



## Full wwPDB EM Validation Report ⓘ

Feb 4, 2025 – 03:59 pm GMT

PDB ID : 8RWG  
EMDB ID : EMD-19547  
Title : PAO1 wild-type ribosome, R, reference map  
Authors : Mesa, P.; Montoya, G.  
Deposited on : 2024-02-04  
Resolution : 2.46 Å (reported)  
Based on initial model : 4YBB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

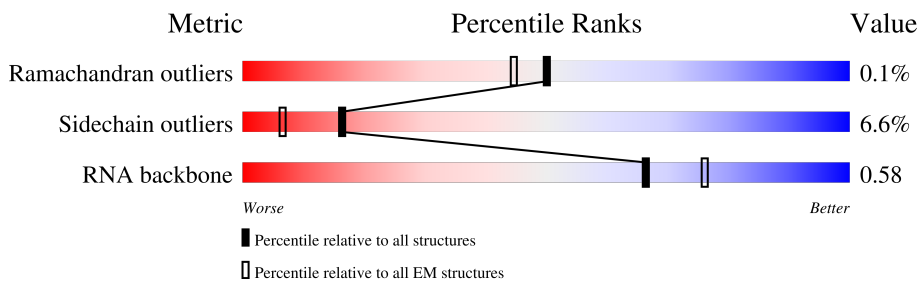
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 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 2.46 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.



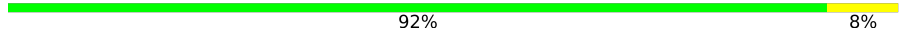


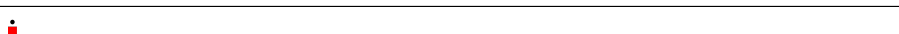
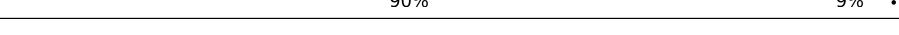
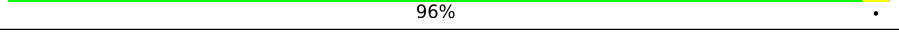
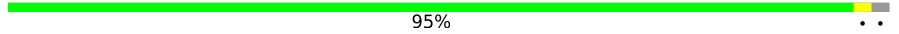
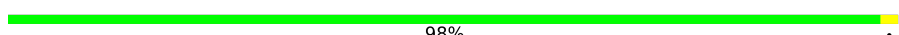

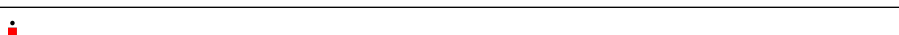
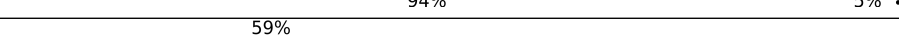

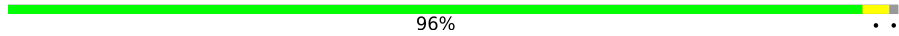
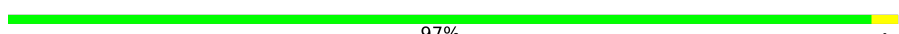

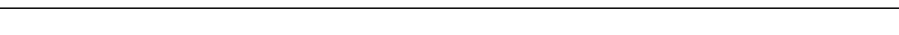
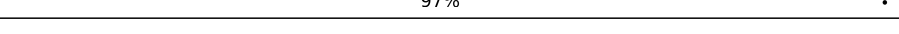


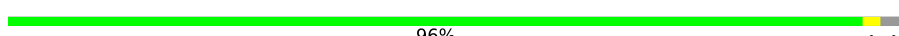


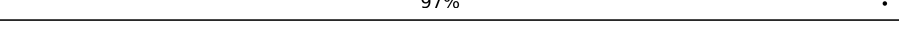
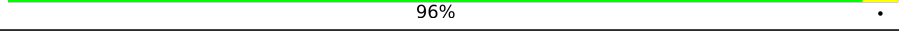

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	1	85	
2	2	78	
3	3	63	
4	4	58	
5	5	60	
6	6	51	
7	7	44	
8	8	64	

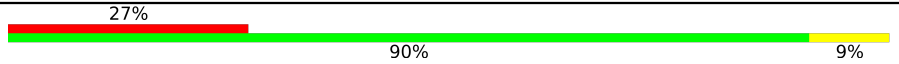










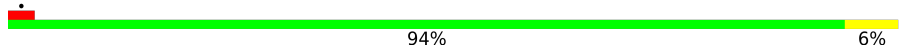
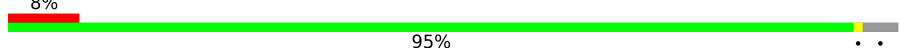



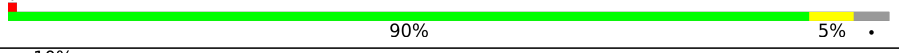

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Mol	Chain	Length	Quality of chain
9	9	38	 92% 8%
10	A	2891	 83% 14%
11	B	1536	 85% 14% 6%
12	C	121	 90% 9%
13	D	273	 96%
14	E	211	 95%
15	F	200	 98%
16	G	179	 90% 9%
17	H	177	 94% 5%
18	I	148	 89% 8% 5%
19	J	142	 96%
20	K	122	 97%
21	L	144	 97%
22	M	137	 97%
23	N	129	 89% 8%
24	O	116	 91% 7%
25	P	116	 96%
26	Q	118	 97%
27	R	103	 97%
28	S	110	 96%
29	T	99	 90% 7%
30	U	104	 93% 6%
31	V	204	 89% 7%
32	a	246	 85% 7% 28%
33	b	228	 82% 9% 44%

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Mol	Chain	Length	Quality of chain
34	c	206	
35	d	166	
36	e	139	
37	f	156	
38	g	130	
39	h	130	
40	i	103	
41	j	129	
42	k	123	
43	l	118	
44	m	101	
45	n	89	
46	o	83	
47	p	88	
48	q	76	
49	r	91	
50	s	91	
51	t	71	

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140256 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 L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1	75	569	361	110	98	0	0

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	77	630	391	134	103	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	62	494	303	97	92	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	56	440	275	86	77	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	55	433	261	93	78	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	50	416	266	76	73	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	44	365	222	87	54	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	63	506	314	108	81	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	38	306	186	69	47	4	0	0

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	2805	60189	26855	11041	19488	2805	0	0

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	B	1527	32768	14616	6016	10610	1526	0	0

- Molecule 12 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	C	120	2555	1141	455	839	120	0	0

- Molecule 13 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	272	2071	1276	426	363	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	206	1552	961	296	290	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	200	1524	956	283	282	3	0	0

- Molecule 16 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	177	1393	892	249	248	4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	174	1316	829	242	243	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	I	136	945	598	175	171	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	141	1122	713	205	201	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	K	122	938	587	180	165	6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	L	144	1066	654	215	194	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	M	137	1085	689	211	181	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	N	119	952	595	191	161	5	0	0

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	O	114	875	541	173	159	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	P	113	894	563	170	160	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Q	117	935	592	196	147	0	0

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	103	822	521	156	143	2	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein uL22.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	S	110	833	515	161	153	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	T	92	720	459	132	128	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	U	103	791	497	152	141	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	V	190	1434	908	260	263	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	224	1725	1092	309	314	10	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	208	1660	1050	314	290	6	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	205	1627	1003	316	303	5	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	155	Total	C	N	O	S	0	0
			1142	717	211	208	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	103	Total	C	N	O	S	0	0
			845	525	155	159	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	153	Total	C	N	O	S	0	0
			1199	752	232	210	5		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	128	Total	C	N	O	S	0	0
			976	615	172	183	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	126	Total	C	N	O	S	0	0
			994	616	198	179	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	101	Total	C	N	O	S	0	0
			810	505	154	150	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	118	Total	C	N	O	S	0	0
			873	540	170	161	2		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	k	121	949	582	196	167	4	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	l	116	904	553	184	163	4	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	m	100	804	496	167	138	3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	n	89	711	439	140	130	2	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	80	631	394	124	112	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	p	80	645	404	124	115	2	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	q	59	466	297	83	86	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	82	Total	C	N	O	S	0	0
			658	419	128	108	3		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	87	Total	C	N	O	S	0	0
			671	414	138	117	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	55	Total	C	N	O	S	0	0
			447	280	90	76	1		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	9	1	Total	Zn	0
			1	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	175	Total	Mg	0
			175	175	
53	C	5	Total	Mg	0
			5	5	
53	E	1	Total	Mg	0
			1	1	
53	N	2	Total	Mg	0
			2	2	
53	T	1	Total	Mg	0
			1	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	A	383	Total	O	0
			383	383	
54	D	4	Total	O	0
			4	4	

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
54	E	3	Total	O	0
			3	3	
54	L	5	Total	O	0
			5	5	

### 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 L27

Chain 1:  84% 5% 12%



- Molecule 2: 50S ribosomal protein L28

Chain 2:  95% ..




- Molecule 3: 50S ribosomal protein L29

Chain 3:  97% ..




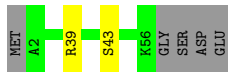
- Molecule 4: 50S ribosomal protein L30

Chain 4:  91% 5% .



- Molecule 5: 50S ribosomal protein L32

Chain 5:  88% . 8%



- Molecule 6: Large ribosomal subunit protein bL33

Chain 6:  94%



- Molecule 7: 50S ribosomal protein L34

Chain 7:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 50S ribosomal protein L35

Chain 8:  91%




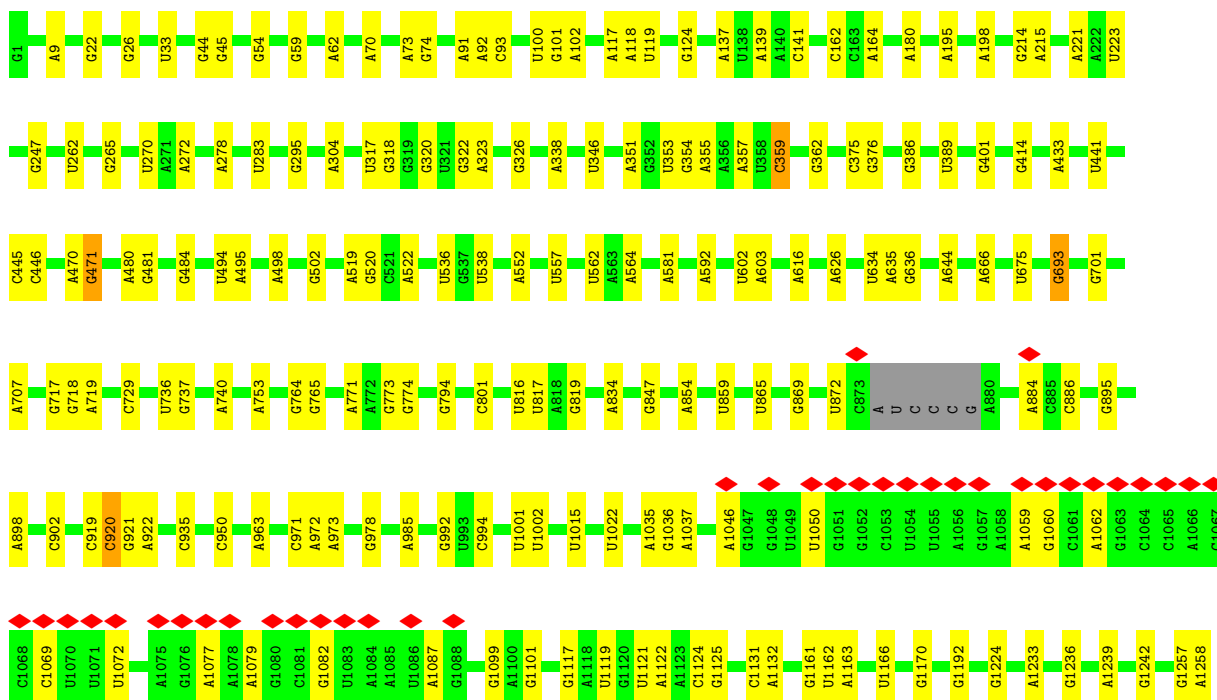
- Molecule 9: 50S ribosomal protein L36

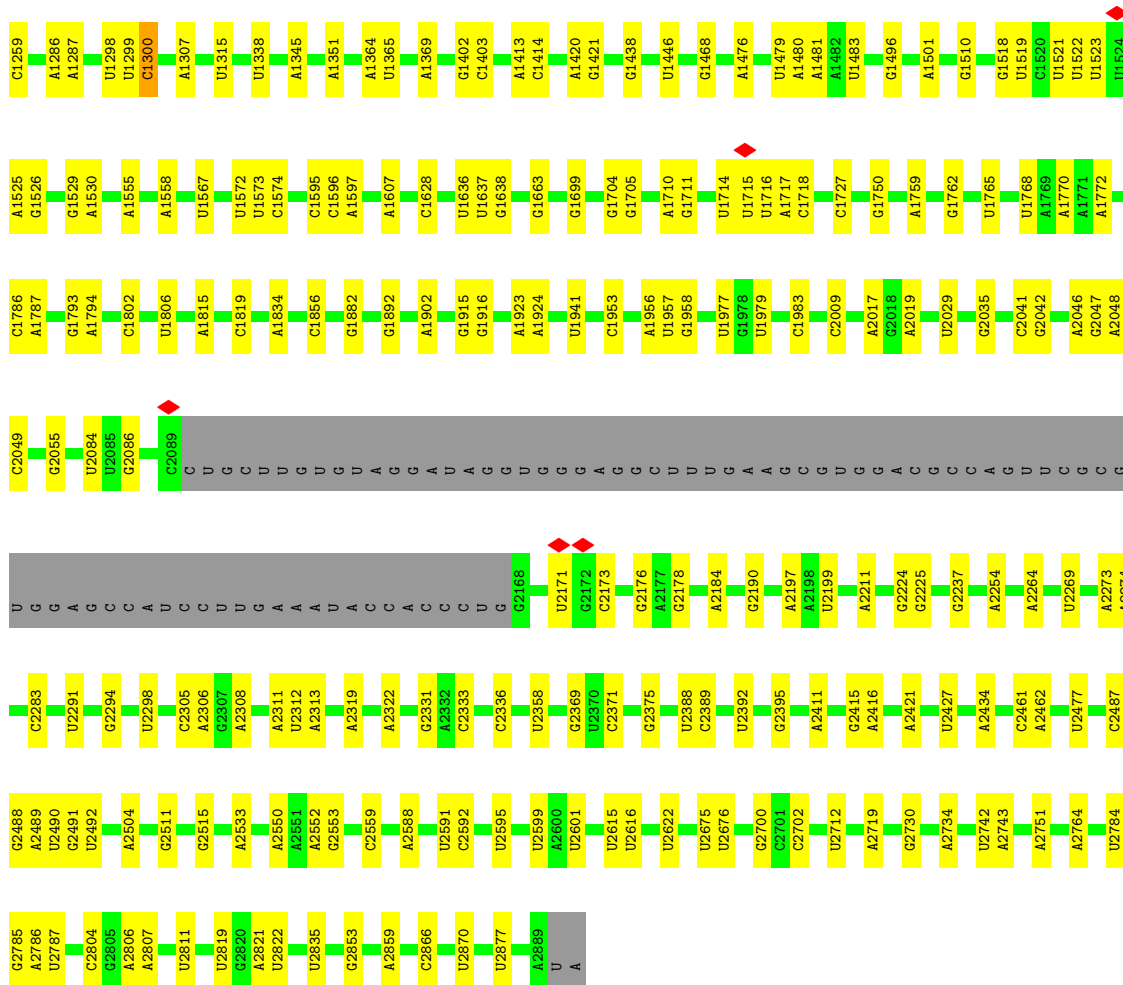
Chain 9:  92%



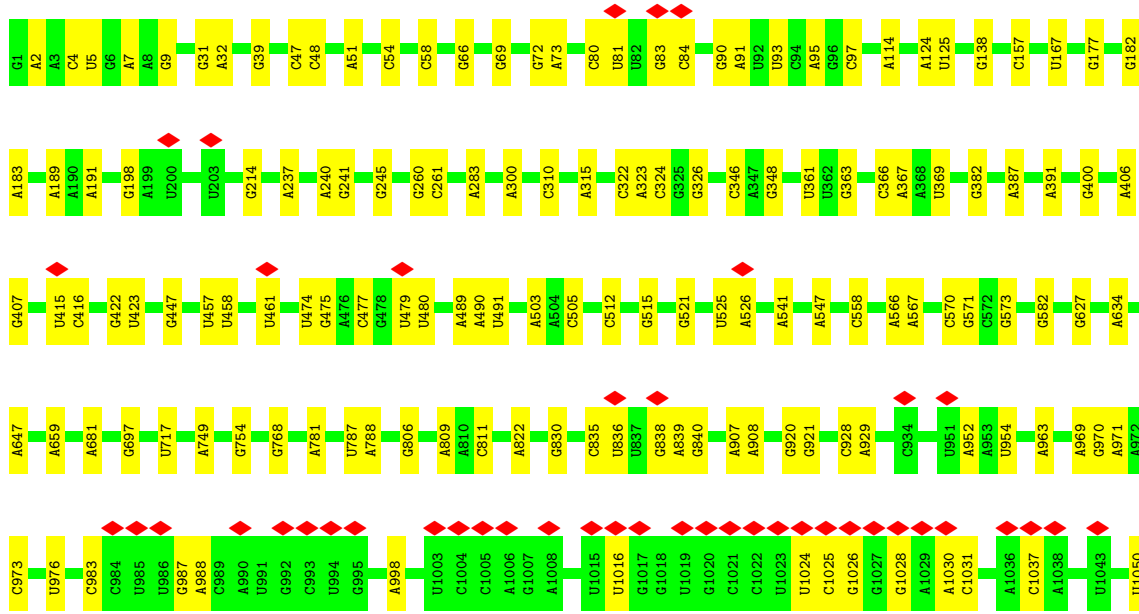
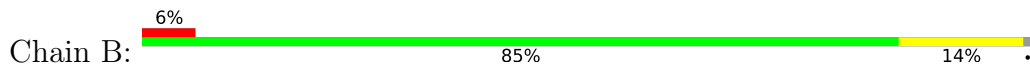
- Molecule 10: 23S ribosomal RNA

Chain A:  83%

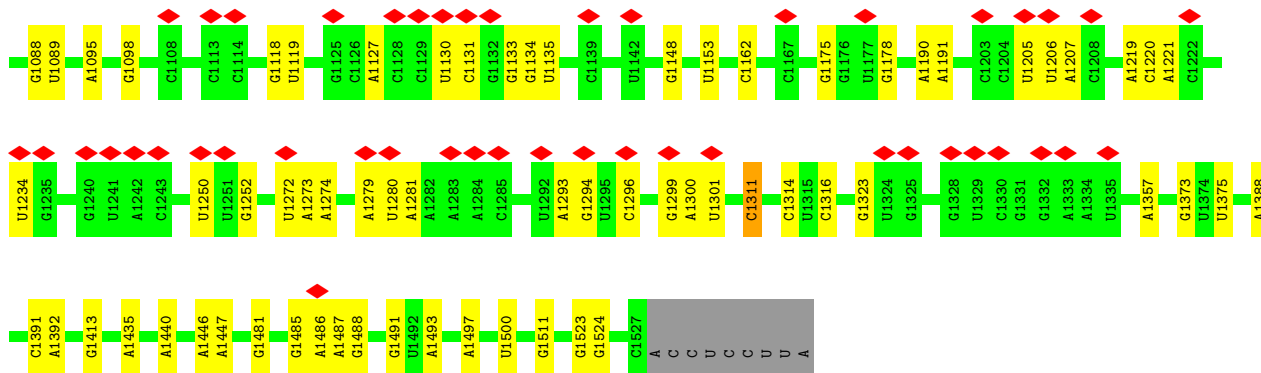




• Molecule 11: 16S ribosomal RNA







• Molecule 12: 5S ribosomal RNA



• Molecule 13: 50S ribosomal protein L2



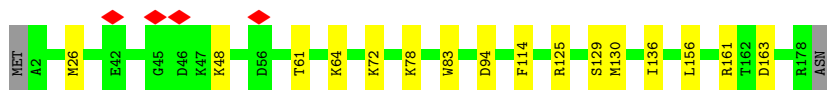
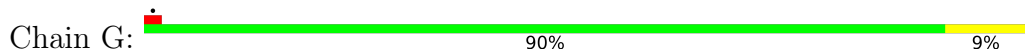
• Molecule 14: 50S ribosomal protein L3



• Molecule 15: 50S ribosomal protein L4

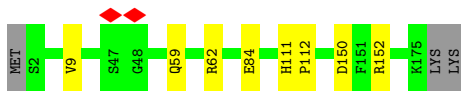


• Molecule 16: 50S ribosomal protein L5

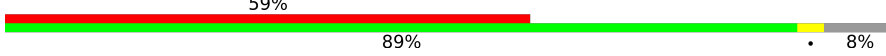


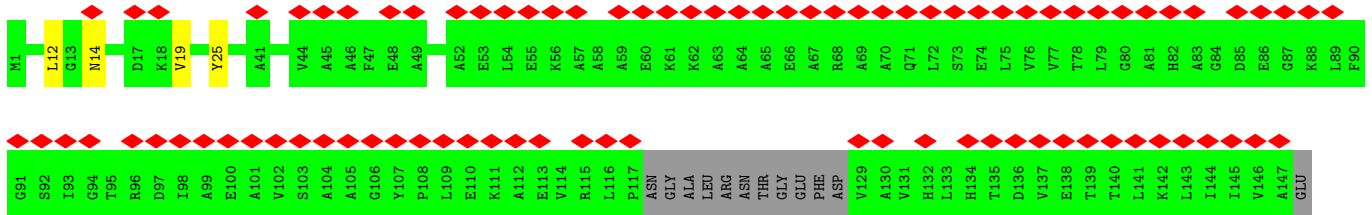
• Molecule 17: 50S ribosomal protein L6

Chain H:  94% 5%



- Molecule 18: 50S ribosomal protein L9

Chain I:  59% 89% 8%



- Molecule 19: 50S ribosomal protein L13

Chain J:  96%



- Molecule 20: 50S ribosomal protein L14

Chain K:  97%



- Molecule 21: 50S ribosomal protein L15

Chain L:  97%



- Molecule 22: 50S ribosomal protein L16

Chain M:  97%



- Molecule 23: 50S ribosomal protein L17

Chain N:  89% 8%



- Molecule 24: 50S ribosomal protein L18



- Molecule 25: 50S ribosomal protein L19



- Molecule 26: 50S ribosomal protein L20



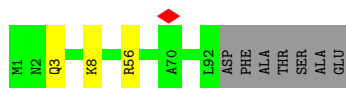
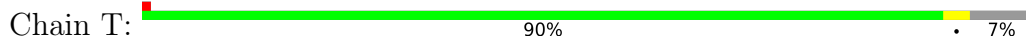
- Molecule 27: 50S ribosomal protein L21



- Molecule 28: Large ribosomal subunit protein uL22



- Molecule 29: 50S ribosomal protein L23



- Molecule 30: 50S ribosomal protein L24





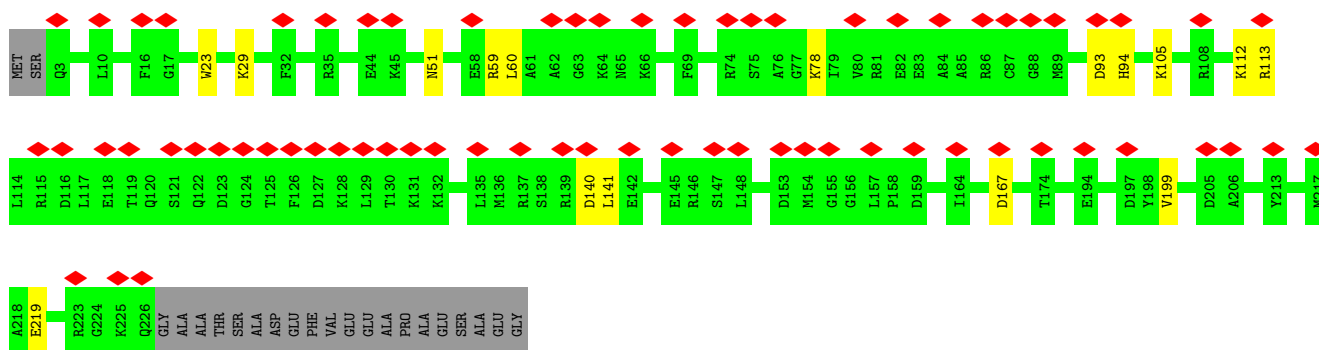
- Molecule 31: 50S ribosomal protein L25

Chain V: 89% 7%



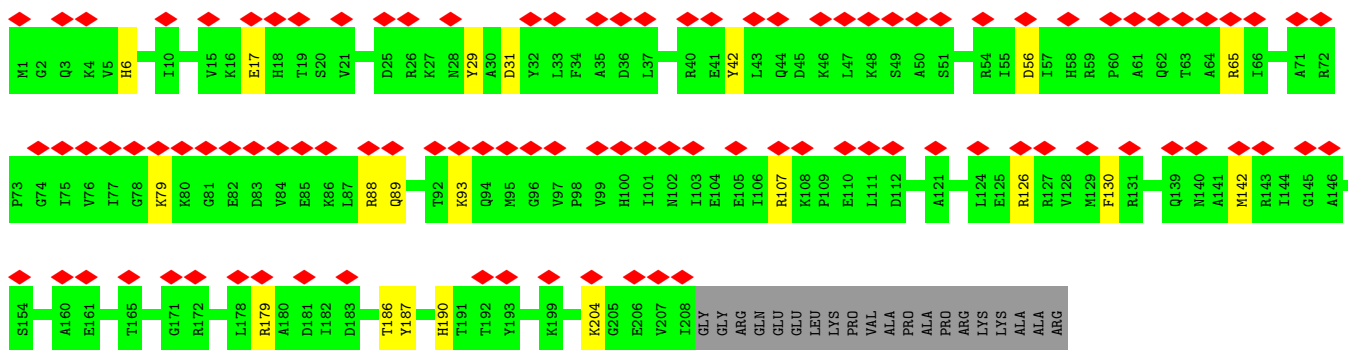
- Molecule 32: 30S ribosomal protein S2

Chain a: 28% 85% 7% 9%



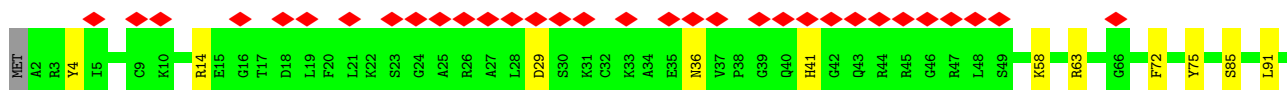
- Molecule 33: 30S ribosomal protein S3

Chain b: 44% 82% 9% 9%

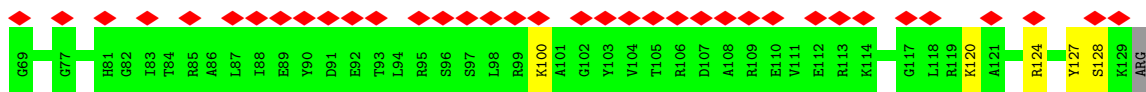


- Molecule 34: 30S ribosomal protein S4

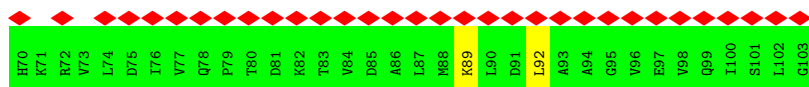
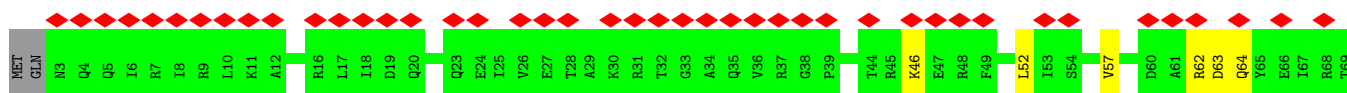
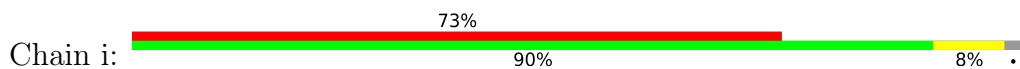
Chain c: 27% 90% 9%



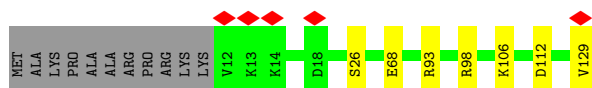
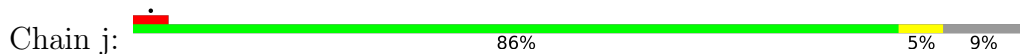




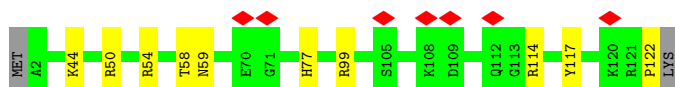
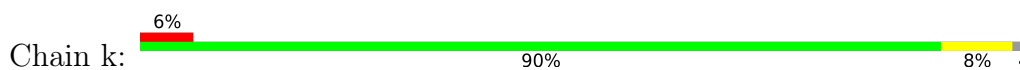
- Molecule 40: 30S ribosomal protein S10



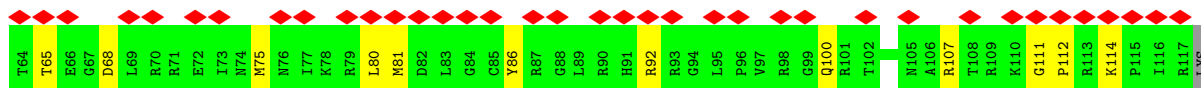
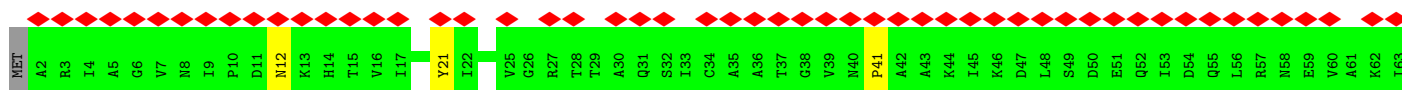
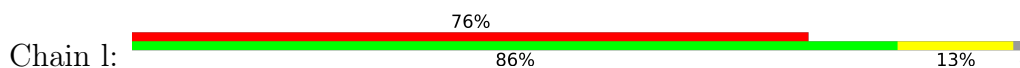
- Molecule 41: 30S ribosomal protein S11



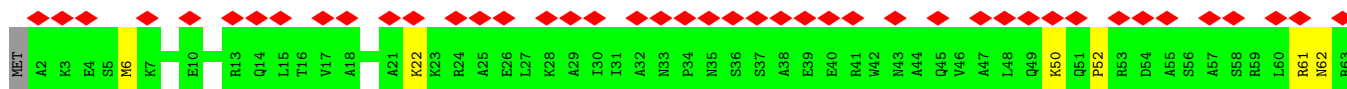
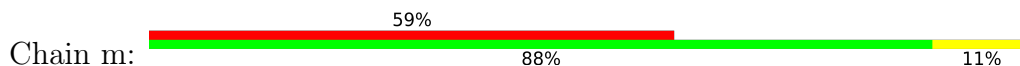
- Molecule 42: 30S ribosomal protein S12

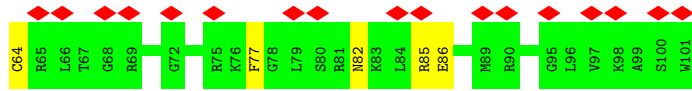


- Molecule 43: 30S ribosomal protein S13

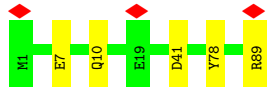


- Molecule 44: 30S ribosomal protein S14

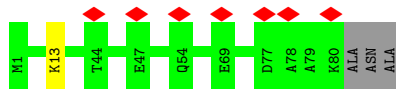




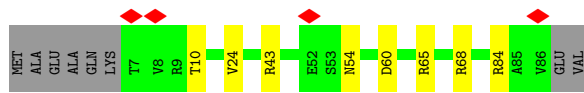
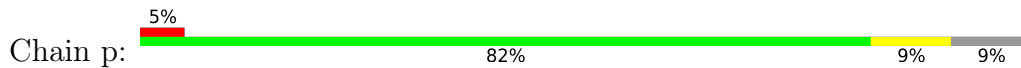
• Molecule 45: 30S ribosomal protein S15



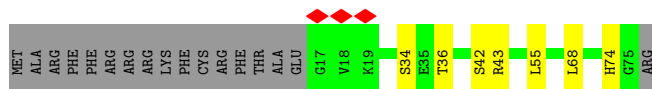
• Molecule 46: 30S ribosomal protein S16



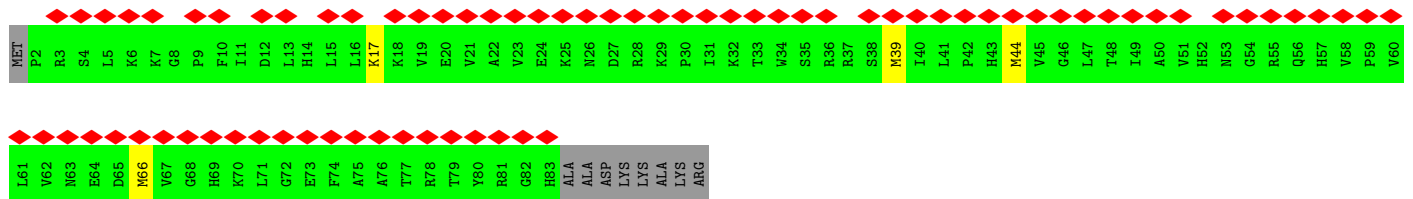
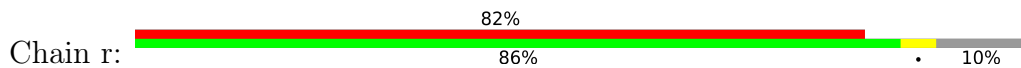
• Molecule 47: 30S ribosomal protein S17



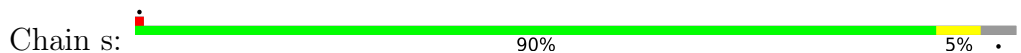
• Molecule 48: 30S ribosomal protein S18

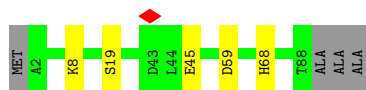


• Molecule 49: 30S ribosomal protein S19

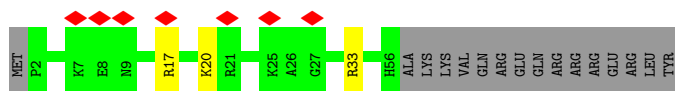
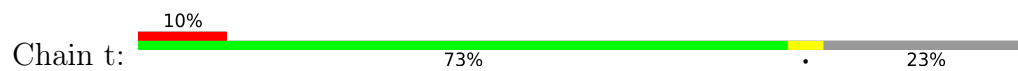


• Molecule 50: 30S ribosomal protein S20





- Molecule 51: 30S ribosomal protein S21





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166770	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.870	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	282.88, 282.88, 282.88	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.37	0/577	0.55	0/767
2	2	0.34	0/641	0.59	0/854
3	3	0.26	0/495	0.49	0/659
4	4	0.31	0/444	0.54	0/597
5	5	0.32	0/439	0.58	0/585
6	6	0.33	0/423	0.51	0/565
7	7	0.35	0/368	0.71	0/482
8	8	0.33	0/511	0.64	0/668
9	9	0.34	0/307	0.62	0/404
10	A	0.75	0/67406	0.83	24/105146 (0.0%)
11	B	0.30	0/36694	0.77	3/57245 (0.0%)
12	C	0.49	0/2855	0.77	0/4447
13	D	0.36	0/2107	0.61	0/2831
14	E	0.36	0/1575	0.57	0/2121
15	F	0.33	0/1544	0.53	0/2079
16	G	0.29	0/1414	0.60	0/1901
17	H	0.93	3/1334 (0.2%)	0.86	6/1797 (0.3%)
18	I	0.27	0/953	0.55	0/1291
19	J	0.38	0/1148	0.51	0/1549
20	K	0.33	0/947	0.59	0/1268
21	L	0.33	0/1078	0.59	0/1436
22	M	0.36	0/1105	0.59	0/1476
23	N	0.35	0/968	0.57	0/1294
24	O	0.29	0/882	0.56	0/1175
25	P	0.34	0/903	0.53	0/1208
26	Q	0.37	0/945	0.58	0/1257
27	R	0.36	0/835	0.56	0/1117
28	S	0.34	0/837	0.54	0/1114
29	T	0.32	0/729	0.55	0/975
30	U	0.30	0/799	0.56	0/1068
31	V	0.29	0/1457	0.54	1/1975 (0.1%)
32	a	0.28	0/1753	0.66	1/2362 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	b	0.27	0/1689	0.63	0/2275
34	c	0.26	0/1646	0.58	0/2201
35	d	0.29	0/1156	0.60	1/1555 (0.1%)
36	e	0.31	0/859	0.70	1/1156 (0.1%)
37	f	0.28	0/1217	0.66	0/1627
38	g	0.27	0/987	0.55	0/1324
39	h	0.26	0/1006	0.66	1/1347 (0.1%)
40	i	0.27	0/820	0.72	1/1106 (0.1%)
41	j	0.28	0/889	0.57	0/1202
42	k	0.29	0/963	0.70	1/1292 (0.1%)
43	l	0.63	2/913 (0.2%)	0.99	6/1227 (0.5%)
44	m	0.28	0/816	0.74	1/1087 (0.1%)
45	n	0.26	0/718	0.57	0/957
46	o	0.28	0/642	0.63	0/863
47	p	0.29	0/653	0.65	0/881
48	q	0.27	0/473	0.55	1/637 (0.2%)
49	r	0.24	0/673	0.59	0/905
50	s	0.25	0/678	0.53	0/904
51	t	0.27	0/454	0.62	0/603
All	All	0.56	5/151725 (0.0%)	0.76	48/226862 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	112	PRO	CG-CD	-27.13	0.61	1.50
17	H	112	PRO	CB-CG	14.32	2.21	1.50
43	l	112	PRO	CG-CD	-13.91	1.04	1.50
17	H	112	PRO	N-CD	9.21	1.60	1.47
43	l	112	PRO	N-CD	7.61	1.58	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	112	PRO	N-CD-CG	-15.08	80.58	103.20
43	l	112	PRO	N-CD-CG	-14.70	81.15	103.20
17	H	112	PRO	CB-CG-CD	-13.26	54.78	106.50
17	H	112	PRO	CA-N-CD	-12.26	94.34	111.50
43	l	41	PRO	CA-N-CD	-11.97	94.74	111.50
42	k	122	PRO	CA-N-CD	-11.39	95.56	111.50
17	H	112	PRO	CA-CB-CG	-11.07	82.97	104.00
43	l	112	PRO	CA-N-CD	-10.84	96.33	111.50
10	A	502	G	O4'-C1'-N9	10.41	116.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	l	112	PRO	CA-CB-CG	-8.88	87.12	104.00
44	m	52	PRO	CA-N-CD	-8.60	99.45	111.50
10	A	920	C	C2-N1-C1'	8.26	127.89	118.80
17	H	112	PRO	N-CA-CB	-7.94	93.77	103.30
10	A	920	C	N1-C2-O2	7.70	123.52	118.90
17	H	111	HIS	C-N-CD	7.54	144.23	128.40
10	A	1299	U	C2-N1-C1'	6.95	126.04	117.70
10	A	1069	C	N3-C2-O2	-6.78	117.15	121.90
43	l	111	GLY	C-N-CD	6.50	142.04	128.40
10	A	920	C	N3-C2-O2	-6.42	117.41	121.90
35	d	76	ASP	CB-CG-OD1	6.38	124.05	118.30
10	A	2490	U	N3-C2-O2	-6.37	117.74	122.20
32	a	141	LEU	CA-CB-CG	6.25	129.69	115.30
10	A	737	G	O4'-C1'-N9	6.16	113.13	108.20
43	l	41	PRO	N-CD-CG	-5.85	94.42	103.20
36	e	76	ASP	CB-CG-OD1	5.81	123.53	118.30
10	A	693	G	O4'-C1'-N9	5.74	112.79	108.20
10	A	920	C	C6-N1-C1'	-5.70	113.96	120.80
10	A	1299	U	N1-C2-O2	5.70	126.79	122.80
39	h	52	LEU	CA-CB-CG	5.61	128.20	115.30
10	A	920	C	C6-N1-C2	-5.44	118.12	120.30
11	B	1301	U	C2-N1-C1'	5.43	124.21	117.70
11	B	973	C	C6-N1-C2	-5.42	118.13	120.30
10	A	359	C	C2-N1-C1'	5.40	124.74	118.80
10	A	1299	U	N3-C2-O2	-5.37	118.44	122.20
10	A	2490	U	C2-N1-C1'	5.36	124.13	117.70
10	A	471	G	O4'-C1'-N9	5.30	112.44	108.20
10	A	2487	C	C2-N1-C1'	-5.28	112.99	118.80
10	A	1069	C	N1-C2-O2	5.26	122.06	118.90
10	A	2811	U	C2-N1-C1'	5.26	124.01	117.70
10	A	718	G	O4'-C1'-N9	5.26	112.41	108.20
40	i	92	LEU	CA-CB-CG	5.22	127.30	115.30
11	B	1311	C	N1-C2-O2	5.21	122.02	118.90
10	A	26	G	O4'-C1'-N9	5.17	112.34	108.20
31	V	53	LEU	CA-CB-CG	5.11	127.05	115.30
10	A	1765	U	O4'-C1'-N1	5.10	112.28	108.20
10	A	359	C	C6-N1-C2	-5.07	118.27	120.30
48	q	55	LEU	CA-CB-CG	5.07	126.95	115.30
10	A	1300	C	C2-N1-C1'	5.01	124.31	118.80

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 [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	
1	1	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
2	2	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	3	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
4	4	54/58 (93%)	54 (100%)	0	0	100	100
5	5	53/60 (88%)	52 (98%)	1 (2%)	0	100	100
6	6	48/51 (94%)	48 (100%)	0	0	100	100
7	7	42/44 (96%)	42 (100%)	0	0	100	100
8	8	61/64 (95%)	57 (93%)	4 (7%)	0	100	100
9	9	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	D	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
14	E	204/211 (97%)	193 (95%)	11 (5%)	0	100	100
15	F	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
16	G	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	22	28
17	H	172/177 (97%)	163 (95%)	8 (5%)	1 (1%)	22	28
18	I	132/148 (89%)	122 (92%)	10 (8%)	0	100	100
19	J	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
20	K	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
21	L	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
22	M	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	19	24
23	N	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
24	O	112/116 (97%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	P	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
26	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
27	R	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
28	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
29	T	90/99 (91%)	77 (86%)	13 (14%)	0	100	100
30	U	101/104 (97%)	96 (95%)	5 (5%)	0	100	100
31	V	188/204 (92%)	175 (93%)	12 (6%)	1 (0%)	25	32
32	a	222/246 (90%)	205 (92%)	17 (8%)	0	100	100
33	b	206/228 (90%)	196 (95%)	10 (5%)	0	100	100
34	c	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
35	d	153/166 (92%)	143 (94%)	10 (6%)	0	100	100
36	e	101/139 (73%)	93 (92%)	8 (8%)	0	100	100
37	f	151/156 (97%)	143 (95%)	8 (5%)	0	100	100
38	g	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
39	h	124/130 (95%)	113 (91%)	11 (9%)	0	100	100
40	i	99/103 (96%)	90 (91%)	8 (8%)	1 (1%)	13	14
41	j	116/129 (90%)	112 (97%)	4 (3%)	0	100	100
42	k	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
43	l	114/118 (97%)	105 (92%)	9 (8%)	0	100	100
44	m	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
45	n	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
46	o	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
47	p	78/88 (89%)	74 (95%)	4 (5%)	0	100	100
48	q	57/76 (75%)	55 (96%)	2 (4%)	0	100	100
49	r	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
50	s	85/91 (93%)	84 (99%)	0	1 (1%)	11	11
51	t	53/71 (75%)	53 (100%)	0	0	100	100
All	All	5582/5937 (94%)	5316 (95%)	260 (5%)	6 (0%)	50	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	G	136	ILE

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Mol	Chain	Res	Type
17	H	59	GLN
22	M	29	PHE
31	V	152	ALA
40	i	57	VAL
50	s	68	HIS

### 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	1	56/61 (92%)	52 (93%)	4 (7%)	12 15
2	2	66/67 (98%)	63 (96%)	3 (4%)	23 34
3	3	54/55 (98%)	53 (98%)	1 (2%)	52 67
4	4	48/49 (98%)	45 (94%)	3 (6%)	15 20
5	5	46/52 (88%)	44 (96%)	2 (4%)	25 37
6	6	46/47 (98%)	44 (96%)	2 (4%)	25 37
7	7	37/37 (100%)	37 (100%)	0	100 100
8	8	54/55 (98%)	49 (91%)	5 (9%)	7 7
9	9	34/34 (100%)	31 (91%)	3 (9%)	8 8
13	D	212/213 (100%)	203 (96%)	9 (4%)	25 38
14	E	159/162 (98%)	154 (97%)	5 (3%)	35 50
15	F	158/158 (100%)	155 (98%)	3 (2%)	52 67
16	G	144/153 (94%)	129 (90%)	15 (10%)	5 5
17	H	137/141 (97%)	132 (96%)	5 (4%)	30 44
18	I	82/107 (77%)	78 (95%)	4 (5%)	21 30
19	J	118/119 (99%)	114 (97%)	4 (3%)	32 46
20	K	102/102 (100%)	98 (96%)	4 (4%)	27 41
21	L	106/106 (100%)	102 (96%)	4 (4%)	28 41
22	M	110/110 (100%)	107 (97%)	3 (3%)	40 55
23	N	98/104 (94%)	94 (96%)	4 (4%)	26 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	O	85/87 (98%)	77 (91%)	8 (9%)	7	7
25	P	95/98 (97%)	93 (98%)	2 (2%)	48	64
26	Q	87/88 (99%)	84 (97%)	3 (3%)	32	46
27	R	86/86 (100%)	83 (96%)	3 (4%)	31	45
28	S	87/87 (100%)	83 (95%)	4 (5%)	23	33
29	T	77/82 (94%)	74 (96%)	3 (4%)	27	41
30	U	85/88 (97%)	79 (93%)	6 (7%)	12	15
31	V	151/164 (92%)	144 (95%)	7 (5%)	23	33
32	a	178/202 (88%)	163 (92%)	15 (8%)	9	9
33	b	171/187 (91%)	151 (88%)	20 (12%)	4	3
34	c	173/174 (99%)	154 (89%)	19 (11%)	5	4
35	d	114/124 (92%)	103 (90%)	11 (10%)	7	6
36	e	89/119 (75%)	81 (91%)	8 (9%)	8	8
37	f	119/122 (98%)	104 (87%)	15 (13%)	3	3
38	g	107/109 (98%)	96 (90%)	11 (10%)	6	5
39	h	102/106 (96%)	91 (89%)	11 (11%)	5	4
40	i	90/92 (98%)	84 (93%)	6 (7%)	13	17
41	j	90/98 (92%)	83 (92%)	7 (8%)	10	12
42	k	105/107 (98%)	96 (91%)	9 (9%)	8	9
43	l	96/99 (97%)	84 (88%)	12 (12%)	3	3
44	m	81/82 (99%)	71 (88%)	10 (12%)	4	3
45	n	75/75 (100%)	70 (93%)	5 (7%)	13	17
46	o	64/65 (98%)	63 (98%)	1 (2%)	58	72
47	p	73/79 (92%)	65 (89%)	8 (11%)	5	4
48	q	49/64 (77%)	43 (88%)	6 (12%)	4	3
49	r	72/78 (92%)	68 (94%)	4 (6%)	17	24
50	s	69/70 (99%)	65 (94%)	4 (6%)	17	23
51	t	45/60 (75%)	42 (93%)	3 (7%)	13	17
All	All	4582/4824 (95%)	4278 (93%)	304 (7%)	16	17

All (304) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	1	11	ARG
1	1	41	ARG
1	1	43	THR
1	1	68	LYS
2	2	22	HIS
2	2	71	LEU
2	2	76	GLU
3	3	19	LEU
4	4	11	SER
4	4	18	ASN
4	4	57	GLU
5	5	39	ARG
5	5	43	SER
6	6	24	ARG
6	6	29	LYS
8	8	29	SER
8	8	30	HIS
8	8	39	ARG
8	8	48	MET
8	8	56	ARG
9	9	11	CYS
9	9	12	ARG
9	9	20	ASP
13	D	43	ARG
13	D	79	GLU
13	D	133	ARG
13	D	139	SER
13	D	177	ARG
13	D	194	GLU
13	D	203	ARG
13	D	252	GLN
13	D	256	LYS
14	E	56	ARG
14	E	118	PHE
14	E	128	ARG
14	E	149	CYS
14	E	169	ARG
15	F	106	SER
15	F	143	LYS
15	F	172	GLN
16	G	26	MET
16	G	48	LYS
16	G	61	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	G	64	LYS
16	G	72	LYS
16	G	78	LYS
16	G	83	TRP
16	G	94	ASP
16	G	114	PHE
16	G	125	ARG
16	G	129	SER
16	G	130	MET
16	G	156	LEU
16	G	161	ARG
16	G	163	ASP
17	H	9	VAL
17	H	62	ARG
17	H	84	GLU
17	H	150	ASP
17	H	152	ARG
18	I	12	LEU
18	I	14	ASN
18	I	19	VAL
18	I	25	TYR
19	J	12	GLN
19	J	62	VAL
19	J	71	ASP
19	J	111	LYS
20	K	40	LYS
20	K	49	ARG
20	K	56	GLN
20	K	112	MET
21	L	15	GLU
21	L	85	VAL
21	L	111	MET
21	L	123	LYS
22	M	6	ARG
22	M	28	SER
22	M	68	VAL
23	N	14	SER
23	N	85	LYS
23	N	100	CYS
23	N	118	ARG
24	O	10	ARG
24	O	19	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	O	32	SER
24	O	58	ASP
24	O	60	ARG
24	O	72	LYS
24	O	82	LYS
24	O	87	THR
25	P	40	ARG
25	P	53	ASN
26	Q	51	ARG
26	Q	78	ARG
26	Q	112	LYS
27	R	31	GLU
27	R	37	ARG
27	R	70	ASP
28	S	1	MET
28	S	49	LYS
28	S	70	LYS
28	S	92	ARG
29	T	3	GLN
29	T	8	LYS
29	T	56	ARG
30	U	8	ASP
30	U	30	ASP
30	U	43	ARG
30	U	57	ILE
30	U	77	SER
30	U	78	LYS
31	V	11	ARG
31	V	44	THR
31	V	48	ARG
31	V	141	LYS
31	V	176	LEU
31	V	186	ASN
31	V	188	HIS
32	a	23	TRP
32	a	29	LYS
32	a	51	ASN
32	a	59	ARG
32	a	60	LEU
32	a	78	LYS
32	a	93	ASP
32	a	94	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	a	105	LYS
32	a	112	LYS
32	a	113	ARG
32	a	140	ASP
32	a	167	ASP
32	a	199	VAL
32	a	219	GLU
33	b	6	HIS
33	b	17	GLU
33	b	29	TYR
33	b	31	ASP
33	b	42	TYR
33	b	56	ASP
33	b	65	ARG
33	b	79	LYS
33	b	88	ARG
33	b	89	GLN
33	b	93	LYS
33	b	107	ARG
33	b	126	ARG
33	b	130	PHE
33	b	142	MET
33	b	179	ARG
33	b	186	THR
33	b	187	TYR
33	b	190	HIS
33	b	204	LYS
34	c	4	TYR
34	c	14	ARG
34	c	29	ASP
34	c	36	ASN
34	c	41	HIS
34	c	58	LYS
34	c	63	ARG
34	c	72	PHE
34	c	75	TYR
34	c	85	SER
34	c	91	LEU
34	c	94	LEU
34	c	105	MET
34	c	136	GLN
34	c	148	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	c	150	LYS
34	c	154	ARG
34	c	165	ARG
34	c	190	ASP
35	d	12	TYR
35	d	37	LEU
35	d	53	LYS
35	d	78	ASN
35	d	80	THR
35	d	82	LEU
35	d	87	LYS
35	d	122	GLN
35	d	142	PHE
35	d	161	SER
35	d	164	GLU
36	e	1	MET
36	e	13	ASP
36	e	16	GLU
36	e	17	GLN
36	e	31	GLU
36	e	35	LYS
36	e	56	LYS
36	e	103	LEU
37	f	3	ARG
37	f	10	ARG
37	f	26	PHE
37	f	27	MET
37	f	31	MET
37	f	41	ARG
37	f	61	THR
37	f	67	ASP
37	f	76	LYS
37	f	97	ASN
37	f	116	MET
37	f	124	LEU
37	f	131	LYS
37	f	136	LYS
37	f	139	GLU
38	g	52	SER
38	g	74	GLU
38	g	79	SER
38	g	80	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	g	87	LYS
38	g	96	ARG
38	g	102	SER
38	g	107	ASN
38	g	111	MET
38	g	112	THR
38	g	113	ASP
39	h	4	THR
39	h	25	THR
39	h	27	LYS
39	h	39	PHE
39	h	46	MET
39	h	52	LEU
39	h	100	LYS
39	h	120	LYS
39	h	124	ARG
39	h	127	TYR
39	h	128	SER
40	i	46	LYS
40	i	52	LEU
40	i	62	ARG
40	i	63	ASP
40	i	64	GLN
40	i	89	LYS
41	j	26	SER
41	j	68	GLU
41	j	93	ARG
41	j	98	ARG
41	j	106	LYS
41	j	112	ASP
41	j	129	VAL
42	k	44	LYS
42	k	50	ARG
42	k	54	ARG
42	k	58	THR
42	k	59	ASN
42	k	77	HIS
42	k	99	ARG
42	k	114	ARG
42	k	117	TYR
43	l	12	ASN
43	l	21	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	l	65	THR
43	l	68	ASP
43	l	75	MET
43	l	80	LEU
43	l	81	MET
43	l	86	TYR
43	l	92	ARG
43	l	100	GLN
43	l	107	ARG
43	l	114	LYS
44	m	6	MET
44	m	22	LYS
44	m	50	LYS
44	m	61	ARG
44	m	62	ASN
44	m	64	CYS
44	m	77	PHE
44	m	82	ASN
44	m	85	ARG
44	m	86	GLU
45	n	7	GLU
45	n	10	GLN
45	n	41	ASP
45	n	78	TYR
45	n	89	ARG
46	o	13	LYS
47	p	10	THR
47	p	24	VAL
47	p	43	ARG
47	p	54	ASN
47	p	60	ASP
47	p	65	ARG
47	p	68	ARG
47	p	84	ARG
48	q	34	SER
48	q	36	THR
48	q	42	SER
48	q	43	ARG
48	q	68	LEU
48	q	74	HIS
49	r	17	LYS
49	r	39	MET

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Mol	Chain	Res	Type
49	r	44	MET
49	r	66	MET
50	s	8	LYS
50	s	19	SER
50	s	45	GLU
50	s	59	ASP
51	t	17	ARG
51	t	20	LYS
51	t	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
14	E	102	GLN
15	F	2	GLN
17	H	73	ASN
20	K	91	GLN
29	T	90	GLN
33	b	118	GLN
38	g	18	GLN
38	g	85	GLN
38	g	107	ASN
44	m	49	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2802/2891 (96%)	387 (13%)	7 (0%)
11	B	1526/1536 (99%)	213 (13%)	4 (0%)
12	C	119/121 (98%)	11 (9%)	0
All	All	4447/4548 (97%)	611 (13%)	11 (0%)

All (611) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	9	A
10	A	22	G
10	A	33	U
10	A	44	G
10	A	45	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	54	G
10	A	59	G
10	A	62	A
10	A	70	A
10	A	73	A
10	A	74	G
10	A	91	A
10	A	92	A
10	A	93	C
10	A	100	U
10	A	101	G
10	A	102	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	124	G
10	A	137	A
10	A	139	A
10	A	141	C
10	A	162	C
10	A	164	A
10	A	180	A
10	A	195	A
10	A	198	A
10	A	214	G
10	A	215	A
10	A	221	A
10	A	223	U
10	A	247	G
10	A	262	U
10	A	265	G
10	A	270	U
10	A	272	A
10	A	278	A
10	A	283	U
10	A	295	G
10	A	304	A
10	A	317	U
10	A	318	G
10	A	320	G
10	A	322	G
10	A	323	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	326	G
10	A	338	A
10	A	346	U
10	A	351	A
10	A	354	G
10	A	355	A
10	A	357	A
10	A	359	C
10	A	362	G
10	A	375	C
10	A	376	G
10	A	386	G
10	A	389	U
10	A	401	G
10	A	414	G
10	A	433	A
10	A	441	U
10	A	445	C
10	A	446	C
10	A	470	A
10	A	471	G
10	A	480	A
10	A	481	G
10	A	484	G
10	A	494	U
10	A	495	A
10	A	498	A
10	A	519	A
10	A	520	G
10	A	522	A
10	A	536	U
10	A	538	U
10	A	552	A
10	A	557	U
10	A	562	U
10	A	564	A
10	A	581	A
10	A	592	A
10	A	602	U
10	A	603	A
10	A	616	A
10	A	626	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	634	U
10	A	635	A
10	A	636	G
10	A	644	A
10	A	666	A
10	A	675	U
10	A	693	G
10	A	701	G
10	A	707	A
10	A	717	G
10	A	719	A
10	A	729	C
10	A	736	U
10	A	740	A
10	A	753	A
10	A	764	G
10	A	765	G
10	A	771	A
10	A	773	G
10	A	774	G
10	A	794	G
10	A	801	C
10	A	816	U
10	A	817	U
10	A	819	G
10	A	834	A
10	A	847	G
10	A	854	A
10	A	859	U
10	A	865	U
10	A	869	G
10	A	872	U
10	A	884	A
10	A	886	C
10	A	895	G
10	A	898	A
10	A	902	C
10	A	919	C
10	A	920	C
10	A	921	G
10	A	922	A
10	A	935	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	950	C
10	A	963	A
10	A	971	C
10	A	972	A
10	A	973	A
10	A	978	G
10	A	985	A
10	A	992	G
10	A	994	C
10	A	1001	U
10	A	1002	U
10	A	1015	U
10	A	1022	U
10	A	1035	A
10	A	1036	G
10	A	1037	A
10	A	1046	A
10	A	1050	U
10	A	1059	A
10	A	1060	G
10	A	1062	A
10	A	1072	U
10	A	1077	A
10	A	1079	A
10	A	1082	G
10	A	1087	A
10	A	1099	G
10	A	1101	G
10	A	1117	G
10	A	1119	U
10	A	1121	U
10	A	1122	A
10	A	1124	C
10	A	1125	G
10	A	1131	C
10	A	1132	A
10	A	1161	G
10	A	1162	U
10	A	1163	A
10	A	1166	U
10	A	1170	G
10	A	1192	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	1224	G
10	A	1233	A
10	A	1236	G
10	A	1239	A
10	A	1242	G
10	A	1257	G
10	A	1258	A
10	A	1259	C
10	A	1286	A
10	A	1287	A
10	A	1298	U
10	A	1300	C
10	A	1307	A
10	A	1315	U
10	A	1338	U
10	A	1345	A
10	A	1351	A
10	A	1364	A
10	A	1365	U
10	A	1369	A
10	A	1402	G
10	A	1403	C
10	A	1413	A
10	A	1414	C
10	A	1420	A
10	A	1421	G
10	A	1438	G
10	A	1446	U
10	A	1468	G
10	A	1476	A
10	A	1479	U
10	A	1480	A
10	A	1481	A
10	A	1483	U
10	A	1496	G
10	A	1501	A
10	A	1510	G
10	A	1518	G
10	A	1519	U
10	A	1521	U
10	A	1522	U
10	A	1523	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	1525	A
10	A	1526	G
10	A	1529	G
10	A	1530	A
10	A	1555	A
10	A	1558	A
10	A	1567	U
10	A	1572	U
10	A	1573	U
10	A	1574	C
10	A	1595	C
10	A	1596	C
10	A	1597	A
10	A	1607	A
10	A	1628	C
10	A	1636	U
10	A	1637	U
10	A	1638	G
10	A	1663	G
10	A	1699	G
10	A	1704	G
10	A	1705	G
10	A	1710	A
10	A	1711	G
10	A	1714	U
10	A	1715	U
10	A	1716	U
10	A	1717	A
10	A	1718	C
10	A	1727	C
10	A	1750	G
10	A	1759	A
10	A	1762	G
10	A	1768	U
10	A	1770	A
10	A	1772	A
10	A	1786	C
10	A	1787	A
10	A	1793	G
10	A	1794	A
10	A	1802	C
10	A	1806	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	1815	A
10	A	1819	C
10	A	1834	A
10	A	1856	C
10	A	1882	G
10	A	1892	G
10	A	1902	A
10	A	1915	G
10	A	1916	G
10	A	1923	A
10	A	1924	A
10	A	1941	U
10	A	1953	C
10	A	1956	A
10	A	1957	U
10	A	1958	G
10	A	1977	U
10	A	1979	U
10	A	1983	C
10	A	2009	C
10	A	2017	A
10	A	2019	A
10	A	2029	U
10	A	2035	G
10	A	2041	C
10	A	2042	G
10	A	2046	A
10	A	2047	G
10	A	2048	A
10	A	2049	C
10	A	2055	G
10	A	2084	U
10	A	2086	G
10	A	2171	U
10	A	2173	C
10	A	2176	G
10	A	2178	G
10	A	2184	A
10	A	2190	G
10	A	2197	A
10	A	2199	U
10	A	2211	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	2224	G
10	A	2225	G
10	A	2237	G
10	A	2254	A
10	A	2264	A
10	A	2269	U
10	A	2273	A
10	A	2274	A
10	A	2283	C
10	A	2291	U
10	A	2294	G
10	A	2298	U
10	A	2305	C
10	A	2306	A
10	A	2308	A
10	A	2311	A
10	A	2312	U
10	A	2313	A
10	A	2319	A
10	A	2322	A
10	A	2331	G
10	A	2333	C
10	A	2336	C
10	A	2358	U
10	A	2369	G
10	A	2371	C
10	A	2375	G
10	A	2388	U
10	A	2389	C
10	A	2392	U
10	A	2395	G
10	A	2411	A
10	A	2415	G
10	A	2416	A
10	A	2421	A
10	A	2427	U
10	A	2434	A
10	A	2461	C
10	A	2462	A
10	A	2477	U
10	A	2488	G
10	A	2489	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	2491	G
10	A	2492	U
10	A	2504	A
10	A	2511	G
10	A	2515	G
10	A	2533	A
10	A	2550	A
10	A	2552	A
10	A	2553	G
10	A	2559	C
10	A	2588	A
10	A	2591	U
10	A	2592	C
10	A	2595	U
10	A	2599	U
10	A	2601	U
10	A	2615	U
10	A	2616	U
10	A	2622	U
10	A	2675	U
10	A	2676	U
10	A	2700	G
10	A	2702	C
10	A	2712	U
10	A	2719	A
10	A	2730	G
10	A	2734	A
10	A	2743	A
10	A	2751	A
10	A	2764	A
10	A	2784	U
10	A	2785	G
10	A	2786	A
10	A	2787	U
10	A	2804	C
10	A	2806	A
10	A	2807	A
10	A	2819	U
10	A	2821	A
10	A	2822	U
10	A	2835	U
10	A	2853	G

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	A	2859	A
10	A	2866	C
10	A	2870	U
10	A	2877	U
11	B	2	A
11	B	4	C
11	B	5	U
11	B	7	A
11	B	9	G
11	B	31	G
11	B	32	A
11	B	39	G
11	B	47	C
11	B	48	C
11	B	51	A
11	B	54	C
11	B	58	C
11	B	66	G
11	B	69	G
11	B	72	G
11	B	73	A
11	B	81	U
11	B	83	G
11	B	84	C
11	B	90	G
11	B	91	A
11	B	93	U
11	B	95	A
11	B	97	C
11	B	114	A
11	B	124	A
11	B	125	U
11	B	138	G
11	B	157	C
11	B	167	U
11	B	177	G
11	B	182	G
11	B	183	A
11	B	189	A
11	B	191	A
11	B	198	G
11	B	214	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	B	237	A
11	B	240	A
11	B	241	G
11	B	245	G
11	B	260	G
11	B	261	C
11	B	283	A
11	B	300	A
11	B	310	C
11	B	315	A
11	B	322	C
11	B	323	A
11	B	324	C
11	B	326	G
11	B	346	C
11	B	348	G
11	B	361	U
11	B	363	G
11	B	366	C
11	B	367	A
11	B	369	U
11	B	382	G
11	B	387	A
11	B	391	A
11	B	400	G
11	B	406	A
11	B	407	G
11	B	415	U
11	B	416	C
11	B	423	U
11	B	447	G
11	B	458	U
11	B	461	U
11	B	474	U
11	B	475	G
11	B	477	C
11	B	479	U
11	B	480	U
11	B	489	A
11	B	490	A
11	B	491	U
11	B	503	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	B	505	C
11	B	512	C
11	B	515	G
11	B	521	G
11	B	525	U
11	B	526	A
11	B	541	A
11	B	547	A
11	B	558	C
11	B	566	A
11	B	567	A
11	B	570	C
11	B	571	G
11	B	573	G
11	B	582	G
11	B	627	G
11	B	634	A
11	B	647	A
11	B	659	A
11	B	681	A
11	B	697	G
11	B	717	U
11	B	749	A
11	B	754	G
11	B	768	G
11	B	781	A
11	B	787	U
11	B	788	A
11	B	806	G
11	B	809	A
11	B	811	C
11	B	822	A
11	B	830	G
11	B	835	C
11	B	836	U
11	B	838	G
11	B	839	A
11	B	840	G
11	B	907	A
11	B	908	A
11	B	920	G
11	B	921	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	B	928	C
11	B	929	A
11	B	952	A
11	B	954	U
11	B	963	A
11	B	969	A
11	B	970	G
11	B	971	A
11	B	976	U
11	B	983	C
11	B	987	G
11	B	988	A
11	B	998	A
11	B	1016	U
11	B	1024	U
11	B	1025	C
11	B	1026	G
11	B	1028	G
11	B	1030	A
11	B	1031	C
11	B	1037	C
11	B	1050	U
11	B	1059	U
11	B	1064	U
11	B	1067	U
11	B	1079	U
11	B	1088	G
11	B	1089	U
11	B	1095	A
11	B	1098	G
11	B	1118	G
11	B	1119	U
11	B	1127	A
11	B	1130	U
11	B	1131	C
11	B	1133	G
11	B	1134	G
11	B	1135	U
11	B	1148	G
11	B	1153	U
11	B	1162	C
11	B	1175	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	B	1178	G
11	B	1190	A
11	B	1191	A
11	B	1206	U
11	B	1207	A
11	B	1219	A
11	B	1220	C
11	B	1221	A
11	B	1234	U
11	B	1250	U
11	B	1252	G
11	B	1272	U
11	B	1273	A
11	B	1274	A
11	B	1279	A
11	B	1280	U
11	B	1281	A
11	B	1293	A
11	B	1294	G
11	B	1296	C
11	B	1299	G
11	B	1300	A
11	B	1311	C
11	B	1314	C
11	B	1316	C
11	B	1323	G
11	B	1357	A
11	B	1373	G
11	B	1375	U
11	B	1388	A
11	B	1391	C
11	B	1392	A
11	B	1413	G
11	B	1435	A
11	B	1440	A
11	B	1446	A
11	B	1447	A
11	B	1481	G
11	B	1485	G
11	B	1486	A
11	B	1487	A
11	B	1488	G

*Continued on next page...*

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Mol	Chain	Res	Type
11	B	1491	G
11	B	1493	A
11	B	1497	A
11	B	1500	U
11	B	1511	G
11	B	1523	G
11	B	1524	G
12	C	13	A
12	C	24	G
12	C	35	U
12	C	44	G
12	C	56	G
12	C	67	U
12	C	88	C
12	C	89	U
12	C	91	C
12	C	105	G
12	C	109	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	353	U
10	A	602	U
10	A	773	G
10	A	1480	A
10	A	2416	A
10	A	2591	U
10	A	2742	U
11	B	80	C
11	B	422	G
11	B	457	U
11	B	1205	U

#### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 185 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.



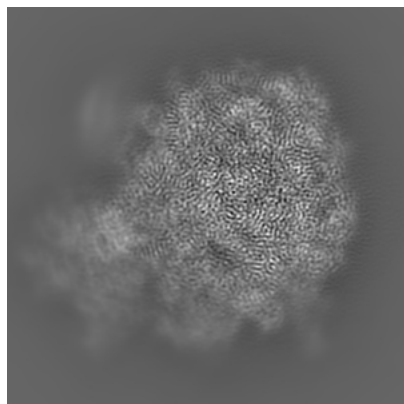
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19547. These allow visual inspection of the internal detail of the map and identification of artifacts.

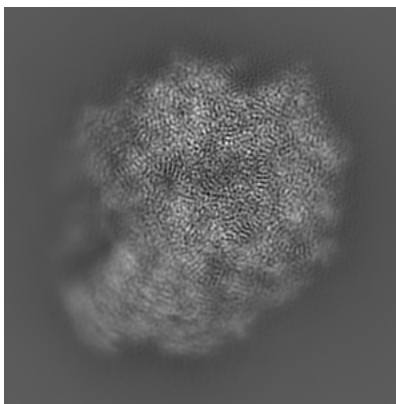
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

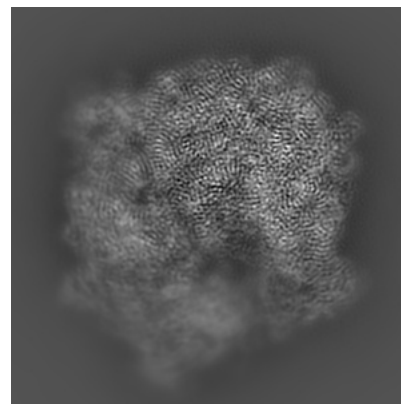
#### 6.1.1 Primary map



X

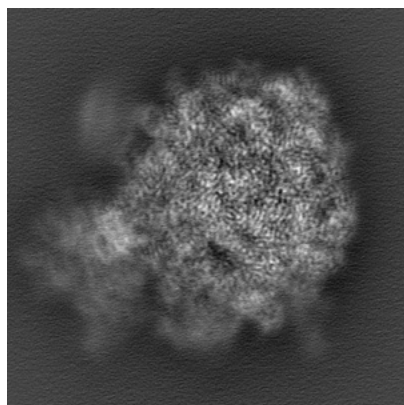


Y

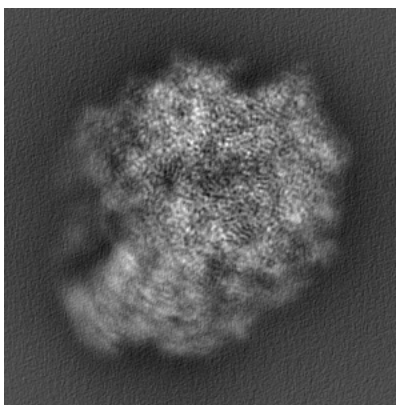


Z

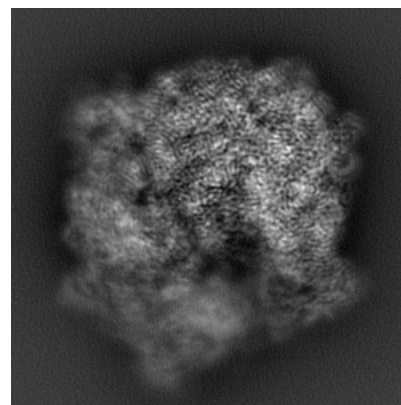
#### 6.1.2 Raw map



X



Y

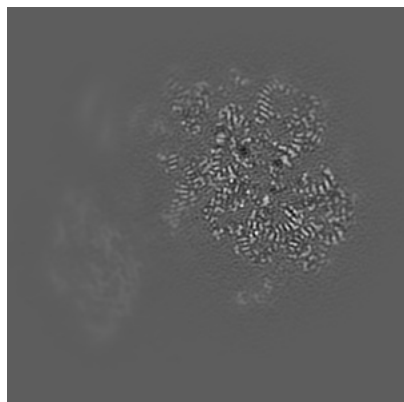


Z

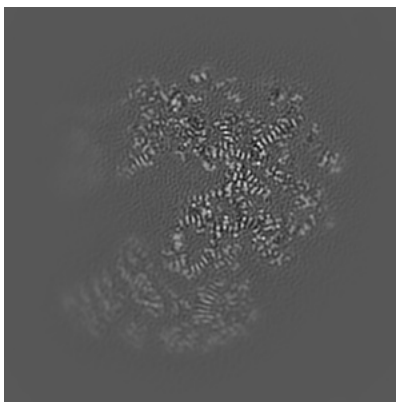
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

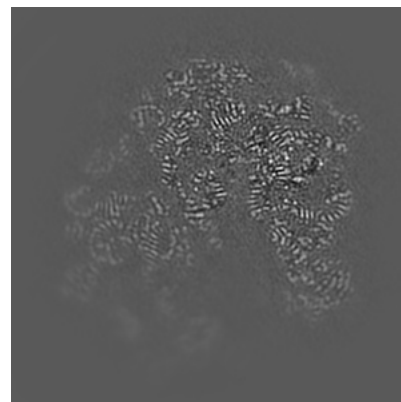
### 6.2.1 Primary map



X Index: 170

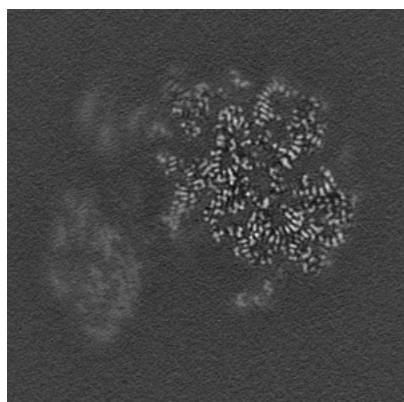


Y Index: 170

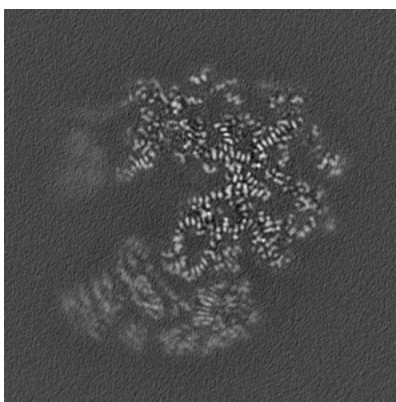


Z Index: 170

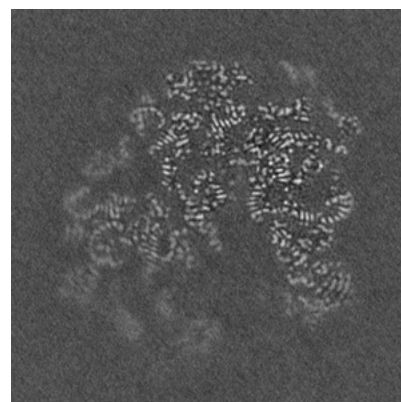
### 6.2.2 Raw map



X Index: 170



Y Index: 170

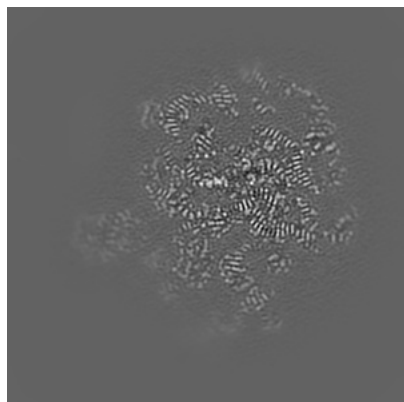


Z Index: 170

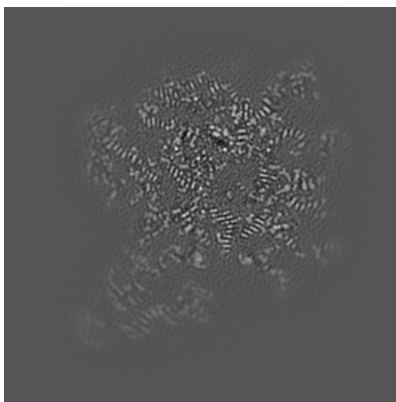
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

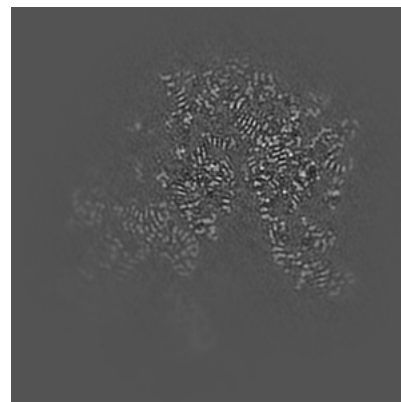
### 6.3.1 Primary map



X Index: 228

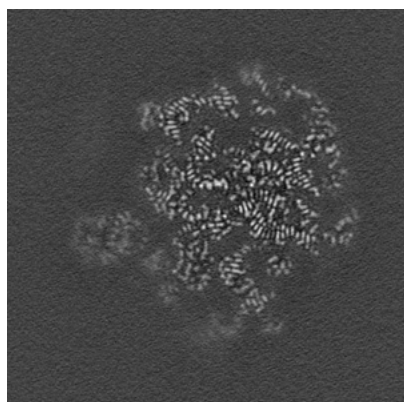


Y Index: 217

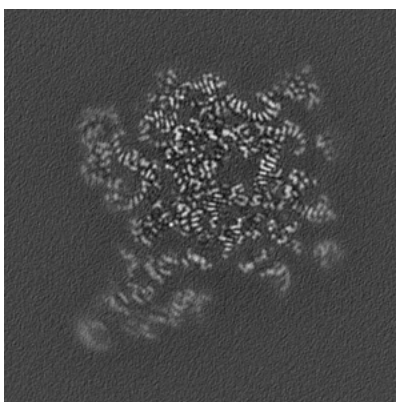


Z Index: 182

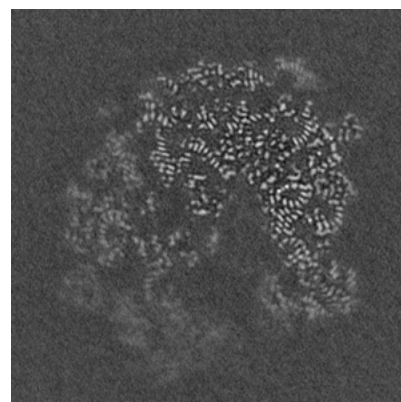
### 6.3.2 Raw map



X Index: 228



Y Index: 221

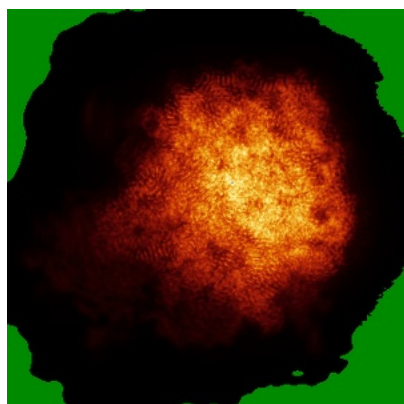


Z Index: 163

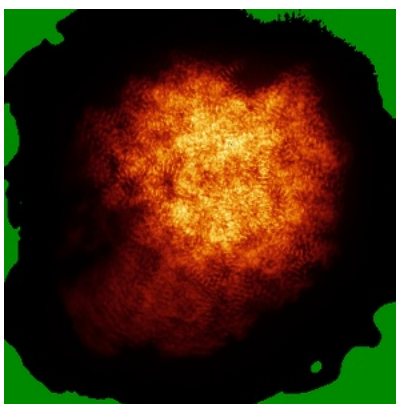
The images above show the largest variance slices of the map in three orthogonal directions.

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

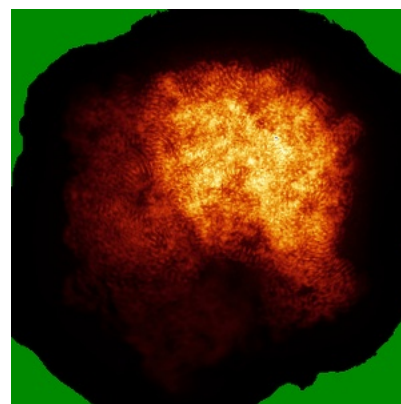
### 6.4.1 Primary map



X

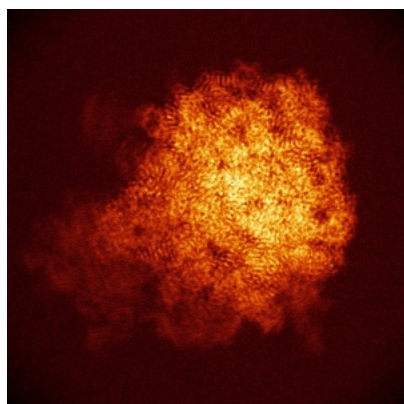


Y

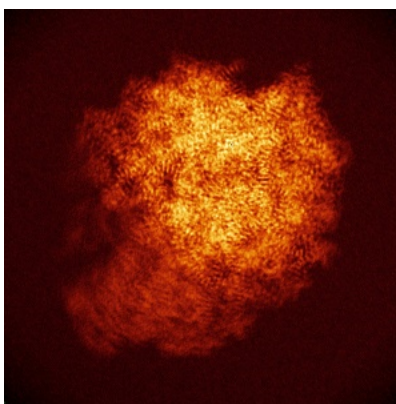


Z

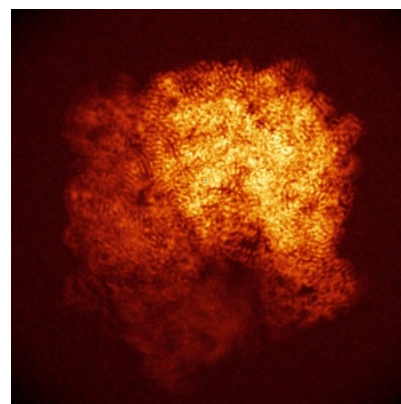
### 6.4.2 Raw map



X



Y

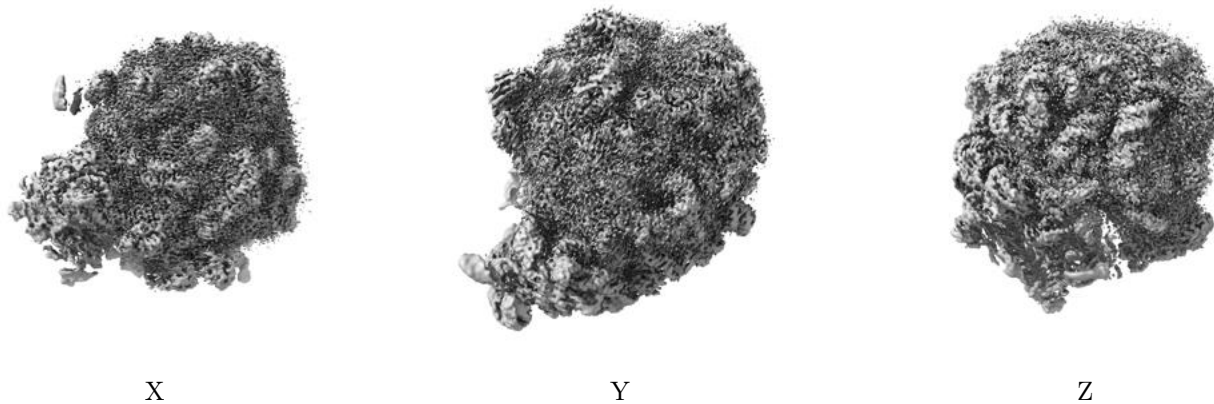


Z

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.

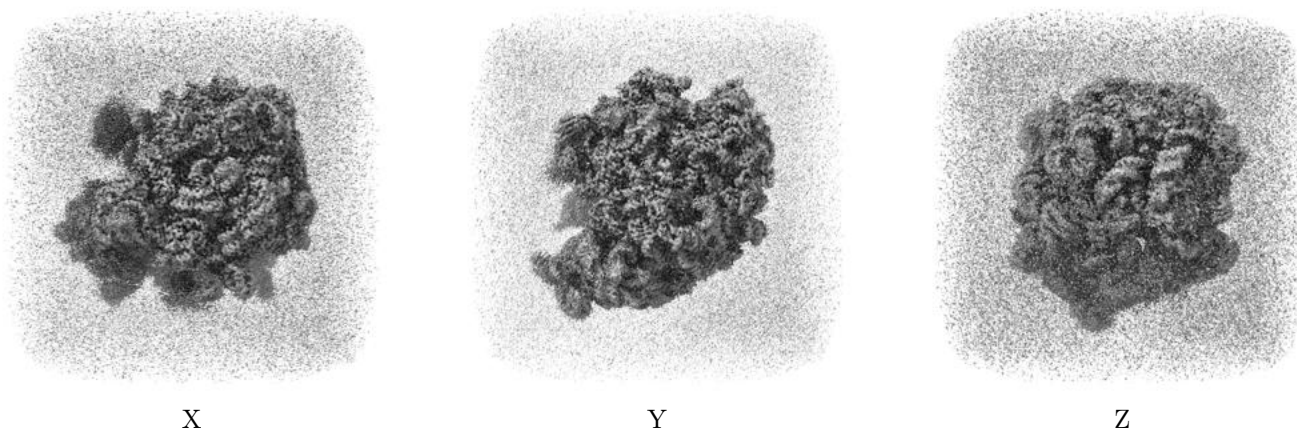
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

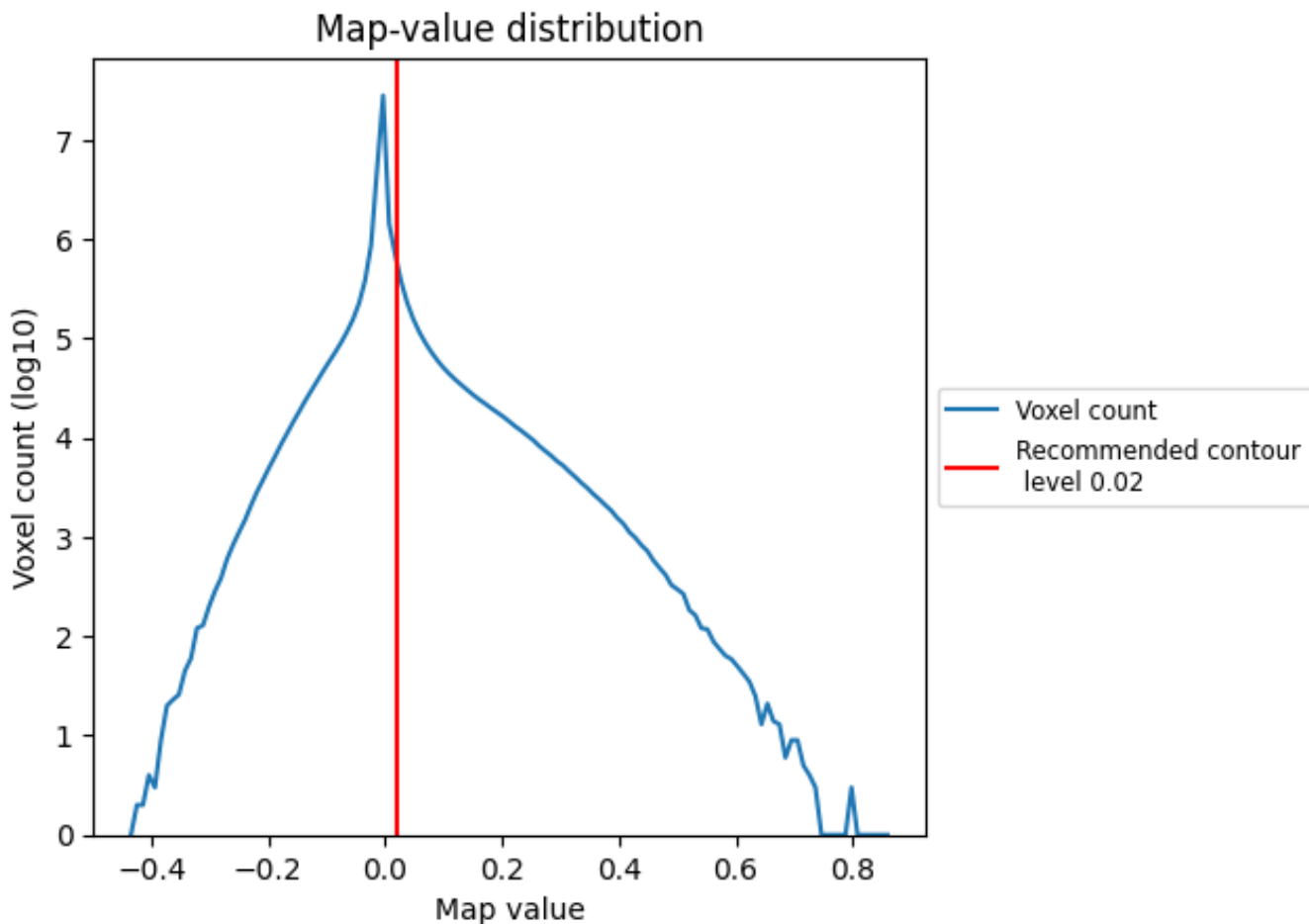
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

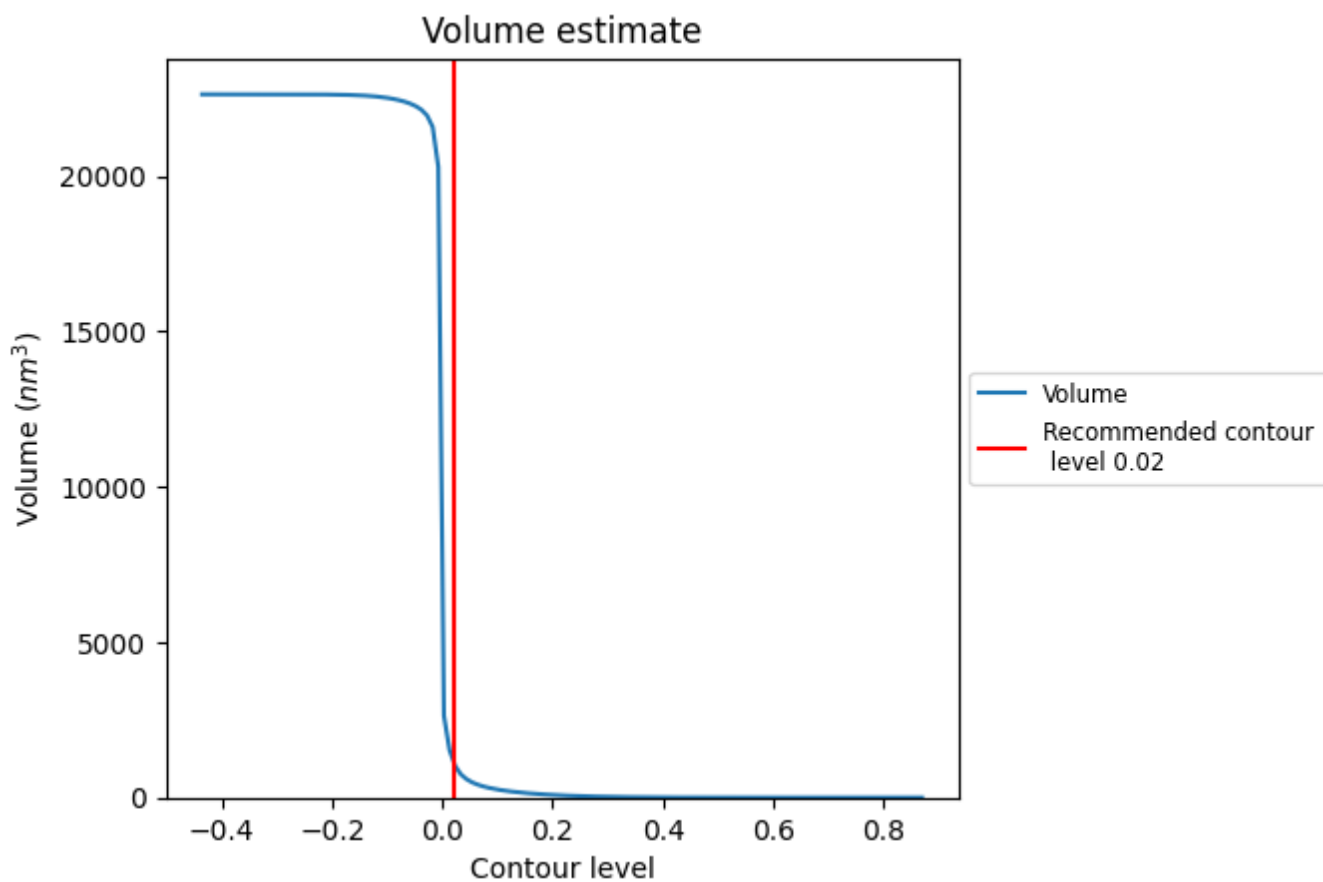
This section contains the results of statistical analysis of the map.

### 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.

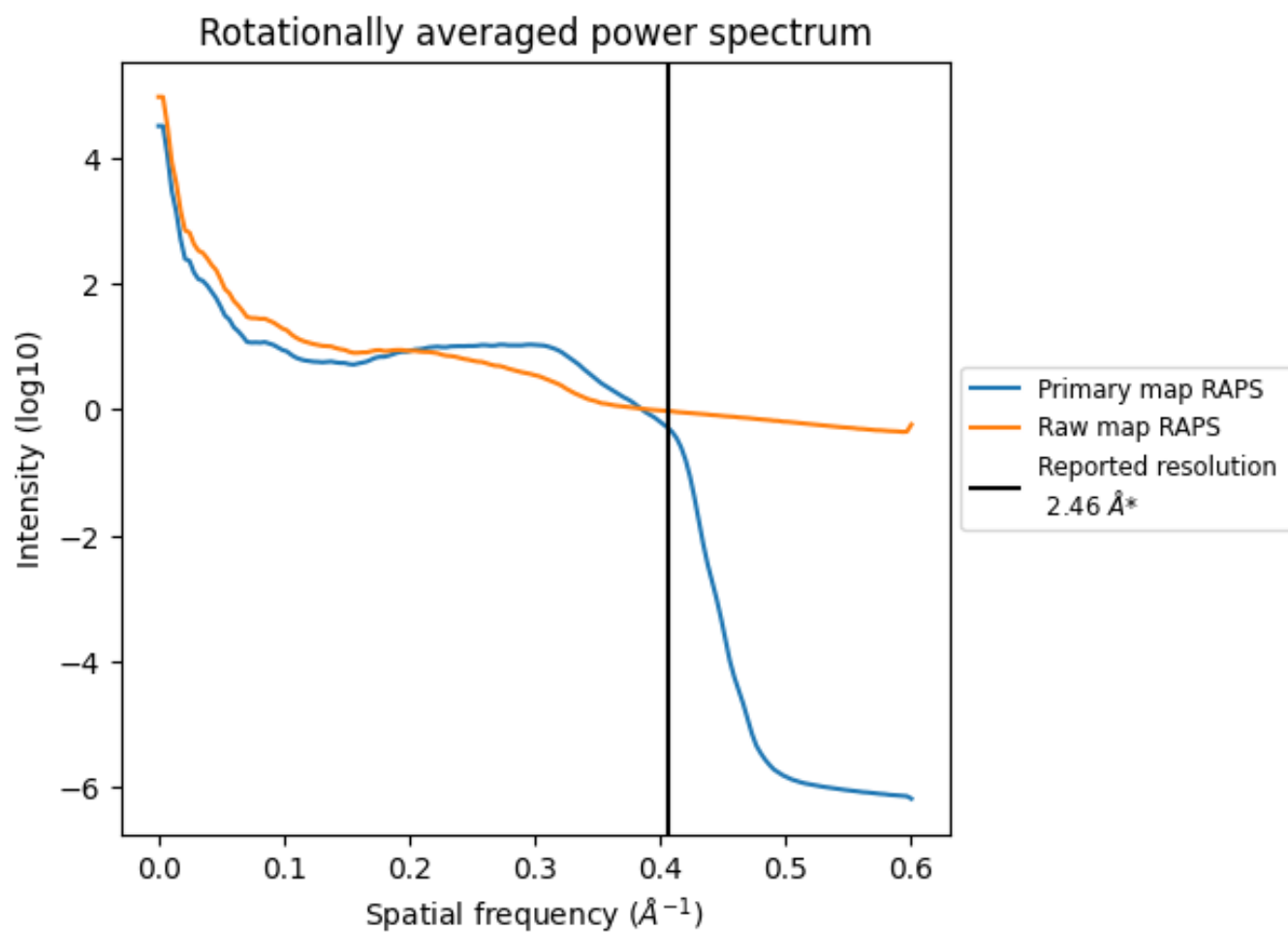
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192  $\text{nm}^3$ ; this corresponds to an approximate mass of 1077 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



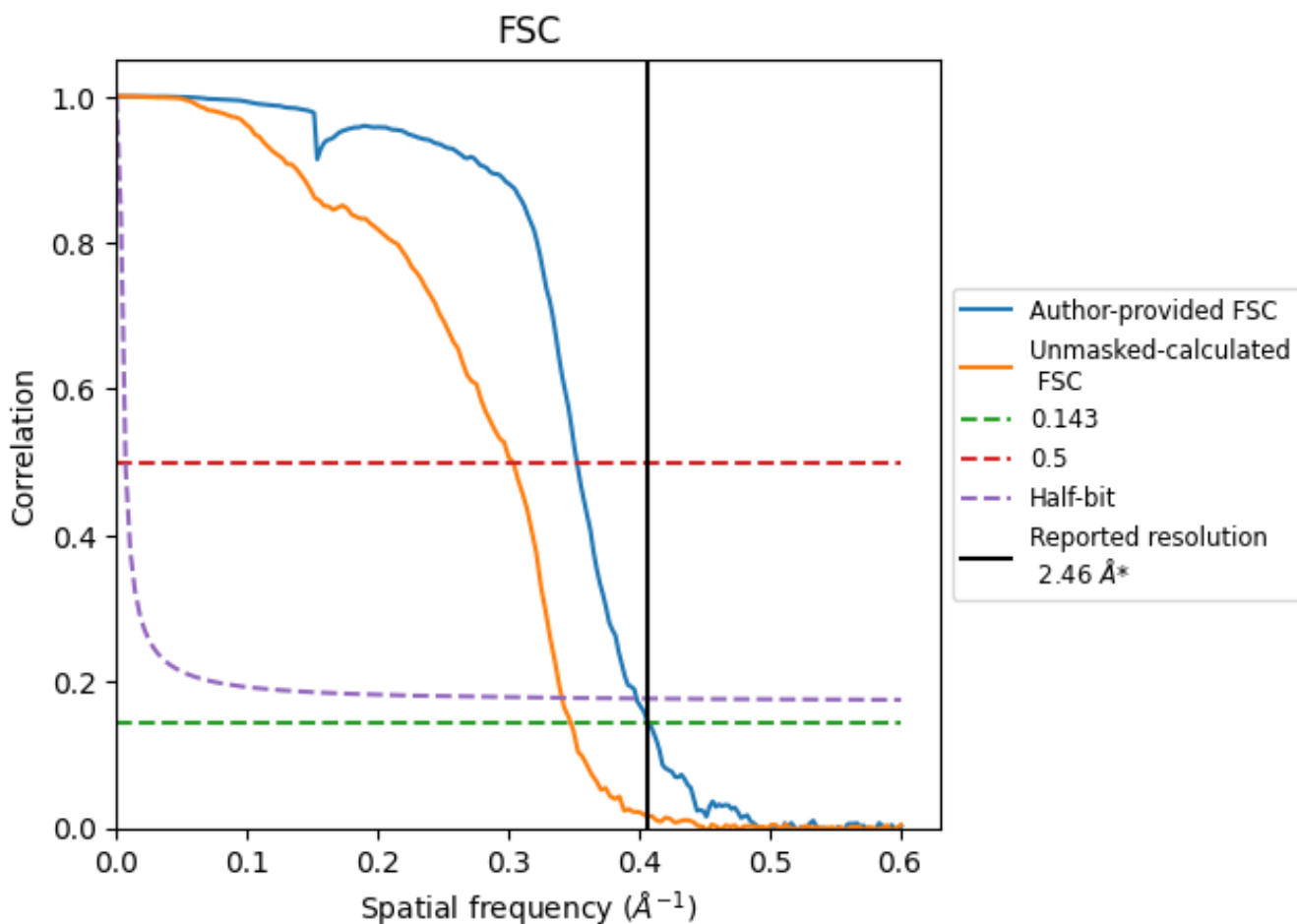
\*Reported resolution corresponds to spatial frequency of 0.407 Å<sup>-1</sup>



## 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 0.407 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

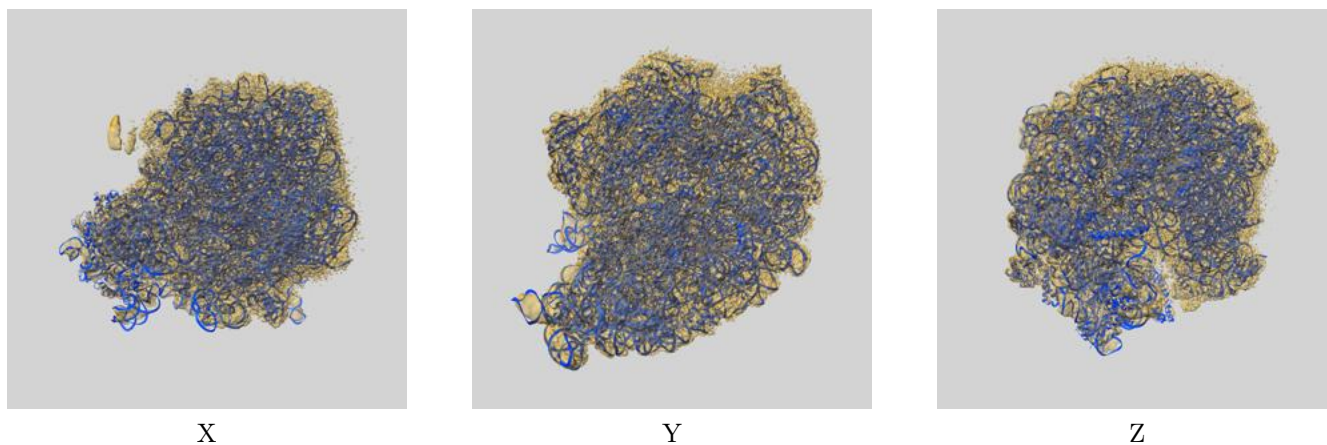
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	2.45	2.84	2.51
Unmasked-calculated*	2.87	3.29	2.93

\*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 2.87 differs from the reported value 2.46 by more than 10 %

## 9 Map-model fit [i](#)

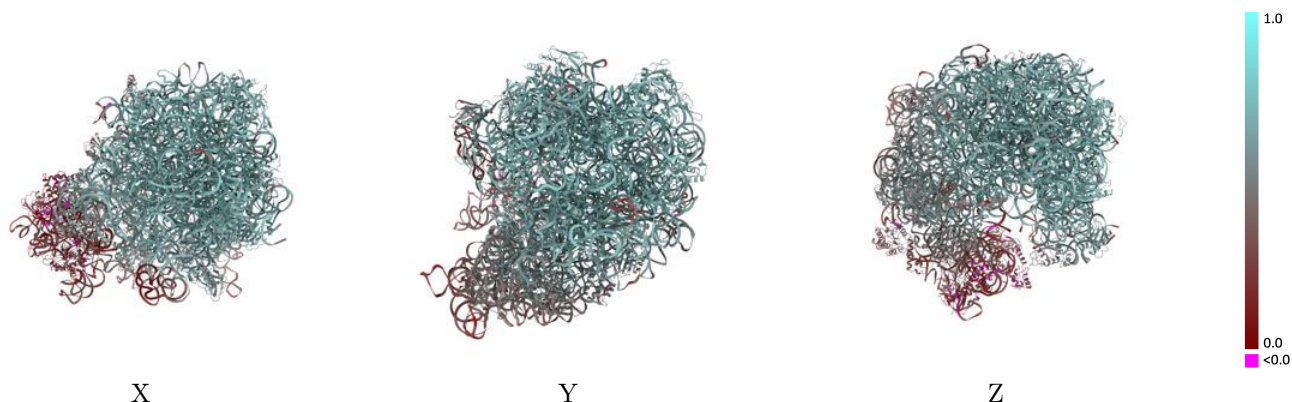
This section contains information regarding the fit between EMDB map EMD-19547 and PDB model 8RWG. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



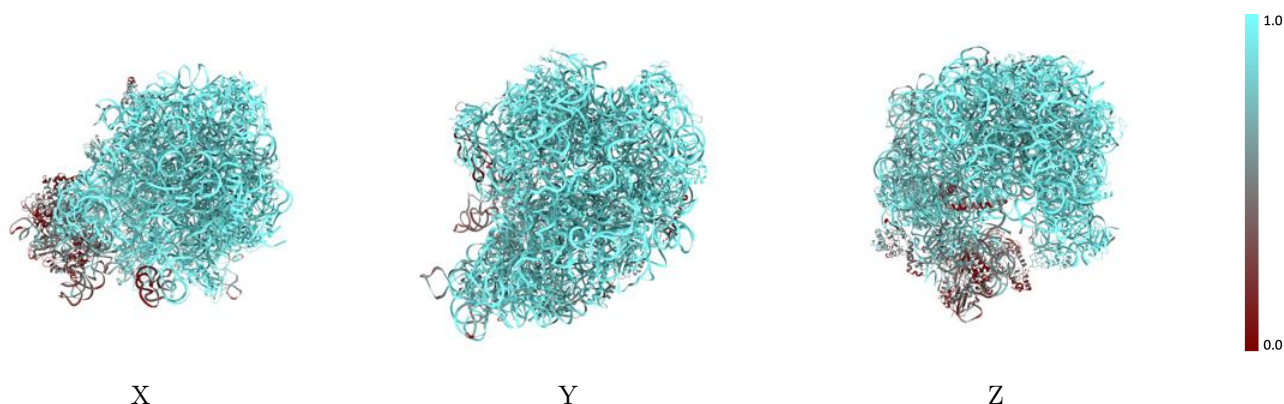
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



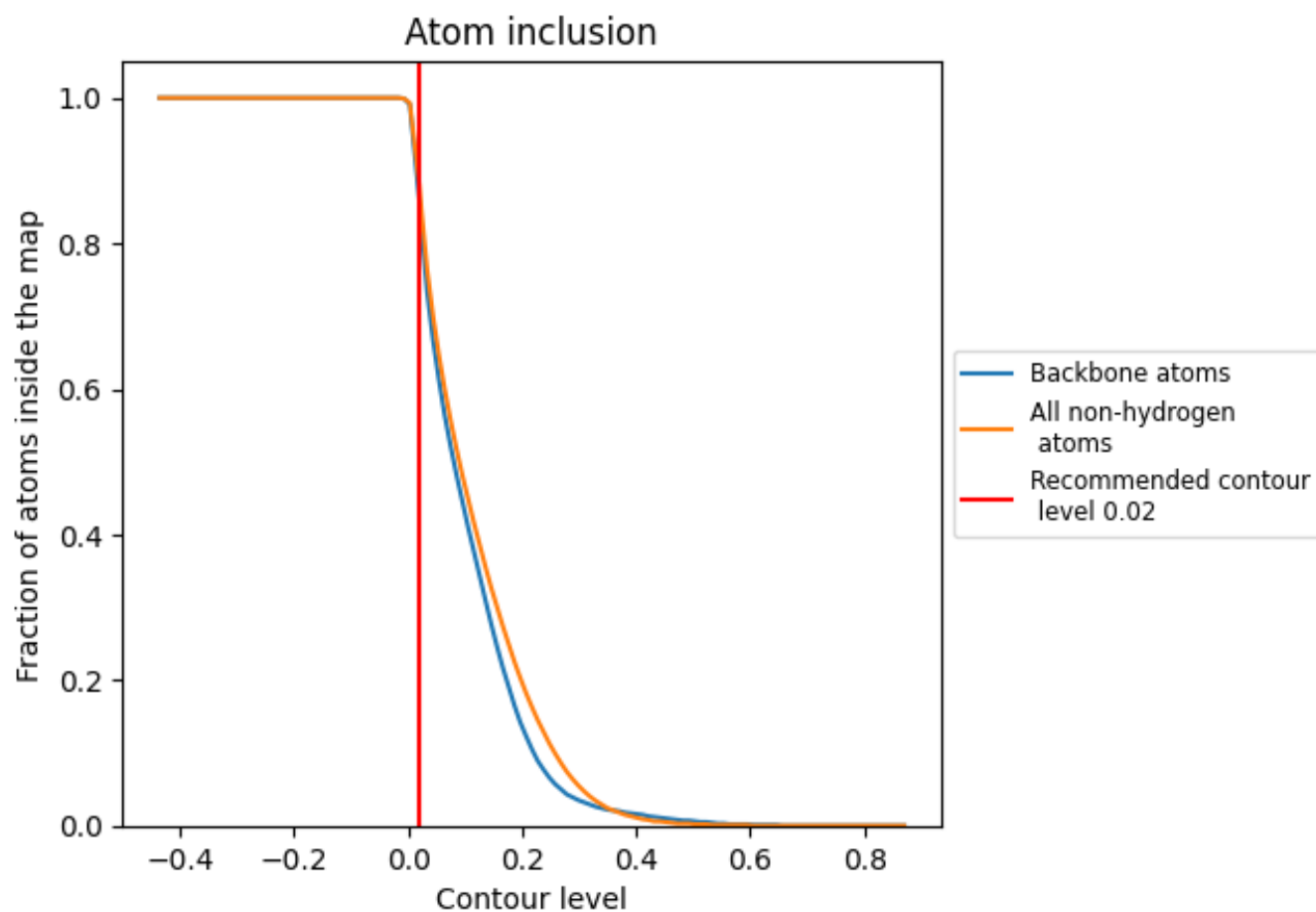
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary



































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

Chain	Atom inclusion	Q-score
All	 0.8800	 0.5540
1	 0.9950	 0.6740
2	 0.9670	 0.6510
3	 0.9690	 0.6180
4	 0.9950	 0.6640
5	 0.9710	 0.6580
6	 0.9730	 0.6310
7	 0.9940	 0.7060
8	 0.9920	 0.6790
9	 0.9830	 0.6500
A	 0.9740	 0.6430
B	 0.8330	 0.4280
C	 0.9780	 0.5870
D	 0.9850	 0.6690
E	 0.9880	 0.6770
F	 0.9830	 0.6610
G	 0.8410	 0.4850
H	 0.9260	 0.5710
I	 0.3590	 0.4250
J	 0.9830	 0.6640
K	 0.9790	 0.6620
L	 0.9770	 0.6620
M	 0.9810	 0.6540
N	 0.9900	 0.6810
O	 0.9570	 0.5950
P	 0.9840	 0.6580
Q	 0.9910	 0.6880
R	 0.9730	 0.6490
S	 0.9870	 0.6720
T	 0.9650	 0.6270
U	 0.9590	 0.6050
V	 0.9080	 0.5920
a	 0.5170	 0.3480
b	 0.4150	 0.3520
c	 0.5660	 0.3760



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Chain	Atom inclusion	Q-score
d	 0.7760	 0.4890
e	 0.8030	 0.4980
f	 0.2030	 0.2060
g	 0.8200	 0.4980
h	 0.2920	 0.1840
i	 0.2410	 0.2340
j	 0.8230	 0.5110
k	 0.7520	 0.5030
l	 0.2110	 0.1460
m	 0.3770	 0.2920
n	 0.8680	 0.5260
o	 0.7570	 0.4570
p	 0.8110	 0.4840
q	 0.8030	 0.5120
r	 0.1110	 0.1560
s	 0.8810	 0.5030
t	 0.6930	 0.4970