wwPDB EM Validation Summary Report (i)

Feb 24, 2024 – 10:12 PM EST

PDB ID	:	7M4V
EMDB ID	:	EMD-23667
Title	:	A. baumannii Ribosome-Eravacycline complex: 50S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-03-22
Resolution	:	2.54 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

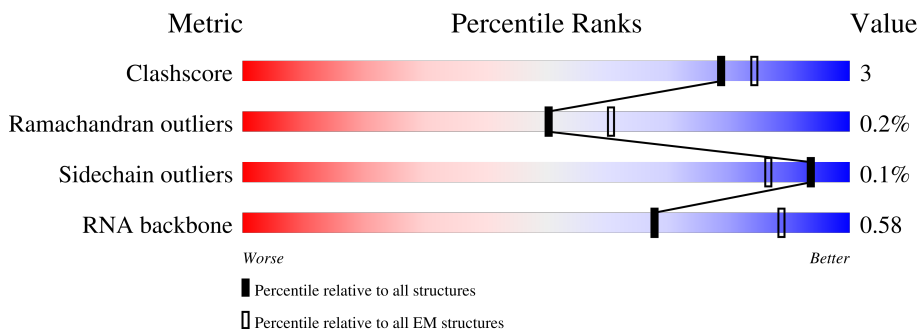|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.54 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.
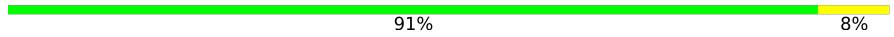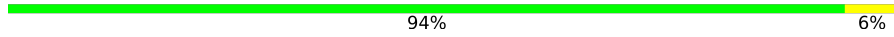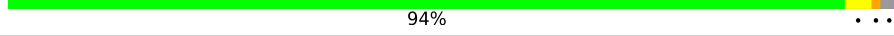
Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		0.1%
RNA backbone		0.58

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
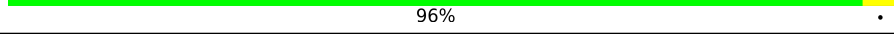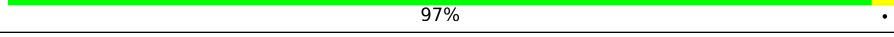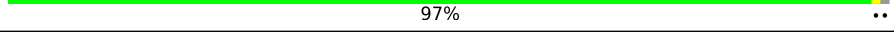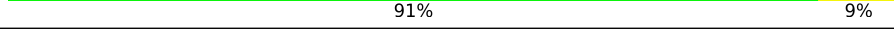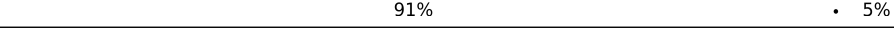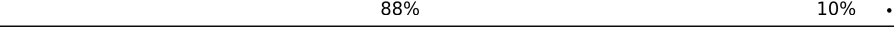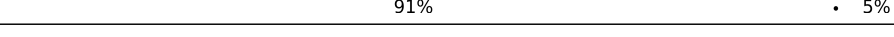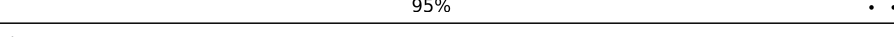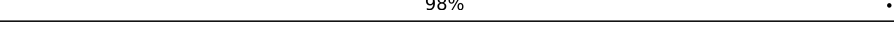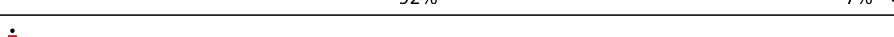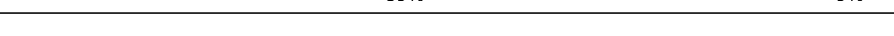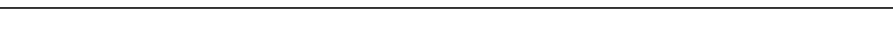
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	51	84% 16%
2	1	44	100%
3	2	64	91% 8%
4	3	38	84% 11% 5%
5	A	2918	70% 21% 6%
6	B	115	73% 21% 6%
7	C	274	93% 7%

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Mol	Chain	Length	Quality of chain
8	D	212	91% 8%
9	E	200	94% 6%
10	F	178	72% / 69% 29%
11	G	177	94%
12	H	148	23% / 30% 9% 59%
13	I	142	96%
14	J	122	97%
15	K	146	97%
16	L	137	91% 9%
17	M	125	91% 5%
18	N	116	88% 10%
19	O	122	91% 5%
20	P	119	95%
21	Q	103	98%
22	R	109	89% 11%
23	S	106	79% 7% 14%
24	T	105	10% / 88% 10%
25	U	98	92% 7%
26	V	85	89% 9%
27	W	78	96%
28	X	65	86% 6% 8%
29	Y	58	95%
30	Z	61	5% / 79% 11% 10%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 86404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2732	Total	C	N	O	P	0	0
			58607	26163	10731	18982	2731		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total 946	C 592	N 180	O 169	S 5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	144	Total 1071	C 663	N 213	O 195	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total 1087	C 687	N 210	O 185	S 5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total 942	C 590	N 186	O 163	S 3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total 857	C 528	N 173	O 155	S 1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	116	Total 913	C 575	N 176	O 162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	118	Total 942	C 594	N 198	O 147	S 3	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total 807	C 506	N 155	O 143	S 3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total 826	C 514	N 158	O 150	S 4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total 710	C 452	N 128	O 129	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	103	Total 766	C 476	N 142	O 148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total 760	C 477	N 143	O 139	S 1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	77	Total 585	C 363	N 112	O 108	S 2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total 632	C 395	N 130	O 105	S 2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	3	1	Total	Zn	0
			1	1	

- Molecule 32 is Eravacycline (three-letter code: YQM) (formula: $C_{27}H_{31}FN_4O_8$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	F	N	O	0
			40	27	1	4	8	

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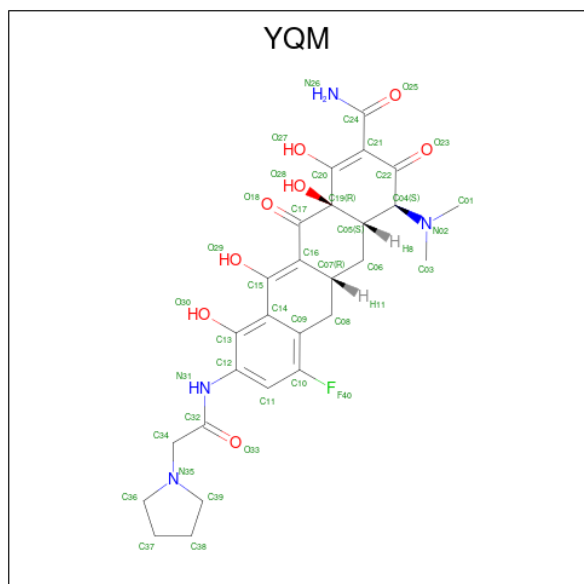
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
32	A	1	40	27	1	4	8	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	A	157	157	157	0
33	B	1	Total 1	Mg 1	0
33	K	1	Total 1	Mg 1	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
34	1	1	1	1	0
34	2	3	Total 3	O 3	0
34	A	759	Total 759	O 759	0
34	B	5	Total 5	O 5	0
34	C	9	Total 9	O 9	0
34	D	4	Total 4	O 4	0
34	E	4	Total 4	O 4	0
34	K	5	Total 5	O 5	0
34	P	3	Total 3	O 3	0
34	R	2	Total 2	O 2	0
34	S	3	Total 3	O 3	0
34	U	1	Total 1	O 1	0
34	W	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
34	Z	2	Total 2	O 2	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 50S ribosomal protein L33

Chain 0:

84%   16%
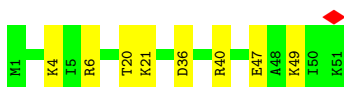
• Molecule 2: 50S ribosomal protein L34

Chain 1:

100%

There are no outlier residues recorded for this chain.

• Molecule 3: 50S ribosomal protein L35

Chain 2:

91%   8%

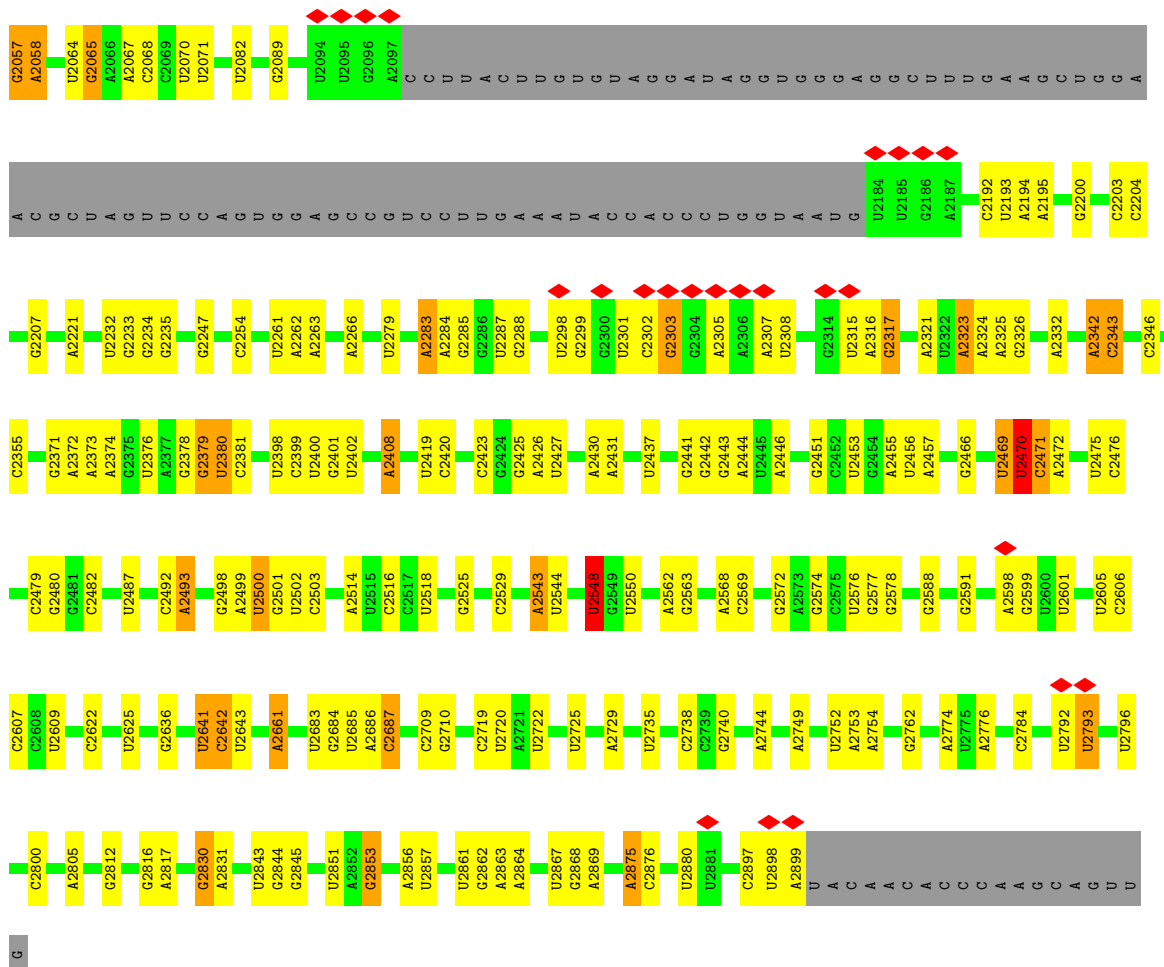• Molecule 4: 50S ribosomal protein L36

Chain 3:

84%   11%   5%

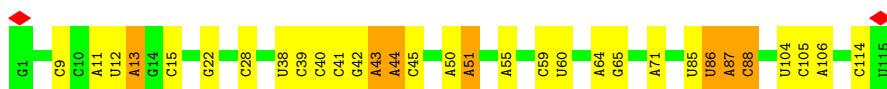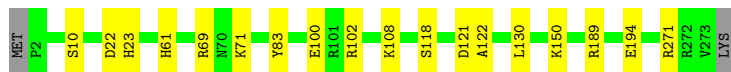• Molecule 5: 23s ribosomal RNA

Chain A:

70%   21%   6%
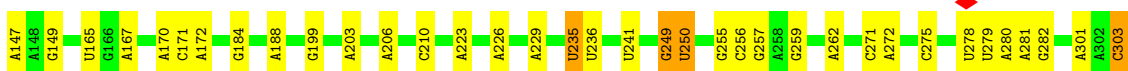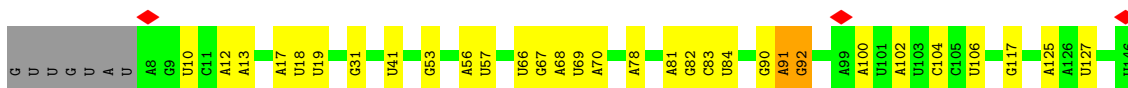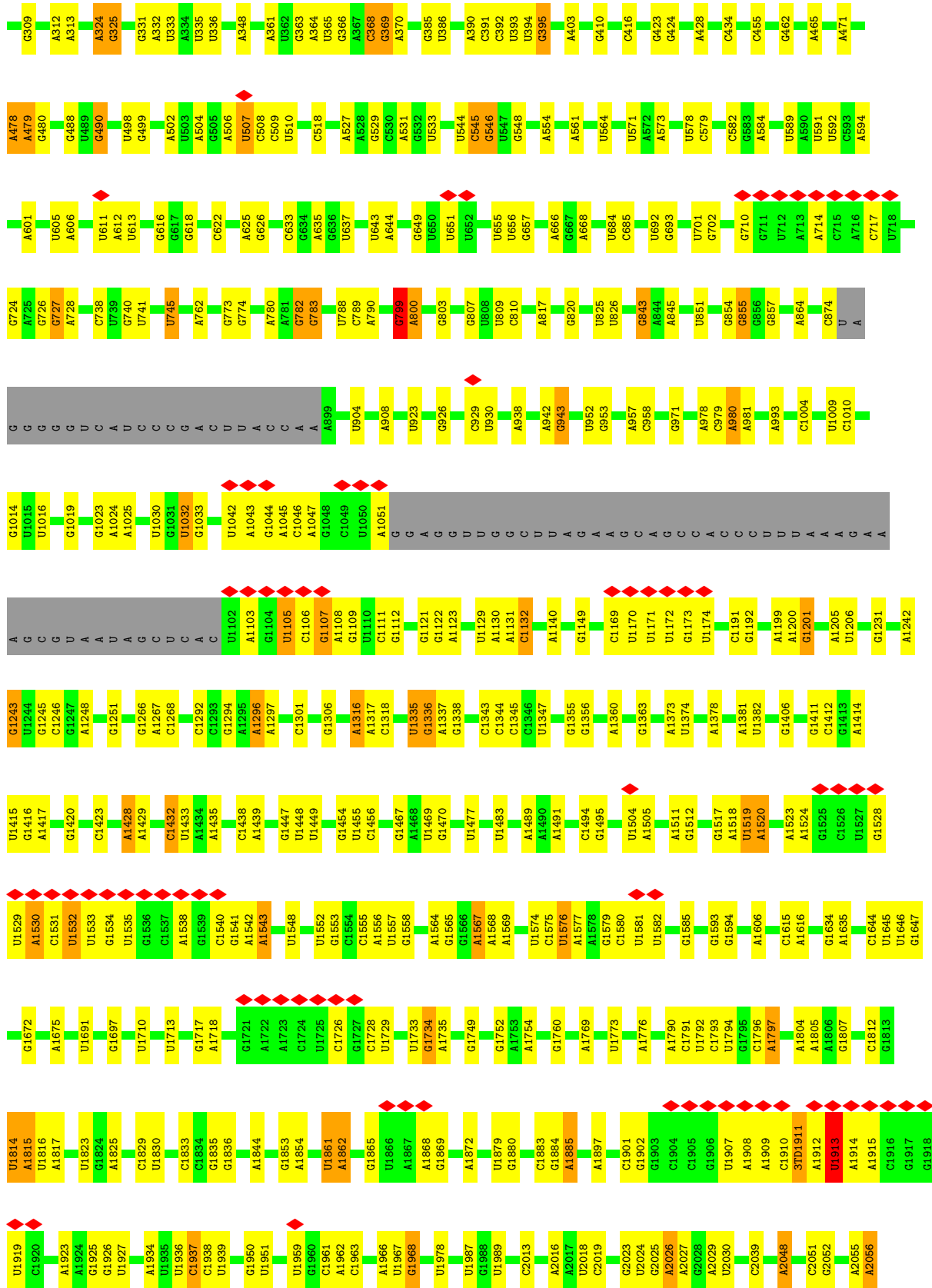
• Molecule 6: 5s ribosomal RNA

Chain B:

• Molecule 7: 50S ribosomal protein L2

Chain C:

• Molecule 8: 50S ribosomal protein L3

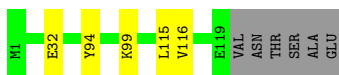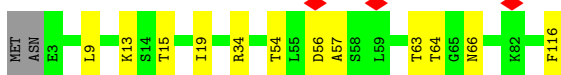Chain D:

• Molecule 9: 50S ribosomal protein L4

Chain E:

94% 6%

M1 S14 Q40 G41 T42 H45 R87 V152 L156 V168 V169 D170 A171 E196 G200

• Molecule 10: 50S ribosomal protein L5

Chain F:

72%
69% 29%

MET ALA ARG L4 K5 A6 R7 Y8 N9 D10 E11 L12 K13 A14 K15 L16 Q17 E18 E19 L20 S21 I22 K23 N24 E27 R30 I31 I34 T35 L36 N37 M38 G39 V40 G41 A42 A43 A44 T45 D46 K47 K48 L49 L50 D51 G52 A53 V54 A55 D56 M57 Q58 L59 I60 A61 G62 Q63

K64 P65 L69 A70 R71 K72 S73 I74 A75 G76 F77 K78 I79 R80 D81 G82 W83 P84 I85 K88 V89 T90 L91 R92 G93 D94 Q95 M96 Y97 E98 F99 L100 D101 R102 L103 I104 S105 I106 A107 I108 P109 R110 I111 R112 D113 F114 R115 G116 F117 S118 A119 K120 S121 F122 D123 G124 R125 G126

N127 Y128 S129 M130 G131 L132 K133 E134 Q135 I136 V137 F138 P139 E140 I141 D142 F143 D144 K145 I146 D147 R148 I149 R150 G151 I154 T155 I156 T157 T158 T159 A160 R161 T162 D163 D164 E165 G166 R167 A168 L169 M170 R171 A172 F173 G174 F175 P176 F177 LYS

• Molecule 11: 50S ribosomal protein L6

Chain G:

94%

MET S2 P12 N13 G14 E46 E47 G48 K49 E57 V71 L75 G78 V79 S80 E81 T101 K175 LYS LYS

• Molecule 12: 50S ribosomal protein L9

Chain H:

23%
30% 9% 59%

M1 I4 L5 L6 Q7 R8 I9 K10 N11 L12 G13 K14 L15 G16 D17 K18 I31 P32 A38 A39 T40 E41 A42 N43 T44 A45 A46 F47 E48 A49 R50 R51 A52 E53 L54 E55 K56 Q57 E58 A59 E60 VAL LEU ALA ALA ALA GLN ALA ARG ALA GLU GLN LEU ASN GLU VAL ASN

ILE VAL ILE THR ALA LYS ALA GLY ASP GLU GLY LYS LEU PHE GLY SER ILE GLY THR ARG ASP ILE ALA ASP ALA LEU THR ASN ALA GLY LEU THR VAL ASP ARG ALA GLU VAL ARG LEU PRO ASN GLY ALA LEU ARG HIS THR GLY GLU PHE ASN ILE ALA ILE GLN LEU HIS HIS ASP

VAL VAL ALA GLU LEU VAL THR ILE VAL SER GLU

• Molecule 13: 50S ribosomal protein L13

Chain I:

96%

M1 V11 Q12 H13 K73 E86 E98 D141 I142

• Molecule 14: 50S ribosomal protein L14

Chain J:

97%

• Molecule 15: 50S ribosomal protein L15

Chain K:

97%

• Molecule 16: 50S ribosomal protein L16

Chain L:

91%   9%

• Molecule 17: 50S ribosomal protein L17

Chain M:

91%   5%

• Molecule 18: 50S ribosomal protein L18

Chain N:

88%   10%

• Molecule 19: 50S ribosomal protein L19

Chain O:

91%   5%

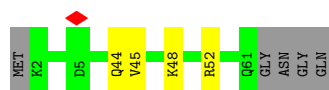• Molecule 20: 50S ribosomal protein L20

Chain P:

95%

• Molecule 21: 50S ribosomal protein L21

Chain Q:
98%

M1 A51 P52 G103

• Molecule 22: 50S ribosomal protein L22

Chain R:
89%   11%

M1 E2 V3 D22 R25 G26 K27 L33 N37 A58 V66 L69 E78 R92 A93 D94 V109

• Molecule 23: 50S ribosomal protein L23

Chain S:
79%   7%   14%

M1 R5 V9 I35 N36 T60 T66 K67 R68 F69 G70 R71 D91 VAL GLU MET ALA ASP LEU GLY ASP THR ALA GLU SER ALA ALA GLU

• Molecule 24: 50S ribosomal protein L24

10%

Chain T:
88%   10%

MET A2 Q9 T23 S28 E29 D30 N47 R48 V49 T50 G51 A52 E53 I65 I86 D87 G88 V89 K90 Y94 G98 A104 LYS

• Molecule 25: 50S ribosomal protein L25

Chain U:
92%   7%

MET A2 N3 G37 N38 E66 I67 K68 V69 G70 D71 R83 N88 A98

• Molecule 26: 50S ribosomal protein L27

Chain V:
89%   9%

MET ALA THR LYS LYS ALA GLY GLY S9 T43 V85

• Molecule 27: 50S ribosomal protein L28

Chain W:
96%

MET S2 I64 V68 I78

• Molecule 28: 50S ribosomal protein L29

Chain X:

86%   6%   8%

MET K2 D5 Q44 V45 K48 R52 Q61 GLY ASN GLY GLN

• Molecule 29: 50S ribosomal protein L30

Chain Y:

95%

MET K2 L23 M53 E58

• Molecule 30: 50S ribosomal protein L32

5%

Chain Z:

79%   11%   10%

MET A2 V3 Q4 E24 D30 G34 D45 Q52 L53 F54 A55 K56 ALA ALA ASP ALA GLU
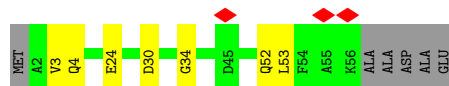
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.051	Depositor
Minimum map value	-1.693	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YQM, OMU, PSU, 2MA, ZN, MG, 5MU, 2MG, 7MG, OMG, 3TD, 6MZ

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	0.26	0/434	0.52	0/573
2	1	0.24	0/367	0.66	0/481
3	2	0.24	0/515	0.61	0/678
4	3	0.25	0/296	0.59	0/389
5	A	0.21	0/65276	0.76	7/101810 (0.0%)
6	B	0.20	0/2739	0.76	0/4266
7	C	0.24	0/2152	0.57	0/2891
8	D	0.24	0/1590	0.56	0/2142
9	E	0.25	0/1537	0.52	0/2073
10	F	0.27	0/1390	0.55	0/1863
11	G	0.25	0/1337	0.50	0/1807
12	H	0.26	0/461	0.55	0/616
13	I	0.25	0/1151	0.47	0/1551
14	J	0.25	0/956	0.58	0/1286
15	K	0.24	0/1079	0.57	0/1439
16	L	0.25	0/1104	0.57	0/1475
17	M	0.25	0/956	0.57	0/1282
18	N	0.24	0/865	0.56	0/1156
19	O	0.24	0/925	0.56	0/1241
20	P	0.26	0/955	0.58	0/1272
21	Q	0.24	0/818	0.54	0/1094
22	R	0.24	0/831	0.51	0/1113
23	S	0.26	0/716	0.51	0/957
24	T	0.23	0/770	0.50	0/1034
25	U	0.24	0/770	0.53	0/1036
26	V	0.24	0/593	0.55	0/793
27	W	0.22	0/642	0.54	0/856
28	X	0.24	0/487	0.48	0/646
29	Y	0.24	0/460	0.54	0/614
30	Z	0.23	0/462	0.63	0/615
All	All	0.22	0/92634	0.71	7/139049 (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
4	3	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1105	U	O4'-C1'-N1	11.66	117.53	108.20
5	A	727	G	O4'-C1'-N9	5.97	112.97	108.20
5	A	1105	U	N1-C1'-C2'	5.61	121.30	114.00
5	A	2470	U	C2-N1-C1'	5.50	124.29	117.70
5	A	788	U	C2-N1-C1'	5.45	124.24	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Peptide

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	427	0	462	4	0
2	1	363	0	401	0	0
3	2	509	0	566	3	0
4	3	295	0	326	7	0
5	A	58607	0	29474	228	0
6	B	2450	0	1241	17	0
7	C	2111	0	2176	12	0
8	D	1572	0	1610	13	0
9	E	1516	0	1569	6	0
10	F	1370	0	1420	38	0
11	G	1318	0	1373	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	458	0	480	17	0
13	I	1125	0	1148	5	0
14	J	946	0	1007	2	0
15	K	1071	0	1140	1	0
16	L	1087	0	1162	9	0
17	M	942	0	987	3	0
18	N	857	0	899	9	0
19	O	913	0	968	4	0
20	P	942	0	1009	6	0
21	Q	807	0	842	3	0
22	R	826	0	894	8	0
23	S	710	0	768	4	0
24	T	766	0	816	6	0
25	U	760	0	783	5	0
26	V	585	0	589	2	0
27	W	632	0	667	1	0
28	X	486	0	528	3	0
29	Y	455	0	476	2	0
30	Z	456	0	448	4	0
31	3	1	0	0	0	0
32	A	80	0	0	1	0
33	A	157	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
34	1	1	0	0	0	0
34	2	3	0	0	0	0
34	A	759	0	0	34	0
34	B	5	0	0	0	0
34	C	9	0	0	0	0
34	D	4	0	0	1	0
34	E	4	0	0	0	0
34	K	5	0	0	0	0
34	P	3	0	0	0	0
34	R	2	0	0	0	0
34	S	3	0	0	0	0
34	U	1	0	0	0	0
34	W	1	0	0	0	0
34	Z	2	0	0	0	0
All	All	86404	0	56229	396	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 3.

The worst 5 of 396 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)
5:A:799:G:O2'	5:A:800:A:OP1	1.81	0.97
19:O:91:ARG:NH2	19:O:113:ILE:O	2.01	0.93
10:F:9:ASN:OD1	10:F:13:LYS:NZ	2.02	0.92
5:A:84:U:OP1	28:X:52:ARG:NH1	2.03	0.90
5:A:1938:C:OP2	5:A:1939:U:O2'	1.91	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	35 (97%)	0	1 (3%)	5	4
7	C	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
8	D	209/212 (99%)	198 (95%)	10 (5%)	1 (0%)	29	40
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	153 (89%)	19 (11%)	0	100	100
11	G	172/177 (97%)	168 (98%)	2 (1%)	2 (1%)	13	17
12	H	58/148 (39%)	57 (98%)	1 (2%)	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	134 (99%)	0	1 (1%)	22	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	117/125 (94%)	113 (97%)	4 (3%)	0	100	100
18	N	112/116 (97%)	112 (100%)	0	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	116/119 (98%)	116 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
All	All	3072/3283 (94%)	2997 (98%)	70 (2%)	5 (0%)	50	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	101	VAL
11	G	81	GLU
16	L	79	LEU
11	G	13	ASN
4	3	37	GLN

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	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	218 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	143 (99%)	1 (1%)	84	90
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	44 (98%)	1 (2%)	52	66
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	86/86 (100%)	86 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	76 (99%)	1 (1%)	69	80
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
All	All	2531/2646 (96%)	2528 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	F	112	ARG

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Mol	Chain	Res	Type
12	H	8	ARG
23	S	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	D	137	HIS
13	I	13	HIS
30	Z	52	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2725/2918 (93%)	431 (15%)	26 (0%)
6	B	114/115 (99%)	19 (16%)	2 (1%)
All	All	2839/3033 (93%)	450 (15%)	28 (0%)

5 of 450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	41	U
5	A	53	G
5	A	56	A
5	A	57	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1296	A
6	B	87	A
5	A	1448	U
5	A	2419	U
5	A	1337	A

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

15 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	#$|Z| > 2$
5	PSU	A	1907	5	18,21,22	1.11	1 (5%)	22,30,33	1.79	5 (22%)
5	PSU	A	2500	5	18,21,22	1.10	1 (5%)	22,30,33	1.75	3 (13%)
5	PSU	A	2453	5	18,21,22	1.10	1 (5%)	22,30,33	1.81	5 (22%)
5	6MZ	A	2026	5	18,25,26	1.89	3 (16%)	16,36,39	3.30	4 (25%)
5	OMU	A	2548	5	19,22,23	3.09	8 (42%)	26,31,34	1.67	4 (15%)
5	3TD	A	1911	5	18,22,23	4.42	7 (38%)	22,32,35	1.70	2 (9%)
5	PSU	A	952	5	18,21,22	1.07	1 (5%)	22,30,33	1.74	3 (13%)
5	OMG	A	2247	5	18,26,27	1.10	2 (11%)	19,38,41	0.88	1 (5%)
5	PSU	A	2576	5	18,21,22	1.13	1 (5%)	22,30,33	1.82	5 (22%)
5	PSU	A	2601	5	18,21,22	1.06	1 (5%)	22,30,33	1.81	5 (22%)
5	PSU	A	1913	5	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
5	2MA	A	2499	33,5	17,25,26	2.51	5 (29%)	17,37,40	1.40	3 (17%)
5	5MU	A	1935	5	19,22,23	0.42	0	28,32,35	0.53	0
5	7MG	A	2065	5	22,26,27	1.22	1 (4%)	29,39,42	0.83	2 (6%)
5	2MG	A	2441	5	18,26,27	1.13	2 (11%)	16,38,41	0.86	1 (6%)

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
5	PSU	A	1907	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	1/5/27/28	0/3/3/3
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2
5	3TD	A	1911	5	-	4/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	0/5/27/28	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	A	1913	5	-	1/7/25/26	0/2/2/2
5	2MA	A	2499	33,5	-	3/3/25/26	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
5	2MG	A	2441	5	-	2/5/27/28	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	12.92	1.50	1.35
5	A	1911	3TD	C2-N1	10.25	1.50	1.37
5	A	2548	OMU	C2-N1	7.34	1.50	1.38
5	A	2499	2MA	C2-N3	7.26	1.46	1.31
5	A	2548	OMU	C2-N3	6.90	1.50	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2026	6MZ	C1'-N9-C4	-11.30	106.80	126.64
5	A	2026	6MZ	N3-C2-N1	-5.32	120.37	128.68
5	A	1911	3TD	N1-C2-N3	5.20	120.25	116.14
5	A	2548	OMU	C4-N3-C2	-5.15	119.79	126.58
5	A	2601	PSU	C4-N3-C2	-4.70	119.57	126.34

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1911	3TD	C2'-C1'-C5-C4
5	A	1911	3TD	C2'-C1'-C5-C6
5	A	1913	PSU	O4'-C1'-C5-C6
5	A	2548	OMU	O4'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2026	6MZ	2	0
5	A	2548	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1911	3TD	2	0
5	A	1913	PSU	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 162 ligands modelled in this entry, 160 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	$\#|Z| > 2$
32	YQM	A	3201	33	42,44,44	3.65	21 (50%)	47,69,69	2.91	21 (44%)
32	YQM	A	3202	33	42,44,44	3.44	22 (52%)	47,69,69	2.83	21 (44%)

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
32	YQM	A	3201	33	-	4/16/81/81	0/5/5/5
32	YQM	A	3202	33	-	5/16/81/81	0/5/5/5

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	3201	YQM	C19-C20	14.37	1.64	1.52
32	A	3202	YQM	C19-C20	13.43	1.63	1.52
32	A	3201	YQM	C19-C17	8.29	1.66	1.55
32	A	3202	YQM	C19-C17	8.00	1.65	1.55
32	A	3201	YQM	C21-C24	5.76	1.59	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	3201	YQM	C34-C32-N31	7.24	127.74	114.12
32	A	3202	YQM	C34-C32-N31	7.19	127.64	114.12
32	A	3201	YQM	C34-N35-C39	-7.05	103.89	113.25
32	A	3202	YQM	C34-N35-C39	-6.17	105.06	113.25
32	A	3201	YQM	C11-C12-C13	-5.95	114.58	120.49

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	3202	YQM	C20-C21-C24-N26
32	A	3202	YQM	C20-C21-C24-O25
32	A	3201	YQM	C11-C12-N31-C32
32	A	3201	YQM	C13-C12-N31-C32
32	A	3202	YQM	C13-C12-N31-C32

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	3201	YQM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand YQM A 3201

Bond lengths

Bond angles

Torsions

Rings

Ligand YQM A 3202

Bond lengths

Bond angles

Torsions

Rings
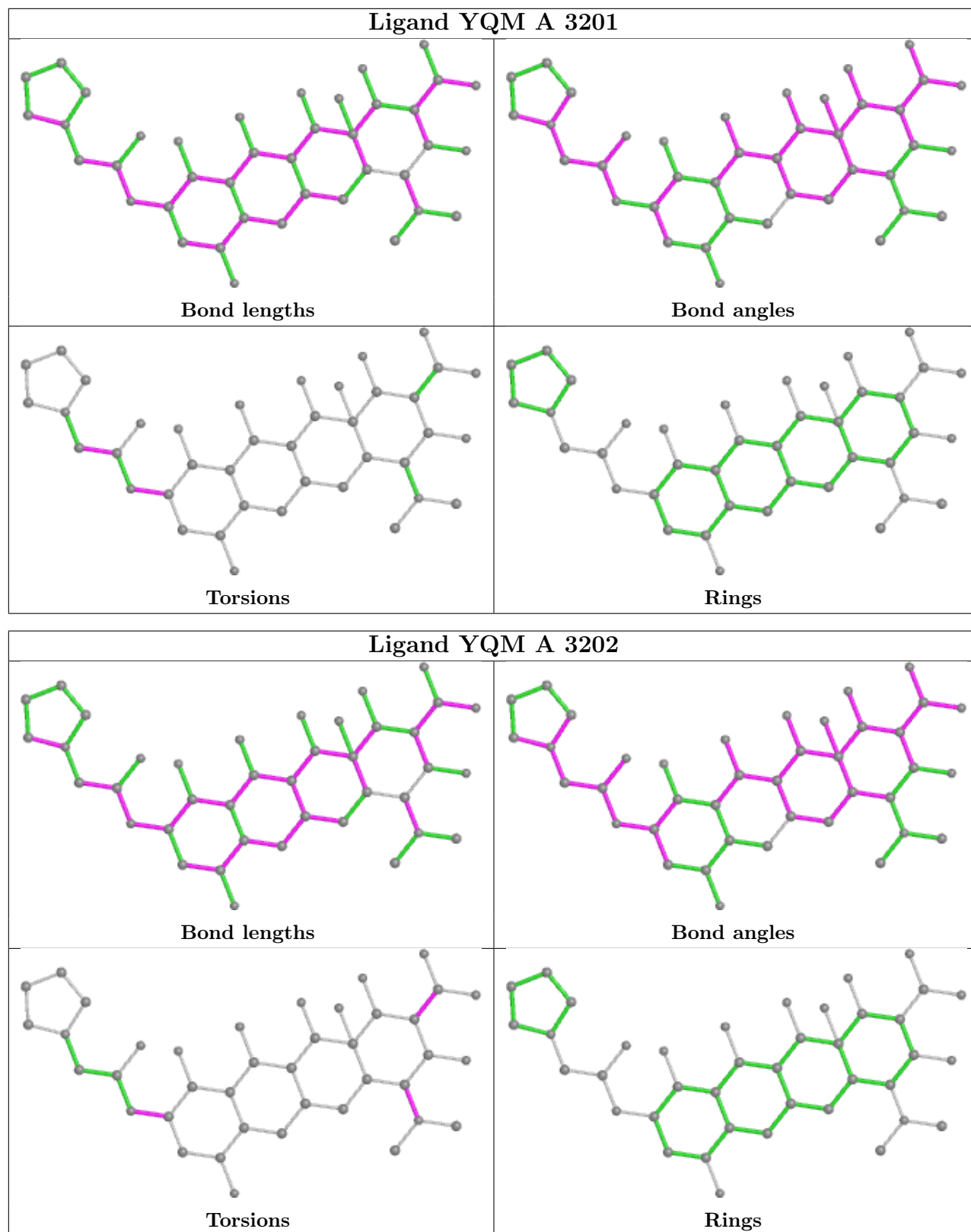
5.7 Other polymers ⓘ

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 ⓘ

This section contains visualisations of the EMDB entry EMD-23667. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1   Orthogonal projections ⓘ

6.1.1   Primary map

| X | Y | Z |
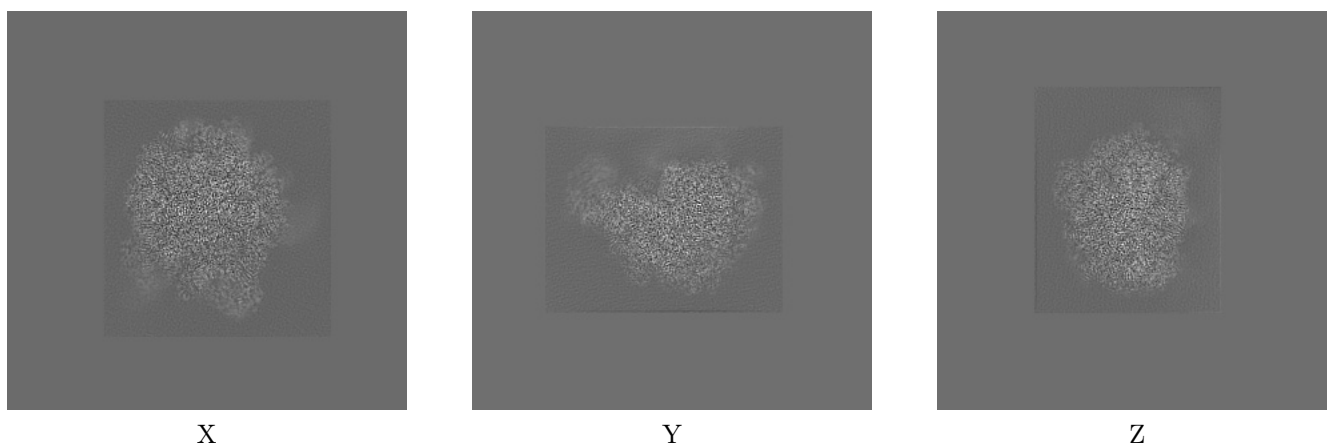
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ

6.2.1   Primary map

| X Index: 256 | Y Index: 256 | Z Index: 256 |
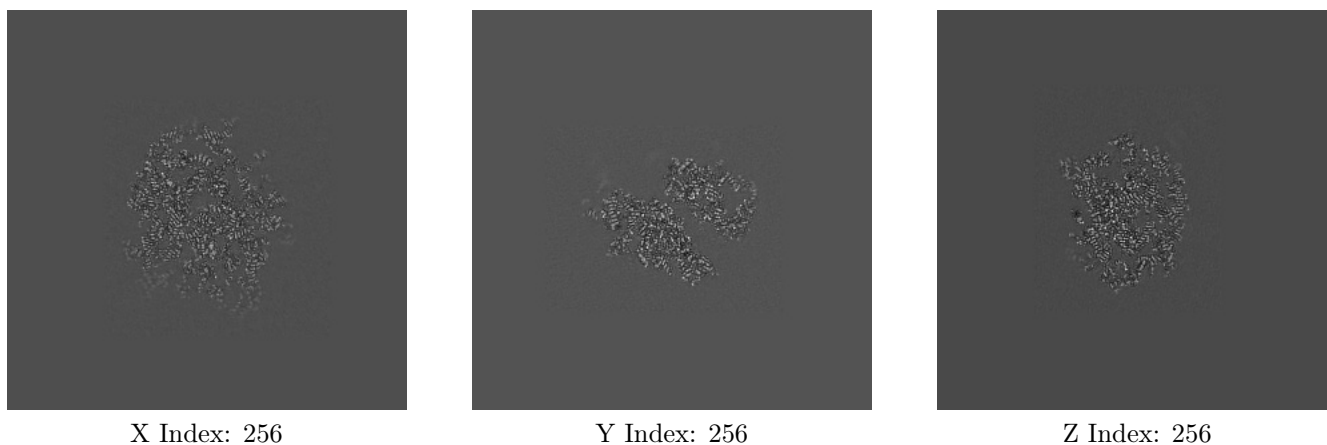
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

<div align="center">
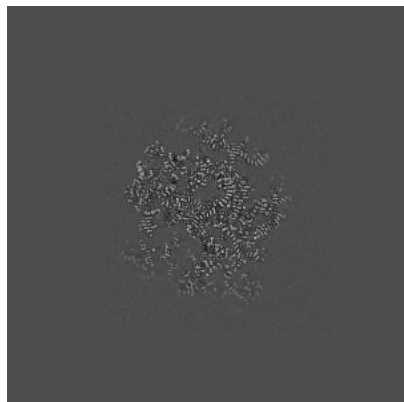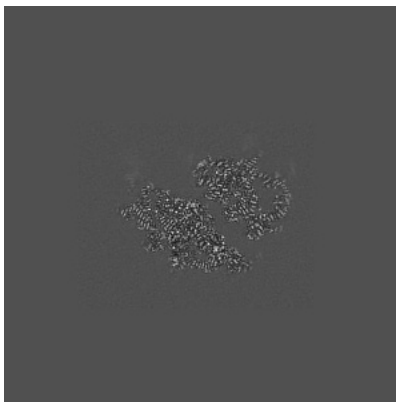
X Index: 247   Y Index: 250   Z Index: 264
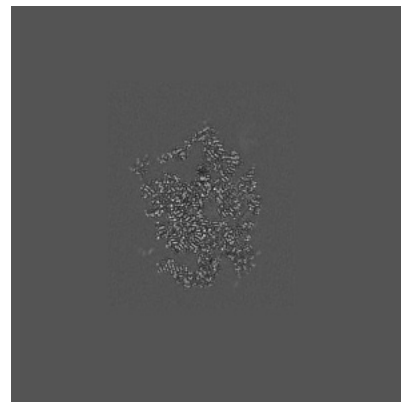
</div>

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

<div align="center">

X   Y   Z

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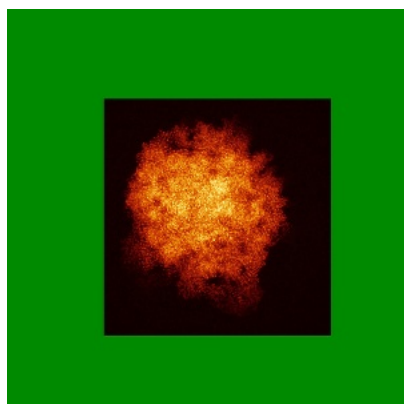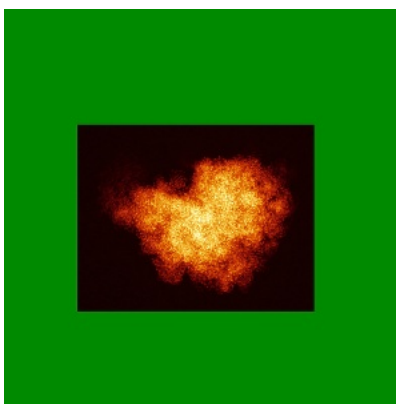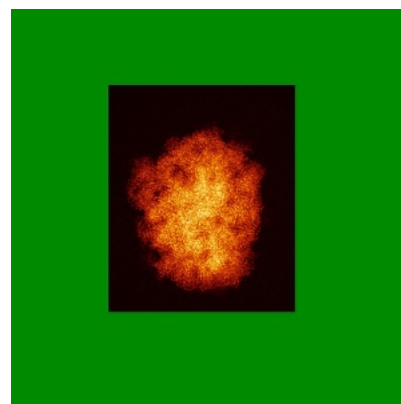
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views ⓘ

6.5.1   Primary map

| X | Y | Z |
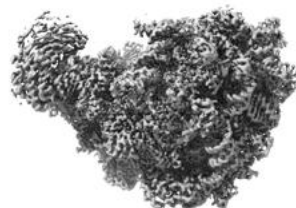
The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6   Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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 ⓘ
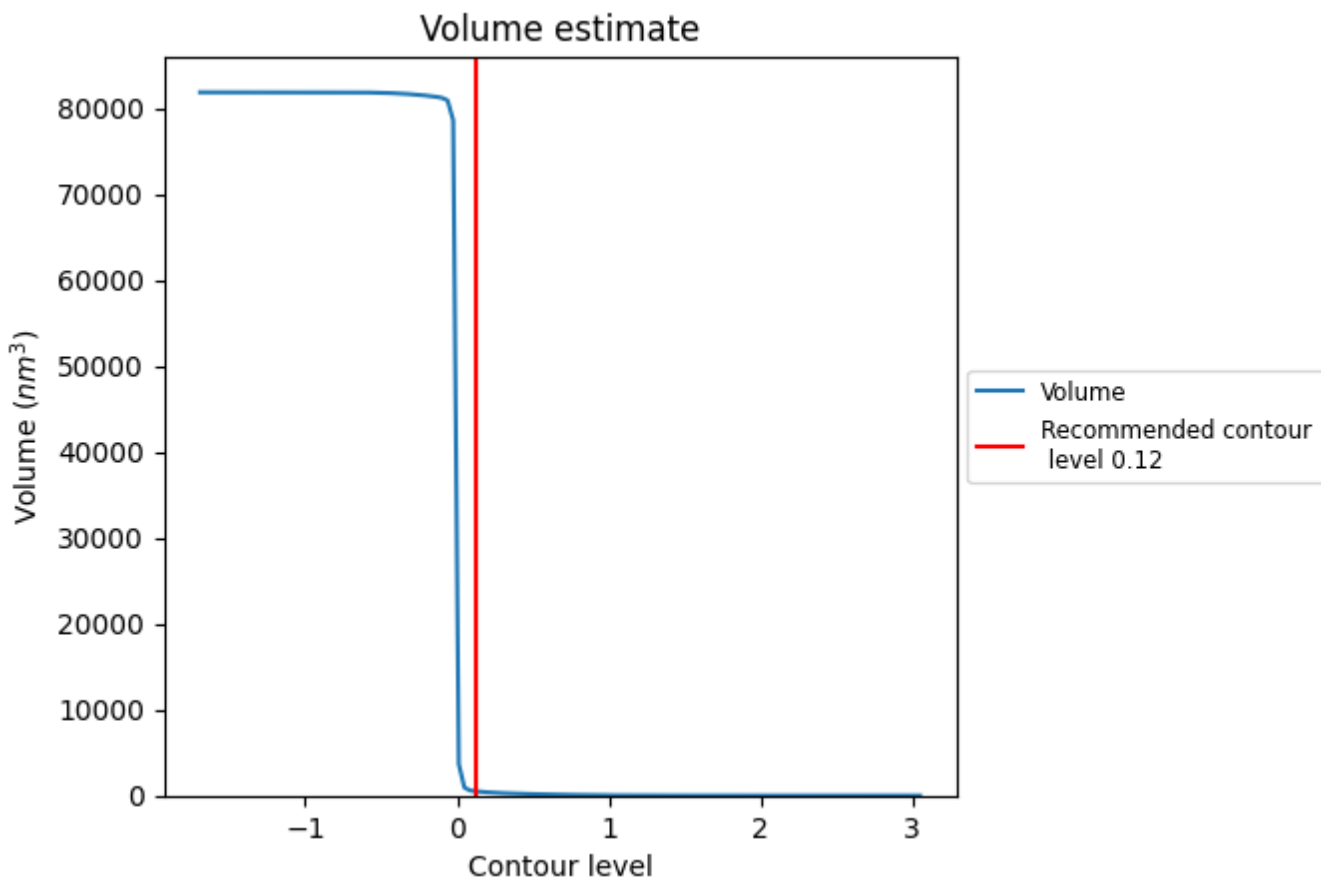
The volume at the recommended contour level is 508 nm^3; this corresponds to an approximate mass of 459 kDa.

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 ⓘ
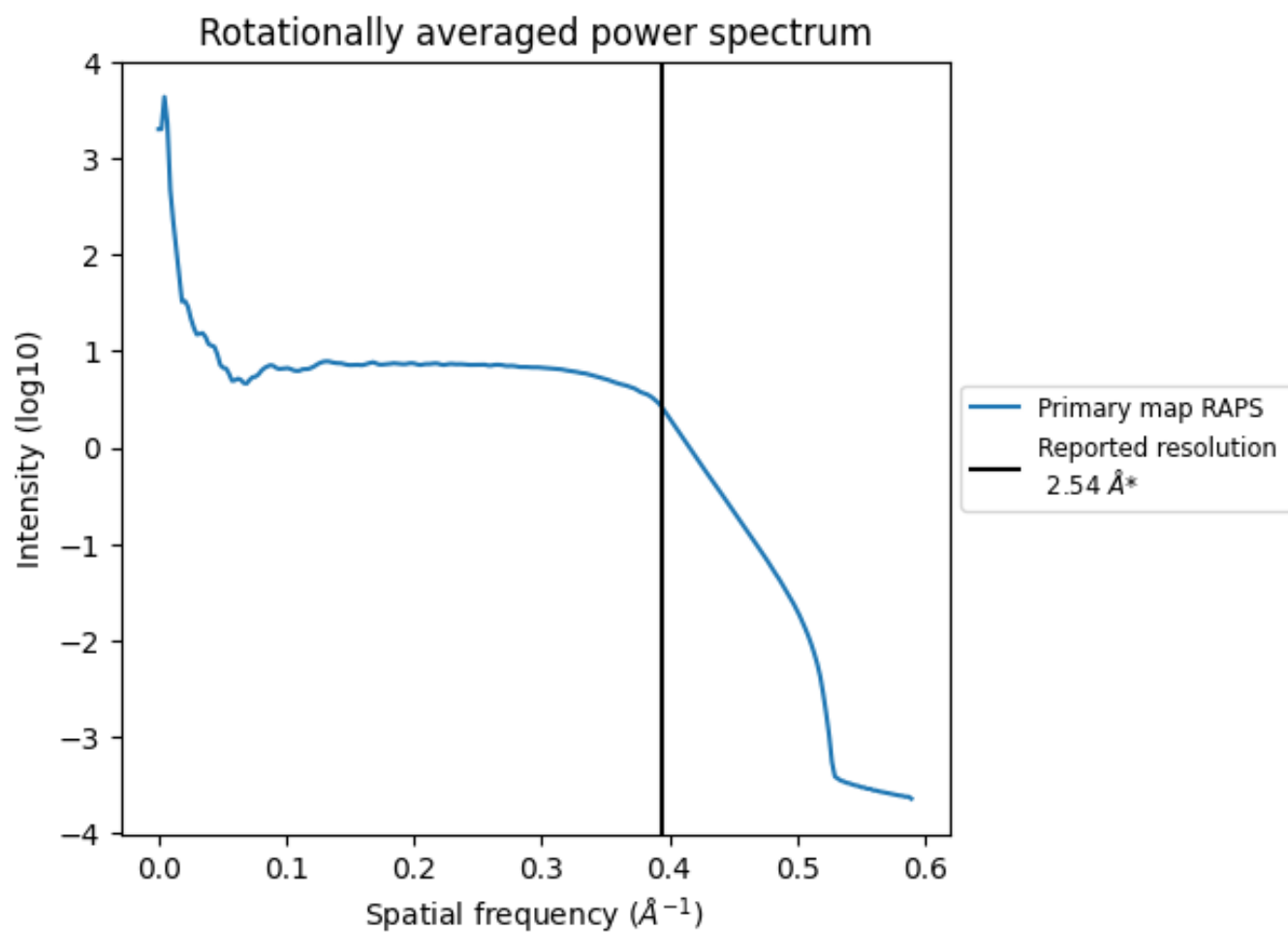
*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

8   Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23667 and PDB model 7M4V. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

X   Y   Z
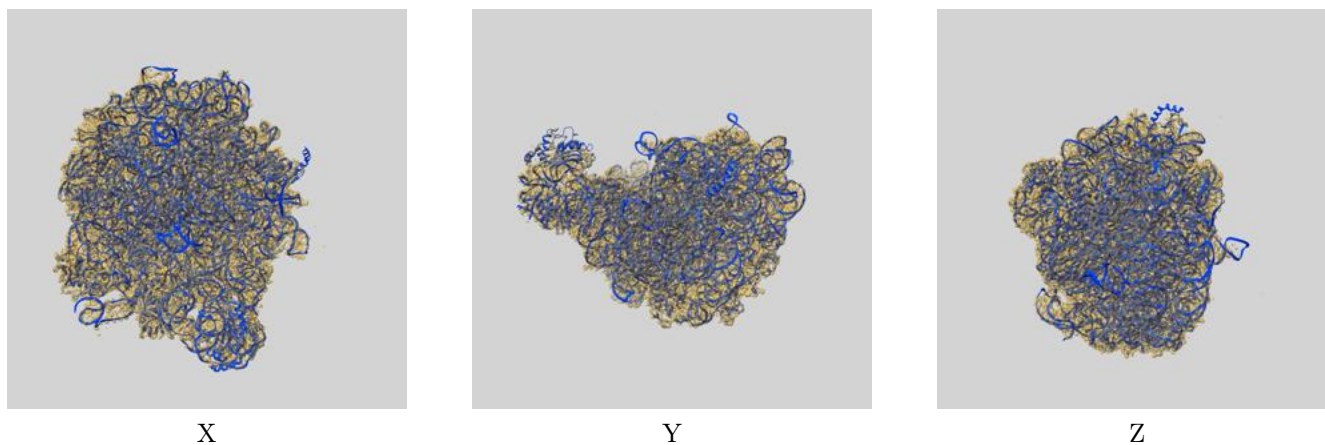
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
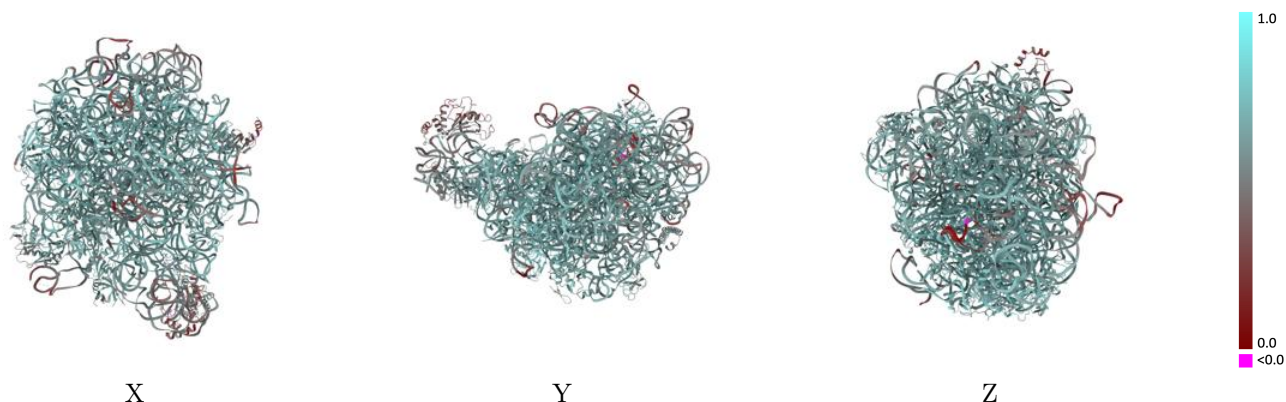
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
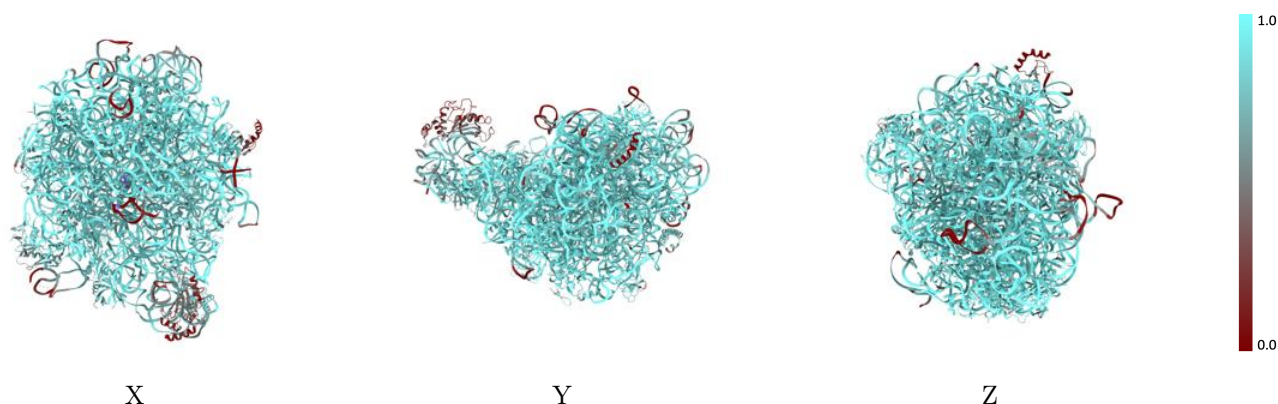
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4　Atom inclusion ⓘ
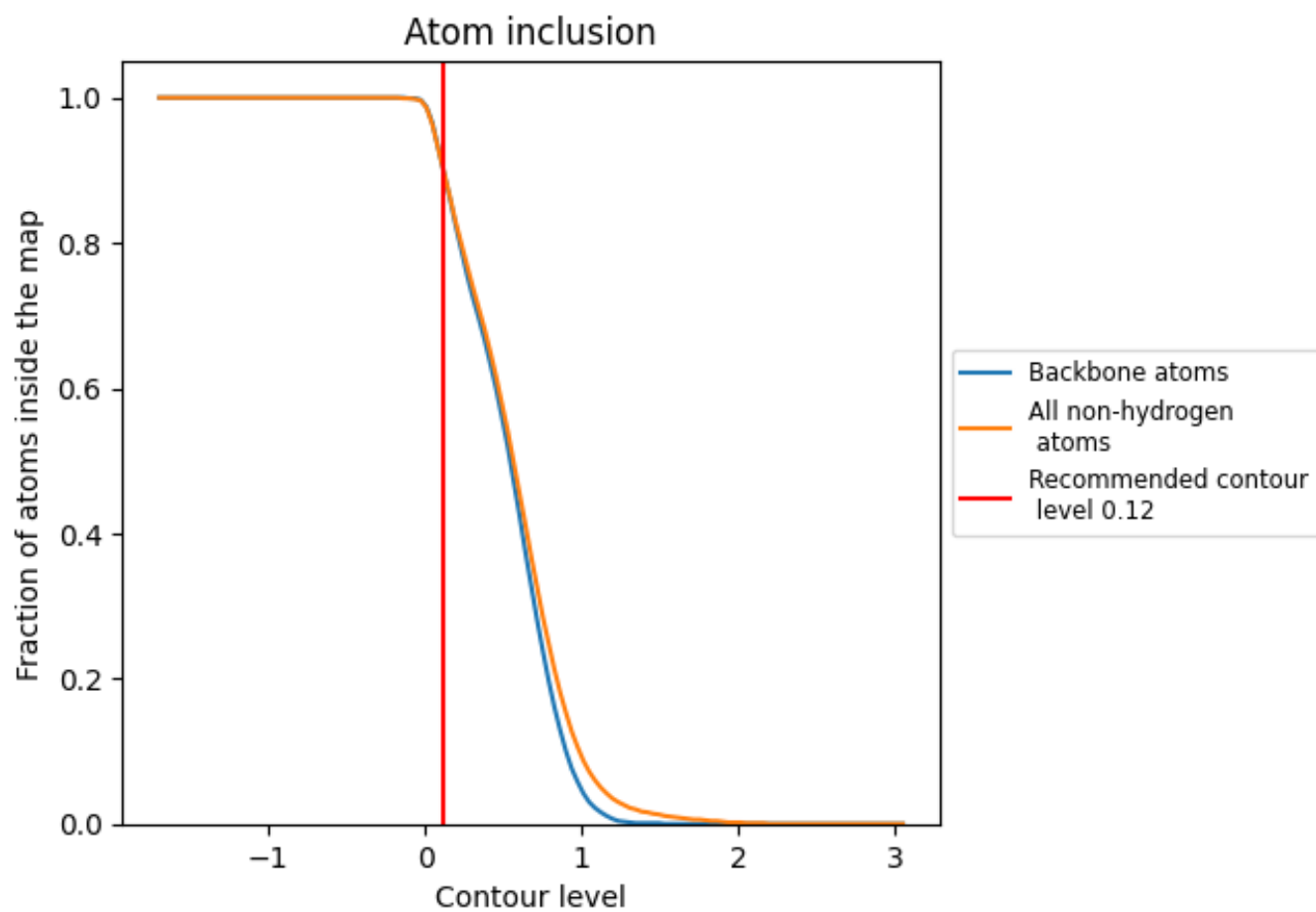
At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.6320
0	0.8680	0.6400
1	0.9740	0.7060
2	0.9840	0.7030
3	0.9160	0.6450
A	0.9230	0.6360
B	0.8150	0.5480
C	0.9470	0.6720
D	0.9520	0.6900
E	0.9030	0.6550
F	0.2470	0.3670
G	0.7260	0.5490
H	0.3540	0.3910
I	0.9500	0.6770
J	0.9190	0.6640
K	0.9550	0.6860
L	0.9070	0.6500
M	0.9760	0.6970
N	0.7600	0.5540
O	0.8890	0.6540
P	0.9760	0.6960
Q	0.9310	0.6670
R	0.9540	0.6870
S	0.8570	0.6180
T	0.7820	0.5910
U	0.8360	0.6090
V	0.9480	0.6850
W	0.9150	0.6630
X	0.7650	0.5490
Y	0.9350	0.6710
Z	0.8870	0.6620

1.0

0.0
<0.0