



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:34 PM UTC

PDB ID : 6YAN / pdb_00006yan
EMDB ID : EMD-10762
Title : Mammalian 48S late-stage translation initiation complex with histone 4 mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.48 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 ⓘ 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:

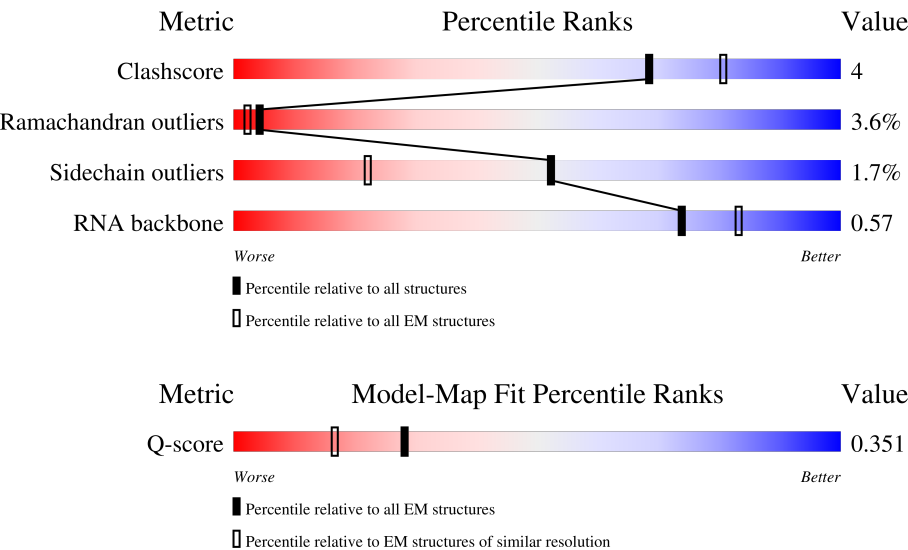
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.48 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.



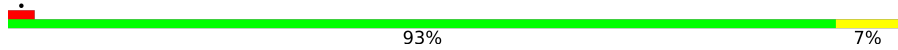
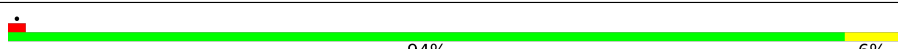
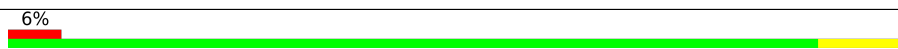
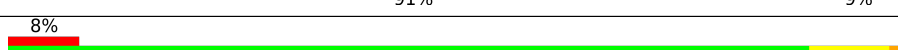
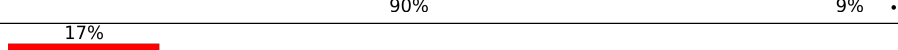
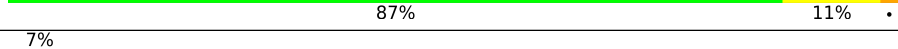
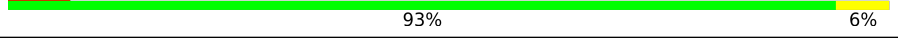
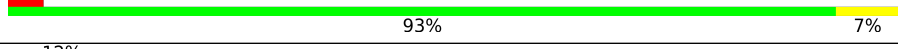
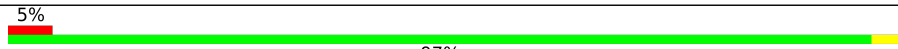
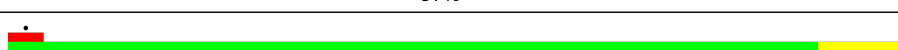
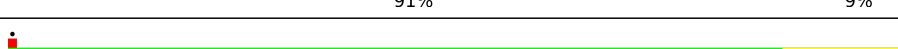
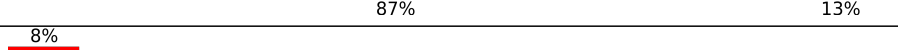
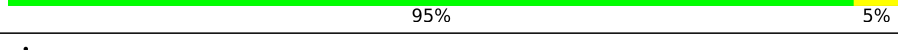
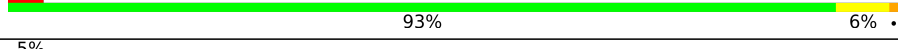
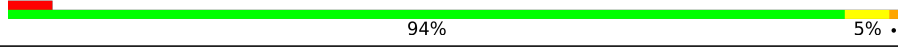
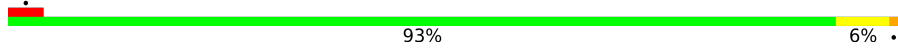
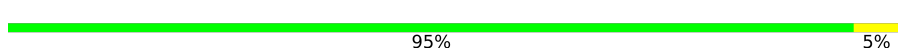
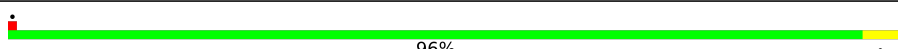
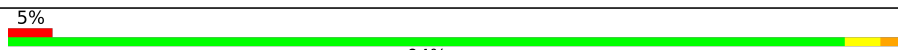
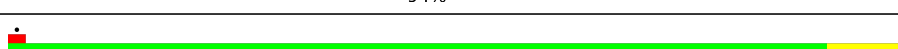
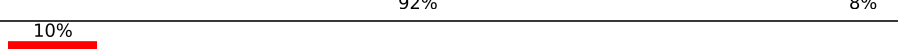
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13672 (2.98 - 3.98)

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	l	25	16% 88% 12%
2	C	208	92% 8%
3	D	215	90% 8%

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Mol	Chain	Length	Quality of chain
4	E	226	
5	F	227	
6	G	263	
7	H	191	
8	I	237	
9	J	190	
10	K	206	
11	L	182	
12	M	98	
13	N	158	
14	O	124	
15	P	150	
16	Q	136	
17	S	141	
18	T	126	
19	V	141	
20	W	104	
21	X	82	
22	Y	129	
23	Z	142	
24	a	126	
25	b	99	
26	c	84	
27	d	64	
28	e	53	

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Mol	Chain	Length	Quality of chain
29	f	71	
30	g	313	
31	h	75	
32	i	59	
33	2	1863	
34	3	36	
35	A	266	
36	B	422	
37	U	142	
38	R	135	
39	1	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	C4J	2	1244	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 84251 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 3 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	215	Total	C	N	O	S	0	0
			1742	1107	309	311	15		

- Molecule 4 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 9 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 12 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 15 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 16 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 18 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	126	Total	C	N	O	S	0	0
			1020	639	188	188	5		

- Molecule 19 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 20 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 22 is a protein called Ribosomal protein S15a.

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

- Molecule 23 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	126	Total	C	N	O	S	0	0
			1022	645	198	174	5		

- Molecule 25 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	99	Total	C	N	O	S	0	0
			790	491	162	131	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 27 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	64	Total	C	N	O	S	0	0
			507	308	102	95	2		

- Molecule 28 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 29 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 30 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 31 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 33 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	1744	Total	C	N	O	P	0	0
			37202	16613	6663	12186	1740		

- Molecule 34 is a RNA chain called histone 4 (H4) mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	36	Total	C	N	O	P	0	0
			774	346	144	249	35		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 36 is a protein called eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	142	Total	C	N	O	S	0	0
			1172	733	239	199	1		

- Molecule 38 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	135	Total	C	N	O	S	0	0
			1111	704	211	189	7		

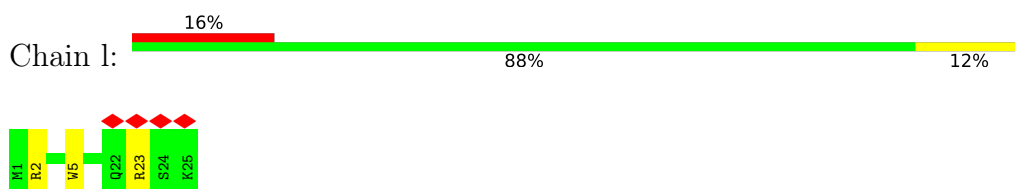
- Molecule 39 is a RNA chain called initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

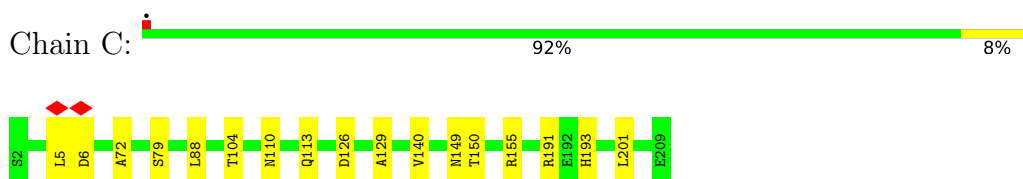
3 Residue-property plots

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.

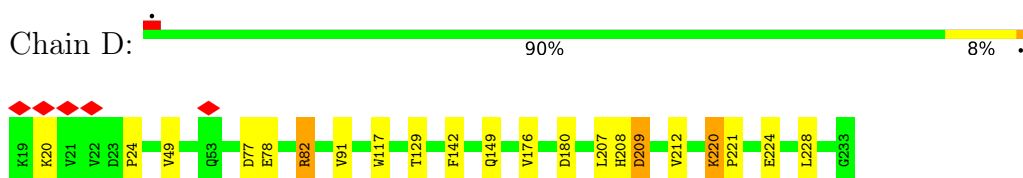
- Molecule 1: 60s ribosomal protein l41



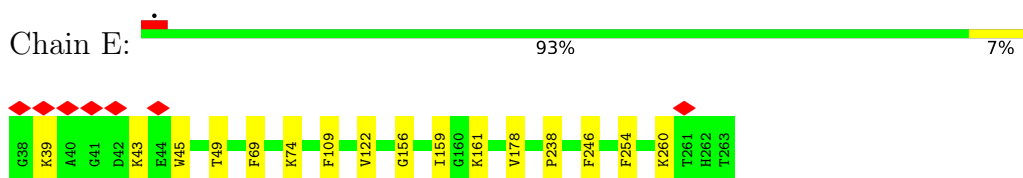
- Molecule 2: 40S ribosomal protein SA



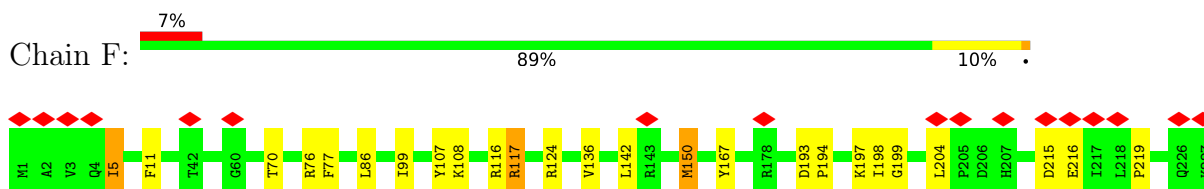
- Molecule 3: ribosomal protein eS1



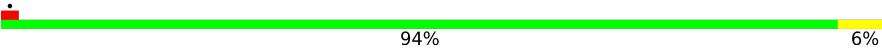
- Molecule 4: 40S ribosomal protein uS5

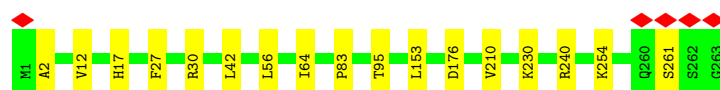


- Molecule 5: Ribosomal protein S3

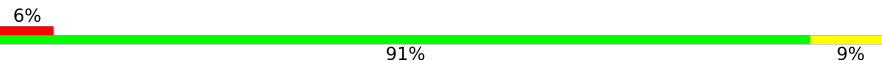


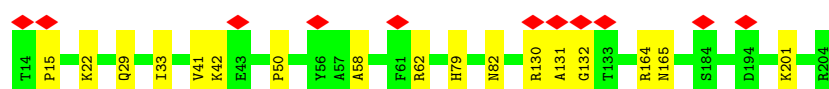
- Molecule 6: 40S ribosomal protein S4

Chain G:  94% 6%



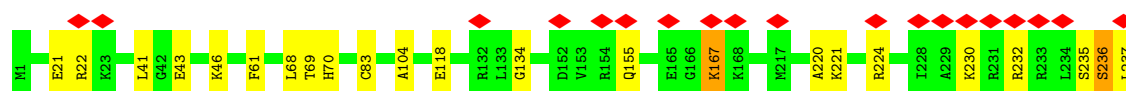
- Molecule 7: Ribosomal protein S5

Chain H:  6% 91% 9%



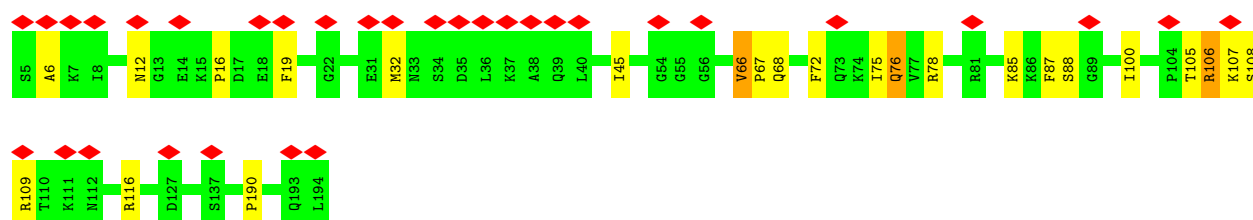
- Molecule 8: 40S ribosomal protein S6

Chain I:  8% 90% 9%

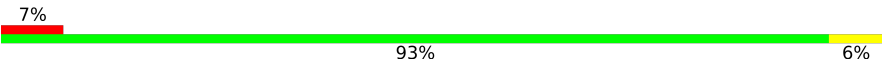


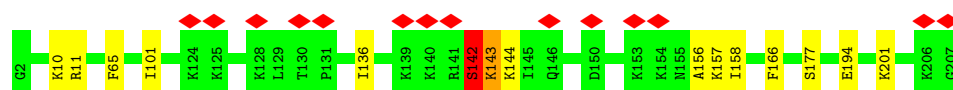
- Molecule 9: ribosomal protein eS7

Chain J:  17% 87% 11%

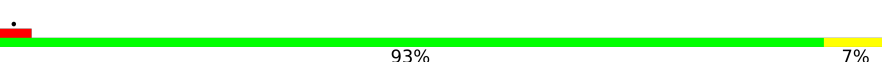


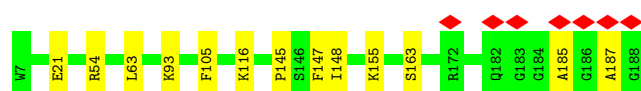
- Molecule 10: 40S ribosomal protein S8

Chain K:  7% 93% 6%

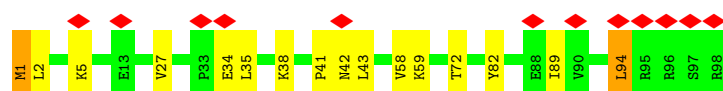
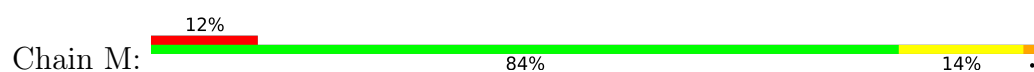


- Molecule 11: Ribosomal protein S9 (Predicted)

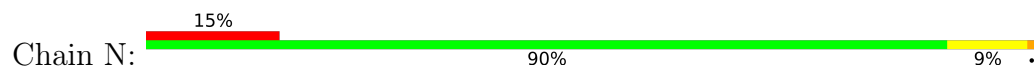
Chain L:  93% 7%



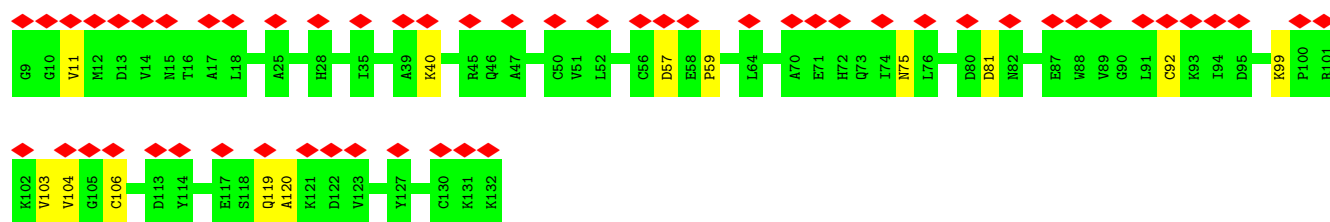
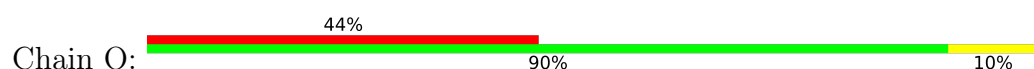
- Molecule 12: 40S ribosomal protein eS10



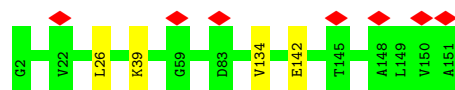
- Molecule 13: Ribosomal protein S11



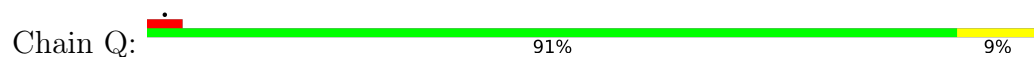
- Molecule 14: 40S ribosomal protein S12



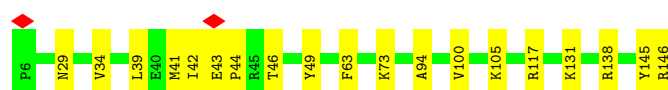
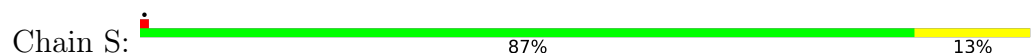
- Molecule 15: ribosomal protein uS15



- Molecule 16: 40S ribosomal protein uS11

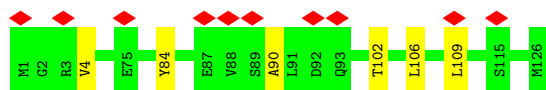


- Molecule 17: ribosomal protein uS9

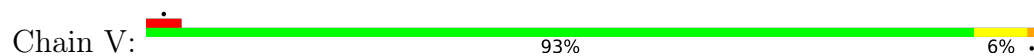


- Molecule 18: ribosomal protein eS17

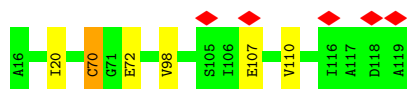
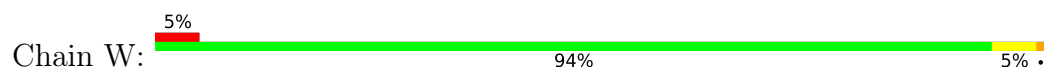




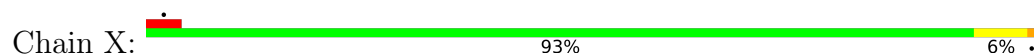
- Molecule 19: 40S ribosomal protein eS19



- Molecule 20: Ribosomal_S10 domain-containing protein



- Molecule 21: 40S ribosomal protein S21



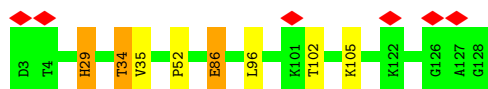
- Molecule 22: Ribosomal protein S15a



- Molecule 23: 40S ribosomal protein uS12

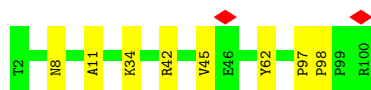


- Molecule 24: 40S ribosomal protein S24

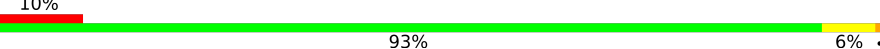


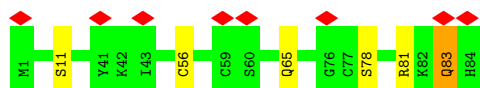
- Molecule 25: 40S ribosomal protein eS26

Chain b:  92% 8%

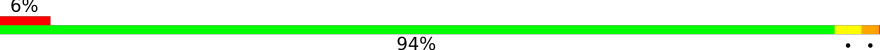


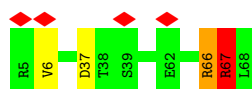
- Molecule 26: 40S ribosomal protein S27

Chain c:  10% 93% 6%



- Molecule 27: ribosomal protein eS28

Chain d:  6% 94%



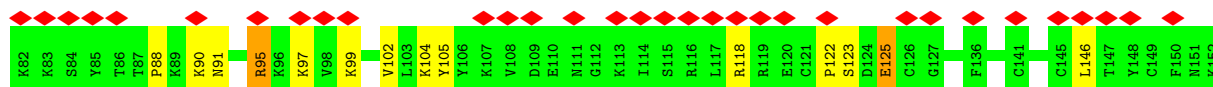
- Molecule 28: ribosomal protein uS14

Chain e:  85% 15%

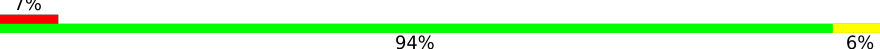


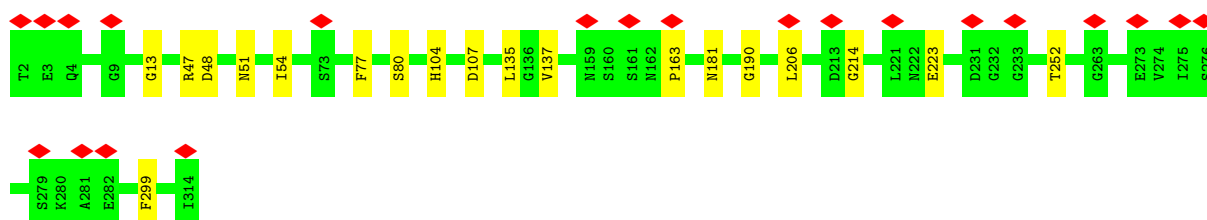
- Molecule 29: ribosomal protein eS31

Chain f:  45% 80% 17%



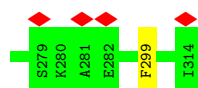
- Molecule 30: ribosomal protein RACK1

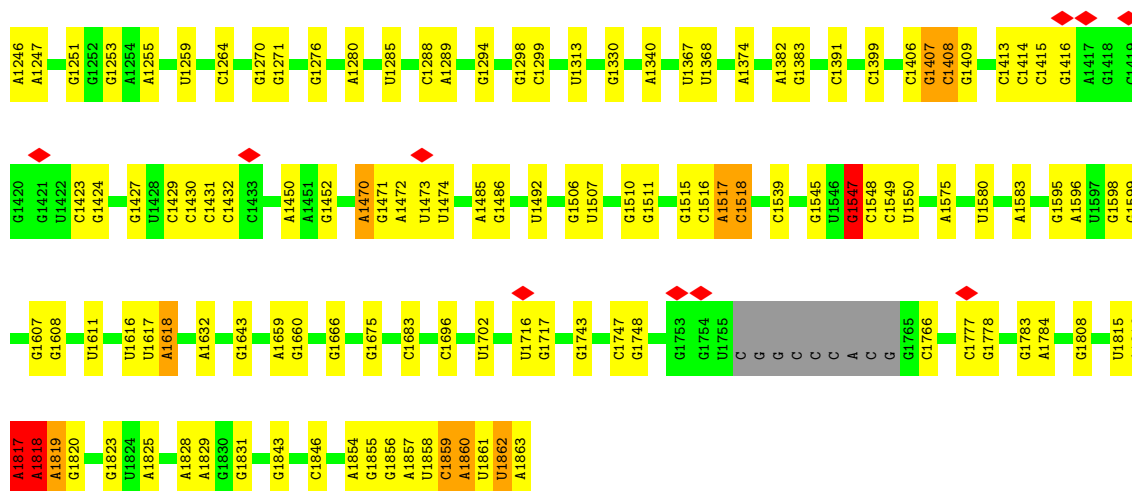
Chain g:  7% 94% 6%



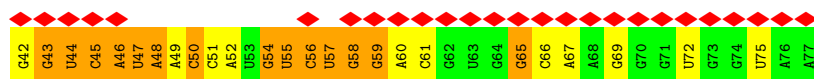
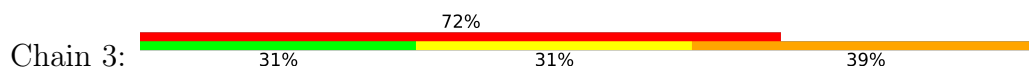
- Molecule 31: ribosomal protein eS25

Chain h:  12% 85% 13%

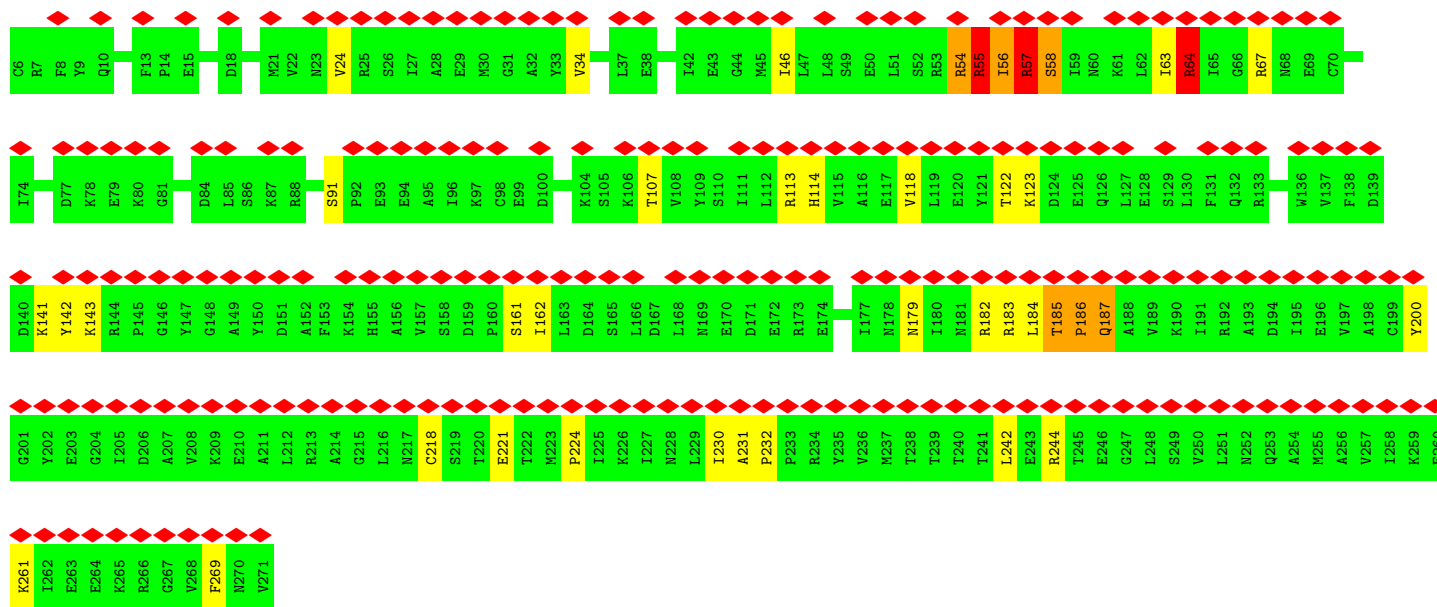
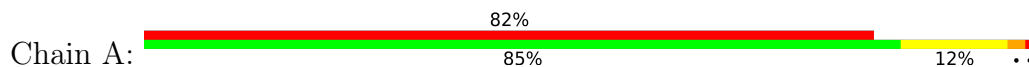




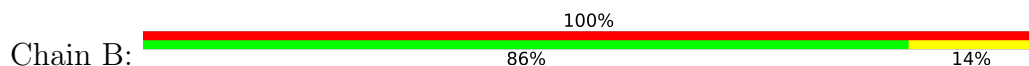
• Molecule 34: histone 4 (H4) mRNA

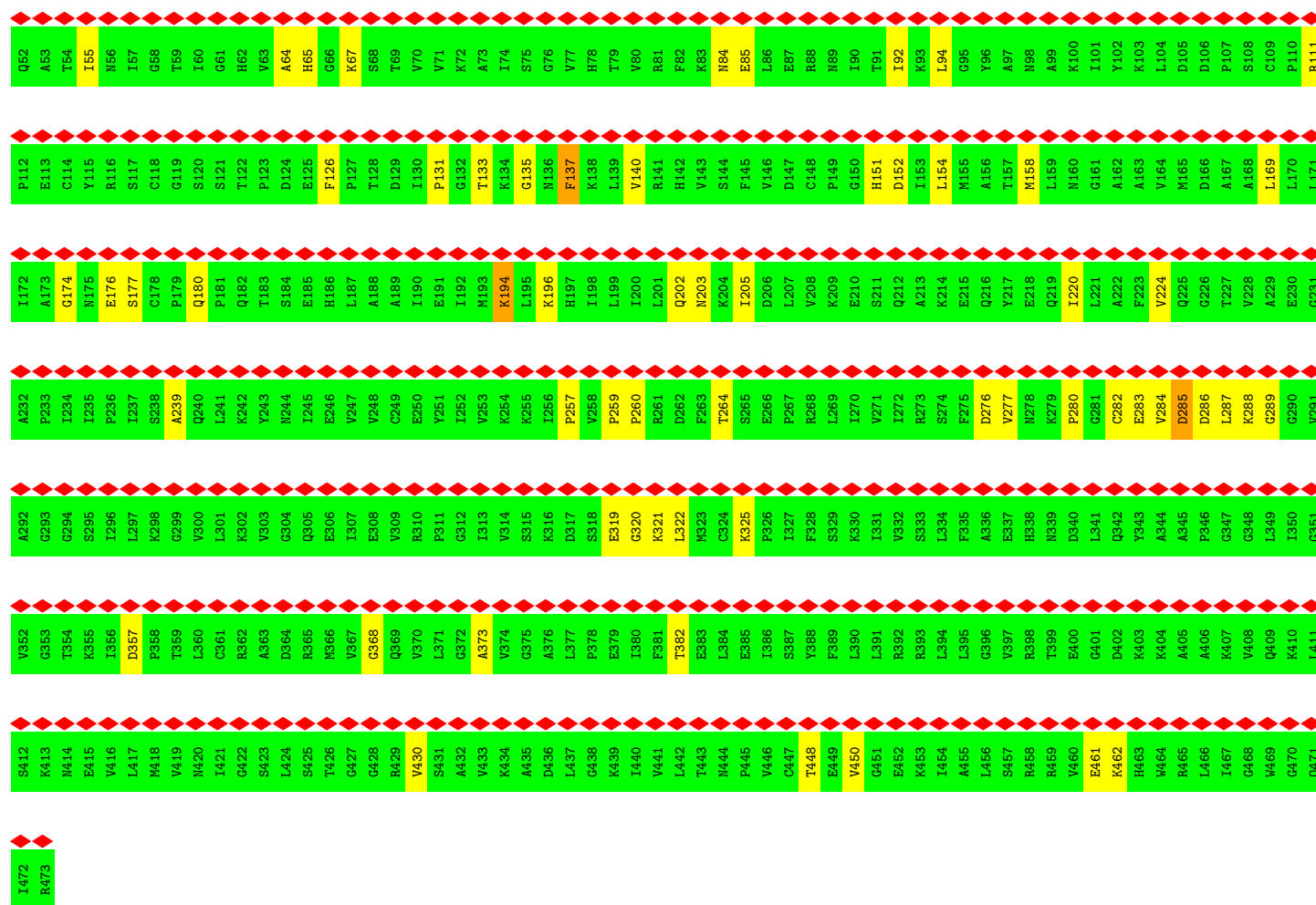


• Molecule 35: Eukaryotic translation initiation factor 2 subunit 1

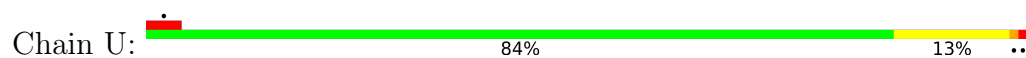


• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma

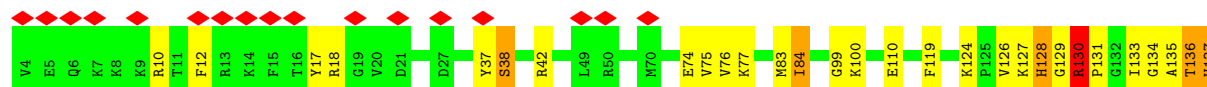
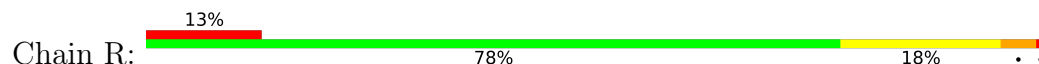




- Molecule 37: 40S ribosomal protein uS13

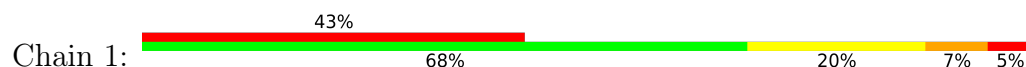


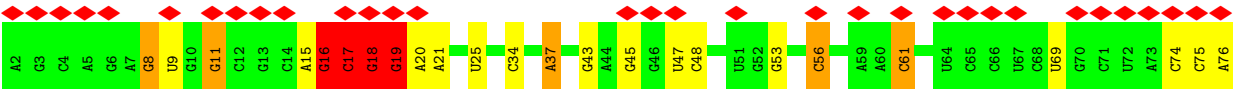
- Molecule 38: Ribosomal protein S15



S138

- Molecule 39: initiator methionylated tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	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	0.110	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0109	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, C4J

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	I	1.58	0/241	1.45	0/305
2	C	1.26	0/1680	1.42	3/2283 (0.1%)
3	D	1.23	0/1770	1.47	13/2367 (0.5%)
4	E	1.22	0/1779	1.37	10/2399 (0.4%)
5	F	1.27	0/1793	1.45	7/2412 (0.3%)
6	G	1.29	0/2125	1.42	9/2856 (0.3%)
7	H	1.28	0/1531	1.44	5/2059 (0.2%)
8	I	1.37	0/1946	1.44	18/2587 (0.7%)
9	J	1.26	0/1553	1.46	9/2079 (0.4%)
10	K	1.32	0/1709	1.44	7/2278 (0.3%)
11	L	1.36	0/1523	1.45	3/2031 (0.1%)
12	M	1.27	0/852	1.52	6/1147 (0.5%)
13	N	1.30	0/1319	1.36	6/1761 (0.3%)
14	O	1.20	0/968	1.68	12/1296 (0.9%)
15	P	1.25	0/1232	1.50	3/1656 (0.2%)
16	Q	1.32	0/1029	1.47	7/1380 (0.5%)
17	S	1.30	0/1141	1.47	6/1528 (0.4%)
18	T	1.27	0/1032	1.43	3/1383 (0.2%)
19	V	1.26	0/1133	1.53	7/1517 (0.5%)
20	W	1.28	0/832	1.46	3/1117 (0.3%)
21	X	1.33	0/627	1.39	6/839 (0.7%)
22	Y	1.31	0/1051	1.40	6/1406 (0.4%)
23	Z	1.32	0/1125	1.40	0/1500
24	a	1.30	0/1038	1.47	5/1377 (0.4%)
25	b	1.38	0/803	1.44	2/1076 (0.2%)
26	c	1.25	0/673	1.43	5/902 (0.6%)
27	d	1.44	0/509	1.30	1/680 (0.1%)
28	e	1.38	0/455	1.37	2/603 (0.3%)
29	f	1.27	0/594	1.43	4/786 (0.5%)
30	g	1.26	0/2494	1.41	11/3394 (0.3%)
31	h	1.25	0/605	1.48	7/810 (0.9%)
32	i	1.37	0/478	1.47	4/628 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.92	11/41562 (0.0%)	1.06	39/64770 (0.1%)
34	3	0.71	0/867	0.86	0/1352
35	A	1.27	1/2178 (0.0%)	1.62	28/2935 (1.0%)
36	B	1.22	0/3267	1.55	42/4415 (1.0%)
37	U	1.28	0/1190	1.45	3/1592 (0.2%)
38	R	1.24	0/1132	1.38	6/1510 (0.4%)
39	1	1.77	9/1770 (0.5%)	1.64	17/2759 (0.6%)
All	All	1.14	21/89606 (0.0%)	1.27	325/129775 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	1
5	F	0	2
8	I	0	2
9	J	0	2
11	L	0	2
12	M	0	5
17	S	0	2
26	c	0	1
28	e	0	2
29	f	0	1
31	h	0	1
32	i	0	2
33	2	1	64
34	3	1	0
35	A	0	8
36	B	0	11
37	U	0	3
39	1	3	3
All	All	5	113

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	19	G	O3'-P	34.80	2.13	1.61
39	1	16	G	O3'-P	-31.34	1.14	1.61
39	1	17	C	O3'-P	25.68	1.99	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	1815	U	O3'-P	-23.38	1.26	1.61
39	1	17	C	C2'-O2'	-22.58	1.07	1.41

The worst 5 of 325 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	19	G	O3'-P-O5'	40.40	164.60	104.00
39	1	17	C	C4'-C3'-O3'	24.13	145.59	109.40
33	2	797	U	O3'-P-O5'	-22.57	70.15	104.00
33	2	676	U	O3'-P-O5'	-22.25	70.62	104.00
35	A	54	ARG	CA-C-N	21.29	151.05	122.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'
34	3	65	G	C3'
39	1	17	C	C2',C3'
39	1	18	G	C3'

5 of 113 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	193	HIS	Peptide
3	D	208	HIS	Peptide
5	F	107	TYR	Sidechain
5	F	167	TYR	Sidechain
8	I	68	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	240	0	289	0	0
2	C	1643	0	1646	1	0
3	D	1742	0	1815	0	0
4	E	1743	0	1836	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1765	0	1863	23	0
6	G	2083	0	2189	0	0
7	H	1509	0	1563	8	0
8	I	1924	0	2086	12	0
9	J	1530	0	1623	27	0
10	K	1680	0	1762	1	0
11	L	1499	0	1608	0	0
12	M	828	0	854	0	0
13	N	1296	0	1374	0	0
14	O	958	0	993	0	0
15	P	1208	0	1294	1	0
16	Q	1016	0	1039	0	0
17	S	1123	0	1193	2	0
18	T	1020	0	1075	0	0
19	V	1113	0	1149	5	0
20	W	822	0	887	1	0
21	X	620	0	622	0	0
22	Y	1034	0	1080	0	0
23	Z	1107	0	1179	2	0
24	a	1022	0	1084	1	0
25	b	790	0	839	5	0
26	c	659	0	683	0	0
27	d	507	0	536	2	0
28	e	445	0	442	0	0
29	f	582	0	599	1	0
30	g	2437	0	2393	0	0
31	h	599	0	655	17	0
32	i	473	0	524	2	0
33	2	37202	0	18777	315	0
34	3	774	0	390	80	0
35	A	2147	0	2189	26	0
36	B	3214	0	3354	0	0
37	U	1172	0	1226	66	0
38	R	1111	0	1166	58	0
39	1	1614	0	824	59	0
All	All	84251	0	66700	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 545 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:U:147:GLY:CA	38:R:131:PRO:HG3	1.22	1.68
37:U:147:GLY:HA3	38:R:131:PRO:CG	1.34	1.55
39:1:16:G:O3'	39:1:17:C:P	1.14	1.52
33:2:1817:A:C2'	33:2:1818:A:H5'	1.47	1.42
5:F:117:ARG:HH12	34:3:67:A:N6	1.14	1.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	23/25 (92%)	23 (100%)	0	0	100	100
2	C	206/208 (99%)	176 (85%)	21 (10%)	9 (4%)	2	17
3	D	213/215 (99%)	185 (87%)	19 (9%)	9 (4%)	2	18
4	E	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	5	30
5	F	225/227 (99%)	205 (91%)	13 (6%)	7 (3%)	3	25
6	G	261/263 (99%)	229 (88%)	26 (10%)	6 (2%)	5	30
7	H	189/191 (99%)	165 (87%)	16 (8%)	8 (4%)	2	18
8	I	233/237 (98%)	206 (88%)	20 (9%)	7 (3%)	3	25
9	J	188/190 (99%)	162 (86%)	18 (10%)	8 (4%)	2	18
10	K	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	3	26
11	L	180/182 (99%)	167 (93%)	6 (3%)	7 (4%)	2	20
12	M	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	1	12
13	N	156/158 (99%)	130 (83%)	19 (12%)	7 (4%)	2	17
14	O	122/124 (98%)	103 (84%)	15 (12%)	4 (3%)	3	23
15	P	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
16	Q	134/136 (98%)	116 (87%)	11 (8%)	7 (5%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	S	139/141 (99%)	123 (88%)	12 (9%)	4 (3%)	3	26
18	T	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	7	36
19	V	139/141 (99%)	124 (89%)	10 (7%)	5 (4%)	2	21
20	W	102/104 (98%)	95 (93%)	4 (4%)	3 (3%)	3	26
21	X	80/82 (98%)	66 (82%)	13 (16%)	1 (1%)	9	39
22	Y	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	36
23	Z	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	38
24	a	122/126 (97%)	106 (87%)	12 (10%)	4 (3%)	3	23
25	b	97/99 (98%)	81 (84%)	13 (13%)	3 (3%)	3	25
26	c	82/84 (98%)	72 (88%)	8 (10%)	2 (2%)	4	29
27	d	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	2	16
28	e	51/53 (96%)	39 (76%)	8 (16%)	4 (8%)	1	8
29	f	69/71 (97%)	56 (81%)	6 (9%)	7 (10%)	0	6
30	g	311/313 (99%)	273 (88%)	31 (10%)	7 (2%)	5	30
31	h	73/75 (97%)	70 (96%)	2 (3%)	1 (1%)	9	38
32	i	57/59 (97%)	45 (79%)	7 (12%)	5 (9%)	0	7
35	A	264/266 (99%)	225 (85%)	29 (11%)	10 (4%)	2	20
36	B	420/422 (100%)	350 (83%)	48 (11%)	22 (5%)	1	14
37	U	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	2	21
38	R	133/135 (98%)	105 (79%)	18 (14%)	10 (8%)	1	9
All	All	5534/5610 (99%)	4836 (87%)	500 (9%)	198 (4%)	4	21

5 of 198 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	209	ASP
3	D	221	PRO
5	F	193	ASP
5	F	219	PRO
6	G	2	ALA

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	24/24 (100%)	21 (88%)	3 (12%)	4	22
2	C	174/174 (100%)	171 (98%)	3 (2%)	53	69
3	D	196/196 (100%)	192 (98%)	4 (2%)	48	66
4	E	187/187 (100%)	184 (98%)	3 (2%)	55	70
5	F	190/190 (100%)	184 (97%)	6 (3%)	34	59
6	G	225/225 (100%)	222 (99%)	3 (1%)	61	72
7	H	161/161 (100%)	159 (99%)	2 (1%)	63	73
8	I	207/207 (100%)	206 (100%)	1 (0%)	81	80
9	J	170/170 (100%)	165 (97%)	5 (3%)	37	61
10	K	177/177 (100%)	173 (98%)	4 (2%)	44	64
11	L	157/157 (100%)	156 (99%)	1 (1%)	78	79
12	M	89/89 (100%)	86 (97%)	3 (3%)	32	58
13	N	142/142 (100%)	136 (96%)	6 (4%)	26	52
14	O	104/104 (100%)	103 (99%)	1 (1%)	68	75
15	P	130/130 (100%)	129 (99%)	1 (1%)	73	76
16	Q	106/106 (100%)	105 (99%)	1 (1%)	70	75
17	S	117/117 (100%)	112 (96%)	5 (4%)	26	52
18	T	114/114 (100%)	113 (99%)	1 (1%)	70	75
19	V	113/113 (100%)	113 (100%)	0	100	100
20	W	94/94 (100%)	94 (100%)	0	100	100
21	X	67/67 (100%)	65 (97%)	2 (3%)	36	60
22	Y	112/112 (100%)	112 (100%)	0	100	100
23	Z	114/114 (100%)	112 (98%)	2 (2%)	51	69
24	a	108/108 (100%)	107 (99%)	1 (1%)	70	75
25	b	87/87 (100%)	87 (100%)	0	100	100
26	c	76/76 (100%)	75 (99%)	1 (1%)	61	72
27	d	57/57 (100%)	56 (98%)	1 (2%)	51	69
28	e	47/47 (100%)	46 (98%)	1 (2%)	47	66
29	f	64/64 (100%)	60 (94%)	4 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	g	272/272 (100%)	270 (99%)	2 (1%)	76	77
31	h	66/66 (100%)	66 (100%)	0	100	100
32	i	49/49 (100%)	49 (100%)	0	100	100
35	A	238/238 (100%)	234 (98%)	4 (2%)	53	69
36	B	354/354 (100%)	351 (99%)	3 (1%)	73	76
37	U	122/122 (100%)	120 (98%)	2 (2%)	55	70
38	R	121/121 (100%)	116 (96%)	5 (4%)	27	53
All	All	4831/4831 (100%)	4750 (98%)	81 (2%)	52	69

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	a	29	HIS
36	B	137	PHE
27	d	67	ARG
30	g	51	ASN
37	U	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
22	Y	113	HIS
28	e	10	HIS
36	B	203	ASN
23	Z	46	HIS
25	b	72	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1733/1863 (93%)	264 (15%)	11 (0%)
34	3	35/36 (97%)	20 (57%)	5 (14%)
39	1	74/75 (98%)	16 (21%)	5 (6%)
All	All	1842/1974 (93%)	300 (16%)	21 (1%)

5 of 300 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	4	C
33	2	33	G
33	2	41	G
33	2	42	A
33	2	44	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	3	58	G
39	1	16	G
39	1	74	C
39	1	17	C
39	1	8	G

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

2 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	$\# Z > 2$
39	T6A	1	37	39	31,34,35	1.41	4 (12%)	43,49,52	2.50	18 (41%)
33	C4J	2	1244	33	25,29,30	1.04	2 (8%)	28,42,45	2.91	2 (7%)

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
39	T6A	1	37	39	-	6/23/41/42	0/3/3/3
33	C4J	2	1244	33	1/1/7/7	9/16/34/35	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	37	T6A	C5-C4	4.75	1.47	1.39
33	2	1244	C4J	C4-C5	-3.51	1.39	1.47
39	1	37	T6A	C5-C6	2.76	1.48	1.41
39	1	37	T6A	C5-N7	-2.33	1.34	1.39
39	1	37	T6A	C8-N7	2.25	1.36	1.31

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	1244	C4J	C1'-C5-C4	14.41	139.48	117.61
39	1	37	T6A	C12-N11-C10	8.54	136.20	121.99
39	1	37	T6A	C5-C4-N3	-5.55	119.07	126.72
39	1	37	T6A	N3-C4-N9	4.45	134.74	127.17
39	1	37	T6A	C14-C12-C13	3.69	116.47	110.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	2	1244	C4J	C31-C3-N3-C2
33	2	1244	C4J	C31-C3-N3-C4
33	2	1244	C4J	C3-C31-C32-C34
33	2	1244	C4J	C3-C31-C32-N33
39	1	37	T6A	C14-C12-N11-C10

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	37	T6A	4	0
33	2	1244	C4J	3	0

5.5 Carbohydrates

There are no oligosaccharides 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
33	2	6
39	1	5
8	I	1
24	a	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	I	217:MET	C	218:LYS	N	3.94
1	a	9:THR	C	10:ARG	N	3.27
1	1	19:G	O3'	20:A	P	2.13
1	1	17:C	O3'	18:G	P	1.99

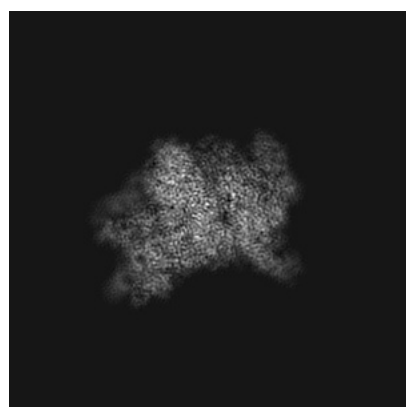
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10762. These allow visual inspection of the internal detail of the map and identification of artifacts.

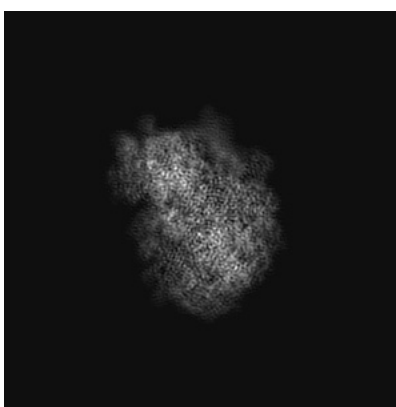
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

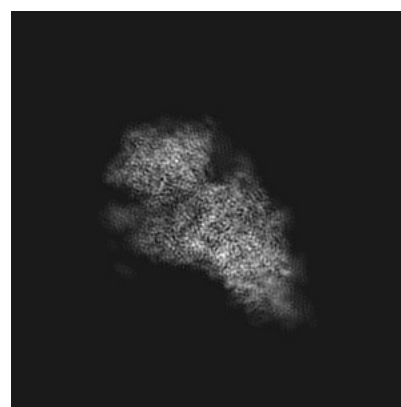
6.1.1 Primary map



X



Y

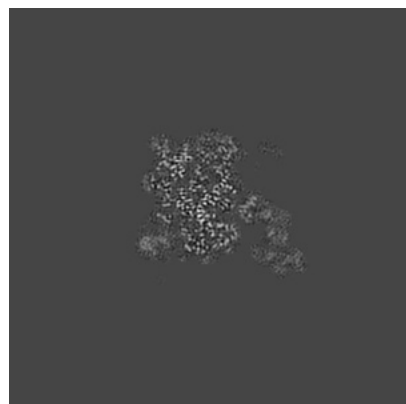


Z

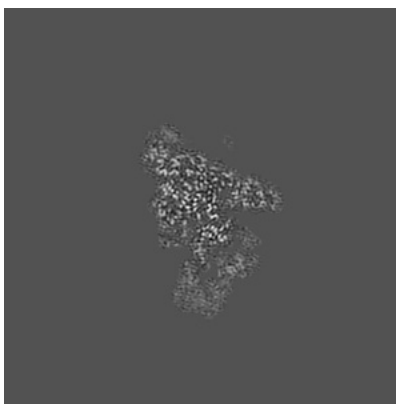
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

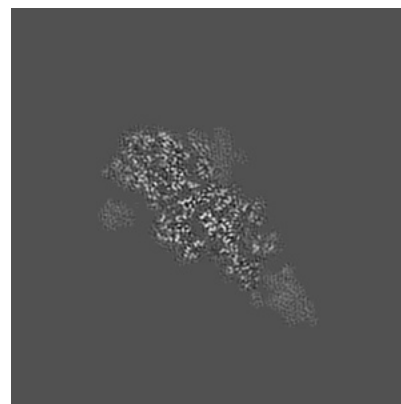
6.2.1 Primary map



X Index: 192



Y Index: 192

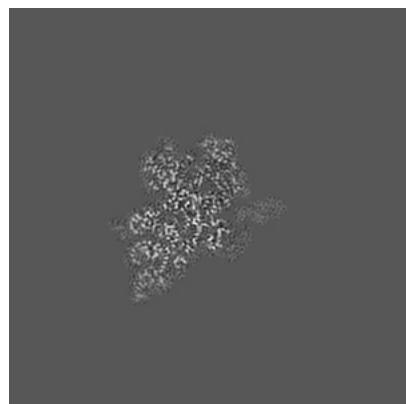


Z Index: 192

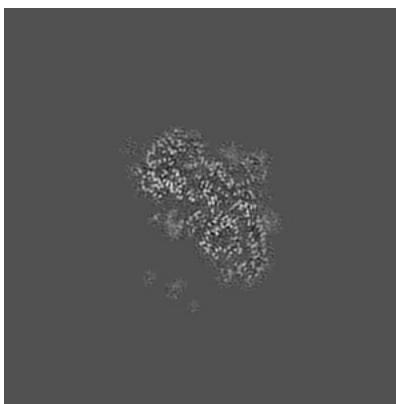
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

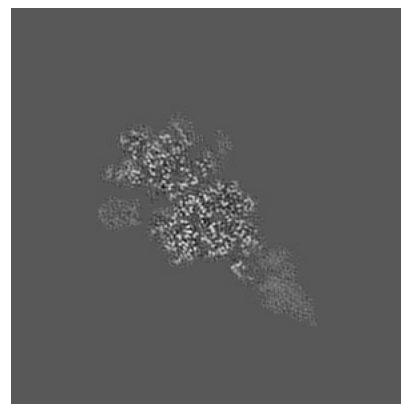
6.3.1 Primary map



X Index: 208



Y Index: 160

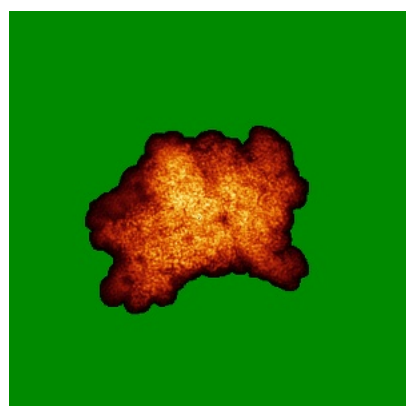


Z Index: 199

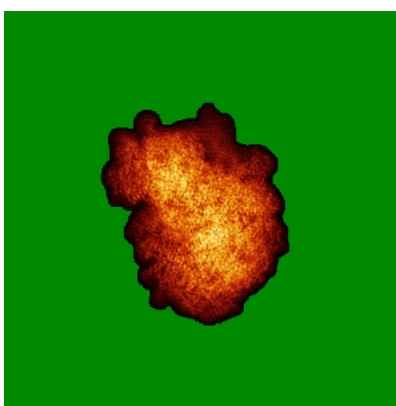
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

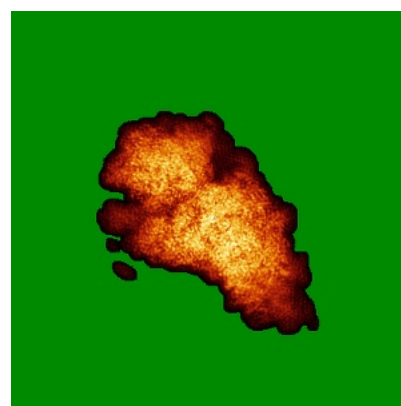
6.4.1 Primary map



X



Y

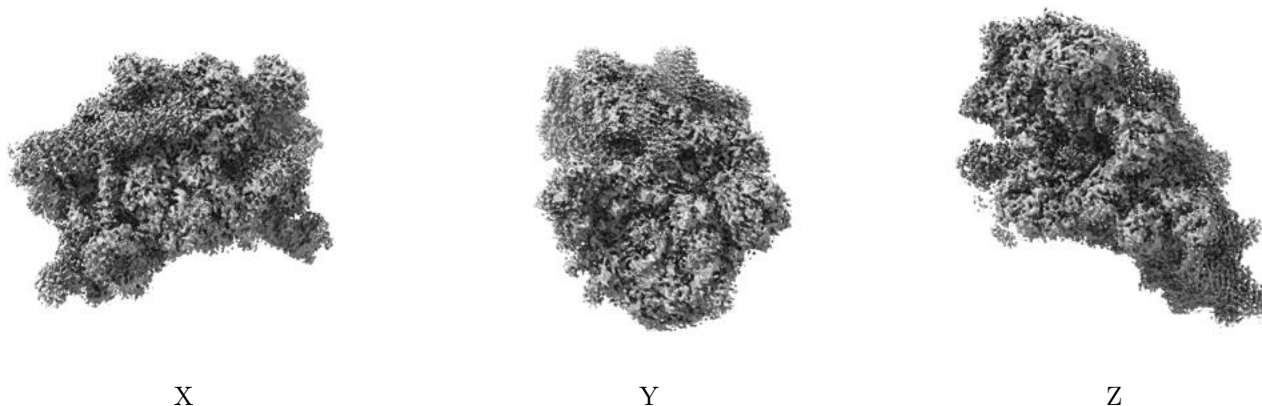


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

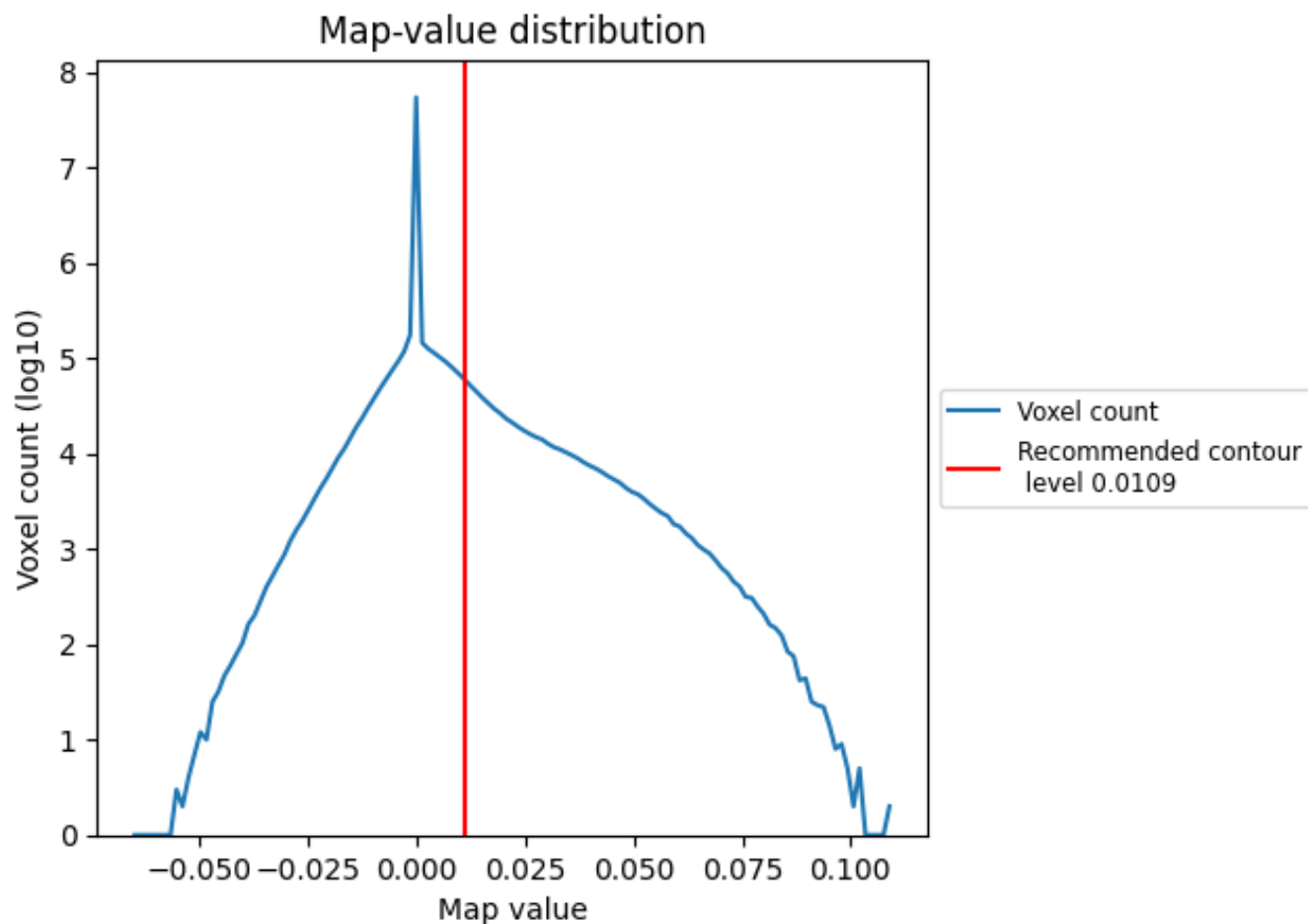
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

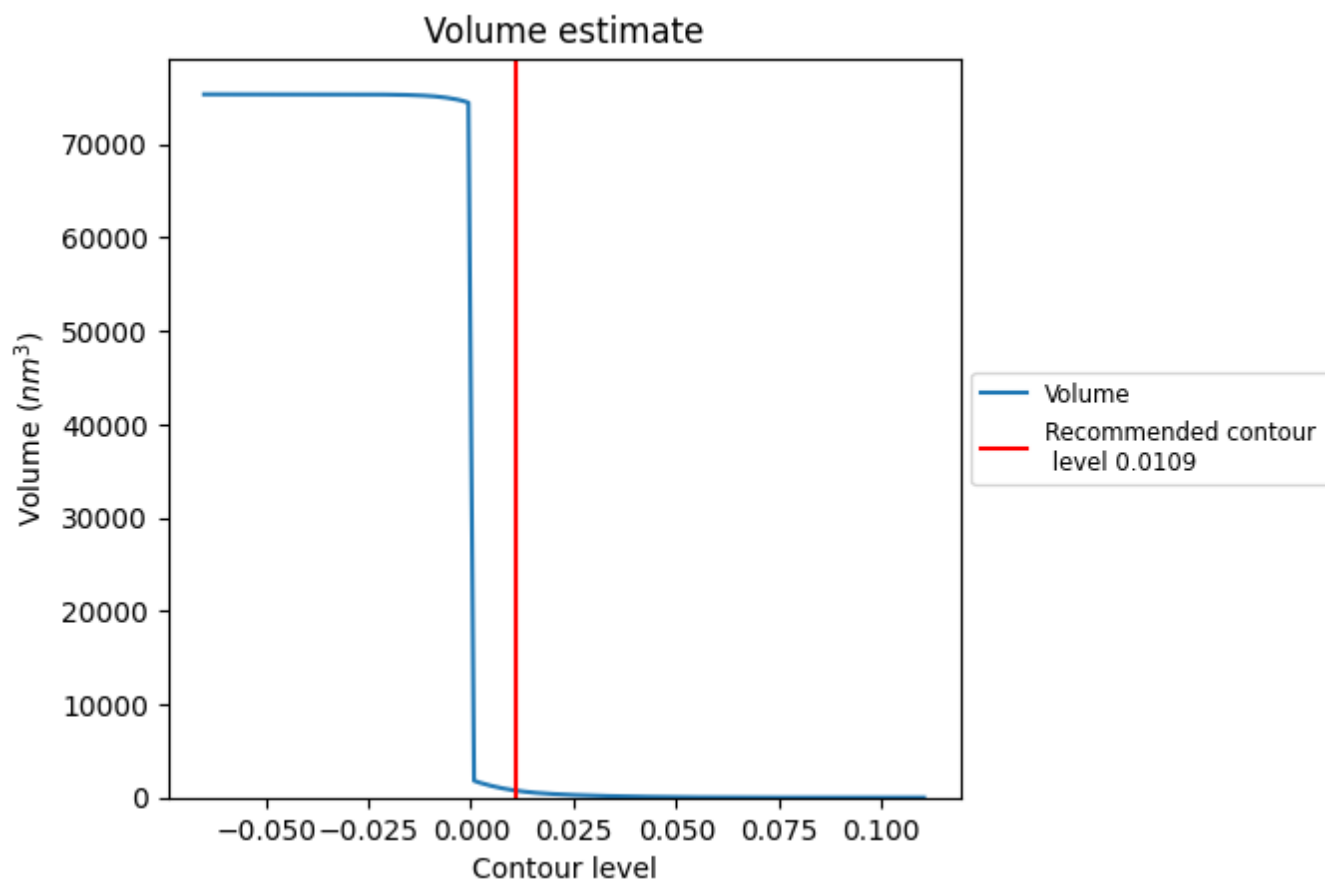
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

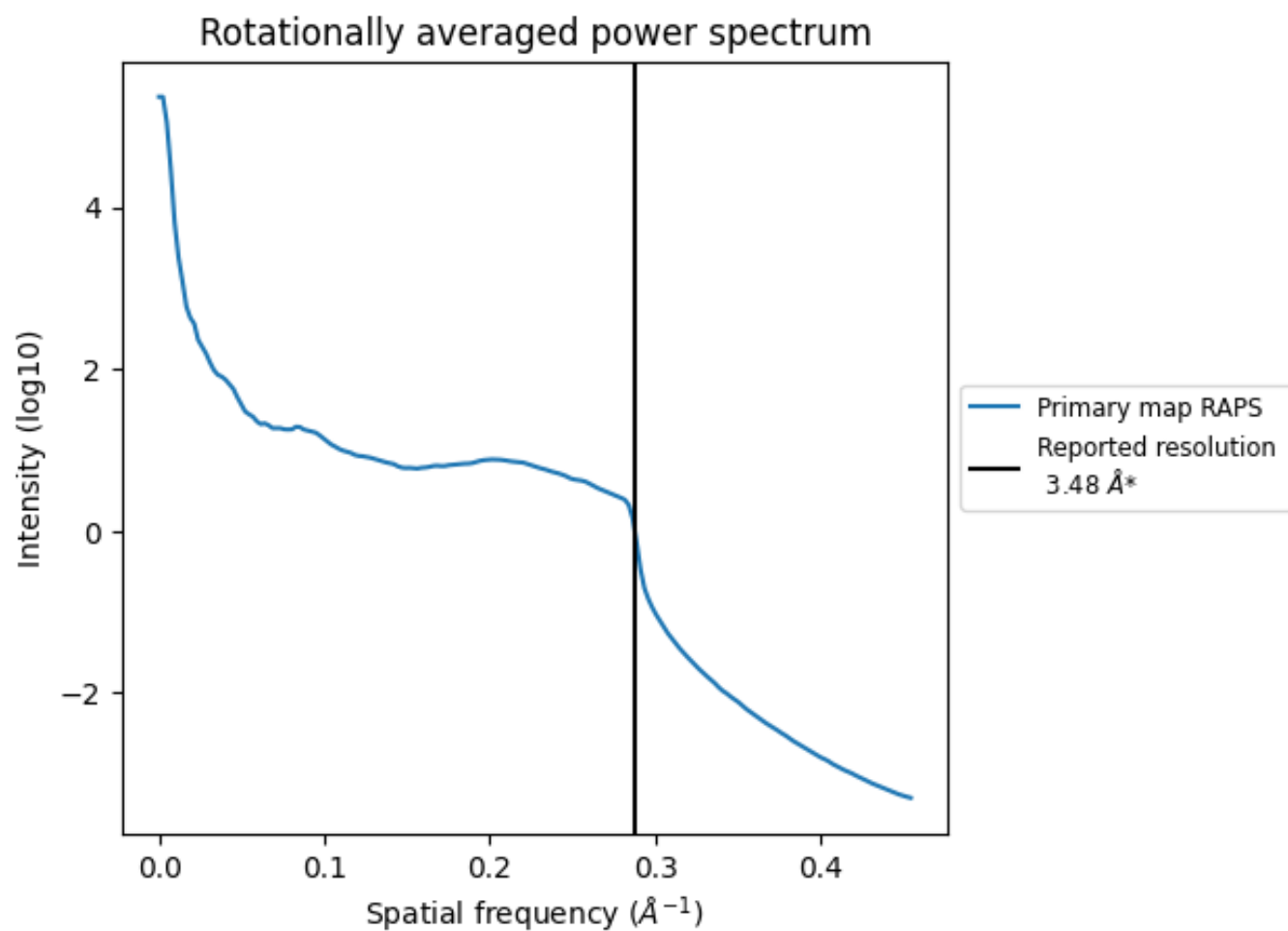
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

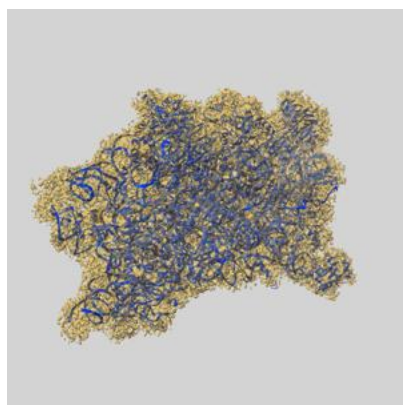
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

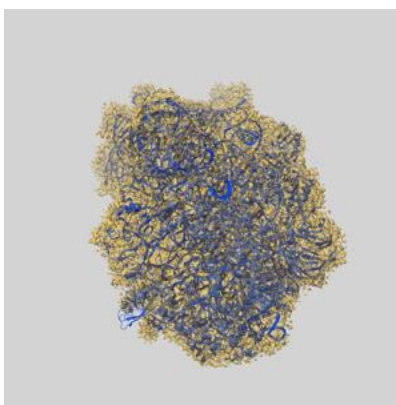
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10762 and PDB model 6YAN. Per-residue inclusion information can be found in section 3 on page 11.

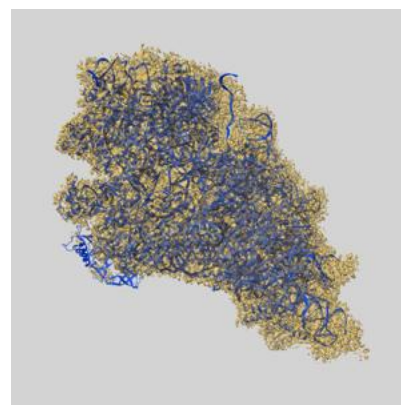
9.1 Map-model overlay [i](#)



X



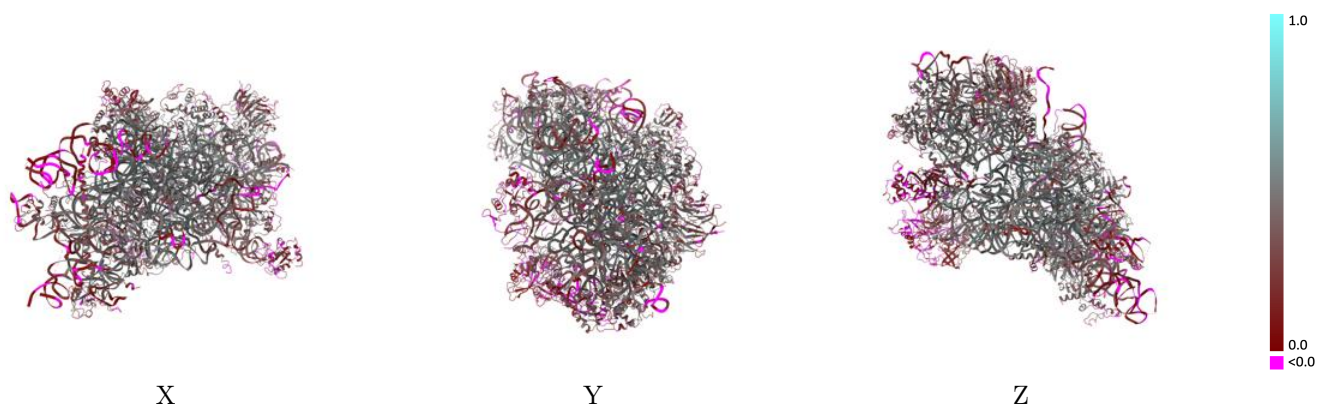
Y



Z

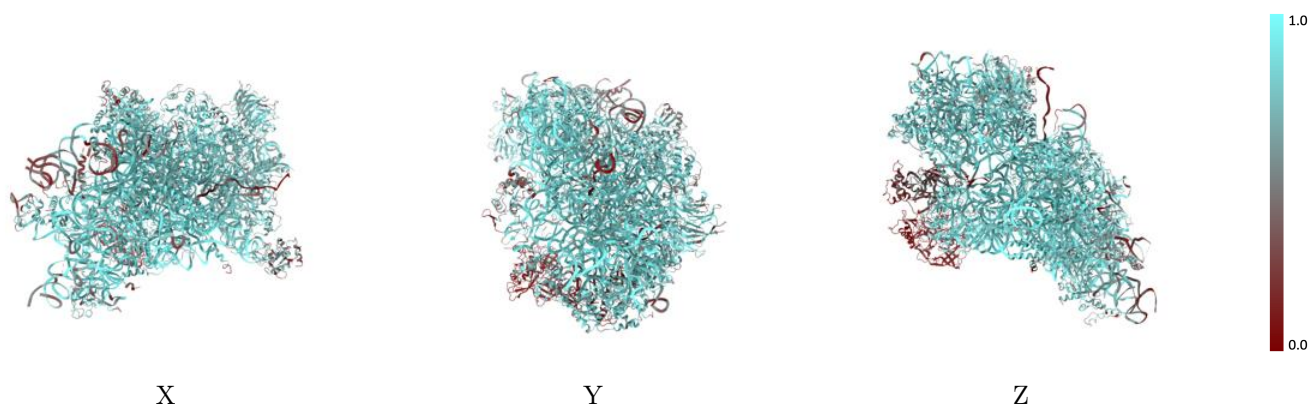
The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



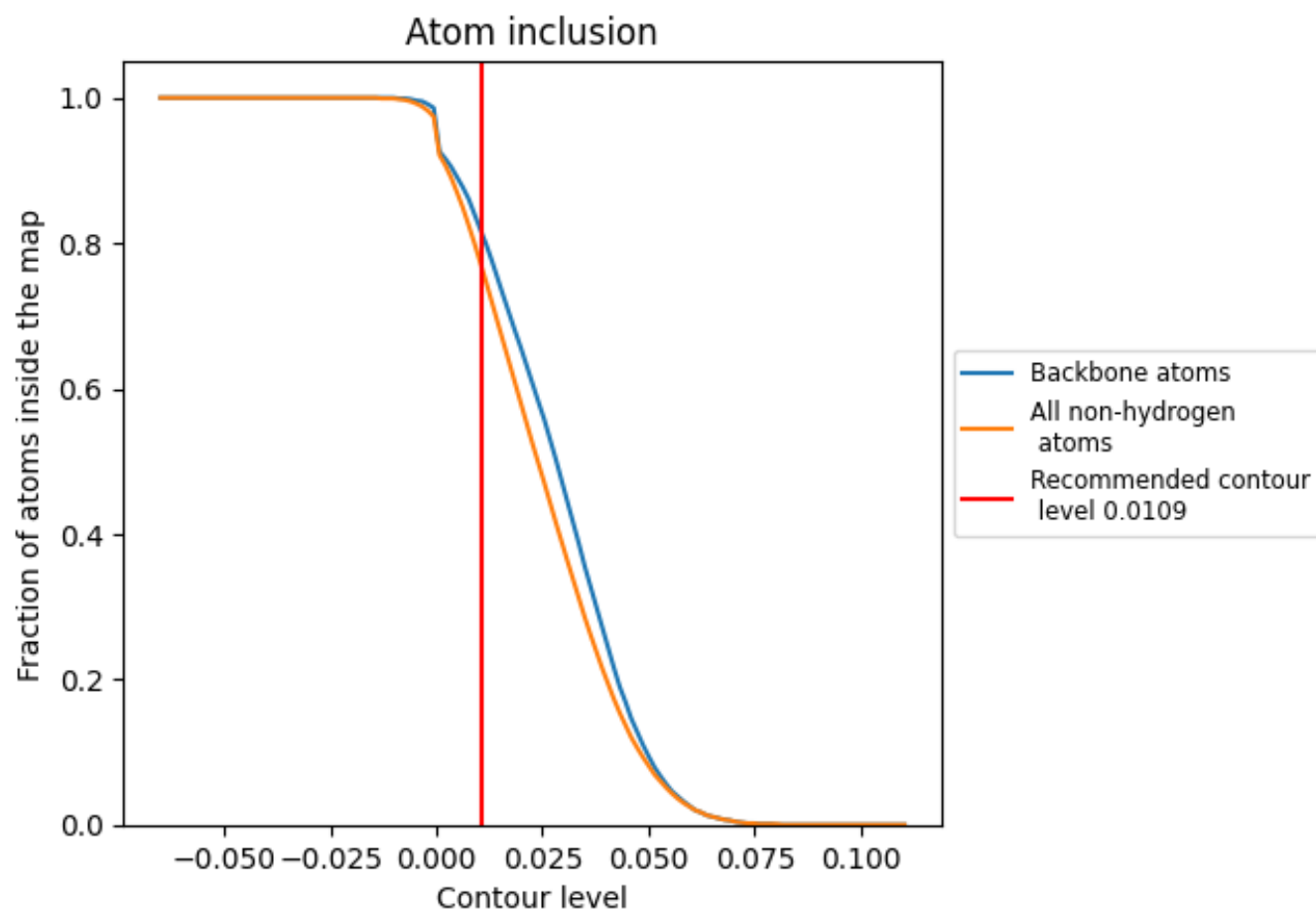
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0109).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.3510
1	 0.5060	 0.1520
2	 0.8840	 0.4010
3	 0.3270	 0.1390
A	 0.1820	 0.0510
B	 0.0080	 -0.0120
C	 0.8300	 0.4210
D	 0.7890	 0.4010
E	 0.8250	 0.4440
F	 0.7360	 0.3530
G	 0.8140	 0.4160
H	 0.7840	 0.3830
I	 0.7260	 0.2980
J	 0.6340	 0.2810
K	 0.7710	 0.3630
L	 0.8230	 0.4160
M	 0.7420	 0.3150
N	 0.7490	 0.3830
O	 0.4360	 0.1240
P	 0.8050	 0.3960
Q	 0.8060	 0.4090
R	 0.7000	 0.3020
S	 0.8140	 0.4180
T	 0.7290	 0.3300
U	 0.7690	 0.3430
V	 0.7770	 0.3790
W	 0.7500	 0.3450
X	 0.7920	 0.3780
Y	 0.8680	 0.4780
Z	 0.8510	 0.4510
a	 0.7970	 0.3730
b	 0.8330	 0.4320
c	 0.7400	 0.3230
d	 0.7540	 0.3660
e	 0.8100	 0.3800



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Chain	Atom inclusion	Q-score
f	 0.4430	 0.0750
g	 0.7390	 0.3250
h	 0.7060	 0.3110
i	 0.6230	 0.2840
l	 0.7670	 0.3910