



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2024 – 02:16 PM EST

PDB ID : 8UU6
EMDB ID : EMD-42561
Title : Cryo-EM structure of the ratcheted *Listeria innocua* 70S ribosome in complex with p/E-tRNA (structure II-A)
Authors : Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on : 2023-10-31
Resolution : 3.30 Å (reported)
Based on initial model : 7NHN

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:

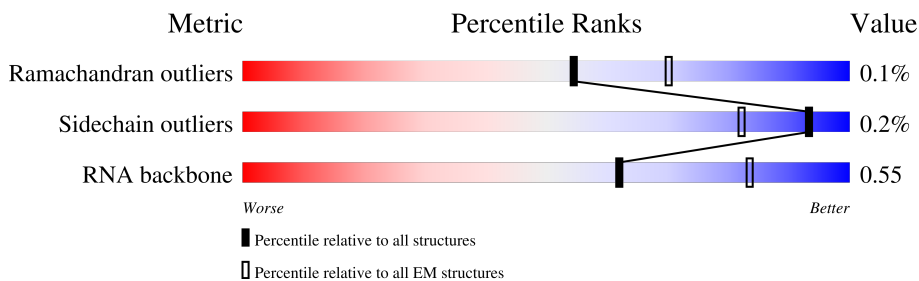
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



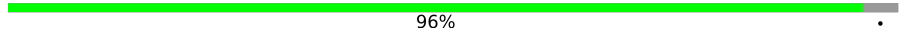
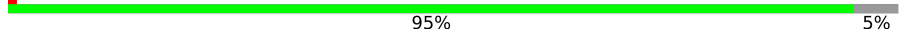

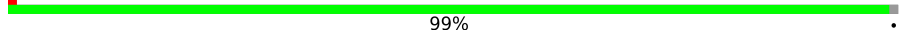
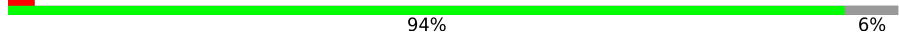
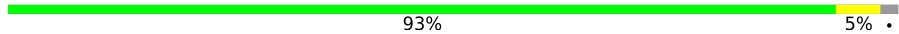
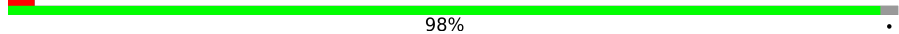
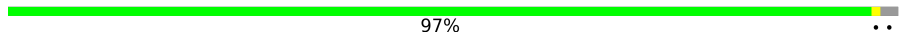



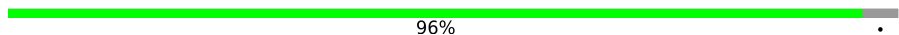




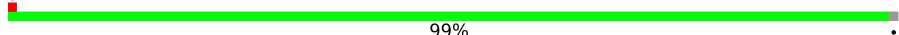
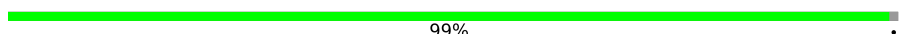
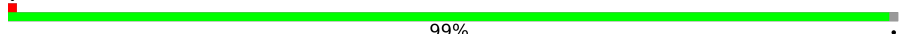


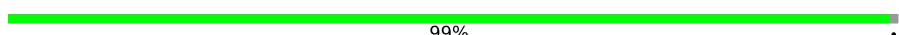
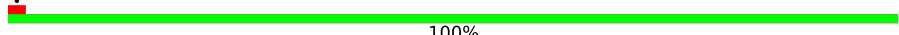
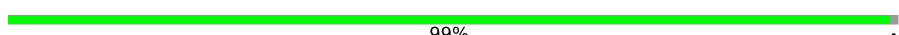
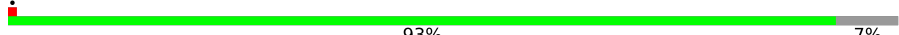
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	a	1550	
2	b	249	
3	c	218	
4	d	200	
5	e	167	
6	f	97	
7	g	156	
8	h	132	


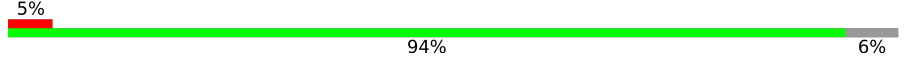
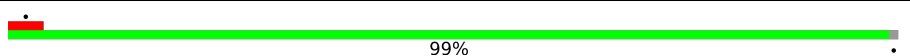
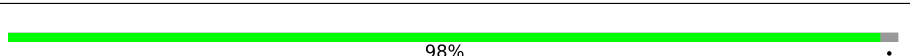
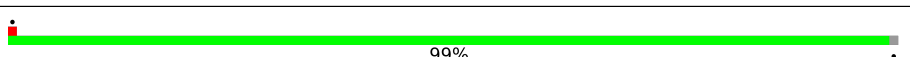
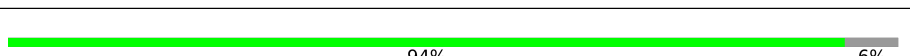
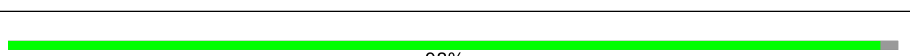
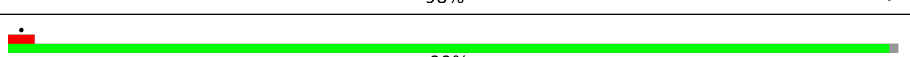
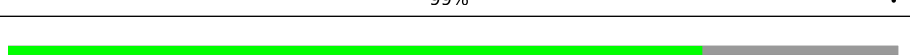
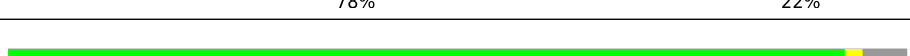
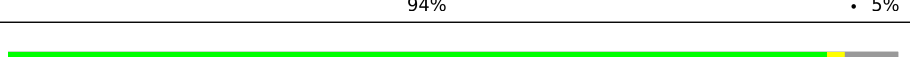
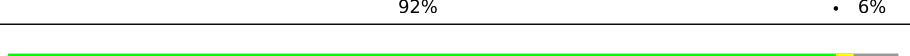

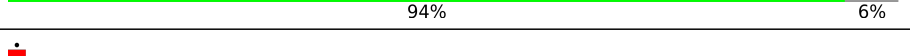
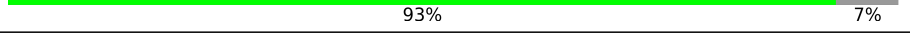
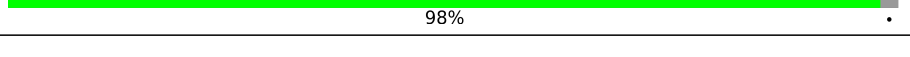
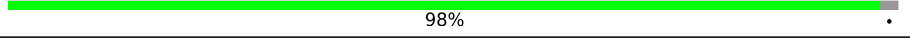
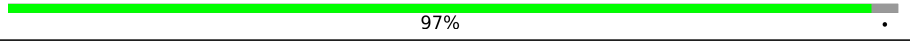
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Mol	Chain	Length	Quality of chain
9	i	130	 96%
10	j	102	 95% 5%
11	k	129	 88% 12%
12	l	137	 99%
13	m	121	 94% 6%
14	n	61	 93% 5%
15	o	89	 98%
16	p	90	 97%
17	q	87	 91% 8%
18	r	79	 80% 19%
19	s	92	 88% 12% 8%
20	t	84	 96%
21	x	76	 58% 36% 14%
22	w	21	 71% 24% 5%
23	A	2932	 81% 18%
24	B	116	 87% 11%
25	C	277	 99%
26	D	209	 99%
27	E	207	 99%
28	F	179	 93% 7% 25%
29	G	178	 90% 10%
30	L	145	 99%
31	M	122	 100%
32	N	146	 99%
33	O	144	 93% 7%

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Mol	Chain	Length	Quality of chain
34	P	135	 90% 10%
35	Q	119	 94% 6%
36	R	114	 99%
37	S	119	 98%
38	T	102	 99%
39	U	118	 94% 6%
40	V	94	 98%
41	W	103	 99%
42	Y	96	 78% 22%
43	Z	62	 94% 5%
44	1	63	 92% 6%
45	2	59	 93% 5%
46	3	81	 48% 94% 6%
47	4	57	 93% 7%
48	5	49	 98%
49	6	44	 98%
50	7	66	 97%
51	8	37	 97%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 136923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1516	32515	14504	5960	10535	1516	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	b	224	1228	757	236	235	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	203	1395	880	254	259	2	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	199	1429	893	269	266	1	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1087	685	196	204	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	93	652	419	117	114	2	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	143	1015	634	191	186	4	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	131	929	597	159	171	2	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	125	920	578	183	158	1	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	97	714	449	129	135	1	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	114	681	415	131	133	2	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	135	935	584	184	166	1	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	780	483	157	139	1	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			463	295	89	74	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			635	393	124	116	2		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	q	80	Total	C	N	O	0	0
			558	350	113	95		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			449	288	84	75	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	81	Total	C	N	O	S	0	0
			502	314	100	87	1		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	t	81	Total	C	N	O	0	0
			493	298	95	100		

- Molecule 21 is a RNA chain called p/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	x	74	Total	C	N	O	P	S	0	0
			1591	713	285	517	74	2		

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	6	Total	C	N	O	P	0	0
			126	57	22	41	6		

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2904	Total	C	N	O	P	0	0
			62385	27841	11542	20098	2904		

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	C	273	Total	C	N	O	S	0	0
			2059	1276	405	371	7		

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	206	Total	C	N	O	S	0	0
			1545	974	287	280	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	E	205	Total	C	N	O	0	0
			1515	960	279	276		

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	F	167	1142	724	195	218	5	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	G	160	1085	684	201	199	1	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	L	143	1084	689	201	191	3	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	M	122	914	566	173	170	5	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	N	145	1022	633	205	184	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	O	134	1025	658	194	167	6	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	P	122	952	596	188	167	1	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Q	112	Total	C	N	O	0	0
			701	431	139	131		

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	R	113	Total	C	N	O	S	0	0
			843	534	161	147	1		

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	S	117	Total	C	N	O	S	0	0
			930	590	181	155	4		

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	T	101	Total	C	N	O	S	0	0
			762	492	131	138	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	U	111	Total	C	N	O	0	0
			843	532	160	151		

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	V	92	Total	C	N	O	S	0	0
			724	460	122	140	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	W	102	Total	C	N	O	S	0	0
			735	464	135	133	3		

- Molecule 42 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	75	Total	C	N	O	S	0	0
			549	338	106	104	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z	59	Total	C	N	O	S	0	0
			439	271	90	76	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	59	Total	C	N	O	S	0	0
			467	286	92	88	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	56	Total	C	N	O	S	0	0
			429	269	81	78	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	3	76	Total	C	N	O	0	0
			529	332	92	105		

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	48	Total	C	N	O	S	0	0
			380	233	75	68	4		

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	43	Total	C	N	O	S	0	0
			361	219	87	53	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	7	64	Total	C	N	O	S	0	0
			512	316	112	79	5		

- Molecule 51 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	8	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	a	18	Total	Mg	0
			18	18	
52	q	1	Total	Mg	0
			1	1	
52	A	78	Total	Mg	0
			78	78	
52	D	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	n	1	Total	Zn	0
			1	1	
53	4	1	Total	Zn	0
			1	1	
53	5	1	Total	Zn	0
			1	1	
53	8	1	Total	Zn	0
			1	1	

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
54	O	1	Total K 1 1	0

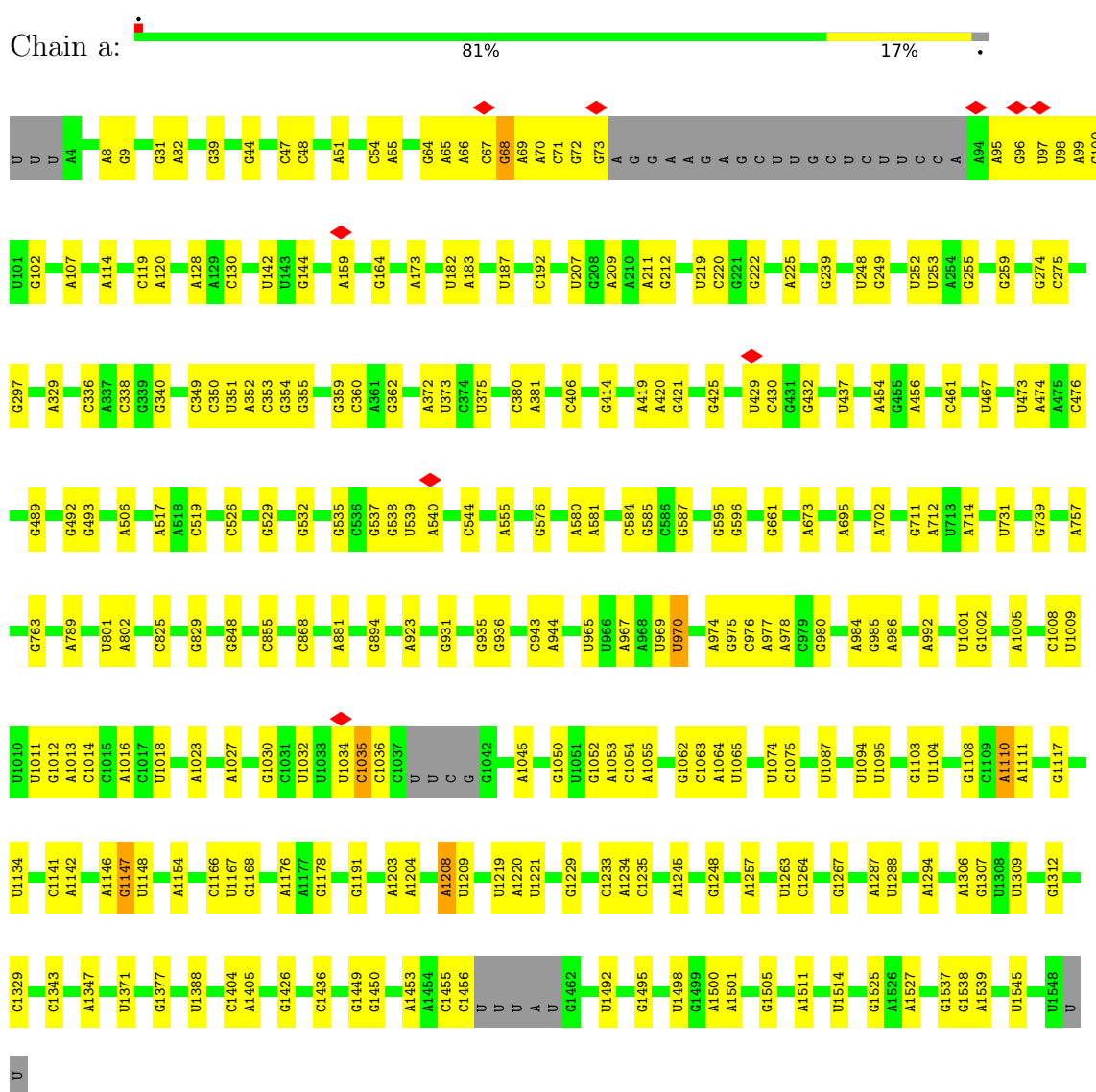
- Molecule 55 is water.

Mol	Chain	Residues	Atoms	AltConf
55	a	2	Total O 2 2	0
55	A	3	Total O 3 3	0

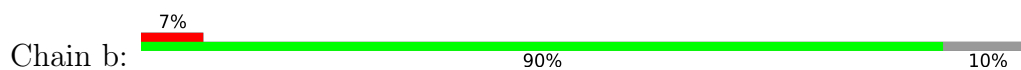
3 Residue-property plots

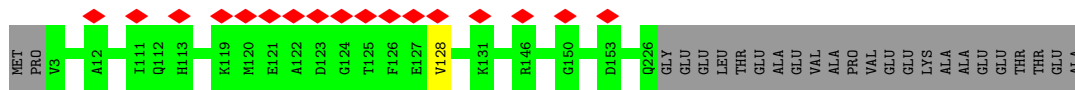
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S Ribosomal RNA

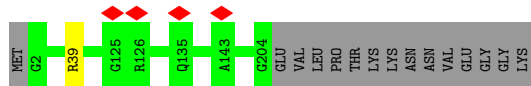
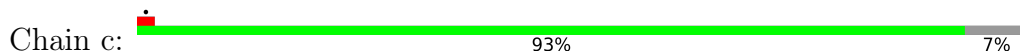


- Molecule 2: Small ribosomal subunit protein uS2

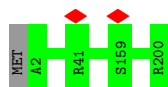




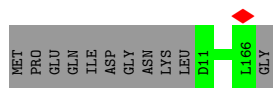
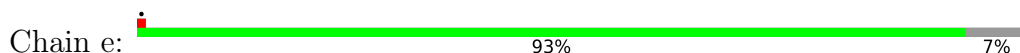
• Molecule 3: Small ribosomal subunit protein uS3



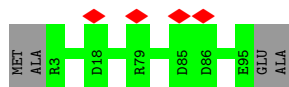
• Molecule 4: Small ribosomal subunit protein uS4



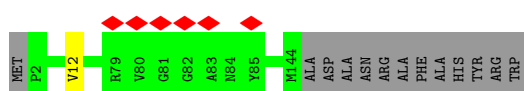
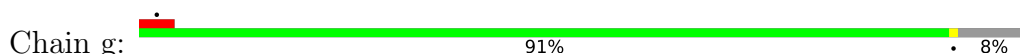
• Molecule 5: Small ribosomal subunit protein uS5



• Molecule 6: Small ribosomal subunit protein bS6



• Molecule 7: Small ribosomal subunit protein uS7

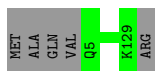


• Molecule 8: Small ribosomal subunit protein uS8



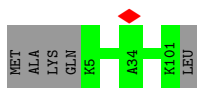
• Molecule 9: Small ribosomal subunit protein uS9

Chain i:  96%




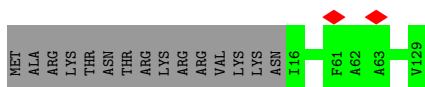
- Molecule 10: Small ribosomal subunit protein uS10

Chain j:  95%



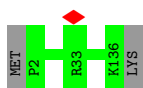
- Molecule 11: Small ribosomal subunit protein uS11

Chain k:  88%



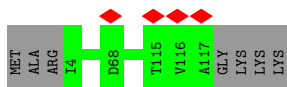
- Molecule 12: Small ribosomal subunit protein uS12

Chain l:  99%



- Molecule 13: Small ribosomal subunit protein uS13

Chain m:  94%



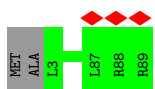
- Molecule 14: Small ribosomal subunit protein uS14

Chain n:  93%



- Molecule 15: Small ribosomal subunit protein uS15

Chain o:  98%



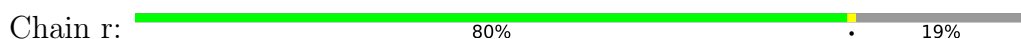
- Molecule 16: Small ribosomal subunit protein bS16



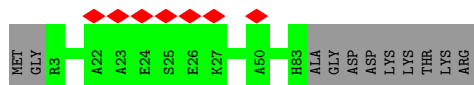
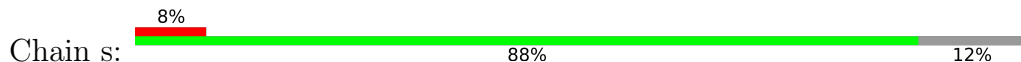
- Molecule 17: Small ribosomal subunit protein uS17



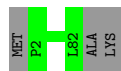
- Molecule 18: Small ribosomal subunit protein bS18



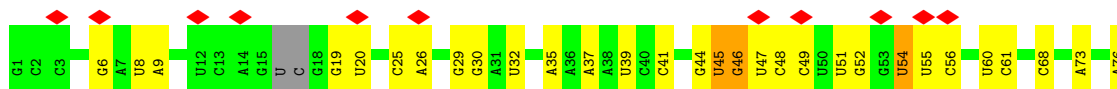
- Molecule 19: Small ribosomal subunit protein uS19



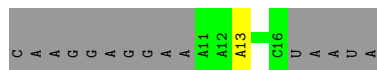
- Molecule 20: Small ribosomal subunit protein bS20




- Molecule 21: p/E Hybrid State Phenylalanine tRNA

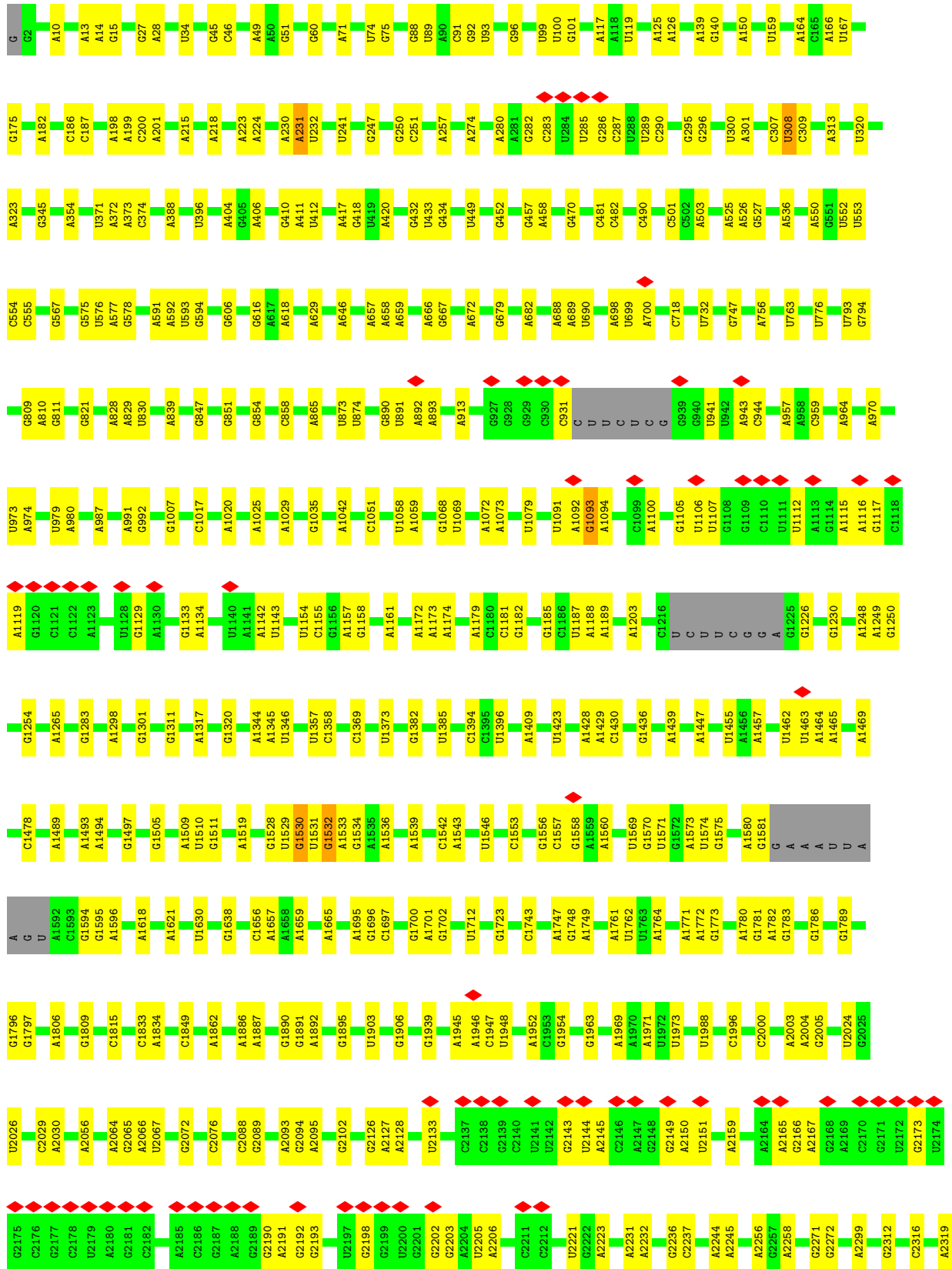


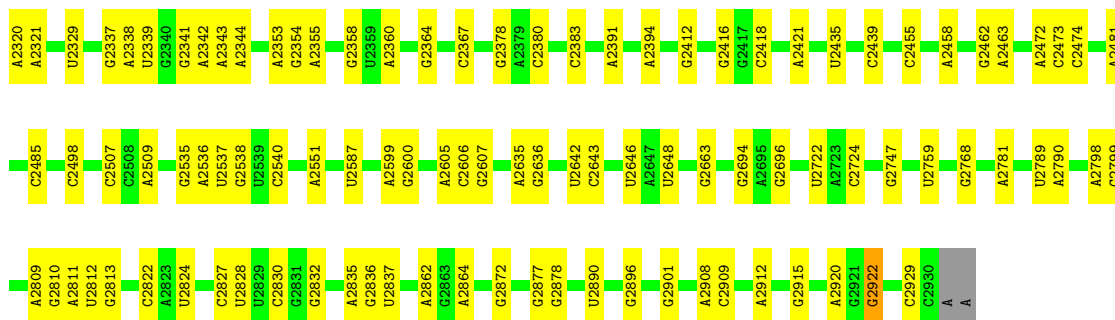
- Molecule 22: F-Stop mRNA



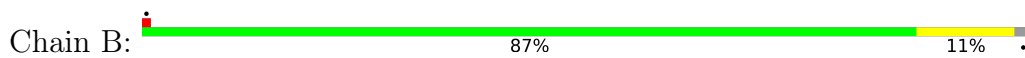
• Molecule 23: 23S Ribosomal RNA

Chain A:  81% 18%

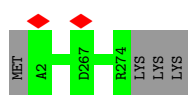




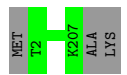
• Molecule 24: 5S Ribosomal RNA



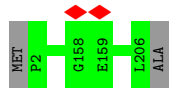
• Molecule 25: Large ribosomal subunit protein uL2



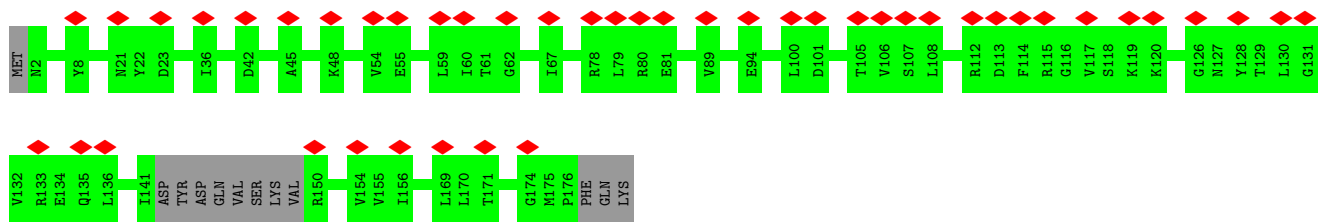
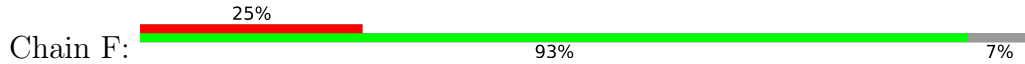
• Molecule 26: Large ribosomal subunit protein uL3




• Molecule 27: Large ribosomal subunit protein uL4

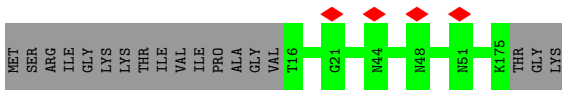


• Molecule 28: Large ribosomal subunit protein uL5



- Molecule 29: Large ribosomal subunit protein uL6

Chain G:  90% 10%



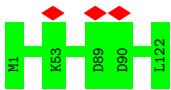
- Molecule 30: Large ribosomal subunit protein uL13

Chain L:  99%



- Molecule 31: Large ribosomal subunit protein uL14

Chain M:  100%



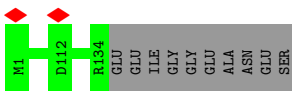
- Molecule 32: Large ribosomal subunit protein uL15

Chain N:  99%




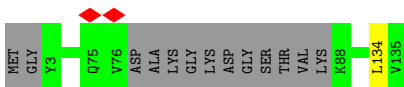
- Molecule 33: Large ribosomal subunit protein uL16

Chain O:  93% 7%



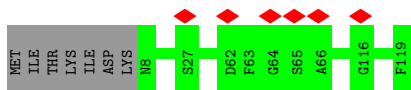
- Molecule 34: Large ribosomal subunit protein bL17

Chain P:  90% 10%



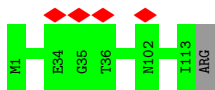
- Molecule 35: Large ribosomal subunit protein uL18

Chain Q:  5% 94% 6%



- Molecule 36: Large ribosomal subunit protein bL19

Chain R: 99%



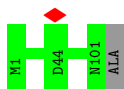
- Molecule 37: Large ribosomal subunit protein bL20

Chain S: 98%



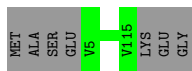
- Molecule 38: Large ribosomal subunit protein bL21

Chain T: 99%



- Molecule 39: Large ribosomal subunit protein uL22

Chain U: 94% 6%



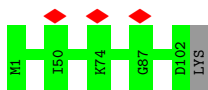
- Molecule 40: Large ribosomal subunit protein uL23

Chain V: 98%

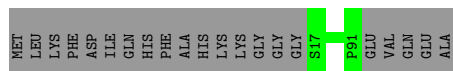
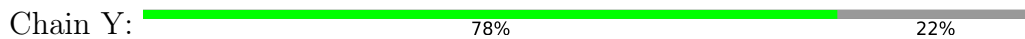


- Molecule 41: Large ribosomal subunit protein uL24

Chain W: 99%



- Molecule 42: Large ribosomal subunit protein bL27



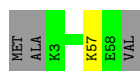
- Molecule 43: Large ribosomal subunit protein bL28



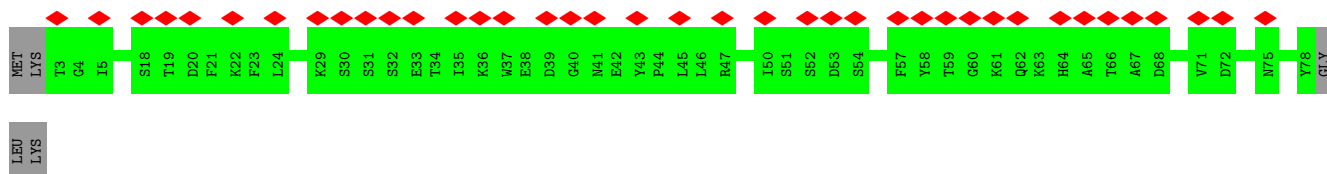
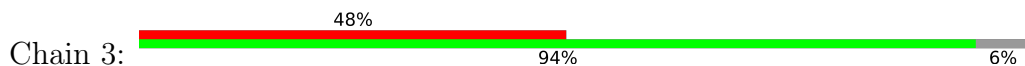
- Molecule 44: Large ribosomal subunit protein uL29



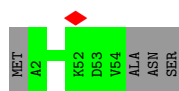
- Molecule 45: Large ribosomal subunit protein uL30



- Molecule 46: Large ribosomal subunit protein bL31B



- Molecule 47: Large ribosomal subunit protein bL32



- Molecule 48: Large ribosomal subunit protein bL33



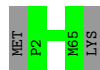
- Molecule 49: Large ribosomal subunit protein bL34

Chain 6:  98%



- Molecule 50: Large ribosomal subunit protein bL35

Chain 7:  97%



- Molecule 51: Large ribosomal subunit protein bL36

Chain 8:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	25.559	Depositor
Minimum map value	-12.278	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.072	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, 5MU, MIA, PSU, 4SU, MG, 7MG

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	a	0.68	1/36403 (0.0%)	0.87	12/56778 (0.0%)
2	b	0.26	0/1241	0.41	0/1721
3	c	0.40	0/1418	0.56	0/1939
4	d	0.34	0/1453	0.53	0/1976
5	e	0.35	0/1100	0.55	0/1496
6	f	0.33	0/663	0.51	0/904
7	g	0.35	0/1028	0.58	1/1396 (0.1%)
8	h	0.39	0/942	0.55	0/1284
9	i	0.40	0/936	0.59	0/1267
10	j	0.42	0/726	0.56	0/988
11	k	0.28	0/691	0.49	0/955
12	l	0.37	0/949	0.57	0/1290
13	m	0.36	0/786	0.57	0/1064
14	n	0.53	0/472	0.60	0/631
15	o	0.32	0/643	0.55	0/872
16	p	0.37	0/654	0.54	0/888
17	q	0.32	0/565	0.58	0/768
18	r	0.37	0/454	0.55	0/613
19	s	0.36	0/514	0.51	0/707
20	t	0.26	0/495	0.43	0/682
21	x	0.39	0/1605	0.87	1/2497 (0.0%)
22	w	0.41	0/140	0.80	0/215
23	A	0.66	0/69894	0.84	9/109035 (0.0%)
24	B	0.42	0/2711	0.79	0/4224
25	C	0.38	0/2095	0.58	0/2821
26	D	0.41	0/1567	0.56	0/2111
27	E	0.37	0/1536	0.56	0/2082
28	F	0.30	0/1156	0.54	0/1579
29	G	0.31	0/1102	0.55	0/1508
30	L	0.37	0/1107	0.52	0/1495
31	M	0.37	0/921	0.57	0/1236
32	N	0.34	0/1032	0.55	0/1381

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	O	0.37	0/1047	0.56	0/1406
34	P	0.37	0/963	0.63	1/1294 (0.1%)
35	Q	0.28	0/709	0.51	0/966
36	R	0.37	0/855	0.56	0/1158
37	S	0.41	0/943	0.56	0/1258
38	T	0.42	0/775	0.52	0/1045
39	U	0.37	0/853	0.55	0/1156
40	V	0.40	0/733	0.54	0/988
41	W	0.33	0/745	0.51	0/1005
42	Y	0.37	0/556	0.58	0/744
43	Z	0.34	0/444	0.62	1/593 (0.2%)
44	1	0.31	0/468	0.57	0/628
45	2	0.34	0/432	0.60	0/581
46	3	0.28	0/542	0.48	0/743
47	4	0.41	0/433	0.58	0/577
48	5	0.33	0/384	0.58	0/518
49	6	0.39	0/364	0.66	0/475
50	7	0.35	0/519	0.63	0/677
51	8	0.36	0/295	0.61	0/387
All	All	0.60	1/149059 (0.0%)	0.79	25/224602 (0.0%)

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
14	n	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	95	A	C1'-N9	-5.05	1.39	1.46

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	12	VAL	C-N-CA	-6.66	105.06	121.70
1	a	970	U	C2-N3-C4	-6.35	123.19	127.00
1	a	544	C	C2-N1-C1'	6.12	125.53	118.80
23	A	1358	C	C2-N1-C1'	5.97	125.37	118.80
23	A	231	A	O4'-C1'-N9	5.93	112.94	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	n	42	ILE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/249 (89%)	202 (91%)	19 (9%)	1 (0%)	29	61
3	c	201/218 (92%)	179 (89%)	22 (11%)	0	100	100
4	d	197/200 (98%)	178 (90%)	19 (10%)	0	100	100
5	e	154/167 (92%)	138 (90%)	16 (10%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	141/156 (90%)	136 (96%)	5 (4%)	0	100	100
8	h	129/132 (98%)	122 (95%)	7 (5%)	0	100	100
9	i	123/130 (95%)	114 (93%)	9 (7%)	0	100	100
10	j	95/102 (93%)	88 (93%)	7 (7%)	0	100	100
11	k	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
12	l	133/137 (97%)	119 (90%)	14 (10%)	0	100	100
13	m	112/121 (93%)	103 (92%)	9 (8%)	0	100	100
14	n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	p	86/90 (96%)	81 (94%)	5 (6%)	0	100	100
17	q	78/87 (90%)	71 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	62/79 (78%)	56 (90%)	5 (8%)	1 (2%)	9	36
19	s	79/92 (86%)	69 (87%)	10 (13%)	0	100	100
20	t	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
25	C	271/277 (98%)	257 (95%)	14 (5%)	0	100	100
26	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100
27	E	203/207 (98%)	193 (95%)	10 (5%)	0	100	100
28	F	163/179 (91%)	151 (93%)	12 (7%)	0	100	100
29	G	158/178 (89%)	149 (94%)	9 (6%)	0	100	100
30	L	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
31	M	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
32	N	143/146 (98%)	131 (92%)	12 (8%)	0	100	100
33	O	132/144 (92%)	127 (96%)	5 (4%)	0	100	100
34	P	118/135 (87%)	108 (92%)	10 (8%)	0	100	100
35	Q	110/119 (92%)	104 (94%)	6 (6%)	0	100	100
36	R	111/114 (97%)	106 (96%)	5 (4%)	0	100	100
37	S	115/119 (97%)	111 (96%)	4 (4%)	0	100	100
38	T	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
39	U	109/118 (92%)	106 (97%)	3 (3%)	0	100	100
40	V	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
41	W	100/103 (97%)	90 (90%)	10 (10%)	0	100	100
42	Y	73/96 (76%)	65 (89%)	8 (11%)	0	100	100
43	Z	57/62 (92%)	49 (86%)	8 (14%)	0	100	100
44	1	57/63 (90%)	54 (95%)	2 (4%)	1 (2%)	8	35
45	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
46	3	74/81 (91%)	58 (78%)	16 (22%)	0	100	100
47	4	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
48	5	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
49	6	41/44 (93%)	40 (98%)	1 (2%)	0	100	100
50	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
51	8	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
All	All	5173/5545 (93%)	4802 (93%)	368 (7%)	3 (0%)	54	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	128	VAL
18	r	14	VAL
44	1	11	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	31/214 (14%)	31 (100%)	0	100	100
3	c	112/177 (63%)	111 (99%)	1 (1%)	78	87
4	d	124/170 (73%)	124 (100%)	0	100	100
5	e	108/131 (82%)	108 (100%)	0	100	100
6	f	49/85 (58%)	49 (100%)	0	100	100
7	g	90/130 (69%)	90 (100%)	0	100	100
8	h	86/110 (78%)	86 (100%)	0	100	100
9	i	85/102 (83%)	85 (100%)	0	100	100
10	j	71/93 (76%)	71 (100%)	0	100	100
11	k	44/100 (44%)	44 (100%)	0	100	100
12	l	83/118 (70%)	83 (100%)	0	100	100
13	m	64/102 (63%)	64 (100%)	0	100	100
14	n	46/52 (88%)	44 (96%)	2 (4%)	29	59
15	o	54/81 (67%)	54 (100%)	0	100	100
16	p	60/80 (75%)	59 (98%)	1 (2%)	60	78
17	q	45/78 (58%)	44 (98%)	1 (2%)	52	74
18	r	39/67 (58%)	39 (100%)	0	100	100
19	s	24/78 (31%)	24 (100%)	0	100	100
20	t	31/66 (47%)	31 (100%)	0	100	100
25	C	209/225 (93%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D	159/171 (93%)	159 (100%)	0	100	100
27	E	156/174 (90%)	156 (100%)	0	100	100
28	F	100/155 (64%)	100 (100%)	0	100	100
29	G	90/147 (61%)	90 (100%)	0	100	100
30	L	109/121 (90%)	109 (100%)	0	100	100
31	M	98/101 (97%)	98 (100%)	0	100	100
32	N	93/115 (81%)	93 (100%)	0	100	100
33	O	98/113 (87%)	98 (100%)	0	100	100
34	P	94/111 (85%)	94 (100%)	0	100	100
35	Q	40/97 (41%)	40 (100%)	0	100	100
36	R	83/99 (84%)	83 (100%)	0	100	100
37	S	92/97 (95%)	92 (100%)	0	100	100
38	T	76/82 (93%)	76 (100%)	0	100	100
39	U	89/97 (92%)	89 (100%)	0	100	100
40	V	76/84 (90%)	76 (100%)	0	100	100
41	W	76/88 (86%)	76 (100%)	0	100	100
42	Y	54/76 (71%)	54 (100%)	0	100	100
43	Z	44/53 (83%)	44 (100%)	0	100	100
44	1	47/55 (86%)	47 (100%)	0	100	100
45	2	49/52 (94%)	48 (98%)	1 (2%)	55	76
46	3	45/73 (62%)	45 (100%)	0	100	100
47	4	47/50 (94%)	47 (100%)	0	100	100
48	5	41/48 (85%)	41 (100%)	0	100	100
49	6	38/39 (97%)	38 (100%)	0	100	100
50	7	52/56 (93%)	52 (100%)	0	100	100
51	8	35/35 (100%)	35 (100%)	0	100	100
All	All	3436/4648 (74%)	3430 (100%)	6 (0%)	93	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	p	71	ARG
17	q	39	ARG

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Mol	Chain	Res	Type
45	2	57	LYS
14	n	25	GLU
3	c	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
36	R	102	ASN
47	4	23	GLN
37	S	52	GLN
41	W	67	ASN
17	q	74	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1512/1550 (97%)	261 (17%)	0
21	x	71/76 (93%)	25 (35%)	0
22	w	5/21 (23%)	1 (20%)	0
23	A	2900/2932 (98%)	507 (17%)	31 (1%)
24	B	113/116 (97%)	13 (11%)	0
All	All	4601/4695 (97%)	807 (17%)	31 (0%)

5 of 807 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	A
1	a	9	G
1	a	31	G
1	a	32	A
1	a	39	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	979	U
23	A	2472	A
23	A	1248	A
23	A	2809	A
23	A	1595	G

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

7 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
21	MIA	x	37	21	24,31,32	2.20	3 (12%)	26,44,47	2.52	9 (34%)
21	5MU	x	54	21	19,22,23	1.32	4 (21%)	28,32,35	2.30	10 (35%)
21	PSU	x	39	21	18,21,22	1.32	2 (11%)	22,30,33	1.97	4 (18%)
21	7MG	x	46	21	22,26,27	1.30	3 (13%)	29,39,42	2.63	8 (27%)
21	4SU	x	8	21	18,21,22	1.80	4 (22%)	26,30,33	2.34	5 (19%)
21	PSU	x	55	21	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
21	PSU	x	32	21	18,21,22	1.36	3 (16%)	22,30,33	1.87	4 (18%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	MIA	x	37	21	-	3/11/33/34	0/3/3/3
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2
21	PSU	x	39	21	-	1/7/25/26	0/2/2/2
21	7MG	x	46	21	-	4/7/37/38	0/3/3/3
21	4SU	x	8	21	-	2/7/25/26	0/2/2/2
21	PSU	x	55	21	-	2/7/25/26	0/2/2/2
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	37	MIA	C13-C14	7.08	1.52	1.32
21	x	37	MIA	C2-S10	-6.91	1.69	1.75
21	x	8	4SU	C4-S4	-4.77	1.59	1.68
21	x	8	4SU	C4-N3	-3.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	55	PSU	C6-C5	3.20	1.39	1.35

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	46	7MG	N9-C4-N3	9.32	139.41	125.47
21	x	37	MIA	C12-C13-C14	-7.79	111.98	127.14
21	x	8	4SU	C4-N3-C2	-7.11	120.43	127.34
21	x	8	4SU	C5-C4-N3	6.42	120.64	114.69
21	x	39	PSU	N1-C2-N3	6.03	121.96	115.13

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C15
21	x	8	4SU	O4'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C8
21	x	46	7MG	O4'-C1'-N9-C4
21	x	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 103 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

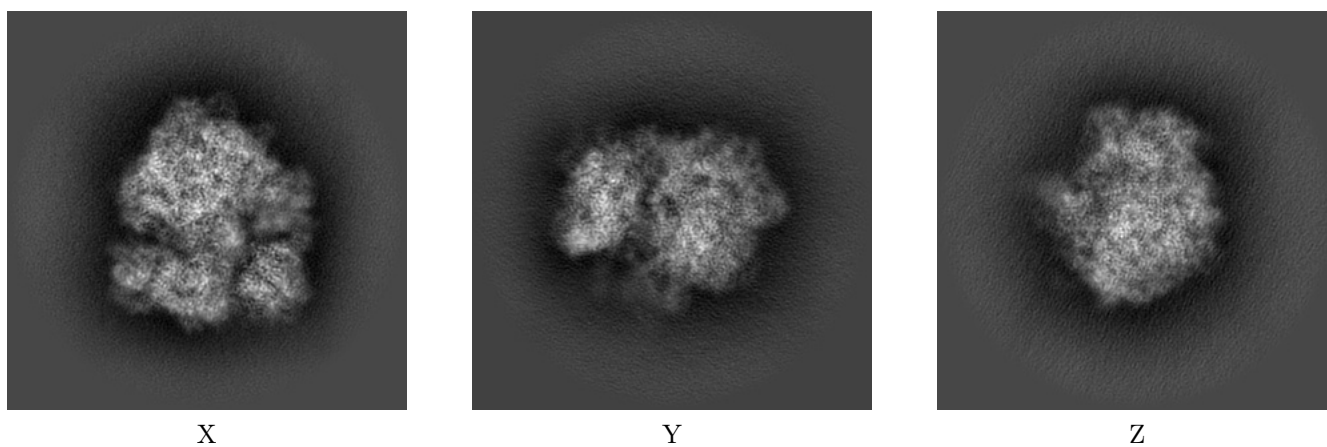
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42561. 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](#)

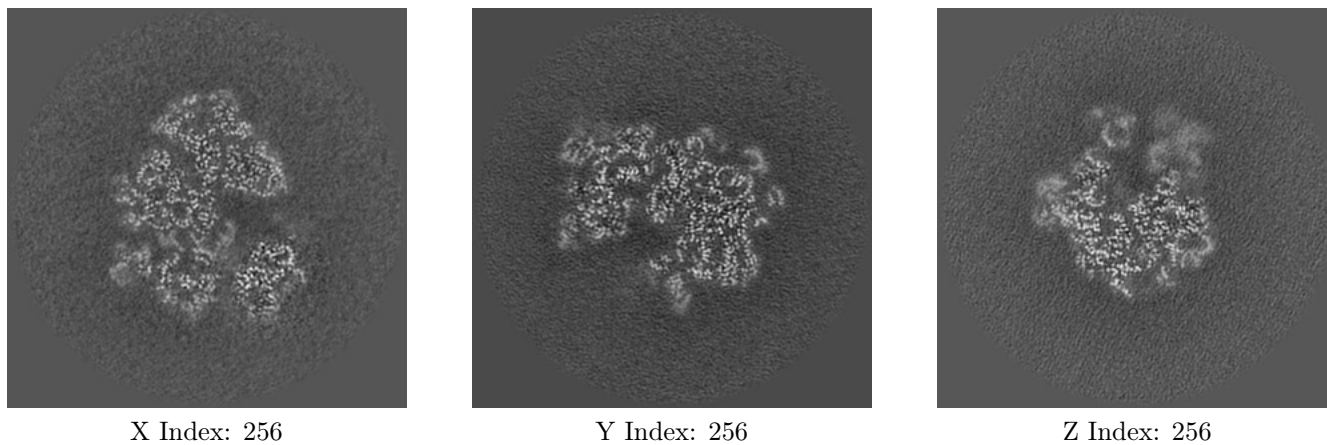
6.1.1 Primary map



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

6.2 Central slices [i](#)

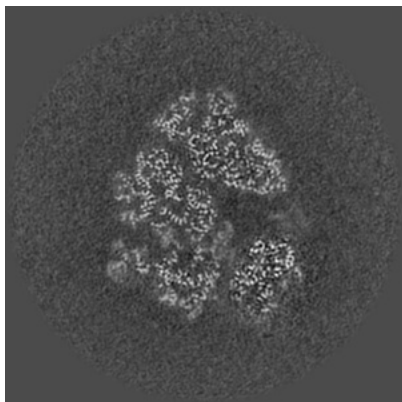
6.2.1 Primary map



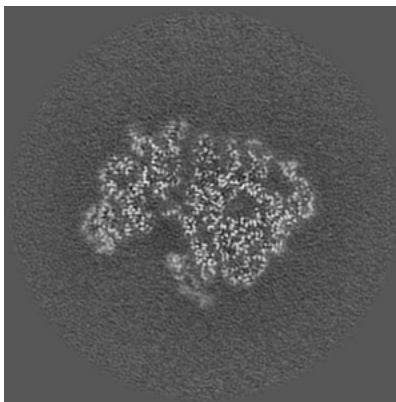
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

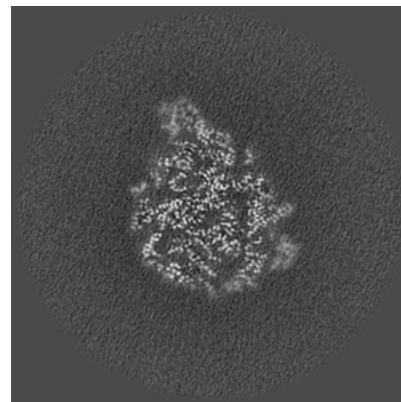
6.3.1 Primary map



X Index: 254



Y Index: 234

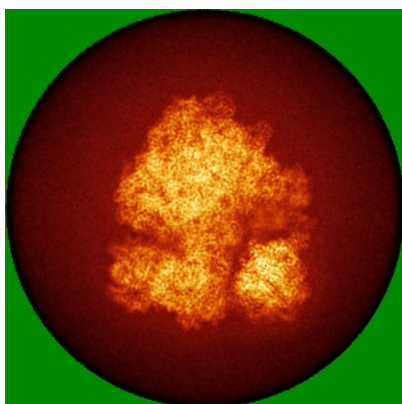


Z Index: 296

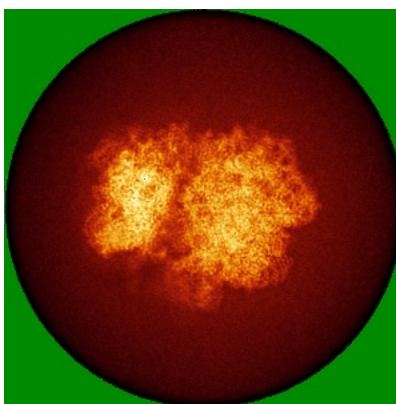
The images above show the largest variance slices of the map in three orthogonal directions.

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

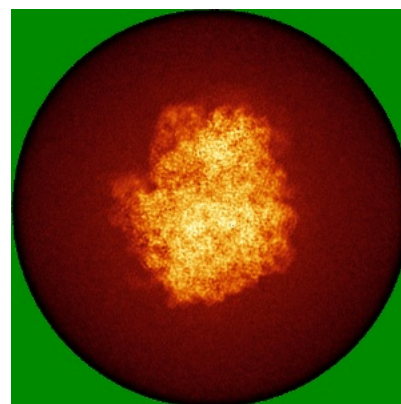
6.4.1 Primary map



X



Y

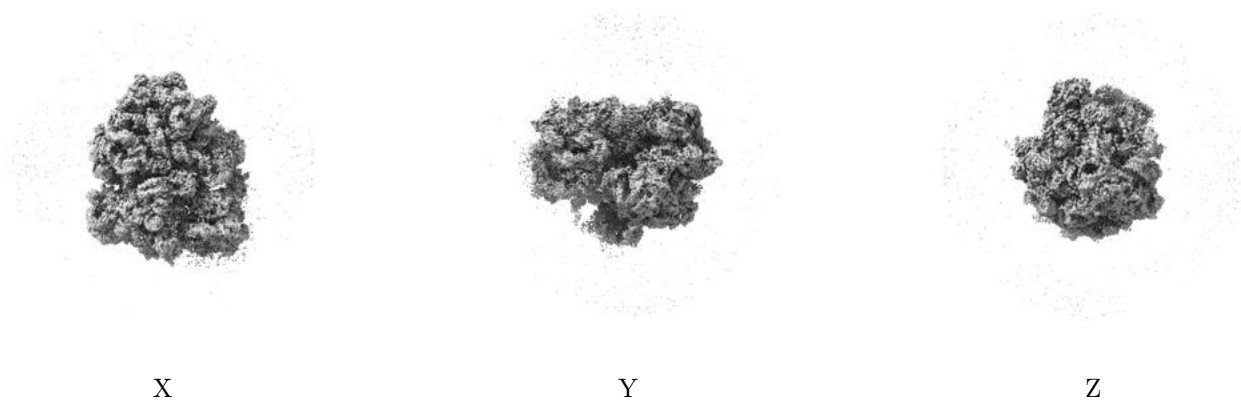


Z

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 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

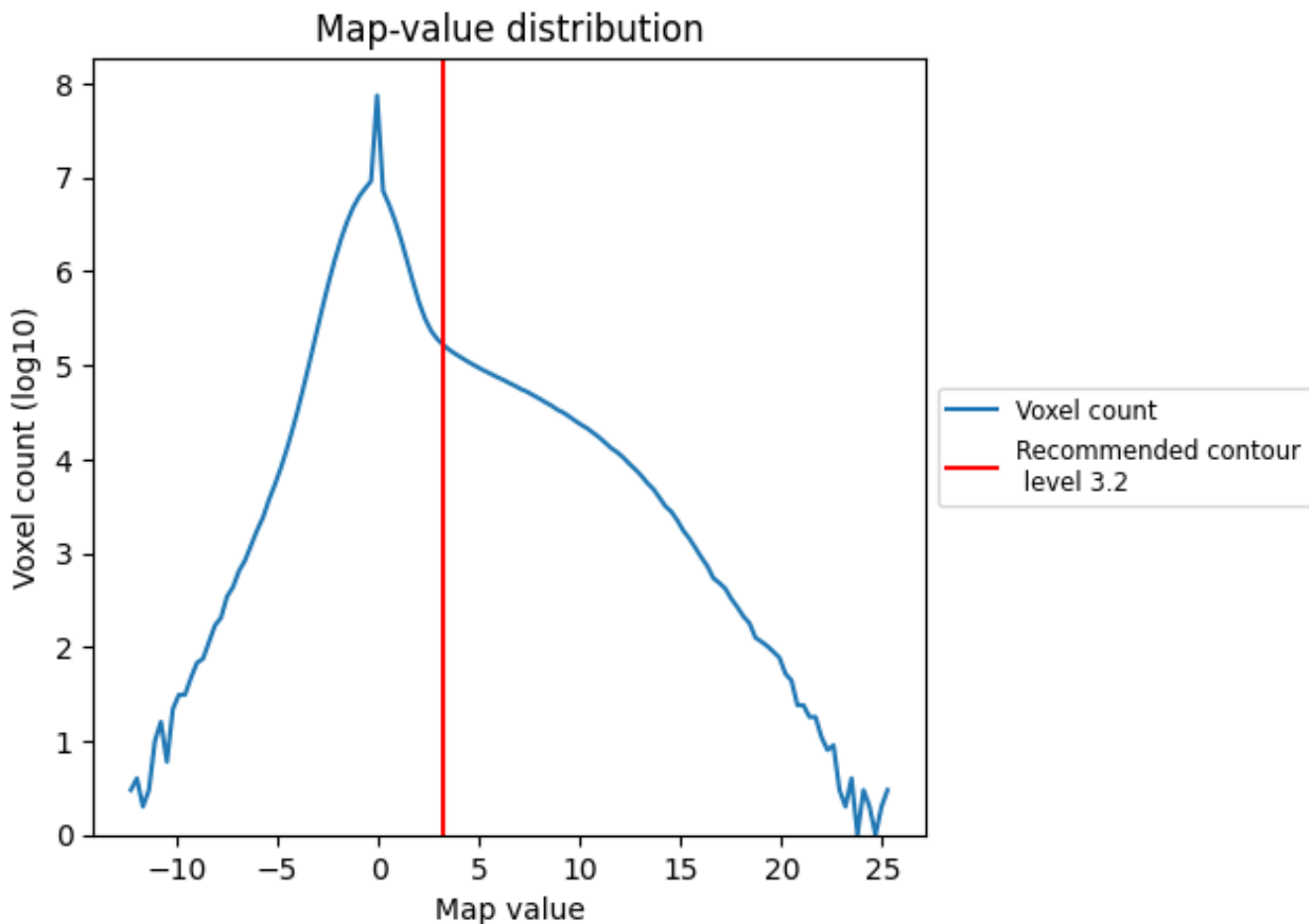
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

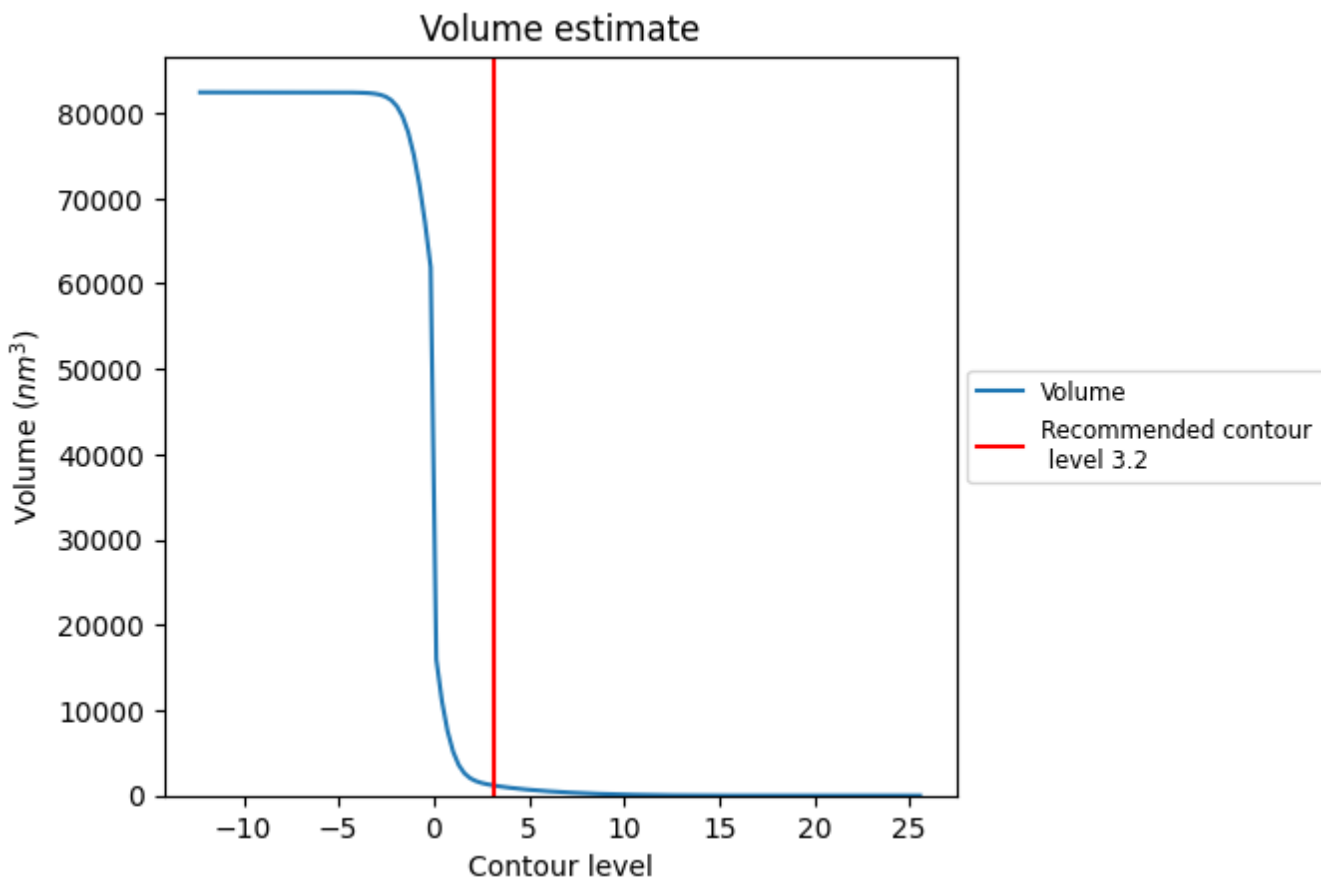
This section contains the results of statistical analysis of the map.

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.

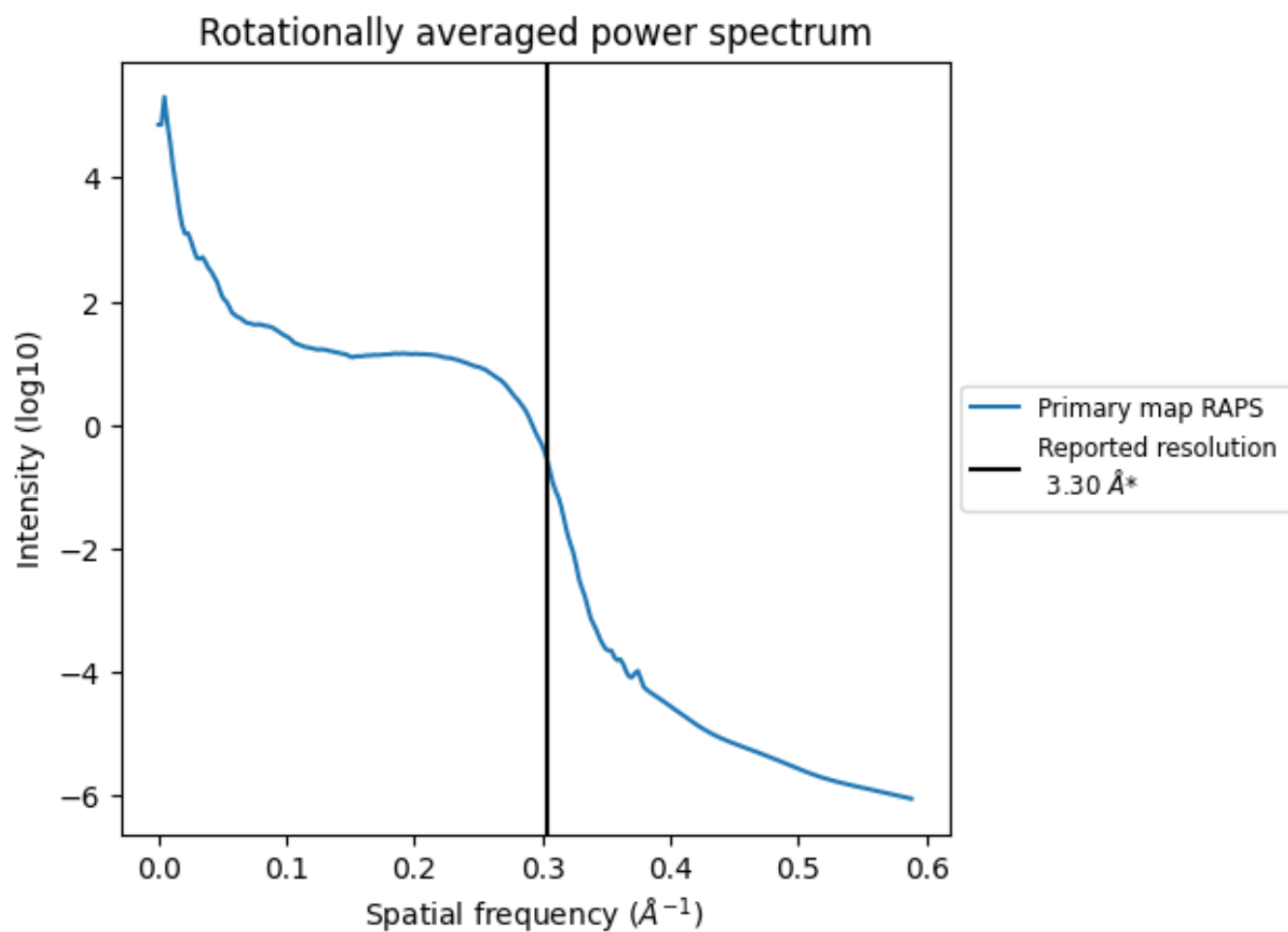
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm³; this corresponds to an approximate mass of 1055 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 0.303\AA^{-1}

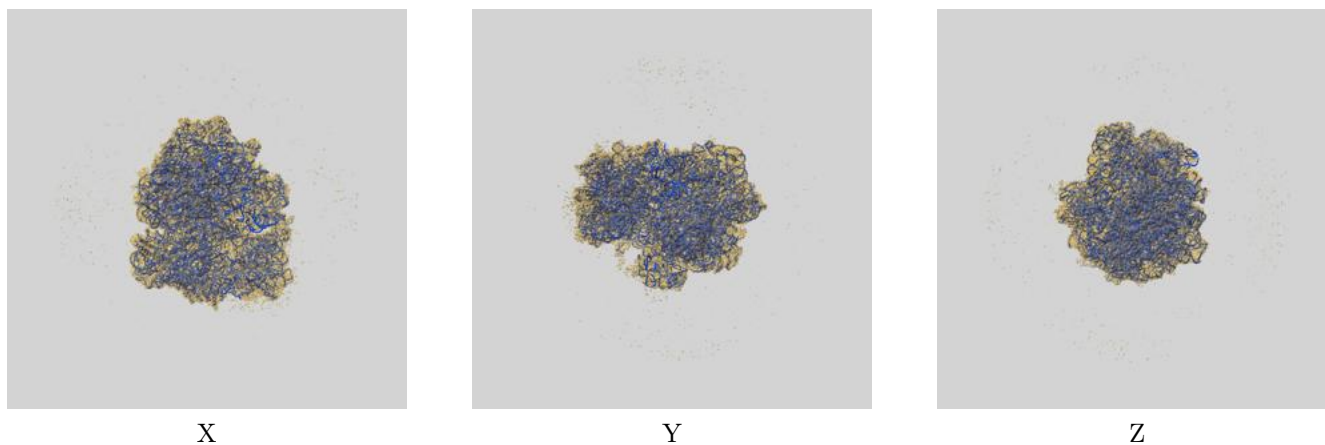
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

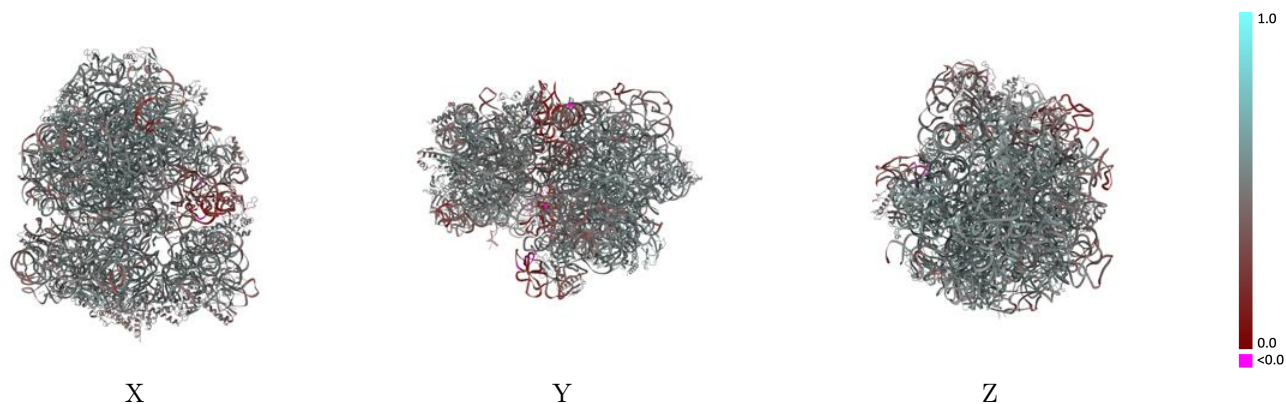
This section contains information regarding the fit between EMDB map EMD-42561 and PDB model 8UU6. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



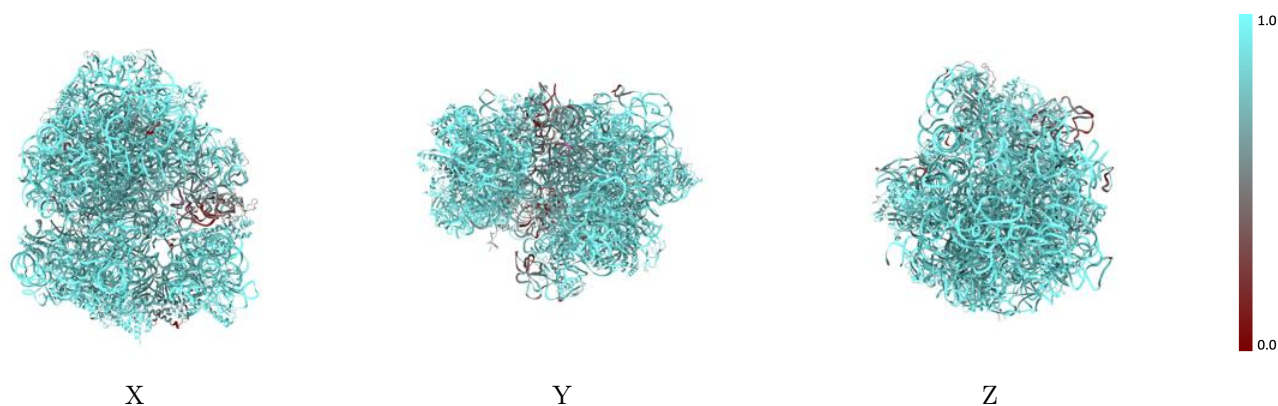
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



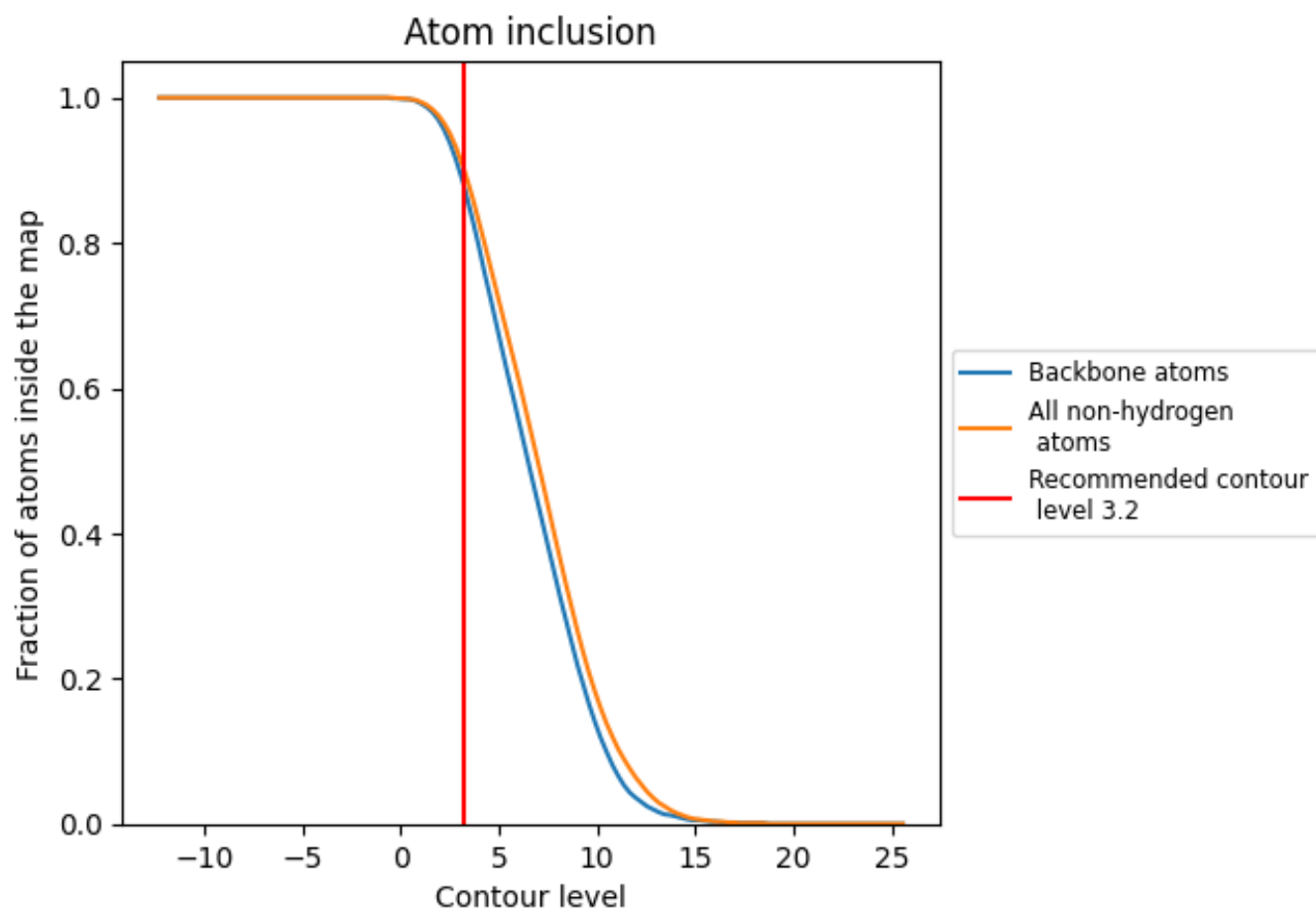
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 90% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.4890
1	 0.8740	 0.4880
2	 0.8650	 0.5280
3	 0.4180	 0.3130
4	 0.8540	 0.5110
5	 0.8500	 0.5350
6	 0.8990	 0.5620
7	 0.9190	 0.5670
8	 0.8220	 0.5480
A	 0.9230	 0.4900
B	 0.9350	 0.4280
C	 0.8570	 0.5560
D	 0.8820	 0.5520
E	 0.8670	 0.5280
F	 0.5630	 0.3370
G	 0.8240	 0.4470
L	 0.9150	 0.5550
M	 0.7640	 0.5390
N	 0.8800	 0.5330
O	 0.8500	 0.5280
P	 0.8810	 0.5350
Q	 0.8440	 0.4580
R	 0.8500	 0.5430
S	 0.9050	 0.5490
T	 0.9020	 0.5490
U	 0.8780	 0.5470
V	 0.8390	 0.5230
W	 0.8370	 0.5090
Y	 0.8930	 0.5530
Z	 0.8880	 0.5500
a	 0.9330	 0.4730
b	 0.8320	 0.4720
c	 0.8820	 0.5100
d	 0.8990	 0.4840
e	 0.8560	 0.5140



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Chain	Atom inclusion	Q-score
f	 0.8610	 0.4800
g	 0.8880	 0.4840
h	 0.9190	 0.5170
i	 0.9560	 0.5090
j	 0.9230	 0.4930
k	 0.8670	 0.4890
l	 0.8810	 0.5290
m	 0.8900	 0.4940
n	 0.9580	 0.5400
o	 0.8230	 0.5070
p	 0.9200	 0.5090
q	 0.9150	 0.5070
r	 0.9180	 0.5100
s	 0.7900	 0.5220
t	 0.9080	 0.4810
w	 0.8250	 0.4920
x	 0.6190	 0.3410