



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 01:34 pm BST

PDB ID : 9TQA / pdb_00009tqa
EMDB ID : EMD-56128
Title : E. coli 70S ribosome, trapped conformational ground state of SSU-h44 apical loop, with A- and P-site tRNA
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.
Deposited on : 2025-12-19
Resolution : 2.06 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

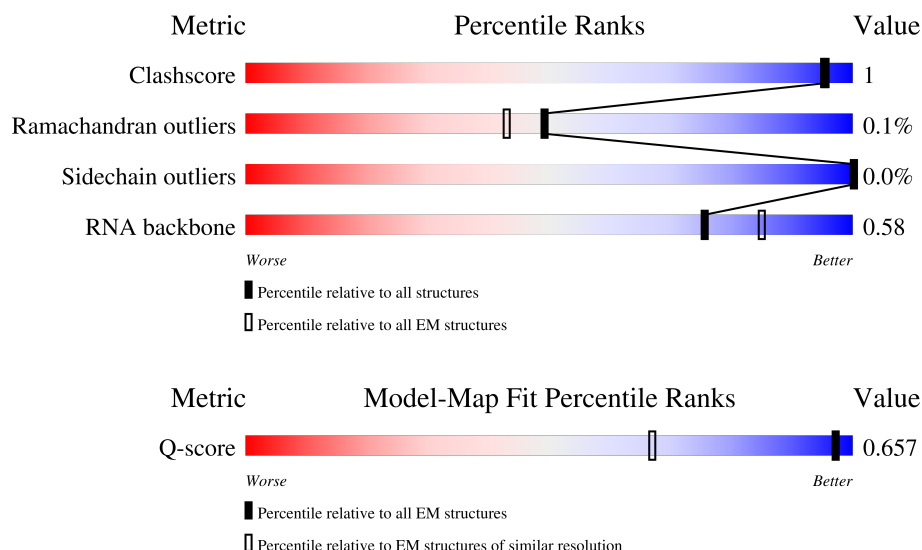
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

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

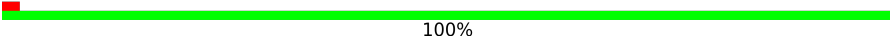
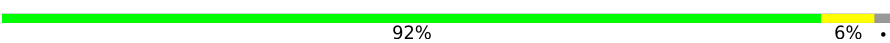
The reported resolution of this entry is 2.06 Å.

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	1895 (1.56 - 2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	

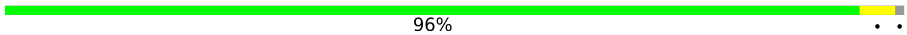
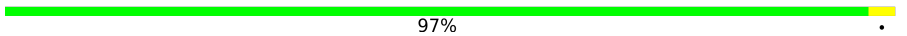
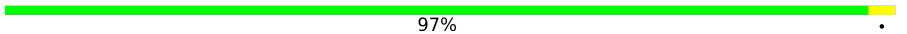
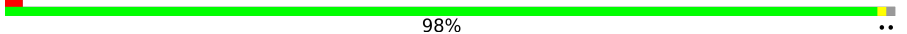
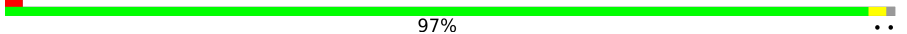
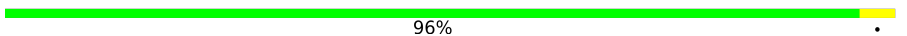
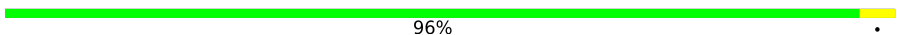
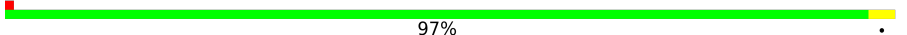
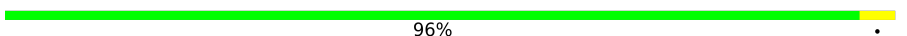
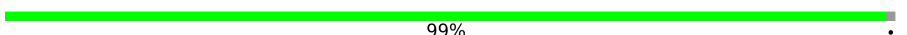
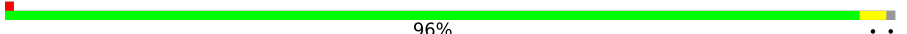
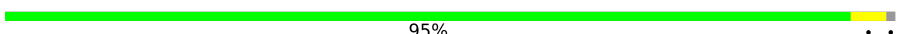
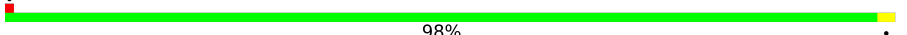
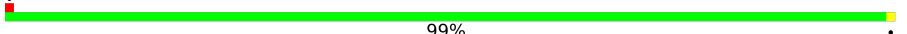
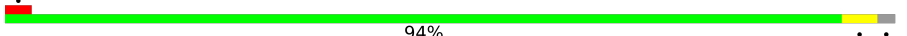
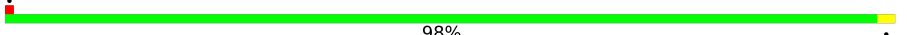
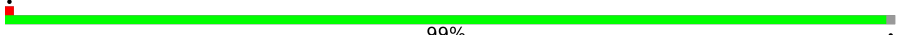
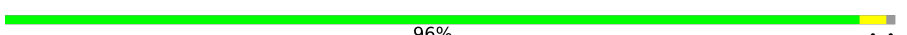
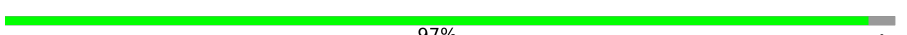
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1544	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	10	
28	Y	76	

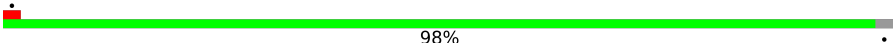
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Mol	Chain	Length	Quality of chain
29	Z	78	
30	a	2904	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

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Mol	Chain	Length	Quality of chain
54	y	59	 98%
55	z	57	 91%7%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151159 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 bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1521	Total	C	N	O	P	0	0
			32655	14571	5994	10569	1521		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1448A	G	-	insertion	GB 2971070070
A	1454A	C	-	insertion	GB 2971070070

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 11 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	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 17 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 27 is a RNA chain called mRNA.

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

- Molecule 28 is a RNA chain called A-site Val-tRNA^{Val}.

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

- Molecule 29 is a RNA chain called P-site tRNA^{fMet}.

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

- Molecule 30 is a RNA chain called 23S rRNA.

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

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

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

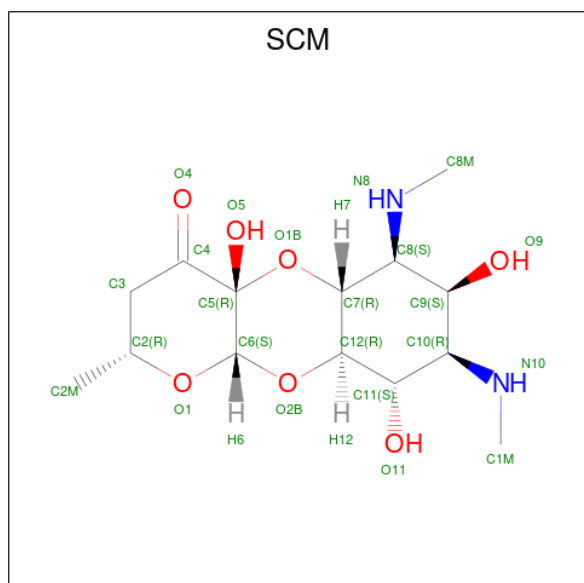
- Molecule 55 is a protein called Large ribosomal subunit protein bL32.

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

- 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 SPECTINOMYCIN (CCD ID: SCM) (formula: C₁₄H₂₄N₂O₇).

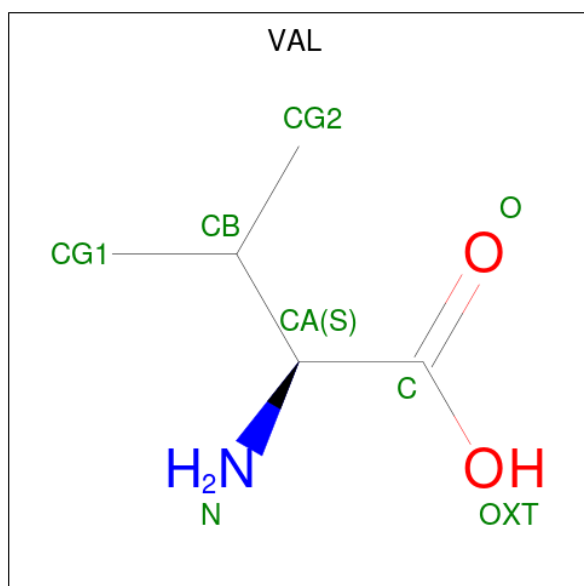


Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	46	Total	Mg	0
			46	46	
58	Z	1	Total	Mg	0
			1	1	
58	a	186	Total	Mg	0
			186	186	
58	b	2	Total	Mg	0
			2	2	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	

- Molecule 59 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



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

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	a	6	Total	K	0
			6	6	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	0	14	Total 14	O 14	0
61	1	21	Total 21	O 21	0
61	2	19	Total 19	O 19	0
61	3	12	Total 12	O 12	0
61	A	1816	Total 1816	O 1816	0
61	B	23	Total 23	O 23	0
61	C	29	Total 29	O 29	0
61	D	29	Total 29	O 29	0
61	E	23	Total 23	O 23	0
61	F	6	Total 6	O 6	0
61	G	17	Total 17	O 17	0
61	H	25	Total 25	O 25	0
61	I	18	Total 18	O 18	0
61	J	16	Total 16	O 16	0
61	K	13	Total 13	O 13	0
61	L	23	Total 23	O 23	0
61	M	16	Total 16	O 16	0
61	N	20	Total 20	O 20	0
61	O	15	Total 15	O 15	0
61	P	13	Total 13	O 13	0
61	Q	13	Total 13	O 13	0
61	R	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
61	S	8	Total 8	O 8	0
61	T	7	Total 7	O 7	0
61	U	16	Total 16	O 16	0
61	X	10	Total 10	O 10	0
61	Y	33	Total 33	O 33	0
61	Z	37	Total 37	O 37	0
61	a	5230	Total 5230	O 5230	0
61	b	142	Total 142	O 142	0
61	c	116	Total 116	O 116	0
61	d	79	Total 79	O 79	0
61	e	70	Total 70	O 70	0
61	f	10	Total 10	O 10	0
61	g	23	Total 23	O 23	0
61	h	19	Total 19	O 19	0
61	i	34	Total 34	O 34	0
61	j	33	Total 33	O 33	0
61	k	54	Total 54	O 54	0
61	l	51	Total 51	O 51	0
61	m	29	Total 29	O 29	0
61	n	13	Total 13	O 13	0
61	o	38	Total 38	O 38	0

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Mol	Chain	Residues	Atoms		AltConf
61	p	51	Total 51	O 51	0
61	q	43	Total 43	O 43	0
61	r	39	Total 39	O 39	0
61	s	20	Total 20	O 20	0
61	t	20	Total 20	O 20	0
61	u	18	Total 18	O 18	0
61	v	31	Total 31	O 31	0
61	w	25	Total 25	O 25	0
61	x	10	Total 10	O 10	0
61	y	21	Total 21	O 21	0
61	z	33	Total 33	O 33	0

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 bL33

Chain 0:  89% 7%

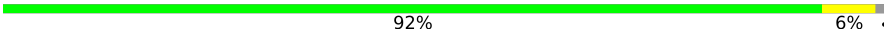


- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  100%

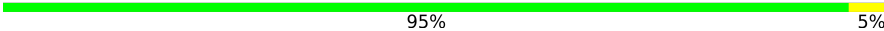


- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  92% 6%



- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  95% 5%



- Molecule 5: Large ribosomal subunit protein bL31

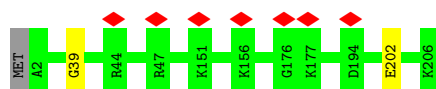
Chain 4:  9% 83% 14%



- Molecule 6: 16S rRNA

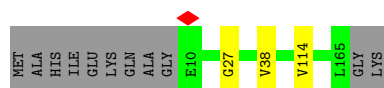


Chain D:  99%



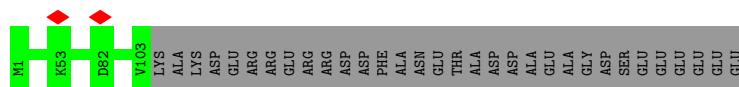
- Molecule 10: Small ribosomal subunit protein uS5

Chain E:  92%



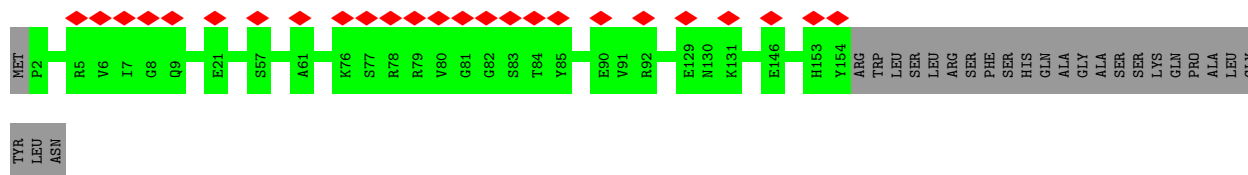
- Molecule 11: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  76%

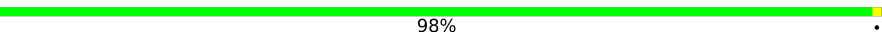


- Molecule 12: Small ribosomal subunit protein uS7

Chain G:  14%



- Molecule 13: Small ribosomal subunit protein uS8

Chain H:  98%



- Molecule 14: Small ribosomal subunit protein uS9

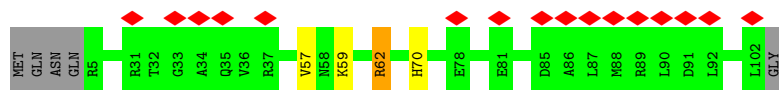
Chain I:  98%



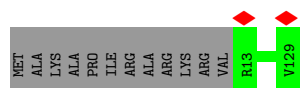
- Molecule 15: Small ribosomal subunit protein uS10

Chain J:  16%

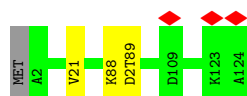
Chain J:  91%



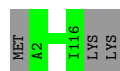
- Molecule 16: Small ribosomal subunit protein uS11



- Molecule 17: Small ribosomal subunit protein uS12



- Molecule 18: Small ribosomal subunit protein uS13



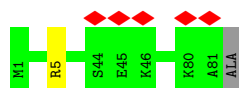
- Molecule 19: Small ribosomal subunit protein uS14



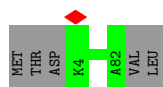
- Molecule 20: Small ribosomal subunit protein uS15



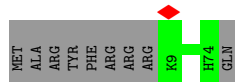
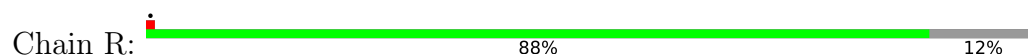
- Molecule 21: Small ribosomal subunit protein bS16



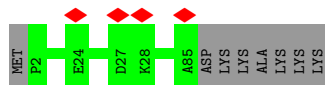
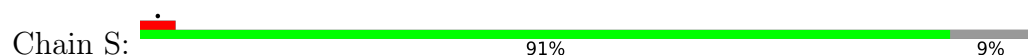
- Molecule 22: Small ribosomal subunit protein uS17



- Molecule 23: Small ribosomal subunit protein bS18



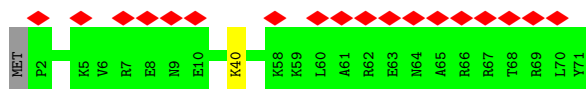
- Molecule 24: Small ribosomal subunit protein uS19



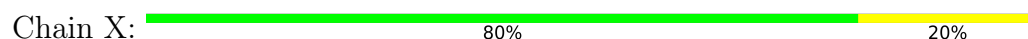
- Molecule 25: Small ribosomal subunit protein bS20



- Molecule 26: Small ribosomal subunit protein bS21



- Molecule 27: mRNA

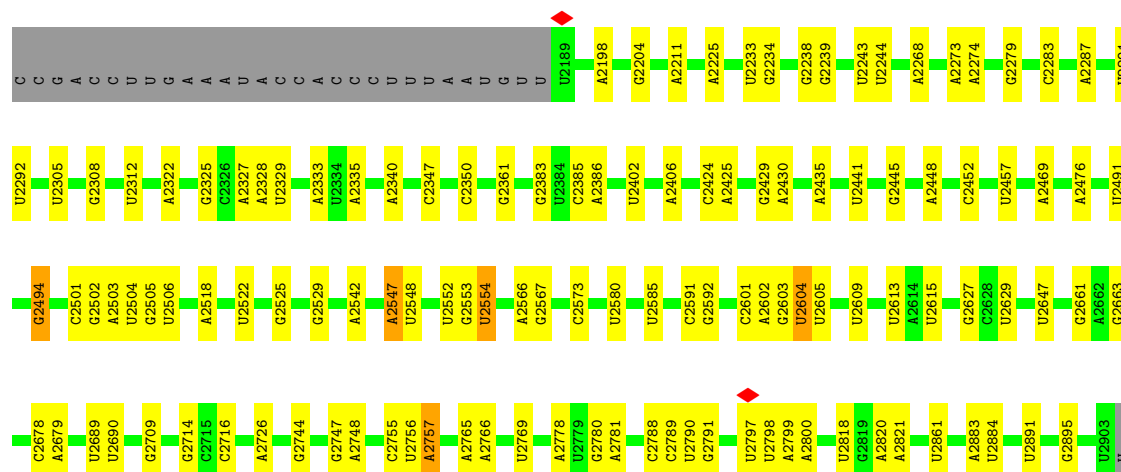


- Molecule 28: A-site Val-tRNA^{Val}



C1		U8	G9		G12	C13	A14	G15	C	C	U	G	G18	G19	A	A21		G46	C	C48		G53	U54	U55		A58		G70	C71		A76
----	--	----	----	--	-----	-----	-----	-----	---	---	---	---	-----	-----	---	-----	--	-----	---	-----	--	-----	-----	-----	--	-----	--	-----	-----	--	-----

G2100	3TD1915	U1729	C1428	U1132	G	C889	U686	G494	A222	G1
A	A1916	C1730	A1133	A1133	G	C390	C687	A502	G248	A10
C	U1917	G1731	A1434	A1134	C	G891	U688	C11	G11	U12
C	C1732	C1732	A1435	C1135	U	U		A503	G263	U34
U	G1929	G1738	G1462	U1141	A	U895	C717	A504	C264	G88
U	G1930	A1754	A1463	A1142	G	A896	C723	A505	A272	A63
G	G1932	A1760	U1474	A1156	A	C897	U724	C509	U276	A71
A	G1933	C1764	G1475	A1171	C	A910	A730	A526	A278	U72
U	U1937	U1778	G1482	C1172	G	A911	G914	G530	A279	A74
U	U1938	A1773	U1490	U	A	C915	G738	C531	A73	A74
U	U1939	A	A	A	C	G916	U746	A532	A282	G75
U	U1955	U	U	U	C	A917	U747	G533	G285	A84
G	A1966	G1177	C1493	G1177	U	A918	A764	U534	U286	G98
G	C1967				C	A919	C765	A538	C287	A101
A			A1508	G1182	A	A927	U775	U545	U288	U102
U	A1970	A1782	A1509	U1183	U	U931	G776	U546	C289	A118
A	U1971	A1784	A1515	U1184	U	C944	G776	A547	U290	A119
G	G1972				U	A945	U761	A548	G548	U120
G					A	C946	A782	G549	C291	G122
G	U1991	G1799	G1529	G1190	A	A945	A781	U558	A299	A131
U	G1992	C1800	U1534	A1205	A	A945	A782	U558	G303	A131
G	U1993	A1801			G	U955	A783	G303	U304	A118
G					A	C961	G784	A563	G121	A119
A	A2000	A1808	A1535	G1239	A	C961	G785	C564	G361	G141
G		A1809	C1536	U1240	A	C961	G785	A575	A362	A142
G			G1537	A1253	U	A996	U811	G579	G386	A165
C	A2014	C1816			C	C974	C812	U850	U395	A181
U					C	A789	A820	A586	G396	G185
U	A2019	A1829	A1569	G1256	G	U990	A821	A404	U405	A196
U	A2020				U	A983	A821	A627	G411	A199
U		A1847	U1578	G1271	U	A984	G805	A412	A119	U200
G	C2023	A1848		A1272	A	C985	C806	G420	A204	A207
A					U	U	U811	U637	C420	C208
A					U	A996	C812	G638	G476	G215
G	A2030	A1853	U1584	A1286	A	U1012	U827	U639	A644	A216
G	A2031	C1585	C1585	A1287	A	C1013	U828	C640	G645	A217
G					G	A1020	U828	U615	G647	A218
G	A2032	C1604	C1604	G1296	C	G1022	U846	A404	A492	A221
G					U	A1028	U847	A654	C493	
G	A2033				C	A1028	U847	A654	A654	
U					U	U1033	G857	G857	A654	
G	A2034	C1607	U1647	A1365	A	U1033	G858	G858	G858	
G	G2038	A1608	U1648	A1378	A	G1047	G859	G859	G859	
G	U2039	G1861	C1649	U1379	A	C1052	U860	C640	G861	
G	G2040	G1862	A1610	G1110	A	C	U860	A644	G861	
C	U2041	G1869		G1111	A	G1047	U860	A644	G861	
C	A2042			G1112	A	C1052	U860	A644	G861	
C					U	C	U860	A644	G861	
C	C2043	A1637	A1637	U1352	G	A	U860</			



• Molecule 31: 5S rRNA



• Molecule 32: Large ribosomal subunit protein uL2



• Molecule 33: Large ribosomal subunit protein uL3

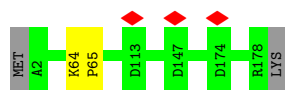


• Molecule 34: Large ribosomal subunit protein uL4



• Molecule 35: Large ribosomal subunit protein uL5





- Molecule 36: Large ribosomal subunit protein uL6

Chain g: 97%



- Molecule 37: Large ribosomal subunit protein bL9

Chain h: 74%
99%



- Molecule 38: Large ribosomal subunit protein uL13

Chain i: 96%



- Molecule 39: Large ribosomal subunit protein uL14

Chain j: 96%



- Molecule 40: Large ribosomal subunit protein uL15

Chain k: 97%



- Molecule 41: Large ribosomal subunit protein uL16

Chain l: 96%



- Molecule 42: Large ribosomal subunit protein bL17

Chain m: 91% 7%



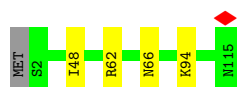
- Molecule 43: Large ribosomal subunit protein uL18

Chain n: 99%



- Molecule 44: Large ribosomal subunit protein bL19

Chain o: 96%



- Molecule 45: Large ribosomal subunit protein bL20

Chain p: 95%



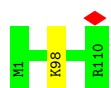
- Molecule 46: Large ribosomal subunit protein bL21

Chain q: 98%



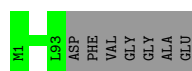
- Molecule 47: Large ribosomal subunit protein uL22

Chain r: 99%



- Molecule 48: Large ribosomal subunit protein uL23

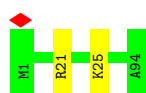
Chain s: 93% 7%



- Molecule 49: Large ribosomal subunit protein uL24



- Molecule 50: Large ribosomal subunit protein bL25



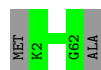
- Molecule 51: Large ribosomal subunit protein bL27



- Molecule 52: Large ribosomal subunit protein bL28



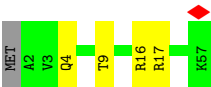
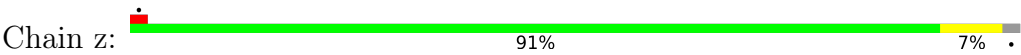
- Molecule 53: Large ribosomal subunit protein uL29



- Molecule 54: Large ribosomal subunit protein uL30



- Molecule 55: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81491	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 ($e^-/\text{\AA}^2$)	51.5	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	0.604	Depositor
Minimum map value	-0.175	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0474	Depositor
Map size (Å)	436.896, 436.896, 436.896	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7585, 0.7585, 0.7585	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.45	0/424	0.78	0/565
2	1	0.47	0/380	0.89	0/498
3	2	0.49	0/513	0.88	0/676
4	3	0.47	0/303	0.85	0/397
5	4	0.47	0/488	0.85	0/649
6	A	0.52	1/36284 (0.0%)	0.79	3/56595 (0.0%)
7	B	0.46	0/1784	0.90	0/2403
8	C	0.46	0/1651	0.85	0/2225
9	D	0.44	0/1665	0.89	0/2227
10	E	0.46	0/1165	0.82	0/1568
11	F	0.46	0/858	0.82	0/1160
12	G	0.46	0/1219	0.93	0/1635
13	H	0.46	0/989	0.85	0/1326
14	I	0.45	0/1034	0.88	0/1375
15	J	0.46	0/796	0.85	0/1077
16	K	0.50	0/884	0.85	0/1191
17	L	0.46	0/960	0.84	0/1286
18	M	0.47	0/900	0.93	0/1204
19	N	0.46	0/817	0.91	0/1088
20	O	0.43	0/722	0.95	0/964
21	P	0.46	0/653	0.85	0/877
22	Q	0.46	0/650	0.79	0/871
23	R	0.45	0/553	0.92	0/742
24	S	0.48	0/685	0.83	0/922
25	T	0.46	0/676	0.98	0/895
26	U	0.46	0/598	0.96	0/792
27	X	0.54	0/242	0.80	0/375
28	Y	0.56	0/1596	0.80	0/2478
29	Z	0.56	1/1608 (0.1%)	0.77	0/2500
30	a	0.49	1/65747 (0.0%)	0.83	6/102563 (0.0%)
31	b	0.52	0/2850	0.79	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.48	0/2121	0.84	0/2852
33	d	0.46	0/1576	0.78	0/2119
34	e	0.45	0/1571	0.84	0/2113
35	f	0.44	0/1434	0.89	0/1926
36	g	0.48	0/1333	0.83	0/1805
37	h	0.46	0/1122	0.82	0/1515
38	i	0.45	0/1152	0.83	0/1551
39	j	0.45	0/956	0.82	0/1279
40	k	0.47	0/1062	0.83	0/1413
41	l	0.45	0/1073	0.84	0/1433
42	m	0.46	0/958	0.90	0/1281
43	n	0.46	0/902	0.89	0/1209
44	o	0.45	0/929	0.75	0/1242
45	p	0.45	0/960	0.90	0/1278
46	q	0.44	0/829	0.72	0/1107
47	r	0.46	0/864	0.83	0/1156
48	s	0.44	0/744	0.79	0/994
49	t	0.46	0/787	0.80	0/1051
50	u	0.45	0/766	0.79	0/1025
51	v	0.46	0/642	0.81	0/848
52	w	0.45	0/635	0.84	0/848
53	x	0.41	0/496	0.90	0/660
54	y	0.45	0/453	0.85	0/605
55	z	0.47	0/450	0.88	0/599
All	All	0.49	3/153509 (0.0%)	0.82	9/229477 (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
3	2	0	1
15	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	527	G7M	O3'-P	5.16	1.61	1.56
30	a	2069	G7M	O3'-P	5.12	1.61	1.56
29	Z	8	4SU	O3'-P	5.02	1.61	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1905	C	O3'-P-O5'	-8.13	91.81	104.00
6	A	572	A	O3'-P-O5'	-7.25	93.13	104.00
30	a	204	A	O3'-P-O5'	-6.73	93.91	104.00
30	a	781	A	O3'-P-O5'	-6.42	94.36	104.00
6	A	563	A	O3'-P-O5'	-5.42	95.86	104.00
30	a	2601	C	O3'-P-O5'	-5.14	96.28	104.00
30	a	1966	A	O3'-P-O5'	-5.13	96.31	104.00
30	a	2501	C	O3'-P-O5'	-5.04	96.45	104.00
6	A	812	G	O3'-P-O5'	-5.01	96.49	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
15	J	62	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	0	417	0	451	1	0
2	1	377	0	418	0	0
3	2	504	0	572	2	0
4	3	302	0	340	1	0
5	4	480	0	478	1	0
6	A	32655	0	16454	41	0
7	B	1753	0	1780	3	0
8	C	1624	0	1696	1	0
9	D	1643	0	1707	2	0
10	E	1152	0	1196	2	0
11	F	839	0	833	0	0
12	G	1203	0	1254	0	0
13	H	979	0	1031	1	0
14	I	1022	0	1070	0	0
15	J	786	0	828	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	877	0	884	0	0
17	L	957	0	1017	2	0
18	M	891	0	952	0	0
19	N	805	0	844	1	0
20	O	714	0	734	0	0
21	P	643	0	661	1	0
22	Q	641	0	682	0	0
23	R	544	0	565	0	0
24	S	668	0	693	0	0
25	T	670	0	719	1	0
26	U	590	0	629	1	0
27	X	216	0	108	0	0
28	Y	1539	0	791	4	0
29	Z	1546	0	794	3	0
30	a	59216	0	29807	115	0
31	b	2549	0	1291	2	0
32	c	2082	0	2154	10	0
33	d	1566	0	1618	4	0
34	e	1552	0	1619	6	0
35	f	1410	0	1444	1	0
36	g	1313	0	1358	5	0
37	h	1111	0	1148	1	0
38	i	1129	0	1162	5	0
39	j	947	0	1023	3	0
40	k	1053	0	1129	4	0
41	l	1075	0	1145	4	0
42	m	945	0	989	2	0
43	n	892	0	923	0	0
44	o	917	0	962	4	0
45	p	947	0	1019	4	0
46	q	816	0	839	2	0
47	r	857	0	922	1	0
48	s	738	0	807	0	0
49	t	779	0	831	2	0
50	u	753	0	780	1	0
51	v	634	0	653	0	0
52	w	625	0	652	1	0
53	x	495	0	526	0	0
54	y	449	0	488	0	0
55	z	444	0	458	4	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	A	23	0	24	2	0
58	A	46	0	0	0	0
58	Z	1	0	0	0	0
58	a	186	0	0	0	0
58	b	2	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	z	1	0	0	0	0
59	Y	7	0	8	3	0
60	a	6	0	0	0	0
61	0	14	0	0	0	0
61	1	21	0	0	0	0
61	2	19	0	0	0	0
61	3	12	0	0	0	0
61	A	1816	0	0	0	0
61	B	23	0	0	0	0
61	C	29	0	0	0	0
61	D	29	0	0	0	0
61	E	23	0	0	0	0
61	F	6	0	0	0	0
61	G	17	0	0	0	0
61	H	25	0	0	0	0
61	I	18	0	0	0	0
61	J	16	0	0	0	0
61	K	13	0	0	0	0
61	L	23	0	0	0	0
61	M	16	0	0	0	0
61	N	20	0	0	0	0
61	O	15	0	0	0	0
61	P	13	0	0	0	0
61	Q	13	0	0	0	0
61	R	8	0	0	0	0
61	S	8	0	0	0	0
61	T	7	0	0	0	0
61	U	16	0	0	0	0
61	X	10	0	0	0	0
61	Y	33	0	0	0	0
61	Z	37	0	0	0	0
61	a	5230	0	0	26	0
61	b	142	0	0	0	0
61	c	116	0	0	3	0
61	d	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	e	70	0	0	1	0
61	f	10	0	0	0	0
61	g	23	0	0	5	0
61	h	19	0	0	0	0
61	i	34	0	0	0	0
61	j	33	0	0	1	0
61	k	54	0	0	2	0
61	l	51	0	0	0	0
61	m	29	0	0	0	0
61	n	13	0	0	0	0
61	o	38	0	0	2	0
61	p	51	0	0	0	0
61	q	43	0	0	1	0
61	r	39	0	0	1	0
61	s	20	0	0	0	0
61	t	20	0	0	0	0
61	u	18	0	0	0	0
61	v	31	0	0	0	0
61	w	25	0	0	0	0
61	x	10	0	0	0	0
61	y	21	0	0	0	0
61	z	33	0	0	2	0
All	All	151159	0	95960	221	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 (221) 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)
30:a:2553:G:H3'	61:a:3532:HOH:O	1.53	1.05
36:g:148:LEU:HD12	61:g:201:HOH:O	1.62	0.99
36:g:133:LEU:HD11	61:g:201:HOH:O	1.82	0.78
30:a:1654:A:H3'	61:a:5692:HOH:O	1.85	0.76
44:o:48:ILE:HG12	61:o:201:HOH:O	1.87	0.74
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.70	0.73
36:g:144:VAL:HG12	61:g:201:HOH:O	1.87	0.72
30:a:2054:A:H3'	61:a:3204:HOH:O	1.91	0.69
30:a:12:U:H2'	30:a:12:U:O2	1.96	0.64
38:i:125:TYR:HH	38:i:132:HIS:HE2	1.44	0.64
30:a:2552:OMU:HM22	61:a:3532:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:579:G:H4'	61:a:3205:HOH:O	1.97	0.63
30:a:2445:2MG:O5'	61:a:3201:HOH:O	2.16	0.62
36:g:145:ALA:HA	61:g:201:HOH:O	1.99	0.62
30:a:2494:G:O2'	41:l:79:ALA:HA	2.02	0.60
6:A:823:C:HO2'	13:H:2:SER:N	2.00	0.59
44:o:62:ARG:N	61:o:201:HOH:O	2.35	0.58
30:a:1508:A:O2'	30:a:1509:A:O4'	2.21	0.57
32:c:219:THR:HG22	61:c:435:HOH:O	2.04	0.57
30:a:2056:G:H5''	61:a:3204:HOH:O	2.05	0.57
30:a:2552:OMU:CM2	61:a:3532:HOH:O	2.51	0.57
28:Y:60:C:H5''	28:Y:60:C:H6	1.69	0.57
30:a:2547:A:H2'	30:a:2548:U:C6	2.40	0.57
30:a:1434:A:H2'	30:a:1435:G:C8	2.40	0.57
61:a:3206:HOH:O	32:c:238:ARG:HG3	2.05	0.57
55:z:16:ARG:NE	61:z:201:HOH:O	2.37	0.57
6:A:993:G:O2'	6:A:994:A:N7	2.38	0.56
30:a:580:U:H5''	61:a:3692:HOH:O	2.05	0.56
40:k:41:ARG:NH1	61:k:201:HOH:O	2.39	0.56
32:c:39:LYS:NZ	61:c:401:HOH:O	2.33	0.55
6:A:664:G:H22	6:A:741:G:H1	1.54	0.55
46:q:76:LYS:NZ	61:q:201:HOH:O	2.39	0.55
57:A:1601:SCM:H2M1	10:E:27:GLY:HA2	1.87	0.54
61:a:3709:HOH:O	32:c:242:LYS:HE2	2.07	0.54
6:A:769:G:H4'	6:A:1513:A:H4'	1.89	0.54
6:A:1391:U:H2'	6:A:1392:G:C8	2.43	0.54
47:r:98:LYS:NZ	61:r:201:HOH:O	2.40	0.54
30:a:534:U:O2'	45:p:49:ASP:OD2	2.20	0.54
30:a:1190:G:H5''	40:k:32:GLY:HA2	1.90	0.54
30:a:2627:G:O2'	30:a:2781:A:N1	2.38	0.53
30:a:12:U:O2	30:a:12:U:C2'	2.56	0.53
30:a:565:C:H3'	61:a:4388:HOH:O	2.09	0.53
7:B:94:HIS:O	7:B:95:ARG:C	2.51	0.53
30:a:2747:G:O6	30:a:2755:C:H5''	2.10	0.52
59:Y:101:VAL:N	29:Z:76:A:HO3'	2.07	0.52
61:a:3206:HOH:O	32:c:238:ARG:N	2.41	0.52
30:a:1115:G:O2'	30:a:1116:G:O5'	2.22	0.52
32:c:271:ARG:O	32:c:272:SER:C	2.52	0.52
30:a:2386:A:N7	61:a:3213:HOH:O	2.34	0.51
33:d:121:THR:HB	33:d:127:PHE:CD2	2.46	0.51
6:A:502:A:H2'	6:A:503:C:O4'	2.10	0.51
30:a:1434:A:H2'	30:a:1435:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:162:ALA:HA	61:d:412:HOH:O	2.10	0.51
30:a:493:G:H2'	30:a:494:G:O4'	2.11	0.51
41:l:66:ARG:NH2	41:l:104:GLU:OE2	2.44	0.51
45:p:76:TYR:CZ	45:p:80:ILE:HG13	2.46	0.50
30:a:84:A:N1	30:a:98:G:O2'	2.42	0.49
3:2:54:ASP:HB3	40:k:57:LEU:HD22	1.93	0.49
30:a:476:G:H4'	30:a:502:A:N1	2.27	0.49
30:a:2766:A:H2'	30:a:2766:A:N3	2.27	0.49
6:A:303:A:H2'	6:A:304:U:O4'	2.12	0.49
6:A:1191:A:OP1	8:C:4:LYS:NZ	2.42	0.49
30:a:645:C:H2'	30:a:647:G:C8	2.48	0.49
30:a:944:C:O2'	61:a:3203:HOH:O	2.20	0.49
30:a:1939:5MU:OP1	30:a:2604:PSU:O2'	2.29	0.49
30:a:1778:U:H2'	30:a:1784:A:N6	2.28	0.49
6:A:337:G:H2'	6:A:338:A:C8	2.48	0.49
28:Y:37:6MZ:O2'	30:a:1913:A:N1	2.43	0.49
30:a:806:C:H3'	61:k:201:HOH:O	2.13	0.48
30:a:2273:A:H2'	30:a:2274:A:C8	2.48	0.48
30:a:1637:A:H2'	30:a:1638:C:O4'	2.14	0.48
30:a:2291:U:H2'	30:a:2292:U:C6	2.48	0.48
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.95	0.48
30:a:857:G:H2'	30:a:858:G:O4'	2.14	0.48
30:a:811:U:H2'	40:k:21:ARG:HA	1.95	0.48
30:a:2552:OMU:HM23	30:a:2554:U:C6	2.49	0.47
30:a:2780:G:OP2	38:i:120:ARG:HD3	2.14	0.47
30:a:303:G:H2'	30:a:304:U:C6	2.49	0.47
30:a:2591:C:H2'	30:a:2592:G:C8	2.50	0.47
6:A:928:G:O2'	6:A:1533:C:OP1	2.33	0.47
30:a:1028:A:N6	30:a:1125:G:H2'	2.29	0.47
30:a:1932:A:H2'	30:a:1933:G:O4'	2.14	0.47
30:a:1296:G:OP1	30:a:2709:G:O2'	2.29	0.47
6:A:1402:4OC:O2	6:A:1500:A:N1	2.48	0.47
41:l:53:MET:HE1	41:l:103:TYR:CG	2.49	0.47
30:a:2060:A:N6	61:a:3348:HOH:O	2.48	0.47
34:e:58:LYS:NZ	61:e:301:HOH:O	2.43	0.47
6:A:1526:G:N7	26:U:40:LYS:NZ	2.62	0.46
30:a:747:5MU:O2	30:a:2014:A:H1'	2.15	0.46
6:A:673:A:H2'	6:A:674:G:C8	2.51	0.46
30:a:207:A:H2'	30:a:208:C:O4'	2.15	0.46
61:a:3692:HOH:O	45:p:33:ARG:HD2	2.15	0.46
6:A:553:A:H5''	17:L:21:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1156:A:C8	45:p:51:ARG:HG2	2.50	0.46
36:g:144:VAL:C	61:g:201:HOH:O	2.58	0.46
30:a:639:U:H2'	30:a:640:C:C6	2.51	0.46
30:a:945:A:H2'	61:a:3673:HOH:O	2.14	0.46
30:a:1021:A:N3	30:a:1021:A:H3'	2.30	0.46
33:d:156:PHE:CE1	38:i:81:ILE:HD13	2.51	0.46
30:a:1676:A:H2'	30:a:1677:A:O4'	2.16	0.46
7:B:28:LYS:N	7:B:29:PRO:CD	2.79	0.45
30:a:723:C:H2'	30:a:724:U:O4'	2.16	0.45
30:a:2019:A:P	61:a:3205:HOH:O	2.74	0.45
19:N:73:PHE:CZ	19:N:78:GLY:HA2	2.52	0.45
30:a:1754:A:C8	44:o:94:LYS:CE	3.00	0.45
30:a:2000:C:OP1	42:m:5:LYS:NZ	2.40	0.45
6:A:293:G:H4'	6:A:609:A:N1	2.32	0.45
6:A:1486:G:H2'	6:A:1487:G:O4'	2.17	0.45
10:E:38:VAL:HG11	10:E:114:VAL:HG22	1.98	0.45
15:J:59:LYS:HE2	15:J:62:ARG:NH1	2.31	0.45
30:a:785:G:P	61:a:3268:HOH:O	2.74	0.45
39:j:107:LEU:O	39:j:109:SER:N	2.50	0.45
55:z:17:ARG:HG3	61:z:201:HOH:O	2.16	0.45
59:Y:101:VAL:HG11	30:a:2452:C:O4'	2.16	0.45
30:a:644:A:H2'	30:a:645:C:O4'	2.17	0.45
52:w:3:ARG:O	52:w:12:PRO:HD3	2.17	0.45
6:A:1218:C:H2'	6:A:1219:A:C8	2.53	0.44
30:a:2327:A:H2'	30:a:2328:A:C8	2.52	0.44
33:d:62:LYS:N	33:d:63:PRO:HD2	2.32	0.44
34:e:41:GLN:HG2	34:e:43:THR:HG23	1.98	0.44
6:A:1356:G:H2'	6:A:1357:A:C8	2.53	0.44
30:a:1607:C:H4'	30:a:1608:A:O5'	2.16	0.44
32:c:221:ARG:HG3	61:c:435:HOH:O	2.16	0.44
30:a:2233:U:H2'	30:a:2234:G:C8	2.53	0.44
6:A:49:U:O2	6:A:362:G:H1'	2.18	0.44
59:Y:101:VAL:HG21	61:a:7835:HOH:O	2.17	0.44
61:a:3337:HOH:O	34:e:72:SER:HB3	2.16	0.44
6:A:533:A:O2'	6:A:535:A:OP2	2.25	0.44
6:A:1064:G:N7	57:A:1601:SCM:O11	2.44	0.44
30:a:1799:G:O2'	32:c:180:GLU:OE2	2.34	0.44
30:a:2038:G:H2'	30:a:2039:U:O4'	2.18	0.44
38:i:125:TYR:OH	38:i:132:HIS:NE2	2.37	0.44
30:a:120:U:H5''	30:a:122:G:OP2	2.17	0.44
30:a:918:A:O2'	31:b:96:G:N2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:977:A:H1'	6:A:982:U:O4	2.17	0.43
30:a:1311:G:N7	61:a:3216:HOH:O	2.36	0.43
30:a:2020:A:H5'	55:z:9:THR:CG2	2.49	0.43
30:a:185:G:H4'	30:a:218:A:H4'	2.00	0.43
6:A:109:A:C6	6:A:326:G:C6	3.07	0.43
6:A:965:U:O4'	6:A:969:A:H1'	2.19	0.43
30:a:1183:U:H2'	30:a:1184:U:C6	2.54	0.43
30:a:2469:A:H4'	41:l:55:ARG:HD2	2.00	0.43
37:h:31:VAL:N	37:h:32:PRO:HD2	2.34	0.43
6:A:244:U:O4	6:A:906:A:H1'	2.18	0.43
30:a:788:A:OP1	30:a:790:U:H5	2.02	0.43
30:a:1508:A:HO2'	30:a:1509:A:C4'	2.30	0.43
30:a:1637:A:H5'	30:a:1760:C:O2'	2.19	0.43
46:q:74:ILE:N	46:q:74:ILE:HD12	2.34	0.43
30:a:1474:U:C4	30:a:1475:G:C6	3.07	0.43
5:4:40:CYS:O	5:4:40:CYS:SG	2.76	0.43
6:A:1053:G:N7	6:A:1200:C:H5''	2.34	0.43
6:A:757:U:H2'	6:A:758:C:O4'	2.18	0.43
30:a:2522:U:O2'	30:a:2647:U:OP1	2.32	0.43
6:A:1148:U:H2'	6:A:1149:C:O4'	2.19	0.43
30:a:2040:G:H2'	30:a:2041:U:O4'	2.18	0.43
6:A:526:C:OP2	17:L:88:LYS:HE3	2.18	0.42
30:a:263:G:H2'	30:a:264:C:O4'	2.18	0.42
30:a:1859:U:H2'	30:a:1860:G:C8	2.54	0.42
30:a:1916:A:H2'	30:a:1917:PSU:O4'	2.19	0.42
6:A:8:A:N6	9:D:202:GLU:O	2.52	0.42
29:Z:8:4SU:H6	29:Z:8:4SU:O5'	2.19	0.42
29:Z:12:G:H5''	30:a:1908:C:O2'	2.19	0.42
30:a:1853:A:N1	30:a:2087:G:H1'	2.33	0.42
28:Y:60:C:H5'	28:Y:61:C:H5	1.85	0.42
30:a:1141:U:H4'	30:a:1142:A:O4'	2.19	0.42
30:a:1205:A:C6	34:e:165:HIS:HB2	2.55	0.42
30:a:1405:U:H2'	30:a:1406:U:C6	2.55	0.42
30:a:687:C:H2'	30:a:688:U:O4'	2.20	0.42
30:a:861:A:C2	30:a:917:A:C4	3.07	0.42
30:a:2328:A:H2'	30:a:2329:U:C6	2.54	0.42
30:a:1378:A:O2'	30:a:1380:G:N7	2.52	0.42
1:0:13:SER:OG	1:0:40:ASP:OD2	2.33	0.42
6:A:1408:A:O2'	30:a:1916:A:N1	2.48	0.42
30:a:2506:U:C2	30:a:2585:U:O4	2.72	0.42
30:a:2678:C:H2'	30:a:2679:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2788:C:H2'	30:a:2789:C:C6	2.54	0.42
50:u:21:ARG:HA	50:u:25:LYS:O	2.20	0.42
30:a:1604:C:O2'	30:a:1610:A:N1	2.47	0.42
61:a:3348:HOH:O	34:e:69:ARG:NH1	2.53	0.42
30:a:558:U:OP1	38:i:113:PRO:HD2	2.20	0.42
30:a:1808:A:H3'	30:a:1809:A:C8	2.55	0.42
7:B:130:THR:O	7:B:132:LYS:N	2.52	0.41
30:a:101:A:H2'	30:a:101:A:N3	2.35	0.41
4:3:16:ILE:HD13	4:3:25:VAL:HG22	2.01	0.41
6:A:918:A:H2'	6:A:919:A:O4'	2.21	0.41
30:a:2243:U:H2'	30:a:2244:U:C6	2.55	0.41
39:j:101:GLY:HA2	44:o:66:ASN:HB2	2.02	0.41
6:A:376:G:H5''	21:P:5:ARG:HB2	2.02	0.41
30:a:1779:U:H1'	61:a:3268:HOH:O	2.19	0.41
6:A:607:A:H2'	6:A:608:A:C8	2.55	0.41
6:A:1098:C:H2'	6:A:1099:G:O4'	2.20	0.41
30:a:395:U:O2'	30:a:396:G:N7	2.47	0.41
30:a:820:A:H2'	30:a:821:A:O4'	2.20	0.41
30:a:910:A:H2'	30:a:911:A:C8	2.55	0.41
30:a:2756:U:H1'	30:a:2757:A:H5''	2.02	0.41
6:A:896:C:H2'	6:A:897:C:O4'	2.20	0.41
30:a:2542:A:H5''	30:a:2766:A:O2'	2.20	0.41
3:2:27:ALA:O	3:2:28:ASN:HB2	2.21	0.41
30:a:1182:G:H2'	30:a:1183:U:O4'	2.21	0.41
35:f:64:LYS:HA	35:f:65:PRO:HD3	1.93	0.41
6:A:542:G:H5'	9:D:39:GLY:HA3	2.03	0.41
6:A:1152:A:OP1	15:J:70:HIS:ND1	2.51	0.41
25:T:55:GLN:N	25:T:56:PRO:HD2	2.36	0.41
30:a:1902:C:H4'	32:c:242:LYS:O	2.21	0.41
30:a:2615:U:C2	55:z:4:GLN:HA	2.56	0.41
42:m:56:LYS:HE2	42:m:87:PHE:O	2.21	0.41
30:a:278:A:O2'	30:a:279:A:P	2.79	0.40
30:a:1239:G:H2'	30:a:1240:U:O4'	2.20	0.40
61:a:3337:HOH:O	34:e:75:SER:HB2	2.20	0.40
6:A:1074:G:O2'	6:A:1101:A:N1	2.50	0.40
28:Y:8:4SU:H6	28:Y:8:4SU:O5'	2.20	0.40
30:a:1020:A:C2	30:a:1141:U:C2	3.10	0.40
30:a:2800:A:C2	30:a:2895:G:H1'	2.55	0.40
49:t:10:GLU:HG3	49:t:73:PHE:HB3	2.03	0.40
49:t:54:GLN:N	49:t:55:PRO:CD	2.84	0.40
31:b:106:G:H2'	31:b:107:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:58:G:O2'	30:a:73:A:N1	2.45	0.40
30:a:299:A:N1	30:a:322:A:O2'	2.46	0.40
6:A:867:G:O2'	6:A:873:A:N1	2.47	0.40
6:A:892:A:H2'	6:A:893:C:O4'	2.22	0.40
39:j:2:ILE:HG22	61:j:231:HOH:O	2.22	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	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
7	B	222/241 (92%)	211 (95%)	10 (4%)	1 (0%)	24	17
8	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
9	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
10	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
11	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
12	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
13	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
15	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	5
16	K	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
17	L	120/124 (97%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
19	N	98/101 (97%)	98 (100%)	0	0	100	100
20	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
21	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
22	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
23	R	64/75 (85%)	64 (100%)	0	0	100	100
24	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
25	T	84/87 (97%)	84 (100%)	0	0	100	100
26	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
32	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
33	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
34	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
35	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
36	g	173/177 (98%)	170 (98%)	3 (2%)	0	100	100
37	h	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
38	i	140/142 (99%)	140 (100%)	0	0	100	100
39	j	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	8
40	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
41	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
42	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
43	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
46	q	101/103 (98%)	101 (100%)	0	0	100	100
47	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
48	s	91/100 (91%)	91 (100%)	0	0	100	100
49	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
50	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
51	v	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	59/63 (94%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5593/5913 (95%)	5440 (97%)	150 (3%)	3 (0%)	49	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	J	57	VAL
39	j	108	ARG
7	B	131	LYS

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	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	51
7	B	186/199 (94%)	186 (100%)	0	100	100
8	C	170/190 (90%)	170 (100%)	0	100	100
9	D	172/173 (99%)	172 (100%)	0	100	100
10	E	119/126 (94%)	119 (100%)	0	100	100
11	F	90/116 (78%)	90 (100%)	0	100	100
12	G	126/147 (86%)	126 (100%)	0	100	100
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	105/107 (98%)	105 (100%)	0	100	100
15	J	86/90 (96%)	86 (100%)	0	100	100
16	K	89/98 (91%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L	102/103 (99%)	102 (100%)	0	100	100
18	M	93/96 (97%)	93 (100%)	0	100	100
19	N	83/84 (99%)	83 (100%)	0	100	100
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	65/65 (100%)	65 (100%)	0	100	100
22	Q	73/78 (94%)	73 (100%)	0	100	100
23	R	57/65 (88%)	57 (100%)	0	100	100
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	60 (100%)	0	100	100
32	c	216/218 (99%)	216 (100%)	0	100	100
33	d	163/163 (100%)	163 (100%)	0	100	100
34	e	165/165 (100%)	165 (100%)	0	100	100
35	f	148/150 (99%)	148 (100%)	0	100	100
36	g	136/138 (99%)	136 (100%)	0	100	100
37	h	114/114 (100%)	114 (100%)	0	100	100
38	i	116/116 (100%)	116 (100%)	0	100	100
39	j	104/104 (100%)	104 (100%)	0	100	100
40	k	103/103 (100%)	103 (100%)	0	100	100
41	l	107/107 (100%)	107 (100%)	0	100	100
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	86 (100%)	0	100	100
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	84 (100%)	0	100	100
47	r	93/93 (100%)	93 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	83/85 (98%)	83 (100%)	0	100	100
50	u	78/78 (100%)	78 (100%)	0	100	100
51	v	62/63 (98%)	62 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4657/4825 (96%)	4656 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	6	GLN
7	B	58	ASN
7	B	103	ASN
9	D	40	GLN
10	E	73	ASN
10	E	132	ASN
11	F	17	GLN
11	F	37	HIS
11	F	46	GLN
12	G	9	GLN
12	G	68	ASN
14	I	4	ASN
14	I	75	GLN
20	O	40	GLN
23	R	52	GLN
26	U	56	HIS
26	U	64	ASN
32	c	90	ASN
32	c	153	GLN
34	e	94	GLN
34	e	136	GLN
34	e	165	HIS
35	f	21	ASN
36	g	22	GLN
36	g	73	ASN
36	g	104	ASN
37	h	33	GLN

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Mol	Chain	Res	Type
37	h	66	ASN
37	h	119	ASN
37	h	145	ASN
38	i	58	ASN
38	i	80	HIS
38	i	128	ASN
40	k	35	HIS
41	l	3	GLN
41	l	97	GLN
42	m	9	GLN
44	o	10	GLN
45	p	52	GLN
45	p	81	ASN
46	q	86	GLN
50	u	12	GLN
52	w	17	ASN
52	w	20	HIS
53	x	58	ASN
54	y	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	9/10 (90%)	2 (22%)	0
28	Y	68/76 (89%)	14 (20%)	0
29	Z	68/78 (87%)	9 (13%)	0
30	a	2753/2904 (94%)	288 (10%)	0
31	b	118/120 (98%)	9 (7%)	0
6	A	1518/1544 (98%)	184 (12%)	23 (1%)
All	All	4534/4732 (95%)	506 (11%)	23 (0%)

All (506) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	6	G
6	A	22	G
6	A	32	A
6	A	39	G
6	A	47	C
6	A	48	C

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Mol	Chain	Res	Type
6	A	50	A
6	A	51	A
6	A	71	A
6	A	83	C
6	A	85	U
6	A	86	G
6	A	87	C
6	A	95	C
6	A	120	A
6	A	131	A
6	A	144	G
6	A	149	A
6	A	163	C
6	A	164	G
6	A	181	A
6	A	182	A
6	A	197	A
6	A	204	G
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	289	G
6	A	321	A
6	A	328	C
6	A	329	A
6	A	339	C
6	A	347	G
6	A	352	C
6	A	354	G
6	A	367	U
6	A	368	U
6	A	372	C
6	A	384	G
6	A	398	U
6	A	406	G
6	A	411	A
6	A	412	A
6	A	413	G

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Mol	Chain	Res	Type
6	A	414	A
6	A	429	U
6	A	436	C
6	A	438	U
6	A	439	U
6	A	451	A
6	A	453	G
6	A	457	G
6	A	467	U
6	A	468	A
6	A	469	C
6	A	479	U
6	A	481	G
6	A	484	G
6	A	486	U
6	A	499	A
6	A	511	C
6	A	518	C
6	A	531	U
6	A	547	A
6	A	559	A
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	588	G
6	A	633	G
6	A	650	G
6	A	653	U
6	A	665	A
6	A	723	U
6	A	724	G
6	A	734	G
6	A	747	A
6	A	748	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	802	A
6	A	815	A
6	A	817	C

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Mol	Chain	Res	Type
6	A	832	G
6	A	836	G
6	A	847	G
6	A	849	G
6	A	851	G
6	A	887	G
6	A	890	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	942	G
6	A	960	U
6	A	966	2MG
6	A	969	A
6	A	975	A
6	A	976	G
6	A	977	A
6	A	993	G
6	A	1003	G
6	A	1004	A
6	A	1009	U
6	A	1020	G
6	A	1030	U
6	A	1031	C
6	A	1033	G
6	A	1036	A
6	A	1037	C
6	A	1039	G
6	A	1053	G
6	A	1065	U
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1099	G
6	A	1101	A
6	A	1124	G
6	A	1125	U
6	A	1132	C
6	A	1137	C
6	A	1139	G
6	A	1140	C

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Mol	Chain	Res	Type
6	A	1159	U
6	A	1171	A
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1211	U
6	A	1212	U
6	A	1213	A
6	A	1225	A
6	A	1226	C
6	A	1227	A
6	A	1238	A
6	A	1248	A
6	A	1253	G
6	A	1256	A
6	A	1257	A
6	A	1260	G
6	A	1275	A
6	A	1280	A
6	A	1285	A
6	A	1286	U
6	A	1287	A
6	A	1300	G
6	A	1302	C
6	A	1317	C
6	A	1319	A
6	A	1320	C
6	A	1338	G
6	A	1340	A
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1368	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1397	C
6	A	1398	A
6	A	1419	G
6	A	1429	A
6	A	1450	U
6	A	1452	C

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Mol	Chain	Res	Type
6	A	1487	G
6	A	1492	A
6	A	1497	G
6	A	1503	A
6	A	1505	G
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
27	X	14	A
27	X	15	A
28	Y	5	G
28	Y	7	U
28	Y	8	4SU
28	Y	19	G
28	Y	22	G
28	Y	25	C
28	Y	45	G
28	Y	46	G7M
28	Y	49	G
28	Y	50	G
28	Y	60	C
28	Y	70	C
28	Y	73	A
28	Y	74	C
29	Z	9	G
29	Z	14	A
29	Z	19	G
29	Z	46	G7M
29	Z	53	G
29	Z	58	A
29	Z	70	G
29	Z	71	C
29	Z	76	A
30	a	10	A
30	a	34	U
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	102	U

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Mol	Chain	Res	Type
30	a	118	A
30	a	119	A
30	a	120	U
30	a	131	A
30	a	139	U
30	a	140	C
30	a	142	A
30	a	165	A
30	a	181	A
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	272	A
30	a	276	U
30	a	278	A
30	a	279	A
30	a	282	A
30	a	285	G
30	a	287	G
30	a	288	U
30	a	289	G
30	a	291	G
30	a	311	A
30	a	330	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	404	A
30	a	405	U
30	a	411	G
30	a	412	A
30	a	420	C
30	a	451	U
30	a	481	G
30	a	491	G
30	a	503	A
30	a	504	A

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Mol	Chain	Res	Type
30	a	505	A
30	a	509	C
30	a	526	A
30	a	530	G
30	a	532	A
30	a	533	G
30	a	538	A
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	563	A
30	a	573	U
30	a	574	A
30	a	575	A
30	a	586	A
30	a	603	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	654	A
30	a	655	A
30	a	686	U
30	a	717	C
30	a	730	A
30	a	738	G
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	846	U

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Mol	Chain	Res	Type
30	a	847	U
30	a	859	G
30	a	881	G
30	a	883	G
30	a	888	C
30	a	890	C
30	a	891	G
30	a	895	U
30	a	896	A
30	a	897	C
30	a	910	A
30	a	914	G
30	a	915	C
30	a	927	A
30	a	931	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1033	U
30	a	1047	G
30	a	1108	U
30	a	1110	G
30	a	1111	A
30	a	1112	G
30	a	1116	G
30	a	1128	G
30	a	1129	A
30	a	1132	U
30	a	1133	A
30	a	1134	A
30	a	1135	C
30	a	1142	A
30	a	1171	G
30	a	1172	C
30	a	1253	A

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Mol	Chain	Res	Type
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1286	A
30	a	1287	A
30	a	1300	G
30	a	1301	A
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1380	G
30	a	1383	A
30	a	1416	G
30	a	1428	C
30	a	1452	G
30	a	1453	A
30	a	1482	G
30	a	1490	A
30	a	1493	C
30	a	1508	A
30	a	1515	A
30	a	1529	G
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1569	A
30	a	1578	U
30	a	1584	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1732	C
30	a	1738	G
30	a	1764	C
30	a	1773	A

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Mol	Chain	Res	Type
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1809	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1862	G
30	a	1869	G
30	a	1872	A
30	a	1873	G
30	a	1906	G
30	a	1907	G
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2198	A
30	a	2204	G
30	a	2211	A
30	a	2225	A
30	a	2238	G

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Mol	Chain	Res	Type
30	a	2239	G
30	a	2268	A
30	a	2279	G
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2312	U
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2340	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2406	A
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2476	A
30	a	2491	U
30	a	2494	G
30	a	2502	G
30	a	2505	G
30	a	2518	A
30	a	2525	G
30	a	2529	G
30	a	2547	A
30	a	2554	U
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2603	G

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Mol	Chain	Res	Type
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2661	G
30	a	2663	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2757	A
30	a	2765	A
30	a	2769	U
30	a	2778	A
30	a	2790	U
30	a	2791	G
30	a	2797	U
30	a	2798	U
30	a	2799	A
30	a	2818	U
30	a	2820	A
30	a	2821	A
30	a	2861	U
30	a	2883	A
30	a	2884	U
30	a	2891	U
31	b	9	G
31	b	35	C
31	b	36	C
31	b	45	A
31	b	56	G
31	b	89	U
31	b	90	C
31	b	105	G
31	b	109	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A

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Mol	Chain	Res	Type
6	A	13	U
6	A	119	A
6	A	181	A
6	A	199	A
6	A	367	U
6	A	438	U
6	A	481	G
6	A	574	A
6	A	587	G
6	A	776	G
6	A	793	U
6	A	858	G
6	A	884	U
6	A	1035	A
6	A	1046	A
6	A	1124	G
6	A	1211	U
6	A	1225	A
6	A	1281	C
6	A	1319	A
6	A	1397	C
6	A	1505	G

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	$\# Z > 2$
29	G7M	Z	46	29	23,26,27	0.73	1 (4%)	35,39,42	0.54	0
6	G7M	A	527	6	23,26,27	0.73	1 (4%)	35,39,42	0.68	0
16	IAS	K	119	16	6,7,8	0.88	0	6,8,10	0.99	0
28	4SU	Y	8	28	18,21,22	0.37	0	26,30,33	1.20	3 (11%)
29	4SU	Z	8	29	18,21,22	0.36	0	26,30,33	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	2MG	a	2445	30	23,26,27	0.39	0	32,38,41	0.44	0
6	4OC	A	1402	6	20,23,24	0.35	0	26,32,35	0.58	0
30	PSU	a	746	58,30	18,21,22	0.90	1 (5%)	22,30,33	0.61	0
30	5MU	a	747	30	19,22,23	0.26	0	28,32,35	0.38	0
30	5MC	a	1962	30	18,22,23	0.31	0	26,32,35	0.49	0
30	PSU	a	1917	30	18,21,22	0.91	1 (5%)	22,30,33	0.65	0
6	UR3	A	1498	6	19,22,23	0.27	0	26,32,35	0.67	0
30	6MZ	a	1618	30	22,25,26	0.33	0	30,36,39	0.55	0
28	6MZ	Y	37	28	22,25,26	0.33	0	30,36,39	0.49	0
28	PSU	Y	55	28	18,21,22	0.90	1 (5%)	22,30,33	0.61	0
6	MA6	A	1518	6	23,26,27	0.24	0	34,38,41	0.70	1 (2%)
29	5MU	Z	54	29	19,22,23	0.27	0	28,32,35	0.38	0
30	2MA	a	2503	60,58,30	22,25,26	0.88	1 (4%)	33,37,40	1.10	4 (12%)
17	D2T	L	89	17	7,9,10	0.91	0	6,11,13	1.73	2 (33%)
30	5MU	a	1939	30	19,22,23	0.30	0	28,32,35	0.40	0
30	PSU	a	2604	30	18,21,22	0.90	1 (5%)	22,30,33	0.77	1 (4%)
28	5MU	Y	54	28	19,22,23	0.25	0	28,32,35	0.30	0
41	4D4	l	81	41	9,11,12	0.46	0	8,13,15	0.71	0
29	PSU	Z	55	29	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
6	5MC	A	967	6	18,22,23	0.31	0	26,32,35	0.56	0
30	OMC	a	2498	58,30	19,22,23	0.29	0	26,31,34	0.46	0
28	G7M	Y	46	28	23,26,27	0.72	1 (4%)	35,39,42	0.56	0
6	2MG	A	1516	6	23,26,27	0.38	0	32,38,41	0.54	0
33	MEQ	d	150	33	8,9,10	0.43	0	5,10,12	0.60	0
41	MS6	l	82	41	5,7,8	0.18	0	2,7,9	0.03	0
6	MA6	A	1519	6	23,26,27	0.25	0	34,38,41	0.78	1 (2%)
30	PSU	a	2605	30	18,21,22	0.95	1 (5%)	22,30,33	0.79	0
30	1MG	a	745	30	22,26,27	0.48	0	33,39,42	0.53	0
30	OMU	a	2552	30	19,22,23	0.21	0	26,31,34	0.31	0
6	2MG	A	1207	6	23,26,27	0.39	0	32,38,41	0.46	0
6	PSU	A	516	6	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
30	PSU	a	955	30	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
30	PSU	a	1911	30	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
6	2MG	A	966	6	23,26,27	0.39	0	32,38,41	0.36	0
6	5MC	A	1407	6	18,22,23	0.32	0	26,32,35	0.66	0
30	G7M	a	2069	30	23,26,27	0.71	1 (4%)	35,39,42	0.66	0
30	6MZ	a	2030	30	22,25,26	0.35	0	30,36,39	0.64	0
30	PSU	a	2457	30	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
30	OMG	a	2251	60,30,29	23,26,27	0.32	0	33,38,41	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	H2U	a	2449	30	18,21,22	0.60	0	21,30,33	0.74	0
30	PSU	a	2504	60,30	18,21,22	0.86	1 (5%)	22,30,33	0.79	1 (4%)
30	2MG	a	1835	30	23,26,27	0.37	0	32,38,41	0.42	0
30	PSU	a	2580	30	18,21,22	0.90	1 (5%)	22,30,33	0.77	1 (4%)
30	3TD	a	1915	30	18,22,23	0.97	1 (5%)	22,32,35	0.66	0
29	OMC	Z	32	29	19,22,23	0.27	0	26,31,34	0.40	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
29	G7M	Z	46	29	-	1/7/25/26	0/3/3/3
6	G7M	A	527	6	-	1/7/25/26	0/3/3/3
16	IAS	K	119	16	-	0/7/7/8	-
28	4SU	Y	8	28	-	0/7/25/26	0/2/2/2
29	4SU	Z	8	29	-	0/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	0/9/27/28	0/3/3/3
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2
30	PSU	a	746	58,30	-	1/7/25/26	0/2/2/2
30	5MU	a	747	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	1/7/25/26	0/2/2/2
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
28	6MZ	Y	37	28	-	0/9/27/28	0/3/3/3
28	PSU	Y	55	28	-	2/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
29	5MU	Z	54	29	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	60,58,30	-	3/7/25/26	0/3/3/3
17	D2T	L	89	17	-	4/7/12/14	-
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
28	5MU	Y	54	28	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	0/11/12/14	-
29	PSU	Z	55	29	-	1/7/25/26	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	58,30	-	0/9/27/28	0/2/2/2
28	G7M	Y	46	28	-	3/7/25/26	0/3/3/3
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	MEQ	d	150	33	-	3/8/9/11	-
41	MS6	l	82	41	-	1/4/6/8	-
6	MA6	A	1519	6	-	2/11/29/30	0/3/3/3
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3
6	PSU	A	516	6	-	0/7/25/26	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
30	G7M	a	2069	30	-	2/7/25/26	0/3/3/3
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2251	60,30,29	-	0/9/27/28	0/3/3/3
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	2504	60,30	-	0/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
29	OMC	Z	32	29	-	0/9/27/28	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1915	3TD	C6-C5	3.68	1.39	1.35
6	A	516	PSU	C6-C5	3.61	1.39	1.35
30	a	2605	PSU	C6-C5	3.59	1.39	1.35
28	Y	55	PSU	C6-C5	3.58	1.39	1.35
30	a	955	PSU	C6-C5	3.58	1.39	1.35
30	a	746	PSU	C6-C5	3.56	1.39	1.35
30	a	2580	PSU	C6-C5	3.55	1.39	1.35
29	Z	55	PSU	C6-C5	3.54	1.39	1.35
30	a	1917	PSU	C6-C5	3.53	1.39	1.35
30	a	2457	PSU	C6-C5	3.52	1.39	1.35
30	a	1911	PSU	C6-C5	3.52	1.39	1.35
30	a	2604	PSU	C6-C5	3.51	1.39	1.35
30	a	2504	PSU	C6-C5	3.32	1.39	1.35
6	A	527	G7M	C8-N7	2.67	1.37	1.33
29	Z	46	G7M	C8-N7	2.65	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2069	G7M	C8-N7	2.62	1.37	1.33
28	Y	46	G7M	C8-N7	2.56	1.37	1.33
30	a	2503	2MA	C6-N6	-2.41	1.28	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z	8	4SU	C4-N3-C2	-4.36	123.11	127.34
28	Y	8	4SU	C4-N3-C2	-4.35	123.11	127.34
6	A	1518	MA6	C2-N1-C6	2.97	118.76	111.75
30	a	2503	2MA	C5-C4-N3	-2.95	123.87	127.19
6	A	1519	MA6	C2-N1-C6	2.91	118.63	111.75
28	Y	8	4SU	C5-C4-N3	2.74	117.23	114.69
29	Z	8	4SU	C5-C4-N3	2.74	117.23	114.69
30	a	2503	2MA	CM2-C2-N1	2.65	121.28	117.15
17	L	89	D2T	OD1-CG-CB	-2.62	116.94	122.44
30	a	2503	2MA	C2-N1-C6	2.43	121.87	118.08
30	a	2580	PSU	C3'-C2'-C1'	2.43	104.47	101.64
30	a	2503	2MA	N3-C2-N1	-2.27	121.54	125.72
28	Y	8	4SU	N3-C2-N1	2.25	117.87	114.89
30	a	2604	PSU	C2'-C3'-C4'	-2.24	98.29	102.64
29	Z	8	4SU	N3-C2-N1	2.24	117.86	114.89
17	L	89	D2T	OD2-CG-CB	2.14	117.78	113.15
30	a	2504	PSU	C2'-C3'-C4'	-2.05	98.66	102.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD2
28	Y	46	G7M	O4'-C4'-C5'-O5'
28	Y	46	G7M	C3'-C4'-C5'-O5'
6	A	1519	MA6	O4'-C4'-C5'-O5'
30	a	2030	6MZ	O4'-C4'-C5'-O5'
6	A	1519	MA6	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
33	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	C3'-C4'-C5'-O5'
28	Y	46	G7M	C4'-C5'-O5'-P
33	d	150	MEQ	C-CA-CB-CG
41	l	82	MS6	CB-CG-SD-CE
17	L	89	D2T	CA-CB-CG-OD1

Continued on next page...

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Mol	Chain	Res	Type	Atoms
29	Z	46	G7M	C4'-C5'-O5'-P
30	a	2069	G7M	C4'-C5'-O5'-P
28	Y	55	PSU	O4'-C1'-C5-C4
17	L	89	D2T	SB-CB-CG-OD2
17	L	89	D2T	CG-CB-SB-CB1
28	Y	55	PSU	O4'-C1'-C5-C6
29	Z	55	PSU	O4'-C1'-C5-C6
30	a	746	PSU	O4'-C1'-C5-C6
6	A	527	G7M	C4'-C5'-O5'-P
30	a	2503	2MA	C4'-C5'-O5'-P
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	2503	2MA	O4'-C1'-N9-C8

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Y	8	4SU	1	0
29	Z	8	4SU	1	0
30	a	2445	2MG	1	0
6	A	1402	4OC	1	0
30	a	747	5MU	1	0
30	a	1917	PSU	1	0
28	Y	37	6MZ	1	0
30	a	1939	5MU	1	0
30	a	2604	PSU	1	0
30	a	2552	OMU	3	0
30	a	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 248 ligands modelled in this entry, 246 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	$\# Z > 2$
57	SCM	A	1601	-	23,25,25	0.27	0	26,39,39	0.64	0
59	VAL	Y	101	28	4,6,7	0.57	0	6,7,9	0.80	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
57	SCM	A	1601	-	-	0/4/57/57	0/3/3/3
59	VAL	Y	101	28	-	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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	1601	SCM	2	0
59	Y	101	VAL	3	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.

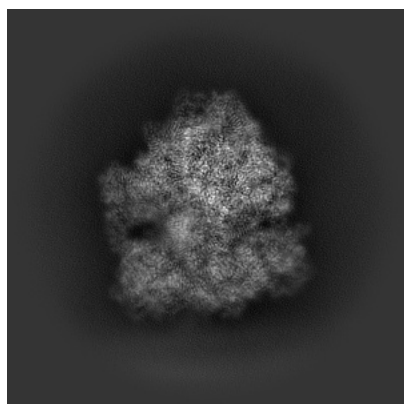
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56128. These allow visual inspection of the internal detail of the map and identification of artifacts.

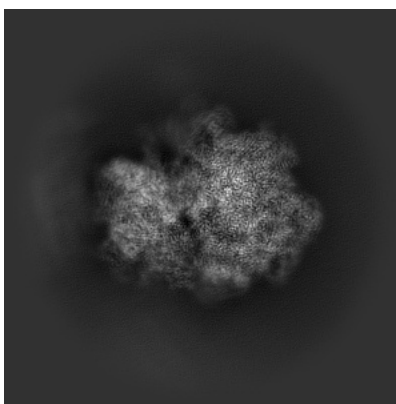
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

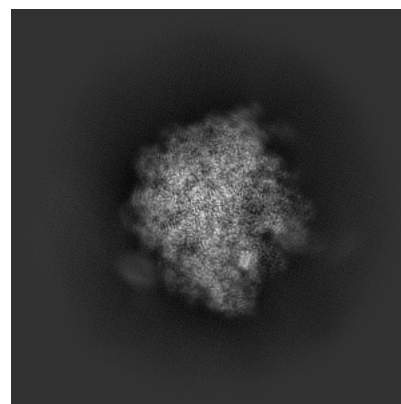
6.1.1 Primary map



X

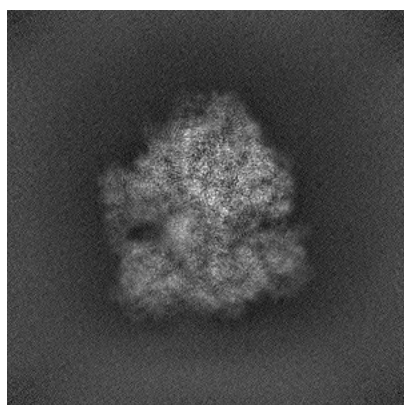


Y

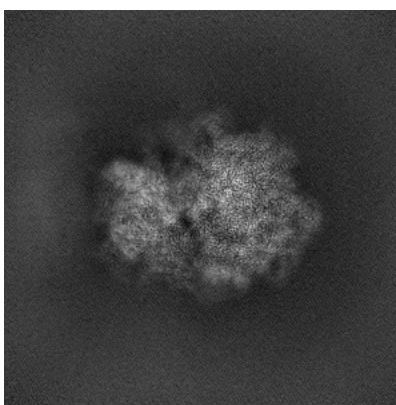


Z

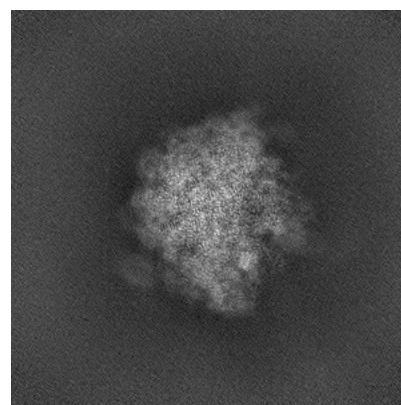
6.1.2 Raw map



X



Y

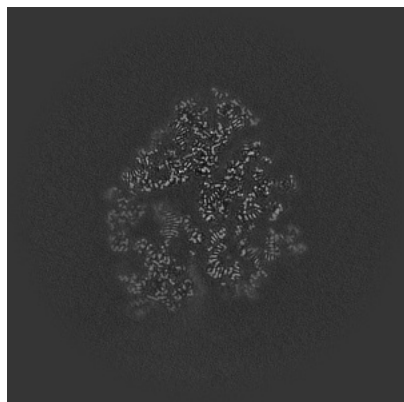


Z

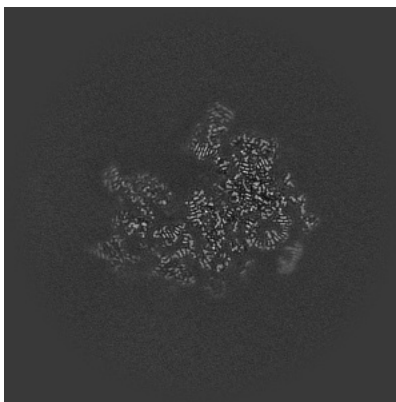
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

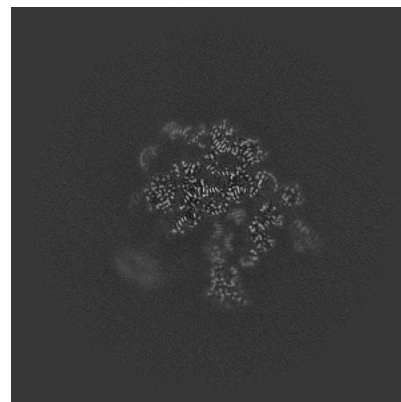
6.2.1 Primary map



X Index: 288

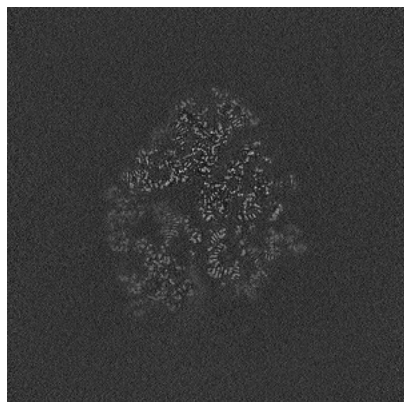


Y Index: 288

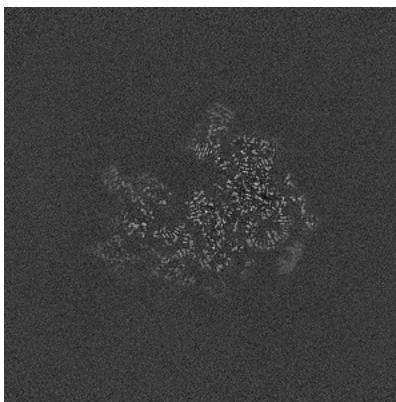


Z Index: 288

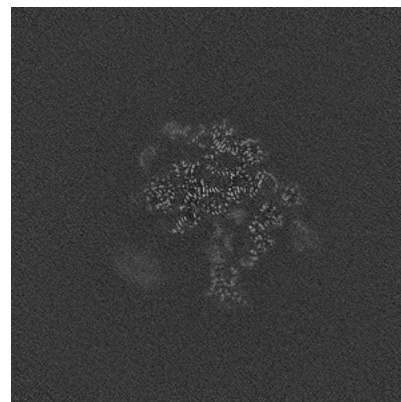
6.2.2 Raw map



X Index: 288



Y Index: 288

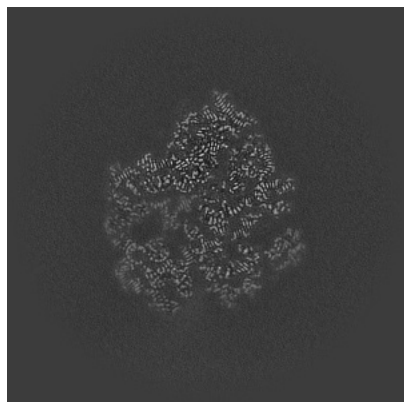


Z Index: 288

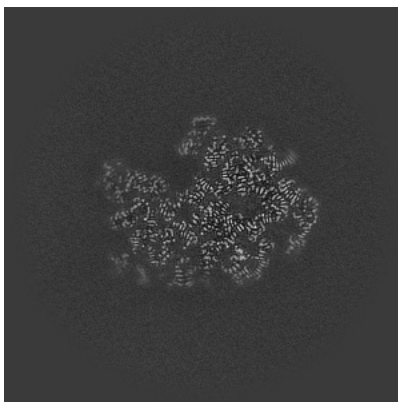
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

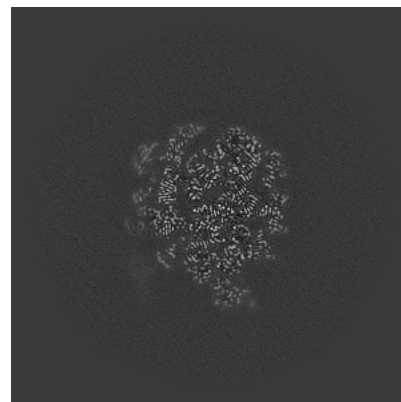
6.3.1 Primary map



X Index: 297

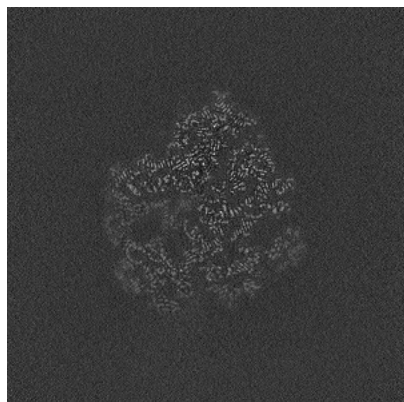


Y Index: 306

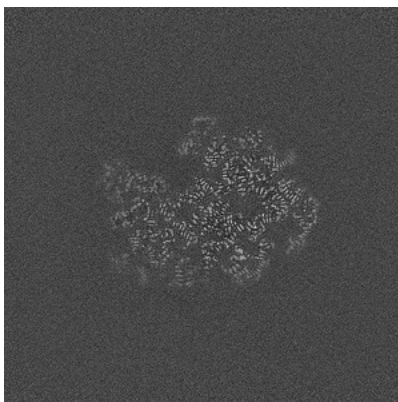


Z Index: 342

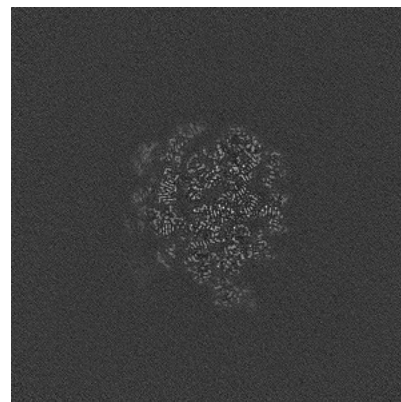
6.3.2 Raw map



X Index: 296



Y Index: 306

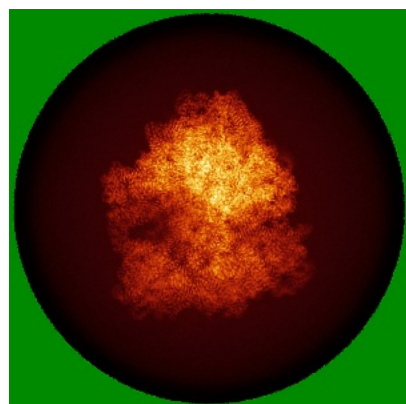


Z Index: 342

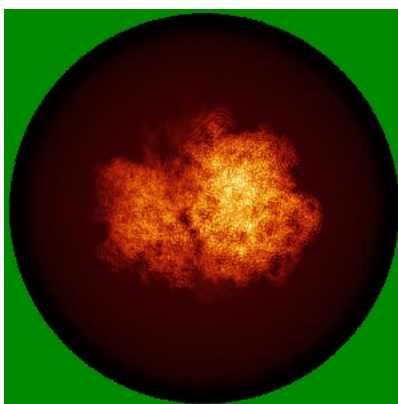
The images above show the largest variance slices of the map in three orthogonal directions.

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

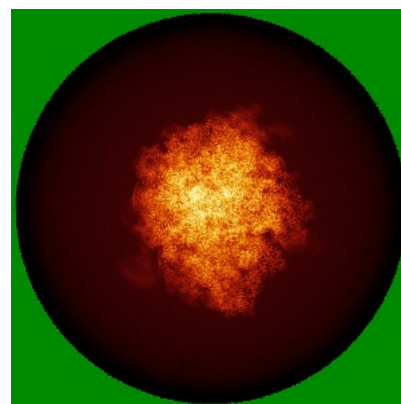
6.4.1 Primary map



X

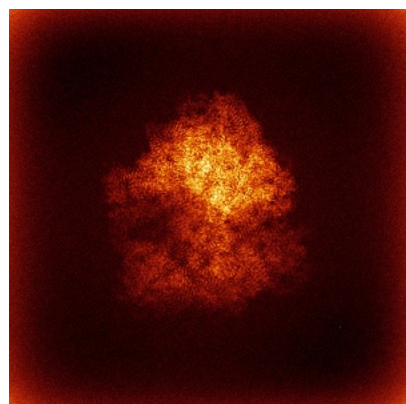


Y

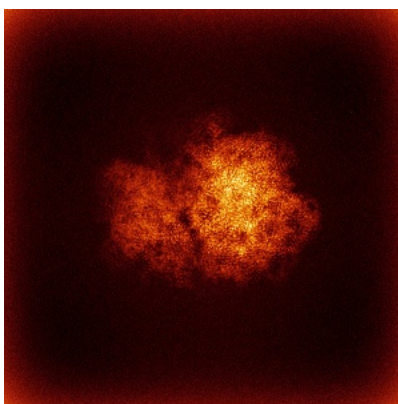


Z

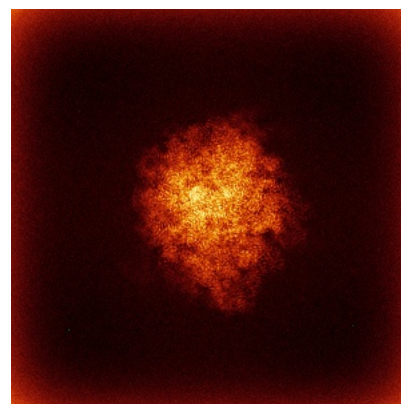
6.4.2 Raw map



X



Y

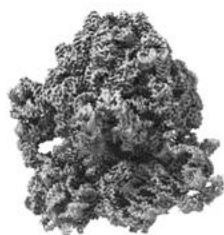


Z

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](#)

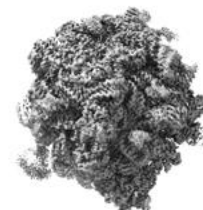
6.5.1 Primary map



X



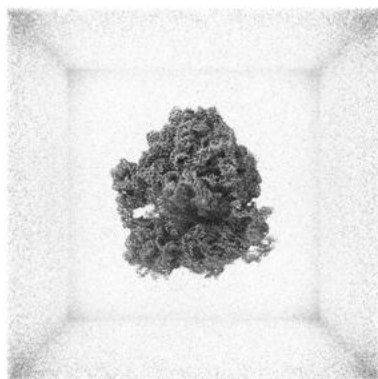
Y



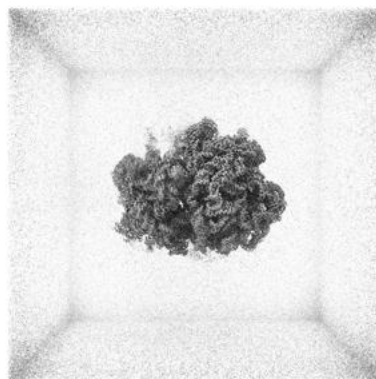
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0474. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

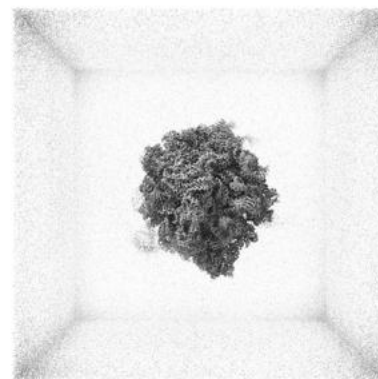
6.5.2 Raw map



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.

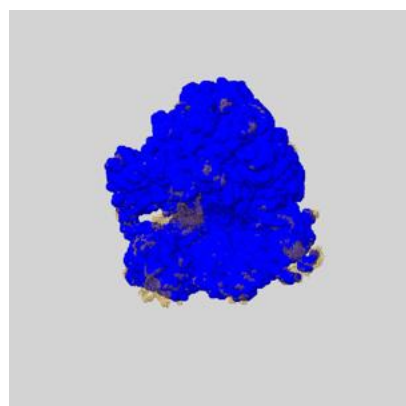
6.6 Mask visualisation [i](#)

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

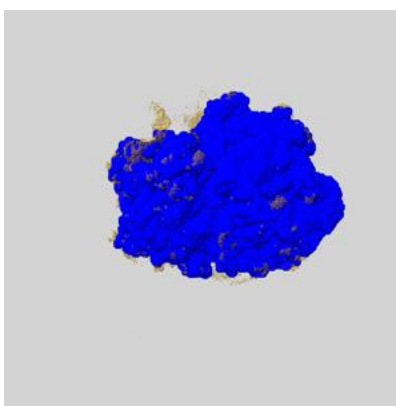
A mask typically either:

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

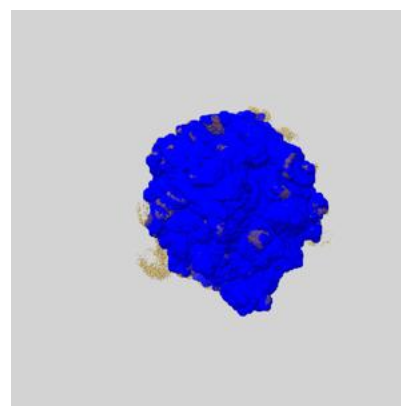
6.6.1 emd_56128_msk_1.map [i](#)



X



Y

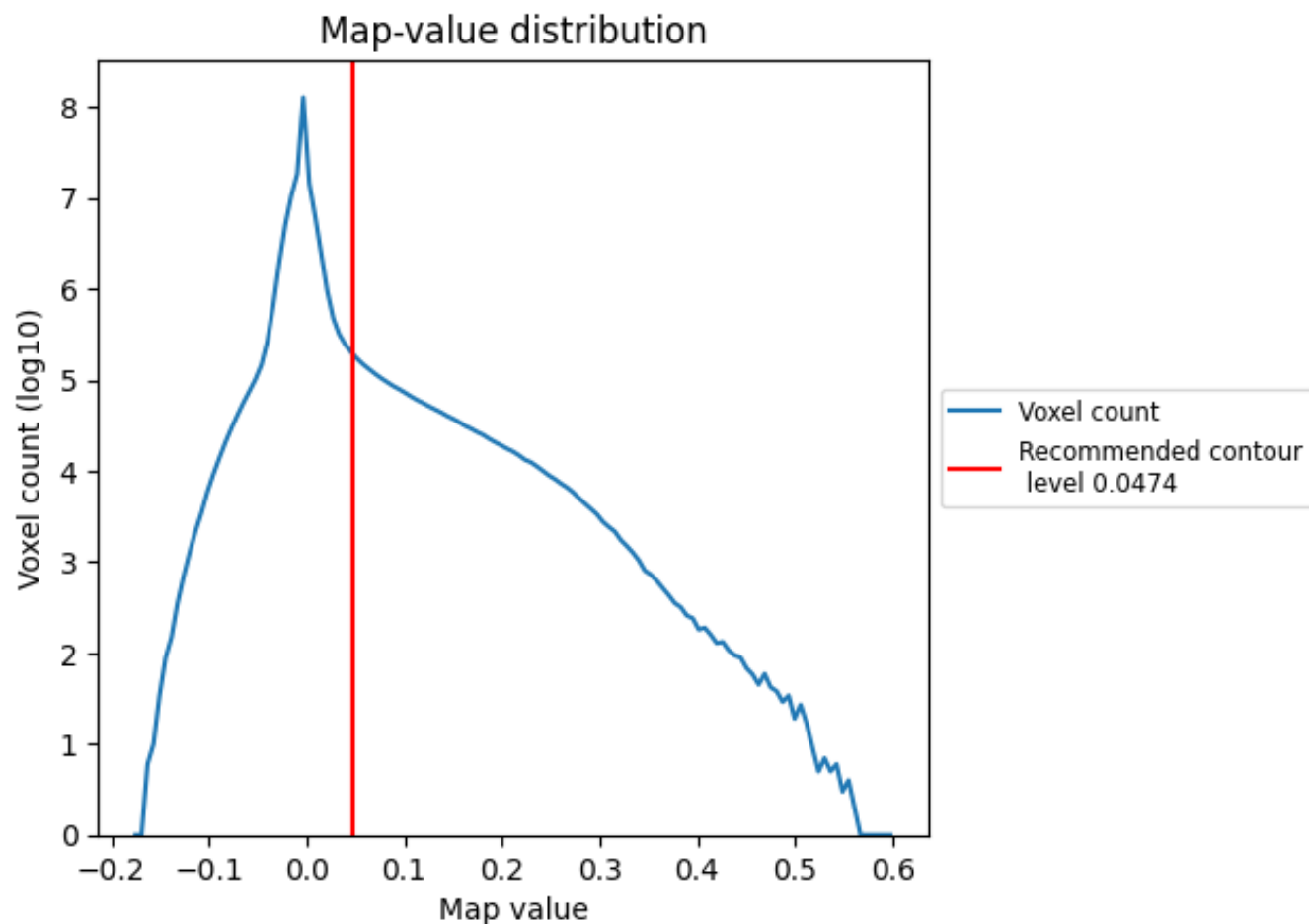


Z

7 Map analysis [i](#)

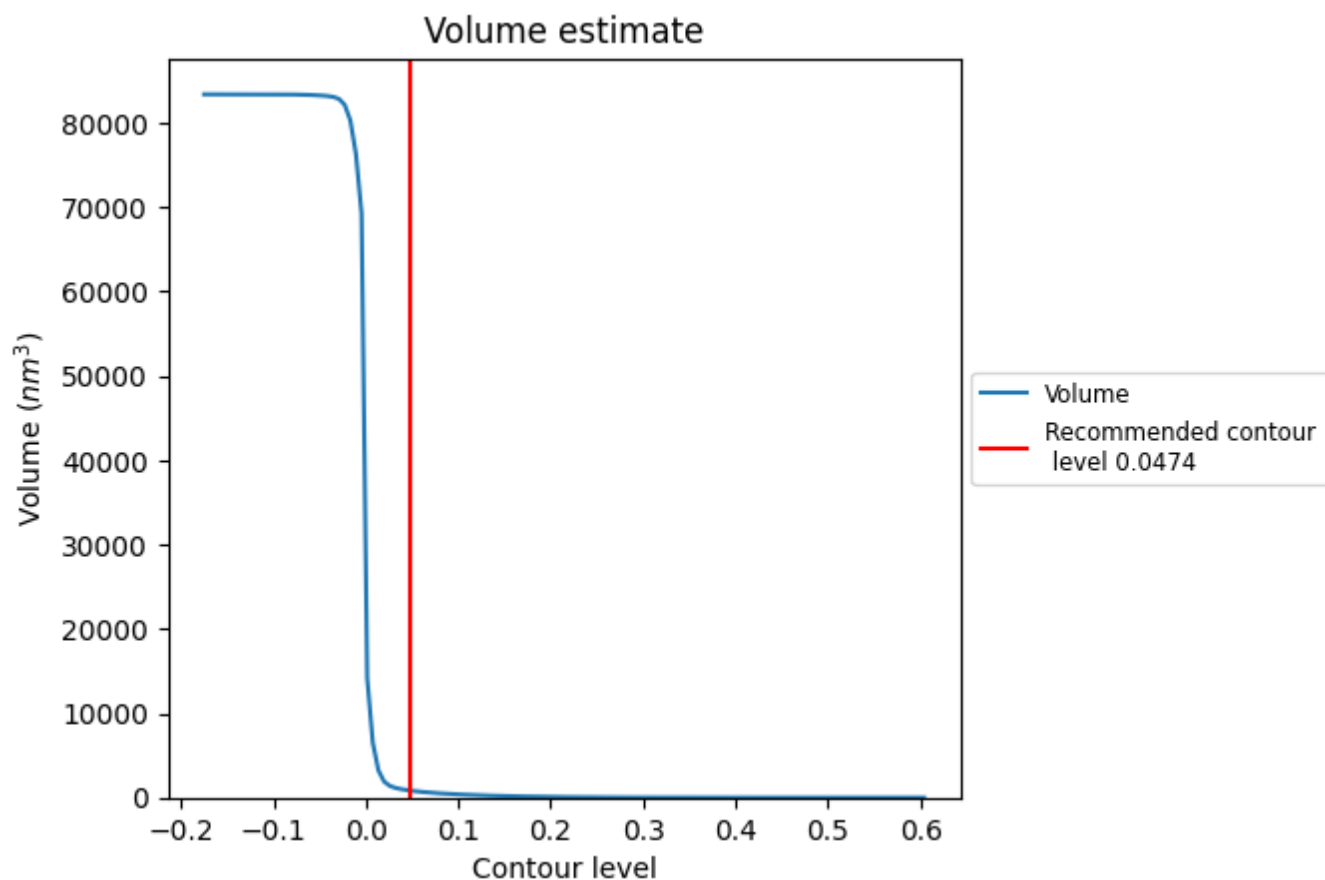
This section contains the results of statistical analysis of the map.

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.

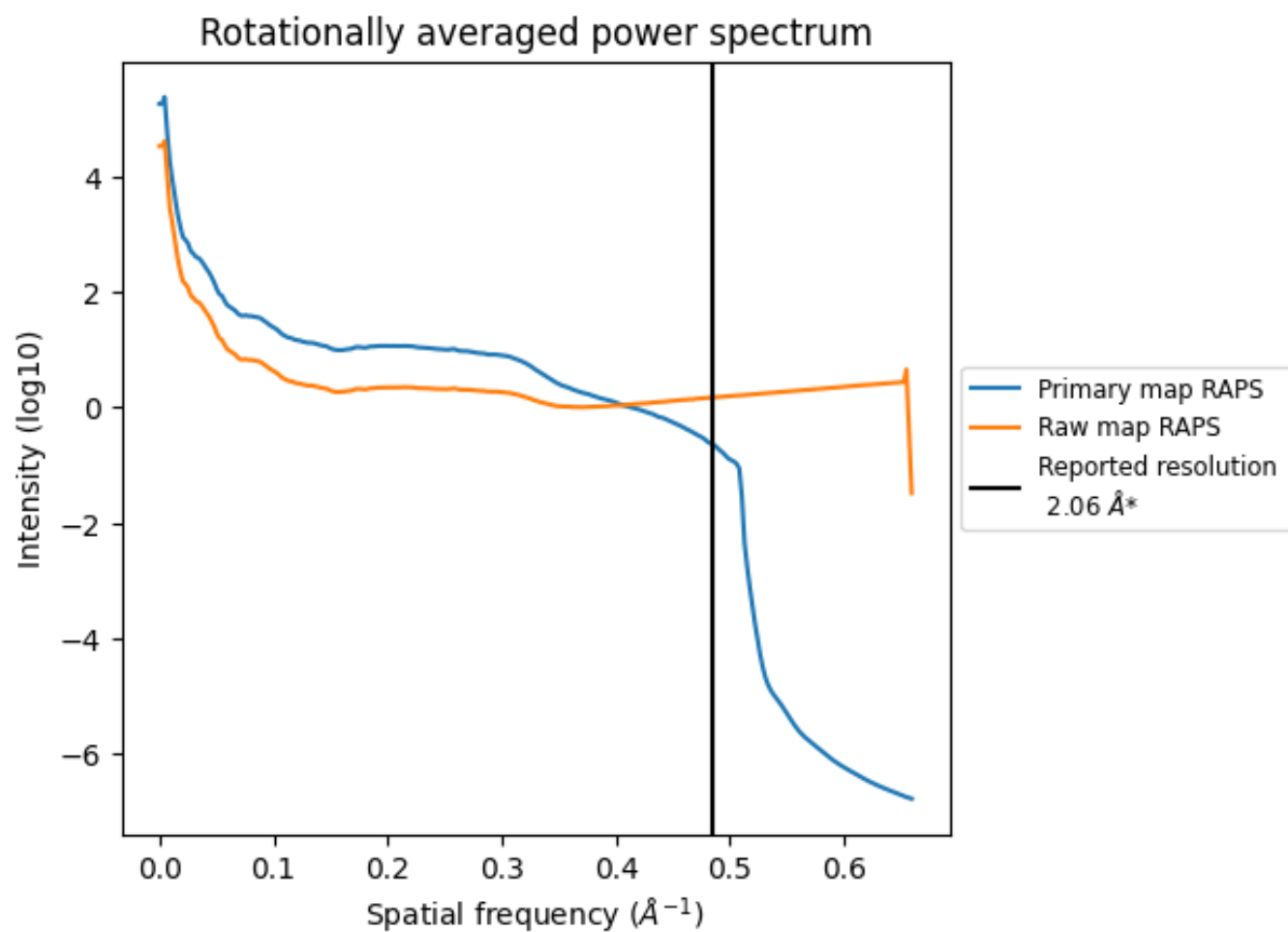
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 841 nm³; this corresponds to an approximate mass of 760 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 ⓘ

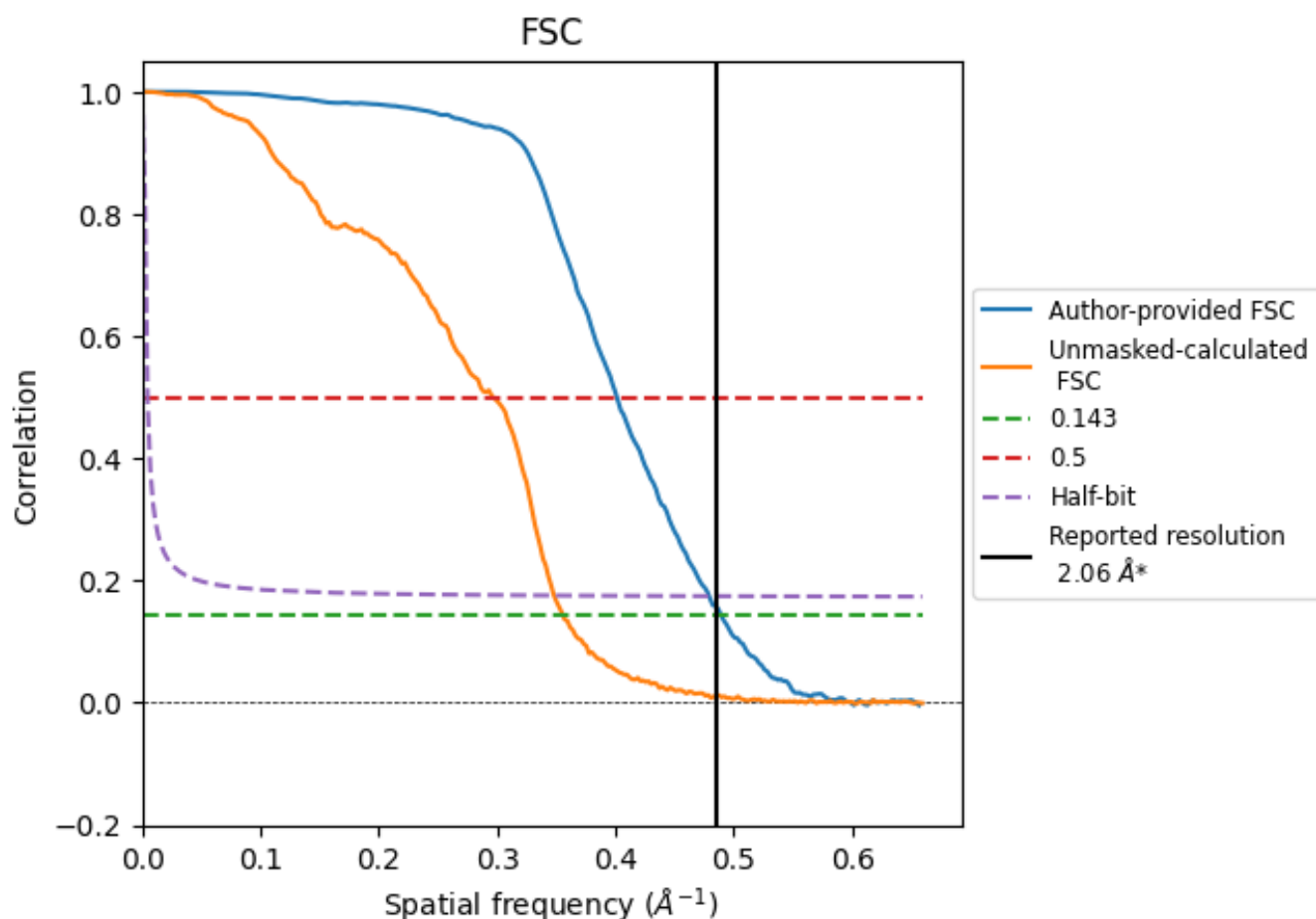


*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.485 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

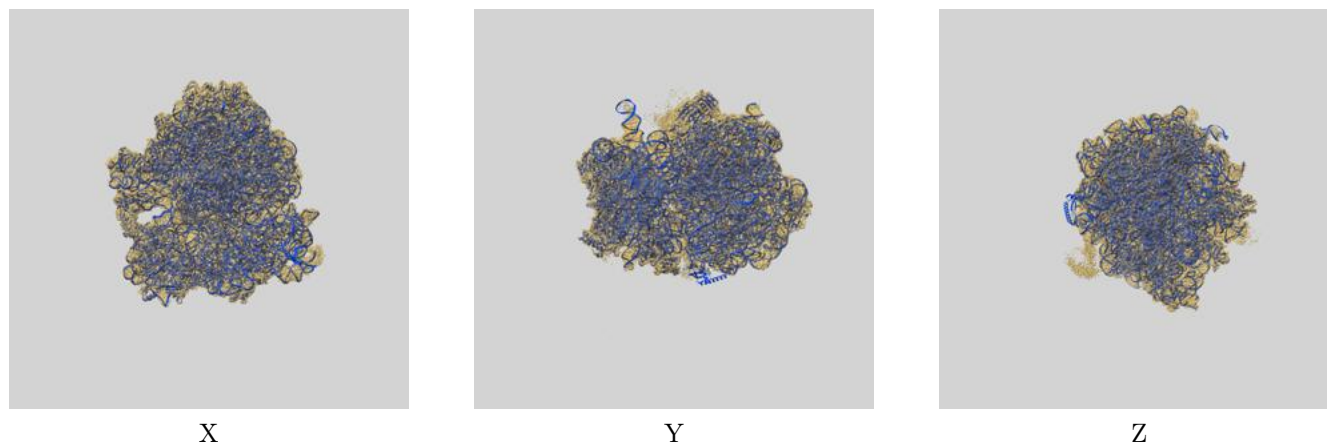
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.04	2.49	2.09
Unmasked-calculated*	2.81	3.37	2.87

*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 2.81 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

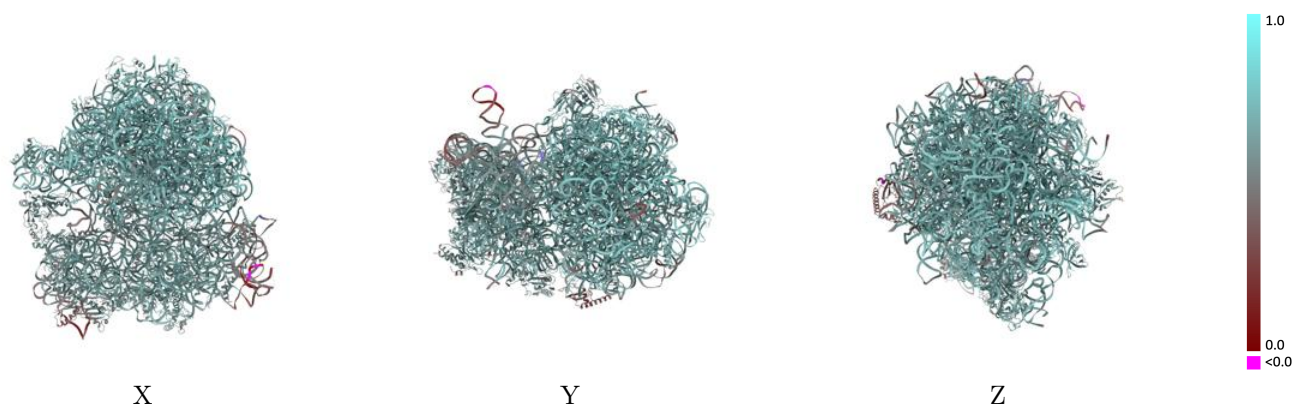
This section contains information regarding the fit between EMDB map EMD-56128 and PDB model 9TQA. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



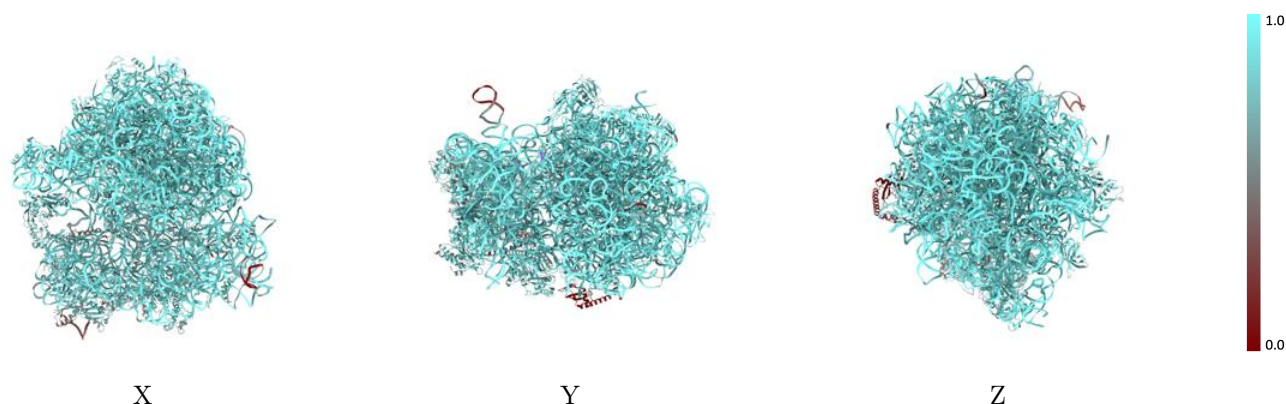
The images above show the 3D surface view of the map at the recommended contour level 0.0474 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



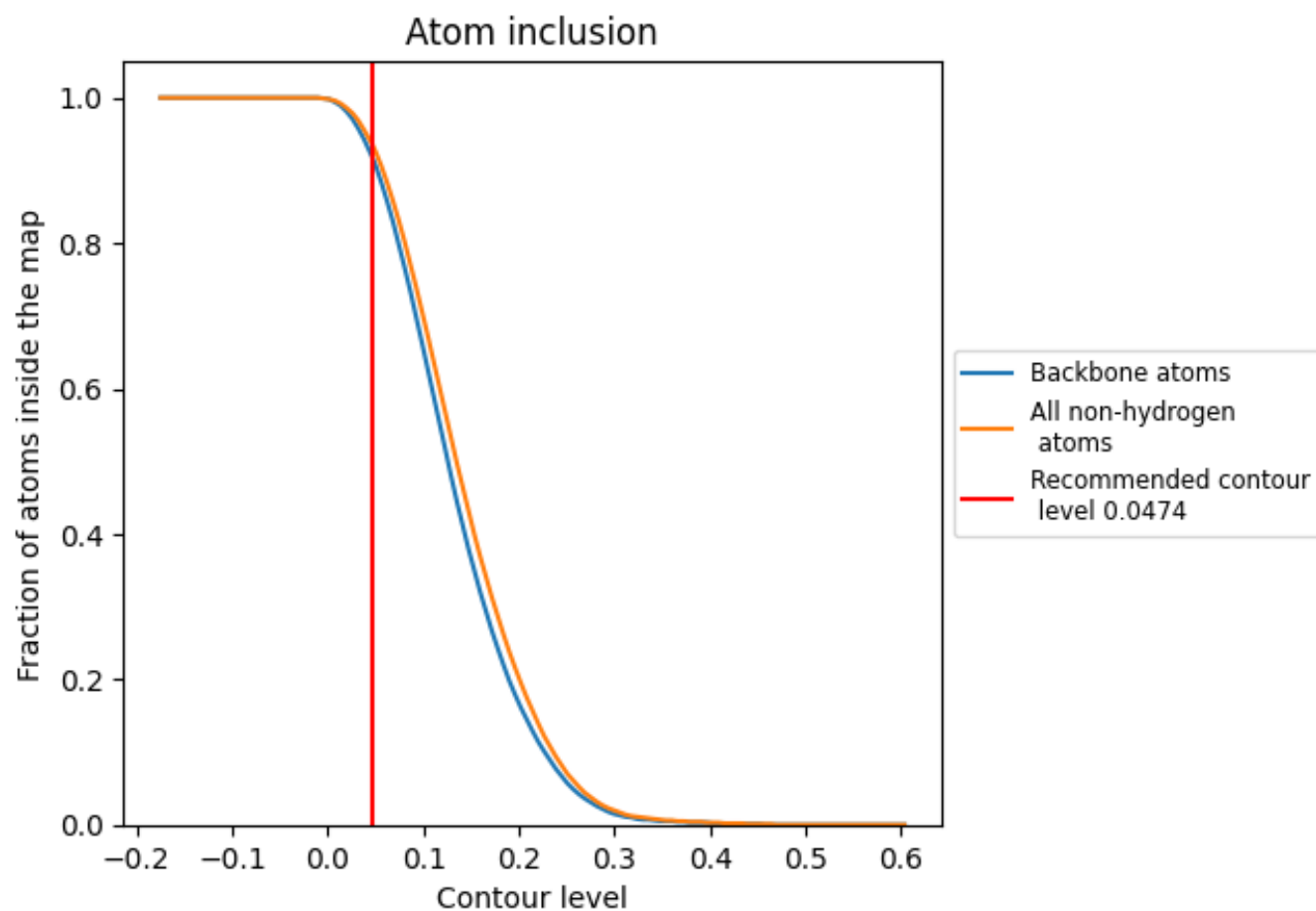
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0474).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (0.0474) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6570
0	 0.9090	 0.6800
1	 0.9720	 0.7330
2	 0.9800	 0.7310
3	 0.9450	 0.7030
4	 0.6950	 0.5150
A	 0.9480	 0.6260
B	 0.7480	 0.5680
C	 0.8540	 0.6250
D	 0.8040	 0.5980
E	 0.9150	 0.6670
F	 0.8170	 0.5850
G	 0.6280	 0.5280
H	 0.9170	 0.6620
I	 0.8280	 0.5960
J	 0.7040	 0.5350
K	 0.8550	 0.6240
L	 0.9010	 0.6710
M	 0.8170	 0.6030
N	 0.8700	 0.6310
O	 0.8770	 0.6370
P	 0.8330	 0.5980
Q	 0.8500	 0.6130
R	 0.8700	 0.6240
S	 0.8050	 0.5980
T	 0.8140	 0.5800
U	 0.5930	 0.5110
X	 0.9210	 0.6320
Y	 0.9110	 0.6070
Z	 0.8870	 0.6000
a	 0.9830	 0.6870
b	 0.9780	 0.6530
c	 0.9610	 0.7200
d	 0.9580	 0.7130
e	 0.9210	 0.6790



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Chain	Atom inclusion	Q-score
f	 0.8260	 0.5900
g	 0.8470	 0.5970
h	 0.2730	 0.4160
i	 0.9540	 0.7090
j	 0.9520	 0.7090
k	 0.9530	 0.7010
l	 0.9520	 0.7120
m	 0.9860	 0.7280
n	 0.9180	 0.6470
o	 0.9210	 0.6940
p	 0.9810	 0.7310
q	 0.9350	 0.6990
r	 0.9380	 0.7010
s	 0.9100	 0.6710
t	 0.9140	 0.6570
u	 0.8980	 0.6570
v	 0.9240	 0.7050
w	 0.9500	 0.7000
x	 0.8840	 0.6370
y	 0.9290	 0.6960
z	 0.9420	 0.7020