wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 04:36 am GMT

PDB ID	:	6Y7C
EMDB ID	:	EMD-10713
Title	:	Early cytoplasmic yeast pre-40S particle (purified with Tsr1 as bait)
Authors	:	Shayan, R.; Plassart, L.; Plisson-Chastang, C.
Deposited on	:	2020-02-28
Resolution	:	3.80 Å(reported)
Based on initial model	:	6FAI

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 ⓘ 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:

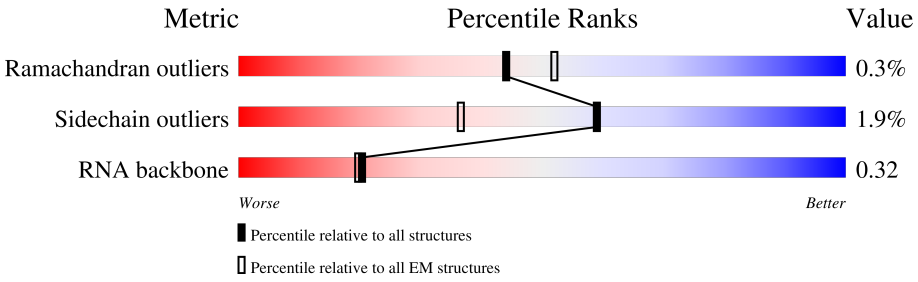
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.80 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)
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	1735	13% 46% 46% 8%
2	A	252	79% 18%
3	B	255	11% 81% 16%
4	C	254	7% 84% 13%
5	E	261	98%
6	F	225	17% 88% 8%
7	G	236	6% 93%
8	H	190	17% 85% 12%

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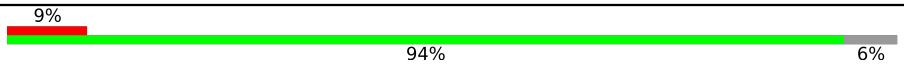
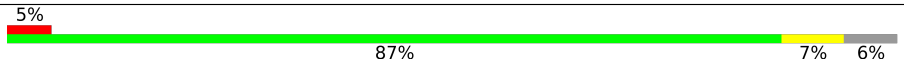
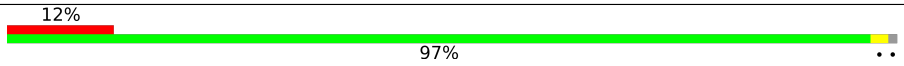
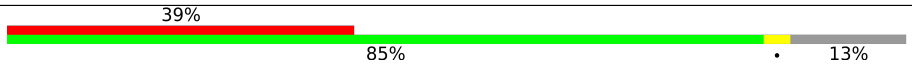
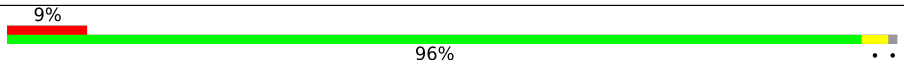
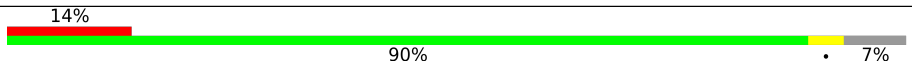
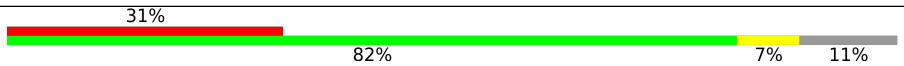
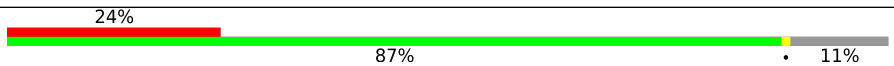
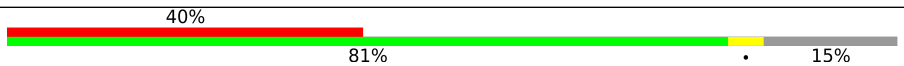
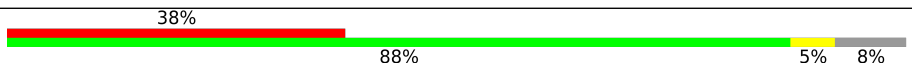
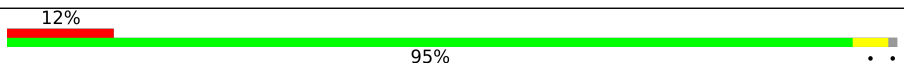
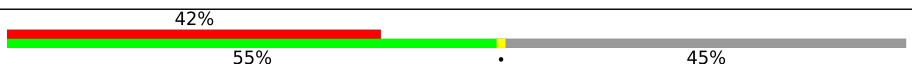
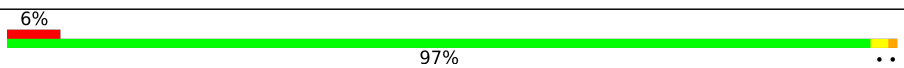
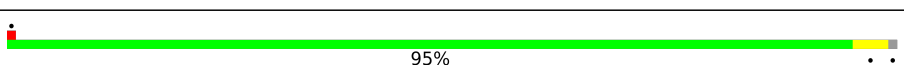
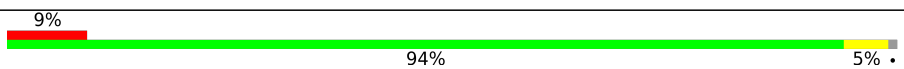
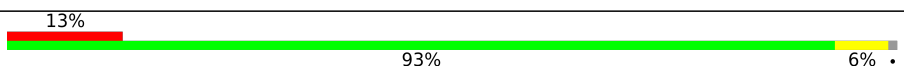
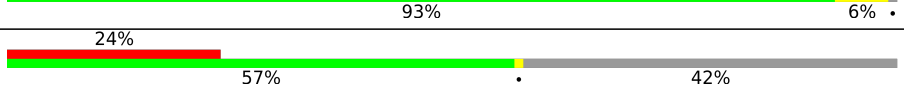
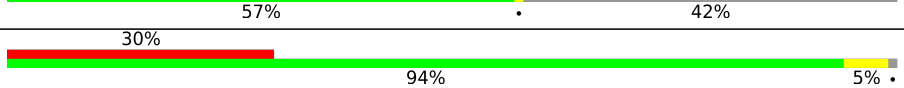
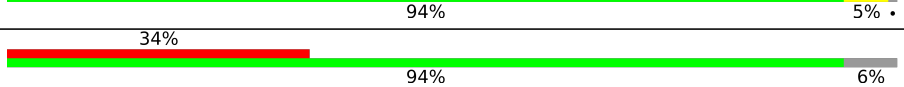
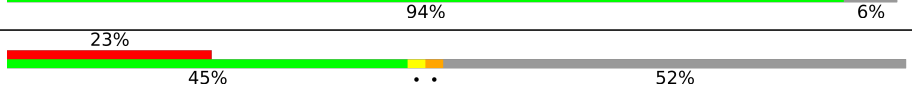
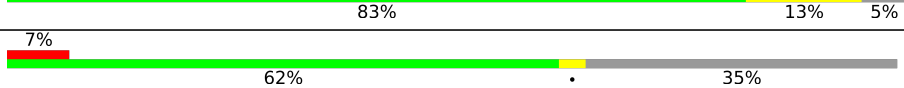
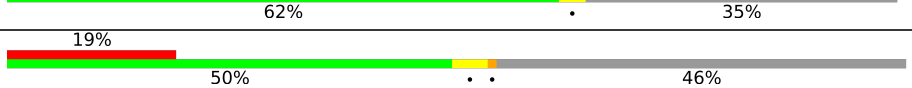
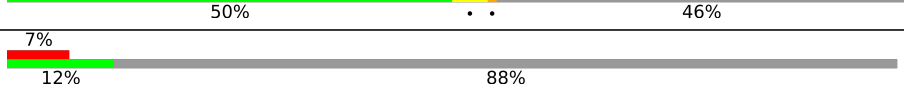
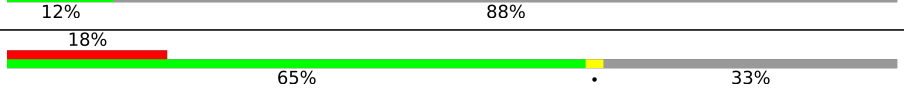
Mol	Chain	Length	Quality of chain
9	I	200	
10	J	197	
11	L	156	
12	M	143	
13	N	151	
14	O	137	
15	P	142	
16	Q	143	
17	R	136	
18	S	146	
19	T	144	
20	U	121	
21	V	87	
22	W	130	
23	X	145	
24	Y	135	
25	Z	108	
26	b	82	
27	c	67	
28	d	56	
29	e	63	
30	h	274	
31	i	483	
32	j	463	
33	l	425	

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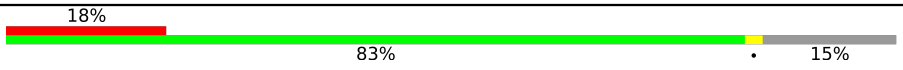
Mol	Chain	Length	Quality of chain
34	t	788	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 79690 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 20S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1735	36965	16530	6537	12163	1735	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1614	1039	284	289	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 3 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	220	1662	1065	295	300	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 6 is a protein called 40S ribosomal protein S5.

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

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	168	Total	C	N	O	0	0
			1362	880	239	243		

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 12 is a protein called 40S ribosomal protein S12.

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

- 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
			1193	759	224	208	2		

- Molecule 14 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	128	Total	C	N	O	S	0	0
			950	582	188	177	3		

- Molecule 15 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	127	Total	C	N	O	S	0	0
			1001	637	186	171	7		

- Molecule 16 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 17 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	115	Total	C	N	O	S	0	0
			924	575	173	174	2		

- Molecule 18 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	135	Total	C	N	O	S	0	0
			1110	696	215	197	2		

- Molecule 19 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 20 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	67	Total	C	N	O	0	0
			541	344	102	95		

- Molecule 21 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	87	Total	C	N	O	S	0	0
			685	420	125	138	2		

- Molecule 22 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	129	Total	C	N	O	S	0	0
			1019	650	188	178	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	51	VAL	GLU	conflict	UNP P0C0W1

- Molecule 23 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 25 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	81	Total	C	N	O	S	0	0
			611	382	110	114	5		

- Molecule 27 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 28 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	27	Total	C	N	O	S	0	0
			219	133	46	36	4		

- Molecule 29 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	179	Total	C	N	O	S	0	0
			1416	906	256	250	4		

- Molecule 31 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	261	Total	C	N	O	S	0	0
			2125	1384	363	375	3		

- Molecule 32 is a protein called Protein LTV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	55	Total	C	N	O	S	0	0
			465	283	66	113	3		

- Molecule 33 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	286	Total	C	N	O	S	0	0
			2322	1464	410	430	18		

- Molecule 34 is a protein called Ribosome biogenesis protein TSR1.

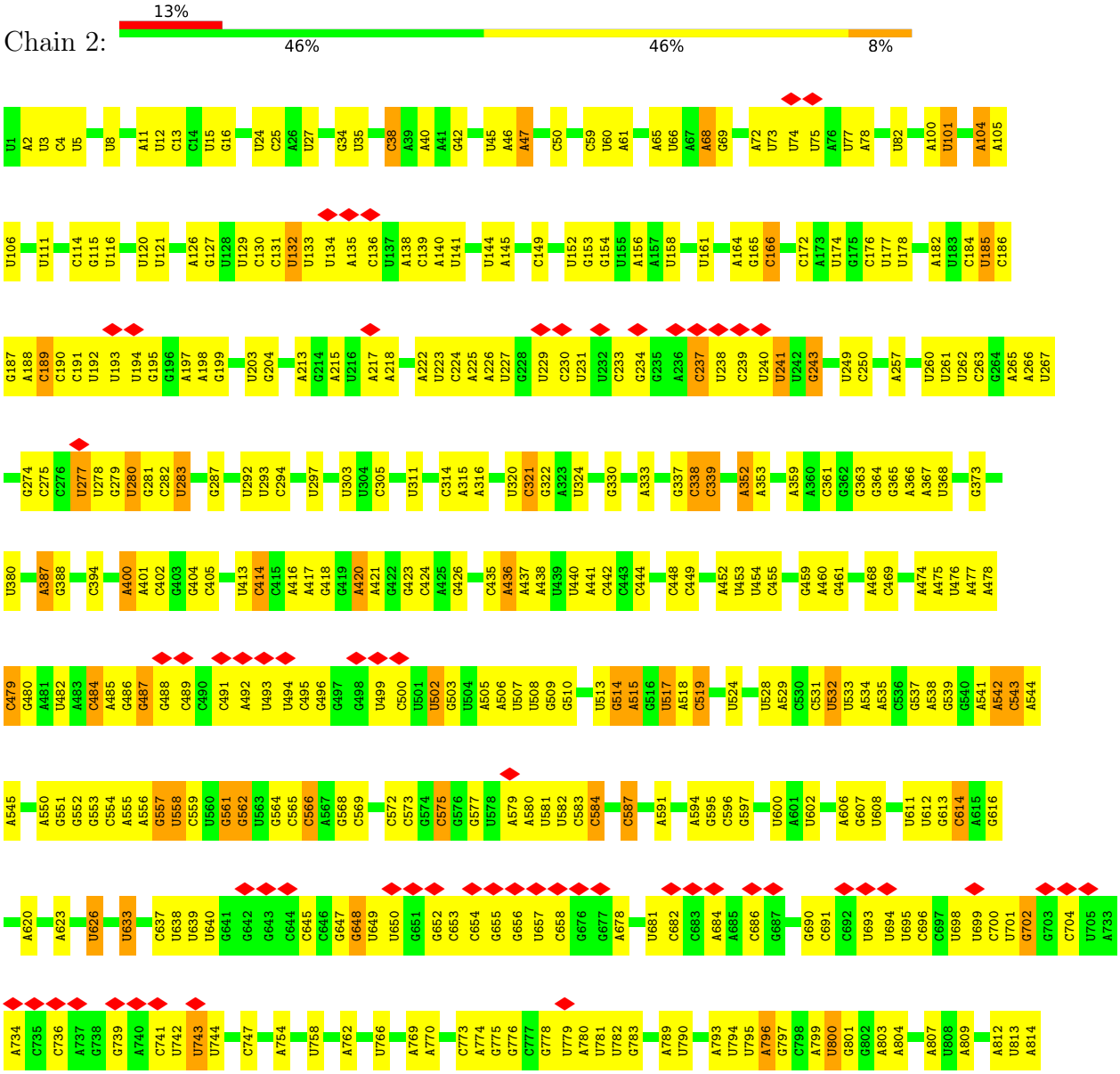
Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	667	Total	C	N	O	S	0	0
			5401	3447	932	1008	14		

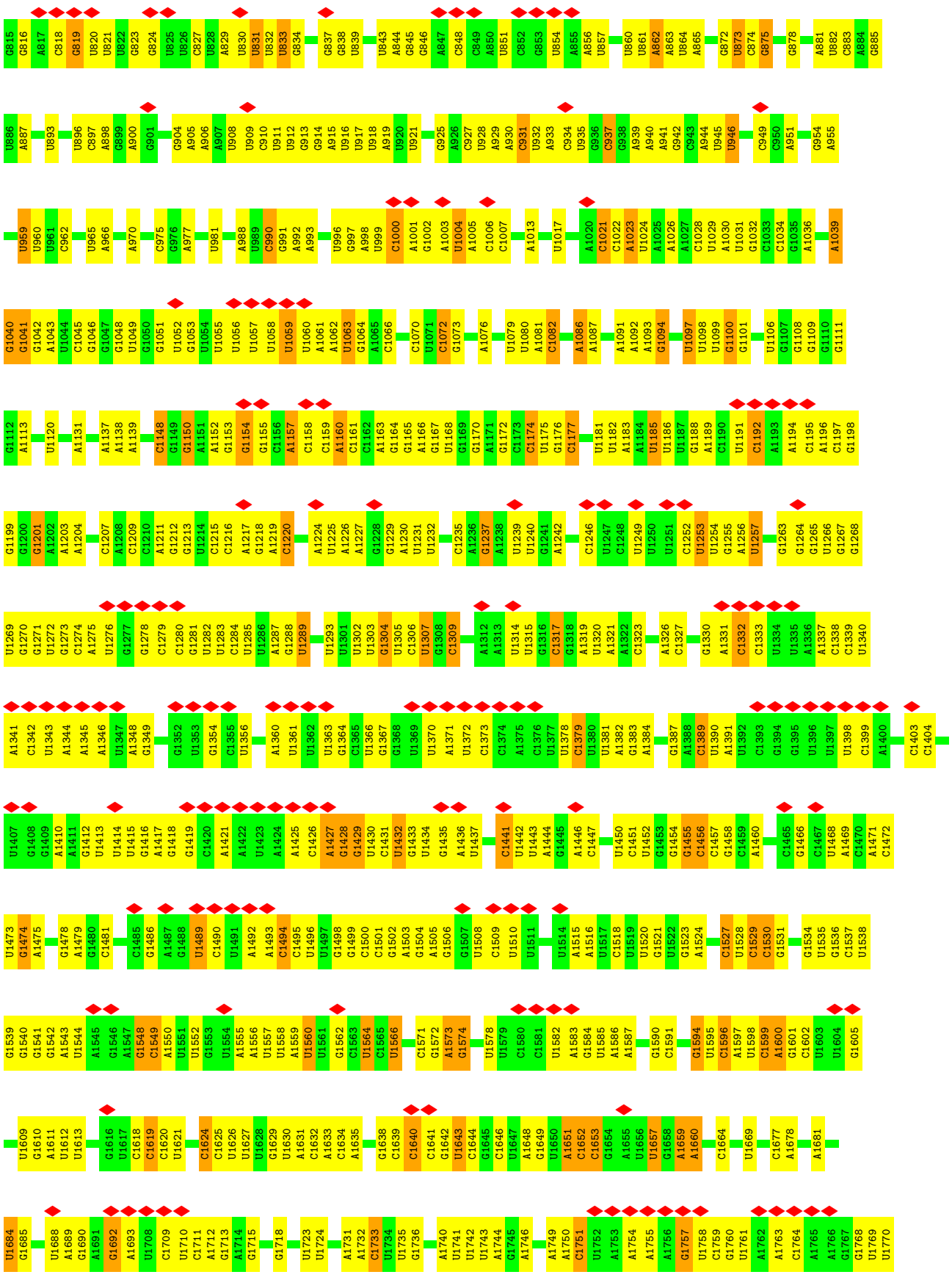
3 Residue-property plots (i)

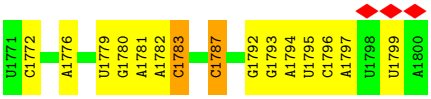
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 20S ribosomal RNA

Chain 2:

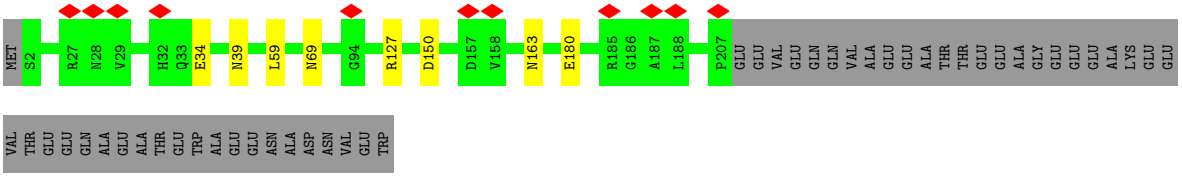






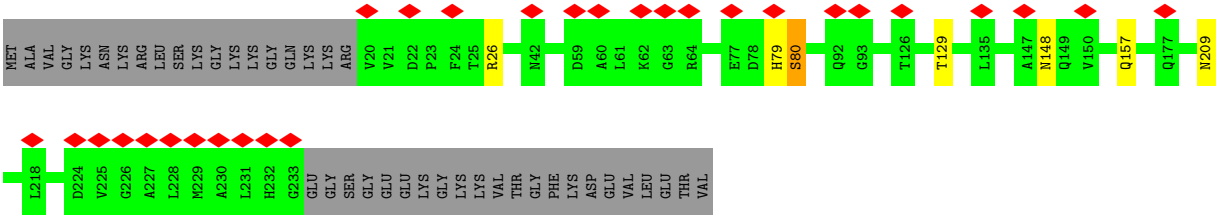
• Molecule 2: 40S ribosomal protein S0-A

Chain A:



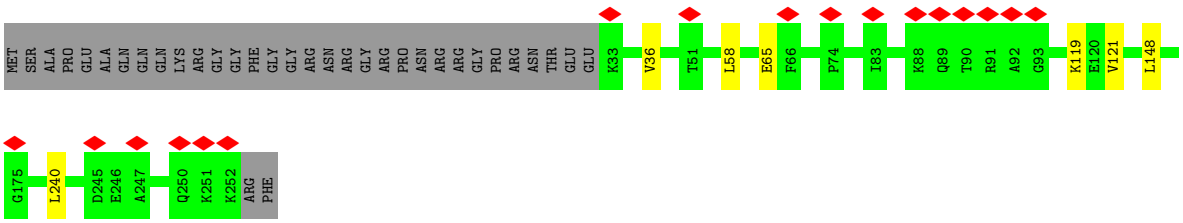
• Molecule 3: 40S ribosomal protein S1-A

Chain B:



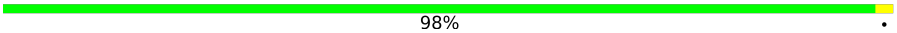
• Molecule 4: 40S ribosomal protein S2

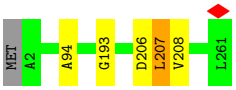
Chain C:



• Molecule 5: 40S ribosomal protein S4-A

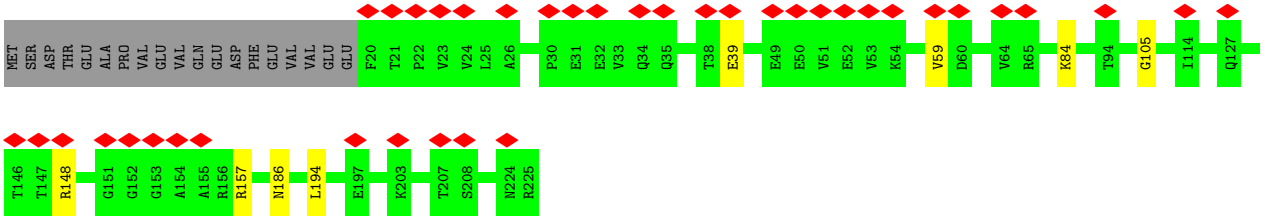
Chain E:



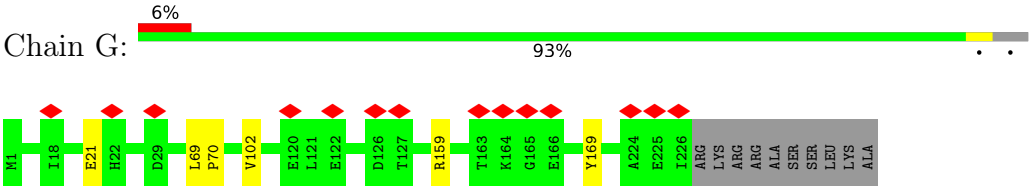


• Molecule 6: 40S ribosomal protein S5

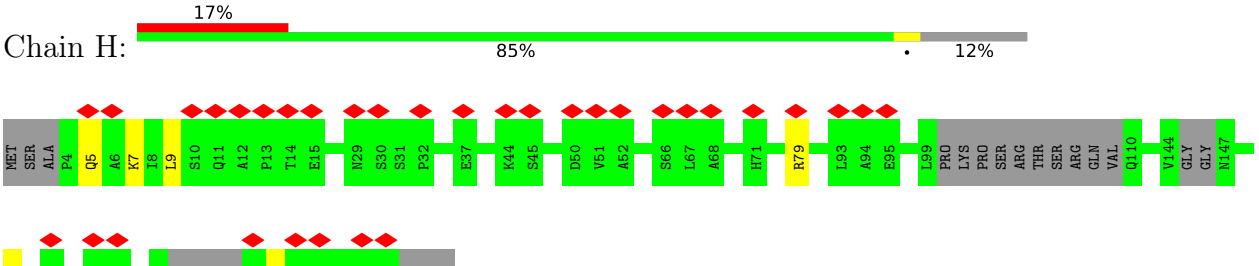
Chain F:



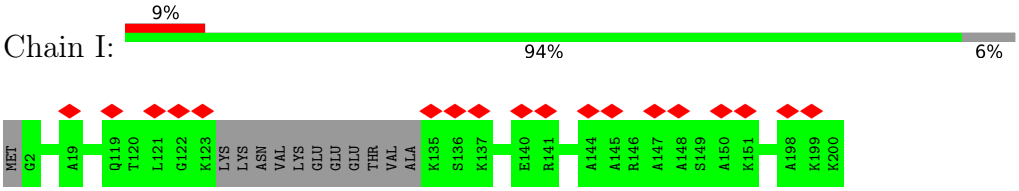
• Molecule 7: 40S ribosomal protein S6-A



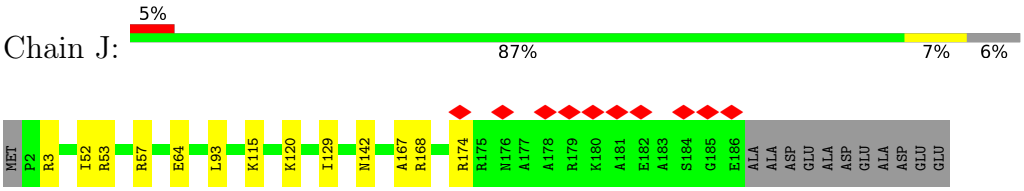
• Molecule 8: 40S ribosomal protein S7-A



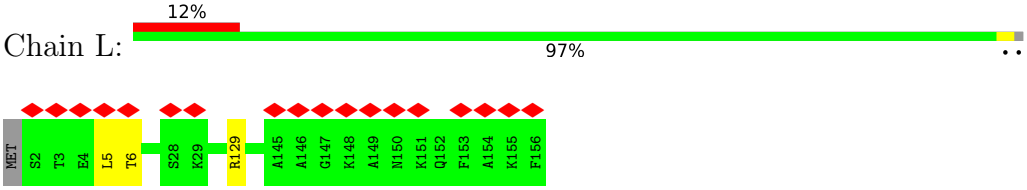
• Molecule 9: 40S ribosomal protein S8-A



• Molecule 10: 40S ribosomal protein S9-A

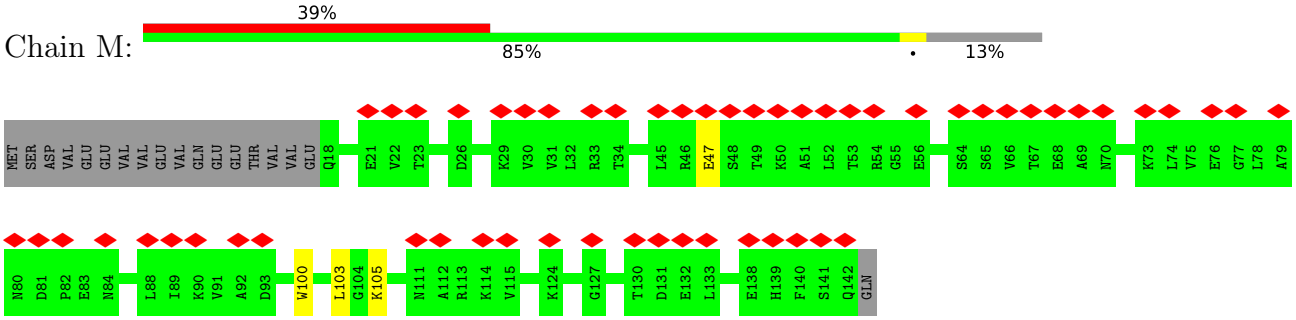


• Molecule 11: 40S ribosomal protein S11-A



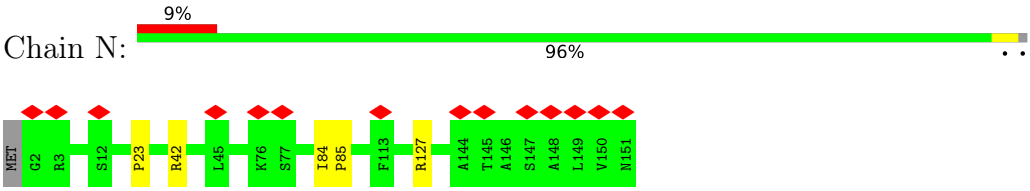
• Molecule 12: 40S ribosomal protein S12

Chain M:



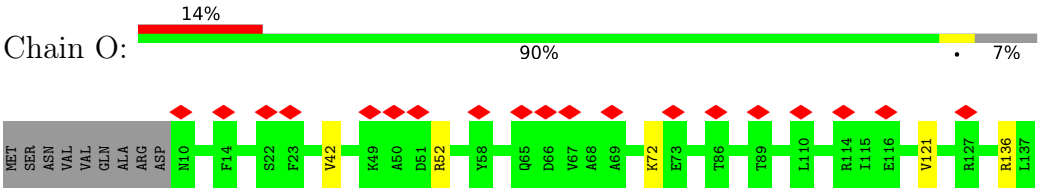
• Molecule 13: 40S ribosomal protein S13

Chain N:



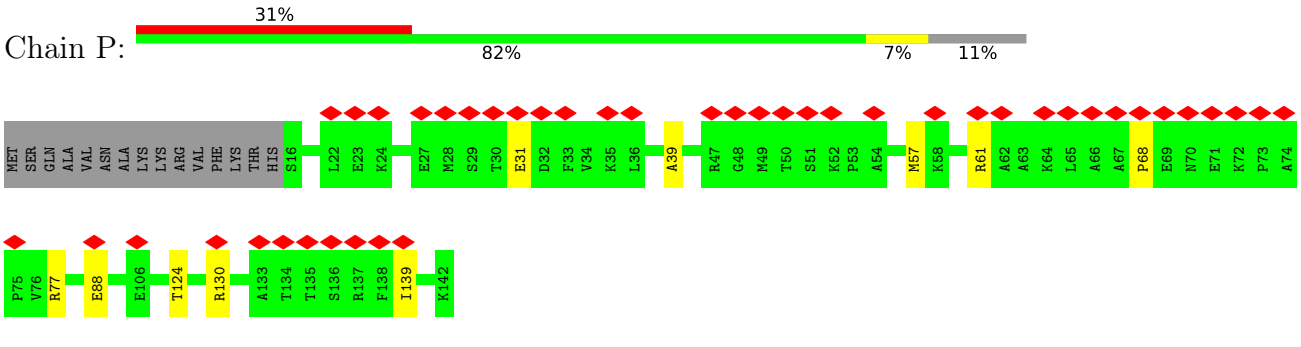
• Molecule 14: 40S ribosomal protein S14-A

Chain O:



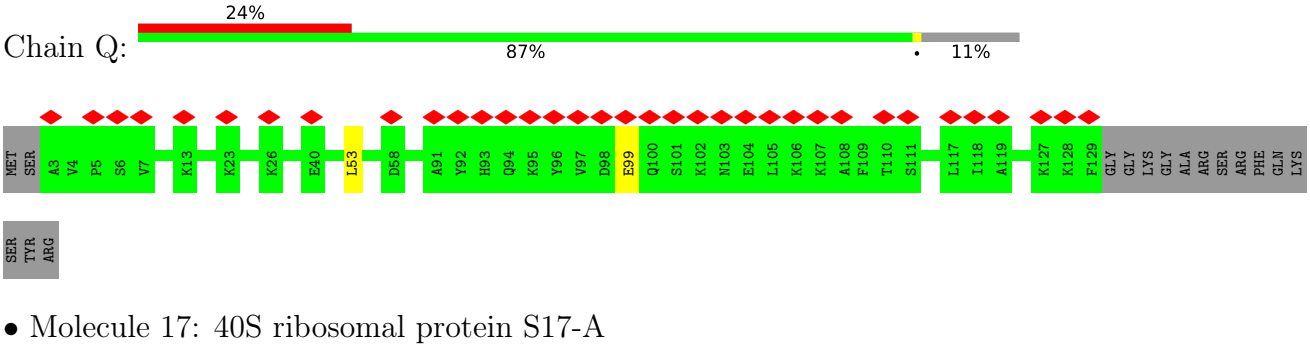
• Molecule 15: 40S ribosomal protein S15

Chain P:



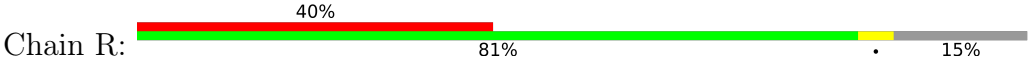
• Molecule 16: 40S ribosomal protein S16-A

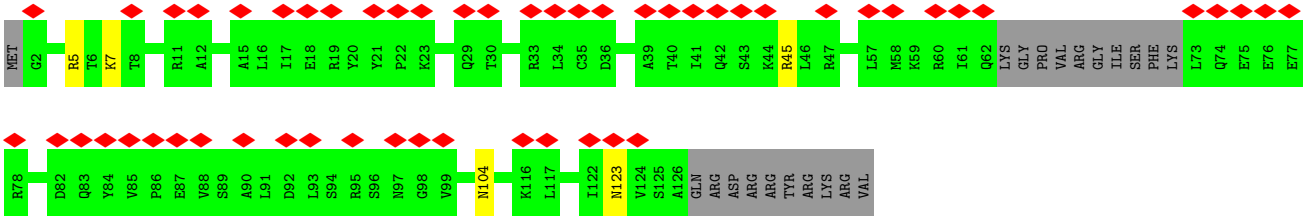
Chain Q:



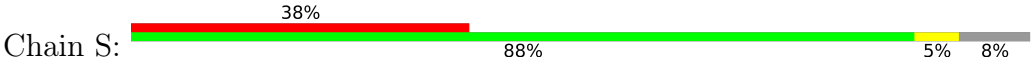
• Molecule 17: 40S ribosomal protein S17-A

Chain R:

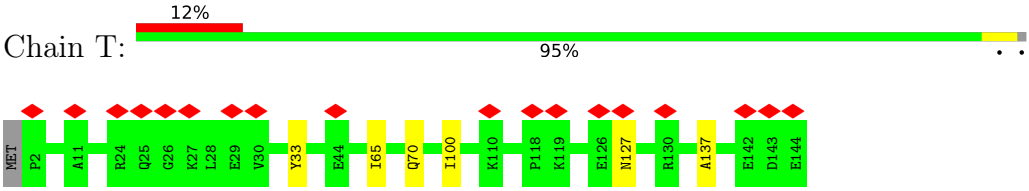




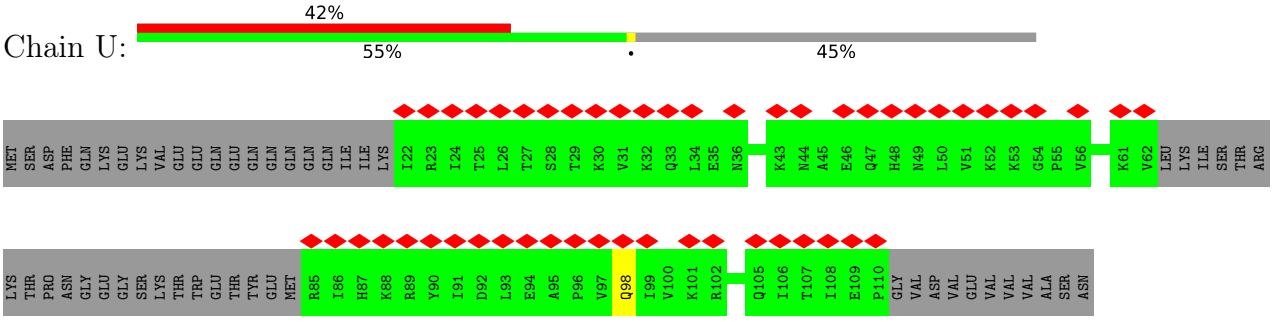
• Molecule 18: 40S ribosomal protein S18-A



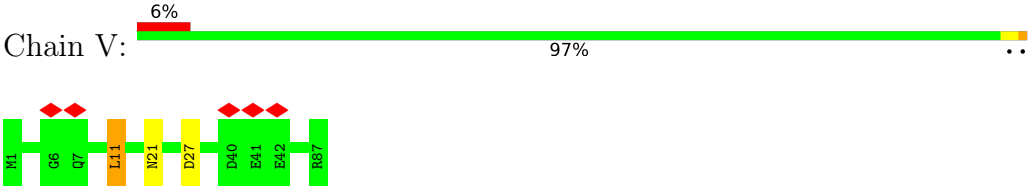
• Molecule 19: 40S ribosomal protein S19-A



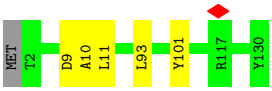
• Molecule 20: 40S ribosomal protein S20



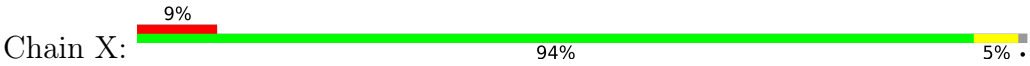
• Molecule 21: 40S ribosomal protein S21-A

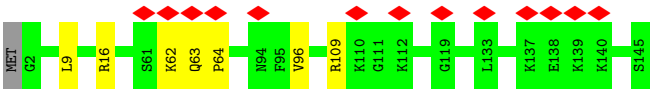


• Molecule 22: 40S ribosomal protein S22-A

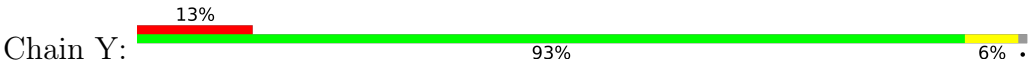


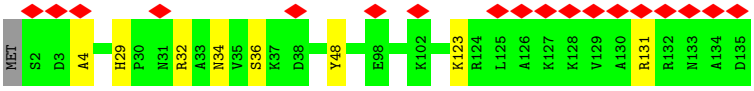
• Molecule 23: 40S ribosomal protein S23-A



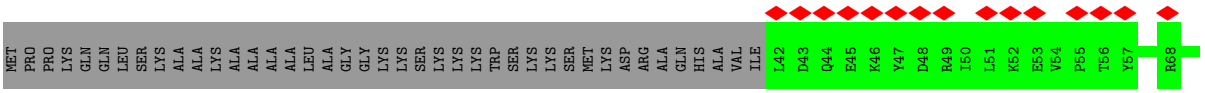


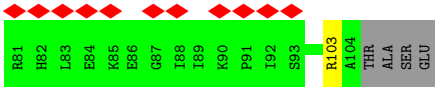
• Molecule 24: 40S ribosomal protein S24-A



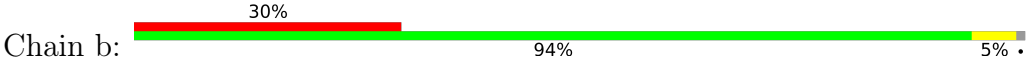


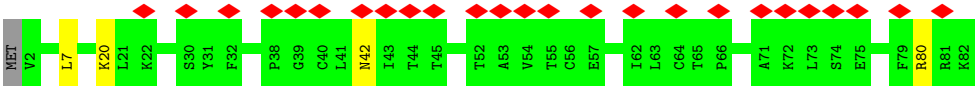
• Molecule 25: 40S ribosomal protein S25-A



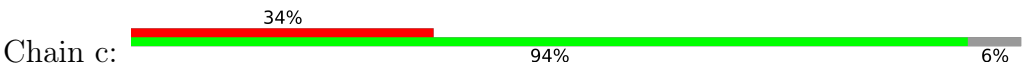


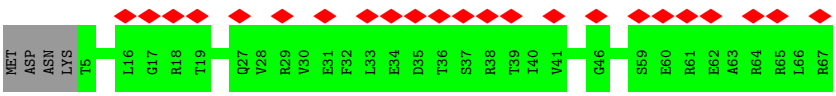
• Molecule 26: 40S ribosomal protein S27-A



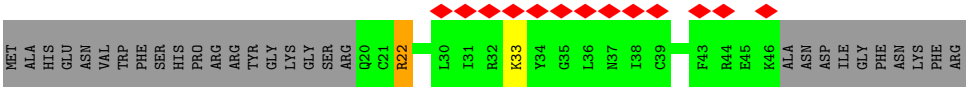


• Molecule 27: 40S ribosomal protein S28-A



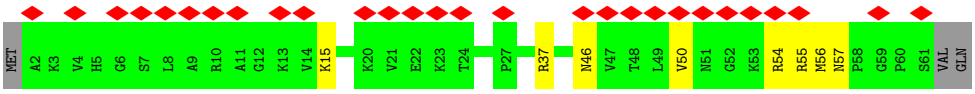


• Molecule 28: 40S ribosomal protein S29-A



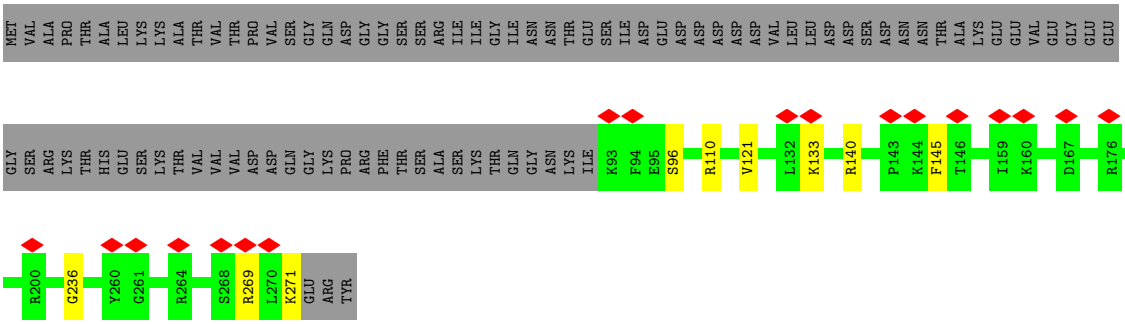
• Molecule 29: 40S ribosomal protein S30-A

Chain e:



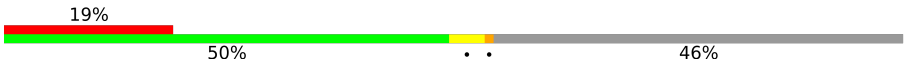
• Molecule 30: Pre-rRNA-processing protein PNO1

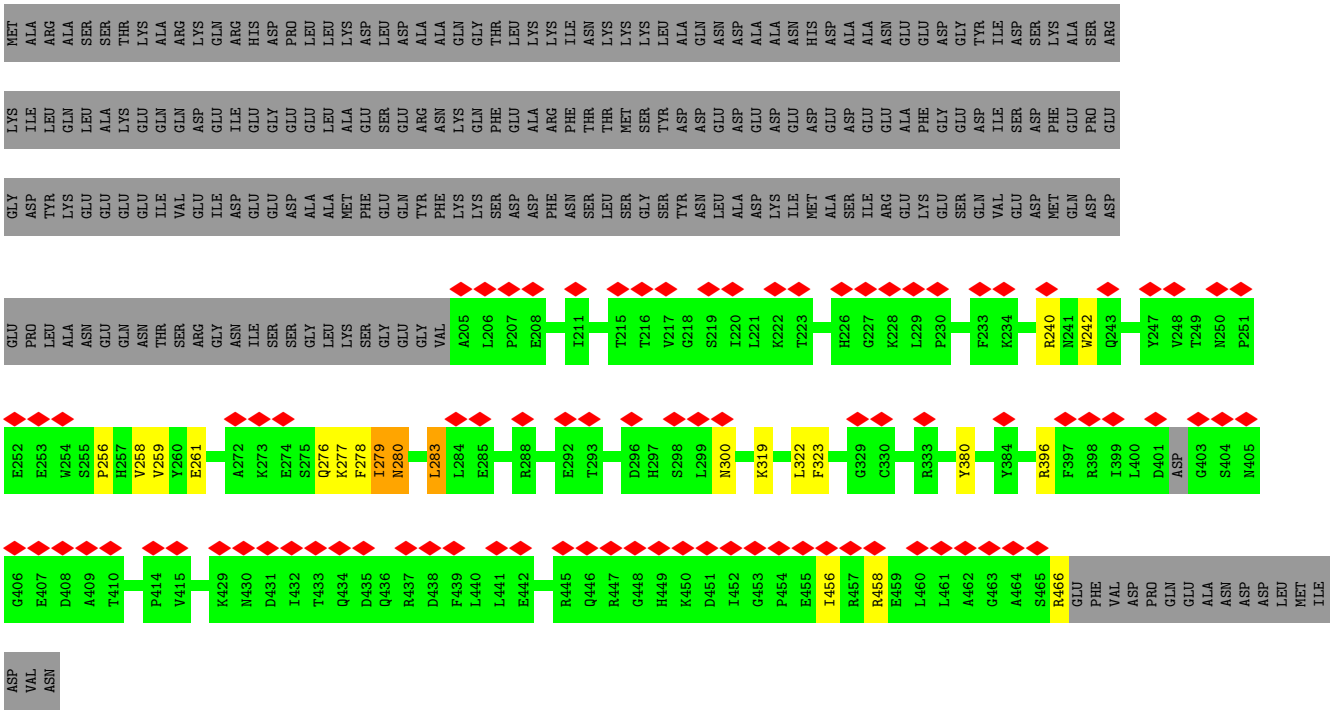
Chain h:



• Molecule 31: Essential nuclear protein 1

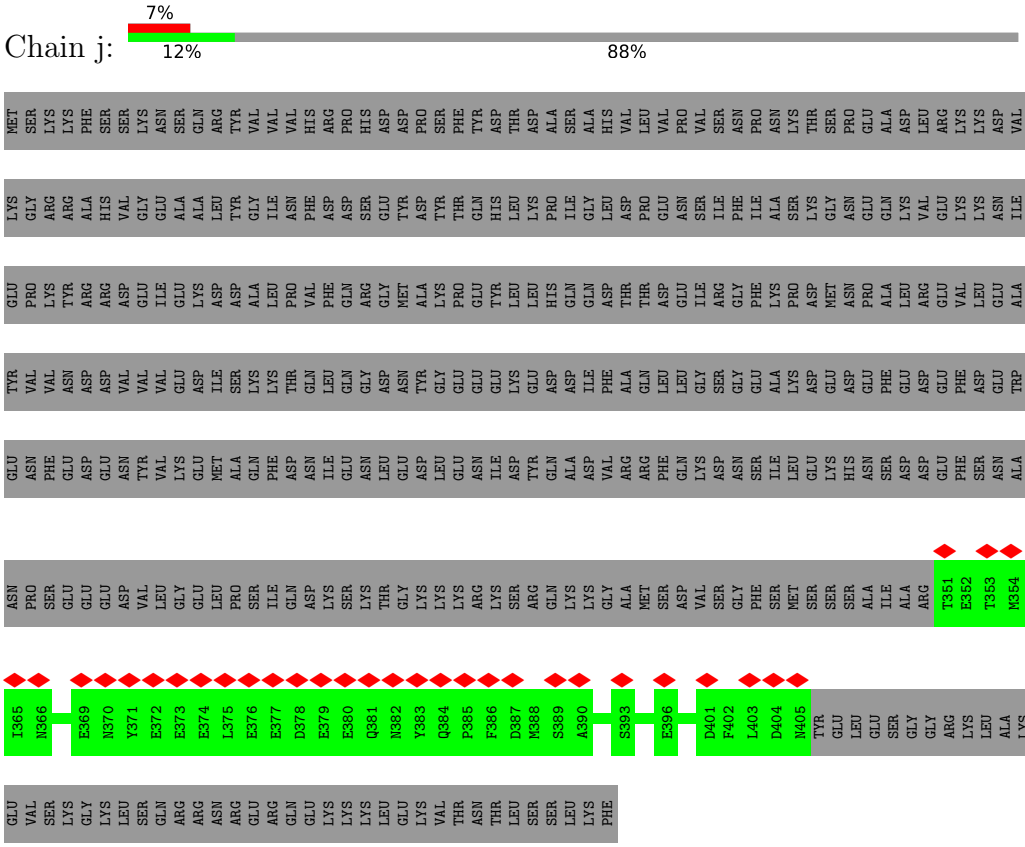
Chain i:





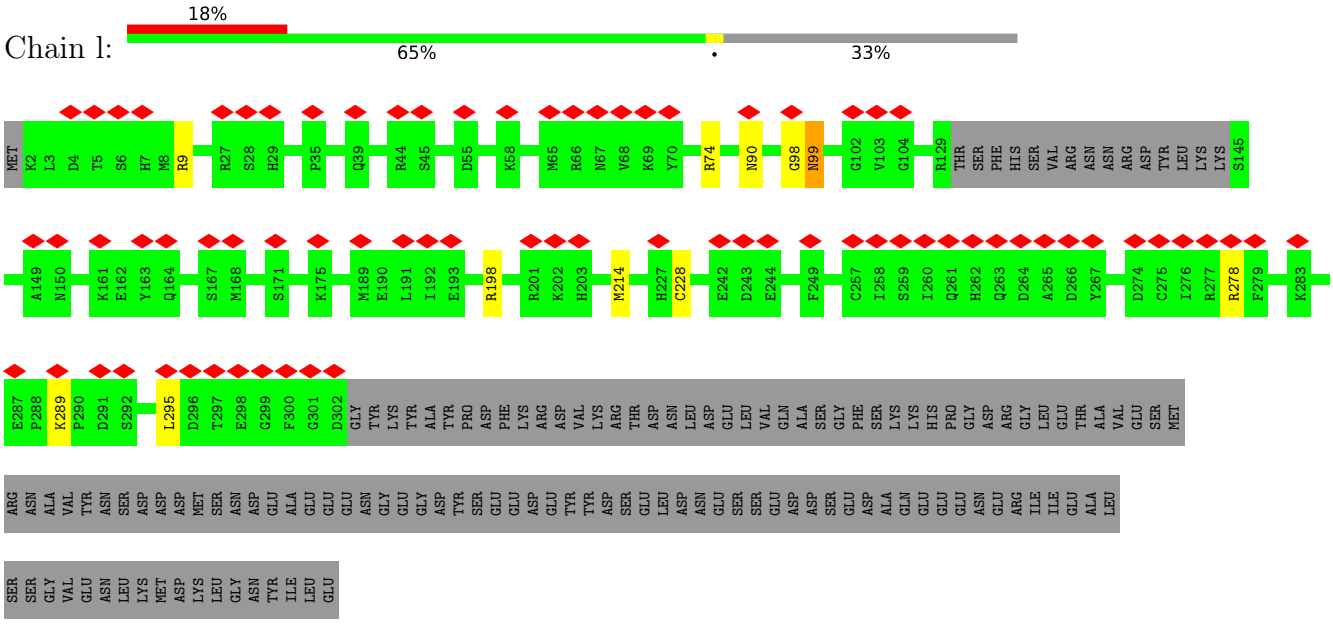
• Molecule 32: Protein LTV1

Chain j:



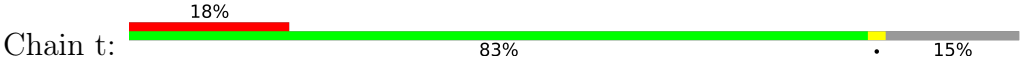
• Molecule 33: Serine/threonine-protein kinase RIO2

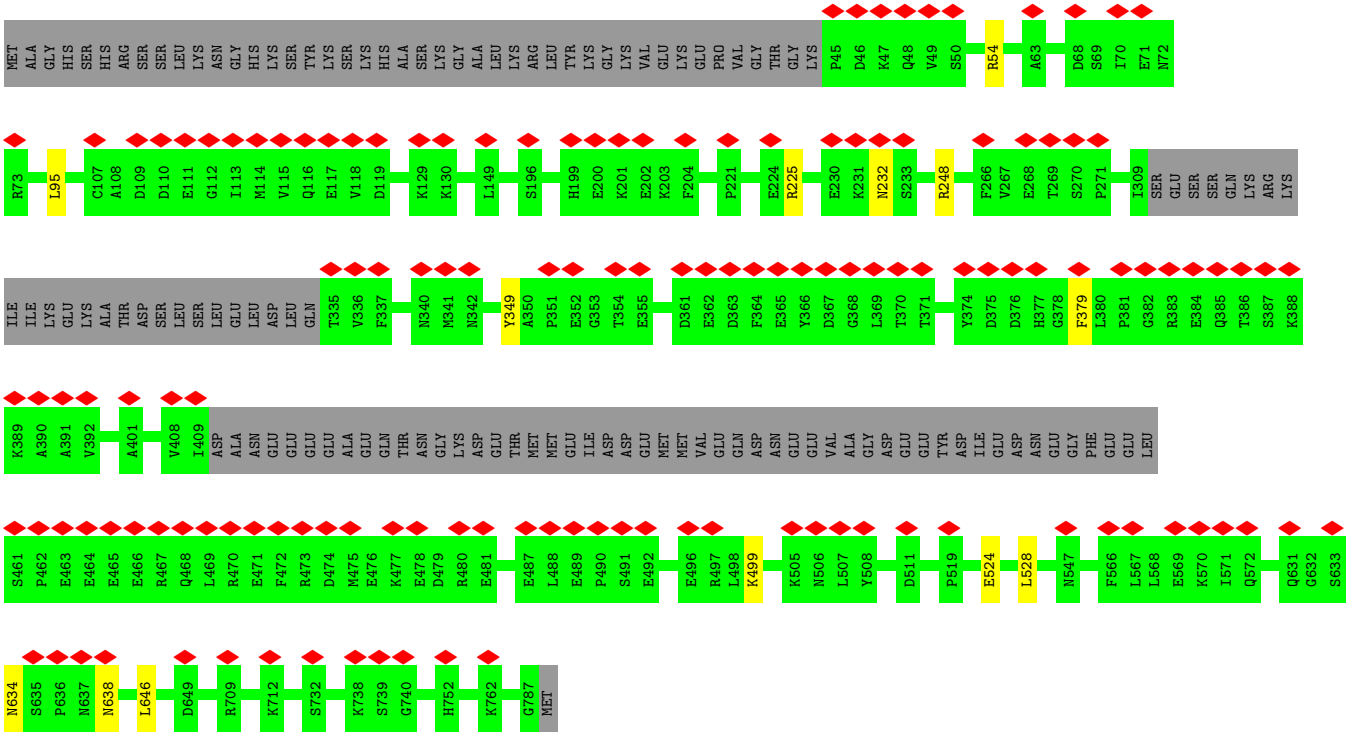
Chain l:



• Molecule 34: Ribosome biogenesis protein TSR1

Chain t:




MET ALA GLY HIS SER HIS ARG SER SER LEU LYS ASN GLY HIS LYS SER TYR LYS SER LYS HIS ALA SER LYS GLY ALA LEU LYS ARG LEU TYR LYS GLY LYS VAL GLU LYS GLU PRO VAL GLY THR GLY LYS P45 D46 K47 Q48 V49 S50 R54 A63 D68 S69 I70 E71 N72
R73 L95 C107 A108 D109 D110 E111 G112 I113 M114 V115 Q116 E117 V118 D119 K129 K130 L149 S196 H199 E200 K201 E202 K203 F204 P221 E224 R225 E230 K231 N232 S233 R248 F266 V267 E268 T269 S270 P271 I309 SER GLU SER SER GLN LYS ARG LYS
ILE ILE LYS GLU LYS ALA THR ASP SER LEU SER LEU GLU LEU ASP LEU GLN T335 V336 F337 N340 M341 N342 Y349 A350 P351 E352 G353 T354 E355 D361 E362 D363 F364 E365 Y366 D367 G368 L369 T370 T371 Y374 D375 D376 H377 G378 F379 L380 P381 G382 R383 E384 Q385 T386 S387 K388
K389 A390 A391 V392 A401 V408 I409 ASP ALA ASN GLU GLU GLU GLU ALA GLU GLN THR ASN GLY LYS ASP GLU THR MET MET GLU ILE ASP ASP GLU MET MET VAL GLU GLN ASP ASN GLU GLU VAL ALA GLY ASP GLU GLU TYR ASP ILE GLU GLU ASP ASN GLU GLY PHE GLU GLU LEU
S461 P462 E463 E464 E465 E466 R467 Q468 L469 R470 E471 F472 R473 D474 M475 E476 K477 E478 D479 R480 E481 E487 L488 E489 P490 S491 E492 E496 R497 L498 K499 K505 N506 L507 Y508 D511 P519 E524 L528 N547 F566 L567 L568 E569 K570 I571 Q572 Q631 G632 S633
N634 S635 P636 N637 N638 L646 D649 R709 K712 S732 K738 S739 G740 H752 K762 G787 MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19564	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 ($e^-/Å^2$)	29.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.410	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	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)

Bond lengths and bond angles in the following residue types are not validated in this section: A2M

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	0.78	6/41219 (0.0%)	1.41	607/64175 (0.9%)
2	A	0.33	0/1656	0.63	1/2264 (0.0%)
3	B	0.31	0/1733	0.68	0/2329
4	C	0.32	0/1692	0.66	2/2296 (0.1%)
5	E	0.38	0/2109	0.72	1/2839 (0.0%)
6	F	0.29	0/1629	0.65	0/2202
7	G	0.33	0/1823	0.63	0/2439
8	H	0.32	0/1382	0.73	1/1857 (0.1%)
9	I	0.38	0/1514	0.65	0/2021
10	J	0.33	0/1519	0.72	1/2035 (0.0%)
11	L	0.43	0/1239	0.60	0/1673
12	M	0.31	0/942	0.70	0/1263
13	N	0.32	0/1216	0.66	0/1638
14	O	0.31	0/961	0.63	0/1290
15	P	0.37	0/1020	0.66	0/1367
16	Q	0.36	0/1011	0.78	0/1362
17	R	0.27	0/931	0.65	0/1249
18	S	0.30	0/1128	0.72	0/1518
19	T	0.31	0/1129	0.60	0/1514
20	U	0.27	0/545	0.59	0/733
21	V	0.33	0/693	0.66	0/932
22	W	0.35	0/1036	0.68	0/1393
23	X	0.36	0/1139	0.79	2/1518 (0.1%)
24	Y	0.40	0/1087	0.73	0/1449
25	Z	0.27	0/519	0.55	0/696
26	b	0.30	0/621	0.64	0/838
27	c	0.28	0/499	0.61	0/670
28	d	0.29	0/221	0.69	0/291
29	e	0.35	0/483	0.72	0/643
30	h	0.31	0/1441	0.69	0/1940
31	i	0.36	0/2179	0.76	1/2956 (0.0%)
32	j	0.29	0/470	0.64	0/632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	l	0.32	0/2364	0.63	1/3169 (0.0%)
34	t	2.60	7/5520 (0.1%)	0.64	4/7456 (0.1%)
All	All	0.89	13/84670 (0.0%)	1.12	621/122647 (0.5%)

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	1
3	B	0	4
4	C	0	2
5	E	0	3
6	F	0	3
7	G	0	2
8	H	0	3
10	J	0	4
11	L	0	2
12	M	0	2
13	N	0	1
14	O	0	2
15	P	0	6
16	Q	0	1
17	R	0	1
18	S	0	6
19	T	0	5
20	U	0	1
21	V	0	1
22	W	0	2
23	X	0	2
24	Y	0	4
26	b	0	1
29	e	0	6
30	h	0	4
31	i	0	13
33	l	0	4
34	t	0	5
All	All	0	91

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	t	524	GLU	CB-CG	157.17	4.50	1.52
1	2	436	A2M	O3'-P	-83.60	0.60	1.61
1	2	420	A2M	O3'-P	-60.90	0.88	1.61
34	t	349	TYR	CD1-CE1	58.33	2.26	1.39
34	t	349	TYR	CD2-CE2	57.92	2.26	1.39

The worst 5 of 621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	420	A2M	P-O3'-C3'	-62.56	44.63	119.70
1	2	796	A2M	OP2-P-O3'	-35.31	27.51	105.20
1	2	436	A2M	O3'-P-O5'	-31.29	44.55	104.00
1	2	420	A2M	OP1-P-O3'	-29.92	39.37	105.20
1	2	436	A2M	P-O3'-C3'	-29.56	84.23	119.70

There are no chirality outliers.

5 of 91 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	34	GLU	Peptide
3	B	129	THR	Peptide
3	B	157	GLN	Peptide
3	B	79	HIS	Peptide
3	B	80	SER	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	
2	A	204/252 (81%)	184 (90%)	20 (10%)	0	100	100
3	B	208/255 (82%)	174 (84%)	33 (16%)	1 (0%)	29	66
4	C	218/254 (86%)	191 (88%)	27 (12%)	0	100	100
5	E	258/261 (99%)	218 (84%)	38 (15%)	2 (1%)	19	57
6	F	204/225 (91%)	168 (82%)	36 (18%)	0	100	100
7	G	224/236 (95%)	200 (89%)	22 (10%)	2 (1%)	17	54
8	H	160/190 (84%)	130 (81%)	30 (19%)	0	100	100
9	I	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
10	J	183/197 (93%)	149 (81%)	33 (18%)	1 (0%)	29	66
11	L	153/156 (98%)	126 (82%)	27 (18%)	0	100	100
12	M	111/143 (78%)	83 (75%)	28 (25%)	0	100	100
13	N	148/151 (98%)	133 (90%)	13 (9%)	2 (1%)	11	46
14	O	126/137 (92%)	108 (86%)	18 (14%)	0	100	100
15	P	121/142 (85%)	96 (79%)	25 (21%)	0	100	100
16	Q	125/143 (87%)	93 (74%)	32 (26%)	0	100	100
17	R	111/136 (82%)	98 (88%)	13 (12%)	0	100	100
18	S	133/146 (91%)	112 (84%)	21 (16%)	0	100	100
19	T	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
20	U	61/121 (50%)	56 (92%)	5 (8%)	0	100	100
21	V	83/87 (95%)	66 (80%)	16 (19%)	1 (1%)	13	50
22	W	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	9	44
23	X	142/145 (98%)	123 (87%)	18 (13%)	1 (1%)	22	60
24	Y	132/135 (98%)	107 (81%)	24 (18%)	1 (1%)	19	57
25	Z	61/108 (56%)	55 (90%)	6 (10%)	0	100	100
26	b	79/82 (96%)	70 (89%)	8 (10%)	1 (1%)	12	48
27	c	61/67 (91%)	52 (85%)	9 (15%)	0	100	100
28	d	25/56 (45%)	23 (92%)	1 (4%)	1 (4%)	3	28
29	e	58/63 (92%)	41 (71%)	17 (29%)	0	100	100
30	h	176/274 (64%)	157 (89%)	19 (11%)	0	100	100
31	i	257/483 (53%)	200 (78%)	55 (21%)	2 (1%)	19	57
32	j	51/463 (11%)	42 (82%)	9 (18%)	0	100	100
33	l	274/425 (64%)	241 (88%)	33 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	t	649/788 (82%)	577 (89%)	72 (11%)	0	100 100
All	All	5246/6795 (77%)	4478 (85%)	751 (14%)	17 (0%)	44 74

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	207	LEU
5	E	208	VAL
22	W	11	LEU
31	i	279	ILE
3	B	80	SER

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	172/210 (82%)	166 (96%)	6 (4%)	36 64
3	B	191/224 (85%)	188 (98%)	3 (2%)	62 79
4	C	179/205 (87%)	176 (98%)	3 (2%)	60 78
5	E	221/222 (100%)	221 (100%)	0	100 100
6	F	173/191 (91%)	168 (97%)	5 (3%)	42 67
7	G	188/201 (94%)	186 (99%)	2 (1%)	73 85
8	H	151/170 (89%)	149 (99%)	2 (1%)	69 82
9	I	150/161 (93%)	150 (100%)	0	100 100
10	J	158/166 (95%)	151 (96%)	7 (4%)	28 57
11	L	129/137 (94%)	128 (99%)	1 (1%)	81 89
12	M	101/119 (85%)	99 (98%)	2 (2%)	55 75
13	N	127/128 (99%)	125 (98%)	2 (2%)	62 79
14	O	97/105 (92%)	94 (97%)	3 (3%)	40 65
15	P	105/118 (89%)	101 (96%)	4 (4%)	33 61
16	Q	107/119 (90%)	106 (99%)	1 (1%)	78 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	R	105/124 (85%)	101 (96%)	4 (4%)	33 61
18	S	120/129 (93%)	119 (99%)	1 (1%)	81 89
19	T	115/116 (99%)	114 (99%)	1 (1%)	78 88
20	U	64/114 (56%)	64 (100%)	0	100 100
21	V	74/74 (100%)	72 (97%)	2 (3%)	44 69
22	W	110/111 (99%)	109 (99%)	1 (1%)	78 88
23	X	119/120 (99%)	117 (98%)	2 (2%)	60 78
24	Y	112/113 (99%)	109 (97%)	3 (3%)	44 69
25	Z	56/89 (63%)	55 (98%)	1 (2%)	59 77
26	b	70/71 (99%)	68 (97%)	2 (3%)	42 67
27	c	56/60 (93%)	56 (100%)	0	100 100
28	d	25/49 (51%)	23 (92%)	2 (8%)	12 42
29	e	51/54 (94%)	49 (96%)	2 (4%)	32 60
30	h	156/238 (66%)	151 (97%)	5 (3%)	39 65
31	i	233/424 (55%)	225 (97%)	8 (3%)	37 64
32	j	53/419 (13%)	52 (98%)	1 (2%)	57 76
33	l	260/384 (68%)	253 (97%)	7 (3%)	44 69
34	t	582/703 (83%)	577 (99%)	5 (1%)	78 88
All	All	4610/5868 (79%)	4522 (98%)	88 (2%)	59 76

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	b	80	ARG
31	i	300	ASN
28	d	33	LYS
30	h	269	ARG
32	j	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	127	HIS
34	t	144	ASN
22	W	56	HIS

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Mol	Chain	Res	Type
34	t	127	HIS
34	t	290	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1711/1735 (98%)	821 (47%)	28 (1%)

5 of 821 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	8	U
1	2	11	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	819	G
1	2	1652	C
1	2	1086	A
1	2	1573	A
1	2	1041	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	2	796	1	18,25,26	1.79	4 (22%)	18,36,39	1.98	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	2	420	1	18,25,26	1.25	3 (16%)	18,36,39	2.19	4 (22%)
1	A2M	2	100	1	18,25,26	1.65	5 (27%)	18,36,39	2.18	8 (44%)
1	A2M	2	436	1	18,25,26	1.47	4 (22%)	18,36,39	1.91	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	2	796	1	-	2/5/27/28	0/3/3/3
1	A2M	2	420	1	-	0/5/27/28	0/3/3/3
1	A2M	2	100	1	-	2/5/27/28	0/3/3/3
1	A2M	2	436	1	-	0/5/27/28	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	796	A2M	C5-C4	3.55	1.50	1.40
1	2	436	A2M	C5-C4	3.54	1.50	1.40
1	2	100	A2M	C5-C4	3.33	1.49	1.40
1	2	796	A2M	C2-N3	3.06	1.37	1.32
1	2	420	A2M	O4'-C1'	3.05	1.45	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	420	A2M	C5-C6-N6	-5.46	112.05	120.35
1	2	100	A2M	O5'-C5'-C4'	4.97	125.89	108.99
1	2	420	A2M	N6-C6-N1	4.70	128.33	118.57
1	2	420	A2M	N3-C2-N1	-4.28	121.99	128.68
1	2	436	A2M	N3-C2-N1	-4.01	122.41	128.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	100	A2M	O4'-C4'-C5'-O5'
1	2	100	A2M	C3'-C4'-C5'-O5'
1	2	796	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	796	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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
1	2	28
12	M	7
34	t	6
33	l	4
32	j	2
15	P	2
3	B	2
30	h	1
19	T	1
20	U	1
21	V	1

The worst 5 of 55 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1293:U	O3'	1301:U	P	19.14
1	2	658:C	O3'	676:G	P	16.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1693:A	O3'	1708:U	P	10.88
1	2	705:U	O3'	733:A	P	9.46
1	2	1508:U	O3'	1509:C	P	9.19

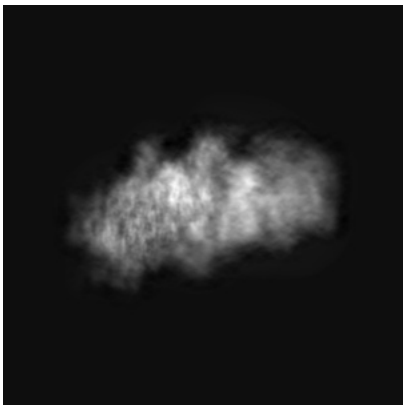
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10713. These allow visual inspection of the internal detail of the map and identification of artifacts.

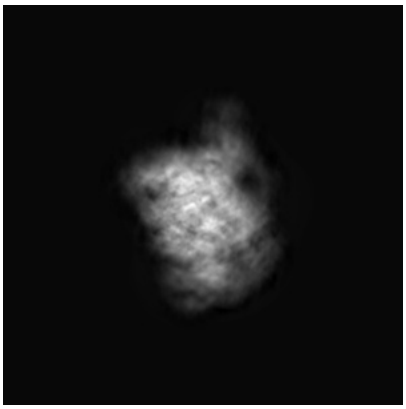
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

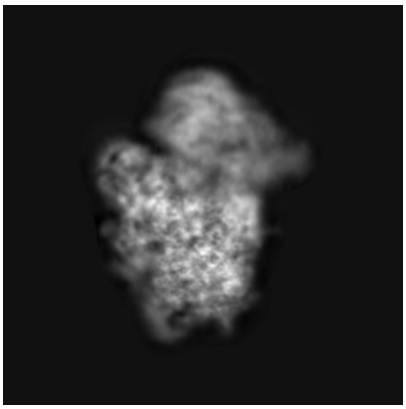
6.1.1 Primary map



X

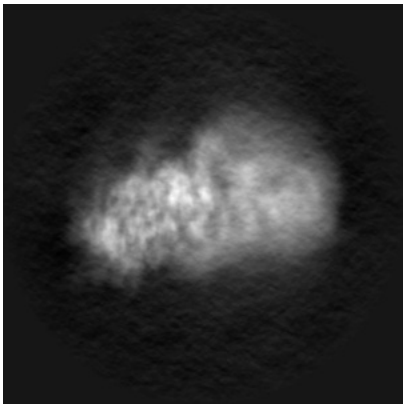


Y

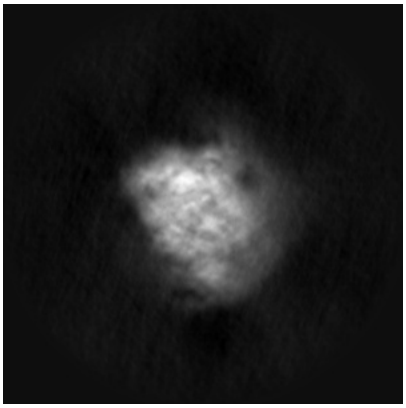


Z

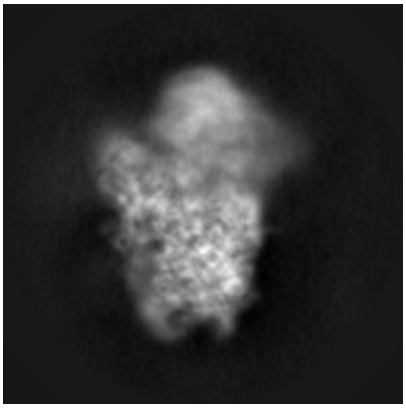
6.1.2 Raw map



X



Y

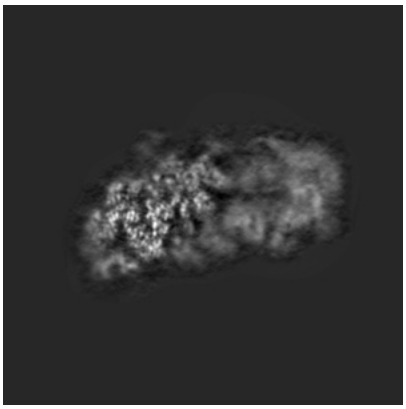


Z

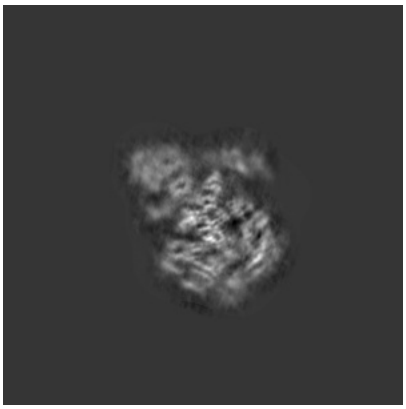
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

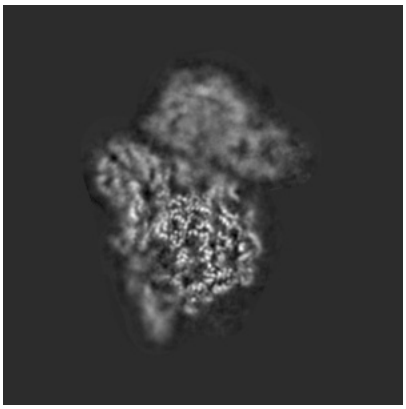
6.2.1 Primary map



X Index: 180

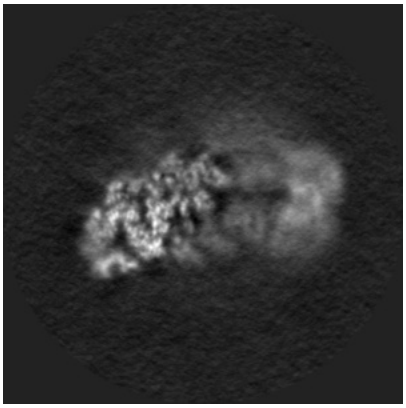


Y Index: 180

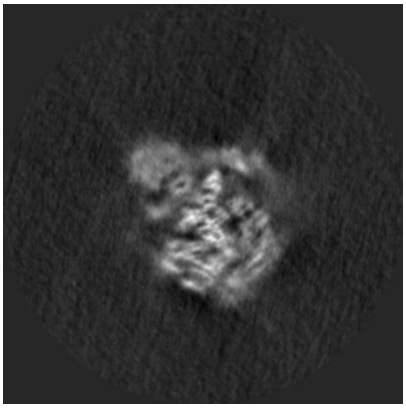


Z Index: 180

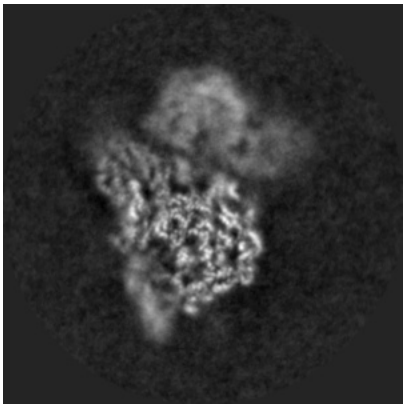
6.2.2 Raw map



X Index: 180



Y Index: 180

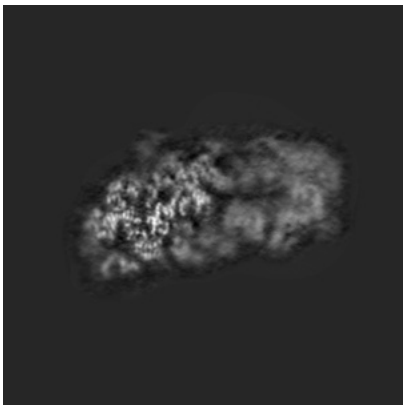


Z Index: 180

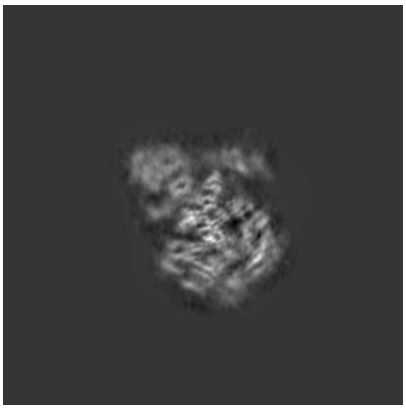
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

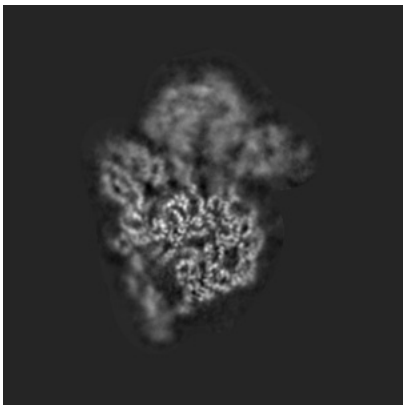
6.3.1 Primary map



X Index: 178

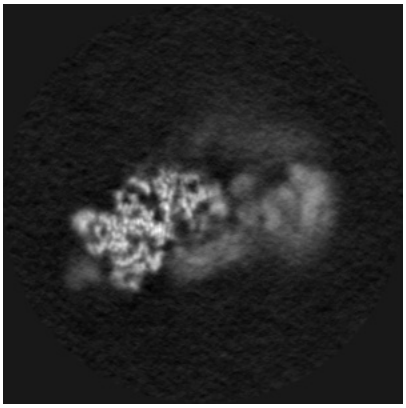


Y Index: 180

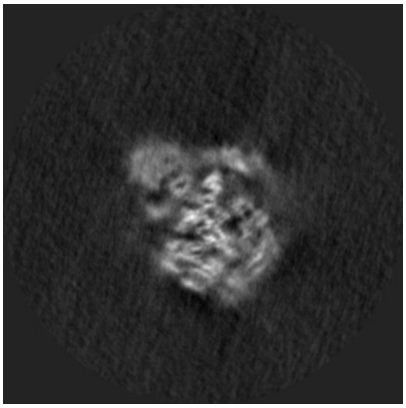


Z Index: 185

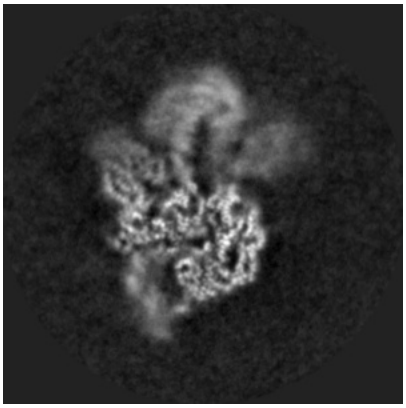
6.3.2 Raw map



X Index: 202



Y Index: 179



Z Index: 187

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 0.085. 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.

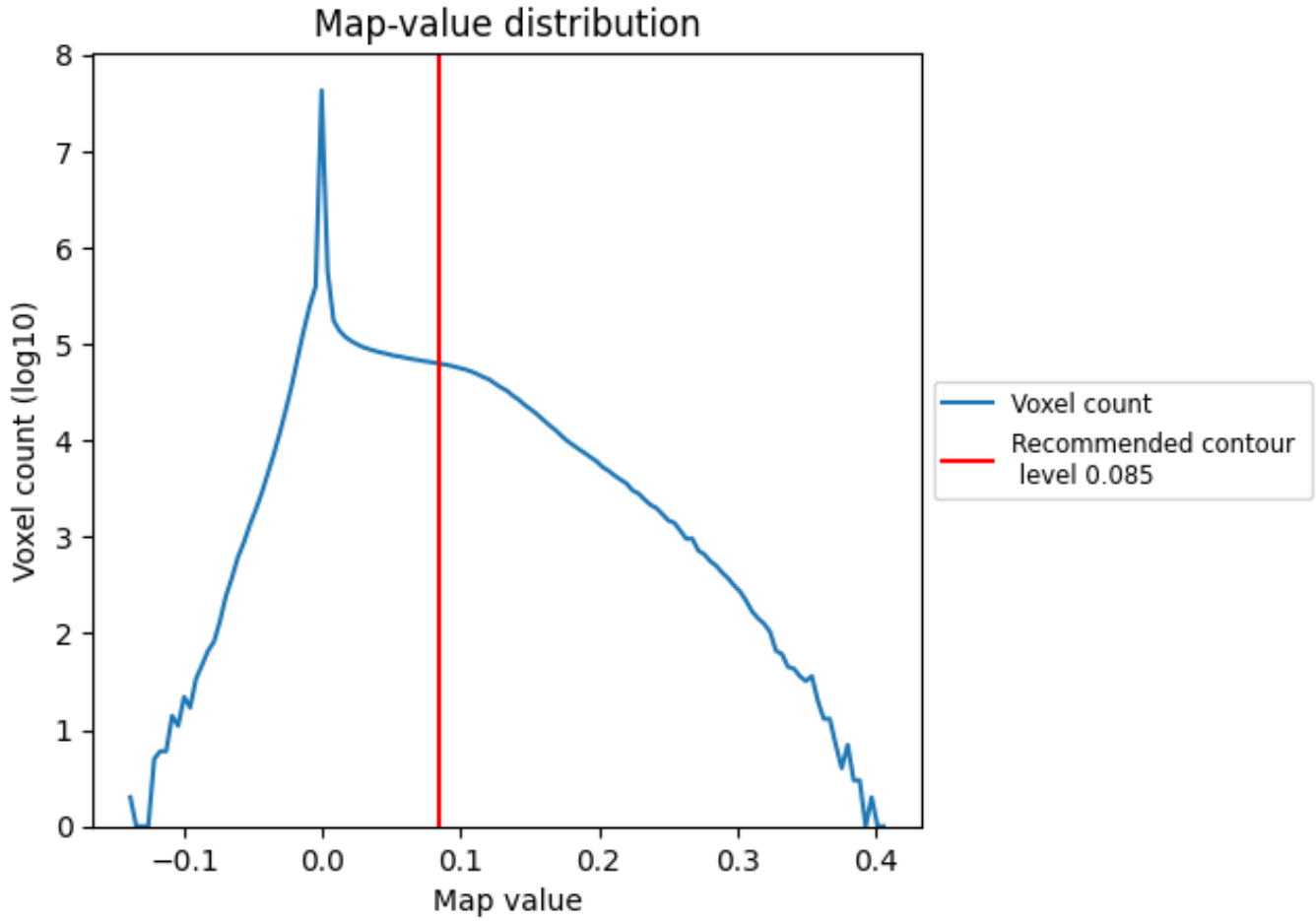
6.5 Mask visualisation (i)

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

7 Map analysis

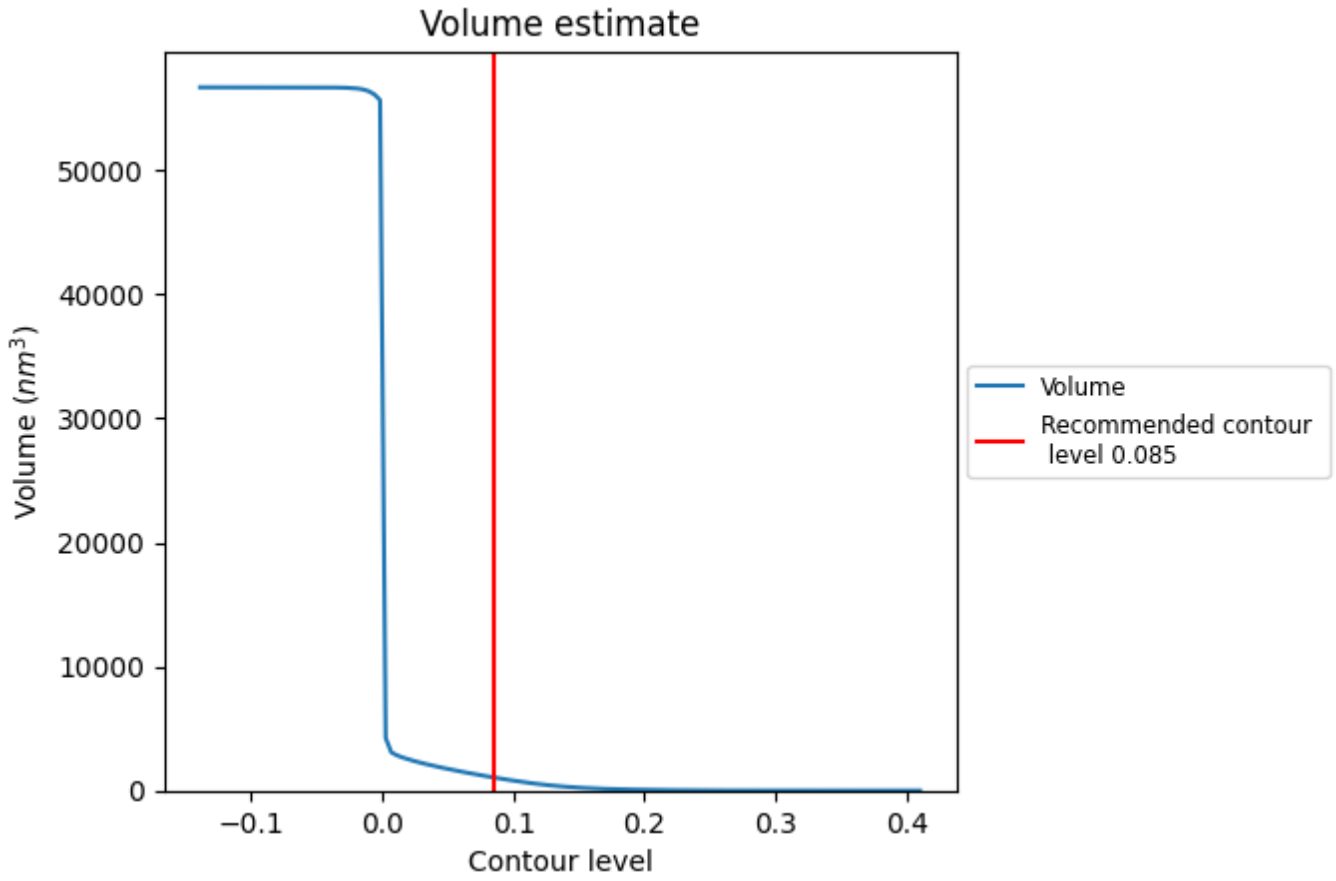
This section contains the results of statistical analysis of the map.

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.

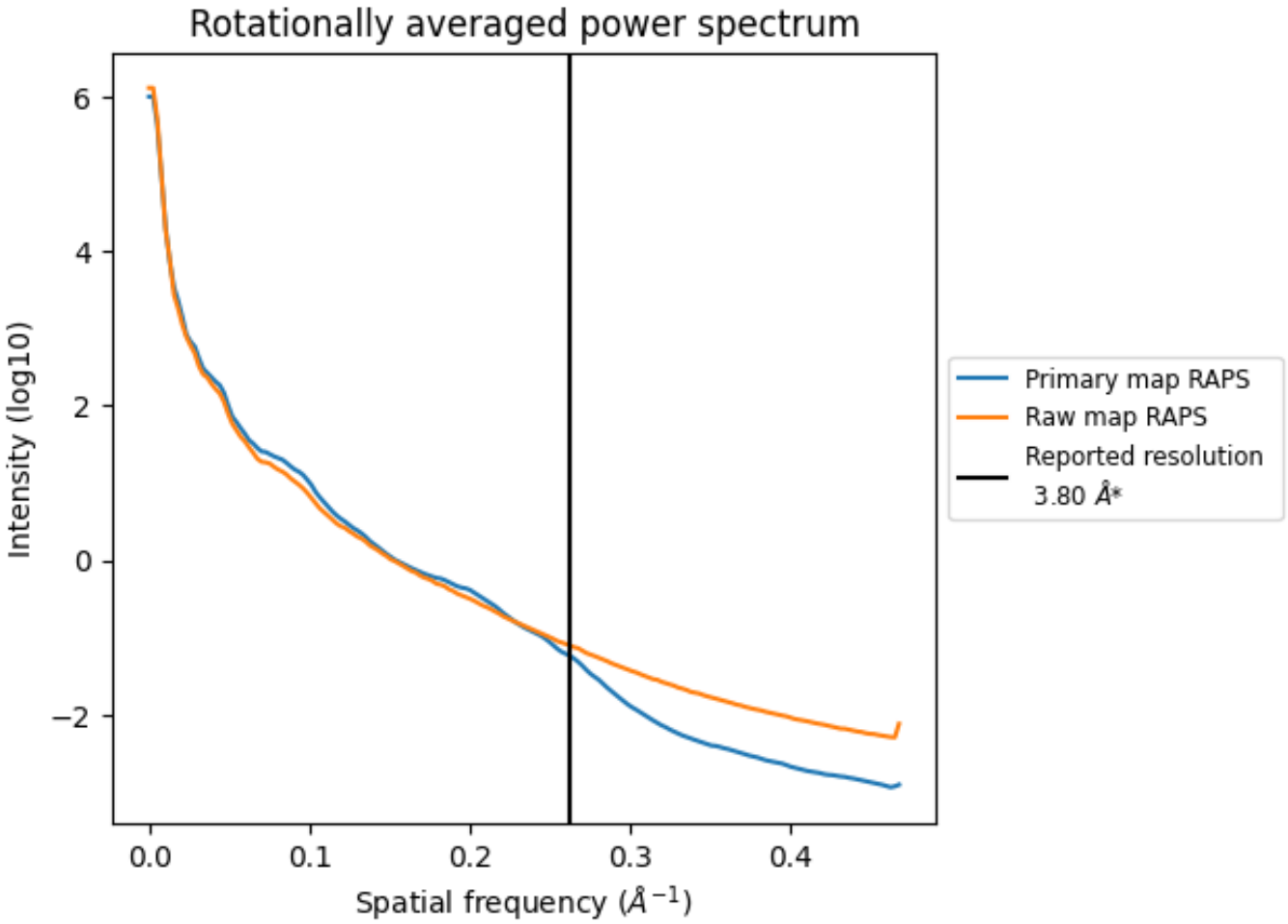
7.2 Volume estimate (i)



The volume at the recommended contour level is 1058 nm^3; this corresponds to an approximate mass of 955 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)

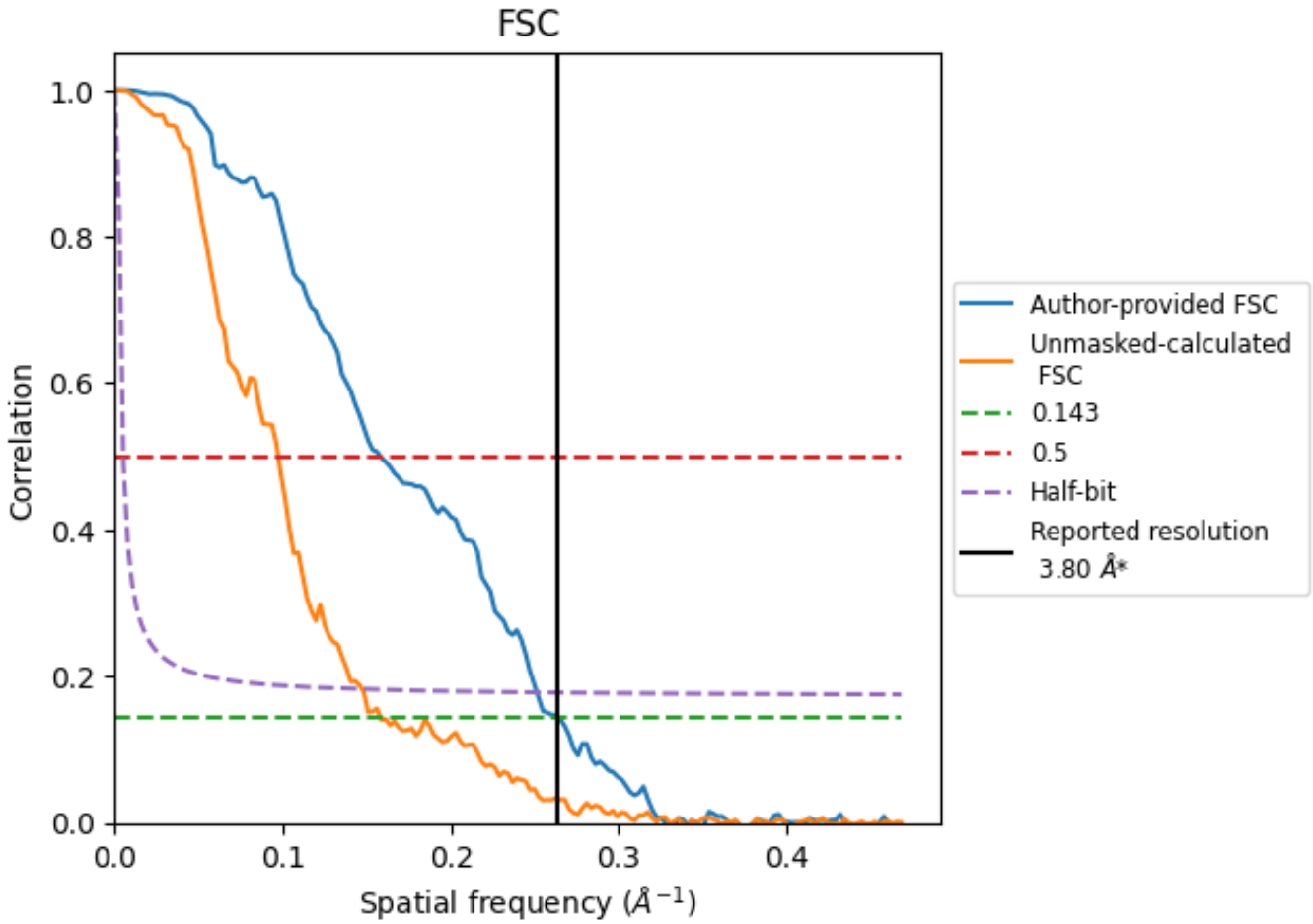


*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

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)

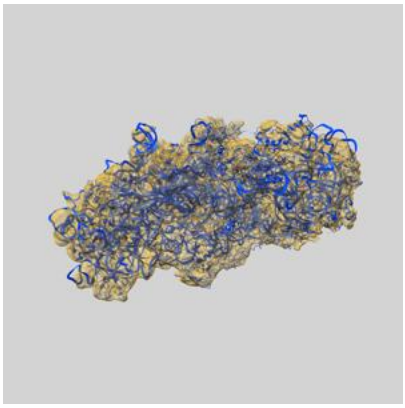
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	6.33	3.97
Unmasked-calculated*	6.31	10.27	6.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.31 differs from the reported value 3.8 by more than 10 %

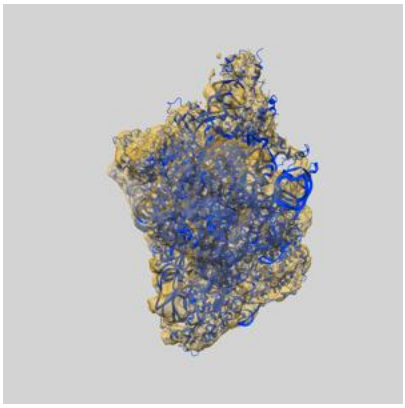
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10713 and PDB model 6Y7C. Per-residue inclusion information can be found in section 3 on page 11.

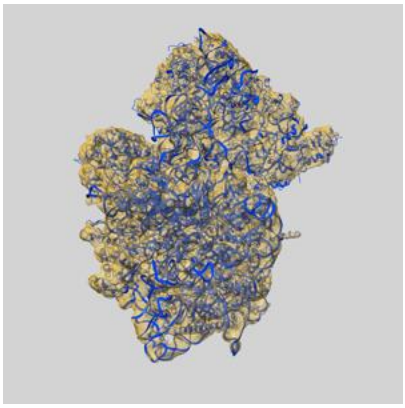
9.1 Map-model overlay



X



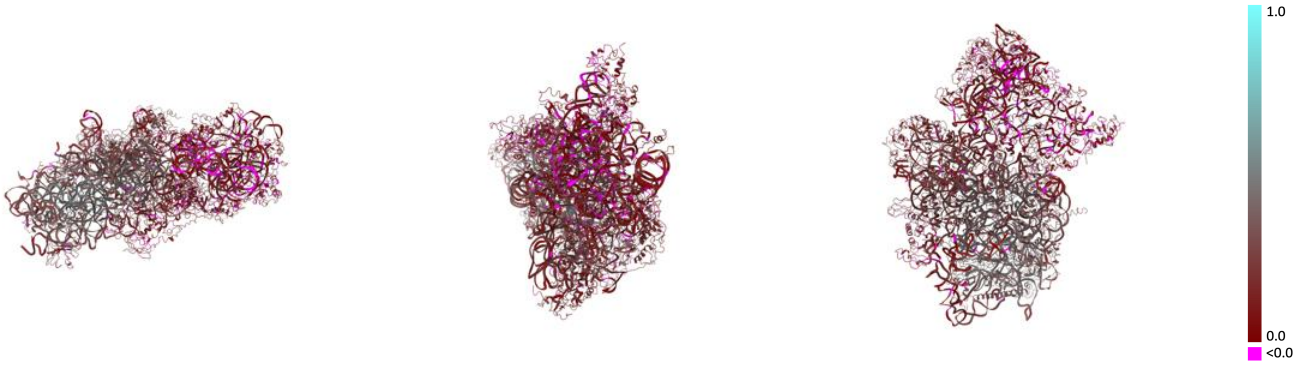
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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.

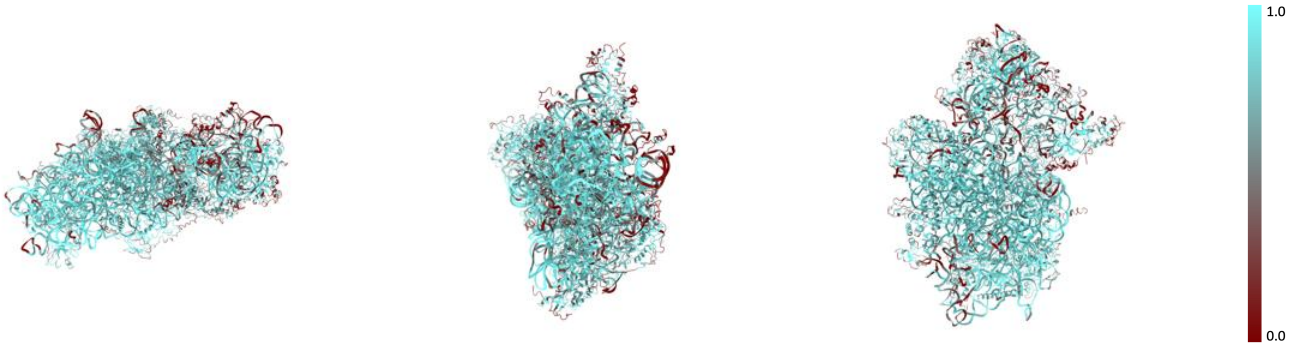
9.2 Q-score mapped to coordinate model



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.

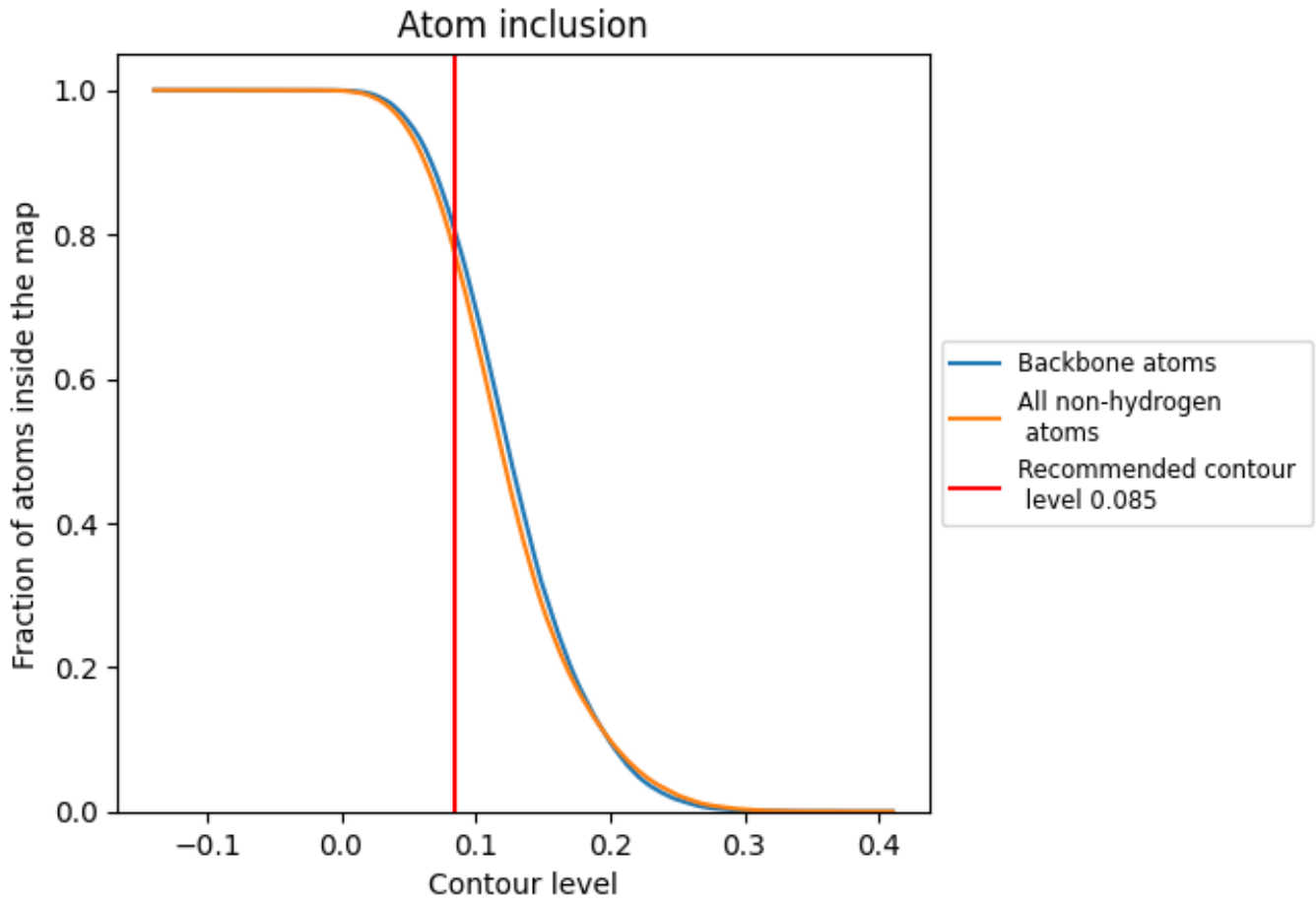
9.3 Atom inclusion mapped to coordinate model



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 (0.085).

9.4 Atom inclusion (i)



At the recommended contour level, 80% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.2350
2	0.8228	0.2550
A	0.8483	0.2370
B	0.7457	0.2040
C	0.8232	0.2960
E	0.9106	0.3860
F	0.7486	0.1460
G	0.8133	0.2940
H	0.7180	0.1730
I	0.8252	0.3600
J	0.8537	0.3110
L	0.8393	0.4070
M	0.4973	0.1130
N	0.7820	0.2340
O	0.7522	0.1890
P	0.6138	0.1420
Q	0.6622	0.1260
R	0.4555	0.1930
S	0.5677	0.1420
T	0.8085	0.1350
U	0.2226	0.1450
V	0.8677	0.2430
W	0.9217	0.3060
X	0.8172	0.2890
Y	0.7646	0.3030
Z	0.5242	0.1520
b	0.5963	0.2230
c	0.5702	0.1390
d	0.3286	0.1210
e	0.4641	0.2070
h	0.7637	0.2230
i	0.6182	0.1120
j	0.3290	0.1540
l	0.6651	0.1440
t	0.7203	0.1630