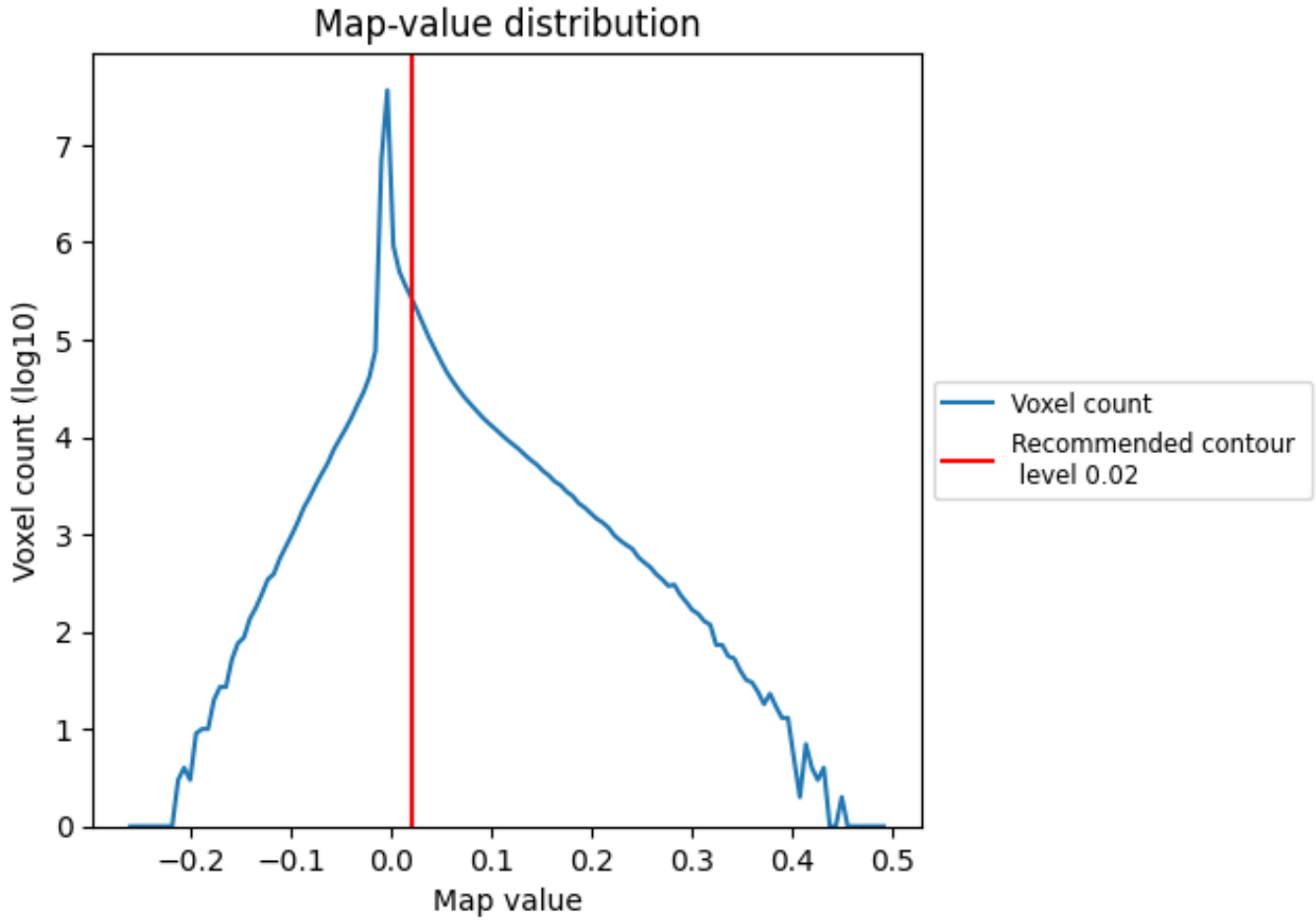
6.5 Mask visualisation (i)

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

7 Map analysis

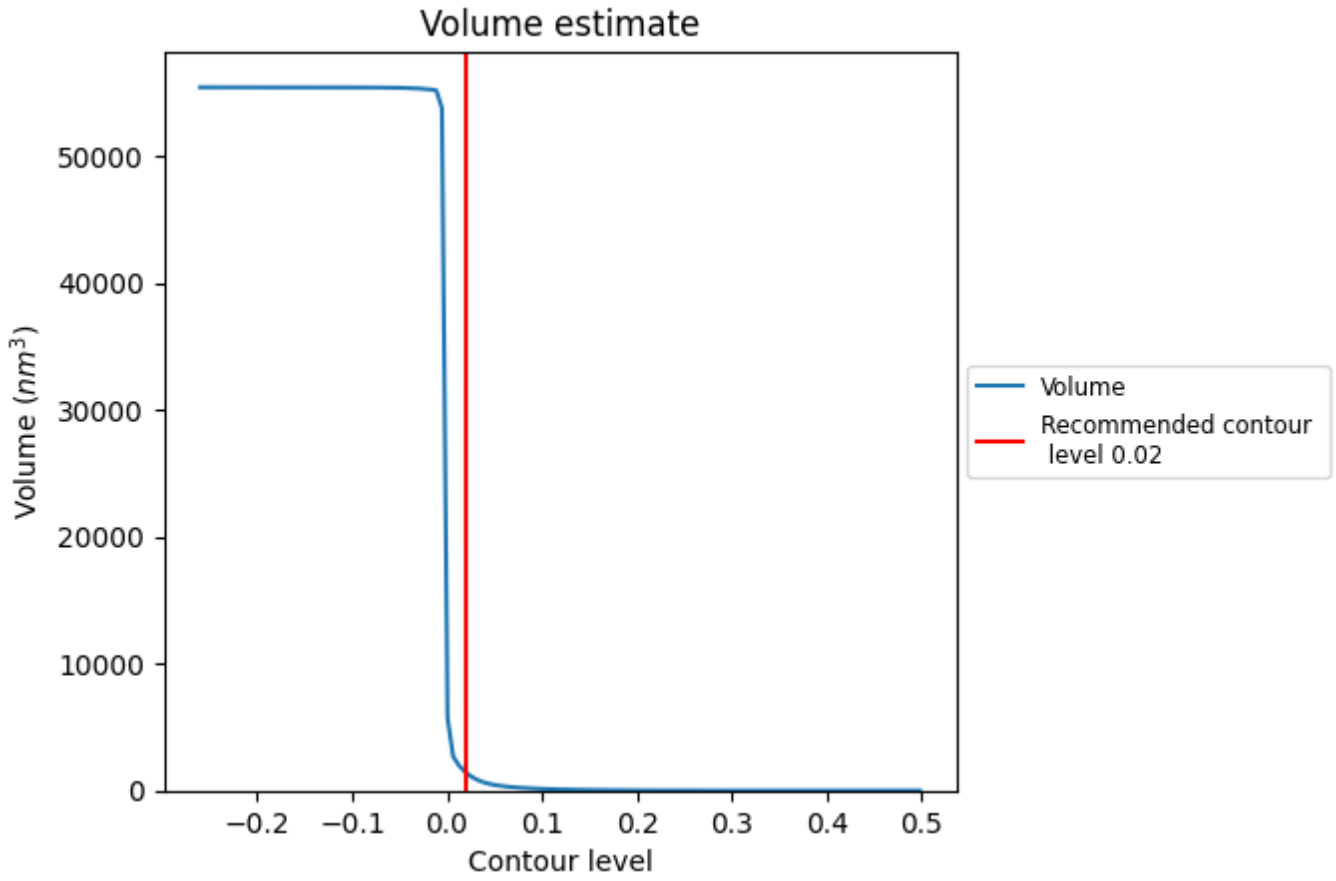
This section contains the results of statistical analysis of the map.

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.

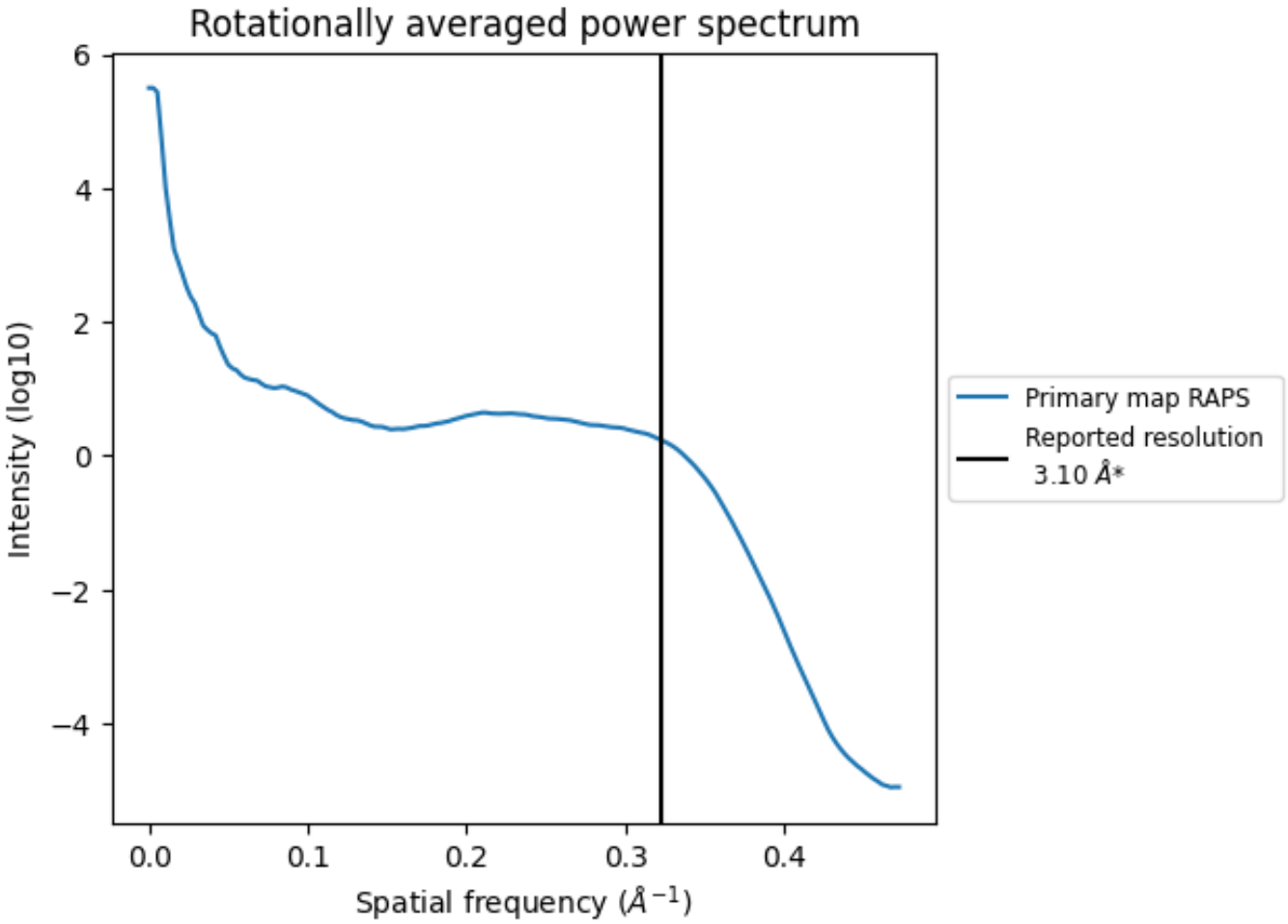
7.2 Volume estimate (i)



The volume at the recommended contour level is 1418 nm^3; this corresponds to an approximate mass of 1281 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)

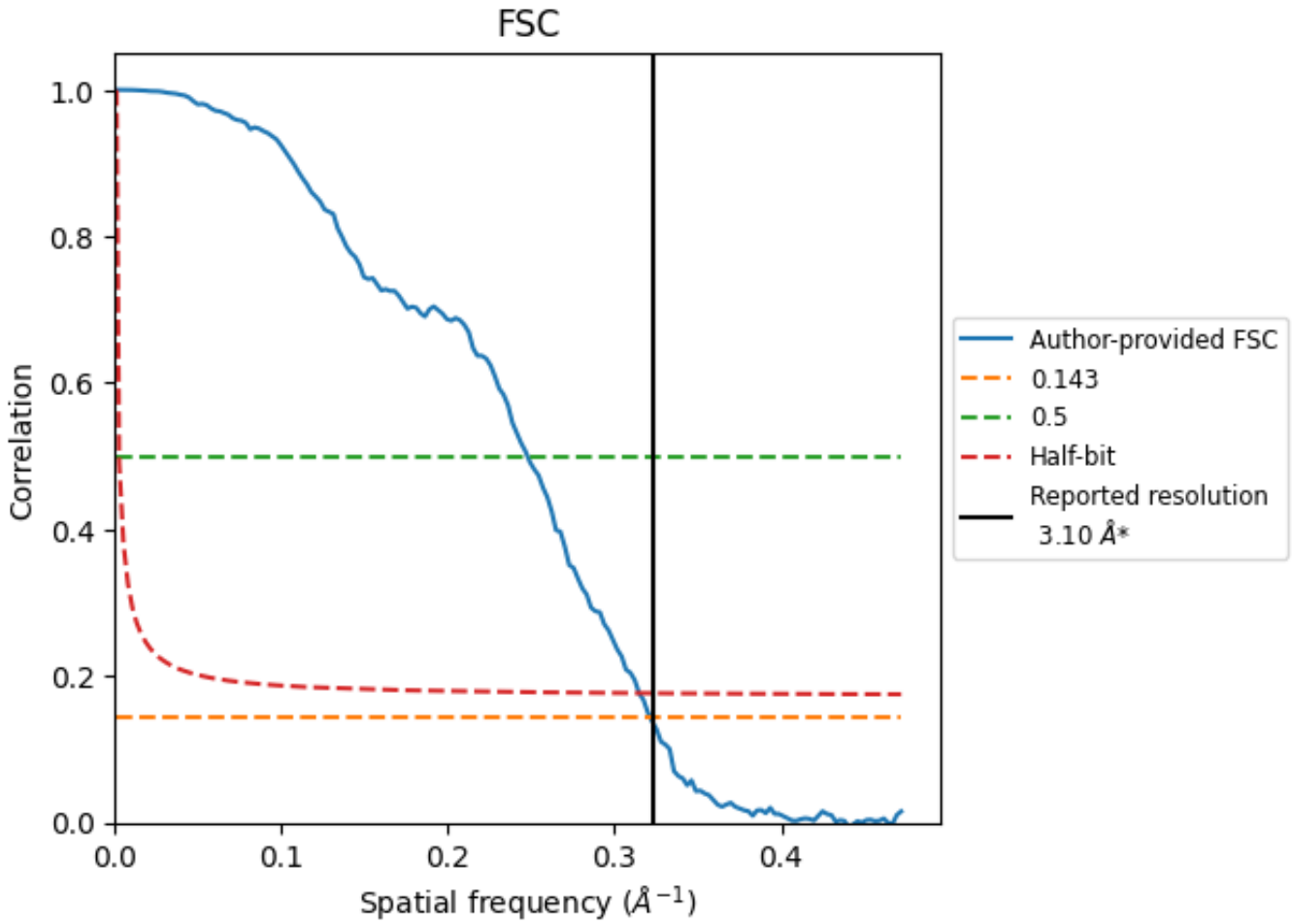


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

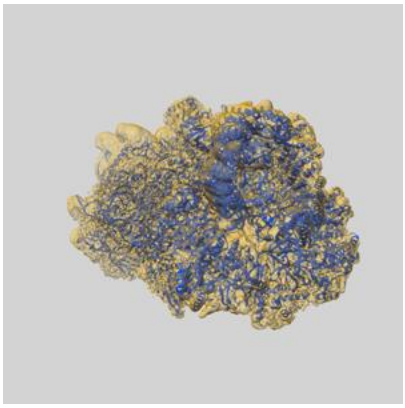
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	4.04	3.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

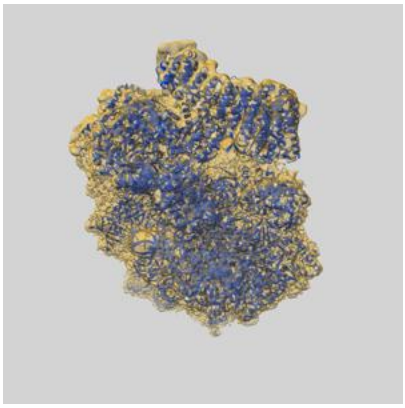
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32804 and PDB model 7WTX. Per-residue inclusion information can be found in section 3 on page 11.

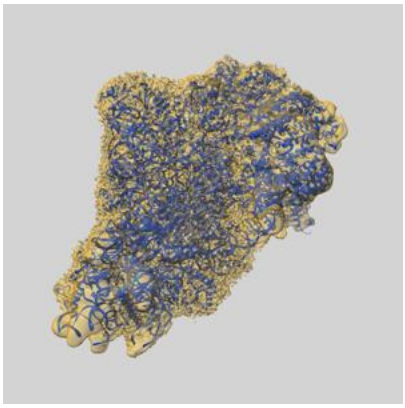
9.1 Map-model overlay



X



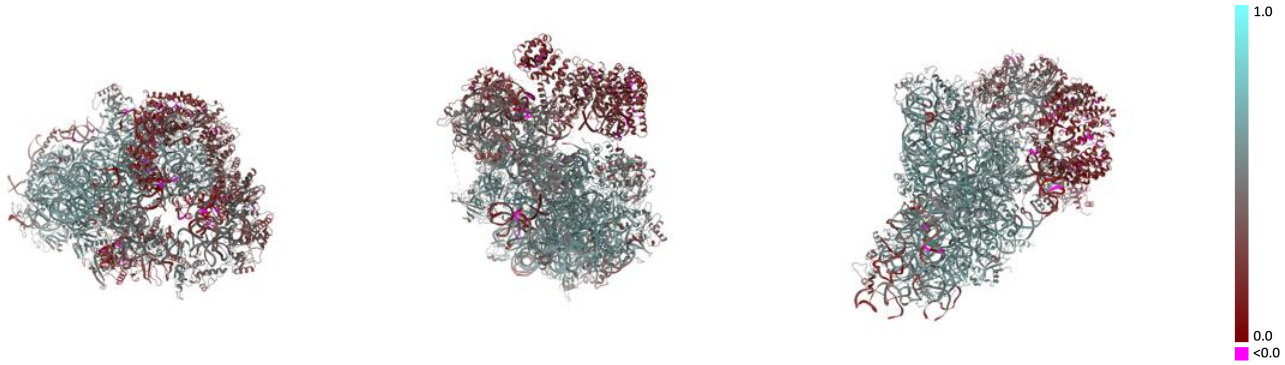
Y



Z

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

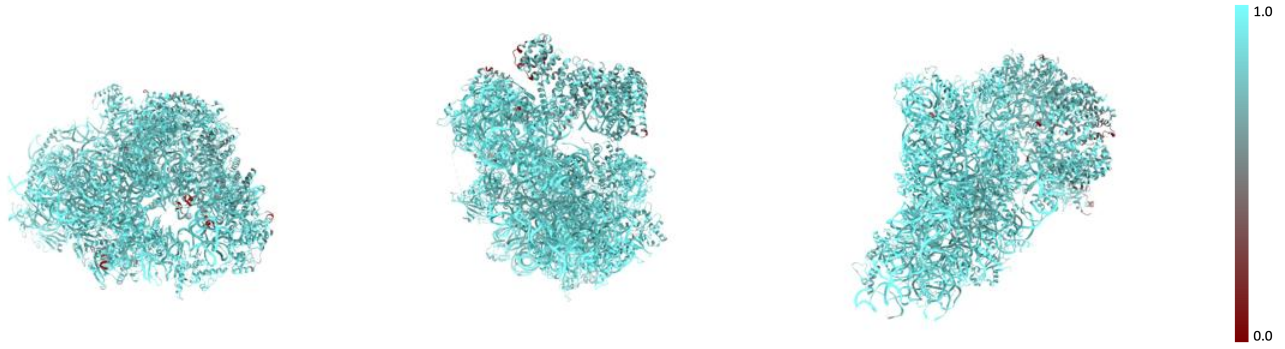
9.2 Q-score mapped to coordinate model



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.

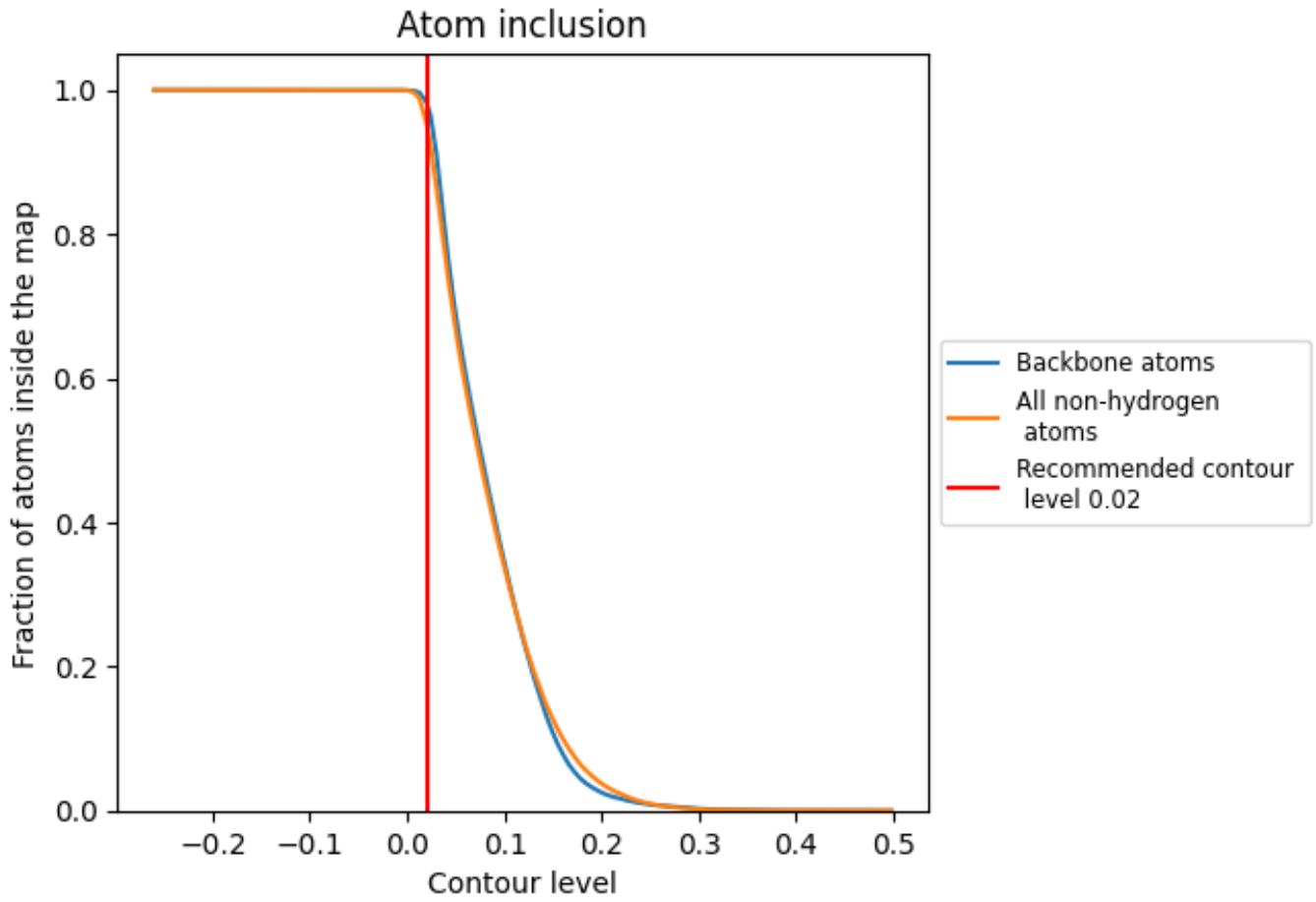
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9537	0.4780
2	0.9875	0.5110
A	0.9826	0.5700
B	0.9729	0.5390
C	0.9879	0.5800
E	0.9837	0.5910
F	0.9443	0.4290
G	0.9617	0.5040
H	0.9389	0.4720
I	0.9600	0.5260
J	0.9937	0.6000
K	0.7863	0.1970
L	0.9606	0.5710
M	0.7220	0.2250
N	0.9931	0.5760
O	0.9694	0.5220
P	0.9392	0.4610
Q	0.8937	0.4160
R	0.9119	0.3240
S	0.9109	0.4010
T	0.8864	0.3800
V	0.9804	0.5730
W	0.9911	0.6160
X	0.9981	0.6220
Y	0.9929	0.5730
Z	0.8414	0.3270
b	0.9857	0.5550
c	0.9492	0.4070
e	0.9480	0.5300
f	0.8992	0.2570
t	0.9518	0.4070
u	0.9776	0.5400
w	0.9405	0.4050
x	0.9883	0.5620
y	0.9426	0.4510