



## Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 11:49 pm BST

PDB ID : 28UM / pdb\_000028um  
EMDB ID : EMD-56832  
Title : E. coli 70S ribosome, conformational excited state mutation in SSU-h41, with A- and P-site tRNA  
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.  
Deposited on : 2026-02-20  
Resolution : 2.15 Å(reported)  
Based on initial model : 7K00

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:

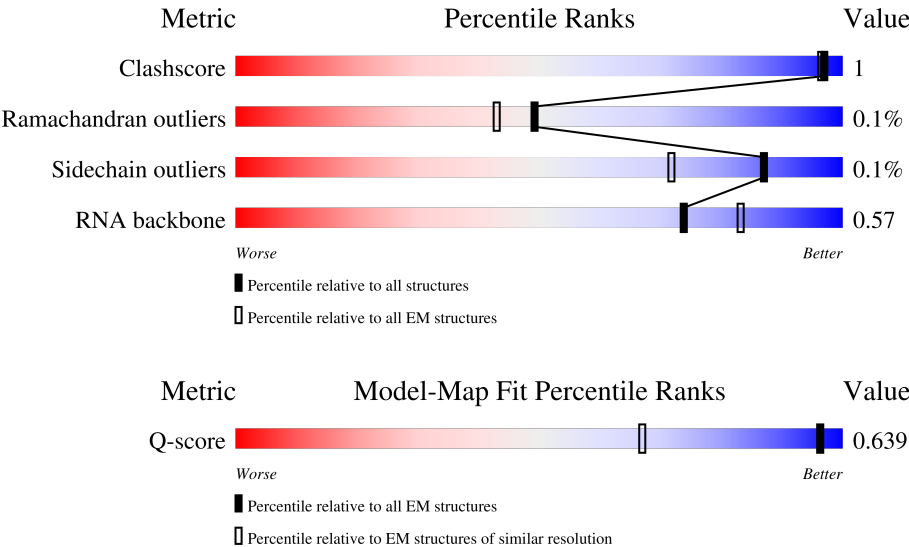
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




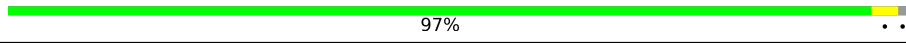
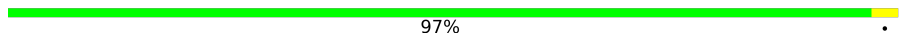
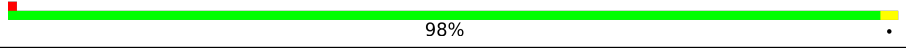
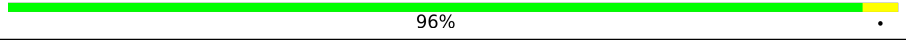
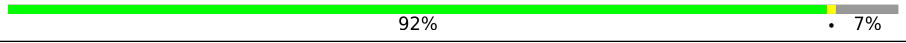
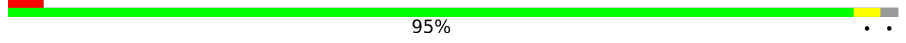
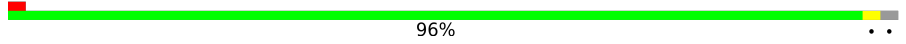
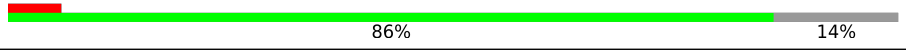


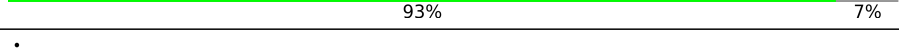
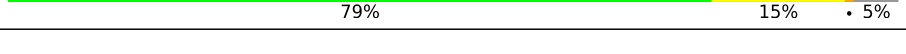
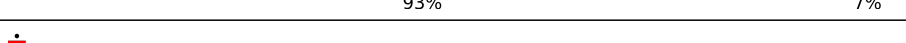
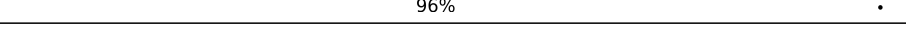
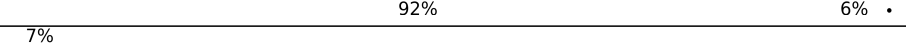
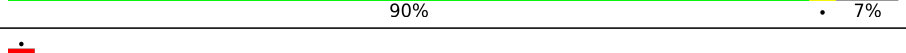

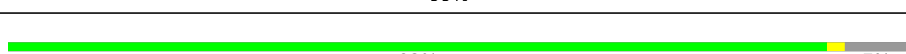
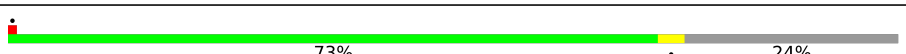

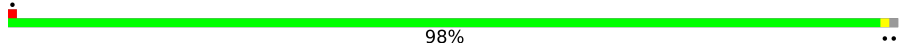
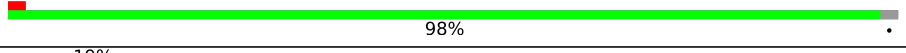
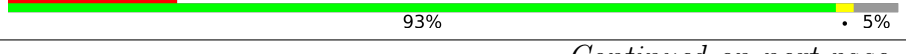
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2551 ( 1.66 - 2.65 )

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	3	38	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> </div>
2	K	129	<div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> </div>
3	L	124	<div> <div style="width: 98%;"></div> <div style="width: 2%;"></div> </div>

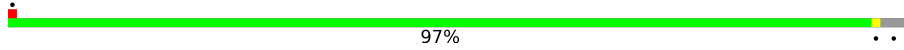
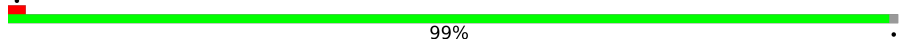
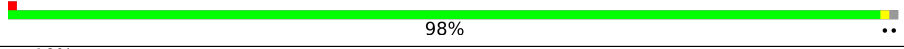
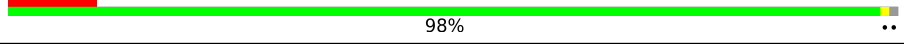
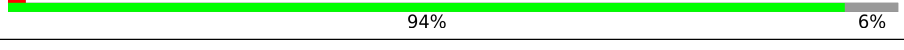

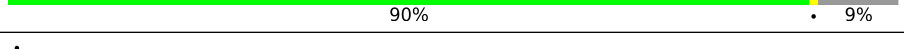
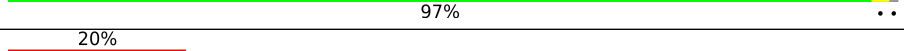
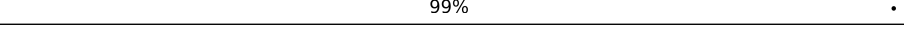
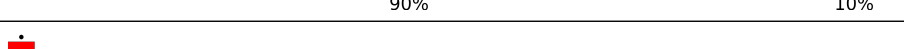
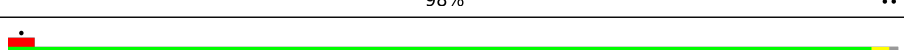
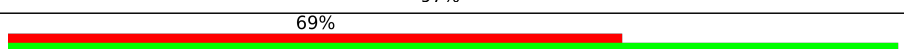
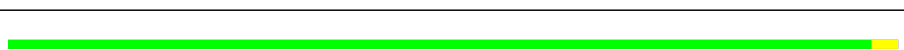
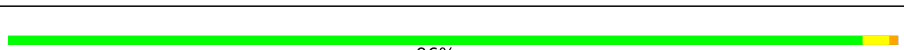
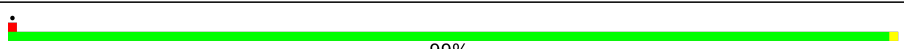
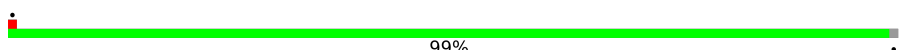
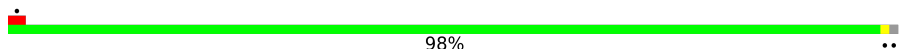
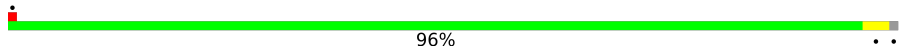
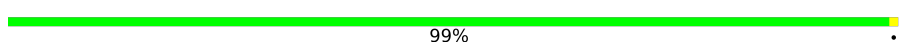
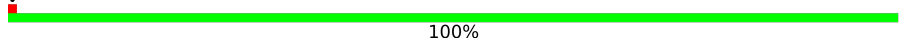
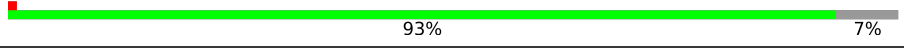
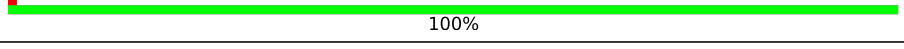
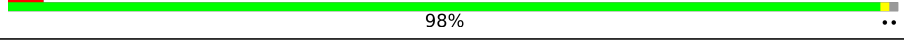
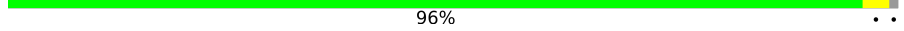

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Mol	Chain	Length	Quality of chain
4	b	120	
5	c	273	
6	d	209	
7	e	201	
8	l	136	
9	m	127	
10	t	104	
11	z	57	
12	4	70	
13	A	1542	
14	Y	76	
15	Z	78	
16	a	2904	
17	0	55	
18	1	46	
19	2	65	
20	B	241	
21	C	233	
22	D	206	
23	E	167	
24	F	135	
25	G	179	
26	H	130	
27	I	130	
28	J	103	

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Mol	Chain	Length	Quality of chain
29	M	118	
30	N	101	
31	O	89	
32	P	82	
33	Q	84	
34	R	75	
35	S	92	
36	T	87	
37	U	71	
38	X	10	
39	f	179	
40	g	177	
41	h	149	
42	i	142	
43	j	123	
44	k	144	
45	n	117	
46	o	115	
47	p	118	
48	q	103	
49	r	110	
50	s	100	
51	u	94	
52	v	85	
53	w	78	

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Mol	Chain	Length	Quality of chain
54	x	63	<div><div></div><div>97%</div><div></div></div>
55	y	59	<div><div></div><div>98%</div><div></div></div>

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148229 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 Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 3 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 9 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 11 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 12 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 13 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	1519	Total	C	N	O	P	0	0
			32610	14551	5983	10557	1519		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	C	A	engineered mutation	GB 2971391267
A	1262	U	C	engineered mutation	GB 2971391267

- Molecule 14 is a RNA chain called A-site Val-tRNA<sup>Val</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Y	72	Total	C	N	O	P	S	0	0
			1539	689	280	498	71	1		

- Molecule 15 is a RNA chain called P-site tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Z	72	Total	C	N	O	P	S	0	0
			1546	690	285	498	72	1		

- Molecule 16 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	2757	Total	C	N	O	P	0	0
			59216	26422	10911	19126	2757		

- Molecule 17 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 18 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 19 is a protein called Large ribosomal subunit protein bL35.



Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 20 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 21 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 23 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 24 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 25 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 26 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 27 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 28 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 29 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 30 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 31 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 32 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 34 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 35 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 37 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	X	10	Total	C	N	O	P	0	0
			216	97	41	68	10		

- Molecule 39 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 41 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 42 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 43 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 44 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	116	Total	C	N	O	S	0	0
			892	552	178	162			

- Molecule 46 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	p	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 48 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 50 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 55 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	b	7	Total	Mg	0
			7	7	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	44	Total	Mg	0
			44	44	
57	Z	1	Total	Mg	0
			1	1	
57	a	182	Total	Mg	0
			182	182	
57	p	1	Total	Mg	0
			1	1	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

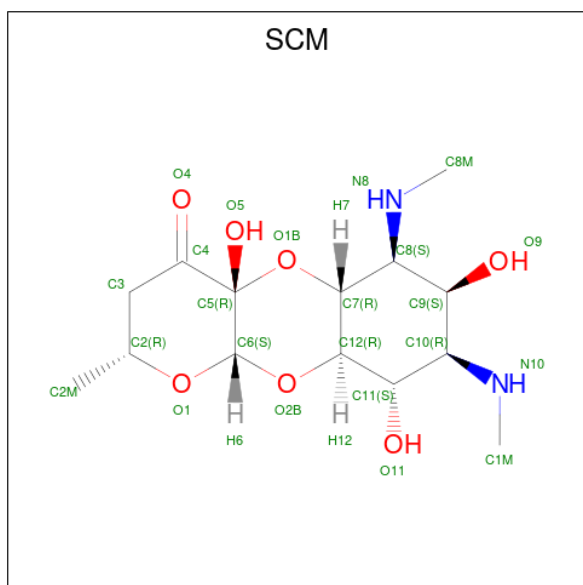
Mol	Chain	Residues	Atoms		AltConf
58	c	3	Total	K	0
			3	3	

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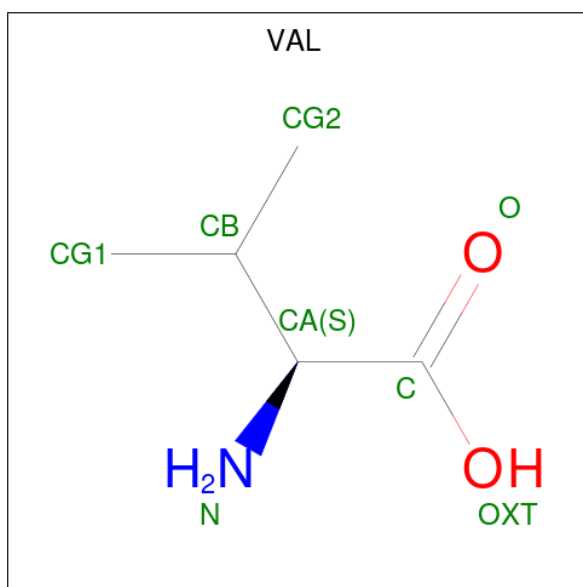
Mol	Chain	Residues	Atoms		AltConf
58	A	21	Total	K	0
			21	21	
58	a	85	Total	K	0
			85	85	

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula:  $C_{14}H_{24}N_2O_7$ ).



Mol	Chain	Residues	Atoms				AltConf
59	A	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 60 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
60	Y	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	3	5	Total	O	0
			5	5	
61	K	13	Total	O	0
			13	13	
61	L	17	Total	O	0
			17	17	
61	b	87	Total	O	0
			87	87	
61	c	78	Total	O	0
			78	78	
61	d	51	Total	O	0
			51	51	
61	e	52	Total	O	0
			52	52	
61	l	26	Total	O	0
			26	26	
61	m	21	Total	O	0
			21	21	
61	t	9	Total	O	0
			9	9	
61	z	26	Total	O	0
			26	26	

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Mol	Chain	Residues	Atoms		AltConf
61	4	1	Total 1	O 1	0
61	A	1120	Total 1120	O 1120	0
61	Y	25	Total 25	O 25	0
61	Z	21	Total 21	O 21	0
61	a	3543	Total 3543	O 3543	0
61	0	8	Total 8	O 8	0
61	1	9	Total 9	O 9	0
61	2	17	Total 17	O 17	0
61	B	9	Total 9	O 9	0
61	C	10	Total 10	O 10	0
61	D	22	Total 22	O 22	0
61	E	9	Total 9	O 9	0
61	F	4	Total 4	O 4	0
61	G	3	Total 3	O 3	0
61	H	15	Total 15	O 15	0
61	I	1	Total 1	O 1	0
61	J	14	Total 14	O 14	0
61	M	6	Total 6	O 6	0
61	N	10	Total 10	O 10	0
61	O	5	Total 5	O 5	0
61	P	7	Total 7	O 7	0

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Mol	Chain	Residues	Atoms		AltConf
61	Q	5	Total 5	O 5	0
61	R	2	Total 2	O 2	0
61	S	3	Total 3	O 3	0
61	T	1	Total 1	O 1	0
61	U	10	Total 10	O 10	0
61	X	8	Total 8	O 8	0
61	f	5	Total 5	O 5	0
61	g	6	Total 6	O 6	0
61	h	8	Total 8	O 8	0
61	i	17	Total 17	O 17	0
61	j	19	Total 19	O 19	0
61	k	38	Total 38	O 38	0
61	n	11	Total 11	O 11	0
61	o	19	Total 19	O 19	0
61	p	34	Total 34	O 34	0
61	q	28	Total 28	O 28	0
61	r	31	Total 31	O 31	0
61	s	12	Total 12	O 12	0
61	u	13	Total 13	O 13	0
61	v	19	Total 19	O 19	0
61	w	16	Total 16	O 16	0

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Mol	Chain	Residues	Atoms		AltConf
61	x	7	Total	O	0
			7	7	
61	y	8	Total	O	0
			8	8	

### 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.

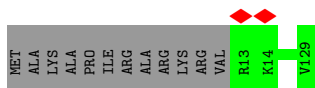
- Molecule 1: Large ribosomal subunit protein bL36A

Chain 3:  89% 11%



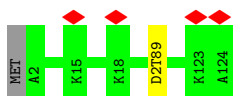
- Molecule 2: Small ribosomal subunit protein uS11

Chain K:  91% 9%




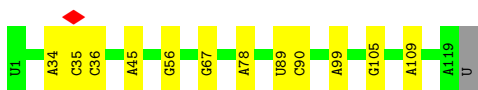
- Molecule 3: Small ribosomal subunit protein uS12

Chain L:  98% ..



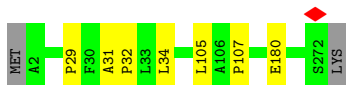
- Molecule 4: 5S rRNA

Chain b:  89% 10% .



- Molecule 5: Large ribosomal subunit protein uL2

Chain c:  97% ..



- Molecule 6: Large ribosomal subunit protein uL3

Chain d:  97%



- Molecule 7: Large ribosomal subunit protein uL4

Chain e:  98%



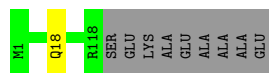
- Molecule 8: Large ribosomal subunit protein uL16

Chain l:  96%



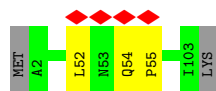
- Molecule 9: Large ribosomal subunit protein bL17

Chain m:  92% 7%



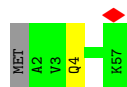
- Molecule 10: Large ribosomal subunit protein uL24

Chain t:  95%




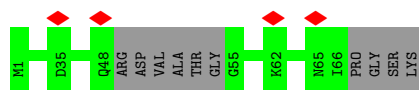
- Molecule 11: Large ribosomal subunit protein bL32

Chain z:  96%

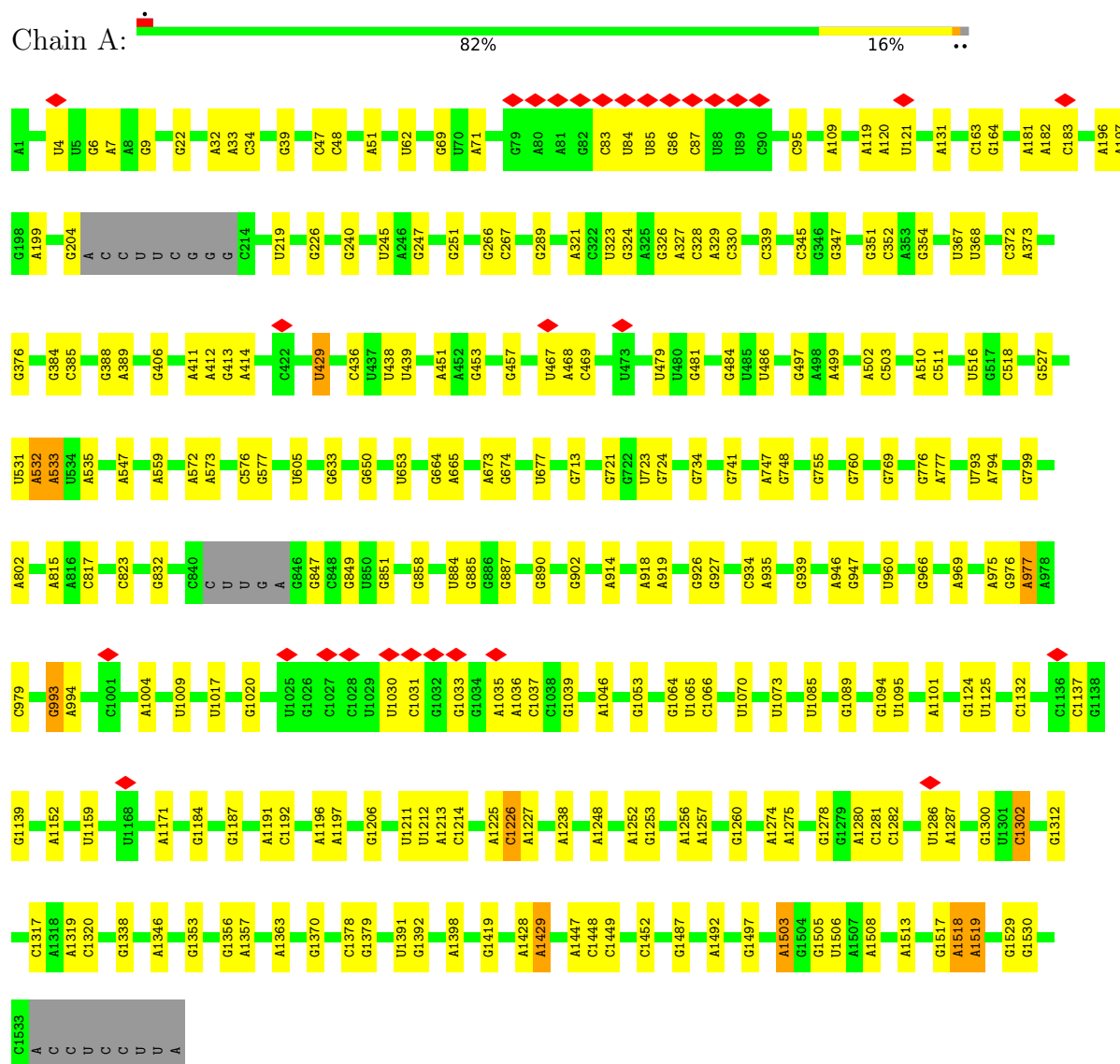


- Molecule 12: Large ribosomal subunit protein bL31

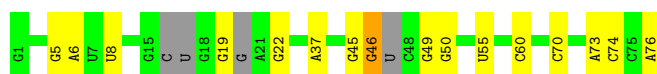
Chain 4:  6% 86% 14%



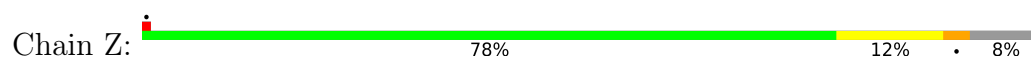
• Molecule 13: 16S rRNA



• Molecule 14: A-site Val-tRNA<sup>Val</sup>



• Molecule 15: P-site tRNA<sup>fMet</sup>

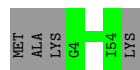






- Molecule 17: Large ribosomal subunit protein bL33

Chain 0: 93% 7%



- Molecule 18: Large ribosomal subunit protein bL34

Chain 1: 96% 4%



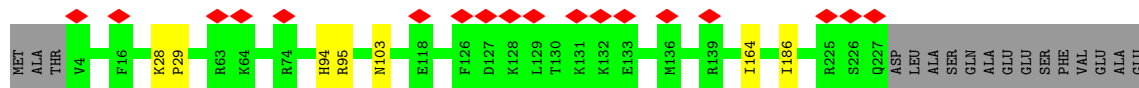
- Molecule 19: Large ribosomal subunit protein bL35

Chain 2: 92% 6%



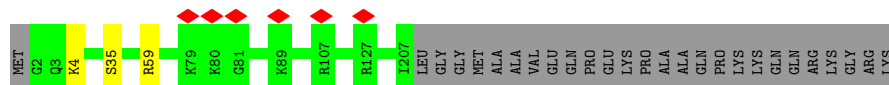
- Molecule 20: Small ribosomal subunit protein uS2

Chain B: 90% 7%



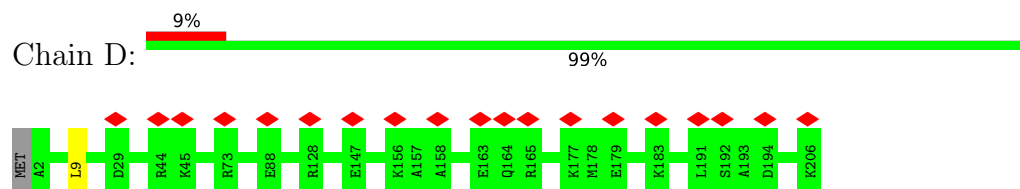
- Molecule 21: Small ribosomal subunit protein uS3

Chain C: 87% 12%

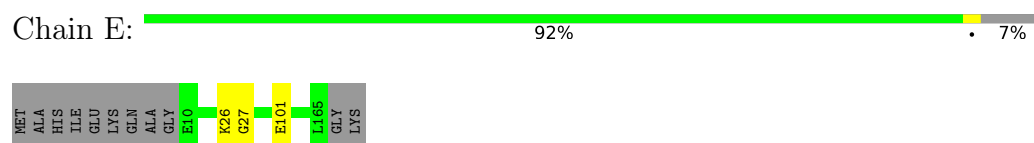




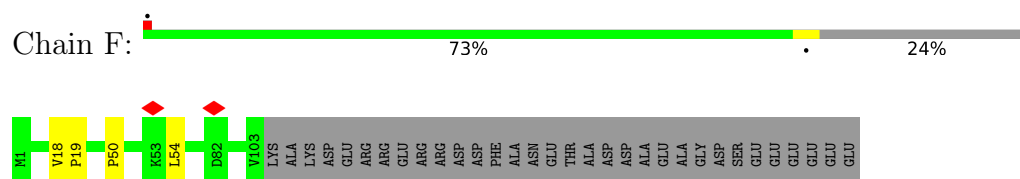
- Molecule 22: Small ribosomal subunit protein uS4



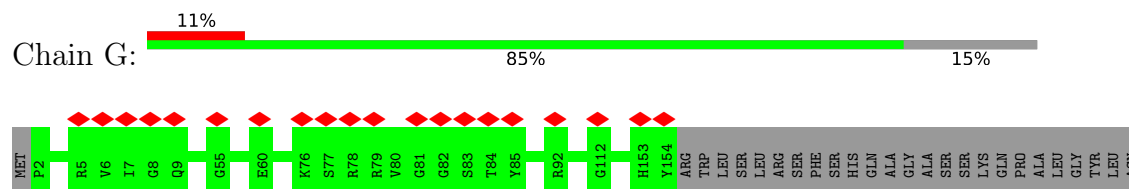
- Molecule 23: Small ribosomal subunit protein uS5



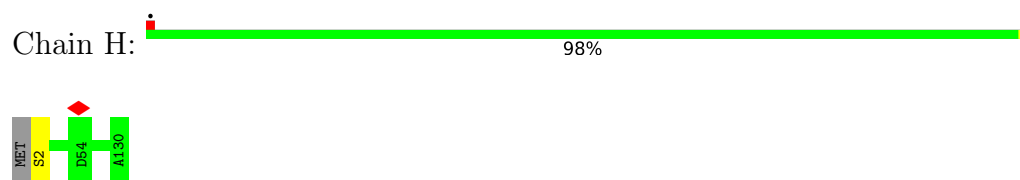
- Molecule 24: Small ribosomal subunit protein bS6, fully modified isoform



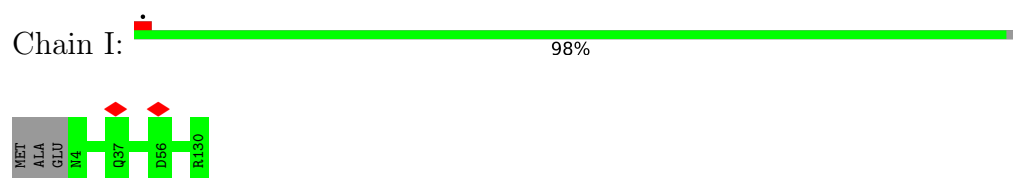
- Molecule 25: Small ribosomal subunit protein uS7



- Molecule 26: Small ribosomal subunit protein uS8



- Molecule 27: Small ribosomal subunit protein uS9

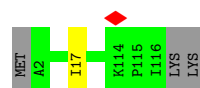


- Molecule 28: Small ribosomal subunit protein uS10

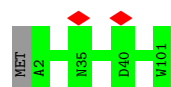




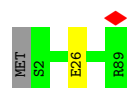
- Molecule 29: Small ribosomal subunit protein uS13



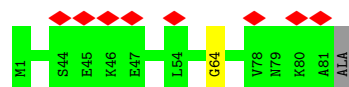
- Molecule 30: Small ribosomal subunit protein uS14



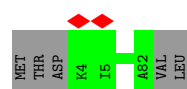
- Molecule 31: Small ribosomal subunit protein uS15



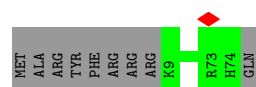
- Molecule 32: Small ribosomal subunit protein bS16




- Molecule 33: Small ribosomal subunit protein uS17

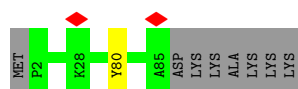


- Molecule 34: Small ribosomal subunit protein bS18



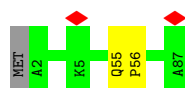
- Molecule 35: Small ribosomal subunit protein uS19

Chain S:  90% 9%



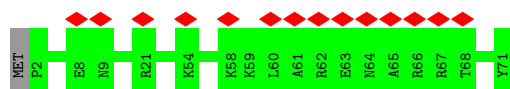
- Molecule 36: Small ribosomal subunit protein bS20

Chain T:  97% ..




- Molecule 37: Small ribosomal subunit protein bS21

Chain U:  20% 99% ..



- Molecule 38: mRNA

Chain X:  90% 10%



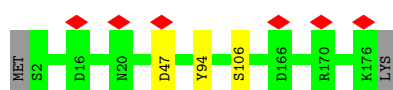
- Molecule 39: Large ribosomal subunit protein uL5

Chain f:  98% ..



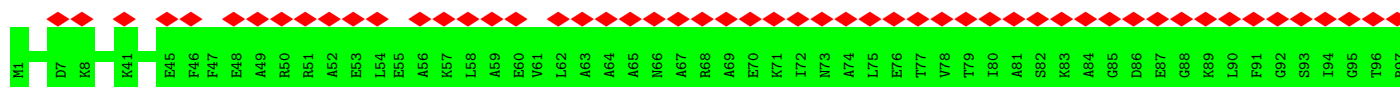
- Molecule 40: Large ribosomal subunit protein uL6

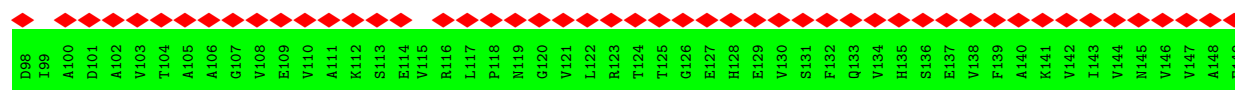
Chain g:  97% ..



- Molecule 41: Large ribosomal subunit protein bL9

Chain h:  69% 100%





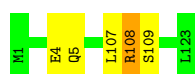
- Molecule 42: Large ribosomal subunit protein uL13

Chain i: 97%



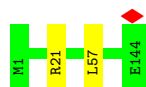
- Molecule 43: Large ribosomal subunit protein uL14

Chain j: 96%



- Molecule 44: Large ribosomal subunit protein uL15

Chain k: 99%



- Molecule 45: Large ribosomal subunit protein uL18

Chain n: 99%



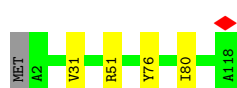
- Molecule 46: Large ribosomal subunit protein bL19

Chain o: 98%



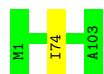
- Molecule 47: Large ribosomal subunit protein bL20

Chain p: 96%



- Molecule 48: Large ribosomal subunit protein bL21

Chain q:  99%



- Molecule 49: Large ribosomal subunit protein uL22

Chain r:  100%



- Molecule 50: Large ribosomal subunit protein uL23

Chain s:  93% 7%



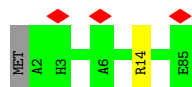
- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  100%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  98%



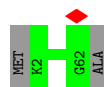
- Molecule 53: Large ribosomal subunit protein bL28

Chain w:  96%



- Molecule 54: Large ribosomal subunit protein uL29

Chain x:  97%



- Molecule 55: Large ribosomal subunit protein uL30

Chain y:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34748	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 ( $e^-/\text{\AA}^2$ )	49.88	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.859	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0748	Depositor
Map size (Å)	436.32, 436.32, 436.32	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7575, 0.7575, 0.7575	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MG, MS6, SCM, ZN, 1MG, OMG, D2T, 2MA, K, OMU, 5MC, 4D4, IAS, 6MZ, G7M, OMC, 4SU, MA6, MEQ, PSU, 2MG, H2U, 5MU, 4OC, 3TD

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	3	0.49	0/303	0.82	0/397
2	K	0.51	0/884	0.83	0/1191
3	L	0.47	0/960	0.83	0/1286
4	b	0.52	0/2850	0.79	0/4444
5	c	0.48	0/2121	0.84	0/2852
6	d	0.46	0/1576	0.79	0/2119
7	e	0.44	0/1571	0.86	0/2113
8	l	0.46	0/1073	0.84	0/1433
9	m	0.45	0/958	0.89	0/1281
10	t	0.47	0/787	0.78	0/1051
11	z	0.48	0/450	0.88	0/599
12	4	0.46	0/488	0.85	0/649
13	A	0.52	0/36233	0.79	0/56515
14	Y	0.56	1/1596 (0.1%)	0.79	0/2478
15	Z	0.57	1/1608 (0.1%)	0.77	0/2500
16	a	0.50	0/65747	0.81	7/102563 (0.0%)
17	0	0.46	0/424	0.80	0/565
18	1	0.47	0/380	0.91	0/498
19	2	0.49	0/513	0.90	0/676
20	B	0.46	0/1784	0.91	0/2403
21	C	0.46	0/1651	0.84	0/2225
22	D	0.44	0/1665	0.90	0/2227
23	E	0.47	0/1165	0.84	0/1568
24	F	0.45	0/858	0.84	0/1160
25	G	0.46	0/1219	0.93	0/1635
26	H	0.46	0/989	0.86	0/1326
27	I	0.46	0/1034	0.89	0/1375
28	J	0.45	0/796	0.86	0/1077
29	M	0.47	0/900	0.94	0/1204
30	N	0.47	0/817	0.91	0/1088
31	O	0.43	0/722	0.97	0/964



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	P	0.47	0/653	0.84	0/877
33	Q	0.46	0/650	0.82	0/871
34	R	0.45	0/553	0.93	0/742
35	S	0.49	0/685	0.84	0/922
36	T	0.46	0/676	0.99	0/895
37	U	0.46	0/598	0.96	0/792
38	X	0.54	0/242	0.80	0/375
39	f	0.45	0/1434	0.89	0/1926
40	g	0.47	0/1333	0.84	0/1805
41	h	0.46	0/1122	0.82	0/1515
42	i	0.45	0/1152	0.84	0/1551
43	j	0.45	0/956	0.82	0/1279
44	k	0.47	0/1062	0.83	0/1413
45	n	0.46	0/902	0.90	0/1209
46	o	0.46	0/929	0.77	0/1242
47	p	0.44	0/960	0.93	0/1278
48	q	0.45	0/829	0.72	0/1107
49	r	0.46	0/864	0.87	0/1156
50	s	0.44	0/744	0.80	0/994
51	u	0.45	0/766	0.81	0/1025
52	v	0.46	0/642	0.80	0/848
53	w	0.46	0/635	0.85	0/848
54	x	0.41	0/496	0.92	0/660
55	y	0.46	0/453	0.86	0/605
All	All	0.50	2/153458 (0.0%)	0.82	7/229397 (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
19	2	0	1
52	v	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Y	8	4SU	O3'-P	5.05	1.61	1.56
15	Z	8	4SU	O3'-P	5.00	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	2546	U	O3'-P-O5'	-7.27	93.09	104.00
16	a	1905	C	O3'-P-O5'	-6.76	93.85	104.00
16	a	2519	U	O3'-P-O5'	-6.12	94.83	104.00
16	a	2501	C	O3'-P-O5'	-5.70	95.46	104.00
16	a	2601	C	O3'-P-O5'	-5.32	96.02	104.00
16	a	781	A	O3'-P-O5'	-5.26	96.12	104.00
16	a	1186	G	O3'-P-O5'	-5.22	96.17	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	2	13	ARG	Sidechain
52	v	14	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	302	0	340	2	0
2	K	877	0	884	0	0
3	L	957	0	1017	0	0
4	b	2549	0	1291	1	0
5	c	2082	0	2153	4	0
6	d	1566	0	1618	4	0
7	e	1552	0	1619	4	0
8	l	1075	0	1145	3	0
9	m	945	0	989	1	0
10	t	779	0	830	1	0
11	z	444	0	458	1	0
12	4	480	0	478	0	0
13	A	32610	0	16428	33	0
14	Y	1539	0	791	2	0
15	Z	1546	0	794	2	0
16	a	59216	0	29780	96	0
17	0	417	0	451	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	1	377	0	417	2	0
19	2	504	0	572	2	0
20	B	1753	0	1780	4	0
21	C	1624	0	1696	2	0
22	D	1643	0	1707	1	0
23	E	1152	0	1196	1	0
24	F	839	0	833	2	0
25	G	1203	0	1254	0	0
26	H	979	0	1031	1	0
27	I	1022	0	1070	0	0
28	J	786	0	828	1	0
29	M	891	0	952	1	0
30	N	805	0	844	0	0
31	O	714	0	734	0	0
32	P	643	0	661	0	0
33	Q	641	0	682	0	0
34	R	544	0	565	0	0
35	S	668	0	693	1	0
36	T	670	0	719	1	0
37	U	590	0	629	0	0
38	X	216	0	108	0	0
39	f	1410	0	1444	1	0
40	g	1313	0	1358	1	0
41	h	1111	0	1148	0	0
42	i	1129	0	1162	2	0
43	j	947	0	1023	3	0
44	k	1053	0	1129	2	0
45	n	892	0	923	0	0
46	o	917	0	962	1	0
47	p	947	0	1019	3	0
48	q	816	0	839	1	0
49	r	857	0	922	0	0
50	s	738	0	807	0	0
51	u	753	0	780	0	0
52	v	634	0	653	0	0
53	w	625	0	652	1	0
54	x	495	0	526	0	0
55	y	449	0	488	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	44	0	0	0	0
57	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	a	182	0	0	0	0
57	b	7	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	p	1	0	0	0	0
57	z	1	0	0	0	0
58	A	21	0	0	0	0
58	a	85	0	0	0	0
58	c	3	0	0	0	0
59	A	23	0	24	4	0
60	Y	7	0	8	2	0
61	0	8	0	0	0	0
61	1	9	0	0	0	0
61	2	17	0	0	0	0
61	3	5	0	0	0	0
61	4	1	0	0	0	0
61	A	1120	0	0	0	0
61	B	9	0	0	0	0
61	C	10	0	0	0	0
61	D	22	0	0	0	0
61	E	9	0	0	0	0
61	F	4	0	0	0	0
61	G	3	0	0	0	0
61	H	15	0	0	0	0
61	I	1	0	0	0	0
61	J	14	0	0	0	0
61	K	13	0	0	0	0
61	L	17	0	0	0	0
61	M	6	0	0	0	0
61	N	10	0	0	0	0
61	O	5	0	0	0	0
61	P	7	0	0	0	0
61	Q	5	0	0	0	0
61	R	2	0	0	0	0
61	S	3	0	0	0	0
61	T	1	0	0	0	0
61	U	10	0	0	0	0
61	X	8	0	0	0	0
61	Y	25	0	0	0	0
61	Z	21	0	0	0	0
61	a	3543	0	0	5	0
61	b	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	c	78	0	0	0	0
61	d	51	0	0	0	0
61	e	52	0	0	0	0
61	f	5	0	0	0	0
61	g	6	0	0	0	0
61	h	8	0	0	0	0
61	i	17	0	0	0	0
61	j	19	0	0	0	0
61	k	38	0	0	0	0
61	l	26	0	0	0	0
61	m	21	0	0	0	0
61	n	11	0	0	0	0
61	o	19	0	0	0	0
61	p	34	0	0	0	0
61	q	28	0	0	0	0
61	r	31	0	0	0	0
61	s	12	0	0	0	0
61	t	9	0	0	0	0
61	u	13	0	0	0	0
61	v	19	0	0	0	0
61	w	16	0	0	0	0
61	x	7	0	0	0	0
61	y	8	0	0	0	0
61	z	26	0	0	0	0
All	All	148229	0	95904	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:12:U:H2'	16:a:12:U:O2	1.92	0.70
16:a:568:U:H1'	16:a:2030:6MZ:H9C1	1.75	0.68
13:A:1391:U:H2'	13:A:1392:G:C8	2.37	0.60
60:Y:101:VAL:N	15:Z:76:A:HO3'	1.99	0.60
13:A:769:G:H4'	13:A:1513:A:H4'	1.85	0.58
20:B:94:HIS:O	20:B:95:ARG:C	2.48	0.56
16:a:12:U:O2	16:a:12:U:C2'	2.54	0.56
13:A:823:C:HO2'	26:H:2:SER:N	2.03	0.56
8:l:66:ARG:NH2	8:l:104:GLU:OE2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1066:C:O2	59:A:1601:SCM:N10	2.36	0.55
16:a:1115:G:O2'	16:a:1116:G:O5'	2.24	0.55
13:A:1064:G:N7	59:A:1601:SCM:O11	2.33	0.54
13:A:502:A:H2'	13:A:503:C:O4'	2.08	0.54
8:l:79:ALA:HA	16:a:2494:G:O2'	2.07	0.54
13:A:1191:A:OP1	21:C:4:LYS:NZ	2.39	0.54
59:A:1601:SCM:H2M1	23:E:27:GLY:HA2	1.89	0.53
16:a:1778:U:H2'	16:a:1784:A:N6	2.24	0.53
13:A:533:A:O2'	13:A:535:A:OP2	2.26	0.53
13:A:376:G:C2	13:A:389:A:C2	2.97	0.53
16:a:210:C:OP1	18:1:29:GLN:NE2	2.41	0.52
16:a:2273:A:H2'	16:a:2274:A:C8	2.44	0.52
13:A:664:G:H22	13:A:741:G:H1	1.57	0.52
13:A:1192:C:N3	59:A:1601:SCM:O5	2.37	0.52
16:a:84:A:N1	16:a:98:G:O2'	2.41	0.51
16:a:620:G:H5'	16:a:620:G:N3	2.26	0.51
16:a:2243:U:H2'	16:a:2244:U:C6	2.46	0.51
19:2:54:ASP:HB3	44:k:57:LEU:HD22	1.94	0.50
16:a:1939:5MU:OP1	16:a:2604:PSU:O2'	2.28	0.49
16:a:2547:A:H2'	16:a:2548:U:C6	2.47	0.49
60:Y:101:VAL:HG11	16:a:2452:C:O4'	2.12	0.49
16:a:811:U:H2'	44:k:21:ARG:HA	1.94	0.49
16:a:2062:A:N7	16:a:2503:2MA:N6	2.61	0.49
8:l:53:MET:HE1	8:l:103:TYR:CG	2.47	0.49
6:d:62:LYS:N	6:d:63:PRO:HD2	2.28	0.49
20:B:164:ILE:O	20:B:186:ILE:HB	2.13	0.48
16:a:451:U:H5''	61:a:3327:HOH:O	2.13	0.48
16:a:1434:A:H2'	16:a:1435:G:C8	2.49	0.48
16:a:1183:U:H2'	16:a:1184:U:C6	2.48	0.48
16:a:2756:U:H1'	16:a:2757:A:H5''	1.96	0.48
42:i:125:TYR:OH	42:i:132:HIS:NE2	2.44	0.48
16:a:120:U:H5''	16:a:122:G:OP2	2.13	0.48
16:a:747:5MU:O2	16:a:2014:A:H1'	2.13	0.48
39:f:62:GLY:O	39:f:95:ARG:NH1	2.47	0.47
16:a:1338:G:O2'	16:a:1393:A:N1	2.44	0.47
16:a:857:G:H2'	16:a:858:G:O4'	2.14	0.47
13:A:677:U:H3	13:A:713:G:H22	1.62	0.47
16:a:2328:A:H2'	16:a:2329:U:C6	2.50	0.47
43:j:107:LEU:O	43:j:109:SER:N	2.48	0.47
16:a:2291:U:H2'	16:a:2292:U:C6	2.49	0.47
13:A:1428:A:H2'	13:A:1429:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:29:PRO:HG2	5:c:34:LEU:HD11	1.97	0.46
7:e:76:PRO:HG2	61:a:3846:HOH:O	2.15	0.46
16:a:1881:C:H2'	16:a:1882:U:O4'	2.15	0.46
16:a:1932:A:H2'	16:a:1933:G:O4'	2.15	0.46
16:a:2327:A:H2'	16:a:2328:A:C8	2.51	0.46
16:a:1026:G:H2'	16:a:1027:A:C8	2.50	0.46
6:d:83:ARG:NH1	16:a:2638:G:OP2	2.49	0.46
48:q:74:ILE:N	48:q:74:ILE:HD12	2.31	0.46
9:m:18:GLN:NE2	16:a:2709:G:OP1	2.49	0.45
16:a:263:G:H2'	16:a:264:C:O4'	2.16	0.45
20:B:28:LYS:N	20:B:29:PRO:CD	2.79	0.45
16:a:1370:C:H2'	16:a:1371:G:O4'	2.16	0.45
16:a:493:G:H2'	16:a:494:G:O4'	2.17	0.45
13:A:1518:MA6:H103	13:A:1519:MA6:H102	1.99	0.45
16:a:2780:G:OP2	42:i:120:ARG:HD3	2.16	0.45
16:a:299:A:N1	16:a:322:A:O2'	2.45	0.45
16:a:1808:A:H3'	16:a:1809:A:C8	2.51	0.45
16:a:1003:G:O2'	16:a:1010:A:N1	2.47	0.45
16:a:2552:OMU:HM23	16:a:2554:U:C6	2.52	0.45
13:A:109:A:C6	13:A:326:G:C6	3.04	0.45
16:a:1405:U:H2'	16:a:1406:U:C6	2.53	0.44
16:a:278:A:O2'	16:a:279:A:P	2.76	0.44
16:a:1378:A:O2'	16:a:1380:G:N7	2.50	0.44
16:a:580:U:O3'	47:p:31:VAL:HG13	2.18	0.44
16:a:1604:C:O2'	16:a:1610:A:N1	2.46	0.44
13:A:993:G:H2'	13:A:993:G:N3	2.33	0.44
16:a:2038:G:H2'	16:a:2039:U:O4'	2.18	0.44
16:a:1188:U:O2'	16:a:1189:A:H5'	2.18	0.44
16:a:1223:G:C6	16:a:1227:G:C6	3.06	0.44
19:2:27:ALA:O	19:2:28:ASN:HB2	2.17	0.44
24:F:18:VAL:HB	24:F:19:PRO:HD3	2.00	0.44
16:a:1637:A:H5'	16:a:1760:C:O2'	2.17	0.44
16:a:26:G:H1'	16:a:514:A:N6	2.33	0.43
16:a:1394:U:H4'	16:a:1603:A:H4'	2.00	0.43
16:a:2591:C:H2'	16:a:2592:G:C8	2.54	0.43
16:a:247:G:H4'	16:a:386:G:C5	2.53	0.43
16:a:1607:C:H4'	16:a:1608:A:O5'	2.18	0.43
5:c:180:GLU:OE2	16:a:1799:G:O2'	2.34	0.43
16:a:1021:A:N3	16:a:1021:A:H3'	2.33	0.43
16:a:655:A:H4'	16:a:656:G:H5'	1.99	0.43
16:a:819:A:C4	16:a:1189:A:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:2850:A:N7	16:a:2868:A:O2'	2.47	0.43
13:A:927:G:O2'	13:A:1503:A:N7	2.46	0.43
16:a:1421:G:C2	16:a:1422:G:C8	3.07	0.43
43:j:107:LEU:O	43:j:108:ARG:C	2.61	0.43
13:A:1252:A:H2'	13:A:1253:G:O4'	2.19	0.42
16:a:1028:A:N6	16:a:1125:G:H2'	2.33	0.42
36:T:55:GLN:N	36:T:56:PRO:HD2	2.34	0.42
13:A:429:U:H3'	22:D:9:LEU:HD12	2.01	0.42
46:o:102:GLU:N	46:o:102:GLU:OE1	2.52	0.42
10:t:54:GLN:N	10:t:55:PRO:HD2	2.35	0.42
13:A:946:A:H2'	13:A:947:G:C8	2.54	0.42
16:a:586:A:N1	16:a:809:G:O2'	2.41	0.42
16:a:700:G:O2'	16:a:1632:A:N3	2.50	0.42
16:a:1141:U:H4'	16:a:1142:A:O4'	2.19	0.42
16:a:2233:U:H2'	16:a:2234:G:C8	2.55	0.42
7:e:49:ARG:HG3	61:a:3995:HOH:O	2.18	0.42
13:A:503:C:O2'	13:A:510:A:N1	2.49	0.42
14:Y:37:6MZ:O2'	16:a:1913:A:N1	2.49	0.42
13:A:1073:U:O2'	20:B:103:ASN:ND2	2.52	0.42
14:Y:76:A:N1	16:a:2583:G:O2'	2.50	0.42
16:a:323:C:C4	16:a:333:G:C8	3.07	0.42
7:e:41:GLN:HG2	7:e:43:THR:HG23	2.00	0.42
16:a:672:C:H4'	61:a:3846:HOH:O	2.18	0.42
6:d:152:PRO:HG3	6:d:156:PHE:CZ	2.54	0.42
16:a:993:G:OP2	47:p:51:ARG:NH1	2.50	0.42
16:a:468:G:N7	18:l:39:ARG:NH1	2.55	0.42
16:a:607:U:O4	16:a:620:G:H5''	2.19	0.42
16:a:1386:C:H2'	16:a:1387:A:C8	2.55	0.42
13:A:323:U:H2'	13:A:324:G:O4'	2.20	0.42
16:a:749:A:H4'	16:a:1271:G:N3	2.35	0.42
16:a:2849:U:H4'	16:a:2868:A:C2	2.55	0.42
16:a:1859:U:H2'	16:a:1860:G:C8	2.55	0.41
16:a:56:A:H2'	16:a:57:C:O4'	2.19	0.41
16:a:566:U:H2'	16:a:567:U:O4'	2.20	0.41
24:F:50:PRO:HA	24:F:54:LEU:O	2.19	0.41
11:z:4:GLN:HA	16:a:2615:U:C2	2.56	0.41
16:a:639:U:H2'	16:a:640:C:C6	2.55	0.41
16:a:2522:U:O2'	16:a:2647:U:OP1	2.35	0.41
13:A:977:A:O2'	13:A:979:C:OP2	2.31	0.41
13:A:1152:A:OP1	28:J:70:HIS:ND1	2.49	0.41
16:a:1026:G:H2'	16:a:1027:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:162:ARG:NH1	16:a:340:A:O2'	2.54	0.41
13:A:532:A:N6	13:A:1206:G:O2'	2.51	0.41
13:A:673:A:H2'	13:A:674:G:C8	2.56	0.41
16:a:948:C:H1'	16:a:984:A:C8	2.55	0.41
16:a:1829:A:H4'	61:a:4253:HOH:O	2.19	0.41
13:A:918:A:H2'	13:A:919:A:O4'	2.21	0.41
16:a:36:G:N3	16:a:450:G:O2'	2.51	0.41
16:a:458:G:O2'	16:a:469:G:O6	2.39	0.41
47:p:76:TYR:CZ	47:p:80:ILE:HG13	2.56	0.41
4:b:78:A:C2	4:b:99:A:C4	3.08	0.41
16:a:565:C:H2'	16:a:566:U:O4'	2.21	0.41
40:g:94:TYR:HA	40:g:106:SER:O	2.21	0.41
13:A:33:A:H2'	13:A:34:C:C6	2.56	0.41
16:a:2627:G:O2'	16:a:2781:A:N1	2.46	0.41
53:w:3:ARG:O	53:w:12:PRO:HD3	2.21	0.41
1:3:36:ARG:NH2	1:3:37:GLN:O	2.53	0.41
5:c:31:ALA:N	5:c:32:PRO:CD	2.83	0.41
13:A:1302:C:C5	29:M:17:ILE:HG13	2.56	0.41
16:a:374:A:C2	16:a:401:A:C4	3.08	0.41
1:3:16:ILE:HD13	1:3:25:VAL:HG22	2.02	0.41
5:c:105:LEU:O	5:c:107:PRO:HD3	2.21	0.41
13:A:62:U:OP1	13:A:385:C:O2'	2.40	0.40
13:A:1356:G:H2'	13:A:1357:A:C8	2.55	0.40
15:Z:12:G:H5''	16:a:1908:C:O2'	2.20	0.40
43:j:4:GLU:O	43:j:5:GLN:HB2	2.21	0.40
16:a:644:A:H2'	16:a:645:C:O4'	2.21	0.40
16:a:1357:C:H2'	16:a:1358:G:O4'	2.21	0.40
6:d:135:GLY:HA2	16:a:743:A:OP1	2.21	0.40
16:a:1266:G:O2'	16:a:2012:G:O6	2.28	0.40
21:C:35:SER:OG	21:C:59:ARG:NH1	2.54	0.40
13:A:1226:C:H4'	35:S:80:TYR:CZ	2.56	0.40
16:a:1182:G:H2'	16:a:1183:U:O4'	2.21	0.40

There are no symmetry-related clashes.

## 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	3	36/38 (95%)	36 (100%)	0	0	100	100
2	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
3	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
5	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
6	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
7	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
8	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
9	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
10	t	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
11	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
12	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
17	0	49/55 (89%)	49 (100%)	0	0	100	100
18	1	44/46 (96%)	44 (100%)	0	0	100	100
19	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
20	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
21	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
22	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
23	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
24	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
25	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
26	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
27	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
28	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	8
29	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
30	N	98/101 (97%)	98 (100%)	0	0	100	100
31	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
32	P	79/82 (96%)	75 (95%)	3 (4%)	1 (1%)	9	5
33	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
34	R	64/75 (85%)	64 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
36	T	84/87 (97%)	84 (100%)	0	0	100	100
37	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
39	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
40	g	173/177 (98%)	165 (95%)	7 (4%)	1 (1%)	21	15
41	h	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
42	i	140/142 (99%)	140 (100%)	0	0	100	100
43	j	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	16	10
44	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
45	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
46	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
47	p	115/118 (98%)	115 (100%)	0	0	100	100
48	q	101/103 (98%)	101 (100%)	0	0	100	100
49	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
50	s	91/100 (91%)	91 (100%)	0	0	100	100
51	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
52	v	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
53	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
54	x	59/63 (94%)	59 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5593/5913 (95%)	5426 (97%)	163 (3%)	4 (0%)	49	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	J	57	VAL
43	j	108	ARG
40	g	47	ASP
32	P	64	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	34/34 (100%)	34 (100%)	0	100	100
2	K	89/98 (91%)	89 (100%)	0	100	100
3	L	102/103 (99%)	102 (100%)	0	100	100
5	c	216/218 (99%)	216 (100%)	0	100	100
6	d	163/163 (100%)	163 (100%)	0	100	100
7	e	165/165 (100%)	165 (100%)	0	100	100
8	l	107/107 (100%)	107 (100%)	0	100	100
9	m	98/103 (95%)	98 (100%)	0	100	100
10	t	83/85 (98%)	82 (99%)	1 (1%)	63	70
11	z	47/48 (98%)	47 (100%)	0	100	100
12	4	55/62 (89%)	55 (100%)	0	100	100
17	0	46/49 (94%)	46 (100%)	0	100	100
18	1	38/38 (100%)	38 (100%)	0	100	100
19	2	51/52 (98%)	51 (100%)	0	100	100
20	B	186/199 (94%)	186 (100%)	0	100	100
21	C	170/190 (90%)	170 (100%)	0	100	100
22	D	172/173 (99%)	172 (100%)	0	100	100
23	E	119/126 (94%)	117 (98%)	2 (2%)	53	60
24	F	90/116 (78%)	90 (100%)	0	100	100
25	G	126/147 (86%)	126 (100%)	0	100	100
26	H	104/105 (99%)	104 (100%)	0	100	100
27	I	105/107 (98%)	105 (100%)	0	100	100
28	J	86/90 (96%)	86 (100%)	0	100	100
29	M	93/96 (97%)	93 (100%)	0	100	100
30	N	83/84 (99%)	83 (100%)	0	100	100
31	O	76/77 (99%)	75 (99%)	1 (1%)	61	68
32	P	65/65 (100%)	65 (100%)	0	100	100
33	Q	73/78 (94%)	73 (100%)	0	100	100
34	R	57/65 (88%)	57 (100%)	0	100	100
35	S	72/79 (91%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	T	65/66 (98%)	65 (100%)	0	100	100
37	U	60/61 (98%)	60 (100%)	0	100	100
39	f	148/150 (99%)	148 (100%)	0	100	100
40	g	136/138 (99%)	136 (100%)	0	100	100
41	h	114/114 (100%)	114 (100%)	0	100	100
42	i	116/116 (100%)	115 (99%)	1 (1%)	70	77
43	j	104/104 (100%)	104 (100%)	0	100	100
44	k	103/103 (100%)	103 (100%)	0	100	100
45	n	86/87 (99%)	86 (100%)	0	100	100
46	o	99/100 (99%)	99 (100%)	0	100	100
47	p	89/90 (99%)	89 (100%)	0	100	100
48	q	84/84 (100%)	84 (100%)	0	100	100
49	r	93/93 (100%)	93 (100%)	0	100	100
50	s	80/84 (95%)	80 (100%)	0	100	100
51	u	78/78 (100%)	78 (100%)	0	100	100
52	v	62/63 (98%)	62 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
All	All	4657/4825 (96%)	4652 (100%)	5 (0%)	87	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	t	52	LEU
23	E	26	LYS
23	E	101	GLU
31	O	26	GLU
42	i	64	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	118	HIS

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Mol	Chain	Res	Type
5	c	86	ASN
5	c	197	ASN
6	d	36	GLN
6	d	185	ASN
7	e	94	GLN
7	e	136	GLN
7	e	165	HIS
8	l	22	GLN
8	l	60	GLN
8	l	97	GLN
11	z	6	ASN
12	4	65	ASN
20	B	19	GLN
20	B	58	ASN
20	B	103	ASN
21	C	139	GLN
22	D	36	GLN
22	D	40	GLN
22	D	89	ASN
23	E	82	GLN
23	E	132	ASN
24	F	3	HIS
24	F	17	GLN
24	F	46	GLN
25	G	68	ASN
25	G	130	ASN
27	I	4	ASN
27	I	126	GLN
28	J	58	ASN
30	N	60	GLN
31	O	50	HIS
32	P	26	ASN
34	R	54	GLN
36	T	20	HIS
37	U	64	ASN
40	g	22	GLN
40	g	30	ASN
40	g	73	ASN
40	g	115	HIS
41	h	66	ASN
41	h	145	ASN
42	i	47	HIS

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Mol	Chain	Res	Type
46	o	7	GLN
46	o	52	ASN
47	p	52	GLN
49	r	9	HIS
49	r	40	ASN
53	w	17	ASN
53	w	36	HIS
54	x	27	ASN
54	x	58	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	A	1516/1542 (98%)	206 (13%)	24 (1%)
14	Y	68/76 (89%)	12 (17%)	0
15	Z	68/78 (87%)	8 (11%)	0
16	a	2753/2904 (94%)	308 (11%)	0
38	X	9/10 (90%)	1 (11%)	0
4	b	118/120 (98%)	10 (8%)	0
All	All	4532/4730 (95%)	545 (12%)	24 (0%)

All (545) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	b	34	A
4	b	35	C
4	b	36	C
4	b	45	A
4	b	56	G
4	b	67	G
4	b	89	U
4	b	90	C
4	b	105	G
4	b	109	A
13	A	4	U
13	A	6	G
13	A	7	A
13	A	9	G
13	A	22	G
13	A	32	A
13	A	39	G

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Mol	Chain	Res	Type
13	A	47	C
13	A	48	C
13	A	51	A
13	A	69	G
13	A	71	A
13	A	83	C
13	A	84	U
13	A	85	U
13	A	86	G
13	A	87	C
13	A	95	C
13	A	119	A
13	A	120	A
13	A	121	U
13	A	131	A
13	A	163	C
13	A	164	G
13	A	181	A
13	A	182	A
13	A	183	C
13	A	197	A
13	A	204	G
13	A	219	U
13	A	226	G
13	A	240	G
13	A	245	U
13	A	247	G
13	A	251	G
13	A	266	G
13	A	267	C
13	A	289	G
13	A	321	A
13	A	327	A
13	A	328	C
13	A	329	A
13	A	330	C
13	A	339	C
13	A	345	C
13	A	347	G
13	A	351	G
13	A	352	C
13	A	354	G

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Mol	Chain	Res	Type
13	A	367	U
13	A	368	U
13	A	372	C
13	A	373	A
13	A	384	G
13	A	388	G
13	A	406	G
13	A	411	A
13	A	412	A
13	A	413	G
13	A	414	A
13	A	429	U
13	A	436	C
13	A	438	U
13	A	439	U
13	A	451	A
13	A	453	G
13	A	457	G
13	A	467	U
13	A	468	A
13	A	469	C
13	A	479	U
13	A	481	G
13	A	484	G
13	A	486	U
13	A	497	G
13	A	499	A
13	A	511	C
13	A	518	C
13	A	531	U
13	A	533	A
13	A	547	A
13	A	559	A
13	A	572	A
13	A	573	A
13	A	576	C
13	A	577	G
13	A	605	U
13	A	633	G
13	A	650	G
13	A	653	U
13	A	665	A

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Mol	Chain	Res	Type
13	A	721	G
13	A	723	U
13	A	724	G
13	A	734	G
13	A	747	A
13	A	748	G
13	A	755	G
13	A	760	G
13	A	777	A
13	A	793	U
13	A	794	A
13	A	799	G
13	A	802	A
13	A	815	A
13	A	817	C
13	A	832	G
13	A	847	G
13	A	849	G
13	A	851	G
13	A	884	U
13	A	885	G
13	A	887	G
13	A	890	G
13	A	902	G
13	A	914	A
13	A	926	G
13	A	934	C
13	A	935	A
13	A	939	G
13	A	960	U
13	A	966	2MG
13	A	969	A
13	A	975	A
13	A	976	G
13	A	977	A
13	A	993	G
13	A	994	A
13	A	1004	A
13	A	1009	U
13	A	1017	U
13	A	1020	G
13	A	1030	U

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Mol	Chain	Res	Type
13	A	1031	C
13	A	1033	G
13	A	1036	A
13	A	1037	C
13	A	1039	G
13	A	1046	A
13	A	1053	G
13	A	1065	U
13	A	1070	U
13	A	1085	U
13	A	1089	G
13	A	1094	G
13	A	1095	U
13	A	1101	A
13	A	1124	G
13	A	1125	U
13	A	1132	C
13	A	1137	C
13	A	1139	G
13	A	1159	U
13	A	1171	A
13	A	1184	G
13	A	1196	A
13	A	1197	A
13	A	1211	U
13	A	1212	U
13	A	1213	A
13	A	1214	C
13	A	1225	A
13	A	1226	C
13	A	1227	A
13	A	1238	A
13	A	1248	A
13	A	1256	A
13	A	1257	A
13	A	1260	G
13	A	1274	A
13	A	1275	A
13	A	1278	G
13	A	1280	A
13	A	1281	C
13	A	1282	C

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Mol	Chain	Res	Type
13	A	1286	U
13	A	1287	A
13	A	1300	G
13	A	1302	C
13	A	1312	G
13	A	1317	C
13	A	1319	A
13	A	1320	C
13	A	1338	G
13	A	1346	A
13	A	1353	G
13	A	1363	A
13	A	1370	G
13	A	1378	C
13	A	1379	G
13	A	1398	A
13	A	1419	G
13	A	1429	A
13	A	1447	A
13	A	1448	C
13	A	1449	C
13	A	1452	C
13	A	1487	G
13	A	1492	A
13	A	1497	G
13	A	1503	A
13	A	1505	G
13	A	1506	U
13	A	1517	G
13	A	1529	G
13	A	1530	G
14	Y	5	G
14	Y	6	A
14	Y	19	G
14	Y	22	G
14	Y	45	G
14	Y	46	G7M
14	Y	49	G
14	Y	50	G
14	Y	60	C
14	Y	70	C
14	Y	73	A

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Mol	Chain	Res	Type
14	Y	74	C
15	Z	9	G
15	Z	19	G
15	Z	46	G7M
15	Z	53	G
15	Z	58	A
15	Z	70	G
15	Z	71	C
15	Z	76	A
16	a	10	A
16	a	12	U
16	a	15	G
16	a	34	U
16	a	45	G
16	a	71	A
16	a	74	A
16	a	75	G
16	a	84	A
16	a	101	A
16	a	102	U
16	a	118	A
16	a	119	A
16	a	120	U
16	a	131	A
16	a	139	U
16	a	140	C
16	a	142	A
16	a	163	C
16	a	165	A
16	a	181	A
16	a	196	A
16	a	199	A
16	a	200	U
16	a	215	G
16	a	216	A
16	a	221	A
16	a	222	A
16	a	248	G
16	a	272	A
16	a	276	U
16	a	278	A
16	a	279	A

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Mol	Chain	Res	Type
16	a	282	A
16	a	287	G
16	a	288	U
16	a	289	G
16	a	310	A
16	a	311	A
16	a	330	A
16	a	361	G
16	a	386	G
16	a	404	A
16	a	405	U
16	a	411	G
16	a	412	A
16	a	451	U
16	a	481	G
16	a	491	G
16	a	503	A
16	a	504	A
16	a	505	A
16	a	509	C
16	a	530	G
16	a	531	C
16	a	532	A
16	a	533	G
16	a	545	U
16	a	547	A
16	a	548	G
16	a	549	G
16	a	563	A
16	a	573	U
16	a	574	A
16	a	575	A
16	a	586	A
16	a	603	A
16	a	615	U
16	a	627	A
16	a	637	A
16	a	645	C
16	a	646	U
16	a	647	G
16	a	653	U
16	a	654	A

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Mol	Chain	Res	Type
16	a	686	U
16	a	717	C
16	a	730	A
16	a	738	G
16	a	747	5MU
16	a	764	A
16	a	765	C
16	a	775	G
16	a	776	G
16	a	777	G
16	a	782	A
16	a	784	G
16	a	785	G
16	a	805	G
16	a	812	C
16	a	827	U
16	a	828	U
16	a	846	U
16	a	847	U
16	a	858	G
16	a	859	G
16	a	869	G
16	a	877	A
16	a	883	G
16	a	888	C
16	a	890	C
16	a	891	G
16	a	895	U
16	a	896	A
16	a	897	C
16	a	905	A
16	a	910	A
16	a	914	G
16	a	915	C
16	a	927	A
16	a	931	U
16	a	946	C
16	a	961	C
16	a	974	G
16	a	983	A
16	a	984	A
16	a	985	C

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Mol	Chain	Res	Type
16	a	996	A
16	a	1012	U
16	a	1013	C
16	a	1022	G
16	a	1033	U
16	a	1040	A
16	a	1047	G
16	a	1108	U
16	a	1110	G
16	a	1111	A
16	a	1112	G
16	a	1116	G
16	a	1128	G
16	a	1129	A
16	a	1132	U
16	a	1133	A
16	a	1134	A
16	a	1135	C
16	a	1142	A
16	a	1172	C
16	a	1187	G
16	a	1188	U
16	a	1253	A
16	a	1256	G
16	a	1271	G
16	a	1272	A
16	a	1273	U
16	a	1286	A
16	a	1287	A
16	a	1300	G
16	a	1301	A
16	a	1303	G
16	a	1352	U
16	a	1365	A
16	a	1379	U
16	a	1383	A
16	a	1386	C
16	a	1416	G
16	a	1420	A
16	a	1428	C
16	a	1452	G
16	a	1453	A

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Mol	Chain	Res	Type
16	a	1458	U
16	a	1482	G
16	a	1490	A
16	a	1493	C
16	a	1497	U
16	a	1498	C
16	a	1508	A
16	a	1509	A
16	a	1515	A
16	a	1529	G
16	a	1535	A
16	a	1536	C
16	a	1537	G
16	a	1569	A
16	a	1578	U
16	a	1583	A
16	a	1584	U
16	a	1585	C
16	a	1608	A
16	a	1609	A
16	a	1610	A
16	a	1644	C
16	a	1647	U
16	a	1648	U
16	a	1649	G
16	a	1674	G
16	a	1715	G
16	a	1729	U
16	a	1730	C
16	a	1732	C
16	a	1738	G
16	a	1764	C
16	a	1773	A
16	a	1782	U
16	a	1800	C
16	a	1801	A
16	a	1808	A
16	a	1809	A
16	a	1816	C
16	a	1829	A
16	a	1842	G
16	a	1848	A

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Mol	Chain	Res	Type
16	a	1858	A
16	a	1862	G
16	a	1872	A
16	a	1873	G
16	a	1906	G
16	a	1907	G
16	a	1915	3TD
16	a	1929	G
16	a	1930	G
16	a	1937	A
16	a	1938	A
16	a	1955	U
16	a	1967	C
16	a	1970	A
16	a	1971	U
16	a	1972	G
16	a	1987	A
16	a	1991	U
16	a	1993	U
16	a	2023	C
16	a	2027	G
16	a	2031	A
16	a	2033	A
16	a	2043	C
16	a	2055	C
16	a	2056	G
16	a	2060	A
16	a	2061	G
16	a	2062	A
16	a	2069	G7M
16	a	2190	G
16	a	2198	A
16	a	2204	G
16	a	2211	A
16	a	2225	A
16	a	2238	G
16	a	2239	G
16	a	2268	A
16	a	2278	A
16	a	2282	G
16	a	2283	C
16	a	2287	A

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Mol	Chain	Res	Type
16	a	2288	A
16	a	2305	U
16	a	2308	G
16	a	2309	A
16	a	2312	U
16	a	2322	A
16	a	2325	G
16	a	2333	A
16	a	2335	A
16	a	2347	C
16	a	2361	G
16	a	2383	G
16	a	2385	C
16	a	2402	U
16	a	2406	A
16	a	2425	A
16	a	2429	G
16	a	2430	A
16	a	2431	U
16	a	2435	A
16	a	2441	U
16	a	2448	A
16	a	2469	A
16	a	2474	U
16	a	2476	A
16	a	2491	U
16	a	2492	U
16	a	2502	G
16	a	2505	G
16	a	2518	A
16	a	2525	G
16	a	2529	G
16	a	2547	A
16	a	2566	A
16	a	2567	G
16	a	2573	C
16	a	2602	A
16	a	2603	G
16	a	2609	U
16	a	2613	U
16	a	2629	U
16	a	2630	G

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Mol	Chain	Res	Type
16	a	2661	G
16	a	2663	G
16	a	2671	G
16	a	2689	U
16	a	2690	U
16	a	2714	G
16	a	2716	C
16	a	2726	A
16	a	2733	A
16	a	2744	G
16	a	2748	A
16	a	2765	A
16	a	2778	A
16	a	2790	U
16	a	2797	U
16	a	2798	U
16	a	2799	A
16	a	2818	U
16	a	2820	A
16	a	2821	A
16	a	2883	A
16	a	2884	U
16	a	2891	U
38	X	15	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	A	7	A
13	A	119	A
13	A	181	A
13	A	196	A
13	A	199	A
13	A	327	A
13	A	367	U
13	A	438	U
13	A	532	A
13	A	653	U
13	A	776	G
13	A	793	U
13	A	858	G
13	A	884	U

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Mol	Chain	Res	Type
13	A	1035	A
13	A	1124	G
13	A	1187	G
13	A	1211	U
13	A	1225	A
13	A	1281	C
13	A	1319	A
13	A	1447	A
13	A	1505	G
13	A	1508	A

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

50 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	$\# Z  > 2$
13	2MG	A	1516	13	23,26,27	0.37	0	32,38,41	0.51	0
16	1MG	a	745	16	22,26,27	0.50	0	33,39,42	0.48	0
3	D2T	L	89	3	7,9,10	0.93	0	6,11,13	1.74	2 (33%)
16	H2U	a	2449	16	18,21,22	0.55	0	21,30,33	0.74	1 (4%)
16	OMU	a	2552	16	19,22,23	0.20	0	26,31,34	0.38	0
16	PSU	a	1911	16	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
8	MS6	l	82	8	5,7,8	0.21	0	2,7,9	0.14	0
16	5MU	a	1939	58,16	19,22,23	0.29	0	28,32,35	0.36	0
16	OMC	a	2498	57,16	19,22,23	0.26	0	26,31,34	0.48	0
16	PSU	a	2580	57,16	18,21,22	0.89	1 (5%)	22,30,33	0.72	1 (4%)
15	PSU	Z	55	15	18,21,22	0.92	1 (5%)	22,30,33	0.64	0
6	MEQ	d	150	6	8,9,10	0.43	0	5,10,12	0.55	0
16	6MZ	a	1618	16	22,25,26	0.35	0	30,36,39	0.60	0
16	PSU	a	2504	58,16	18,21,22	0.86	1 (5%)	22,30,33	0.70	0
16	2MA	a	2503	58,57,16	22,25,26	0.25	0	33,37,40	0.67	2 (6%)
15	OMC	Z	32	15	19,22,23	0.26	0	26,31,34	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	PSU	a	746	57,16	18,21,22	0.91	1 (5%)	22,30,33	0.63	0
16	PSU	a	955	58,16	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
16	2MG	a	2445	16	23,26,27	0.39	0	32,38,41	0.41	0
16	PSU	a	2604	16	18,21,22	0.91	1 (5%)	22,30,33	0.76	1 (4%)
16	OMG	a	2251	58,15,16	23,26,27	0.30	0	33,38,41	0.45	0
13	G7M	A	527	13	23,26,27	0.72	1 (4%)	35,39,42	0.64	0
8	4D4	l	81	8	9,11,12	0.47	0	8,13,15	0.61	0
14	6MZ	Y	37	14	22,25,26	0.33	0	30,36,39	0.54	0
16	5MU	a	747	16	19,22,23	0.27	0	28,32,35	0.41	0
16	5MC	a	1962	58,16	18,22,23	0.33	0	26,32,35	0.45	0
2	IAS	K	119	2	6,7,8	0.89	0	6,8,10	0.97	0
16	G7M	a	2069	16	23,26,27	0.72	1 (4%)	35,39,42	0.64	0
13	UR3	A	1498	13	19,22,23	0.27	0	26,32,35	0.63	0
14	G7M	Y	46	14	23,26,27	0.73	1 (4%)	35,39,42	0.54	0
16	3TD	a	1915	16	18,22,23	0.94	1 (5%)	22,32,35	0.70	0
14	PSU	Y	55	14	18,21,22	0.89	1 (5%)	22,30,33	0.58	0
15	G7M	Z	46	15	23,26,27	0.73	1 (4%)	35,39,42	0.55	0
16	2MG	a	1835	16	23,26,27	0.36	0	32,38,41	0.38	0
13	MA6	A	1519	13	23,26,27	0.25	0	34,38,41	0.76	1 (2%)
13	PSU	A	516	13,58	18,21,22	0.90	1 (5%)	22,30,33	0.66	0
13	2MG	A	966	13	23,26,27	0.38	0	32,38,41	0.35	0
13	2MG	A	1207	13,58	23,26,27	0.38	0	32,38,41	0.41	0
13	5MC	A	1407	13	18,22,23	0.32	0	26,32,35	0.65	0
13	MA6	A	1518	13	23,26,27	0.24	0	34,38,41	0.69	1 (2%)
15	5MU	Z	54	15	19,22,23	0.26	0	28,32,35	0.31	0
16	PSU	a	2457	16	18,21,22	0.94	1 (5%)	22,30,33	0.57	0
14	4SU	Y	8	14	18,21,22	0.37	0	26,30,33	1.20	3 (11%)
14	5MU	Y	54	14	19,22,23	0.27	0	28,32,35	0.30	0
16	PSU	a	1917	16	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
13	4OC	A	1402	13	20,23,24	0.36	0	26,32,35	0.51	0
15	4SU	Z	8	15	18,21,22	0.37	0	26,30,33	1.18	3 (11%)
13	5MC	A	967	13	18,22,23	0.31	0	26,32,35	0.52	0
16	PSU	a	2605	16	18,21,22	0.91	1 (5%)	22,30,33	0.74	0
16	6MZ	a	2030	16	22,25,26	0.32	0	30,36,39	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	2MG	A	1516	13	-	0/9/27/28	0/3/3/3
16	1MG	a	745	16	-	0/7/25/26	0/3/3/3
3	D2T	L	89	3	-	1/7/12/14	-
16	H2U	a	2449	16	-	0/7/38/39	0/2/2/2
16	OMU	a	2552	16	-	0/9/27/28	0/2/2/2
16	PSU	a	1911	16	-	0/7/25/26	0/2/2/2
8	MS6	l	82	8	-	1/4/6/8	-
16	5MU	a	1939	58,16	-	0/7/25/26	0/2/2/2
16	OMC	a	2498	57,16	-	0/9/27/28	0/2/2/2
16	PSU	a	2580	57,16	-	0/7/25/26	0/2/2/2
15	PSU	Z	55	15	-	0/7/25/26	0/2/2/2
6	MEQ	d	150	6	-	2/8/9/11	-
16	6MZ	a	1618	16	-	0/9/27/28	0/3/3/3
16	PSU	a	2504	58,16	-	0/7/25/26	0/2/2/2
16	2MA	a	2503	58,57,16	-	3/7/25/26	0/3/3/3
15	OMC	Z	32	15	-	0/9/27/28	0/2/2/2
16	PSU	a	746	57,16	-	1/7/25/26	0/2/2/2
16	PSU	a	955	58,16	-	0/7/25/26	0/2/2/2
16	2MG	a	2445	16	-	1/9/27/28	0/3/3/3
16	PSU	a	2604	16	-	0/7/25/26	0/2/2/2
16	OMG	a	2251	58,15,16	-	0/9/27/28	0/3/3/3
13	G7M	A	527	13	-	3/7/25/26	0/3/3/3
8	4D4	l	81	8	-	1/11/12/14	-
14	6MZ	Y	37	14	-	0/9/27/28	0/3/3/3
16	5MU	a	747	16	-	1/7/25/26	0/2/2/2
16	5MC	a	1962	58,16	-	1/7/25/26	0/2/2/2
2	IAS	K	119	2	-	0/7/7/8	-
16	G7M	a	2069	16	-	2/7/25/26	0/3/3/3
13	UR3	A	1498	13	-	0/7/25/26	0/2/2/2
14	G7M	Y	46	14	-	3/7/25/26	0/3/3/3
16	3TD	a	1915	16	-	2/7/25/26	0/2/2/2
14	PSU	Y	55	14	-	2/7/25/26	0/2/2/2
15	G7M	Z	46	15	-	1/7/25/26	0/3/3/3
16	2MG	a	1835	16	-	0/9/27/28	0/3/3/3
13	MA6	A	1519	13	-	2/11/29/30	0/3/3/3
13	PSU	A	516	13,58	-	1/7/25/26	0/2/2/2
13	2MG	A	966	13	-	0/9/27/28	0/3/3/3
13	2MG	A	1207	13,58	-	0/9/27/28	0/3/3/3
13	5MC	A	1407	13	-	0/7/25/26	0/2/2/2
13	MA6	A	1518	13	-	0/11/29/30	0/3/3/3
15	5MU	Z	54	15	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PSU	a	2457	16	-	0/7/25/26	0/2/2/2
14	4SU	Y	8	14	-	0/7/25/26	0/2/2/2
14	5MU	Y	54	14	-	0/7/25/26	0/2/2/2
16	PSU	a	1917	16	-	0/7/25/26	0/2/2/2
13	4OC	A	1402	13	-	0/9/29/30	0/2/2/2
15	4SU	Z	8	15	-	0/7/25/26	0/2/2/2
13	5MC	A	967	13	-	0/7/25/26	0/2/2/2
16	PSU	a	2605	16	-	0/7/25/26	0/2/2/2
16	6MZ	a	2030	16	-	2/9/27/28	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Z	55	PSU	C6-C5	3.64	1.39	1.35
16	a	2457	PSU	C6-C5	3.63	1.39	1.35
16	a	955	PSU	C6-C5	3.63	1.39	1.35
16	a	1911	PSU	C6-C5	3.60	1.39	1.35
16	a	1917	PSU	C6-C5	3.59	1.39	1.35
16	a	746	PSU	C6-C5	3.57	1.39	1.35
13	A	516	PSU	C6-C5	3.55	1.39	1.35
16	a	1915	3TD	C6-C5	3.54	1.39	1.35
16	a	2604	PSU	C6-C5	3.54	1.39	1.35
16	a	2605	PSU	C6-C5	3.54	1.39	1.35
14	Y	55	PSU	C6-C5	3.53	1.39	1.35
16	a	2580	PSU	C6-C5	3.53	1.39	1.35
16	a	2504	PSU	C6-C5	3.38	1.39	1.35
15	Z	46	G7M	C8-N7	2.68	1.37	1.33
13	A	527	G7M	C8-N7	2.64	1.37	1.33
14	Y	46	G7M	C8-N7	2.64	1.37	1.33
16	a	2069	G7M	C8-N7	2.63	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Y	8	4SU	C4-N3-C2	-4.36	123.11	127.34
15	Z	8	4SU	C4-N3-C2	-4.32	123.14	127.34
13	A	1518	MA6	C2-N1-C6	2.94	118.70	111.75
13	A	1519	MA6	C2-N1-C6	2.91	118.62	111.75
14	Y	8	4SU	C5-C4-N3	2.80	117.29	114.69
15	Z	8	4SU	C5-C4-N3	2.73	117.23	114.69
3	L	89	D2T	OD1-CG-CB	-2.58	117.05	122.44
16	a	2503	2MA	C5-C4-N3	-2.42	124.47	127.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	2604	PSU	C2'-C3'-C4'	-2.26	98.24	102.64
14	Y	8	4SU	N3-C2-N1	2.20	117.81	114.89
15	Z	8	4SU	N3-C2-N1	2.20	117.81	114.89
3	L	89	D2T	OD2-CG-CB	2.09	117.66	113.15
16	a	2580	PSU	C3'-C2'-C1'	2.05	104.02	101.64
16	a	2449	H2U	O2-C2-N1	-2.03	120.55	123.11
16	a	2503	2MA	N3-C4-N9	2.01	129.79	126.99

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	Y	46	G7M	C3'-C4'-C5'-O5'
16	a	1915	3TD	C3'-C4'-C5'-O5'
16	a	1915	3TD	O4'-C4'-C5'-O5'
13	A	1519	MA6	O4'-C4'-C5'-O5'
14	Y	46	G7M	O4'-C4'-C5'-O5'
16	a	2030	6MZ	O4'-C4'-C5'-O5'
13	A	1519	MA6	C3'-C4'-C5'-O5'
6	d	150	MEQ	NE2-CD-CG-CB
6	d	150	MEQ	OE1-CD-CG-CB
13	A	527	G7M	C3'-C4'-C5'-O5'
16	a	2030	6MZ	C3'-C4'-C5'-O5'
14	Y	46	G7M	C4'-C5'-O5'-P
8	l	82	MS6	CB-CG-SD-CE
16	a	2069	G7M	C4'-C5'-O5'-P
15	Z	46	G7M	C4'-C5'-O5'-P
13	A	527	G7M	O4'-C4'-C5'-O5'
13	A	516	PSU	O4'-C1'-C5-C4
14	Y	55	PSU	O4'-C1'-C5-C4
13	A	527	G7M	C4'-C5'-O5'-P
16	a	2503	2MA	O4'-C1'-N9-C8
16	a	2445	2MG	C3'-C4'-C5'-O5'
16	a	2503	2MA	C4'-C5'-O5'-P
16	a	2069	G7M	O4'-C4'-C5'-O5'
3	L	89	D2T	CG-CB-SB-CB1
14	Y	55	PSU	O4'-C1'-C5-C6
16	a	746	PSU	O4'-C1'-C5-C6
16	a	2503	2MA	O4'-C4'-C5'-O5'
16	a	1962	5MC	O4'-C1'-N1-C6
8	l	81	4D4	O-C-CA-CB
16	a	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	2552	OMU	1	0
16	a	1939	5MU	1	0
16	a	2503	2MA	1	0
16	a	2604	PSU	1	0
14	Y	37	6MZ	1	0
16	a	747	5MU	1	0
13	A	1519	MA6	1	0
13	A	1518	MA6	1	0
16	a	2030	6MZ	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 351 ligands modelled in this entry, 349 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
59	SCM	A	1601	-	23,25,25	0.27	0	26,39,39	0.63	0
60	VAL	Y	101	14	4,6,7	0.58	0	6,7,9	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SCM	A	1601	-	-	0/4/57/57	0/3/3/3
60	VAL	Y	101	14	-	0/5/6/8	-

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	A	1601	SCM	4	0
60	Y	101	VAL	2	0

## 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.

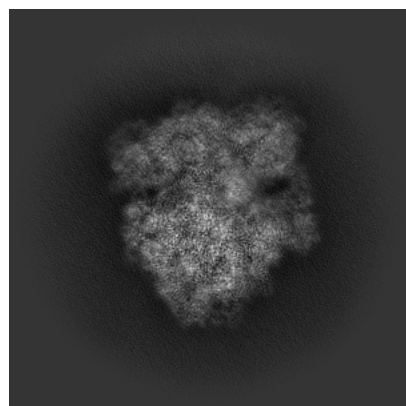
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56832. These allow visual inspection of the internal detail of the map and identification of artifacts.

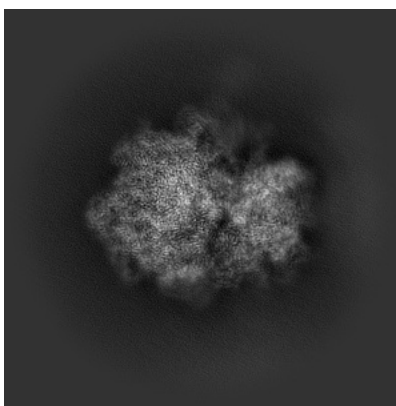
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

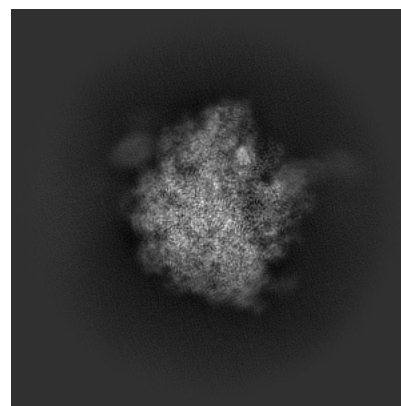
#### 6.1.1 Primary map



X

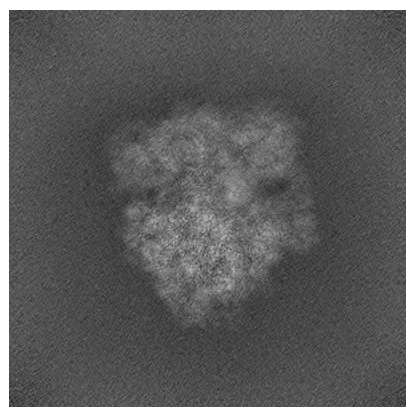


Y

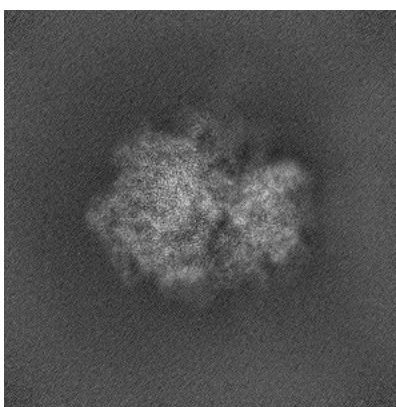


Z

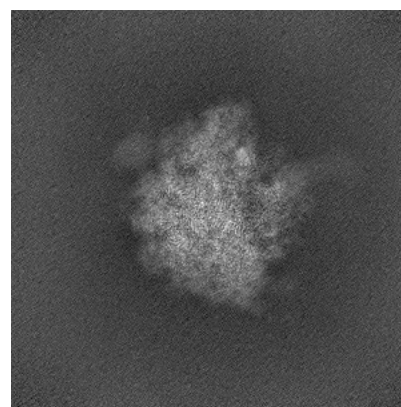
#### 6.1.2 Raw map



X



Y

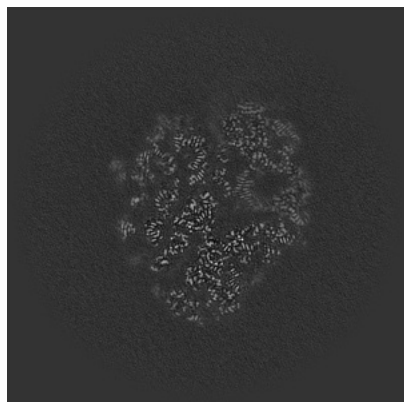


Z

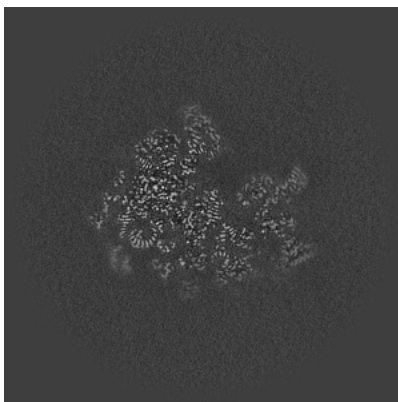
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

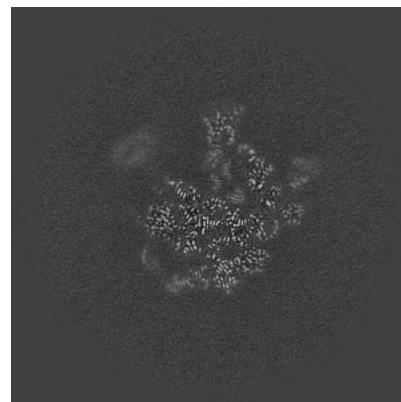
### 6.2.1 Primary map



X Index: 288

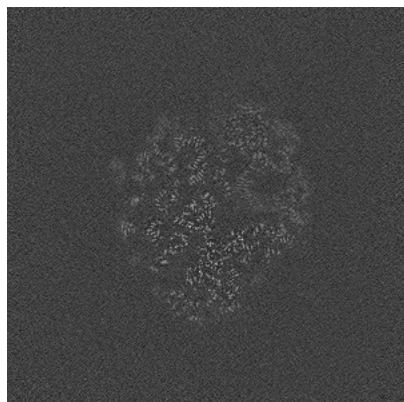


Y Index: 288

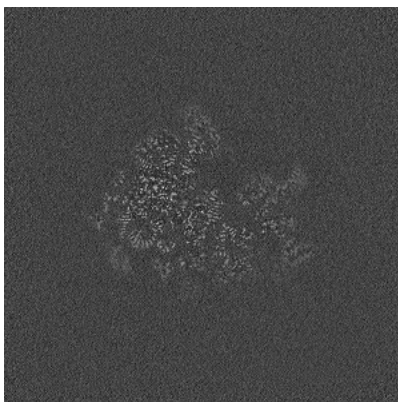


Z Index: 288

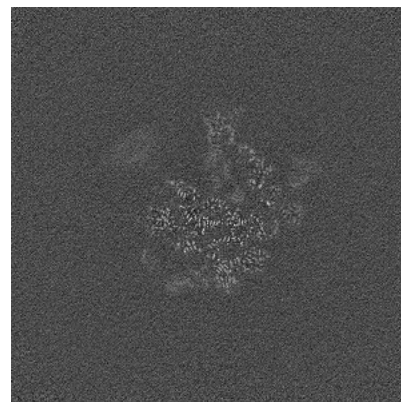
### 6.2.2 Raw map



X Index: 288



Y Index: 288



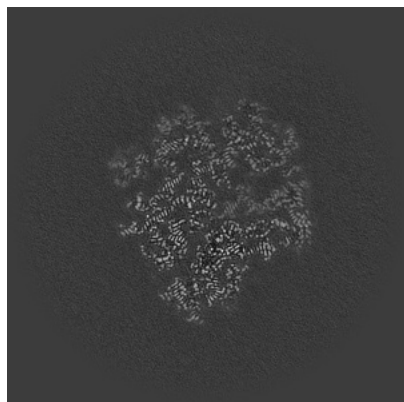
Z Index: 288

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

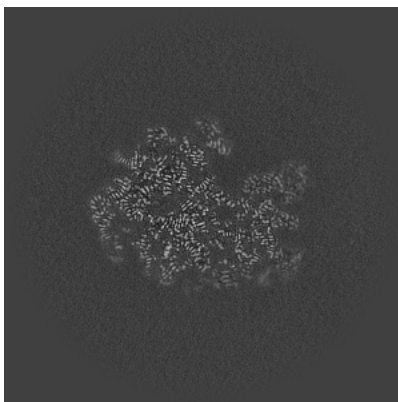


## 6.3 Largest variance slices [i](#)

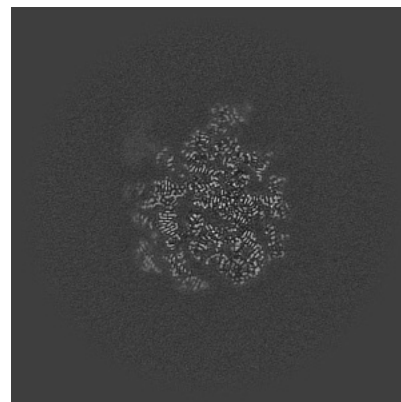
### 6.3.1 Primary map



X Index: 296

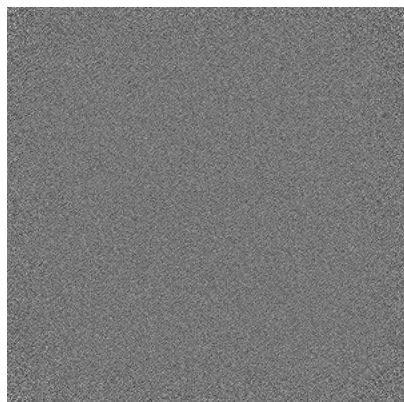


Y Index: 272

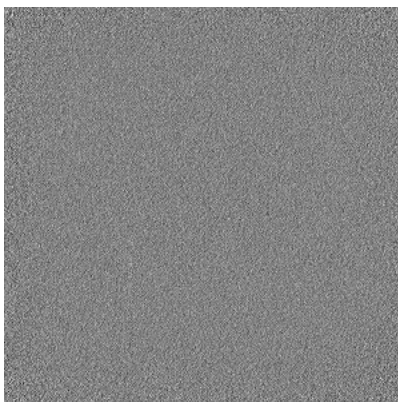


Z Index: 234

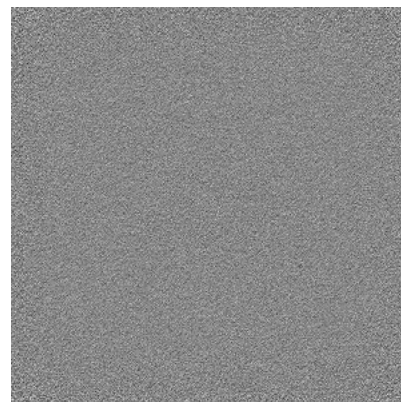
### 6.3.2 Raw map



X Index: 0



Y Index: 0

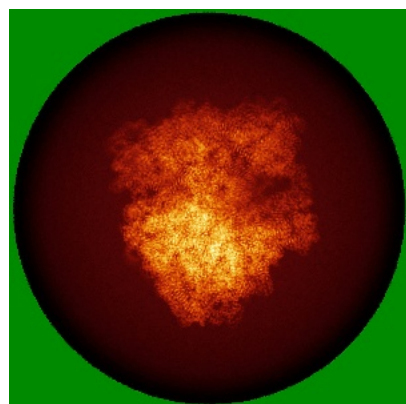


Z Index: 0

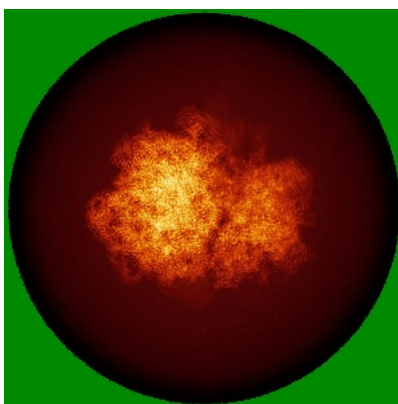
The images above show the largest variance slices of the map in three orthogonal directions.

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

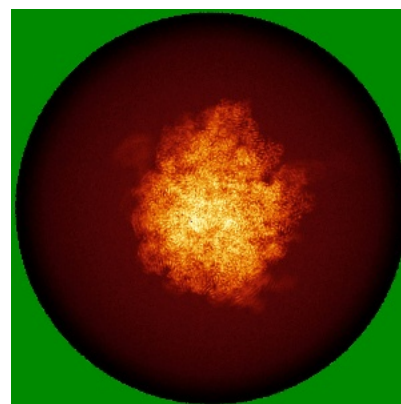
### 6.4.1 Primary map



X

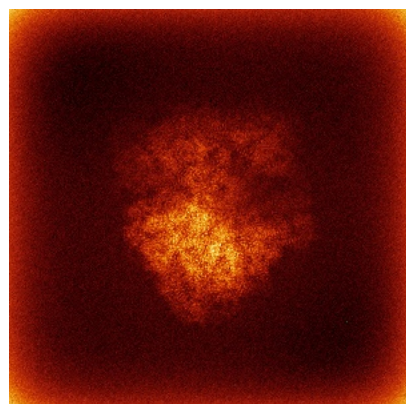


Y

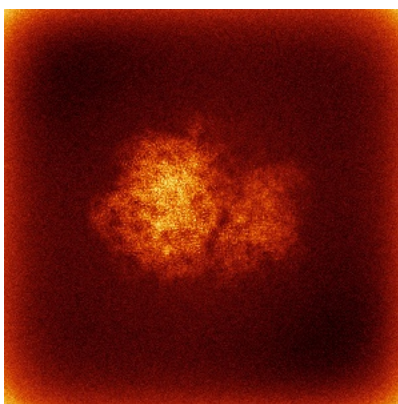


Z

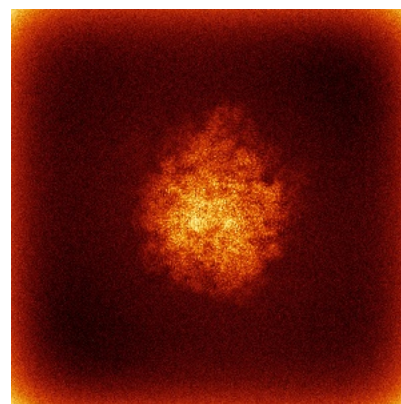
### 6.4.2 Raw map



X



Y



Z

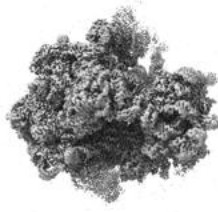
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



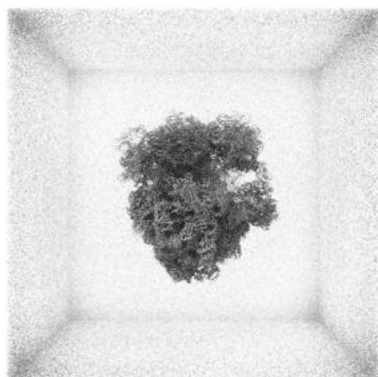
Y



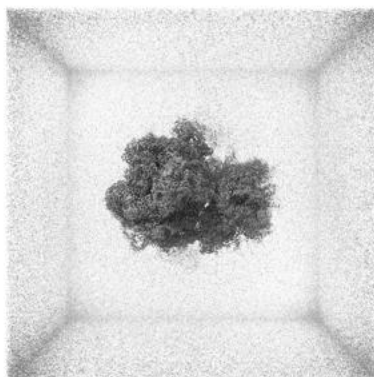
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0748. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

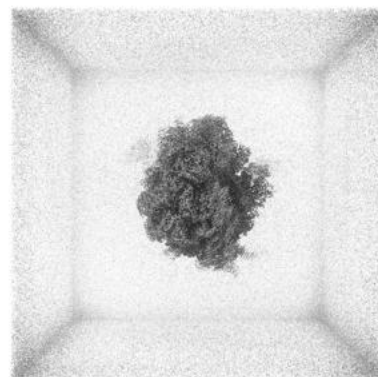
### 6.5.2 Raw map



X



Y



Z

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



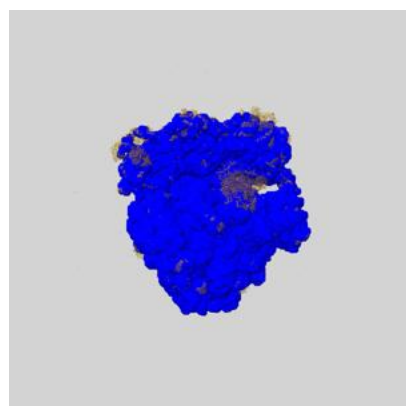
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

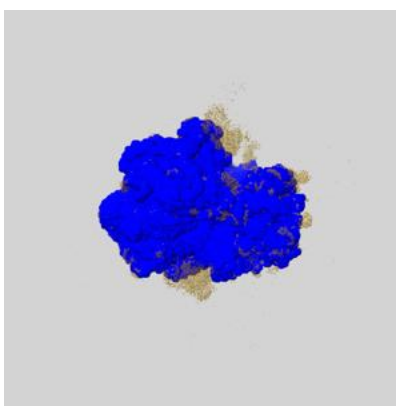
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

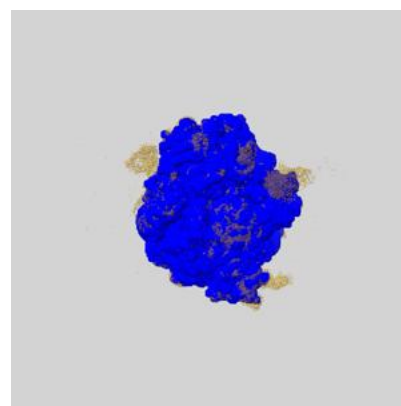
### 6.6.1 emd\_56832\_msk\_1.map [i](#)



X



Y

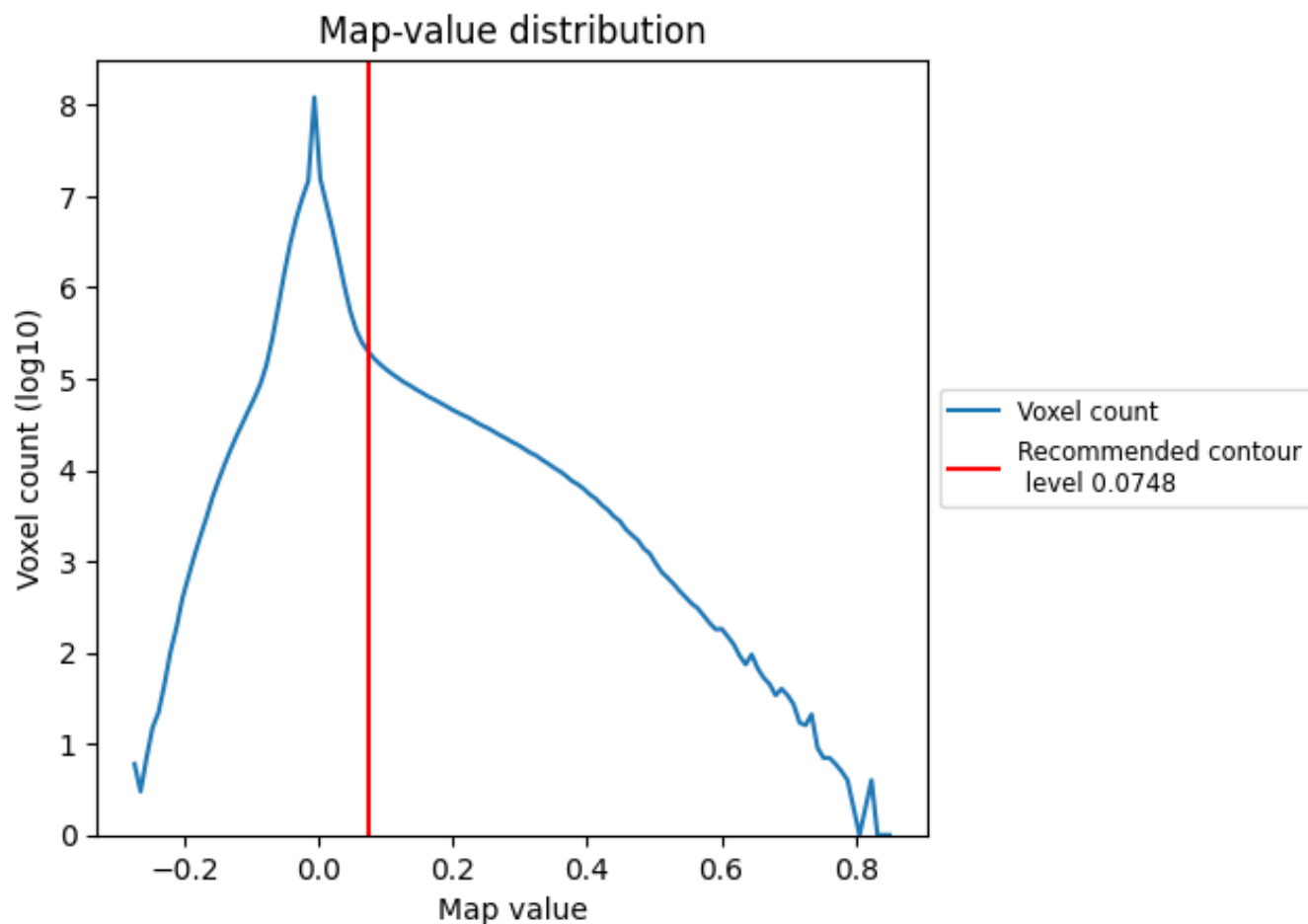


Z

## 7 Map analysis [i](#)

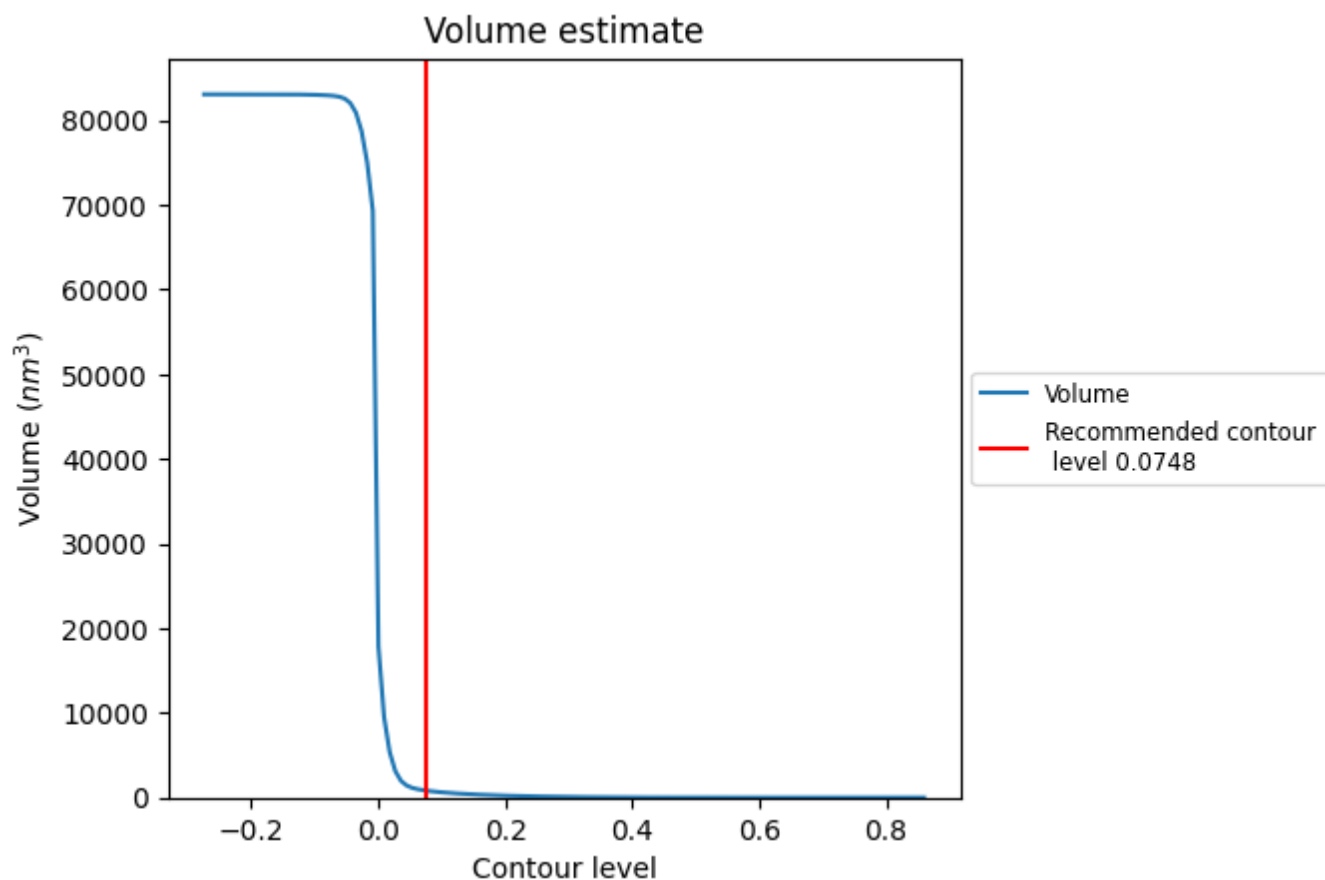
This section contains the results of statistical analysis of the map.

### 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.

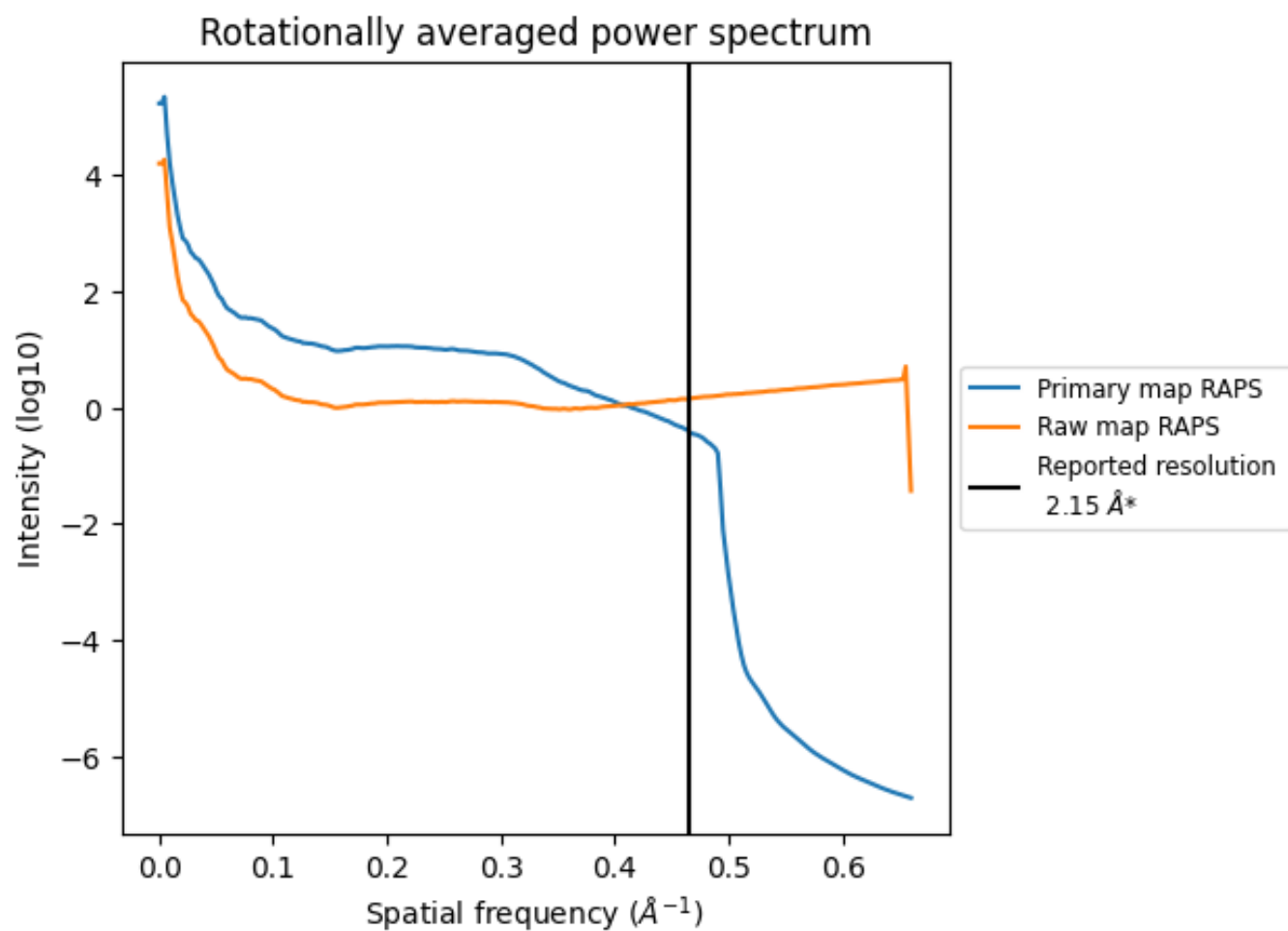
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 832 nm<sup>3</sup>; this corresponds to an approximate mass of 751 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

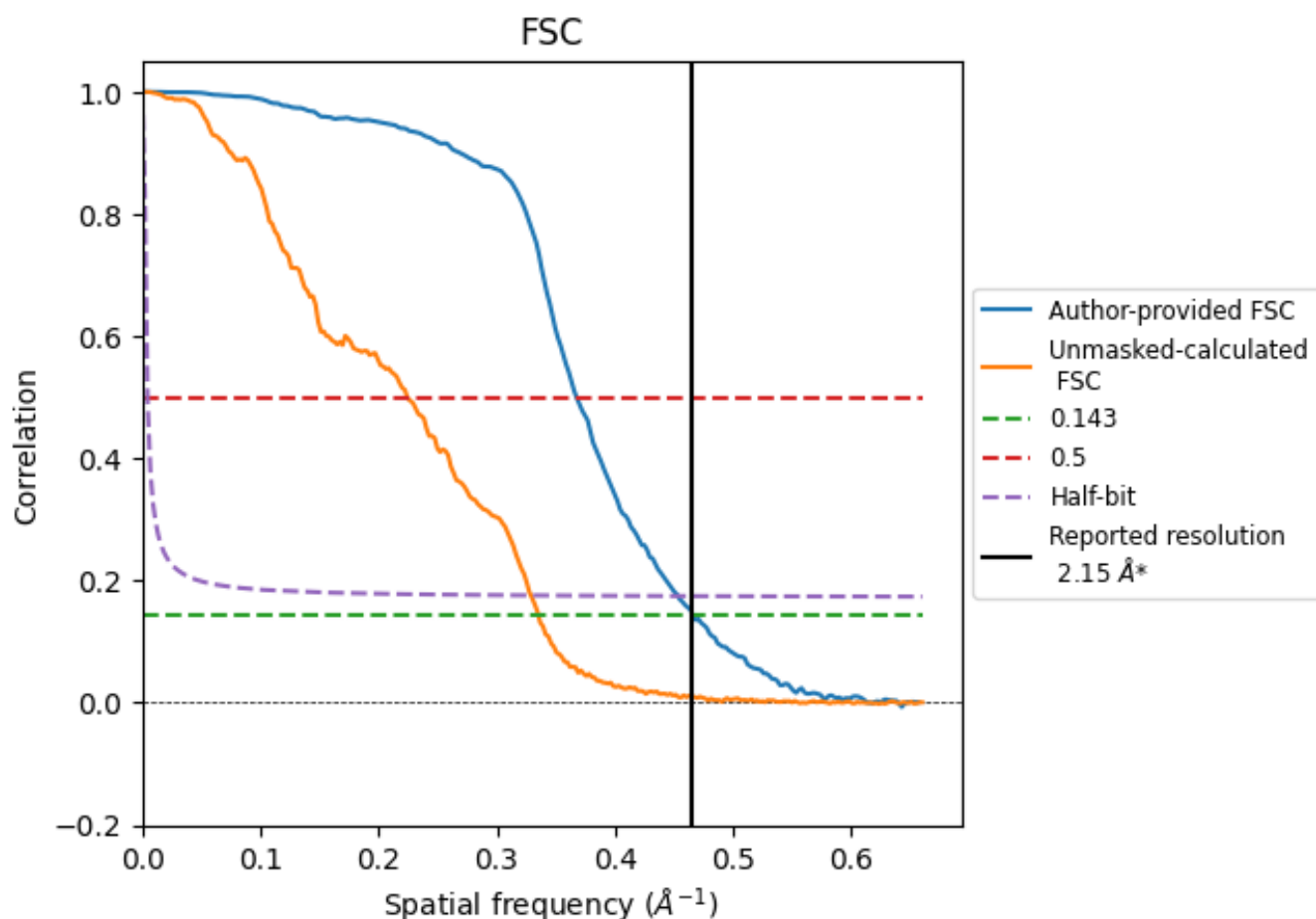


\*Reported resolution corresponds to spatial frequency of 0.465 Å<sup>-1</sup>

## 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 0.465  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

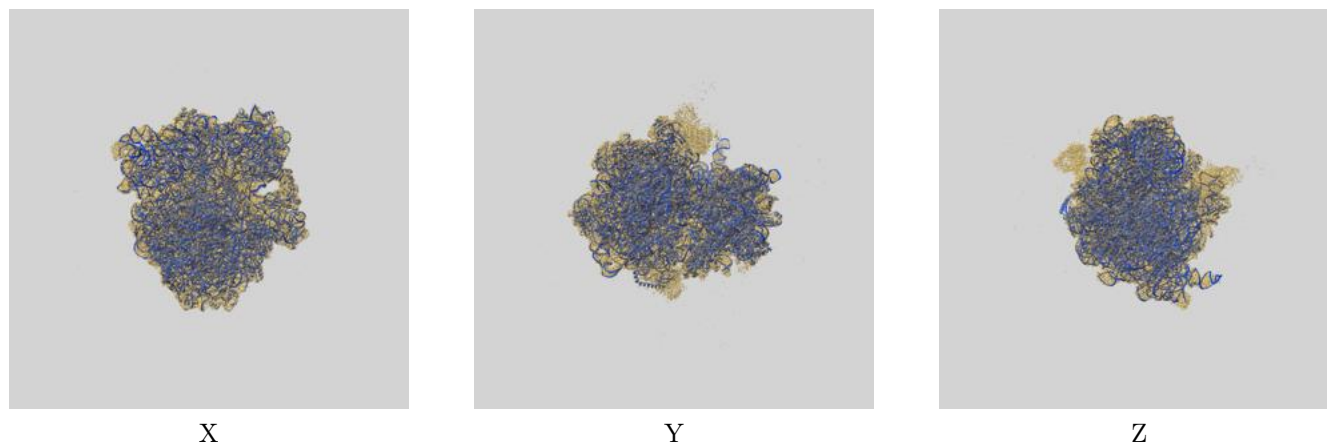
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.15	2.72	2.21
Unmasked-calculated*	2.98	4.46	3.04

\*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 2.98 differs from the reported value 2.15 by more than 10 %

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

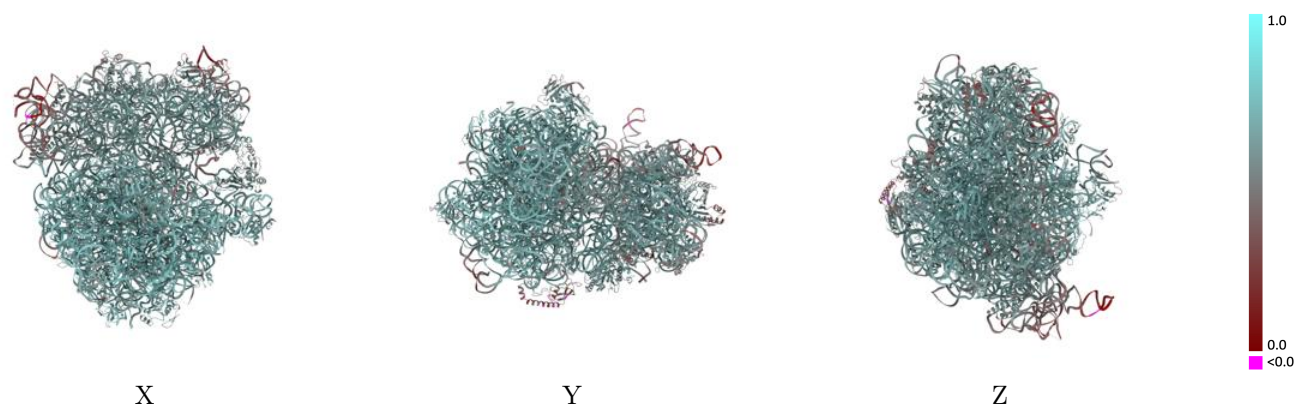
This section contains information regarding the fit between EMDB map EMD-56832 and PDB model 28UM. Per-residue inclusion information can be found in section 3 on page 20.

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



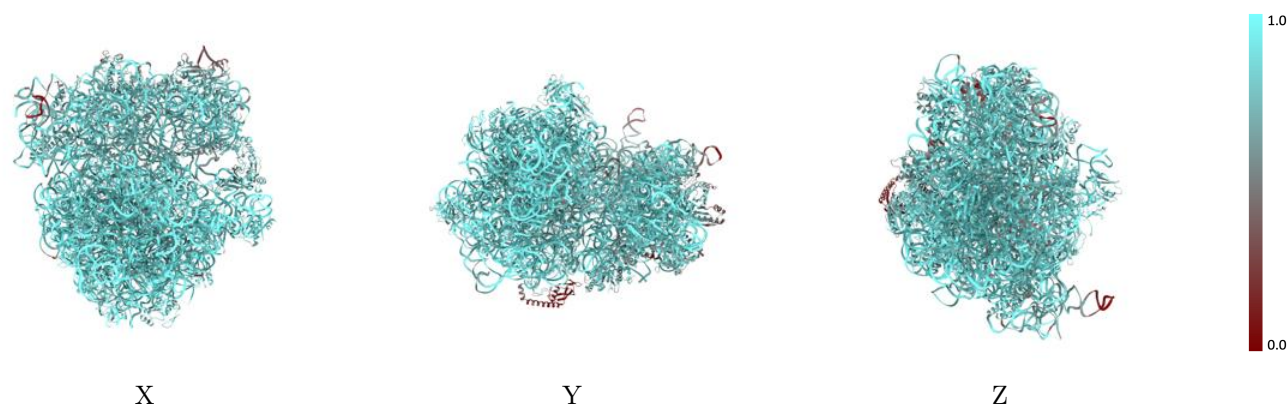
The images above show the 3D surface view of the map at the recommended contour level 0.0748 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

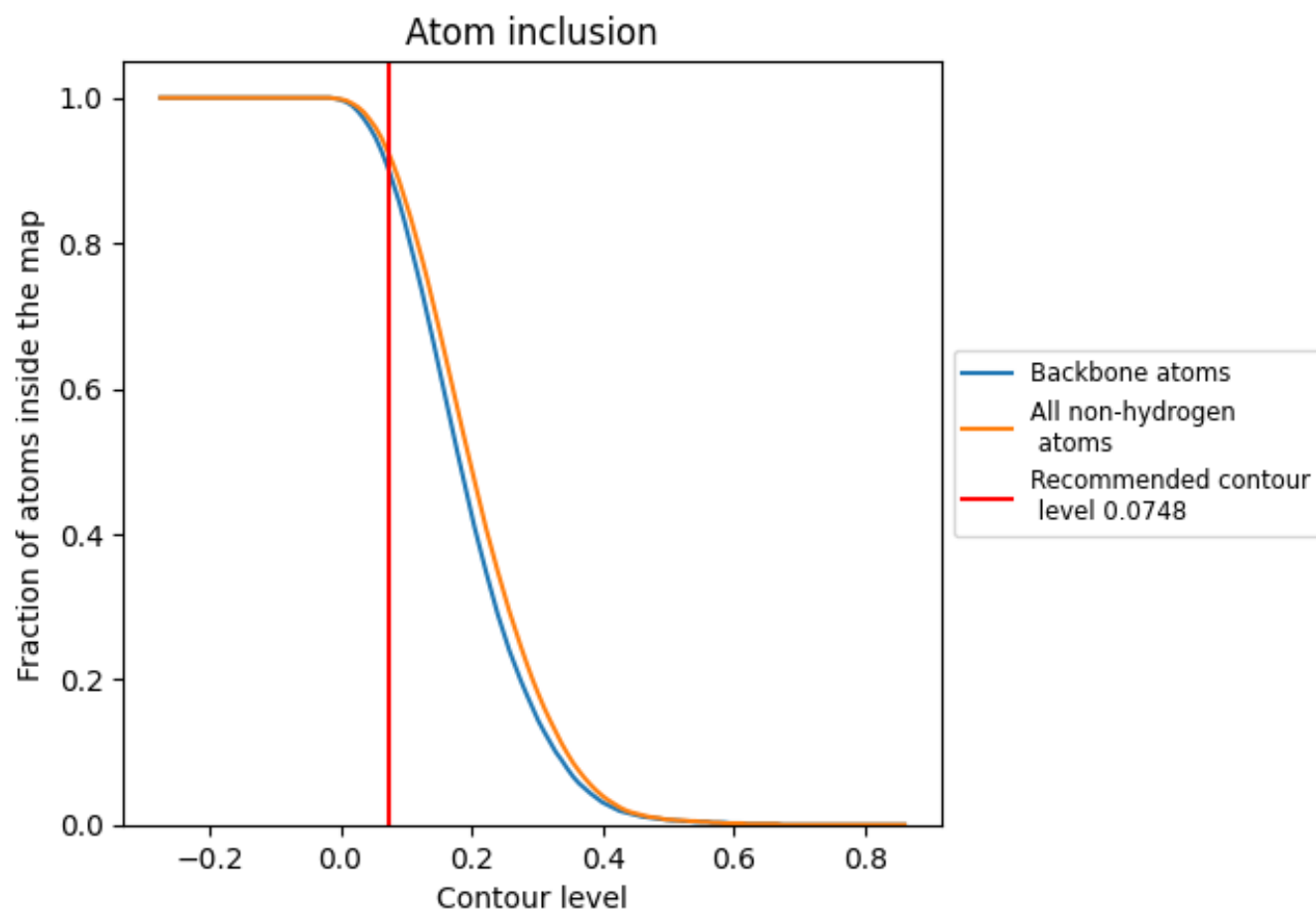
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0748).









































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.0748) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.6390
0	 0.8920	 0.6610
1	 0.9690	 0.7240
2	 0.9720	 0.7140
3	 0.9420	 0.6760
4	 0.7080	 0.5030
A	 0.9270	 0.6030
B	 0.7510	 0.5480
C	 0.8170	 0.6070
D	 0.6980	 0.5260
E	 0.8960	 0.6430
F	 0.8140	 0.5870
G	 0.6730	 0.5140
H	 0.8950	 0.6340
I	 0.7980	 0.5810
J	 0.6670	 0.5120
K	 0.8500	 0.6160
L	 0.8510	 0.6310
M	 0.8200	 0.5860
N	 0.8420	 0.6050
O	 0.8700	 0.6280
P	 0.7120	 0.5310
Q	 0.7840	 0.5740
R	 0.8910	 0.6270
S	 0.8220	 0.5900
T	 0.7590	 0.5390
U	 0.6640	 0.5300
X	 0.8980	 0.6190
Y	 0.8750	 0.5840
Z	 0.8500	 0.5750
a	 0.9790	 0.6750
b	 0.9700	 0.6410
c	 0.9560	 0.7070
d	 0.9460	 0.6940
e	 0.9090	 0.6620



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
f	 0.7960	 0.5620
g	 0.8340	 0.5810
h	 0.2940	 0.3840
i	 0.9410	 0.6920
j	 0.9290	 0.6830
k	 0.9430	 0.6830
l	 0.9360	 0.6900
m	 0.9820	 0.7120
n	 0.8960	 0.6300
o	 0.9000	 0.6790
p	 0.9750	 0.7160
q	 0.9260	 0.6750
r	 0.9290	 0.6900
s	 0.8950	 0.6530
t	 0.8680	 0.6260
u	 0.8830	 0.6340
v	 0.9010	 0.6870
w	 0.9400	 0.6850
x	 0.8800	 0.6230
y	 0.9180	 0.6830
z	 0.9280	 0.6870