



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 08:31 pm BST

PDB ID : 9TMI / pdb_00009tmi
EMDB ID : EMD-56070
Title : E. coli 70S ribosome with A- and P-site tRNA
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.
Deposited on : 2025-12-13
Resolution : 2.08 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:

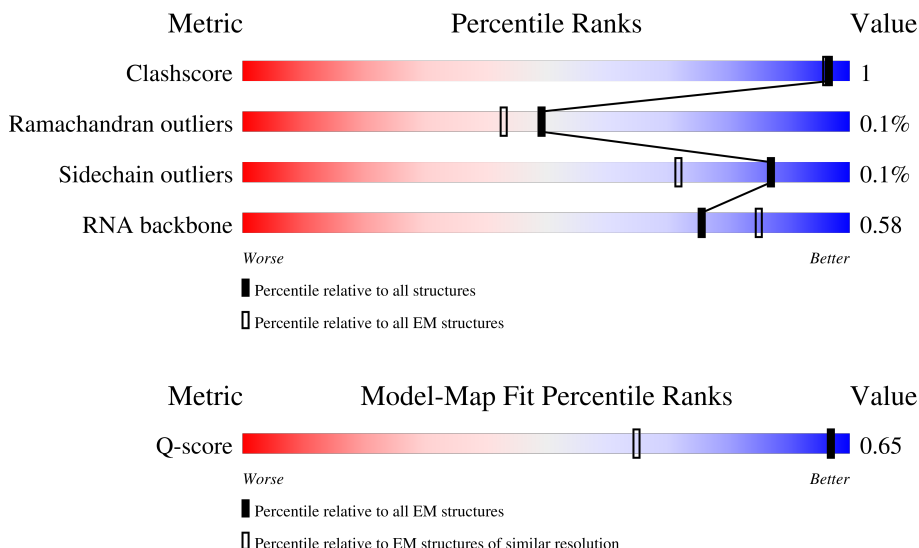
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

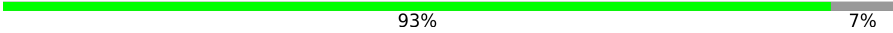
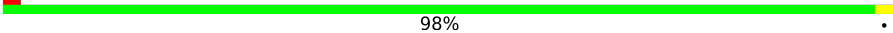
The reported resolution of this entry is 2.08 Å.

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	1976 (1.58 - 2.58)

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	100%
5	B	241	8% 90% 7%
6	C	233	87% 12%
7	D	206	7% 99%
8	E	167	93% 7%
9	F	135	76% 24%
10	G	179	16% 85% 15%
11	H	130	98% ..
12	I	130	96% ..
13	J	103	19% 94% 5%
14	K	129	91% 9%
15	L	124	98% ..
16	M	118	97% .
17	N	101	99% .
18	O	89	99% .
19	P	82	6% 96% ..
20	Q	84	94% 6%
21	R	75	88% 12%
22	S	92	91% 9%
23	T	87	97% ..
24	U	71	28% 97% ..
25	X	10	80% 20%
26	b	120	88% 10% ..
27	c	273	95% ..
28	d	209	94% 6%

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Mol	Chain	Length	Quality of chain
29	e	201	98% .
30	f	179	98% ..
31	g	177	98% ..
32	h	149	66% 100%
33	i	142	97% .
34	j	123	98% .
35	k	144	97% .
36	l	136	96% .
37	m	127	91% 7% .
38	n	117	99% .
39	o	115	97% ..
40	p	118	95% ..
41	q	103	99% .
42	r	110	98% .
43	s	100	92% 7% .
44	t	104	94% . .
45	u	94	100%
46	v	85	95% ..
47	w	78	99% .
48	x	63	97% .
49	y	59	98% .
50	z	57	95% ..
51	4	70	6% 86% 14%
52	A	1542	82% 16% .
53	Y	76	70% 21% 5%

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Mol	Chain	Length	Quality of chain
54	Z	78	74% 14% • • 8%
55	a	2904	79% 14% • 5%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150552 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 Small ribosomal subunit protein uS2.

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

- Molecule 6 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 9 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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	conflict	UNP P0A7R9

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 19 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 25 is a RNA chain called mRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 52 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 53 is a RNA chain called A-site Val-tRNA.

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

- Molecule 54 is a RNA chain called P-site fMet-tRNA.

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

- Molecule 55 is a RNA chain called 23S rRNA.

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

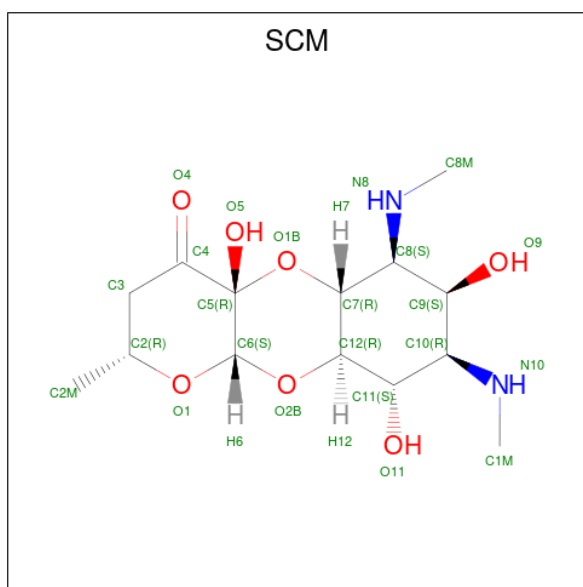
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

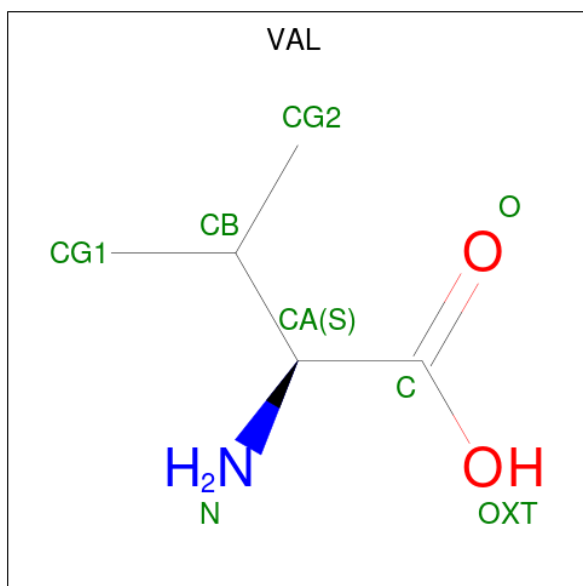
Mol	Chain	Residues	Atoms		AltConf
57	b	4	Total	Mg	0
			4	4	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	47	Total	Mg	0
			47	47	
57	Z	1	Total	Mg	0
			1	1	
57	a	203	Total	Mg	0
			203	203	

- Molecule 58 is SPECTINOMYCIN (CCD ID: SCM) (formula: C₁₄H₂₄N₂O₇).



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

- 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 water.

Mol	Chain	Residues	Atoms		AltConf
60	0	9	Total 9	O 9	0
60	1	18	Total 18	O 18	0
60	2	24	Total 24	O 24	0
60	3	11	Total 11	O 11	0
60	B	16	Total 16	O 16	0
60	C	23	Total 23	O 23	0
60	D	29	Total 29	O 29	0
60	E	18	Total 18	O 18	0
60	F	9	Total 9	O 9	0
60	G	8	Total 8	O 8	0
60	H	23	Total 23	O 23	0
60	I	15	Total 15	O 15	0
60	J	18	Total 18	O 18	0
60	K	20	Total 20	O 20	0
60	L	29	Total 29	O 29	0
60	M	10	Total 10	O 10	0
60	N	12	Total 12	O 12	0
60	O	16	Total 16	O 16	0
60	P	11	Total 11	O 11	0
60	Q	7	Total 7	O 7	0
60	R	9	Total 9	O 9	0
60	S	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
60	T	7	Total 7	O 7	0
60	U	9	Total 9	O 9	0
60	X	9	Total 9	O 9	0
60	b	130	Total 130	O 130	0
60	c	113	Total 113	O 113	0
60	d	77	Total 77	O 77	0
60	e	59	Total 59	O 59	0
60	f	9	Total 9	O 9	0
60	g	30	Total 30	O 30	0
60	h	5	Total 5	O 5	0
60	i	37	Total 37	O 37	0
60	j	36	Total 36	O 36	0
60	k	56	Total 56	O 56	0
60	l	57	Total 57	O 57	0
60	m	31	Total 31	O 31	0
60	n	17	Total 17	O 17	0
60	o	34	Total 34	O 34	0
60	p	41	Total 41	O 41	0
60	q	37	Total 37	O 37	0
60	r	39	Total 39	O 39	0
60	s	30	Total 30	O 30	0

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Mol	Chain	Residues	Atoms		AltConf
60	t	29	Total 29	O 29	0
60	u	22	Total 22	O 22	0
60	v	33	Total 33	O 33	0
60	w	25	Total 25	O 25	0
60	x	10	Total 10	O 10	0
60	y	15	Total 15	O 15	0
60	z	32	Total 32	O 32	0
60	4	3	Total 3	O 3	0
60	A	1657	Total 1657	O 1657	0
60	Y	34	Total 34	O 34	0
60	Z	29	Total 29	O 29	0
60	a	4879	Total 4879	O 4879	0

3 Residue-property plots [i](#)

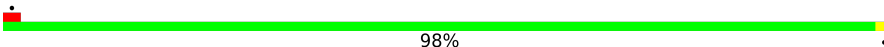
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

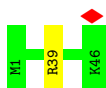
- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  93% 7%



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  98% .



- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  92% 6% .



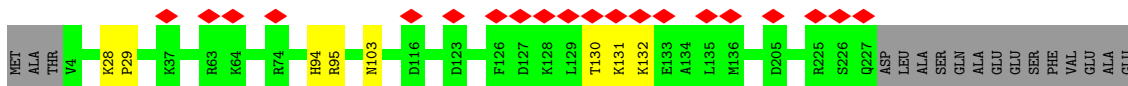
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  100%

There are no outlier residues recorded for this chain.

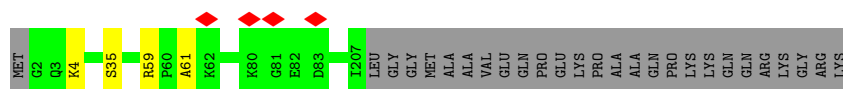
- Molecule 5: Small ribosomal subunit protein uS2

Chain B:  8% 90% . 7%



- Molecule 6: Small ribosomal subunit protein uS3

Chain C:  87% 12%



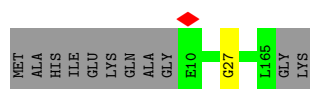
- Molecule 7: Small ribosomal subunit protein uS4

Chain D:  7% 99%



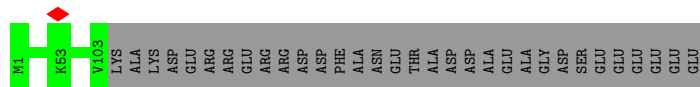
- Molecule 8: Small ribosomal subunit protein uS5

Chain E:  93% 7%



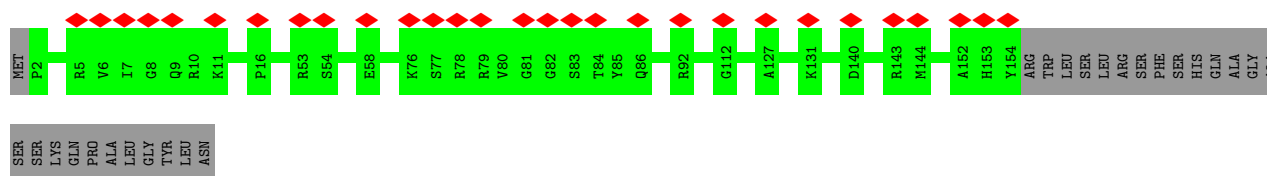
- Molecule 9: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  76% 24%

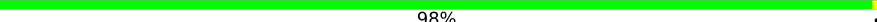


- Molecule 10: Small ribosomal subunit protein uS7

Chain G:  16% 85% 15%



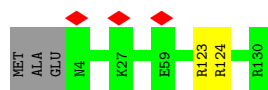
- Molecule 11: Small ribosomal subunit protein uS8

Chain H:  98%

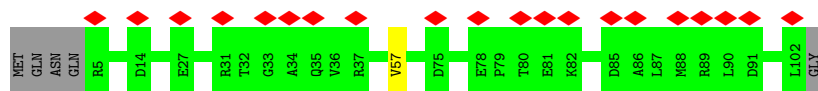
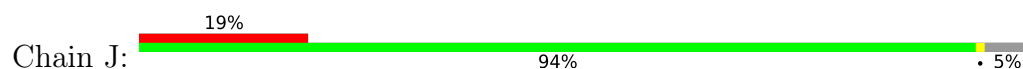


- Molecule 12: Small ribosomal subunit protein uS9

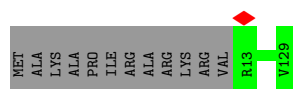
Chain I:  96%



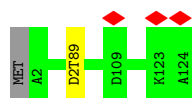
- Molecule 13: Small ribosomal subunit protein uS10



- Molecule 14: Small ribosomal subunit protein uS11



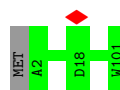
- Molecule 15: Small ribosomal subunit protein uS12



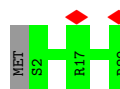
- Molecule 16: Small ribosomal subunit protein uS13



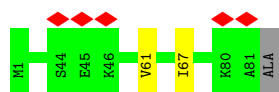
- Molecule 17: Small ribosomal subunit protein uS14



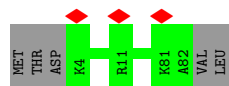
- Molecule 18: Small ribosomal subunit protein uS15



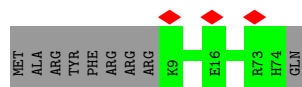
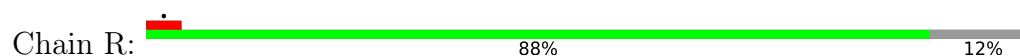
- Molecule 19: Small ribosomal subunit protein bS16



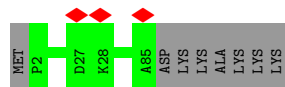
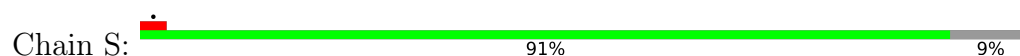
- Molecule 20: Small ribosomal subunit protein uS17



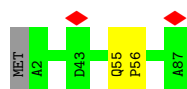
- Molecule 21: Small ribosomal subunit protein bS18



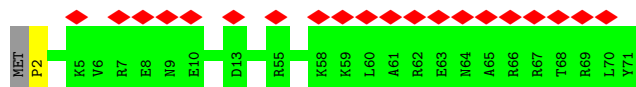
- Molecule 22: Small ribosomal subunit protein uS19



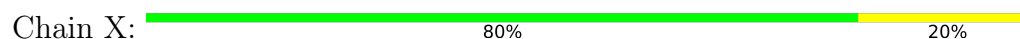
- Molecule 23: Small ribosomal subunit protein bS20



- Molecule 24: Small ribosomal subunit protein bS21

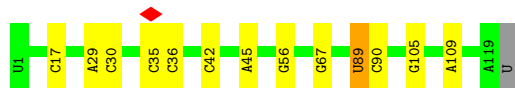


- Molecule 25: mRNA

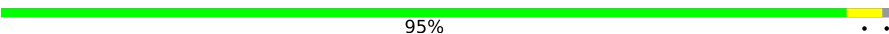


- Molecule 26: 5S rRNA

Chain b:  88% 10% ..

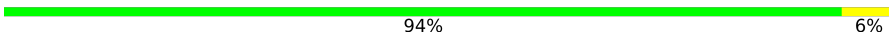


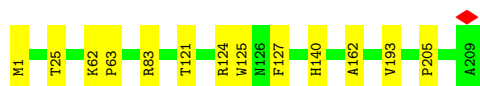
- Molecule 27: Large ribosomal subunit protein uL2

Chain c:  95% ..

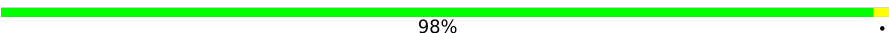


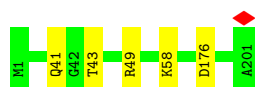
- Molecule 28: Large ribosomal subunit protein uL3

Chain d:  94% 6%

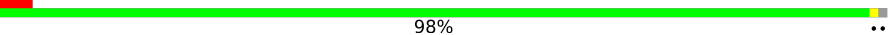


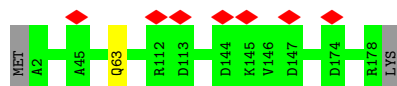
- Molecule 29: Large ribosomal subunit protein uL4

Chain e:  98% .

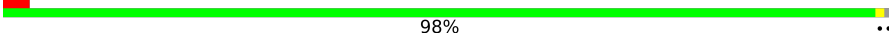


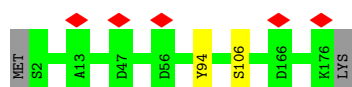
- Molecule 30: Large ribosomal subunit protein uL5

Chain f:  98% ..



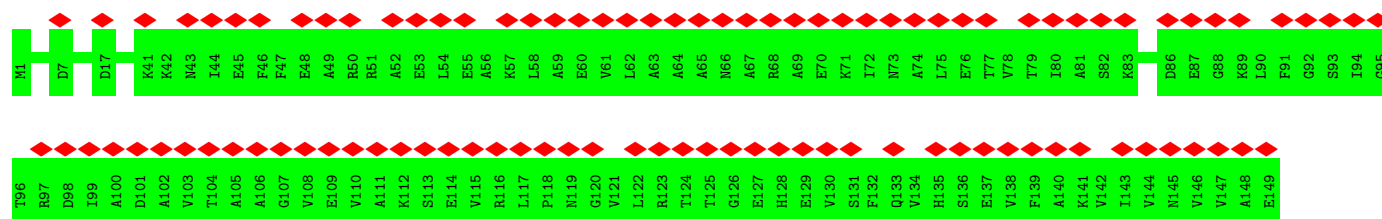
- Molecule 31: Large ribosomal subunit protein uL6

Chain g:  98% ..

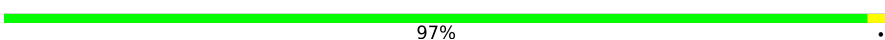


- Molecule 32: Large ribosomal subunit protein bL9

Chain h:  66% 100%

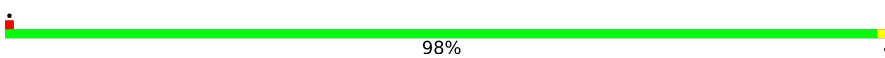


- Molecule 33: Large ribosomal subunit protein uL13

Chain i:  97%

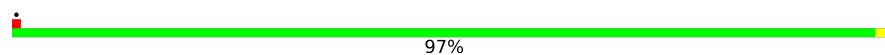


- Molecule 34: Large ribosomal subunit protein uL14

Chain j:  98%

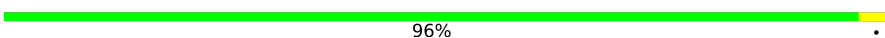


- Molecule 35: Large ribosomal subunit protein uL15

Chain k:  97%

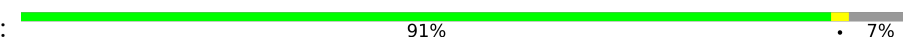


- Molecule 36: Large ribosomal subunit protein uL16

Chain l:  96%

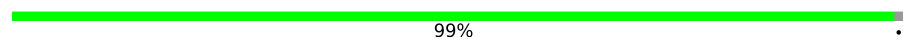


- Molecule 37: Large ribosomal subunit protein bL17

Chain m:  91%

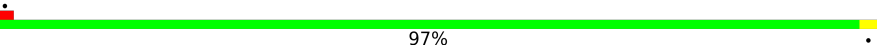


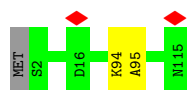
- Molecule 38: Large ribosomal subunit protein uL18

Chain n:  99%

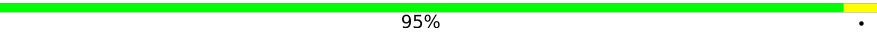


- Molecule 39: Large ribosomal subunit protein bL19

Chain o:  97%

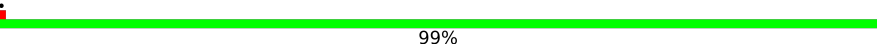


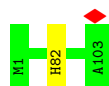
- Molecule 40: Large ribosomal subunit protein bL20

Chain p:  95%

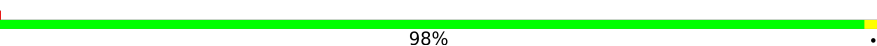


- Molecule 41: Large ribosomal subunit protein bL21

Chain q:  99%



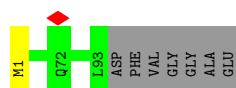
- Molecule 42: Large ribosomal subunit protein uL22

Chain r:  98%



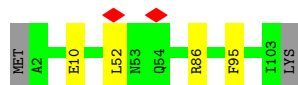
- Molecule 43: Large ribosomal subunit protein uL23

Chain s:  92%

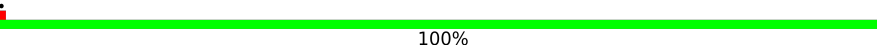


- Molecule 44: Large ribosomal subunit protein uL24

Chain t:  94%



- Molecule 45: Large ribosomal subunit protein bL25

Chain u:  100%



- Molecule 46: Large ribosomal subunit protein bL27

Chain v: 95%



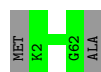
- Molecule 47: Large ribosomal subunit protein bL28

Chain w: 99%



- Molecule 48: Large ribosomal subunit protein uL29

Chain x: 97%



- Molecule 49: Large ribosomal subunit protein uL30

Chain y: 98%



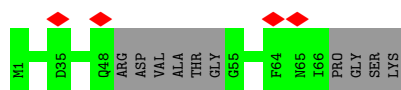
- Molecule 50: Large ribosomal subunit protein bL32

Chain z: 95%

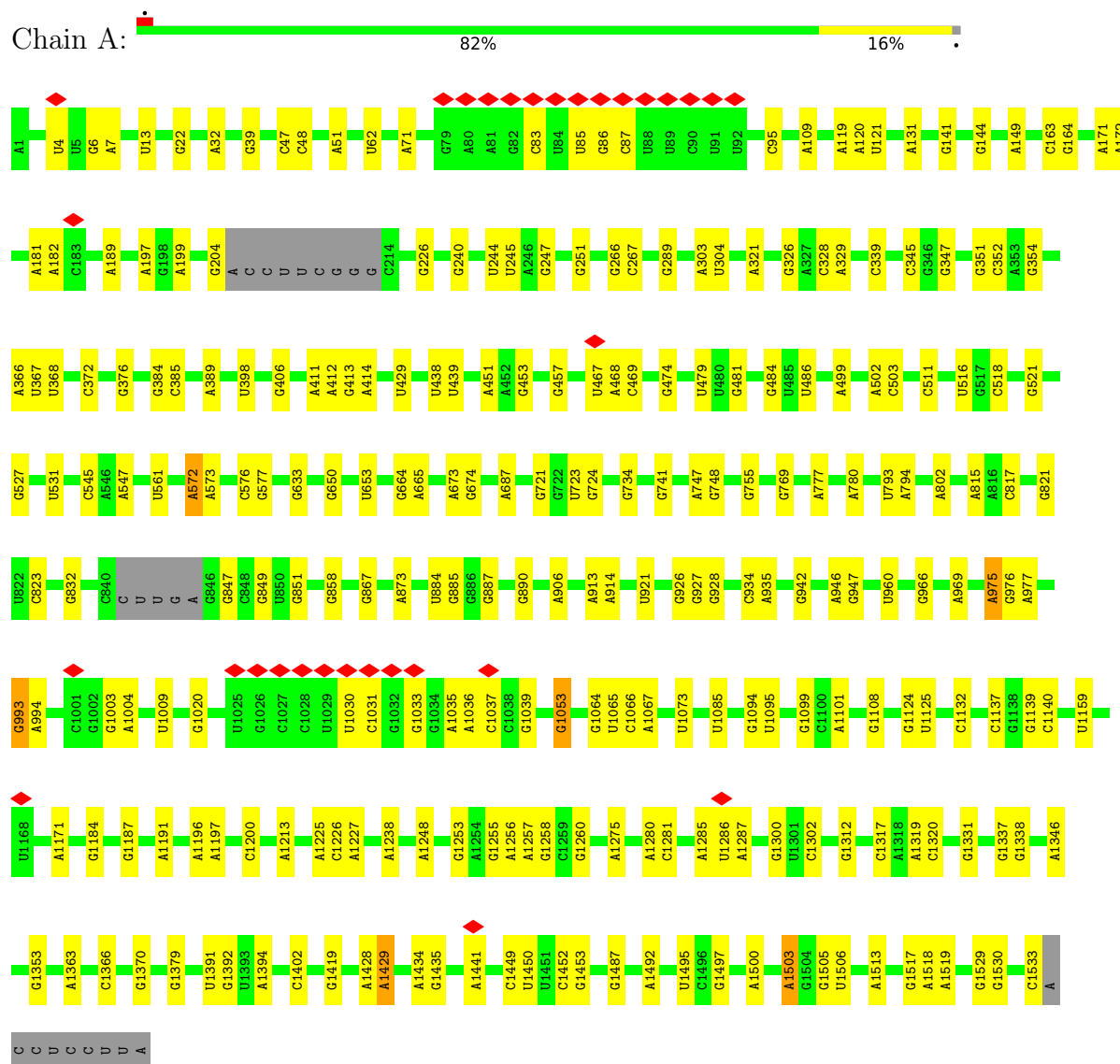


- Molecule 51: Large ribosomal subunit protein bL31A

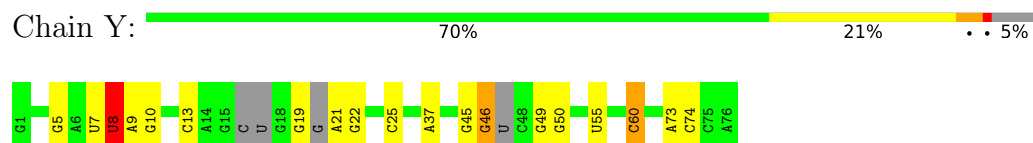
Chain 4: 6% 86% 14%



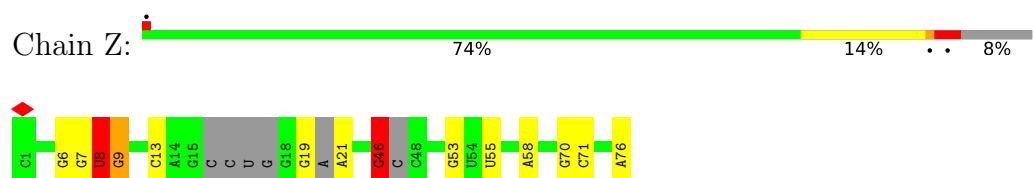
- Molecule 52: 16S rRNA



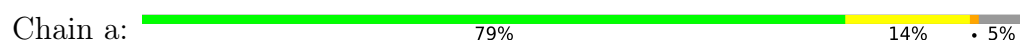
- Molecule 53: A-site Val-tRNA



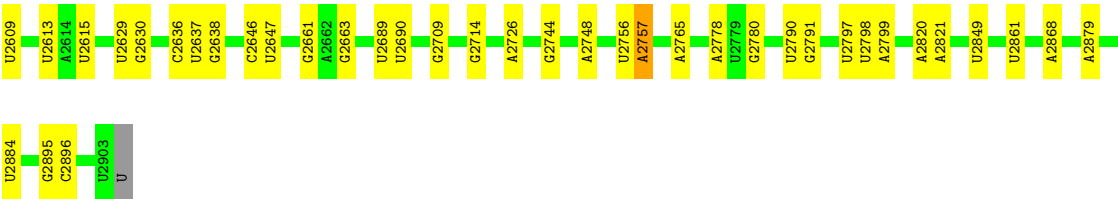
- Molecule 54: P-site fMet-tRNA



- Molecule 55: 23S rRNA



U2431	A2268	C2050	G1873	C1646	A1383	G1112	C1052	A877	G700	A505	C208	G1
A2435	A2273	C2055	C1902	U1647	U1405	G1115	C	G883	C717	C509	G215	A10
U2441	A2274	G2056	C1905	G1649	U1406	G1116	A	U884	U723	G512	A216	C11
A2448	G2277	A2060	G1906	A1650	G1416	G1125	U	U887	U724	G530	A221	U12
U2449	A2278	A2062	G1907	G1674	C1428	G1128	G	C888	G729	C531	A222	U34
C2452	C2282	G2069	U1911	G1715	A1434	A1129	U	C889	A730	A532	G248	G55
U2457	C2283	G2087	A1912	U1729	G1435	U1132	G	G891	G738	G533	G263	G58
A2469	A2287	A	G1913	C1730	G1452	A1133	G	U895	U746	A538	C264	A63
G2470	U2291	G2100	A1914	G1731	A1453	G1134	C	A896	U747	U545	A272	U71
U2474	U2292	A	A1916	C1732	U1458	C1135	U	C897	A749	U546	U276	U72
A2476	U2305	C	U1917	G1738	U1474	U1141	A	A905	A756	A547	G278	A73
G2488	G2308	C	A1919	A1754	G1475	A1142	A	A910	G757	G548	A279	A74
U2489	U2312	U	G1929	U1758	U1482	C1172	C	G914	A761	U558	A282	G75
G2490	U2312	G	U1930	C1764	G1482	U	A	C915	G762	A563	G285	G98
U2491	A2322	A	G1933	A1773	C1493	U	C	A927	G763	G569	U288	A101
G2494	G2325	C	A1937	G1792	U1497	G1177	A	U931	G775	G570	G289	U102
G2502	C2326	U	A1938	U1778	C1498	G1182	U	C946	G776	U573	A310	G110
A2503	A2327	G	U1939	U1782	A1508	U1183	C	U955	A781	A574	A311	A118
U2504	A2328	C	U1955	A1783	A1509	G1186	U	U958	A782	A575	A330	A119
G2505	U2329	C	G1965	A1784	A1515	U	A	C961	A783	G579	G361	U120
U2506	A2333	A	A1966	A1786	G1529	A1189	U	G962	G784	U580	G366	G121
A2518	U2334	U	C1967	G1792	U1534	A1246	G	A973	A788	A586	A404	G124
U2519	A2335	C	A1970	G1799	A1535	G1250	A	G974	U790	A603	U405	A127
U2522	G2340	G	U1971	C1800	A1536	A1253	A	A983	G805	A614	G411	A131
G2529	C2347	C	G1972	A1801	G1537	G1256	C	A984	C806	U615	A412	U139
U2546	C2350	G	A1987	G1807	U1548	U1271	U	C985	G809	A627	U451	G140
A2547	G2361	A	U1991	A1808	A1549	A1272	A	A996	U810	A637	C456	G141
U2548	U2361	C	U1992	U1807	U1562	U1273	A	U1012	C812	G638	G468	A142
U2554	G2382	C	U1993	C1816	U1569	A1274	U	C1013	G818	C640	G476	G178
A2566	U2383	U	A2014	U1825	U1578	G1296	C	A1020	A819	A644	G481	A161
G2567	C2384	U	A2019	G1826	C1584	A1300	U	G1022	U827	C645	U646	A181
C2573	C2385	G	A2020	G1826	C1585	A1301	A	A1027	U828	G647	G491	A196
U2580	G2395	A	C2023	A1829	C1607	U1352	C	A1028	U846	A654	A492	A199
U2585	C2396	C	A2030	C1830	A1608	A1365	G	U1033	U847	A655	G494	U200
A2602	U2402	U	A2031	A1847	A1609	A1373	U	A1040	G857	A502	A504	A204
G2603	A2406	G	G2032	A1848	C1585	U1378	C	G859	U859	A503		
U2604	C2424	C	A2033	A1853	C1607	A1379	A	G1047				
G2605	A2425	A	G2038	A1858	A1609	U1379	G					
	U2429	C	U2039	G1869	A1630		U					
	A2430	C	C2043	A1872	G1645		A					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73907	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 ($e^-/\text{\AA}^2$)	52.5	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	0.801	Depositor
Minimum map value	-0.248	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0683	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: 4SU, 3TD, ZN, 5MC, MG, 4D4, 2MA, OMU, 2MG, G7M, OMG, PSU, SCM, UR3, MEQ, 5MU, D2T, 1MG, MS6, 4OC, OMC, MA6, 6MZ, IAS, H2U

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	0.46	0/424	0.78	0/565
2	1	0.49	0/380	0.91	0/498
3	2	0.49	0/513	0.89	0/676
4	3	0.48	0/303	0.82	0/397
5	B	0.46	0/1784	0.91	0/2403
6	C	0.46	0/1651	0.84	0/2225
7	D	0.44	0/1665	0.90	0/2227
8	E	0.47	0/1165	0.83	0/1568
9	F	0.45	0/858	0.83	0/1160
10	G	0.46	0/1219	0.93	0/1635
11	H	0.46	0/989	0.86	0/1326
12	I	0.45	0/1034	0.90	0/1375
13	J	0.45	0/796	0.84	0/1077
14	K	0.50	0/884	0.83	0/1191
15	L	0.47	0/960	0.83	0/1286
16	M	0.47	0/900	0.93	0/1204
17	N	0.46	0/817	0.91	0/1088
18	O	0.43	0/722	0.95	0/964
19	P	0.46	0/653	0.85	0/877
20	Q	0.45	0/650	0.79	0/871
21	R	0.45	0/553	0.91	0/742
22	S	0.49	0/685	0.83	0/922
23	T	0.46	0/676	0.97	0/895
24	U	0.46	0/598	0.97	0/792
25	X	0.55	0/242	0.80	0/375
26	b	0.52	0/2850	0.79	0/4444
27	c	0.48	0/2121	0.84	0/2852
28	d	0.46	0/1576	0.80	0/2119
29	e	0.45	0/1571	0.85	0/2113
30	f	0.45	0/1434	0.90	0/1926
31	g	0.47	0/1333	0.83	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.46	0/1122	0.82	0/1515
33	i	0.45	0/1152	0.84	0/1551
34	j	0.45	0/956	0.83	0/1279
35	k	0.46	0/1062	0.84	0/1413
36	l	0.46	0/1073	0.85	0/1433
37	m	0.45	0/958	0.87	0/1281
38	n	0.46	0/902	0.89	0/1209
39	o	0.45	0/929	0.77	0/1242
40	p	0.45	0/960	0.90	0/1278
41	q	0.44	0/829	0.72	0/1107
42	r	0.46	0/864	0.84	0/1156
43	s	0.44	0/744	0.79	0/994
44	t	0.47	0/787	0.79	0/1051
45	u	0.45	0/766	0.78	0/1025
46	v	0.47	0/642	0.81	0/848
47	w	0.45	0/635	0.85	0/848
48	x	0.41	0/496	0.91	0/660
49	y	0.45	0/453	0.86	0/605
50	z	0.47	0/450	0.85	0/599
51	4	0.47	0/488	0.85	0/649
52	A	0.52	1/36236 (0.0%)	0.79	6/56520 (0.0%)
53	Y	0.56	1/1596 (0.1%)	0.79	0/2478
54	Z	0.57	0/1608	0.77	0/2500
55	a	0.49	1/65747 (0.0%)	0.83	24/102563 (0.0%)
All	All	0.49	3/153461 (0.0%)	0.83	30/229402 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	527	G7M	O3'-P	5.20	1.61	1.56
55	a	2069	G7M	O3'-P	5.06	1.61	1.56
53	Y	8	4SU	O3'-P	5.04	1.61	1.56

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1905	C	O3'-P-O5'	-8.01	91.99	104.00
55	a	204	A	O3'-P-O5'	-7.88	92.18	104.00
55	a	781	A	O3'-P-O5'	-7.34	92.99	104.00
55	a	2490	G	O3'-P-O5'	-7.34	92.99	104.00
55	a	2278	A	O3'-P-O5'	-6.82	93.77	104.00
55	a	2382	G	O3'-P-O5'	-6.02	94.97	104.00
55	a	2060	A	O3'-P-O5'	-5.75	95.37	104.00
55	a	763	G	O3'-P-O5'	-5.74	95.39	104.00
52	A	366	A	O3'-P-O5'	-5.69	95.47	104.00
55	a	1966	A	O3'-P-O5'	-5.58	95.64	104.00
52	A	572	A	O3'-P-O5'	-5.57	95.65	104.00
55	a	124	G	O3'-P-O5'	-5.54	95.68	104.00
55	a	1373	A	O3'-P-O5'	-5.54	95.70	104.00
55	a	818	G	O3'-P-O5'	-5.53	95.71	104.00
55	a	2519	U	O3'-P-O5'	-5.46	95.80	104.00
55	a	2050	C	O3'-P-O5'	-5.42	95.88	104.00
52	A	913	A	O3'-P-O5'	-5.39	95.92	104.00
55	a	1378	A	O3'-P-O5'	-5.38	95.93	104.00
55	a	2277	G	O3'-P-O5'	-5.35	95.97	104.00
55	a	2879	A	O3'-P-O5'	-5.35	95.98	104.00
55	a	1246	A	O3'-P-O5'	-5.34	95.99	104.00
52	A	780	A	O3'-P-O5'	-5.33	96.01	104.00
55	a	761	A	O3'-P-O5'	-5.27	96.09	104.00
55	a	1186	G	O3'-P-O5'	-5.23	96.15	104.00
55	a	2546	U	O3'-P-O5'	-5.22	96.17	104.00
52	A	561	U	O3'-P-O5'	-5.21	96.18	104.00
55	a	512	G	O4'-C1'-N9	5.17	115.95	108.20
52	A	921	U	O3'-P-O5'	-5.10	96.36	104.00
55	a	1650	A	O3'-P-O5'	-5.03	96.45	104.00
55	a	310	A	O3'-P-O5'	-5.01	96.48	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	0	0
2	1	377	0	418	2	0
3	2	504	0	572	2	0
4	3	302	0	340	0	0
5	B	1753	0	1780	4	0
6	C	1624	0	1696	2	0
7	D	1643	0	1707	1	0
8	E	1152	0	1196	1	0
9	F	839	0	833	0	0
10	G	1203	0	1254	0	0
11	H	979	0	1031	1	0
12	I	1022	0	1070	1	0
13	J	786	0	828	0	0
14	K	877	0	884	0	0
15	L	957	0	1017	0	0
16	M	891	0	952	0	0
17	N	805	0	844	0	0
18	O	714	0	734	0	0
19	P	643	0	661	1	0
20	Q	641	0	682	0	0
21	R	544	0	565	0	0
22	S	668	0	693	0	0
23	T	670	0	719	1	0
24	U	590	0	629	0	0
25	X	216	0	108	0	0
26	b	2549	0	1291	3	0
27	c	2082	0	2154	8	0
28	d	1566	0	1618	10	0
29	e	1552	0	1619	5	0
30	f	1410	0	1444	1	0
31	g	1313	0	1358	1	0
32	h	1111	0	1148	0	0
33	i	1129	0	1162	3	0
34	j	947	0	1023	1	0
35	k	1053	0	1129	5	0
36	l	1075	0	1145	3	0
37	m	945	0	989	1	0
38	n	892	0	923	0	0
39	o	917	0	962	2	0
40	p	947	0	1019	5	0
41	q	816	0	839	1	0
42	r	857	0	922	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	s	738	0	807	1	0
44	t	779	0	831	1	0
45	u	753	0	780	0	0
46	v	634	0	653	1	0
47	w	625	0	652	0	0
48	x	495	0	526	0	0
49	y	449	0	488	0	0
50	z	444	0	458	3	0
51	4	480	0	478	0	0
52	A	32612	0	16432	31	0
53	Y	1539	0	791	4	0
54	Z	1546	0	794	3	0
55	a	59216	0	29809	102	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	47	0	0	0	0
57	Z	1	0	0	0	0
57	a	203	0	0	0	0
57	b	4	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	A	23	0	24	3	0
59	Y	7	0	8	1	0
60	0	9	0	0	0	0
60	1	18	0	0	1	0
60	2	24	0	0	0	0
60	3	11	0	0	0	0
60	4	3	0	0	0	0
60	A	1657	0	0	0	0
60	B	16	0	0	0	0
60	C	23	0	0	0	0
60	D	29	0	0	0	0
60	E	18	0	0	0	0
60	F	9	0	0	0	0
60	G	8	0	0	0	0
60	H	23	0	0	0	0
60	I	15	0	0	0	0
60	J	18	0	0	0	0
60	K	20	0	0	0	0
60	L	29	0	0	0	0
60	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	N	12	0	0	0	0
60	O	16	0	0	0	0
60	P	11	0	0	0	0
60	Q	7	0	0	0	0
60	R	9	0	0	0	0
60	S	8	0	0	0	0
60	T	7	0	0	0	0
60	U	9	0	0	0	0
60	X	9	0	0	0	0
60	Y	34	0	0	0	0
60	Z	29	0	0	0	0
60	a	4879	0	0	13	0
60	b	130	0	0	0	0
60	c	113	0	0	1	0
60	d	77	0	0	4	0
60	e	59	0	0	4	0
60	f	9	0	0	0	0
60	g	30	0	0	0	0
60	h	5	0	0	0	0
60	i	37	0	0	0	0
60	j	36	0	0	0	0
60	k	56	0	0	3	0
60	l	57	0	0	0	0
60	m	31	0	0	0	0
60	n	17	0	0	0	0
60	o	34	0	0	1	0
60	p	41	0	0	3	0
60	q	37	0	0	0	0
60	r	39	0	0	0	0
60	s	30	0	0	0	0
60	t	29	0	0	0	0
60	u	22	0	0	0	0
60	v	33	0	0	0	0
60	w	25	0	0	0	0
60	x	10	0	0	0	0
60	y	15	0	0	0	0
60	z	32	0	0	0	0
All	All	150552	0	95940	187	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 (187) 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)
28:d:121:THR:HA	60:d:401:HOH:O	1.71	0.89
55:a:2019:A:P	60:a:3302:HOH:O	2.33	0.86
55:a:579:G:H4'	60:a:3302:HOH:O	1.80	0.81
55:a:568:U:H1'	55:a:2030:6MZ:H9C1	1.73	0.69
55:a:1646:C:C6	60:a:3438:HOH:O	2.46	0.69
28:d:125:TRP:N	60:d:401:HOH:O	2.26	0.68
55:a:12:U:H2'	55:a:12:U:O2	1.97	0.65
28:d:124:ARG:HB3	60:d:401:HOH:O	1.98	0.64
11:H:2:SER:N	52:A:823:C:HO2'	1.99	0.61
55:a:1274:A:C5	60:a:3438:HOH:O	2.54	0.61
27:c:271:ARG:O	27:c:272:SER:C	2.43	0.61
35:k:41:ARG:NH1	60:k:201:HOH:O	2.33	0.60
36:l:66:ARG:NH2	36:l:104:GLU:OE2	2.36	0.59
52:A:664:G:H22	52:A:741:G:H1	1.51	0.58
36:l:79:ALA:HA	55:a:2494:G:O2'	2.04	0.57
39:o:95:ALA:C	60:o:206:HOH:O	2.48	0.57
55:a:2522:U:O2'	55:a:2647:U:OP1	2.23	0.56
55:a:1645:G:H4'	60:a:3438:HOH:O	2.04	0.56
29:e:49:ARG:NE	60:e:301:HOH:O	2.39	0.55
52:A:769:G:H4'	52:A:1513:A:H4'	1.89	0.55
55:a:810:U:H4'	60:a:3545:HOH:O	2.06	0.55
55:a:1274:A:C6	60:a:3438:HOH:O	2.53	0.55
40:p:6:ARG:NE	60:p:201:HOH:O	2.38	0.55
8:E:27:GLY:HA2	58:A:1601:SCM:H2M1	1.89	0.55
33:i:120:ARG:HD3	55:a:2780:G:OP2	2.07	0.54
52:A:993:G:O2'	52:A:994:A:N7	2.39	0.54
55:a:12:U:O2	55:a:12:U:C2'	2.55	0.54
52:A:1391:U:H2'	52:A:1392:G:C8	2.41	0.54
55:a:788:A:OP1	55:a:790:U:H5	1.91	0.54
35:k:21:ARG:HA	55:a:811:U:H2'	1.89	0.54
55:a:644:A:H2'	55:a:645:C:O4'	2.08	0.53
27:c:180:GLU:OE2	55:a:1799:G:O2'	2.26	0.53
52:A:502:A:H2'	52:A:503:C:O4'	2.09	0.53
55:a:1508:A:HO2'	55:a:1509:A:C4'	2.21	0.53
55:a:1115:G:O2'	55:a:1116:G:O5'	2.24	0.53
55:a:1434:A:H2'	55:a:1435:G:C8	2.44	0.52
50:z:9:THR:CG2	55:a:2020:A:H5'	2.39	0.52
55:a:857:G:H2'	55:a:858:G:O4'	2.09	0.52
54:Z:9:G:O4'	54:Z:46:G7M:H1'	2.10	0.52
36:l:53:MET:HE1	36:l:103:TYR:CG	2.46	0.51
40:p:49:ASP:OD2	55:a:534:U:O2'	2.18	0.51
3:2:54:ASP:HB3	35:k:57:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:29:PRO:HG2	27:c:34:LEU:HD11	1.91	0.51
29:e:49:ARG:CZ	60:e:301:HOH:O	2.59	0.51
28:d:162:ALA:HA	60:d:415:HOH:O	2.12	0.50
52:A:1066:C:O2	58:A:1601:SCM:N10	2.44	0.50
52:A:1064:G:N7	58:A:1601:SCM:O11	2.41	0.50
33:i:125:TYR:OH	33:i:132:HIS:NE2	2.38	0.50
55:a:2273:A:H2'	55:a:2274:A:C8	2.47	0.50
55:a:493:G:H2'	55:a:494:G:O4'	2.13	0.49
50:z:4:GLN:HG3	60:a:3317:HOH:O	2.13	0.49
54:Z:8:4SU:H6	54:Z:8:4SU:O5'	2.12	0.49
55:a:1939:5MU:OP1	55:a:2604:PSU:O2'	2.28	0.49
40:p:31:VAL:HG13	55:a:580:U:O3'	2.12	0.49
29:e:49:ARG:NH2	60:e:303:HOH:O	2.46	0.48
60:k:201:HOH:O	55:a:806:C:H3'	2.12	0.48
55:a:1792:G:O2'	55:a:1830:C:OP1	2.28	0.48
28:d:62:LYS:N	28:d:63:PRO:HD2	2.28	0.48
59:Y:101:VAL:HG11	55:a:2452:C:O4'	2.14	0.48
55:a:1182:G:H2'	55:a:1183:U:O4'	2.13	0.48
35:k:41:ARG:CZ	60:k:201:HOH:O	2.61	0.48
55:a:1020:A:N1	55:a:1141:U:O2'	2.34	0.48
6:C:4:LYS:NZ	52:A:1191:A:OP1	2.44	0.47
39:o:94:LYS:CE	55:a:1754:A:C8	2.97	0.47
55:a:84:A:N1	55:a:98:G:O2'	2.43	0.47
55:a:1853:A:N1	55:a:2087:G:H1'	2.29	0.47
55:a:639:U:H2'	55:a:640:C:C6	2.49	0.47
7:D:58:LYS:NZ	52:A:545:C:OP1	2.48	0.47
55:a:2395:C:H2'	55:a:2396:G:O4'	2.14	0.47
27:c:207:LYS:HB2	55:a:729:G:C6	2.50	0.47
55:a:645:C:H2'	55:a:647:G:C8	2.50	0.47
55:a:2756:U:H1'	55:a:2757:A:H5''	1.96	0.47
40:p:76:TYR:CZ	40:p:80:ILE:HG13	2.50	0.47
55:a:1028:A:N6	55:a:1125:G:H2'	2.30	0.47
55:a:1646:C:N1	60:a:3438:HOH:O	2.48	0.47
2:1:39:ARG:NH1	60:1:101:HOH:O	2.42	0.46
28:d:121:THR:HB	28:d:127:PHE:CD2	2.50	0.46
55:a:55:G:O2'	55:a:127:A:N1	2.46	0.46
55:a:1932:A:H2'	55:a:1933:G:O4'	2.15	0.46
52:A:673:A:H2'	52:A:674:G:C8	2.50	0.46
55:a:2038:G:H2'	55:a:2039:U:O4'	2.15	0.46
55:a:2243:U:H2'	55:a:2244:U:C6	2.51	0.46
37:m:56:LYS:HE2	37:m:87:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Y:37:6MZ:O2'	55:a:1913:A:N1	2.45	0.46
5:B:94:HIS:O	5:B:95:ARG:C	2.57	0.46
52:A:171:A:H2'	52:A:172:A:C8	2.50	0.46
53:Y:60:C:H5''	53:Y:60:C:H6	1.81	0.46
55:a:723:C:H2'	55:a:724:U:O4'	2.16	0.46
52:A:1255:G:O2'	52:A:1258:G:N3	2.41	0.46
55:a:1027:A:C2	55:a:2488:G:H5'	2.51	0.45
2:1:39:ARG:NH1	55:a:468:G:N7	2.58	0.45
52:A:303:A:H2'	52:A:304:U:O4'	2.16	0.45
52:A:946:A:H2'	52:A:947:G:C8	2.52	0.45
55:a:2547:A:H2'	55:a:2548:U:C6	2.50	0.45
55:a:58:G:O2'	55:a:73:A:N1	2.48	0.45
55:a:1778:U:H2'	55:a:1784:A:N6	2.32	0.45
5:B:28:LYS:N	5:B:29:PRO:CD	2.79	0.45
42:r:20:VAL:HG11	42:r:44:ALA:HA	1.97	0.45
52:A:975:A:N1	52:A:1366:C:O2'	2.41	0.45
52:A:1053:G:N7	52:A:1200:C:H5''	2.32	0.45
23:T:55:GLN:N	23:T:56:PRO:HD2	2.32	0.44
60:p:201:HOH:O	55:a:1250:G:H5''	2.17	0.44
52:A:1394:A:N1	52:A:1500:A:O2'	2.49	0.44
55:a:2327:A:H2'	55:a:2328:A:C8	2.53	0.44
5:B:130:THR:O	5:B:132:LYS:N	2.51	0.44
40:p:6:ARG:CZ	60:p:201:HOH:O	2.66	0.44
55:a:2506:U:C2	55:a:2585:U:O4	2.70	0.44
52:A:376:G:C2	52:A:389:A:C2	3.06	0.44
55:a:120:U:H5''	55:a:122:G:OP2	2.17	0.44
3:2:27:ALA:O	3:2:28:ASN:HB2	2.17	0.44
54:Z:21:A:H61	54:Z:46:G7M:H2'	1.83	0.44
55:a:749:A:H4'	55:a:1271:G:N3	2.33	0.44
55:a:1434:A:H2'	55:a:1435:G:H8	1.82	0.44
27:c:242:LYS:O	55:a:1902:C:H4'	2.18	0.44
28:d:140:HIS:HD2	60:a:3568:HOH:O	2.01	0.44
55:a:548:G:H2'	55:a:549:G:O4'	2.18	0.44
55:a:973:A:H1'	60:a:3771:HOH:O	2.18	0.44
55:a:1129:A:N6	55:a:2491:U:OP1	2.50	0.44
55:a:586:A:N1	55:a:809:G:O2'	2.45	0.43
55:a:1405:U:H2'	55:a:1406:U:C6	2.53	0.43
29:e:58:LYS:NZ	60:e:304:HOH:O	2.47	0.43
52:A:62:U:OP1	52:A:385:C:O2'	2.36	0.43
52:A:927:G:O2'	52:A:1503:A:N7	2.44	0.43
52:A:1402:4OC:O2	52:A:1500:A:N1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:43:ARG:HA	27:c:48:ARG:O	2.19	0.43
46:v:37:ILE:HG21	46:v:80:ILE:HG21	2.00	0.43
55:a:1825:U:H5''	60:a:3883:HOH:O	2.18	0.43
28:d:83:ARG:NH1	55:a:2638:G:OP2	2.51	0.43
55:a:747:5MU:O2	55:a:2014:A:H1'	2.19	0.43
31:g:94:TYR:HA	31:g:106:SER:O	2.19	0.42
53:Y:8:4SU:H6	53:Y:8:4SU:O5'	2.19	0.42
52:A:1495:U:O2'	55:a:1919:A:N1	2.47	0.42
55:a:476:G:H4'	55:a:502:A:N1	2.34	0.42
29:e:41:GLN:HG2	29:e:43:THR:HG23	2.01	0.42
55:a:819:A:C4	55:a:1189:A:C2	3.07	0.42
28:d:25:THR:HG21	28:d:193:VAL:HG22	2.01	0.42
55:a:1826:G:P	60:a:3883:HOH:O	2.76	0.42
55:a:2895:G:H2'	55:a:2896:C:C6	2.54	0.42
55:a:263:G:H2'	55:a:264:C:O4'	2.19	0.42
12:I:123:ARG:NH2	12:I:124:ARG:O	2.53	0.42
44:t:86:ARG:HG3	44:t:95:PHE:CD1	2.54	0.42
55:a:2328:A:H2'	55:a:2329:U:C6	2.54	0.42
33:i:113:PRO:HD2	55:a:558:U:OP1	2.20	0.42
34:j:107:LEU:O	34:j:109:SER:N	2.53	0.42
53:Y:8:4SU:O2'	53:Y:21:A:N1	2.53	0.42
26:b:89:U:H1'	55:a:958:U:O2	2.20	0.42
55:a:2646:C:H6	55:a:2646:C:O5'	2.03	0.42
43:s:1:MET:N	55:a:142:A:N3	2.68	0.41
52:A:1428:A:H2'	52:A:1429:A:O4'	2.20	0.41
55:a:118:A:N3	55:a:178:G:H1'	2.35	0.41
55:a:1020:A:C2	55:a:1141:U:C2	3.08	0.41
55:a:1786:A:H1'	55:a:1938:A:N6	2.35	0.41
55:a:278:A:O2'	55:a:279:A:P	2.78	0.41
55:a:784:G:H5'	55:a:785:G:OP1	2.19	0.41
55:a:1508:A:O2'	55:a:1509:A:O4'	2.26	0.41
26:b:42:C:O2'	30:f:63:GLN:HG2	2.21	0.41
52:A:867:G:O2'	52:A:873:A:N1	2.47	0.41
55:a:1296:G:OP1	55:a:2709:G:O2'	2.30	0.41
6:C:35:SER:OG	6:C:59:ARG:NH1	2.54	0.41
27:c:31:ALA:N	27:c:32:PRO:CD	2.83	0.41
52:A:244:U:O4	52:A:906:A:H1'	2.20	0.41
52:A:928:G:O2'	52:A:1533:C:OP1	2.39	0.41
55:a:1548:A:H2'	55:a:1549:A:C8	2.56	0.41
55:a:2636:C:H2'	55:a:2637:U:C6	2.56	0.41
28:d:1:MET:HB3	28:d:205:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:1562:U:H2'	55:a:1563:U:O4'	2.21	0.41
26:b:29:A:H2'	26:b:30:C:O4'	2.21	0.41
27:c:39:LYS:NZ	60:c:408:HOH:O	2.53	0.41
55:a:2849:U:H4'	55:a:2868:A:C2	2.55	0.41
19:P:61:VAL:HG21	19:P:67:ILE:HD11	2.03	0.41
52:A:1434:A:H2'	52:A:1435:G:O4'	2.21	0.41
55:a:645:C:H2'	55:a:647:G:N7	2.36	0.41
35:k:23:ILE:HG12	41:q:82:HIS:CD2	2.56	0.41
50:z:4:GLN:HA	55:a:2615:U:C2	2.56	0.41
55:a:1474:U:C4	55:a:1475:G:C6	3.08	0.41
52:A:1067:A:N1	52:A:1108:G:O2'	2.47	0.40
5:B:103:ASN:ND2	52:A:1073:U:O2'	2.55	0.40
55:a:1607:C:H4'	55:a:1608:A:O5'	2.21	0.40
55:a:2202:U:O2'	55:a:2204:G:OP1	2.34	0.40
55:a:207:A:H2'	55:a:208:C:O4'	2.21	0.40
55:a:1916:A:H2'	55:a:1917:PSU:O4'	2.21	0.40
55:a:2291:U:H2'	55:a:2292:U:C6	2.56	0.40
55:a:2469:A:H2'	55:a:2470:G:O4'	2.20	0.40
52:A:109:A:H2'	52:A:326:G:N2	2.36	0.40
55:a:756:A:H2'	55:a:757:G:O4'	2.22	0.40
55:a:570:G:H2'	55:a:2030:6MZ:N7	2.36	0.40
55:a:700:G:O2'	55:a:1632:A:N3	2.55	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%)	49 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	B	222/241 (92%)	208 (94%)	13 (6%)	1 (0%)	24	21
6	C	204/233 (88%)	197 (97%)	6 (3%)	1 (0%)	24	21
7	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
8	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
9	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
10	G	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
11	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
12	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
13	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	8
14	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
15	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
16	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
17	N	98/101 (97%)	98 (100%)	0	0	100	100
18	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
19	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
20	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
21	R	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
22	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
23	T	84/87 (97%)	84 (100%)	0	0	100	100
24	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
27	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
28	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
29	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
30	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
31	g	173/177 (98%)	170 (98%)	3 (2%)	0	100	100
32	h	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
33	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
34	j	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	12
35	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	18	14
36	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
38	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	q	101/103 (98%)	101 (100%)	0	0	100	100
42	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	s	91/100 (91%)	91 (100%)	0	0	100	100
44	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
45	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	v	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
47	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	x	59/63 (94%)	59 (100%)	0	0	100	100
49	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
51	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5593/5913 (95%)	5432 (97%)	156 (3%)	5 (0%)	49	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	J	57	VAL
34	j	108	ARG
6	C	61	ALA
5	B	131	LYS
35	k	29	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	B	186/199 (94%)	186 (100%)	0	100	100
6	C	170/190 (90%)	170 (100%)	0	100	100
7	D	172/173 (99%)	172 (100%)	0	100	100
8	E	119/126 (94%)	119 (100%)	0	100	100
9	F	90/116 (78%)	90 (100%)	0	100	100
10	G	126/147 (86%)	126 (100%)	0	100	100
11	H	104/105 (99%)	104 (100%)	0	100	100
12	I	105/107 (98%)	105 (100%)	0	100	100
13	J	86/90 (96%)	86 (100%)	0	100	100
14	K	89/98 (91%)	89 (100%)	0	100	100
15	L	102/103 (99%)	102 (100%)	0	100	100
16	M	93/96 (97%)	93 (100%)	0	100	100
17	N	83/84 (99%)	83 (100%)	0	100	100
18	O	76/77 (99%)	76 (100%)	0	100	100
19	P	65/65 (100%)	65 (100%)	0	100	100
20	Q	73/78 (94%)	73 (100%)	0	100	100
21	R	57/65 (88%)	57 (100%)	0	100	100
22	S	72/79 (91%)	72 (100%)	0	100	100
23	T	65/66 (98%)	65 (100%)	0	100	100
24	U	60/61 (98%)	59 (98%)	1 (2%)	53	60
27	c	216/218 (99%)	216 (100%)	0	100	100
28	d	163/163 (100%)	163 (100%)	0	100	100
29	e	165/165 (100%)	164 (99%)	1 (1%)	78	85
30	f	148/150 (99%)	148 (100%)	0	100	100
31	g	136/138 (99%)	136 (100%)	0	100	100
32	h	114/114 (100%)	114 (100%)	0	100	100
33	i	116/116 (100%)	116 (100%)	0	100	100
34	j	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	k	103/103 (100%)	103 (100%)	0	100	100
36	l	107/107 (100%)	107 (100%)	0	100	100
37	m	98/103 (95%)	98 (100%)	0	100	100
38	n	86/87 (99%)	86 (100%)	0	100	100
39	o	99/100 (99%)	99 (100%)	0	100	100
40	p	89/90 (99%)	89 (100%)	0	100	100
41	q	84/84 (100%)	84 (100%)	0	100	100
42	r	93/93 (100%)	93 (100%)	0	100	100
43	s	80/84 (95%)	80 (100%)	0	100	100
44	t	83/85 (98%)	81 (98%)	2 (2%)	43	47
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	62/63 (98%)	61 (98%)	1 (2%)	55	62
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	54/55 (98%)	54 (100%)	0	100	100
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	47/48 (98%)	47 (100%)	0	100	100
51	4	55/62 (89%)	55 (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
24	U	2	PRO
29	e	176	ASP
44	t	10	GLU
44	t	52	LEU
46	v	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	45	GLN
5	B	51	ASN
5	B	58	ASN
5	B	103	ASN

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Mol	Chain	Res	Type
6	C	123	GLN
7	D	40	GLN
7	D	89	ASN
7	D	196	ASN
8	E	82	GLN
8	E	132	ASN
8	E	148	ASN
9	F	3	HIS
9	F	14	GLN
9	F	17	GLN
9	F	46	GLN
9	F	94	HIS
10	G	9	GLN
10	G	68	ASN
10	G	130	ASN
11	H	21	ASN
12	I	4	ASN
14	K	118	HIS
15	L	75	GLN
19	P	26	ASN
19	P	29	ASN
23	T	3	ASN
23	T	48	GLN
23	T	52	ASN
24	U	64	ASN
27	c	86	ASN
27	c	90	ASN
27	c	117	GLN
27	c	153	GLN
27	c	197	ASN
29	e	90	GLN
29	e	94	GLN
30	f	21	ASN
30	f	63	GLN
31	g	22	GLN
31	g	30	ASN
31	g	73	ASN
31	g	104	ASN
32	h	66	ASN
32	h	145	ASN
33	i	47	HIS
33	i	86	GLN

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Mol	Chain	Res	Type
33	i	136	GLN
34	j	3	GLN
36	l	22	GLN
36	l	60	GLN
38	n	100	HIS
39	o	10	GLN
40	p	52	GLN
41	q	86	GLN
42	r	9	HIS
42	r	40	ASN
45	u	12	GLN
47	w	17	ASN
47	w	36	HIS
48	x	27	ASN
48	x	58	ASN
50	z	4	GLN
50	z	6	ASN
51	4	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	X	9/10 (90%)	2 (22%)	0
26	b	118/120 (98%)	10 (8%)	0
52	A	1516/1542 (98%)	189 (12%)	21 (1%)
53	Y	68/76 (89%)	16 (23%)	1 (1%)
54	Z	68/78 (87%)	12 (17%)	0
55	a	2753/2904 (94%)	293 (10%)	0
All	All	4532/4730 (95%)	522 (11%)	22 (0%)

All (522) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	X	14	A
25	X	15	A
26	b	17	C
26	b	35	C
26	b	36	C
26	b	45	A
26	b	56	G
26	b	67	G

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Mol	Chain	Res	Type
26	b	89	U
26	b	90	C
26	b	105	G
26	b	109	A
52	A	4	U
52	A	6	G
52	A	22	G
52	A	32	A
52	A	39	G
52	A	47	C
52	A	48	C
52	A	51	A
52	A	71	A
52	A	83	C
52	A	85	U
52	A	86	G
52	A	87	C
52	A	95	C
52	A	119	A
52	A	120	A
52	A	121	U
52	A	131	A
52	A	141	G
52	A	144	G
52	A	149	A
52	A	163	C
52	A	164	G
52	A	181	A
52	A	182	A
52	A	189	A
52	A	197	A
52	A	204	G
52	A	226	G
52	A	240	G
52	A	245	U
52	A	247	G
52	A	251	G
52	A	266	G
52	A	267	C
52	A	289	G
52	A	321	A
52	A	328	C

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Mol	Chain	Res	Type
52	A	329	A
52	A	339	C
52	A	345	C
52	A	347	G
52	A	351	G
52	A	352	C
52	A	354	G
52	A	367	U
52	A	368	U
52	A	372	C
52	A	384	G
52	A	398	U
52	A	406	G
52	A	411	A
52	A	412	A
52	A	413	G
52	A	414	A
52	A	429	U
52	A	438	U
52	A	439	U
52	A	451	A
52	A	453	G
52	A	457	G
52	A	467	U
52	A	468	A
52	A	469	C
52	A	474	G
52	A	479	U
52	A	481	G
52	A	484	G
52	A	486	U
52	A	499	A
52	A	511	C
52	A	518	C
52	A	521	G
52	A	531	U
52	A	547	A
52	A	572	A
52	A	573	A
52	A	576	C
52	A	577	G
52	A	633	G

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Mol	Chain	Res	Type
52	A	650	G
52	A	653	U
52	A	665	A
52	A	687	A
52	A	721	G
52	A	723	U
52	A	724	G
52	A	734	G
52	A	747	A
52	A	748	G
52	A	755	G
52	A	777	A
52	A	793	U
52	A	794	A
52	A	802	A
52	A	815	A
52	A	817	C
52	A	821	G
52	A	832	G
52	A	847	G
52	A	849	G
52	A	851	G
52	A	884	U
52	A	885	G
52	A	887	G
52	A	890	G
52	A	914	A
52	A	926	G
52	A	934	C
52	A	935	A
52	A	942	G
52	A	960	U
52	A	966	2MG
52	A	969	A
52	A	975	A
52	A	976	G
52	A	977	A
52	A	993	G
52	A	1003	G
52	A	1004	A
52	A	1009	U
52	A	1020	G

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Mol	Chain	Res	Type
52	A	1030	U
52	A	1031	C
52	A	1033	G
52	A	1036	A
52	A	1037	C
52	A	1039	G
52	A	1053	G
52	A	1065	U
52	A	1085	U
52	A	1094	G
52	A	1095	U
52	A	1099	G
52	A	1101	A
52	A	1124	G
52	A	1125	U
52	A	1132	C
52	A	1137	C
52	A	1139	G
52	A	1140	C
52	A	1159	U
52	A	1171	A
52	A	1184	G
52	A	1196	A
52	A	1197	A
52	A	1213	A
52	A	1225	A
52	A	1226	C
52	A	1227	A
52	A	1238	A
52	A	1248	A
52	A	1253	G
52	A	1256	A
52	A	1257	A
52	A	1260	G
52	A	1275	A
52	A	1280	A
52	A	1285	A
52	A	1286	U
52	A	1287	A
52	A	1300	G
52	A	1302	C
52	A	1312	G

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Mol	Chain	Res	Type
52	A	1317	C
52	A	1319	A
52	A	1320	C
52	A	1338	G
52	A	1346	A
52	A	1353	G
52	A	1363	A
52	A	1370	G
52	A	1379	G
52	A	1419	G
52	A	1429	A
52	A	1441	A
52	A	1449	C
52	A	1450	U
52	A	1452	C
52	A	1453	G
52	A	1487	G
52	A	1492	A
52	A	1497	G
52	A	1503	A
52	A	1505	G
52	A	1506	U
52	A	1517	G
52	A	1529	G
52	A	1530	G
53	Y	5	G
53	Y	7	U
53	Y	8	4SU
53	Y	9	A
53	Y	10	G
53	Y	13	C
53	Y	19	G
53	Y	22	G
53	Y	25	C
53	Y	45	G
53	Y	46	G7M
53	Y	49	G
53	Y	50	G
53	Y	60	C
53	Y	73	A
53	Y	74	C
54	Z	6	G

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Mol	Chain	Res	Type
54	Z	7	G
54	Z	8	4SU
54	Z	9	G
54	Z	13	C
54	Z	19	G
54	Z	46	G7M
54	Z	53	G
54	Z	58	A
54	Z	70	G
54	Z	71	C
54	Z	76	A
55	a	10	A
55	a	12	U
55	a	34	U
55	a	63	A
55	a	71	A
55	a	74	A
55	a	75	G
55	a	101	A
55	a	102	U
55	a	110	G
55	a	118	A
55	a	119	A
55	a	120	U
55	a	131	A
55	a	139	U
55	a	140	C
55	a	142	A
55	a	165	A
55	a	181	A
55	a	196	A
55	a	199	A
55	a	200	U
55	a	215	G
55	a	216	A
55	a	221	A
55	a	222	A
55	a	248	G
55	a	272	A
55	a	276	U
55	a	278	A
55	a	279	A

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Mol	Chain	Res	Type
55	a	282	A
55	a	285	G
55	a	288	U
55	a	289	G
55	a	310	A
55	a	311	A
55	a	330	A
55	a	361	G
55	a	386	G
55	a	404	A
55	a	405	U
55	a	411	G
55	a	412	A
55	a	451	U
55	a	456	C
55	a	481	G
55	a	491	G
55	a	503	A
55	a	504	A
55	a	505	A
55	a	509	C
55	a	530	G
55	a	531	C
55	a	532	A
55	a	533	G
55	a	538	A
55	a	545	U
55	a	546	U
55	a	548	G
55	a	549	G
55	a	563	A
55	a	573	U
55	a	574	A
55	a	575	A
55	a	586	A
55	a	603	A
55	a	614	A
55	a	615	U
55	a	627	A
55	a	637	A
55	a	645	C
55	a	646	U

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Mol	Chain	Res	Type
55	a	647	G
55	a	654	A
55	a	655	A
55	a	685	A
55	a	686	U
55	a	717	C
55	a	730	A
55	a	738	G
55	a	747	5MU
55	a	764	A
55	a	765	C
55	a	775	G
55	a	776	G
55	a	782	A
55	a	784	G
55	a	785	G
55	a	805	G
55	a	812	C
55	a	827	U
55	a	828	U
55	a	846	U
55	a	847	U
55	a	858	G
55	a	859	G
55	a	877	A
55	a	883	G
55	a	888	C
55	a	890	C
55	a	891	G
55	a	895	U
55	a	896	A
55	a	897	C
55	a	905	A
55	a	910	A
55	a	914	G
55	a	915	C
55	a	927	A
55	a	931	U
55	a	946	C
55	a	961	C
55	a	962	G
55	a	974	G

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Mol	Chain	Res	Type
55	a	983	A
55	a	984	A
55	a	985	C
55	a	996	A
55	a	1012	U
55	a	1013	C
55	a	1022	G
55	a	1033	U
55	a	1040	A
55	a	1047	G
55	a	1108	U
55	a	1110	G
55	a	1111	A
55	a	1112	G
55	a	1116	G
55	a	1128	G
55	a	1129	A
55	a	1132	U
55	a	1133	A
55	a	1135	C
55	a	1141	U
55	a	1142	A
55	a	1155	A
55	a	1253	A
55	a	1256	G
55	a	1271	G
55	a	1272	A
55	a	1273	U
55	a	1300	G
55	a	1301	A
55	a	1352	U
55	a	1365	A
55	a	1379	U
55	a	1383	A
55	a	1416	G
55	a	1428	C
55	a	1452	G
55	a	1453	A
55	a	1458	U
55	a	1482	G
55	a	1493	C
55	a	1497	U

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Mol	Chain	Res	Type
55	a	1498	C
55	a	1508	A
55	a	1515	A
55	a	1529	G
55	a	1535	A
55	a	1536	C
55	a	1537	G
55	a	1569	A
55	a	1578	U
55	a	1584	U
55	a	1585	C
55	a	1608	A
55	a	1609	A
55	a	1647	U
55	a	1648	U
55	a	1674	G
55	a	1715	G
55	a	1729	U
55	a	1730	C
55	a	1732	C
55	a	1738	G
55	a	1758	U
55	a	1764	C
55	a	1773	A
55	a	1782	U
55	a	1800	C
55	a	1801	A
55	a	1807	G
55	a	1808	A
55	a	1816	C
55	a	1829	A
55	a	1847	A
55	a	1848	A
55	a	1858	A
55	a	1869	G
55	a	1872	A
55	a	1873	G
55	a	1906	G
55	a	1907	G
55	a	1915	3TD
55	a	1929	G
55	a	1930	G

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Mol	Chain	Res	Type
55	a	1937	A
55	a	1938	A
55	a	1955	U
55	a	1965	C
55	a	1967	C
55	a	1970	A
55	a	1971	U
55	a	1972	G
55	a	1987	A
55	a	1991	U
55	a	1993	U
55	a	2023	C
55	a	2031	A
55	a	2033	A
55	a	2043	C
55	a	2055	C
55	a	2056	G
55	a	2060	A
55	a	2061	G
55	a	2062	A
55	a	2069	G7M
55	a	2198	A
55	a	2204	G
55	a	2211	A
55	a	2225	A
55	a	2238	G
55	a	2239	G
55	a	2268	A
55	a	2282	G
55	a	2283	C
55	a	2287	A
55	a	2305	U
55	a	2308	G
55	a	2312	U
55	a	2322	A
55	a	2325	G
55	a	2333	A
55	a	2335	A
55	a	2340	A
55	a	2347	C
55	a	2350	C
55	a	2361	G

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Mol	Chain	Res	Type
55	a	2383	G
55	a	2385	C
55	a	2396	G
55	a	2402	U
55	a	2406	A
55	a	2424	C
55	a	2425	A
55	a	2429	G
55	a	2430	A
55	a	2431	U
55	a	2435	A
55	a	2441	U
55	a	2448	A
55	a	2474	U
55	a	2476	A
55	a	2491	U
55	a	2494	G
55	a	2502	G
55	a	2505	G
55	a	2518	A
55	a	2529	G
55	a	2547	A
55	a	2554	U
55	a	2566	A
55	a	2567	G
55	a	2573	C
55	a	2602	A
55	a	2603	G
55	a	2609	U
55	a	2613	U
55	a	2629	U
55	a	2630	G
55	a	2661	G
55	a	2663	G
55	a	2689	U
55	a	2690	U
55	a	2714	G
55	a	2726	A
55	a	2744	G
55	a	2748	A
55	a	2757	A
55	a	2765	A

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Mol	Chain	Res	Type
55	a	2778	A
55	a	2790	U
55	a	2791	G
55	a	2797	U
55	a	2798	U
55	a	2799	A
55	a	2820	A
55	a	2821	A
55	a	2861	U
55	a	2884	U

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	A	7	A
52	A	13	U
52	A	119	A
52	A	181	A
52	A	199	A
52	A	367	U
52	A	438	U
52	A	793	U
52	A	858	G
52	A	884	U
52	A	1035	A
52	A	1124	G
52	A	1187	G
52	A	1225	A
52	A	1281	C
52	A	1319	A
52	A	1331	G
52	A	1337	G
52	A	1449	C
52	A	1452	C
52	A	1505	G
53	Y	9	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
55	PSU	a	2604	55	18,21,22	0.90	1 (5%)	22,30,33	0.74	1 (4%)
55	PSU	a	2605	55	18,21,22	0.91	1 (5%)	22,30,33	0.82	1 (4%)
55	OMG	a	2251	54,55	23,26,27	0.32	0	33,38,41	0.40	0
52	4OC	A	1402	52	20,23,24	0.38	0	26,32,35	0.54	0
14	IAS	K	119	14	6,7,8	0.89	0	6,8,10	0.96	0
55	6MZ	a	1618	55	22,25,26	0.30	0	30,36,39	0.55	0
55	PSU	a	955	55	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
55	2MG	a	1835	55	23,26,27	0.38	0	32,38,41	0.37	0
53	4SU	Y	8	53	18,21,22	0.36	0	26,30,33	1.23	3 (11%)
52	PSU	A	516	52	18,21,22	0.90	1 (5%)	22,30,33	0.63	0
54	G7M	Z	46	54	23,26,27	0.73	1 (4%)	35,39,42	0.55	0
52	MA6	A	1518	52	23,26,27	0.24	0	34,38,41	0.70	1 (2%)
36	MS6	l	82	36	5,7,8	0.19	0	2,7,9	0.08	0
53	5MU	Y	54	53	19,22,23	0.26	0	28,32,35	0.35	0
55	6MZ	a	2030	55	22,25,26	0.35	0	30,36,39	0.65	0
55	PSU	a	1917	55	18,21,22	0.90	1 (5%)	22,30,33	0.64	0
52	2MG	A	1207	52	23,26,27	0.38	0	32,38,41	0.41	0
55	3TD	a	1915	55	18,22,23	0.94	1 (5%)	22,32,35	0.67	0
52	2MG	A	966	52	23,26,27	0.39	0	32,38,41	0.35	0
55	5MU	a	747	55	19,22,23	0.25	0	28,32,35	0.41	0
55	5MU	a	1939	55	19,22,23	0.33	0	28,32,35	0.42	0
15	D2T	L	89	15	7,9,10	0.94	0	6,11,13	1.80	2 (33%)
54	4SU	Z	8	54	18,21,22	0.38	0	26,30,33	1.16	3 (11%)
55	1MG	a	745	55	22,26,27	0.50	0	33,39,42	0.51	0
55	PSU	a	746	57,55	18,21,22	0.90	1 (5%)	22,30,33	0.61	0
55	PSU	a	1911	55	18,21,22	0.89	1 (5%)	22,30,33	0.64	0
53	G7M	Y	46	53	23,26,27	0.72	1 (4%)	35,39,42	0.55	0
55	2MA	a	2503	57,55	22,25,26	0.88	1 (4%)	33,37,40	1.08	3 (9%)
55	PSU	a	2457	55	18,21,22	0.88	1 (5%)	22,30,33	0.57	0
54	PSU	Z	55	54	18,21,22	0.90	1 (5%)	22,30,33	0.69	0
52	UR3	A	1498	52	19,22,23	0.26	0	26,32,35	0.63	0
53	PSU	Y	55	53	18,21,22	0.90	1 (5%)	22,30,33	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	2MG	a	2445	55	23,26,27	0.38	0	32,38,41	0.43	0
36	4D4	l	81	36	9,11,12	0.50	0	8,13,15	0.60	0
28	MEQ	d	150	28	8,9,10	0.43	0	5,10,12	0.67	0
52	2MG	A	1516	52	23,26,27	0.37	0	32,38,41	0.55	0
53	6MZ	Y	37	53	22,25,26	0.35	0	30,36,39	0.47	0
55	H2U	a	2449	55	18,21,22	0.57	0	21,30,33	0.75	1 (4%)
55	OMU	a	2552	55	19,22,23	0.20	0	26,31,34	0.39	0
52	5MC	A	967	52	18,22,23	0.31	0	26,32,35	0.58	0
55	OMC	a	2498	57,55	19,22,23	0.29	0	26,31,34	0.49	0
55	PSU	a	2580	55	18,21,22	0.92	1 (5%)	22,30,33	0.73	1 (4%)
54	OMC	Z	32	54	19,22,23	0.26	0	26,31,34	0.36	0
55	PSU	a	2504	55	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
55	5MC	a	1962	55	18,22,23	0.34	0	26,32,35	0.48	0
52	5MC	A	1407	52	18,22,23	0.32	0	26,32,35	0.62	0
54	5MU	Z	54	54	19,22,23	0.26	0	28,32,35	0.29	0
52	G7M	A	527	52	23,26,27	0.74	1 (4%)	35,39,42	0.74	1 (2%)
52	MA6	A	1519	52	23,26,27	0.24	0	34,38,41	0.78	1 (2%)
55	G7M	a	2069	55	23,26,27	0.70	1 (4%)	35,39,42	0.67	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
55	PSU	a	2604	55	-	0/7/25/26	0/2/2/2
55	PSU	a	2605	55	-	0/7/25/26	0/2/2/2
55	OMG	a	2251	54,55	-	1/9/27/28	0/3/3/3
52	4OC	A	1402	52	-	0/9/29/30	0/2/2/2
14	IAS	K	119	14	-	0/7/7/8	-
55	6MZ	a	1618	55	-	0/9/27/28	0/3/3/3
55	PSU	a	955	55	-	0/7/25/26	0/2/2/2
55	2MG	a	1835	55	-	0/9/27/28	0/3/3/3
53	4SU	Y	8	53	-	0/7/25/26	0/2/2/2
52	PSU	A	516	52	-	0/7/25/26	0/2/2/2
54	G7M	Z	46	54	-	0/7/25/26	0/3/3/3
52	MA6	A	1518	52	-	0/11/29/30	0/3/3/3
36	MS6	l	82	36	-	1/4/6/8	-
53	5MU	Y	54	53	-	0/7/25/26	0/2/2/2
55	6MZ	a	2030	55	-	1/9/27/28	0/3/3/3
55	PSU	a	1917	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	2MG	A	1207	52	-	0/9/27/28	0/3/3/3
55	3TD	a	1915	55	-	2/7/25/26	0/2/2/2
52	2MG	A	966	52	-	0/9/27/28	0/3/3/3
55	5MU	a	747	55	-	0/7/25/26	0/2/2/2
55	5MU	a	1939	55	-	0/7/25/26	0/2/2/2
15	D2T	L	89	15	-	2/7/12/14	-
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
55	1MG	a	745	55	-	0/7/25/26	0/3/3/3
55	PSU	a	746	57,55	-	1/7/25/26	0/2/2/2
55	PSU	a	1911	55	-	0/7/25/26	0/2/2/2
53	G7M	Y	46	53	-	2/7/25/26	0/3/3/3
55	2MA	a	2503	57,55	-	2/7/25/26	0/3/3/3
55	PSU	a	2457	55	-	0/7/25/26	0/2/2/2
54	PSU	Z	55	54	-	1/7/25/26	0/2/2/2
52	UR3	A	1498	52	-	0/7/25/26	0/2/2/2
53	PSU	Y	55	53	-	0/7/25/26	0/2/2/2
55	2MG	a	2445	55	-	2/9/27/28	0/3/3/3
36	4D4	l	81	36	-	1/11/12/14	-
28	MEQ	d	150	28	-	2/8/9/11	-
52	2MG	A	1516	52	-	0/9/27/28	0/3/3/3
53	6MZ	Y	37	53	-	0/9/27/28	0/3/3/3
55	H2U	a	2449	55	-	0/7/38/39	0/2/2/2
55	OMU	a	2552	55	-	0/9/27/28	0/2/2/2
52	5MC	A	967	52	-	0/7/25/26	0/2/2/2
55	OMC	a	2498	57,55	-	0/9/27/28	0/2/2/2
55	PSU	a	2580	55	-	0/7/25/26	0/2/2/2
54	OMC	Z	32	54	-	0/9/27/28	0/2/2/2
55	PSU	a	2504	55	-	0/7/25/26	0/2/2/2
55	5MC	a	1962	55	-	0/7/25/26	0/2/2/2
52	5MC	A	1407	52	-	0/7/25/26	0/2/2/2
54	5MU	Z	54	54	-	0/7/25/26	0/2/2/2
52	G7M	A	527	52	-	0/7/25/26	0/3/3/3
52	MA6	A	1519	52	-	2/11/29/30	0/3/3/3
55	G7M	a	2069	55	-	2/7/25/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	2580	PSU	C6-C5	3.64	1.39	1.35
55	a	746	PSU	C6-C5	3.58	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1915	3TD	C6-C5	3.57	1.39	1.35
52	A	516	PSU	C6-C5	3.56	1.39	1.35
53	Y	55	PSU	C6-C5	3.56	1.39	1.35
55	a	1917	PSU	C6-C5	3.54	1.39	1.35
54	Z	55	PSU	C6-C5	3.53	1.39	1.35
55	a	1911	PSU	C6-C5	3.53	1.39	1.35
55	a	2605	PSU	C6-C5	3.53	1.39	1.35
55	a	2604	PSU	C6-C5	3.48	1.39	1.35
55	a	2457	PSU	C6-C5	3.46	1.39	1.35
55	a	2504	PSU	C6-C5	3.43	1.39	1.35
55	a	955	PSU	C6-C5	3.40	1.39	1.35
52	A	527	G7M	C8-N7	2.74	1.38	1.33
54	Z	46	G7M	C8-N7	2.64	1.37	1.33
53	Y	46	G7M	C8-N7	2.52	1.37	1.33
55	a	2069	G7M	C8-N7	2.39	1.37	1.33
55	a	2503	2MA	C6-N6	-2.38	1.28	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	Y	8	4SU	C4-N3-C2	-4.27	123.19	127.34
54	Z	8	4SU	C4-N3-C2	-4.14	123.32	127.34
52	A	1518	MA6	C2-N1-C6	2.96	118.74	111.75
52	A	1519	MA6	C2-N1-C6	2.93	118.68	111.75
55	a	2503	2MA	C5-C4-N3	-2.90	123.93	127.19
53	Y	8	4SU	C5-C4-N3	2.70	117.20	114.69
15	L	89	D2T	OD1-CG-CB	-2.61	116.98	122.44
54	Z	8	4SU	C5-C4-N3	2.59	117.09	114.69
55	a	2503	2MA	C2-N1-C6	2.58	122.10	118.08
55	a	2580	PSU	C3'-C2'-C1'	2.35	104.37	101.64
55	a	2503	2MA	N3-C2-N1	-2.28	121.53	125.72
53	Y	8	4SU	N3-C2-N1	2.26	117.89	114.89
55	a	2605	PSU	C2'-C3'-C4'	-2.14	98.47	102.64
54	Z	8	4SU	N3-C2-N1	2.12	117.70	114.89
55	a	2604	PSU	C2'-C3'-C4'	-2.11	98.54	102.64
15	L	89	D2T	OD2-CG-CB	2.10	117.68	113.15
55	a	2449	H2U	O2-C2-N1	-2.08	120.49	123.11
52	A	527	G7M	C2'-C3'-C4'	-2.03	98.71	102.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	a	1915	3TD	C3'-C4'-C5'-O5'
55	a	1915	3TD	O4'-C4'-C5'-O5'
55	a	2251	OMG	C1'-C2'-O2'-CM2
52	A	1519	MA6	O4'-C4'-C5'-O5'
28	d	150	MEQ	NE2-CD-CG-CB
53	Y	46	G7M	C4'-C5'-O5'-P
52	A	1519	MA6	C3'-C4'-C5'-O5'
28	d	150	MEQ	OE1-CD-CG-CB
55	a	2445	2MG	C3'-C4'-C5'-O5'
55	a	2445	2MG	O4'-C4'-C5'-O5'
36	l	82	MS6	CB-CG-SD-CE
55	a	2030	6MZ	O4'-C4'-C5'-O5'
55	a	2503	2MA	C4'-C5'-O5'-P
15	L	89	D2T	SB-CB-CG-OD2
55	a	2069	G7M	O4'-C4'-C5'-O5'
15	L	89	D2T	CG-CB-SB-CB1
54	Z	55	PSU	O4'-C1'-C5-C6
55	a	746	PSU	O4'-C1'-C5-C6
53	Y	46	G7M	C3'-C4'-C5'-O5'
55	a	2503	2MA	O4'-C4'-C5'-O5'
36	l	81	4D4	O-C-CA-CB
55	a	2069	G7M	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	a	2604	PSU	1	0
52	A	1402	4OC	1	0
53	Y	8	4SU	2	0
54	Z	46	G7M	2	0
55	a	2030	6MZ	2	0
55	a	1917	PSU	1	0
55	a	747	5MU	1	0
55	a	1939	5MU	1	0
54	Z	8	4SU	1	0
53	Y	37	6MZ	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 262 ligands modelled in this entry, 260 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	VAL	Y	101	53	4,6,7	0.57	0	6,7,9	0.88	0
58	SCM	A	1601	-	23,25,25	0.27	0	26,39,39	0.62	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	VAL	Y	101	53	-	0/5/6/8	-
58	SCM	A	1601	-	-	0/4/57/57	0/3/3/3

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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	Y	101	VAL	1	0
58	A	1601	SCM	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

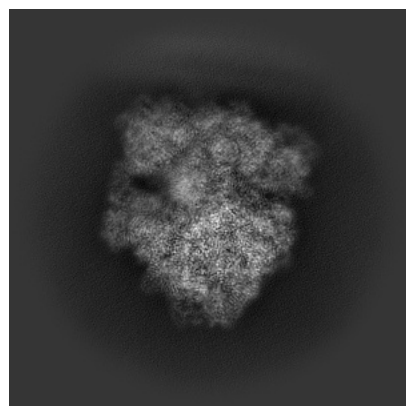
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56070. These allow visual inspection of the internal detail of the map and identification of artifacts.

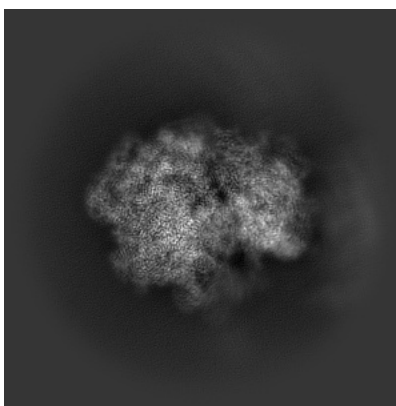
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

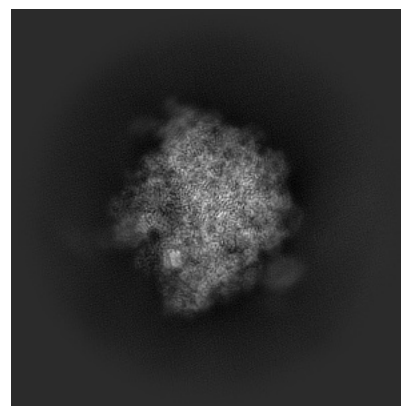
6.1.1 Primary map



X

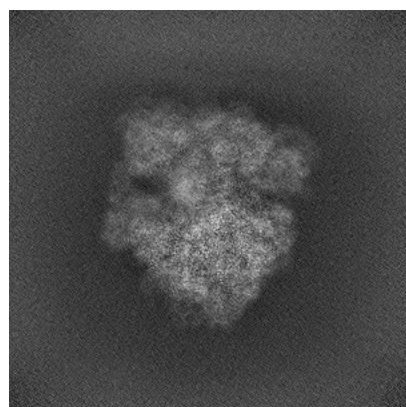


Y

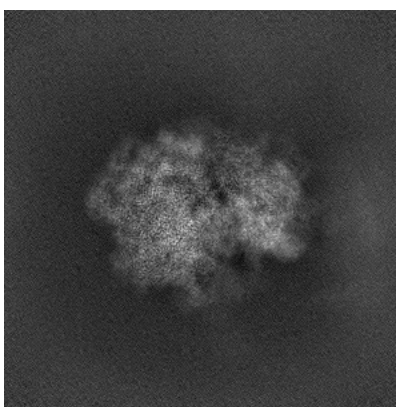


Z

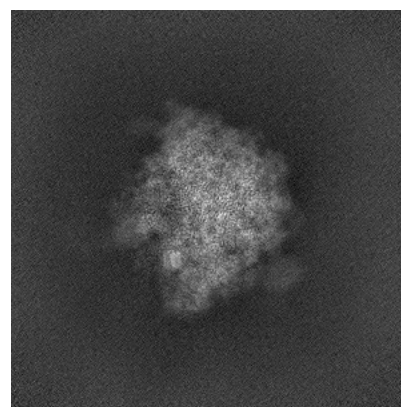
6.1.2 Raw map



X



Y

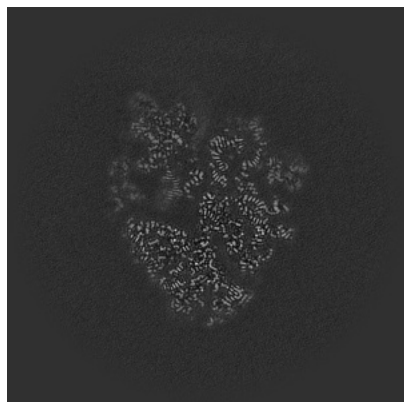


Z

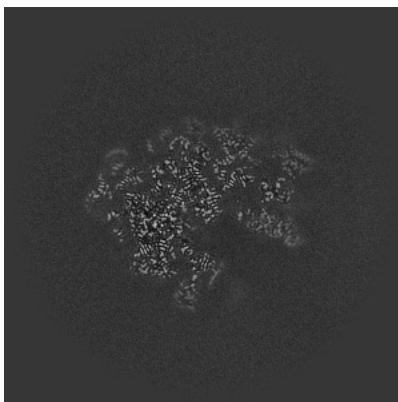
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

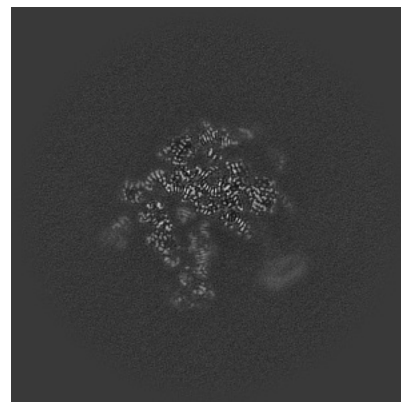
6.2.1 Primary map



X Index: 288

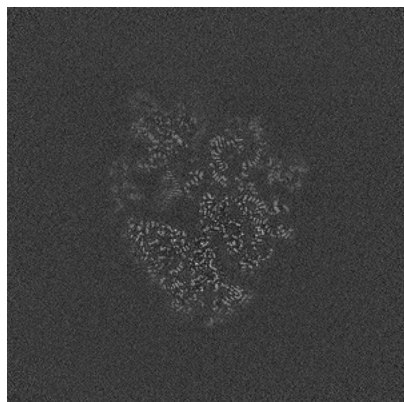


Y Index: 288

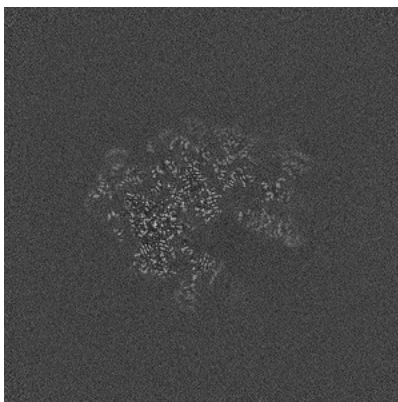


Z Index: 288

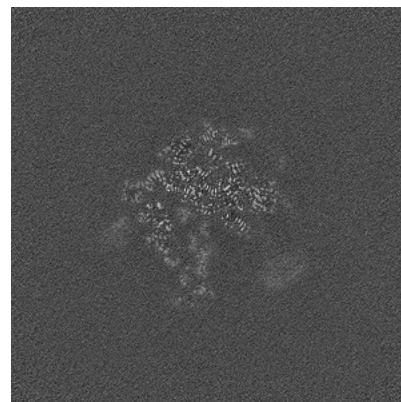
6.2.2 Raw map



X Index: 288



Y Index: 288

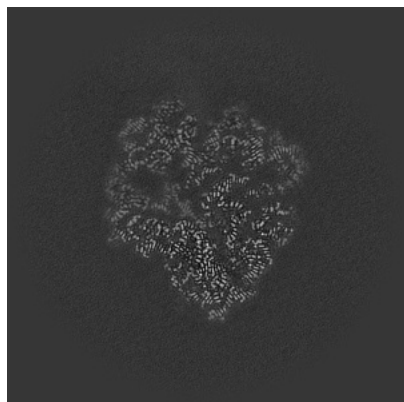


Z Index: 288

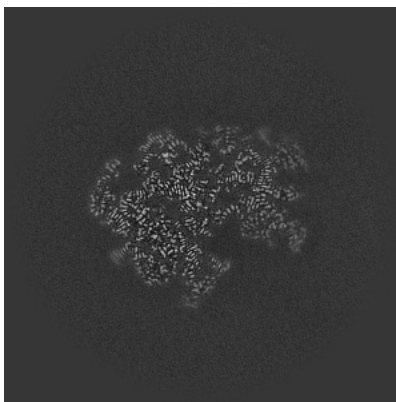
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

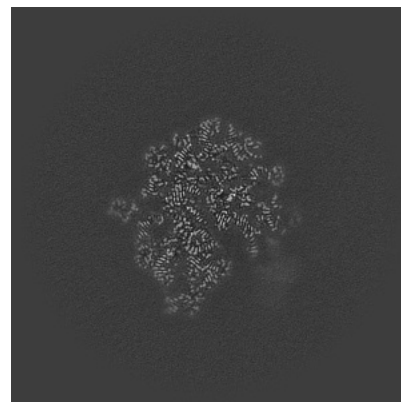
6.3.1 Primary map



X Index: 276

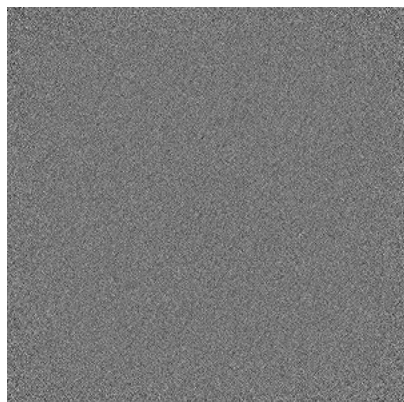


Y Index: 301

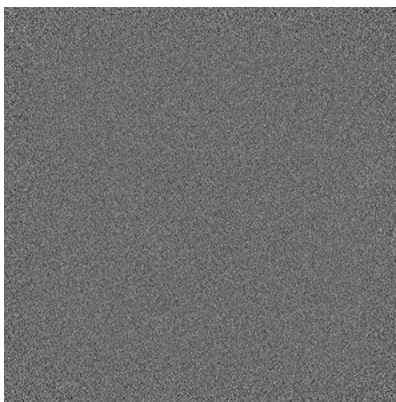


Z Index: 256

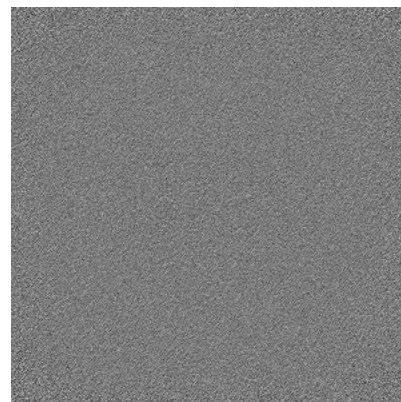
6.3.2 Raw map



X Index: 0



Y Index: 0

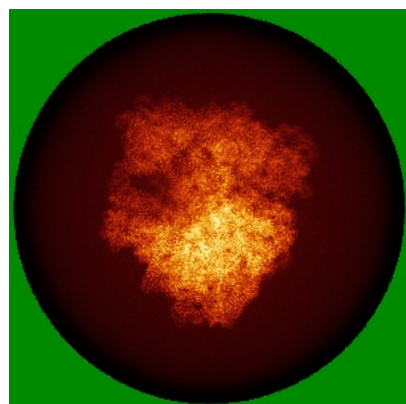


Z Index: 0

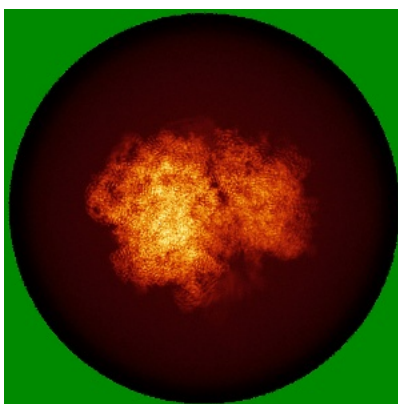
The images above show the largest variance slices of the map in three orthogonal directions.

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

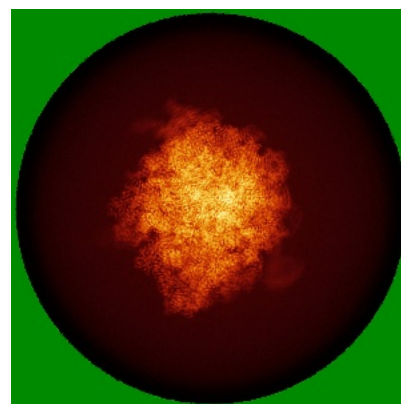
6.4.1 Primary map



X

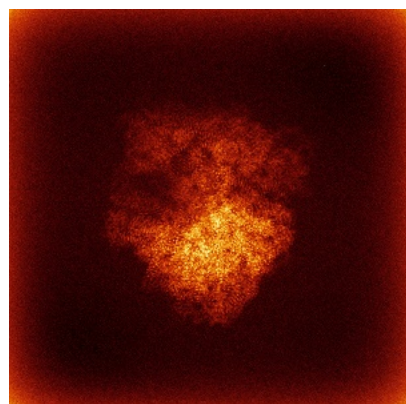


Y

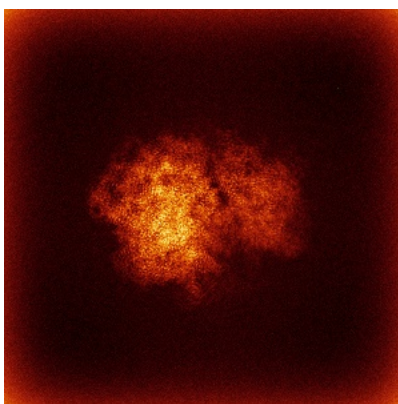


Z

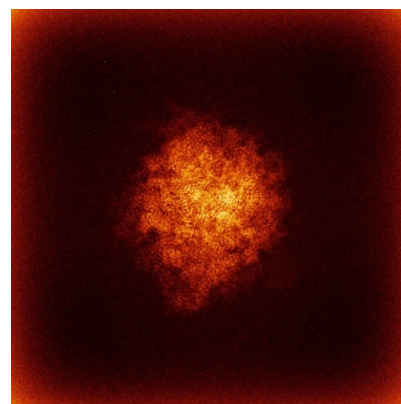
6.4.2 Raw map



X



Y

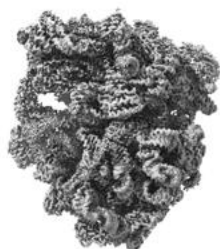


Z

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](#)

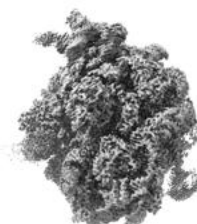
6.5.1 Primary map



X



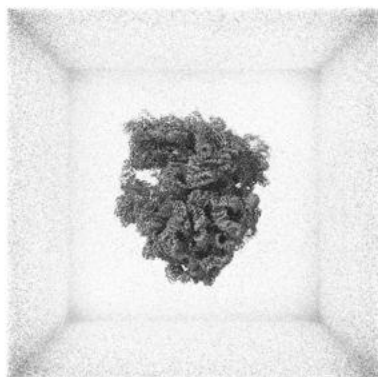
Y



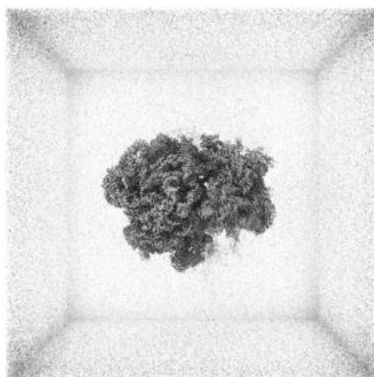
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0683. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

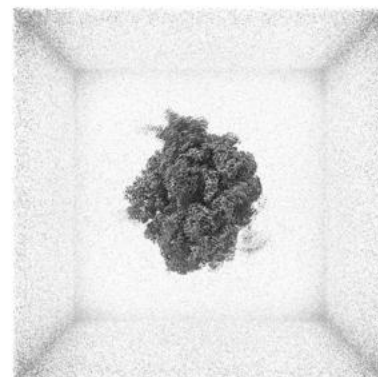
6.5.2 Raw map



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.

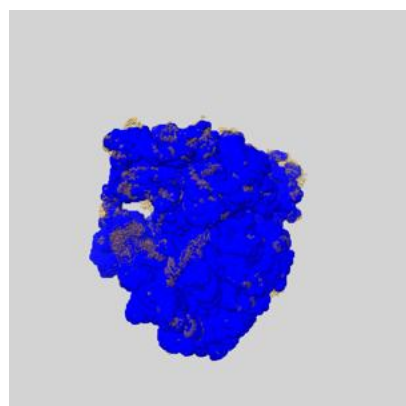
6.6 Mask visualisation [i](#)

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

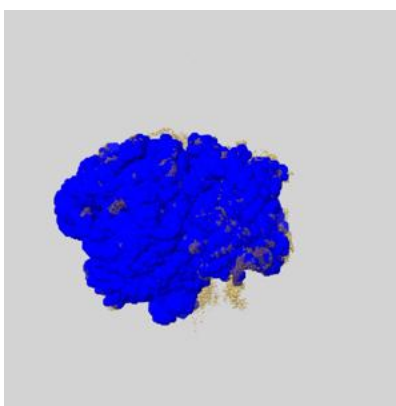
A mask typically either:

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

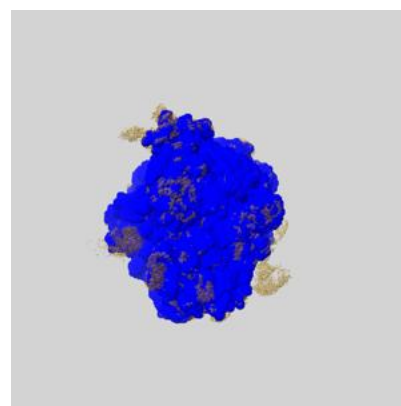
6.6.1 emd_56070_msk_1.map [i](#)



X



Y

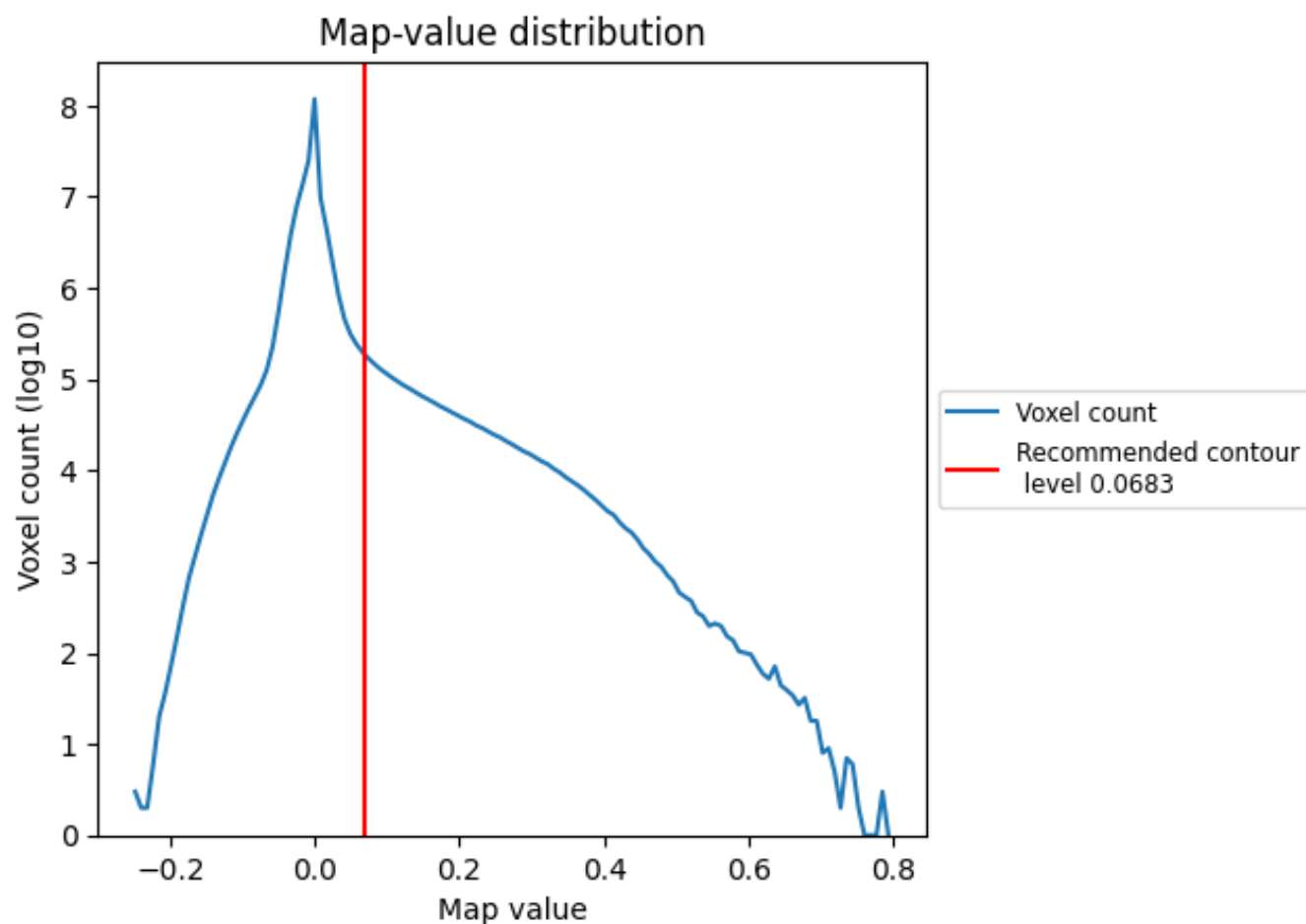


Z

7 Map analysis [i](#)

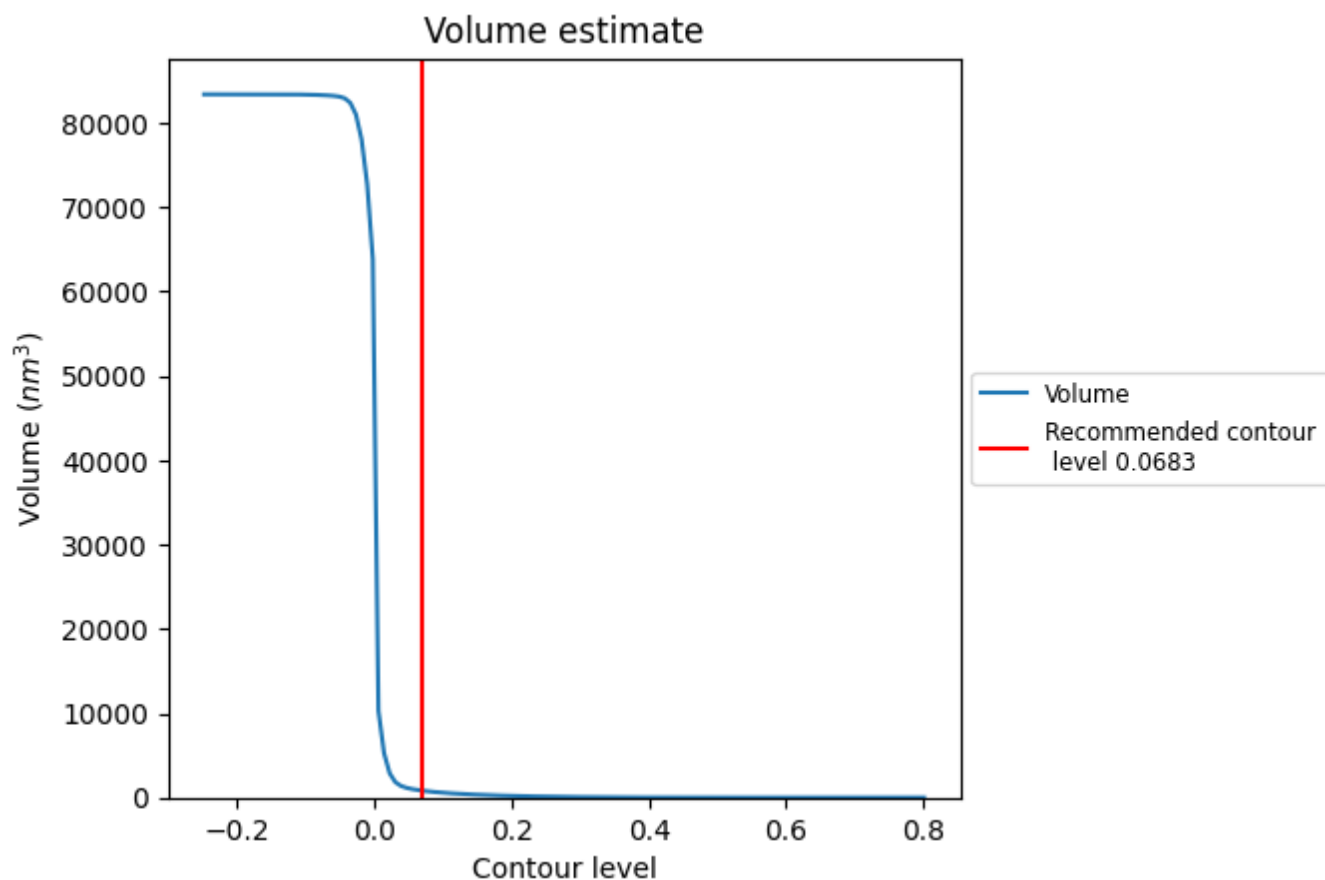
This section contains the results of statistical analysis of the map.

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.

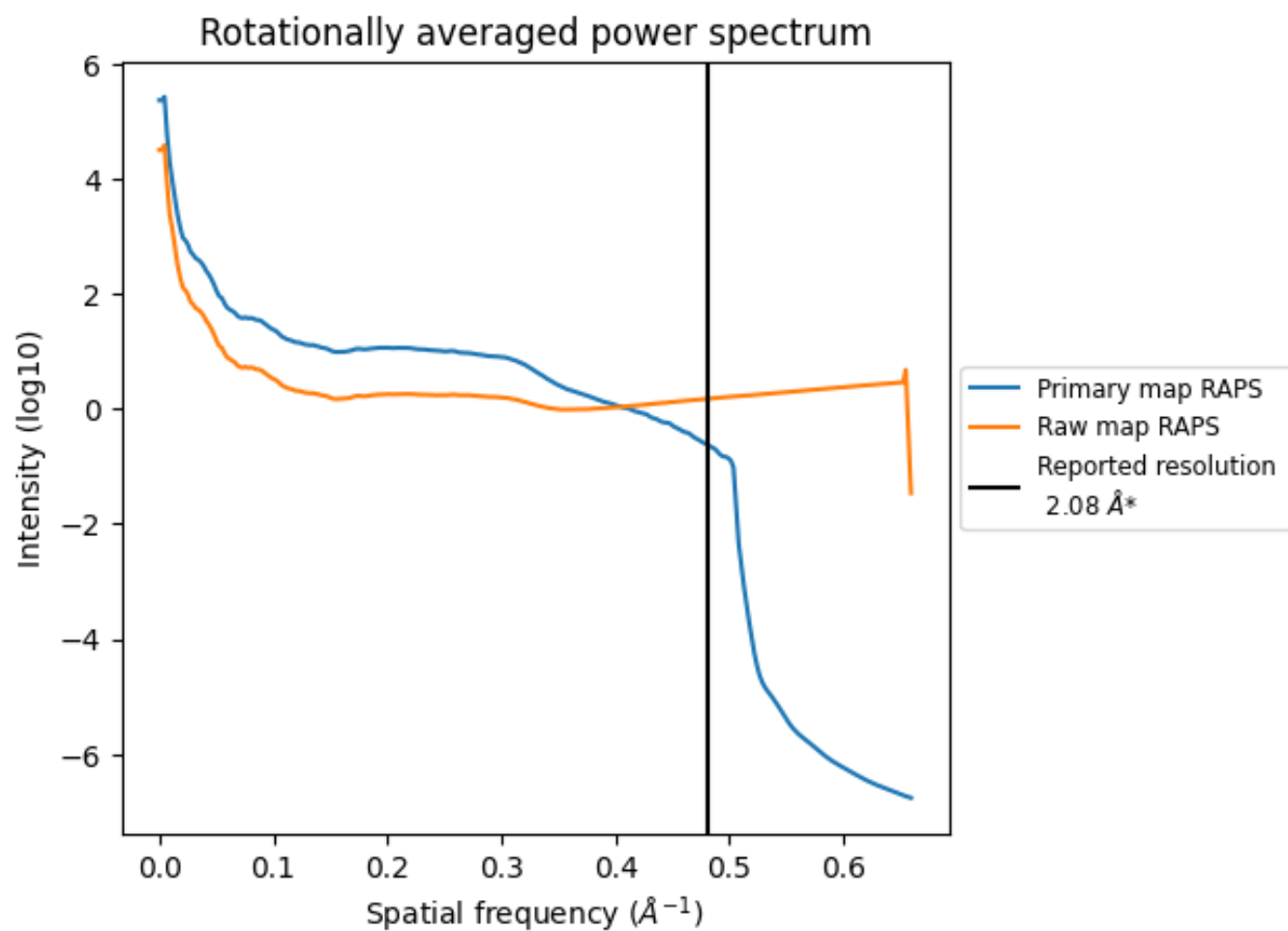
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 838 nm^3 ; this corresponds to an approximate mass of 757 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 ⓘ

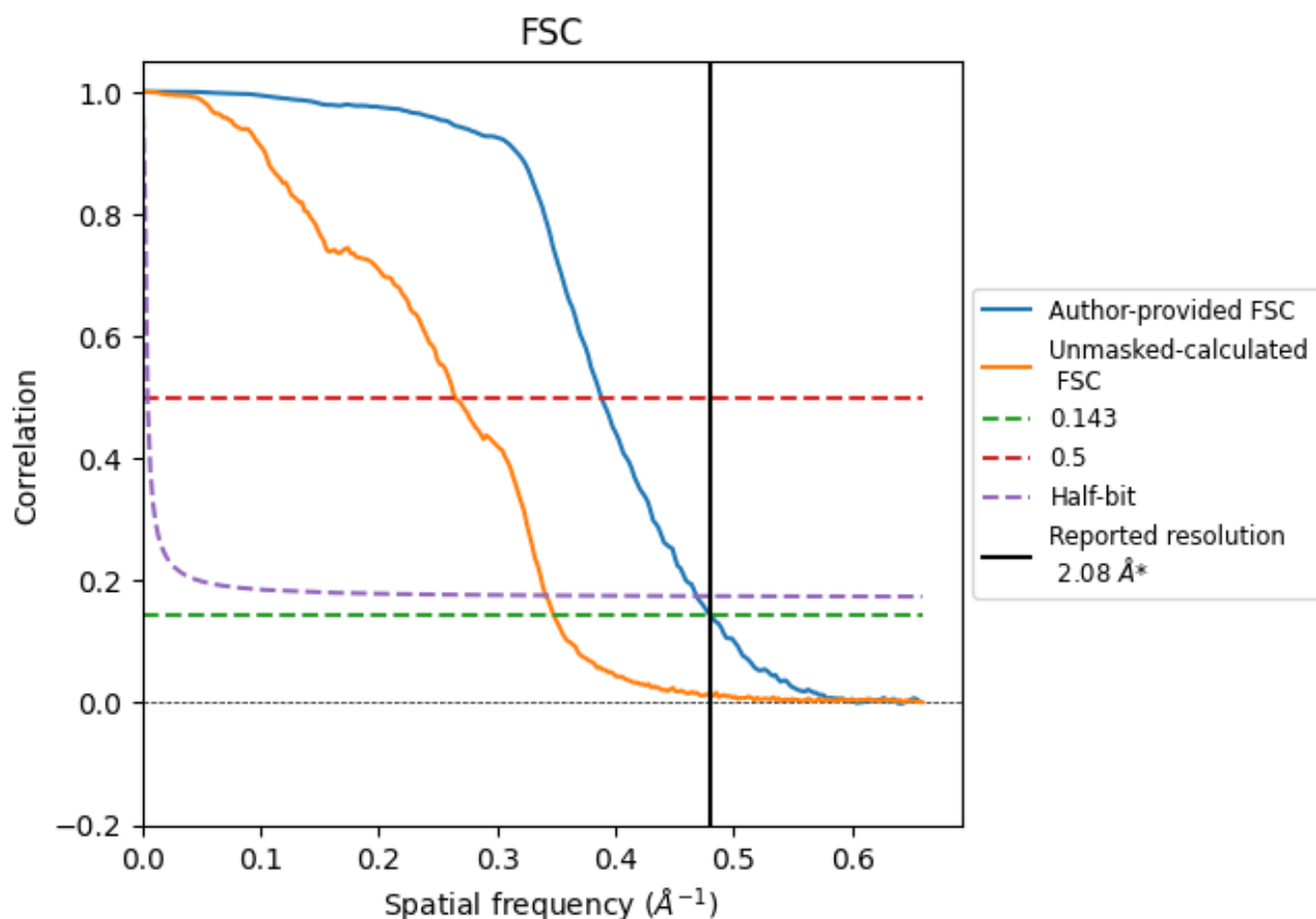


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

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 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates

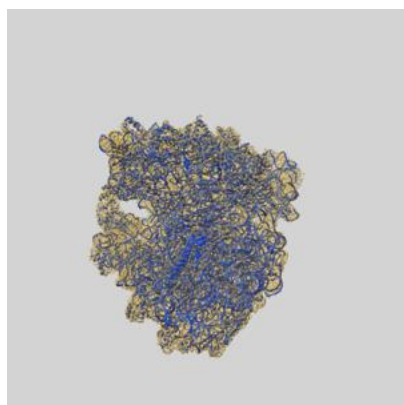
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.58	2.13
Unmasked-calculated*	2.88	3.78	2.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 2.08 by more than 10 %

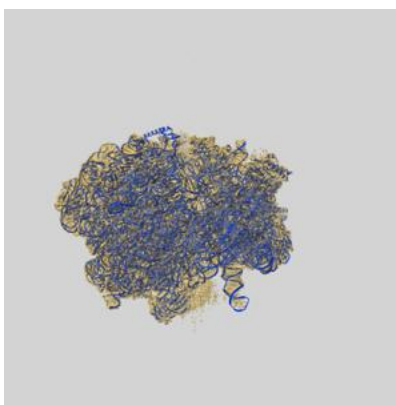
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56070 and PDB model 9TMI. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

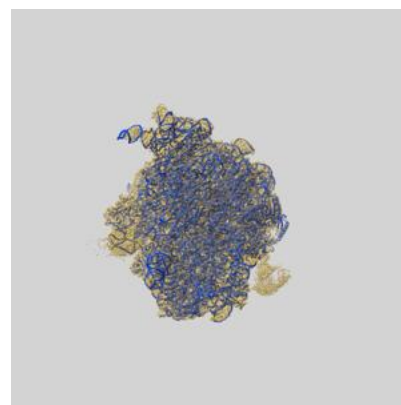
9.1 Map-model overlay [i](#)



X



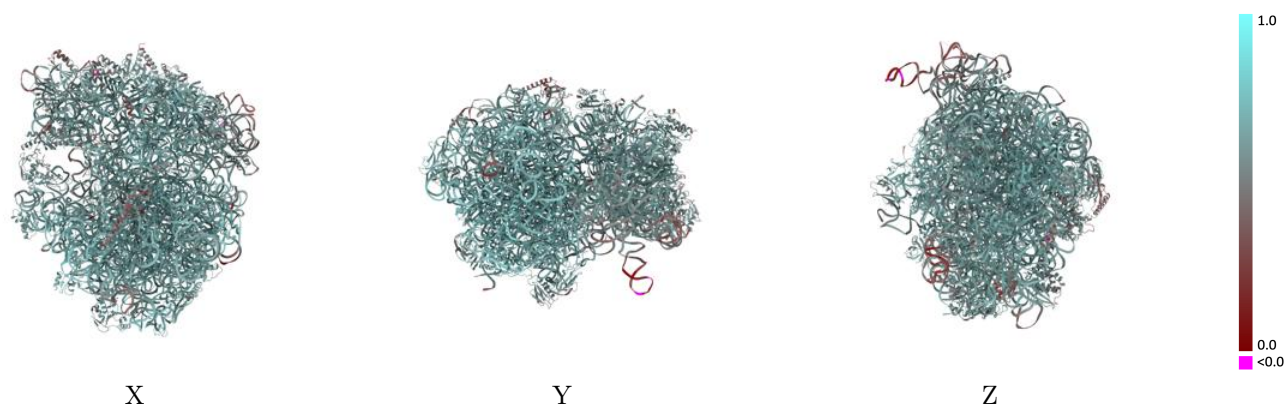
Y



Z

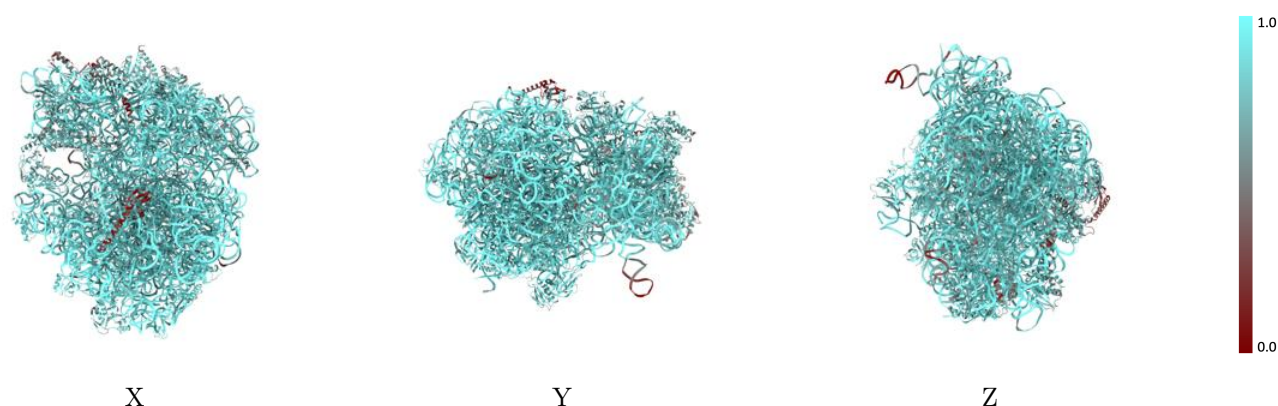
The images above show the 3D surface view of the map at the recommended contour level 0.0683 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



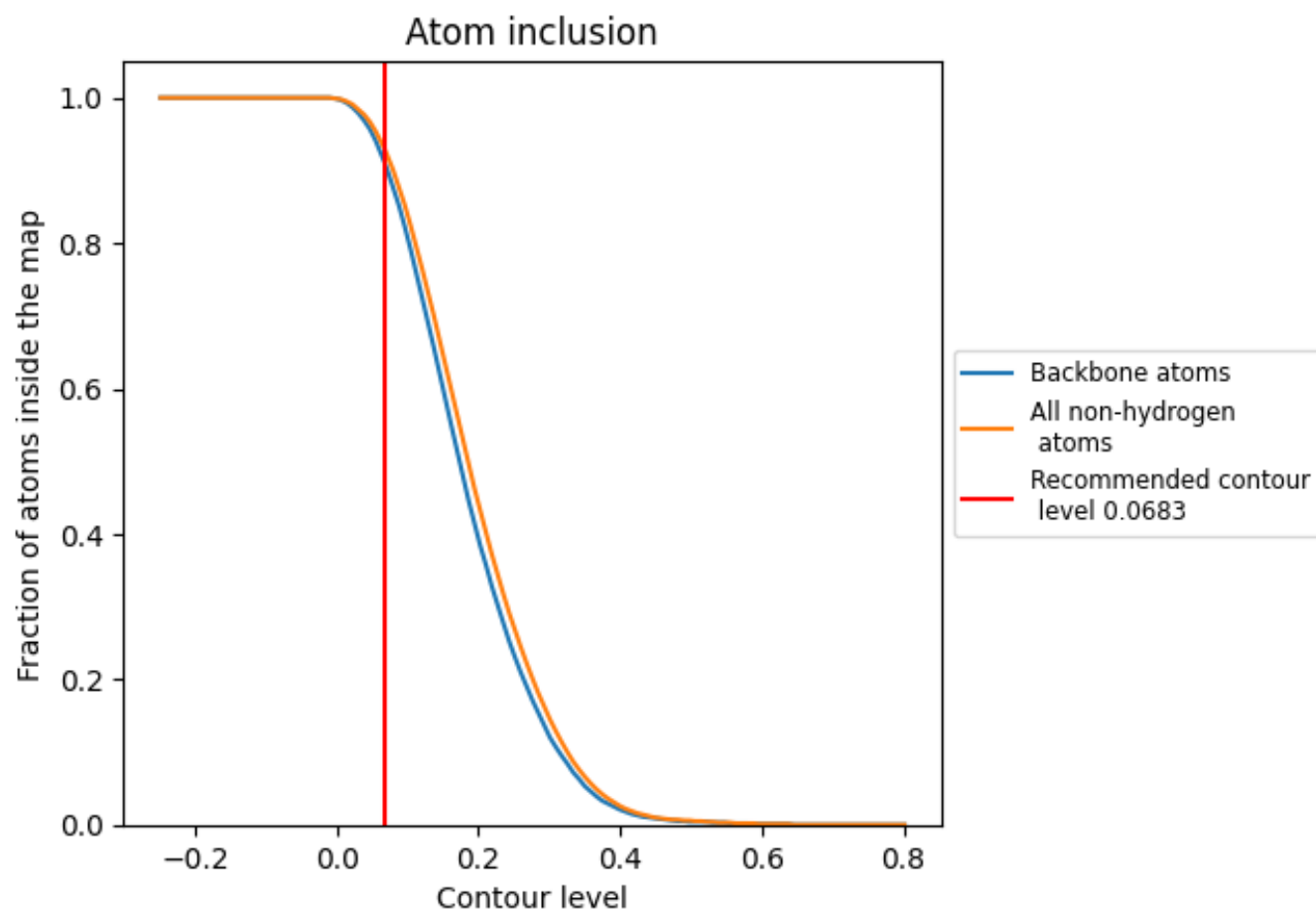
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0683).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.0683) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.6500
0	 0.9020	 0.6760
1	 0.9750	 0.7250
2	 0.9740	 0.7220
3	 0.9420	 0.6910
4	 0.6990	 0.5160
A	 0.9430	 0.6180
B	 0.7300	 0.5600
C	 0.8310	 0.6180
D	 0.7580	 0.5750
E	 0.9010	 0.6630
F	 0.8120	 0.5890
G	 0.6230	 0.5290
H	 0.9090	 0.6470
I	 0.8220	 0.5850
J	 0.6810	 0.5310
K	 0.8340	 0.6170
L	 0.8920	 0.6590
M	 0.8200	 0.6050
N	 0.8620	 0.6150
O	 0.8620	 0.6250
P	 0.8050	 0.5760
Q	 0.8220	 0.5960
R	 0.8410	 0.6040
S	 0.7910	 0.5790
T	 0.7880	 0.5640
U	 0.5790	 0.5120
X	 0.8980	 0.6300
Y	 0.8820	 0.5910
Z	 0.8570	 0.5850
a	 0.9820	 0.6820
b	 0.9730	 0.6470
c	 0.9610	 0.7130
d	 0.9540	 0.7040
e	 0.9160	 0.6700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.8010	 0.5850
g	 0.8490	 0.6010
h	 0.3620	 0.4310
i	 0.9500	 0.7050
j	 0.9390	 0.6960
k	 0.9490	 0.6960
l	 0.9470	 0.6970
m	 0.9810	 0.7200
n	 0.9230	 0.6410
o	 0.9180	 0.6900
p	 0.9780	 0.7240
q	 0.9310	 0.6840
r	 0.9330	 0.7000
s	 0.9030	 0.6670
t	 0.9060	 0.6450
u	 0.8890	 0.6500
v	 0.9170	 0.6940
w	 0.9450	 0.6920
x	 0.8760	 0.6300
y	 0.9240	 0.6880
z	 0.9370	 0.6900