



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2024 – 01:33 PM JST

PDB ID : 8WHX
EMDB ID : EMD-37551
Title : Cryo- EM structure of Mycobacterium smegmatis 70S ribosome and Raff.
Authors : Kumar, N.; Sharma, S.; Kaushal, P.S.
Deposited on : 2023-09-23
Resolution : 2.80 Å (reported)
Based on initial model : 6DZI

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:

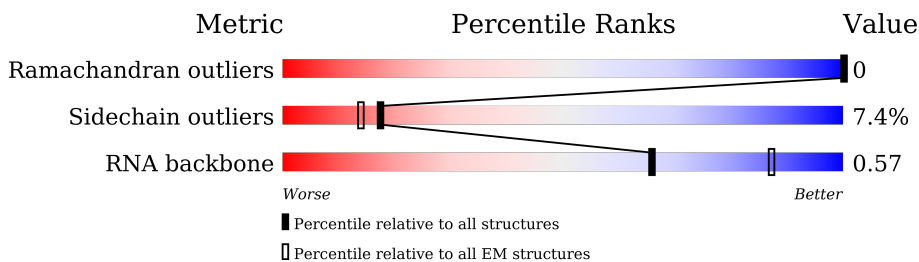
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



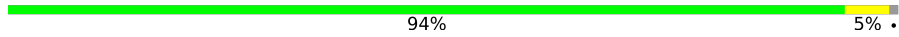

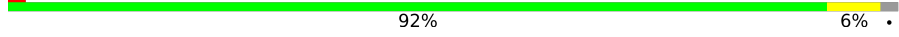

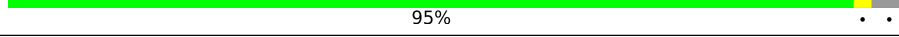
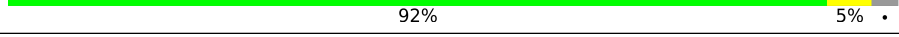

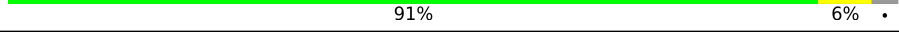
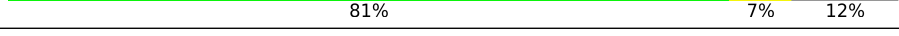

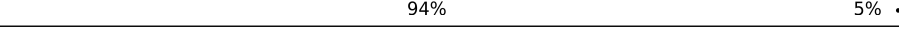
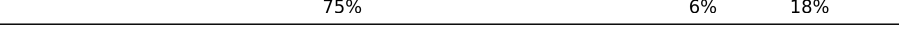

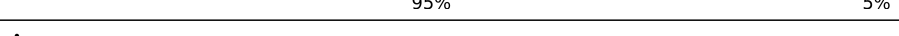


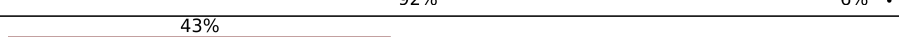

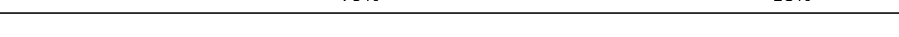






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	E	278	95% . .
2	F	217	94% . .
3	G	215	92% 6% .
4	H	187	7% 91% 6% .
5	I	179	28% 86% 6% 8%
6	J	151	5% 25% . 73%
7	M	147	95% . .
8	N	122	96% .


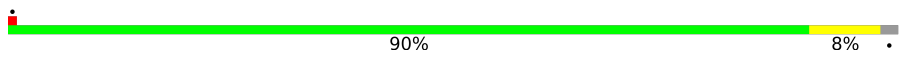
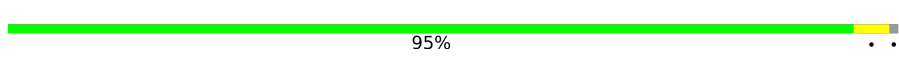

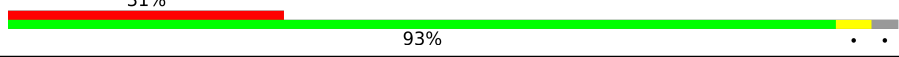

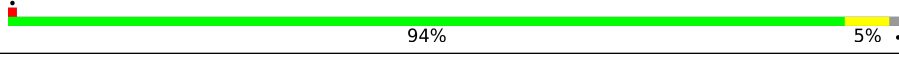

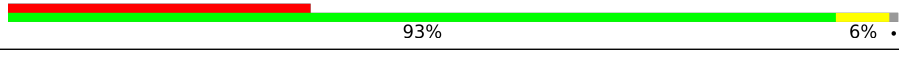
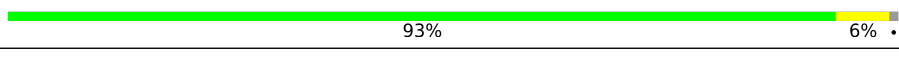
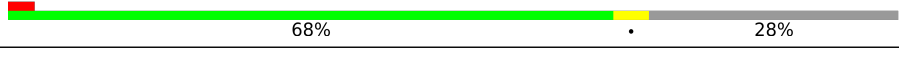
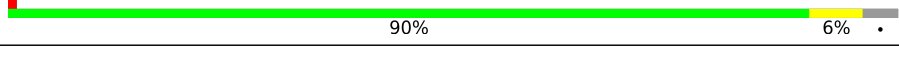


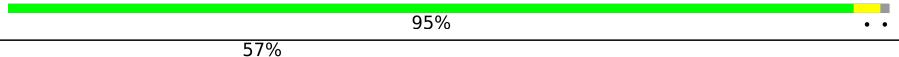


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Mol	Chain	Length	Quality of chain
9	O	147	 94% 5%
10	Q	199	 57% 41%
11	R	127	 92% 6%
12	S	113	 89% 11%
13	T	129	 95%
14	U	103	 92% 5%
15	V	153	 71% 26%
16	W	100	 91% 6%
17	X	105	 81% 7% 12%
18	Z	88	 82% 6% 13%
19	1	64	 94% 5%
20	2	77	 75% 6% 18%
21	3	61	 89% 7% 5%
22	5	57	 95% 5%
23	6	55	 84% 5% 11%
24	7	47	 89% 6%
25	8	64	 92% 6%
26	4	75	 43% 65% 11% 24%
27	A	3119	 79% 18%
28	B	118	 81% 19%
29	a	1528	 81% 18%
30	v	33	 91% 6%
31	d	275	 10% 71% 25%
32	e	201	 95%
33	f	214	 75% 21%

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Mol	Chain	Length	Quality of chain
34	g	96	
35	h	156	
36	i	132	
37	j	150	
38	k	101	
39	l	138	
40	m	124	
41	n	124	
42	o	101	
43	p	89	
44	q	156	
45	r	98	
46	s	84	
47	t	93	
48	u	86	
49	c	277	
50	w	264	

2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 142363 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	275	2110	1298	438	370	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	214	1587	982	310	290	5	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	209	1569	969	295	303	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	181	1436	901	269	260	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	165	1260	792	229	238	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	41	308	195	55	57	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	146	1130	722	207	200	1	0	0

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	122	938	586	179	170	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	145	1078	676	205	194	3	0	0

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	118	928	583	180	163	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	R	124	941	577	195	169	0	0

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	S	113	907	570	171	165	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	T	124	988	613	203	172	0	0

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	113	Total	C	N	O	0	0
			864	538	170	156		

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	W	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	92	Total	C	N	O	S	0	0
			703	439	132	130	2		

- Molecule 18 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Z	77	Total	C	N	O	0	0
			574	355	121	98		

- Molecule 19 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 20 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	63	Total	C	N	O	S	0	0
			527	322	102	102	1		

- Molecule 21 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	3	58	Total	C	N	O	0	0
			470	290	94	86		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 23 is a protein called 50S ribosomal protein L33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7	45	Total	C	N	O	S	0	0
			372	222	96	53	1		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	8	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	57	Total	C	N	O	S	0	0
			445	276	81	83	5		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	3020	Total	C	N	O	P	0	0
			64865	28910	11931	21004	3020		

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	B	117	2502	1117	465	803	117	0	0

- Molecule 29 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	a	1515	32521	14485	5945	10576	1515	0	0

- Molecule 30 is a protein called 30S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	v	31	271	166	69	35	1	0	0

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	207	1656	1034	321	297	4	0	0

- Molecule 32 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	200	1641	1028	316	295	2	0	0

- Molecule 33 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	168	1223	769	230	220	4	0	0

- Molecule 34 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	96	771	486	138	145	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	h	153	1207	751	235	219	2	0	0

- Molecule 36 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	i	131	1010	633	189	187	1	0	0

- Molecule 37 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	j	126	994	630	194	170	0	0

- Molecule 38 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	k	98	784	493	145	143	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	l	115	855	528	170	156	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	m	122	958	594	197	165	2	0	0

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	n	116	935	572	191	169	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	o	100	819	497	183	138	1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	p	88	720	449	147	124		0	0

- Molecule 44 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	q	113	891	570	162	159		0	0

- Molecule 45 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	r	94	748	469	142	135	2	0	0

- Molecule 46 is a protein called 30S ribosomal protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	65	513	318	102	90	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	t	82	662	425	124	112	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	u	85	660	402	139	119		0	0

- Molecule 49 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	c	217	1708	1080	305	316	7	0	0

- Molecule 50 is a protein called Ribosome hibernation promotion factor RaffH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	w	126	1004	609	214	180	1	0	0

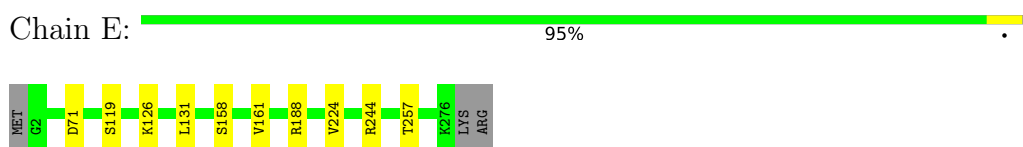
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	259	HIS	-	expression tag	UNP A0QZ86
w	260	HIS	-	expression tag	UNP A0QZ86
w	261	HIS	-	expression tag	UNP A0QZ86
w	262	HIS	-	expression tag	UNP A0QZ86
w	263	HIS	-	expression tag	UNP A0QZ86
w	264	HIS	-	expression tag	UNP A0QZ86

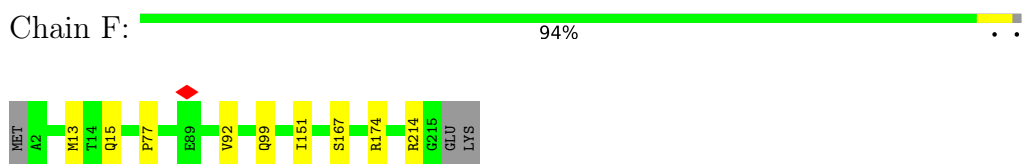
3 Residue-property plots [i](#)

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.

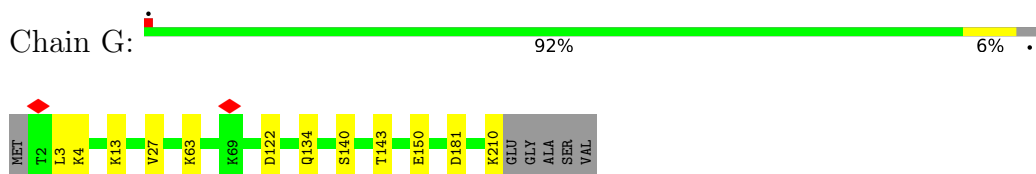
- Molecule 1: 50S ribosomal protein L2



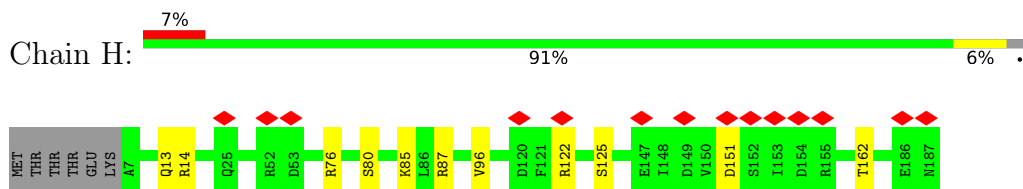
- Molecule 2: 50S ribosomal protein L3



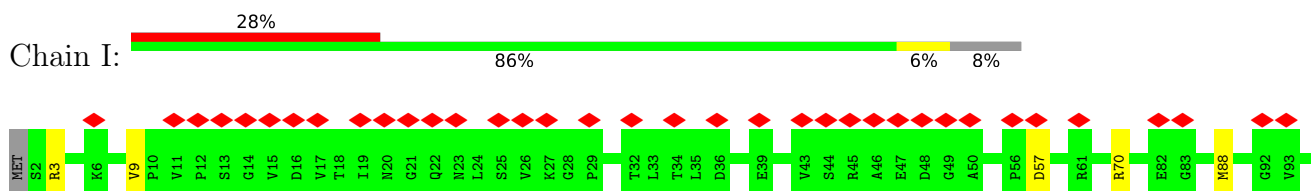
- Molecule 3: 50S ribosomal protein L4

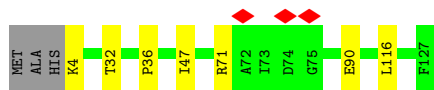


- Molecule 4: 50S ribosomal protein L5

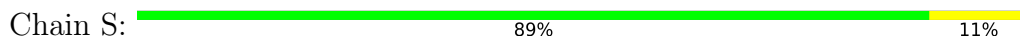


- Molecule 5: 50S ribosomal protein L6

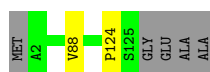




- Molecule 12: 50S ribosomal protein L19



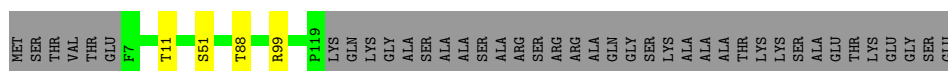
- Molecule 13: 50S ribosomal protein L20



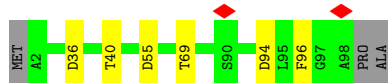
- Molecule 14: 50S ribosomal protein L21



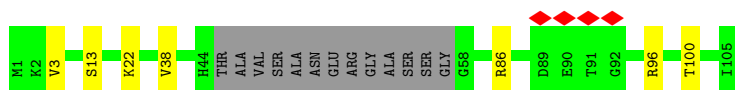
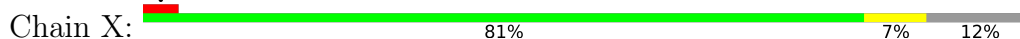
- Molecule 15: 50S ribosomal protein L22



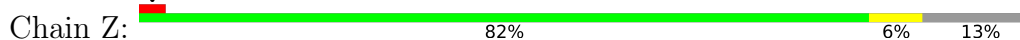
- Molecule 16: 50S ribosomal protein L23

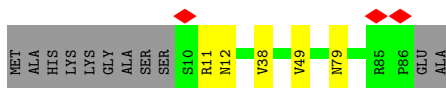


- Molecule 17: 50S ribosomal protein L24



- Molecule 18: 50S ribosomal protein L27

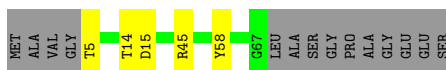
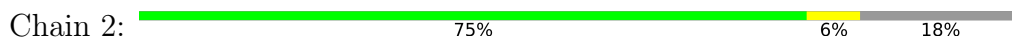




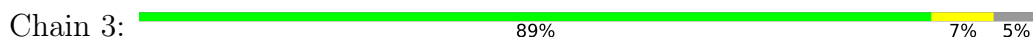
- Molecule 19: 50S ribosomal protein L28



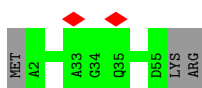
- Molecule 20: 50S ribosomal protein L29



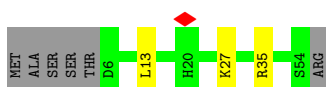
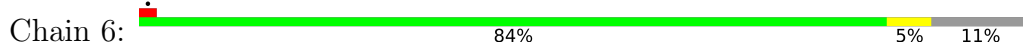
- Molecule 21: 50S ribosomal protein L30



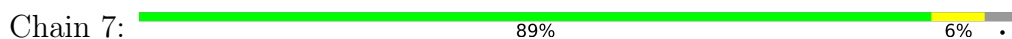
- Molecule 22: 50S ribosomal protein L32



- Molecule 23: 50S ribosomal protein L33A



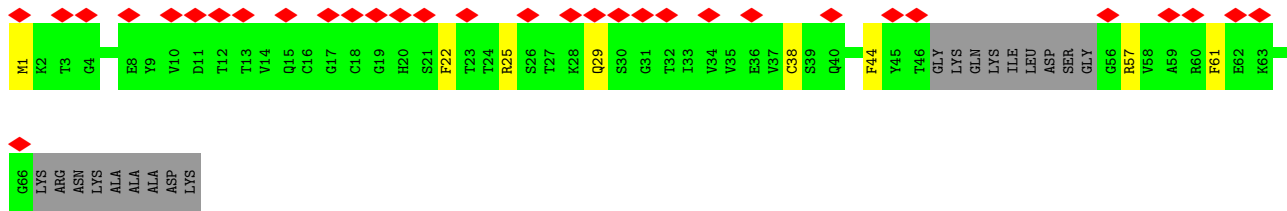
- Molecule 24: 50S ribosomal protein L34



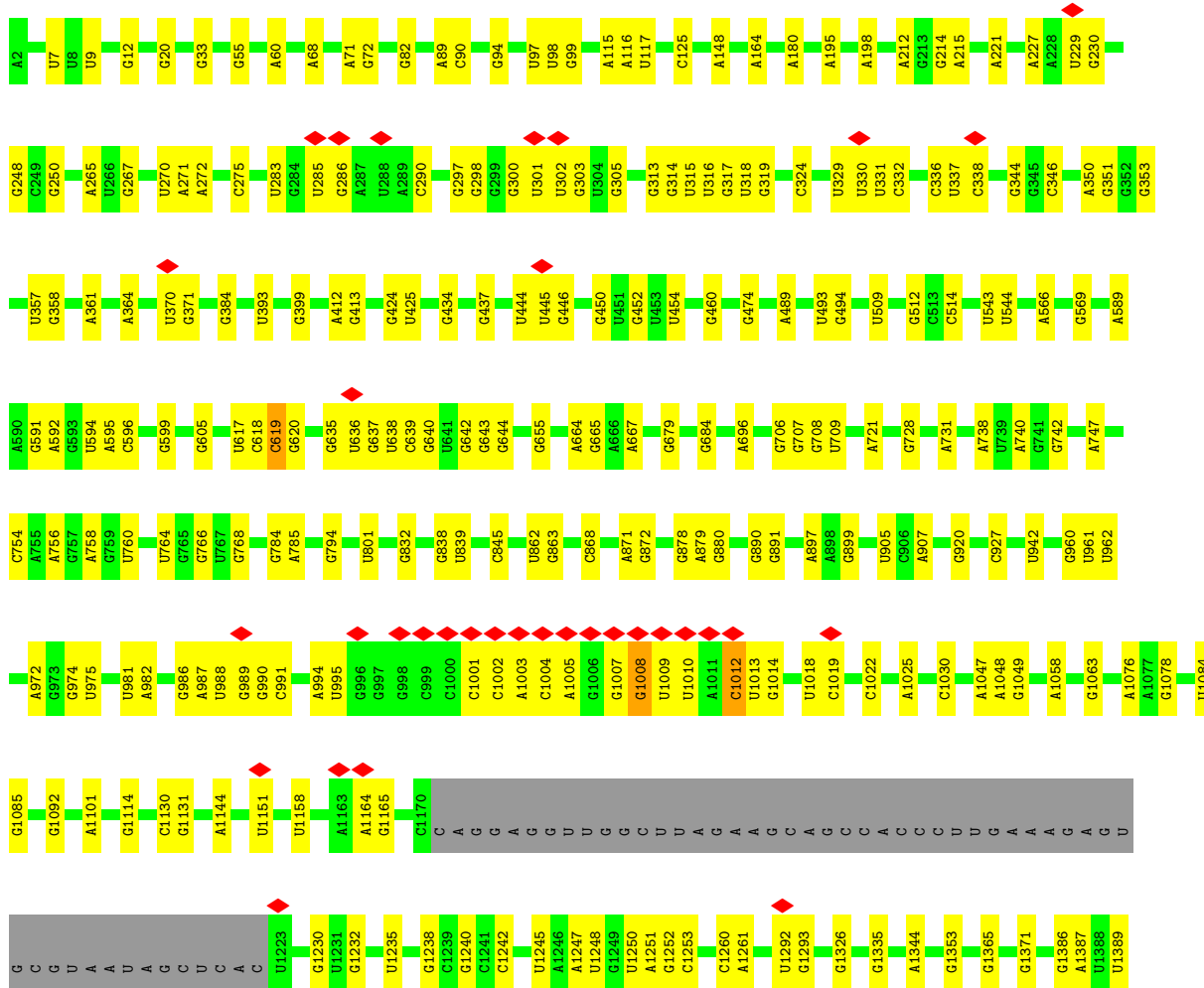
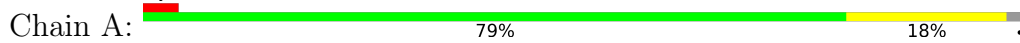
- Molecule 25: 50S ribosomal protein L35

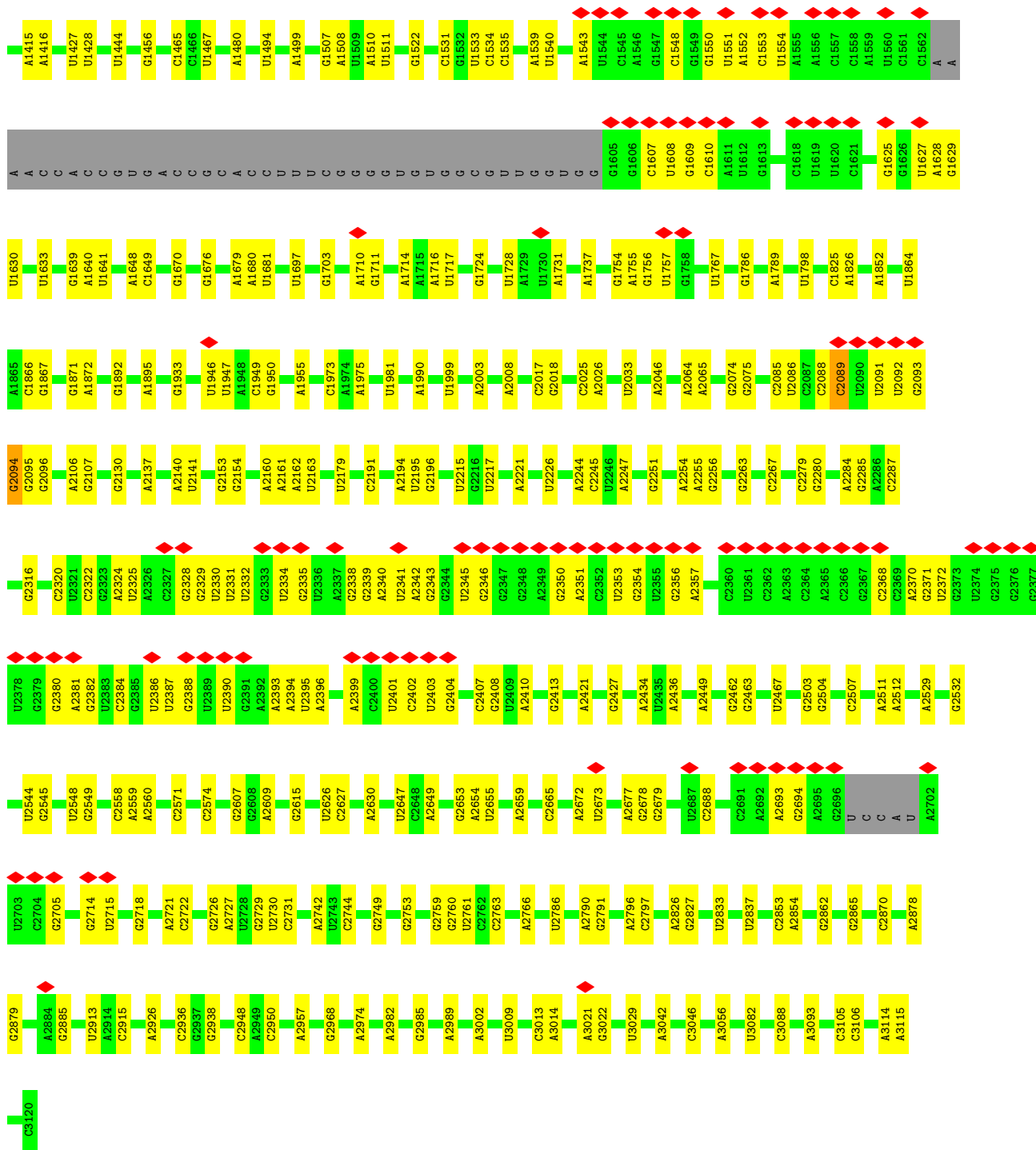


- Molecule 26: 50S ribosomal protein L31

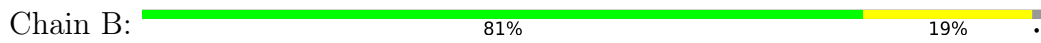


- Molecule 27: 23S rRNA



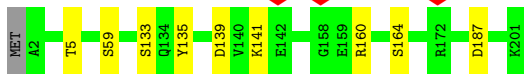


• Molecule 28: 5S rRNA



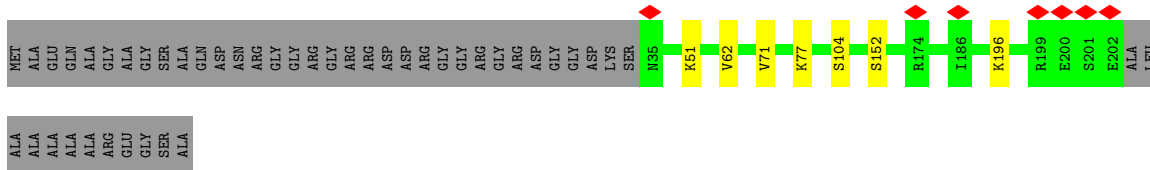
• Molecule 29: 16S rRNA

Chain e:  95%




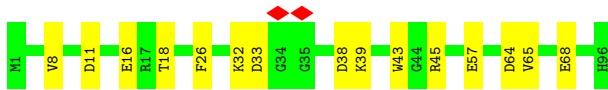
- Molecule 33: 30S ribosomal protein S5

Chain f:  75% 21%




- Molecule 34: 30S ribosomal protein S6

Chain g:  84% 16%



- Molecule 35: 30S ribosomal protein S7

Chain h:  90% 8%




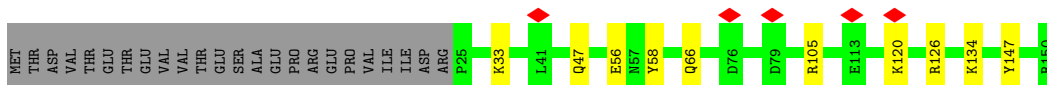
- Molecule 36: 30S ribosomal protein S8

Chain i:  95%




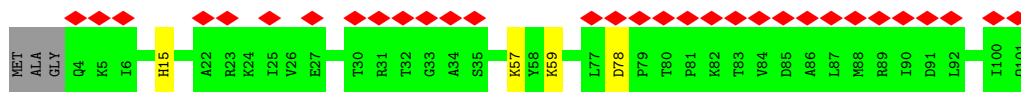
- Molecule 37: 30S ribosomal protein S9

Chain j:  77% 7% 16%

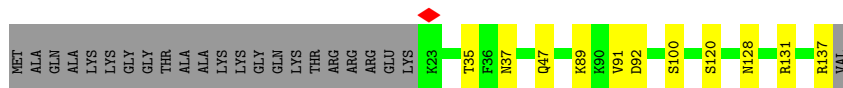


- Molecule 38: 30S ribosomal protein S10

Chain k:  31% 93%



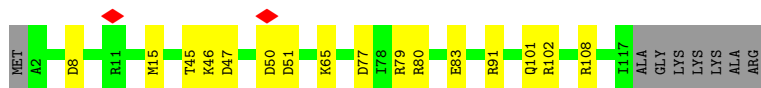
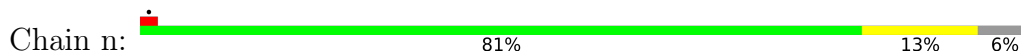
• Molecule 39: 30S ribosomal protein S11



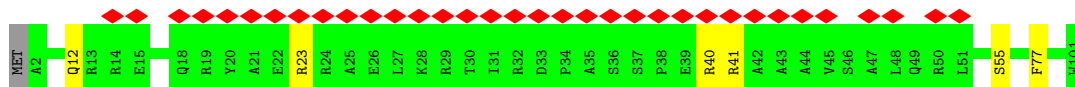
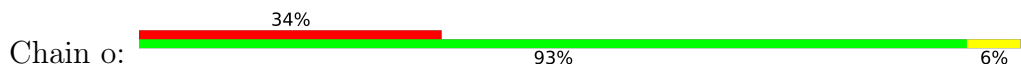
• Molecule 40: 30S ribosomal protein S12



• Molecule 41: 30S ribosomal protein S13



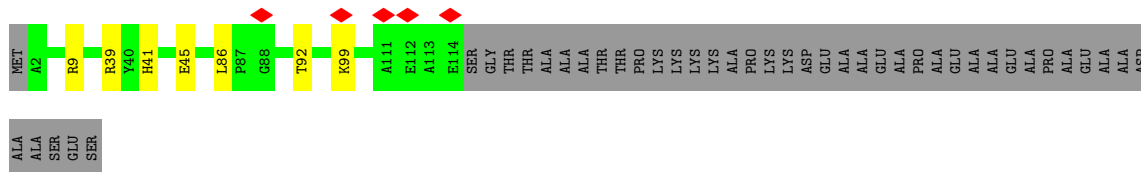
• Molecule 42: 30S ribosomal protein S14A



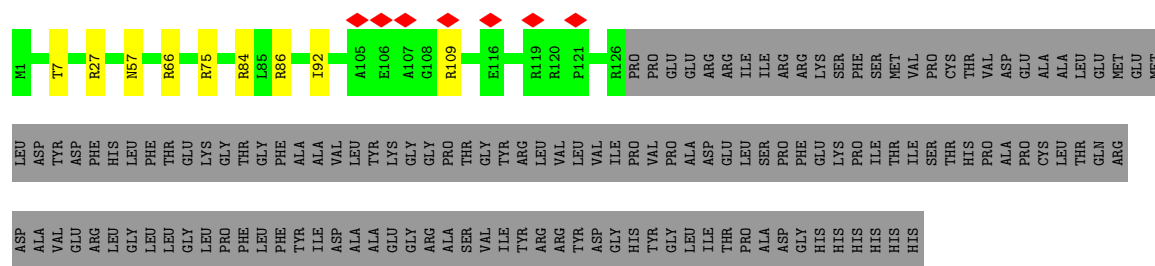
• Molecule 43: 30S ribosomal protein S15



• Molecule 44: 30S ribosomal protein S16



• Molecule 50: Ribosome hibernation promotion factor RafH



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.34	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.045	Depositor
Map size (\AA)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.30	0/2153	0.57	0/2895
2	F	0.32	0/1609	0.59	0/2165
3	G	0.31	0/1592	0.53	0/2153
4	H	0.27	0/1458	0.57	0/1962
5	I	0.27	0/1281	0.60	0/1733
6	J	0.26	0/311	0.59	0/419
7	M	0.29	0/1157	0.48	0/1567
8	N	0.30	0/946	0.55	0/1268
9	O	0.28	0/1091	0.55	0/1457
10	Q	0.30	0/945	0.54	0/1267
11	R	0.30	0/950	0.65	0/1276
12	S	0.31	0/921	0.59	0/1236
13	T	0.30	0/1000	0.56	0/1341
14	U	0.31	0/764	0.51	0/1030
15	V	0.30	0/878	0.57	0/1192
16	W	0.32	0/766	0.53	0/1030
17	X	0.29	0/709	0.55	0/947
18	Z	0.31	0/583	0.58	0/782
19	1	0.28	0/478	0.61	0/641
20	2	0.31	0/530	0.66	0/708
21	3	0.26	0/473	0.56	0/635
22	5	0.24	0/427	0.59	0/572
23	6	0.28	0/413	0.71	0/553
24	7	0.27	0/375	0.68	0/493
25	8	0.29	0/507	0.61	0/672
26	4	0.26	0/454	0.54	0/610
27	A	0.43	0/72631	0.80	22/113324 (0.0%)
28	B	0.30	0/2799	0.81	4/4362 (0.1%)
29	a	0.53	0/36400	0.81	14/56798 (0.0%)
30	v	0.25	0/271	0.71	0/348
31	d	0.30	0/1680	0.58	0/2256
32	e	0.32	0/1672	0.56	0/2251
33	f	0.29	0/1239	0.55	0/1673
34	g	0.43	0/782	0.64	0/1059

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	h	0.30	0/1225	0.58	0/1653
36	i	0.35	0/1025	0.56	0/1385
37	j	0.33	0/1012	0.60	0/1362
38	k	0.30	0/798	0.56	0/1081
39	l	0.32	0/873	0.55	0/1180
40	m	0.34	0/969	0.59	0/1294
41	n	0.34	0/942	0.68	0/1260
42	o	0.27	0/830	0.62	0/1106
43	p	0.33	0/729	0.56	0/977
44	q	0.35	0/908	0.58	0/1226
45	r	0.34	0/759	0.57	0/1016
46	s	0.36	0/518	0.62	0/693
47	t	0.31	0/680	0.59	0/915
48	u	0.30	0/663	0.54	0/882
49	c	0.30	0/1737	0.57	0/2344
50	w	0.29	0/1023	0.60	0/1381
All	All	0.42	0/154936	0.76	40/232430 (0.0%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2089	C	N3-C2-O2	-8.43	116.00	121.90
29	a	1206	U	C2-N1-C1'	7.77	127.03	117.70
27	A	2245	C	C2-N1-C1'	7.69	127.26	118.80
27	A	2245	C	N1-C2-O2	7.40	123.34	118.90
29	a	1017	C	N3-C2-O2	-7.29	116.80	121.90

There are no chirality outliers.

There are no planarity outliers.

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

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	E	273/278 (98%)	260 (95%)	13 (5%)	0	100	100
2	F	212/217 (98%)	203 (96%)	9 (4%)	0	100	100
3	G	207/215 (96%)	202 (98%)	5 (2%)	0	100	100
4	H	179/187 (96%)	169 (94%)	10 (6%)	0	100	100
5	I	163/179 (91%)	162 (99%)	1 (1%)	0	100	100
6	J	39/151 (26%)	39 (100%)	0	0	100	100
7	M	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
8	N	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
9	O	143/147 (97%)	132 (92%)	11 (8%)	0	100	100
10	Q	116/199 (58%)	112 (97%)	4 (3%)	0	100	100
11	R	122/127 (96%)	121 (99%)	1 (1%)	0	100	100
12	S	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
13	T	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
14	U	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
15	V	111/153 (72%)	108 (97%)	3 (3%)	0	100	100
16	W	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
17	X	88/105 (84%)	84 (96%)	4 (4%)	0	100	100
18	Z	75/88 (85%)	69 (92%)	6 (8%)	0	100	100
19	1	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
20	2	61/77 (79%)	60 (98%)	1 (2%)	0	100	100
21	3	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
22	5	52/57 (91%)	52 (100%)	0	0	100	100
23	6	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
24	7	43/47 (92%)	42 (98%)	1 (2%)	0	100	100
25	8	61/64 (95%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	4	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
30	v	29/33 (88%)	29 (100%)	0	0	100	100
31	d	205/275 (74%)	196 (96%)	9 (4%)	0	100	100
32	e	198/201 (98%)	185 (93%)	13 (7%)	0	100	100
33	f	166/214 (78%)	159 (96%)	7 (4%)	0	100	100
34	g	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
35	h	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
36	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
37	j	124/150 (83%)	117 (94%)	7 (6%)	0	100	100
38	k	96/101 (95%)	90 (94%)	6 (6%)	0	100	100
39	l	113/138 (82%)	107 (95%)	6 (5%)	0	100	100
40	m	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
41	n	114/124 (92%)	110 (96%)	4 (4%)	0	100	100
42	o	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
43	p	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
44	q	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
45	r	92/98 (94%)	89 (97%)	3 (3%)	0	100	100
46	s	63/84 (75%)	60 (95%)	3 (5%)	0	100	100
47	t	80/93 (86%)	77 (96%)	3 (4%)	0	100	100
48	u	83/86 (96%)	83 (100%)	0	0	100	100
49	c	215/277 (78%)	199 (93%)	16 (7%)	0	100	100
50	w	124/264 (47%)	116 (94%)	8 (6%)	0	100	100
All	All	5343/6252 (86%)	5127 (96%)	216 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	215/218 (99%)	205 (95%)	10 (5%)	26	59
2	F	160/163 (98%)	151 (94%)	9 (6%)	21	51
3	G	169/173 (98%)	157 (93%)	12 (7%)	14	39
4	H	150/156 (96%)	139 (93%)	11 (7%)	14	38
5	I	139/150 (93%)	128 (92%)	11 (8%)	12	34
6	J	31/116 (27%)	27 (87%)	4 (13%)	4	13
7	M	119/120 (99%)	113 (95%)	6 (5%)	24	56
8	N	100/100 (100%)	95 (95%)	5 (5%)	24	56
9	O	112/114 (98%)	105 (94%)	7 (6%)	18	46
10	Q	97/158 (61%)	93 (96%)	4 (4%)	30	64
11	R	92/94 (98%)	85 (92%)	7 (8%)	13	36
12	S	100/100 (100%)	88 (88%)	12 (12%)	5	15
13	T	97/99 (98%)	95 (98%)	2 (2%)	53	84
14	U	81/83 (98%)	76 (94%)	5 (6%)	18	47
15	V	89/117 (76%)	85 (96%)	4 (4%)	27	60
16	W	83/85 (98%)	77 (93%)	6 (7%)	14	38
17	X	78/86 (91%)	71 (91%)	7 (9%)	9	28
18	Z	56/63 (89%)	51 (91%)	5 (9%)	9	28
19	1	50/51 (98%)	47 (94%)	3 (6%)	19	48
20	2	58/66 (88%)	53 (91%)	5 (9%)	10	30
21	3	52/54 (96%)	48 (92%)	4 (8%)	13	35
22	5	43/46 (94%)	43 (100%)	0	100	100
23	6	47/52 (90%)	44 (94%)	3 (6%)	17	45
24	7	35/36 (97%)	32 (91%)	3 (9%)	10	30
25	8	53/54 (98%)	49 (92%)	4 (8%)	13	37
26	4	50/63 (79%)	42 (84%)	8 (16%)	2	7
30	v	29/31 (94%)	28 (97%)	1 (3%)	37	71
31	d	170/212 (80%)	159 (94%)	11 (6%)	17	44
32	e	175/176 (99%)	166 (95%)	9 (5%)	24	55
33	f	123/147 (84%)	116 (94%)	7 (6%)	20	50
34	g	85/85 (100%)	70 (82%)	15 (18%)	2	5
35	h	129/132 (98%)	117 (91%)	12 (9%)	9	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	i	107/108 (99%)	102 (95%)	5 (5%)	26 59
37	j	102/125 (82%)	92 (90%)	10 (10%)	8 24
38	k	89/90 (99%)	85 (96%)	4 (4%)	27 60
39	l	89/105 (85%)	78 (88%)	11 (12%)	4 14
40	m	103/105 (98%)	97 (94%)	6 (6%)	20 50
41	n	99/104 (95%)	83 (84%)	16 (16%)	2 7
42	o	85/86 (99%)	79 (93%)	6 (7%)	14 39
43	p	76/77 (99%)	71 (93%)	5 (7%)	16 44
44	q	92/118 (78%)	85 (92%)	7 (8%)	13 36
45	r	80/83 (96%)	74 (92%)	6 (8%)	13 37
46	s	55/72 (76%)	54 (98%)	1 (2%)	59 86
47	t	73/84 (87%)	62 (85%)	11 (15%)	3 9
48	u	69/70 (99%)	66 (96%)	3 (4%)	29 62
49	c	182/218 (84%)	162 (89%)	20 (11%)	6 19
50	w	98/215 (46%)	89 (91%)	9 (9%)	9 27
All	All	4466/5060 (88%)	4134 (93%)	332 (7%)	17 37

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	l	35	THR
45	r	72	ASP
39	l	120	SER
41	n	91	ARG
48	u	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
49	c	94	GLN
50	w	95	HIS
32	e	185	GLN
35	h	148	ASN
37	j	47	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	A	3016/3119 (96%)	547 (18%)	17 (0%)
28	B	116/118 (98%)	19 (16%)	1 (0%)
29	a	1514/1528 (99%)	272 (17%)	0
All	All	4646/4765 (97%)	838 (18%)	18 (0%)

5 of 838 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	A	7	U
27	A	9	U
27	A	12	G
27	A	20	G
27	A	33	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	2350	G
28	B	10	G
27	A	2729	G
27	A	1002	C
27	A	2343	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

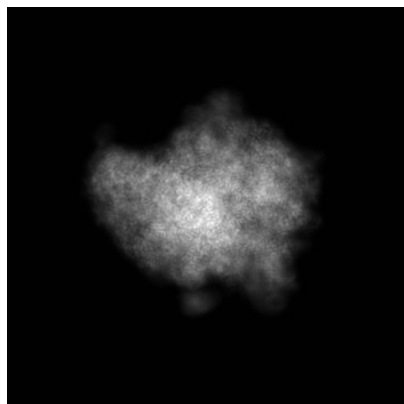
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37551. These allow visual inspection of the internal detail of the map and identification of artifacts.

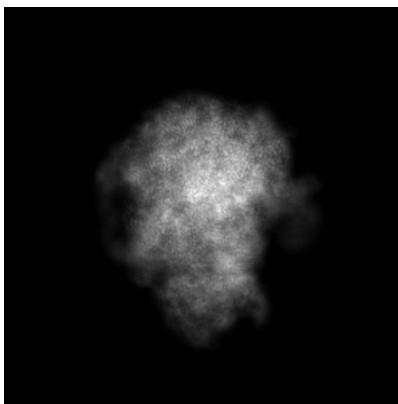
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

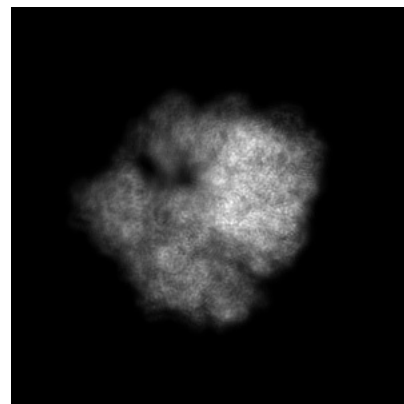
6.1.1 Primary map



X

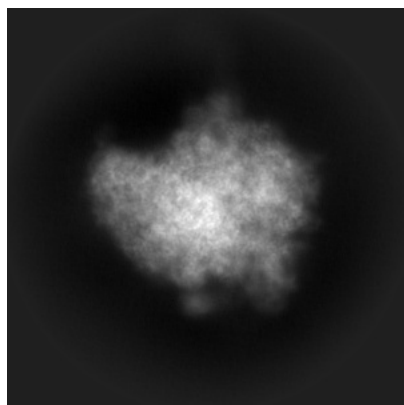


Y

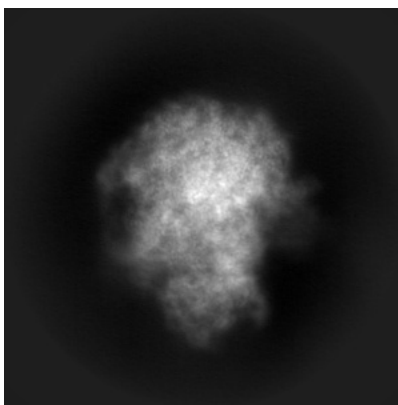


Z

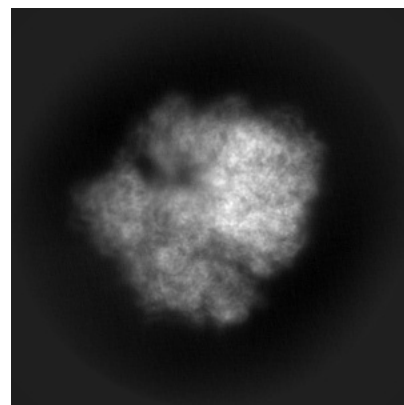
6.1.2 Raw map



X



Y

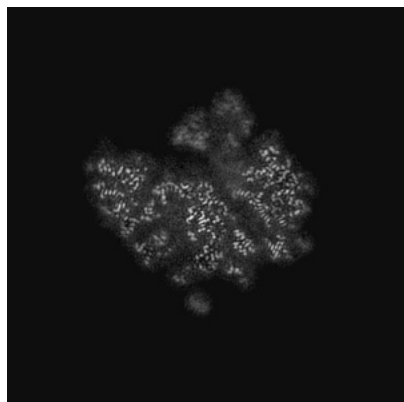


Z

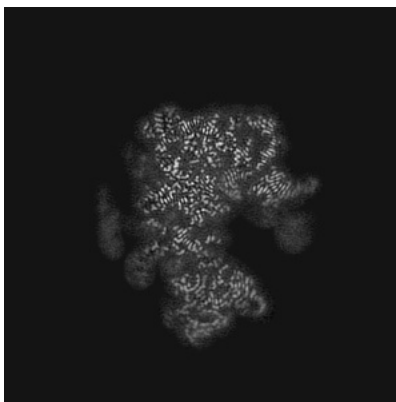
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

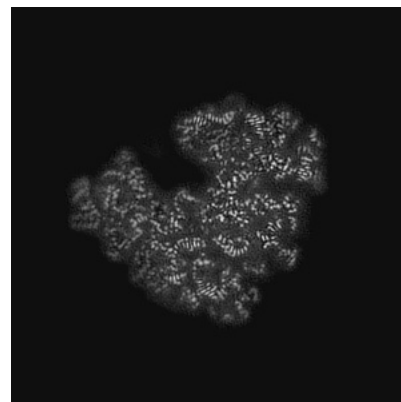
6.2.1 Primary map



X Index: 190

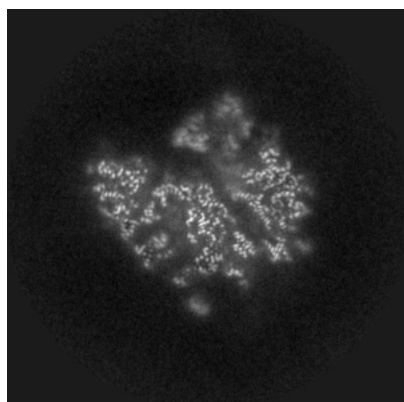


Y Index: 190

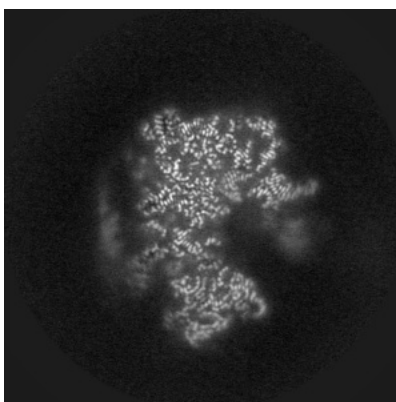


Z Index: 190

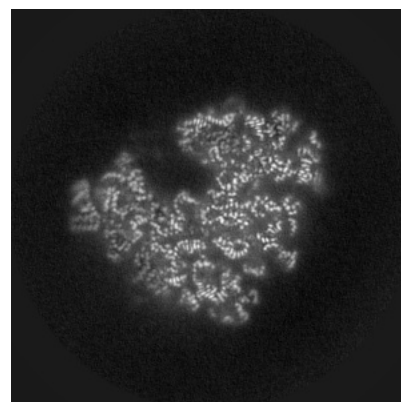
6.2.2 Raw map



X Index: 190



Y Index: 190

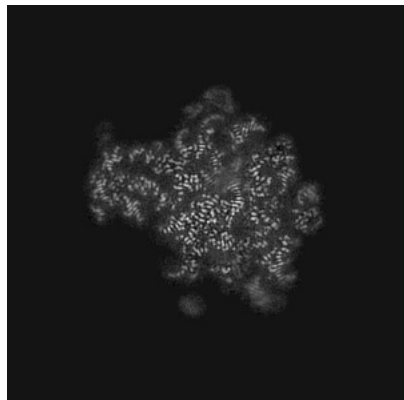


Z Index: 190

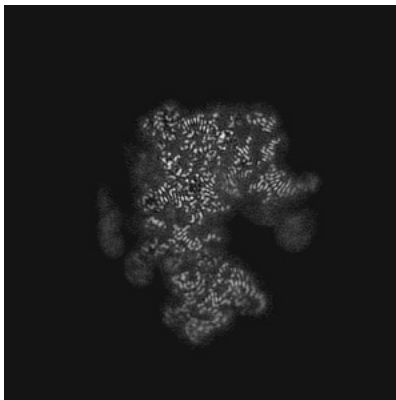
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

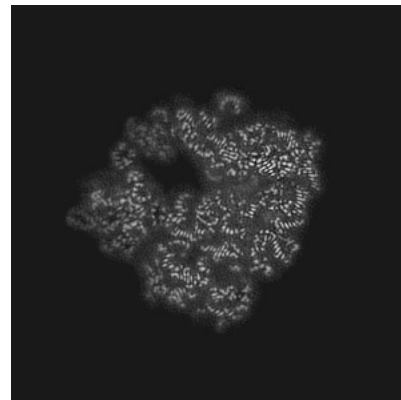
6.3.1 Primary map



X Index: 213

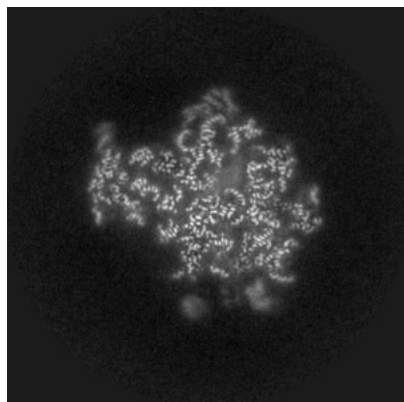


Y Index: 191

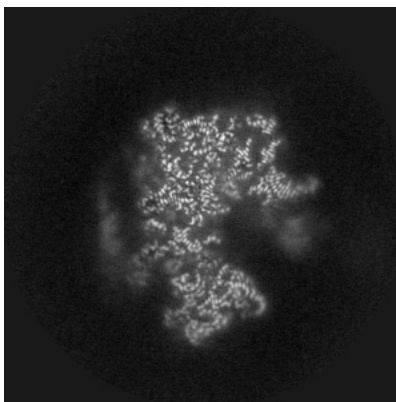


Z Index: 200

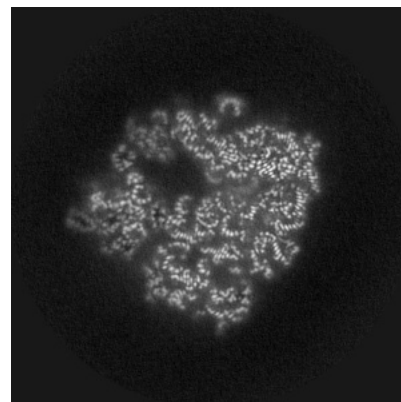
6.3.2 Raw map



X Index: 210



Y Index: 191

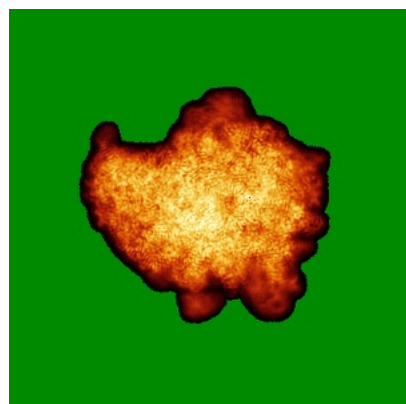


Z Index: 200

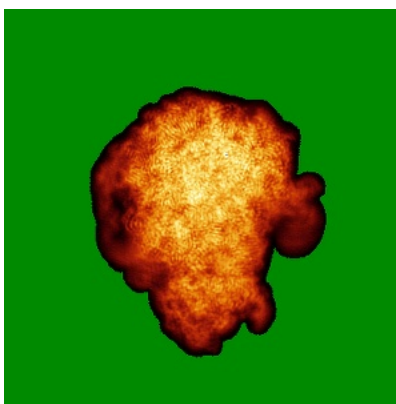
The images above show the largest variance slices of the map in three orthogonal directions.

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

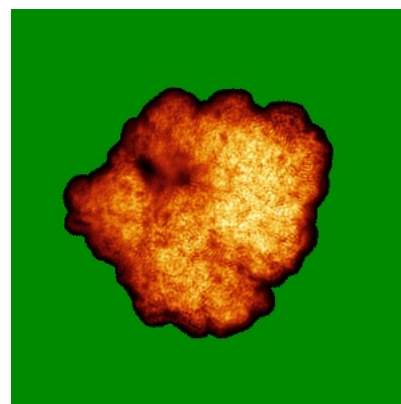
6.4.1 Primary map



X

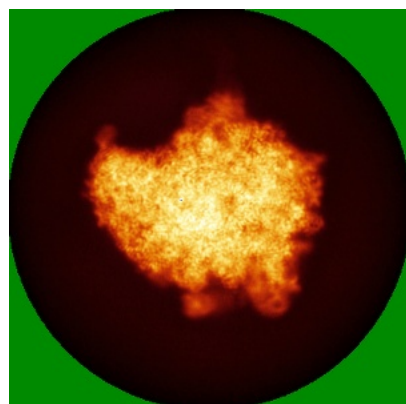


Y

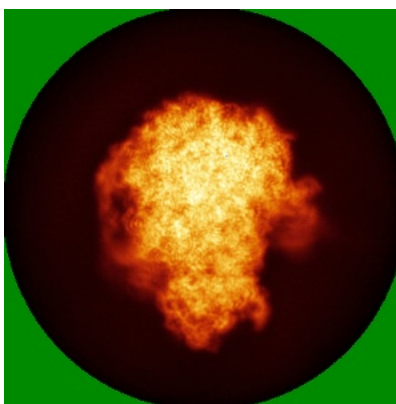


Z

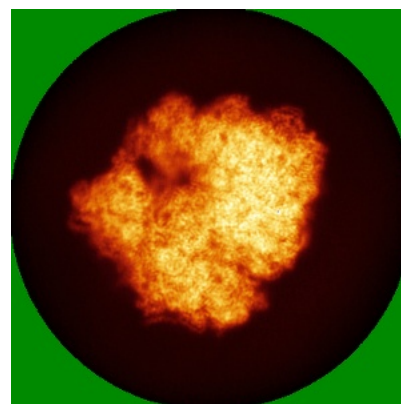
6.4.2 Raw map



X



Y

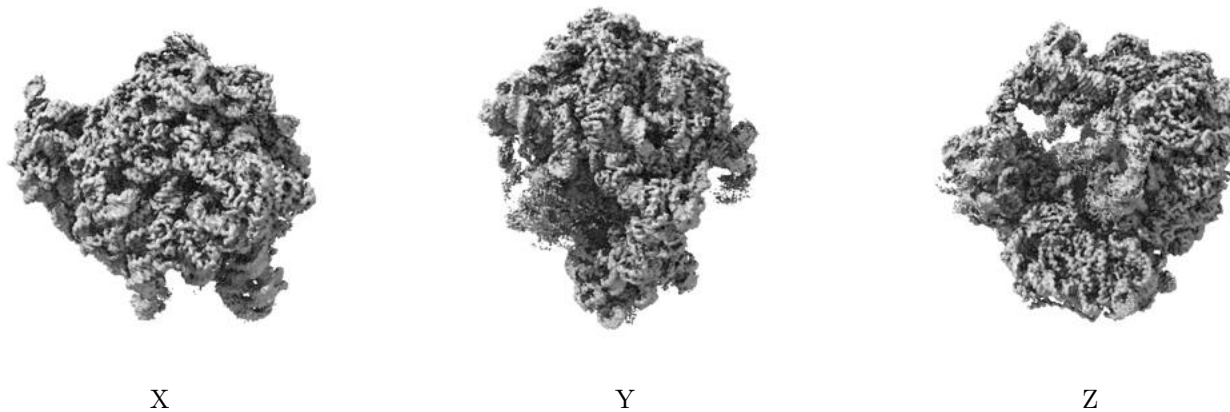


Z

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

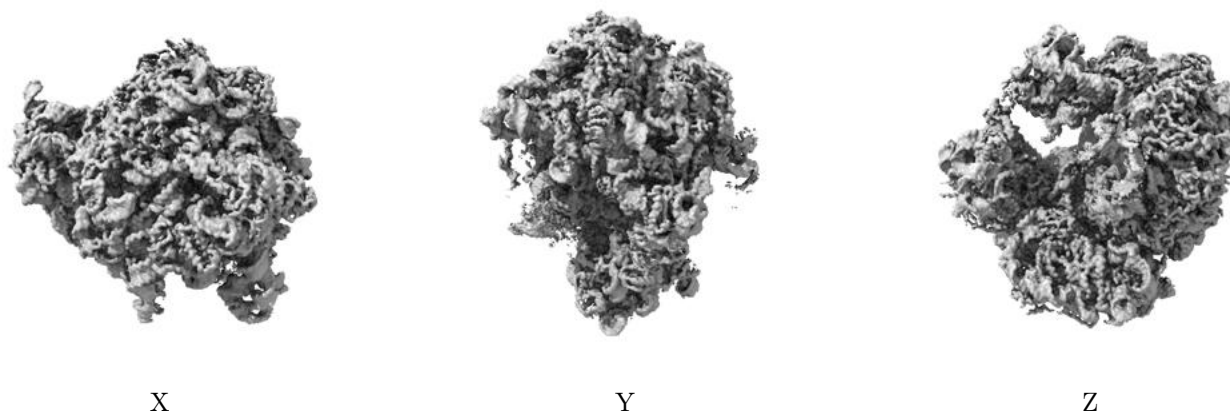
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

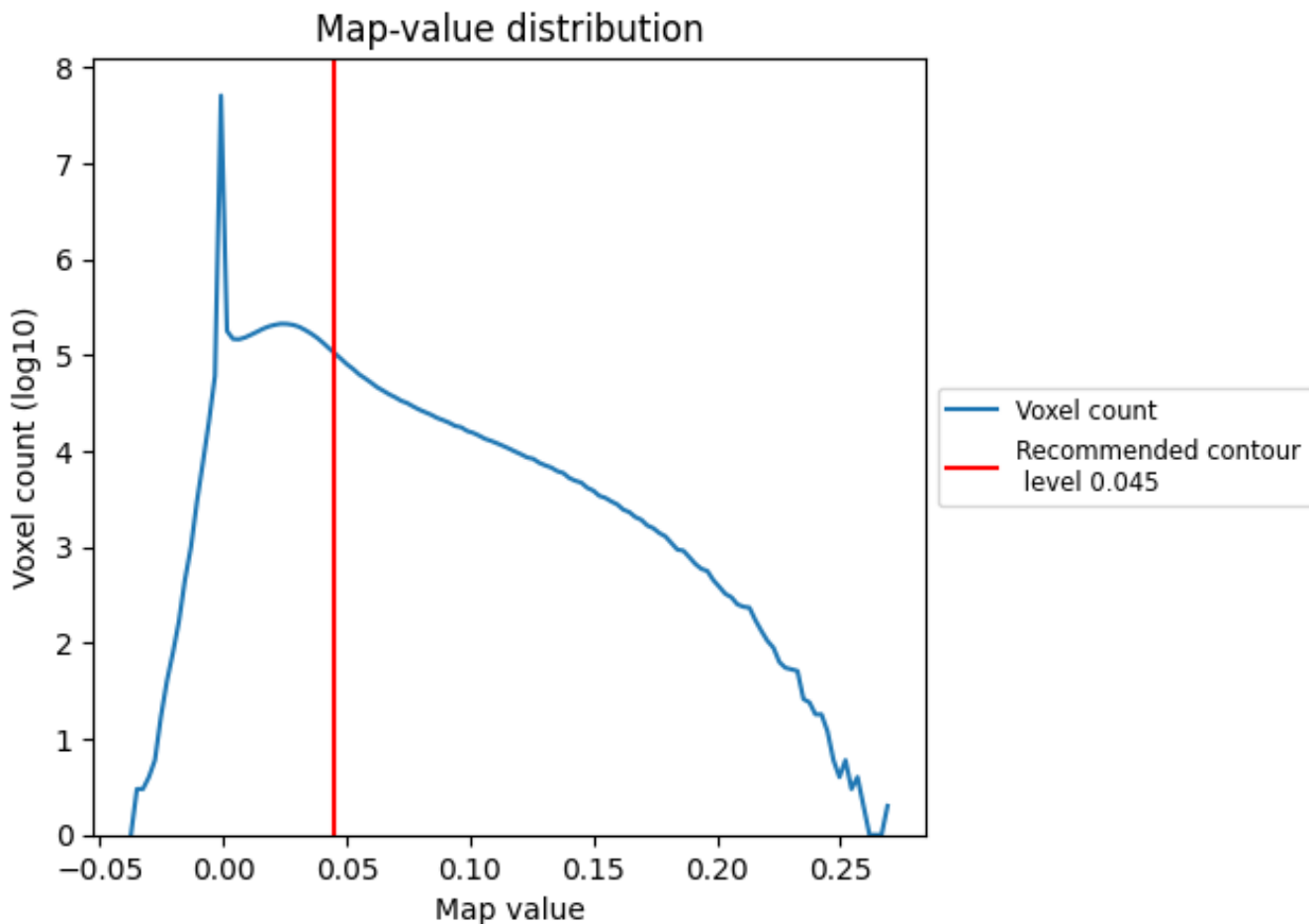
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

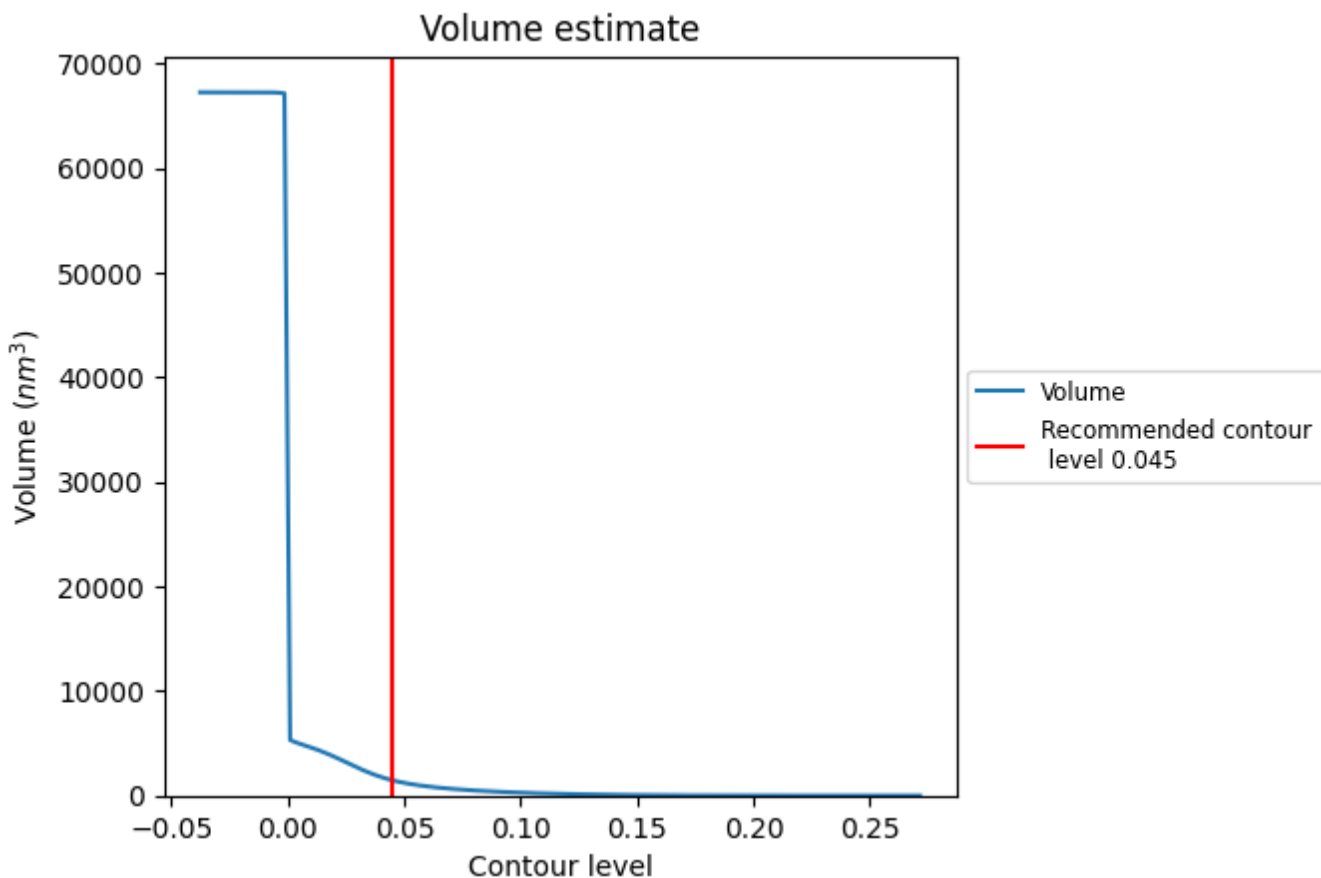
This section contains the results of statistical analysis of the map.

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.

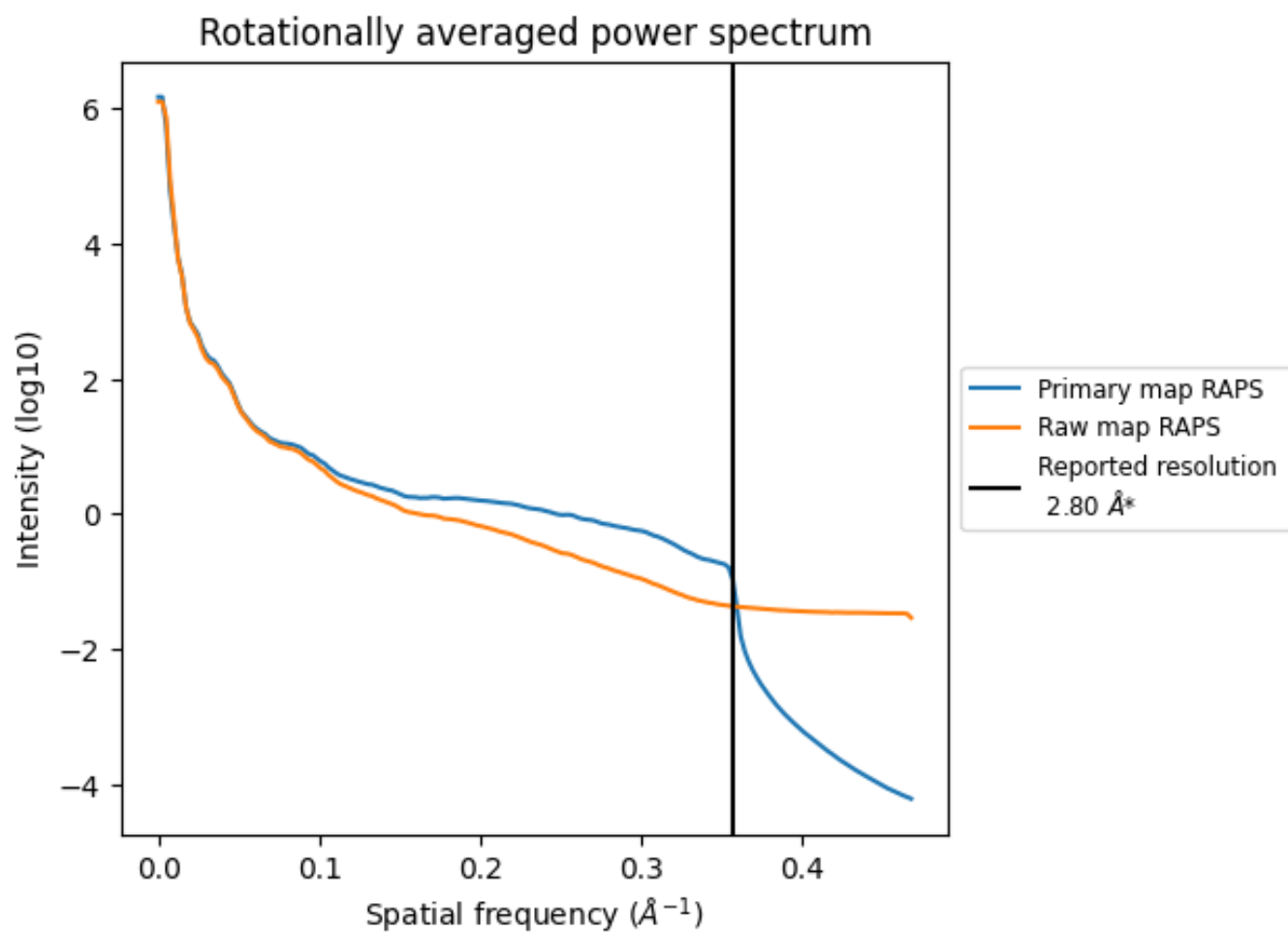
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1462 nm³; this corresponds to an approximate mass of 1321 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

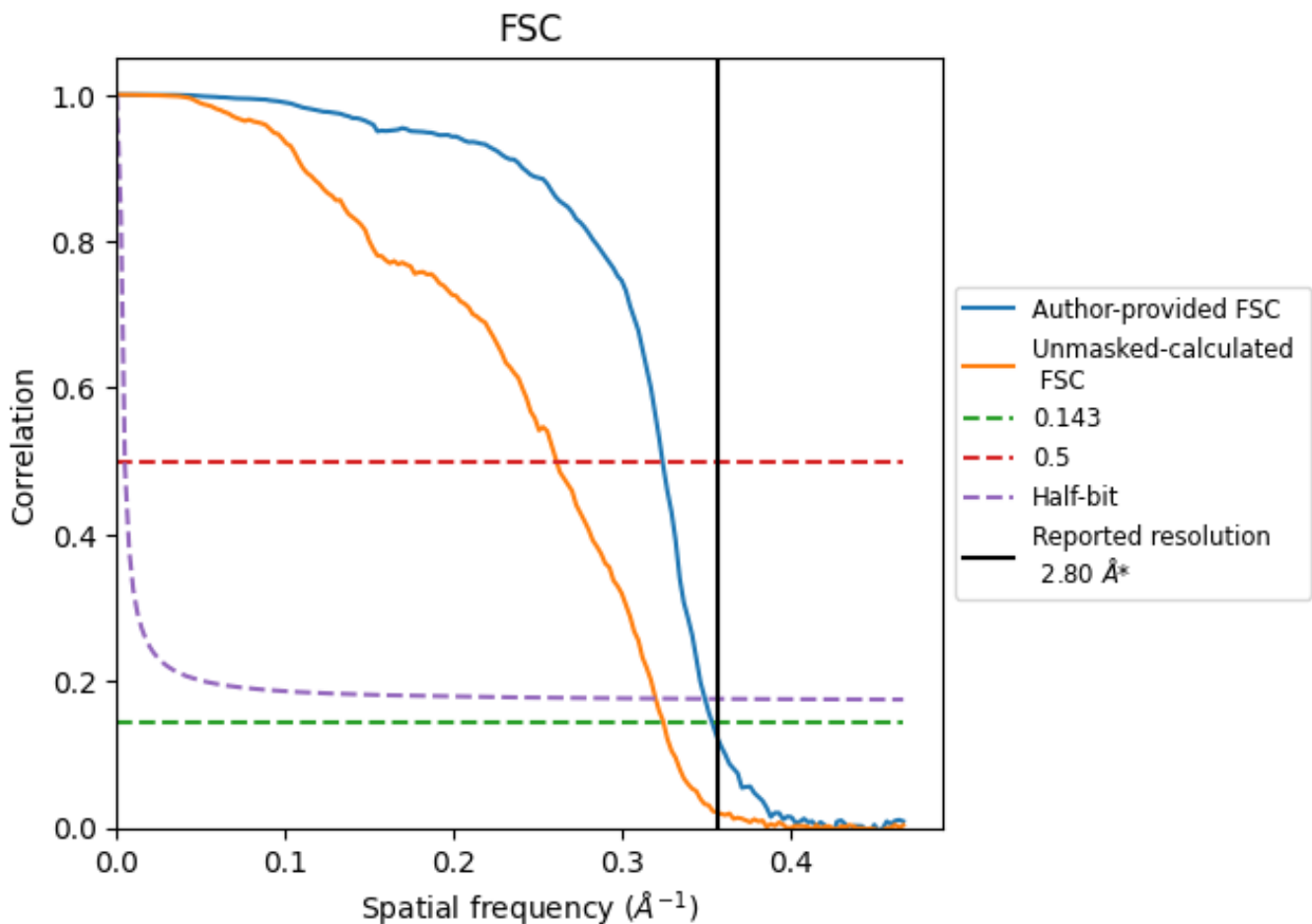


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

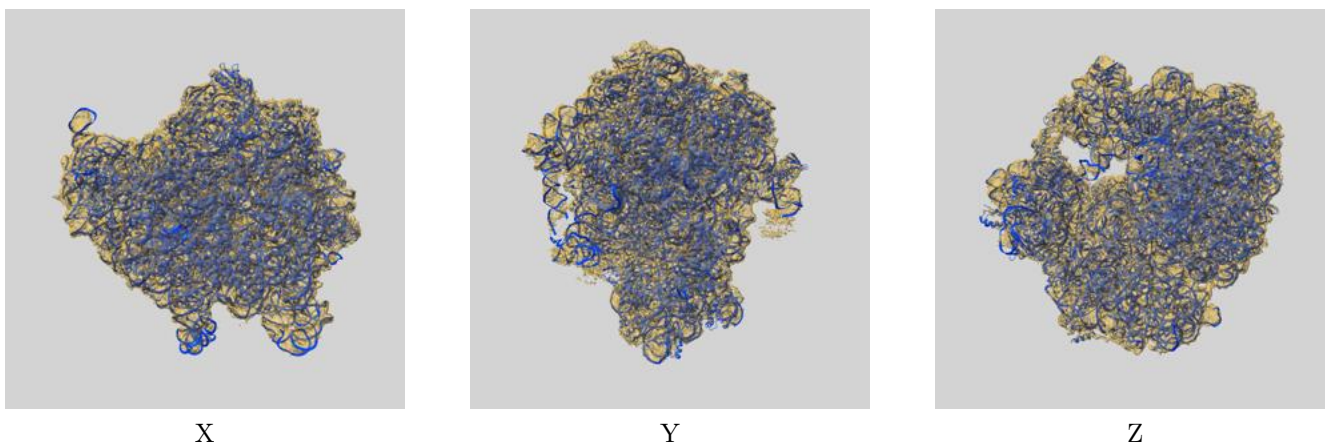
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.08	2.86
Unmasked-calculated*	3.08	3.83	3.12

*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 3.08 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

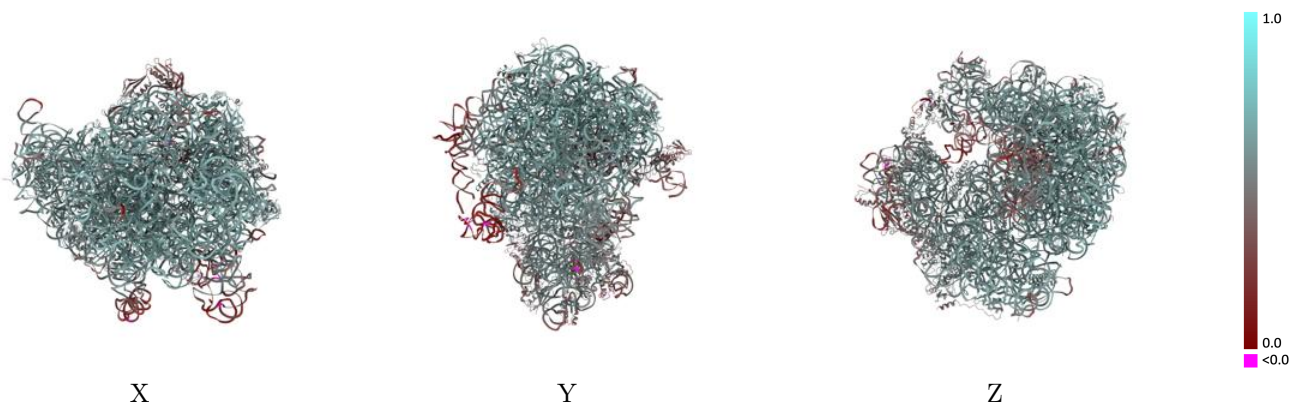
This section contains information regarding the fit between EMDB map EMD-37551 and PDB model 8WHX. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



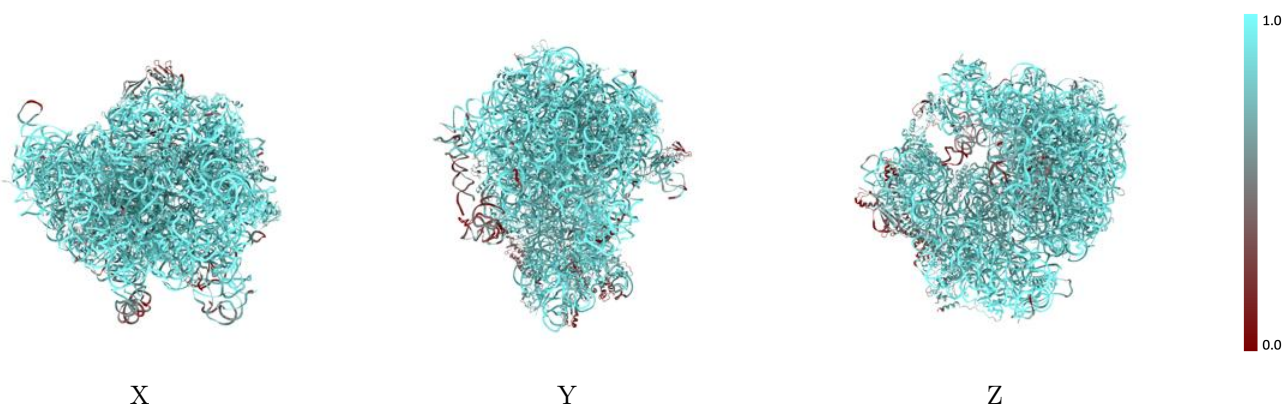
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



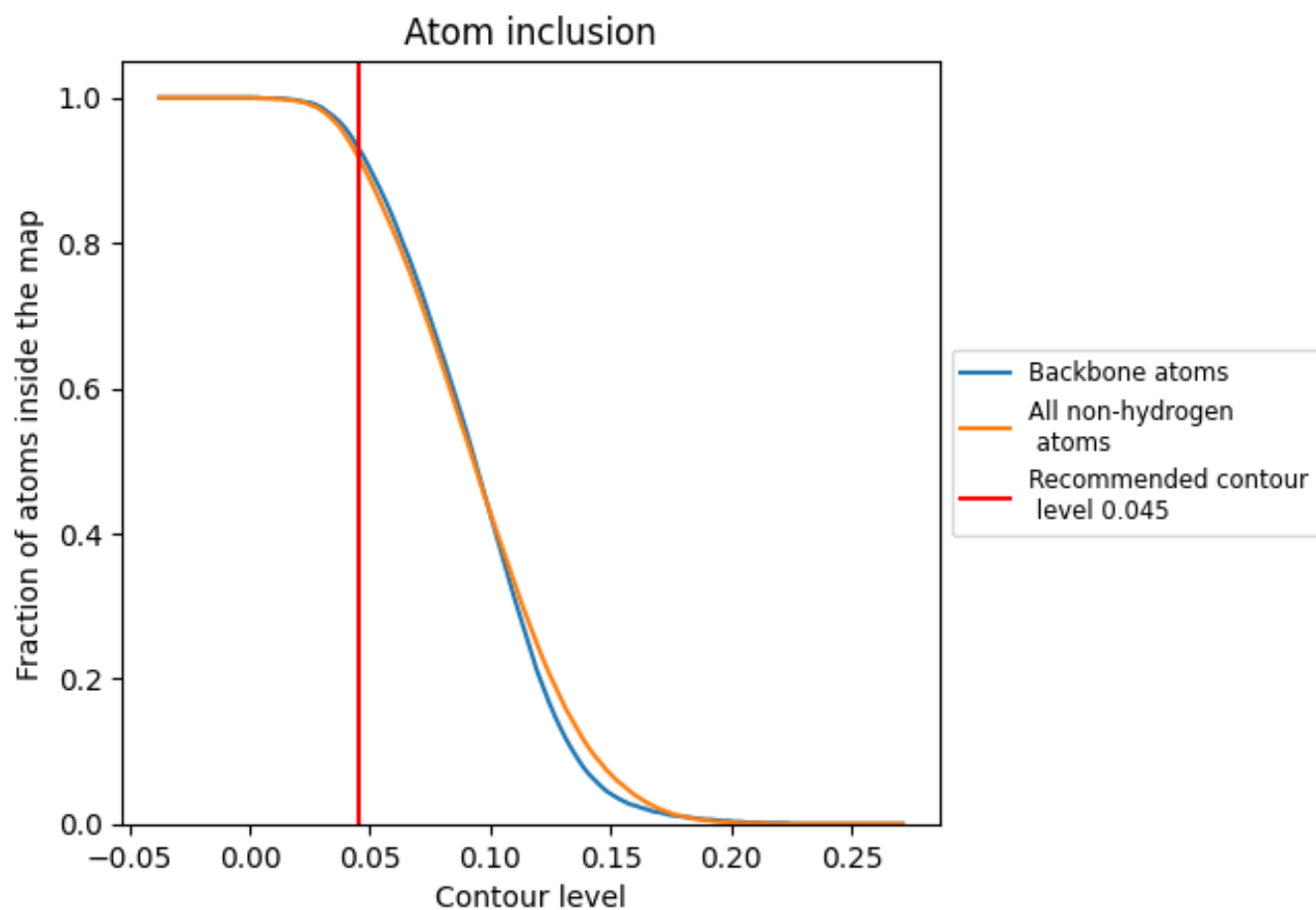
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.5560
1	 0.9090	 0.5710
2	 0.8950	 0.5660
3	 0.9450	 0.6050
4	 0.3640	 0.2580
5	 0.9050	 0.6150
6	 0.7920	 0.5320
7	 0.9970	 0.6380
8	 0.9560	 0.6130
A	 0.9350	 0.5590
B	 0.9650	 0.5210
E	 0.9830	 0.6300
F	 0.9520	 0.6060
G	 0.9190	 0.5830
H	 0.8020	 0.4880
I	 0.5730	 0.3560
J	 0.6470	 0.4860
M	 0.9650	 0.6090
N	 0.9560	 0.6120
O	 0.9340	 0.6010
Q	 0.9750	 0.6240
R	 0.8690	 0.5240
S	 0.9400	 0.5910
T	 0.9700	 0.6140
U	 0.9290	 0.6130
V	 0.9830	 0.6220
W	 0.9350	 0.5970
X	 0.8650	 0.5640
Z	 0.9620	 0.5970
a	 0.9720	 0.5670
c	 0.2550	 0.3730
d	 0.7100	 0.4790
e	 0.8610	 0.5290
f	 0.8090	 0.5500
g	 0.8610	 0.5480



Continued on next page...

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Chain	Atom inclusion	Q-score
h	 0.8660	 0.5090
i	 0.9560	 0.5810
j	 0.8330	 0.4820
k	 0.6060	 0.4630
l	 0.9280	 0.5600
m	 0.9410	 0.5890
n	 0.8710	 0.5060
o	 0.6000	 0.4130
p	 0.9390	 0.5710
q	 0.8940	 0.5510
r	 0.9240	 0.5770
s	 0.9090	 0.5470
t	 0.8460	 0.5110
u	 0.9480	 0.5730
v	 0.9760	 0.5880
w	 0.8970	 0.5370