W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 05:07 AM EST

PDB ID	:	7TTU
EMDB ID	:	EMD-26124
Title	:	50S ribosomal subunit from Staphylococcus aureus (Strain ATCC43300)
Authors	:	Belousoff, M.J.; Piper, S.; Johnson, R.
Deposited on	:	2022-02-01
Resolution	:	3.00 Å(reported)

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 (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:

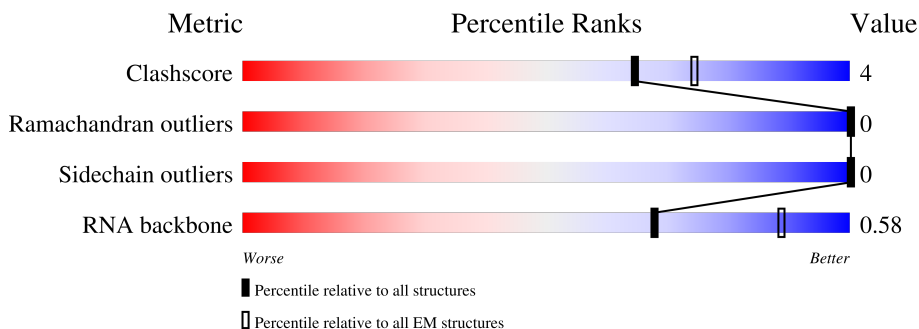|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.00 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		4
Ramachandran outliers		0
Sidechain outliers		0
RNA backbone		0.58

Worse   *Better*

■ Percentile relative to all structures

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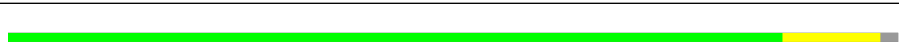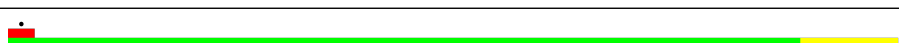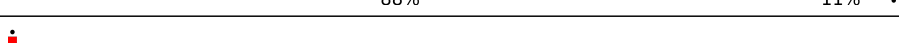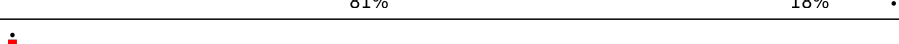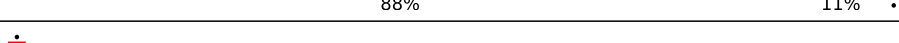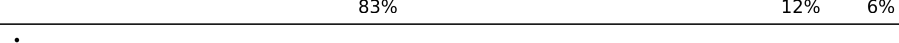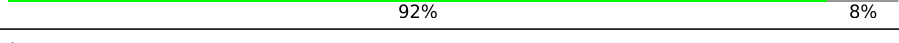
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	116	90% 8% •
2	B	277	85% 14% •
3	C	118	93% 5% •
4	D	102	7% 88% 10% •
5	E	117	80% 15% 5%
6	F	87	92% 8%
7	G	105	72% 13% 14%

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Mol	Chain	Length	Quality of chain
8	H	217	6% · · · 41% · · 57%
9	I	94	74% · 9% · 17%
10	J	61	85% · 11% ·
11	K	73	74% · 10% · 16%
12	L	220	92% · 6% ·
13	M	59	83% · 12% · 5%
14	N	57	75% · 12% · 12%
15	O	49	71% · 24% ·
16	P	45	87% · 11% ·
17	Q	65	95% · · ·
18	R	37	89% · 11%
19	S	207	84% · 9% · 7%
20	V	145	88% · 11% ·
21	W	122	81% · 18% ·
22	X	146	88% · 11% ·
23	Y	144	83% · 12% · 6%
24	Z	122	86% · 13% ·
25	a	119	5% · 92% · 8%
26	1	2923	63% · 25% · 8%
27	2	115	59% · 28% · 10% ·

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 80724 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 L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	113	Total 915	C 576	N 184	O 155	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	273	Total 2085	C 1297	N 413	O 370	S 5	0	0

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total 943	C 593	N 189	O 157	S 4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total 785	C 499	N 139	O 146	S 1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	111	Total 853	C 532	N 163	O 155	S 3	0	0

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total 711	C 447	N 128	O 132	S 4	0	0

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	conflict	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	90	Total	C	N	O	S	0	0
			698	442	128	127	1		

- Molecule 8 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			727	465	129	132	1		

- Molecule 9 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	78	Total	C	N	O	0	0
			597	367	116	114		

- Molecule 10 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

- Molecule 11 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	61	Total	C	N	O	S	0	0
			503	310	95	97	1		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 13 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	56	Total 432	C 269	N 82	O 81	0	0

- Molecule 14 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total 397	C 241	N 83	O 68	S 5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	47	Total 390	C 233	N 79	O 73	S 5	0	0

- Molecule 16 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	44	Total 372	C 228	N 90	O 53	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	64	Total 521	C 324	N 113	O 82	S 2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	37	Total 296	C 186	N 60	O 45	S 5	0	0

- Molecule 19 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	192	Total 1472	C 924	N 271	O 275	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	143	Total 1138	C 710	N 209	O 217	S 2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	121	Total 911	C 566	N 173	O 168	S 4	0	0

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	144	Total 1082	C 669	N 213	O 200	0	0

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	136	Total 1089	C 698	N 206	O 181	S 4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	121	Total 955	C 586	N 183	O 185	S 1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	110	Total 857	C 536	N 165	O 156	0	0

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2684	Total 57543	C 25704	N 10562	O 18603	P 2674	0	0

- Molecule 27 is a RNA chain called 5S rRNA.

| Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	111	Total 2361	C 1057	N 423	O 771	P 110	0	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.
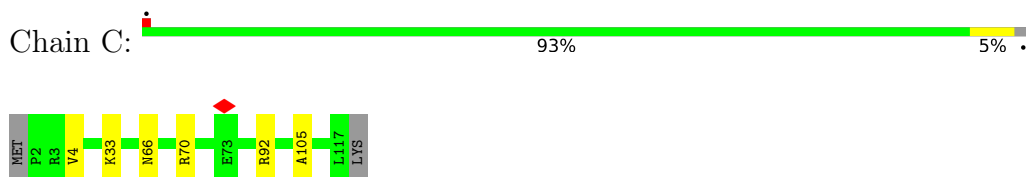
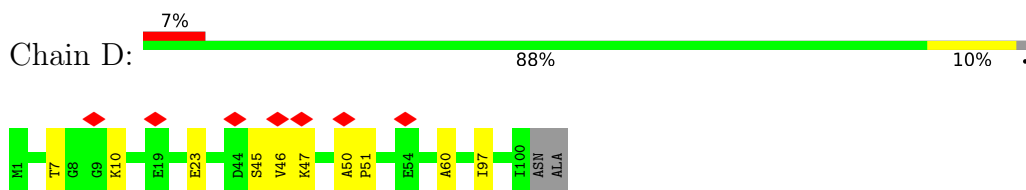- Molecule 1: 50S ribosomal protein L19

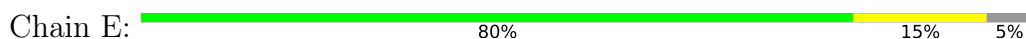Chain A:
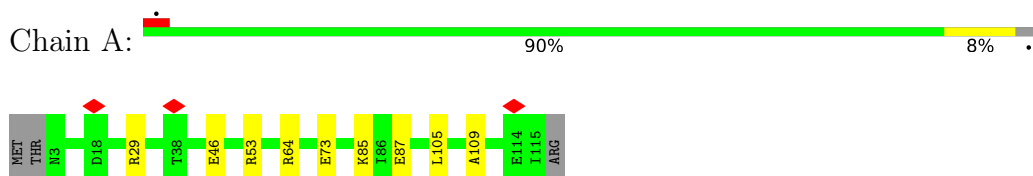
- Molecule 2: 50S ribosomal protein L2

Chain B:
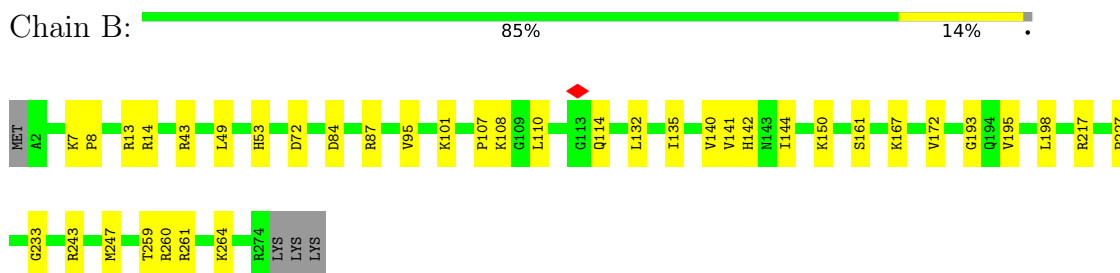
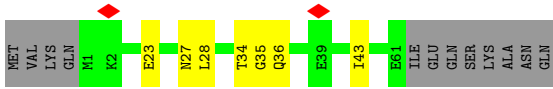

- Molecule 3: 50S ribosomal protein L20
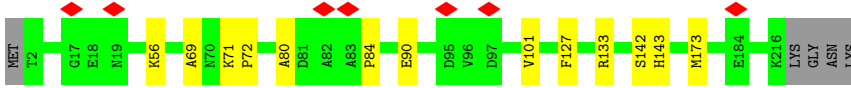
Chain C:

- Molecule 4: 50S ribosomal protein L21
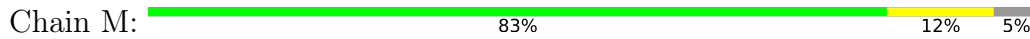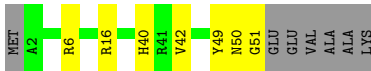
Chain D:

- Molecule 5: 50S ribosomal protein L22

Chain E:

M1 V6 I10 R11 R25 N28 E31 A42 T66 L69 A74 E78 L82 R88 R92 K98 I103 T104 K111 GLU GLU ALA LYS GLU ALA

- Molecule 6: 50S ribosomal protein L23

Chain F: 92% 8%

R4 K39 V48 K49 V50 V53 V80 T81 L82 K83 F90

- Molecule 7: 50S ribosomal protein L24

Chain G: 72% 13% 14%

MET H2 G6 D7 N8 V9 K10 G18 K22 A25 M41 K42 Q45 LYS PRO THR GLN LEU ASN PRO GLU GLY GLY I56 T59 S66 Q69 L70 L71 P78 V86 D87 A94 I101 LYS SER ASN ASN

- Molecule 8: 50S ribosomal protein L25

6%

Chain H: 41% 57%

MET A2 G11 G33 Y34 G35 T36 K37 K50 R53 E54 V55 N58 G59 T69 I70 K71 A75 P81 I94 ASN MET SER GLU GLU ARG THR VAL GLU VAL PRO VAL GLN LEU VAL GLY GLU ALA VAL GLY ALA LYS GLU GLY GLY VAL VAL GLU GLN PRO LEU

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

THR GLU GLU GLU ILE GLU ALA MET GLU GLY GLU GLN GLN THR GLU GLU PRO GLU VAL GLY GLU SER LYS GLU ASP GLU LYS THR GLU GLU

- Molecule 9: 50S ribosomal protein L27

Chain I: 74% 9% 17%

MET LEU LYS LEU ASN LEU GLN PHE PHE ALA SER LYS LYS GLY VAL S16 K19 R22 S26 K27 K80 G81 R82 D83 K84 K85 A93 GLU

- Molecule 10: 50S ribosomal protein L28

Chain J: 85% 11%
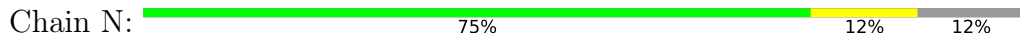
MET G2 K3 Q4 C5 R10 L33 L39 S56 V59 T60 ARG

- Molecule 11: 50S ribosomal protein L29

Chain K: 74% 10% 16%

MET VAL LYS GLN M1 K2 E23 N27 L28 T34 G35 Q36 E39 I43 E61 ILE GLU GLN SER LYS ALA ASN GLN

• Molecule 12: 50S ribosomal protein L3

Chain L:

92%   6% •

MET T2 G17 E18 N19 K56 A69 N70 K71 P72 A80 D81 A82 A83 P84 E90 D95 V96 D97 V101 F127 R133 S142 H143 M173 E184 K216 LYS GLY ASN LYS

• Molecule 13: 50S ribosomal protein L30

Chain M:

83%   12%   5%

MET A2 K3 R15 T18 Q19 R20 K29 K49 E57 GLU LYS
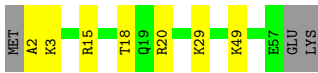
• Molecule 14: 50S ribosomal protein L32

Chain N:

75%   12%   12%

MET A2 R6 R16 H40 R41 V42 Y49 N50 G51 GLU GLU VAL ALA ALA LYS

• Molecule 15: 50S ribosomal protein L33

Chain O:

71%   24%   •

M1 R2 V5 E11 C12 G13 K21 N22 N25 E31 K34 R38 E39 N40 K41 R46 E47 THR LYS

• Molecule 16: 50S ribosomal protein L34

Chain P:

87%   11%   •

MET V2 K3 R4 T25 G28 K41 A45
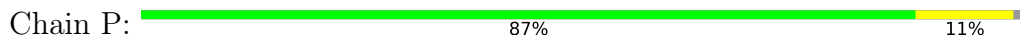
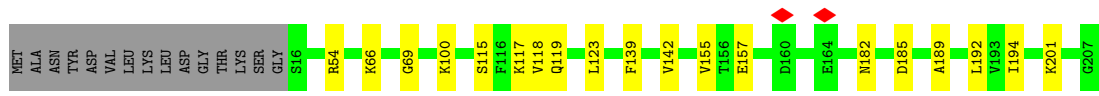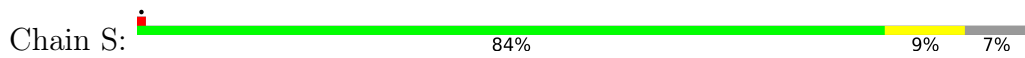• Molecule 17: 50S ribosomal protein L35

Chain Q:

95%   • •

MET P2 K39 R45 K65

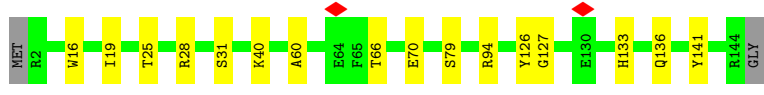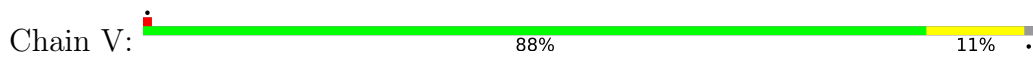• Molecule 18: 50S ribosomal protein L36

Chain R:
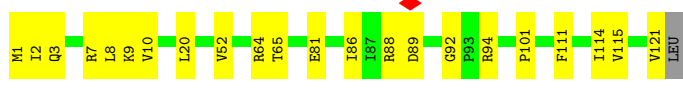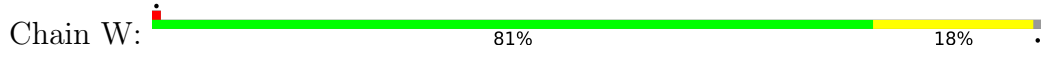
89%   11%

M1 E12 V16 V25 K33 G37
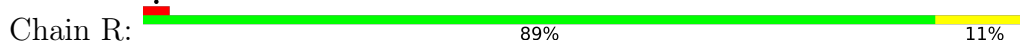
• Molecule 19: 50S ribosomal protein L4

Chain S:
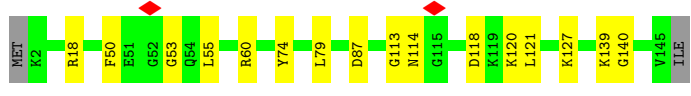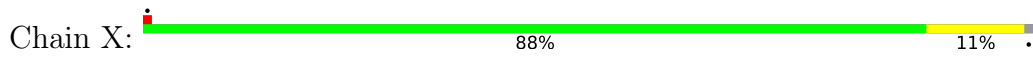84% 9% 7%

MET ALA ASN TYR ASP VAL LEU LYS LEU ASP GLY THR LYS SER GLY S16 R54 K66 G69 K100 S115 F116 K117 V118 Q119 L123 F139 V142 V155 T156 E157 D160 E164 N182 D185 A189 L192 V193 I194 K201 G207

• Molecule 20: 50S ribosomal protein L13

Chain V:
88% 11%

MET R2 W16 I19 T25 R28 S31 K40 A60 E64 F65 T66 E70 S79 R94 Y126 G127 E130 H133 Q136 Y141 R144 GLY

• Molecule 21: 50S ribosomal protein L14

Chain W:
81% 18%

M1 I2 Q3 R7 L8 K9 V10 L20 V52 R64 T65 E81 I86 I87 R88 D89 G92 P93 R94 P101 F111 I114 V115 V121 LEU

• Molecule 22: 50S ribosomal protein L15

Chain X:
88% 11%

MET K2 R18 F50 E51 G52 G53 Q54 L55 R60 Y74 L79 D87 G113 N114 G115 D118 K119 K120 L121 K127 K139 G140 V145 ILE

• Molecule 23: 50S ribosomal protein L16

Chain Y:
83% 12% 6%

M1 K16 T17 T18 T28 F29 Q35 S44 E48 R51 R56 K59 R60 G61 I66 F69 P70 P78 V81 G100 E136 LEU GLY GLY GLU THR ASN GLU SER

• Molecule 24: 50S ribosomal protein L17

Chain Z:
86% 13%

MET G2 T22 S23 L24 I25 I26 I30 T33 E34 A35 R36 A37 K38 E39 V40 N73 E76 I89 R92 R96 R102 K105 V117 V122

• Molecule 25: 50S ribosomal protein L18

Chain a:

5%

92%   8%

MET ILE SER K4 E27 K59 ASP SER ASP ILE ALA THR T66 A67 T68 K69 K87 E114 F119

- Molecule 26: 23S rRNA

Chain 1:

63%   25%   8%

• Molecule 27: 5S rRNA

Chain 2:
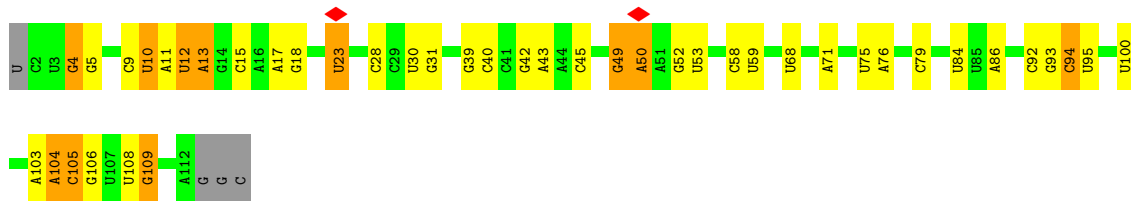
4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/Å^2)$	47.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.353	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	400.96, 400.96, 400.96	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A	0.23	0/927	0.57	0/1239
2	B	0.24	0/2120	0.53	0/2847
3	C	0.23	0/955	0.49	0/1265
4	D	0.24	0/795	0.51	0/1062
5	E	0.23	0/861	0.53	0/1159
6	F	0.24	0/719	0.50	0/959
7	G	0.23	0/704	0.48	0/938
8	H	0.24	0/735	0.47	0/986
9	I	0.25	0/603	0.55	0/801
10	J	0.23	0/469	0.54	0/625
11	K	0.22	0/504	0.53	0/670
12	L	0.25	0/1652	0.50	0/2216
13	M	0.22	0/434	0.51	0/585
14	N	0.24	0/404	0.54	0/537
15	O	0.23	0/393	0.57	0/523
16	P	0.26	0/376	0.59	0/491
17	Q	0.24	0/526	0.55	0/690
18	R	0.22	0/299	0.51	0/393
19	S	0.26	0/1494	0.51	0/2018
20	V	0.23	0/1160	0.48	0/1563
21	W	0.24	0/918	0.56	0/1232
22	X	0.24	0/1096	0.51	0/1461
23	Y	0.24	0/1113	0.53	0/1493
24	Z	0.23	0/959	0.54	0/1282
25	a	0.24	0/865	0.52	0/1154
26	1	0.21	0/64448	0.76	9/100506 (0.0%)
27	2	0.18	0/2640	0.79	3/4112 (0.1%)
All	All	0.21	0/88169	0.71	12/132807 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1865	C	C2-N1-C1'	7.37	126.91	118.80
26	1	1865	C	N1-C2-O2	7.17	123.20	118.90
26	1	1865	C	N3-C2-O2	-5.72	117.89	121.90
27	2	79	C	C2-N1-C1'	5.50	124.85	118.80
26	1	2825	U	N3-C2-O2	-5.45	118.39	122.20
26	1	104	C	C2-N1-C1'	5.44	124.79	118.80
26	1	402	C	C2-N1-C1'	5.32	124.65	118.80
26	1	1351	C	C2-N1-C1'	5.22	124.55	118.80
26	1	402	C	N1-C2-O2	5.14	121.99	118.90
26	1	1865	C	C6-N1-C1'	-5.06	114.73	120.80
27	2	23	U	C2-N1-C1'	5.04	123.75	117.70
27	2	105	C	N1-C2-O2	5.03	121.92	118.90

There are no chirality outliers.

There are no planarity outliers.

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	A	915	0	987	7	0
2	B	2085	0	2192	26	0
3	C	943	0	1014	6	0
4	D	785	0	825	6	0
5	E	853	0	914	11	0
6	F	711	0	743	4	0
7	G	698	0	756	9	0
8	H	727	0	777	3	0
9	I	597	0	607	6	0
10	J	463	0	501	4	0
11	K	503	0	536	4	0
12	L	1628	0	1667	10	0
13	M	432	0	472	5	0
14	N	397	0	407	5	0
15	O	390	0	396	7	0
16	P	372	0	420	4	0
17	Q	521	0	586	2	0
18	R	296	0	340	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	1472	0	1520	11	0
20	V	1138	0	1130	10	0
21	W	911	0	970	15	0
22	X	1082	0	1119	10	0
23	Y	1089	0	1155	12	0
24	Z	955	0	1002	10	0
25	a	857	0	903	0	0
26	1	57543	0	28959	376	0
27	2	2361	0	1197	19	0
All	All	80724	0	52095	533	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 4.

All (533) 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)
9:I:85:LYS:NZ	26:1:902:A:OP1	2.17	0.76
27:2:5:G:H1	27:2:108:U:H3	1.30	0.76
26:1:1862:G:H1	26:1:1932:C:H5	1.33	0.74
2:B:107:PRO:HD2	2:B:110:LEU:HD22	1.70	0.73
27:2:4:G:H22	27:2:109:G:H1	1.35	0.72
2:B:95:VAL:HG22	2:B:101:LYS:HG2	1.72	0.72
21:W:1:MET:HG2	21:W:2:ILE:HG12	1.72	0.72
26:1:2314:A:H62	26:1:2371:U:H3	1.39	0.71
1:A:53:ARG:NH2	26:1:2710:C:OP1	2.23	0.71
14:N:42:VAL:HG12	14:N:49:TYR:HB2	1.73	0.71
26:1:793:G:N2	26:1:796:A:OP2	2.25	0.70
26:1:1806:U:OP2	26:1:1811:A:N6	2.25	0.70
5:E:25:ARG:NH1	5:E:74:ALA:O	2.26	0.69
26:1:330:C:N3	26:1:397:U:O4	2.26	0.69
23:Y:56:ARG:NH1	26:1:2496:A:O2'	2.25	0.69
26:1:2608:G:OP2	26:1:2608:G:N2	2.21	0.68
16:P:41:LYS:HD3	26:1:505:U:H5"	1.75	0.67
26:1:1487:G:H22	26:1:1596:G:H22	1.43	0.67
2:B:150:LYS:NZ	26:1:2231:C:OP2	2.29	0.66
26:1:1514:A:H61	26:1:1566:G:H1	1.44	0.66
26:1:1941:C:O2'	26:1:1943:A:N1	2.29	0.66
26:1:277:C:N3	26:1:278:A:N6	2.44	0.66
26:1:331:G:HO2'	26:1:332:A:H8	1.41	0.66
26:1:2126:C:H42	26:1:2218:G:H1	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1725:G:HO2'	26:1:1789:A:HO2'	1.41	0.65
26:1:944:G:N2	26:1:944:G:OP1	2.29	0.65
26:1:2822:C:H4'	26:1:2823:G:H2'	1.79	0.65
9:I:27:LYS:NZ	26:1:2288:C:OP1	2.29	0.65
21:W:88:ARG:HG2	21:W:89:ASP:H	1.61	0.65
26:1:1515:G:H22	26:1:1565:U:H3	1.43	0.65
24:Z:102:ARG:NH1	26:1:2902:A:OP1	2.29	0.65
23:Y:16:LYS:HG2	23:Y:18:THR:HG22	1.77	0.64
2:B:142:HIS:ND1	2:B:193:GLY:O	2.27	0.64
15:O:34:LYS:NZ	26:1:2374:C:OP1	2.31	0.64
14:N:6:ARG:NH2	26:1:2046:U:OP2	2.28	0.64
27:2:9:C:H42	27:2:104:A:H61	1.45	0.64
26:1:1462:G:OP2	26:1:1462:G:N2	2.25	0.64
6:F:48:VAL:HG11	6:F:82:LEU:HD13	1.80	0.64
19:S:117:LYS:NZ	19:S:189:ALA:O	2.31	0.64
1:A:85:LYS:HZ1	1:A:87:GLU:HG2	1.63	0.64
17:Q:39:LYS:NZ	26:1:2392:G:N7	2.46	0.63
26:1:506:A:C2	26:1:515:G:N2	2.67	0.63
26:1:632:U:H2'	26:1:633:A:H8	1.61	0.63
26:1:721:A:H8	26:1:2096:G:H21	1.45	0.63
26:1:1708:A:H61	26:1:2023:C:H42	1.45	0.63
26:1:2877:G:N2	26:1:2880:A:OP2	2.30	0.63
26:1:591:A:H4'	26:1:592:A:H5'	1.80	0.62
22:X:114:ASN:ND2	26:1:699:U:O4	2.33	0.62
20:V:126:TYR:OH	20:V:133:HIS:NE2	2.29	0.62
26:1:1780:G:N2	26:1:1783:G:OP2	2.30	0.62
20:V:31:SER:HG	26:1:1049:C:HO2'	1.48	0.62
26:1:153:G:H2'	26:1:154:A:H8	1.64	0.61
10:J:5:CYS:HB3	10:J:10:ARG:H	1.65	0.61
7:G:94:ALA:HB2	7:G:101:ILE:HD11	1.83	0.61
15:O:13:GLY:HA3	15:O:38:ARG:HD2	1.82	0.61
2:B:259:THR:HG1	26:1:1824:C:HO2'	1.49	0.60
12:L:71:LYS:HG3	26:1:2814:C:H4'	1.83	0.60
3:C:92:ARG:NH2	26:1:1197:C:OP1	2.33	0.60
14:N:16:ARG:NH2	26:1:1302:G:OP1	2.30	0.60
26:1:2580:G:H8	26:1:2609:G:H21	1.50	0.60
24:Z:105:LYS:HA	24:Z:117:VAL:HG12	1.83	0.60
26:1:200:A:N6	26:1:2457:A:O2'	2.34	0.60
2:B:107:PRO:HA	2:B:195:VAL:HA	1.84	0.60
26:1:221:G:H22	26:1:238:U:H4'	1.67	0.60
2:B:132:LEU:HD23	2:B:135:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:665:G:H4'	26:1:666:A:H5"	1.84	0.59
26:1:304:G:H2'	26:1:305:A:H8	1.65	0.59
26:1:409:G:OP2	26:1:409:G:N2	2.35	0.59
26:1:2355:A:H2'	26:1:2356:A:C8	2.38	0.59
26:1:342:A:N3	26:1:362:C:O2'	2.31	0.59
12:L:90:GLU:OE1	26:1:2662:U:O2'	2.18	0.59
26:1:2885:U:OP2	26:1:2886:G:O2'	2.18	0.59
19:S:182:ASN:ND2	19:S:185:ASP:OD2	2.32	0.59
21:W:64:ARG:NH1	21:W:101:PRO:O	2.33	0.59
26:1:920:A:N6	26:1:944:G:OP2	2.35	0.59
4:D:60:ALA:HB2	4:D:97:ILE:HD13	1.85	0.59
26:1:262:G:H21	26:1:666:A:H8	1.50	0.59
26:1:1512:U:H2'	26:1:1513:A:C8	2.37	0.58
26:1:1881:A:H62	26:1:1915:G:H8	1.49	0.58
9:I:82:ARG:NH2	27:2:10:U:O2'	2.36	0.58
19:S:54:ARG:NH1	26:1:718:C:OP1	2.33	0.58
22:X:55:LEU:HD23	22:X:60:ARG:HB3	1.85	0.58
26:1:1886:A:H62	26:1:1910:G:H8	1.50	0.58
7:G:69:GLN:HE21	26:1:378:C:H4'	1.69	0.58
26:1:320:U:OP1	26:1:325:A:N6	2.34	0.58
26:1:2816:C:H5	26:1:2913:G:H1	1.52	0.58
26:1:1708:A:H61	26:1:2023:C:N4	2.02	0.58
20:V:60:ALA:HB3	20:V:127:GLY:HA2	1.85	0.58
26:1:1522:G:HO2'	26:1:1607:A:HO2'	1.50	0.58
26:1:1482:U:H2'	26:1:1483:A:H8	1.69	0.57
26:1:1915:G:OP2	26:1:1915:G:N2	2.30	0.57
26:1:2824:G:H2'	26:1:2825:U:O2	2.04	0.57
26:1:1357:G:OP2	26:1:1357:G:N2	2.24	0.57
26:1:1422:A:O2'	26:1:1433:U:O2	2.21	0.57
26:1:1479:G:O6	26:1:1605:A:N6	2.37	0.57
7:G:42:LYS:O	26:1:526:A:O2'	2.19	0.57
1:A:85:LYS:NZ	1:A:87:GLU:HG2	2.17	0.57
26:1:331:G:H1	26:1:395:U:H3	1.52	0.57
21:W:3:GLN:NE2	26:1:2022:U:O2	2.38	0.57
26:1:1346:G:H21	26:1:1655:C:H5'	1.70	0.57
7:G:41:MET:SD	7:G:59:THR:OG1	2.63	0.56
26:1:787:U:H2'	26:1:788:A:C8	2.39	0.56
1:A:29:ARG:HG2	1:A:46:GLU:HG2	1.87	0.56
2:B:167:LYS:HG3	2:B:172:VAL:HG12	1.86	0.56
26:1:106:A:H2'	26:1:107:G:H8	1.70	0.56
26:1:1506:C:H2'	26:1:1507:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:629:A:H62	26:1:1289:A:H2	1.53	0.56
26:1:2618:C:H2'	26:1:2619:G:H8	1.70	0.56
19:S:100:LYS:NZ	26:1:651:A:OP1	2.31	0.56
21:W:7:ARG:HE	21:W:20:LEU:HD12	1.69	0.56
21:W:1:MET:HB2	21:W:8:LEU:HD21	1.88	0.55
26:1:2624:G:H2'	26:1:2625:A:C8	2.41	0.55
26:1:1352:C:H2'	26:1:1353:A:H8	1.71	0.55
16:P:2:VAL:N	26:1:1663:G:HO2'	2.03	0.55
2:B:261:ARG:O	2:B:264:LYS:NZ	2.39	0.55
6:F:53:VAL:HG22	6:F:80:VAL:HG12	1.88	0.55
21:W:115:VAL:HG13	21:W:121:VAL:HG21	1.87	0.55
5:E:78:GLU:OE2	26:1:24:G:N2	2.37	0.55
5:E:42:ALA:HB2	26:1:2037:G:H5"	1.88	0.54
26:1:153:G:H2'	26:1:154:A:C8	2.43	0.54
26:1:328:G:H1	26:1:399:U:H3	1.55	0.54
26:1:1522:G:N1	26:1:1523:G:O6	2.40	0.54
26:1:1893:A:N6	26:1:1902:G:O2'	2.41	0.54
26:1:350:G:OP2	26:1:350:G:N2	2.40	0.54
26:1:2881:C:H2'	26:1:2882:A:H8	1.71	0.54
23:Y:56:ARG:HH12	26:1:2496:A:HO2'	1.51	0.54
26:1:2418:G:O2'	26:1:2451:C:N4	2.37	0.54
11:K:23:GLU:O	11:K:27:ASN:ND2	2.41	0.53
2:B:110:LEU:HD12	2:B:114:GLN:HG3	1.90	0.53
10:J:56:SER:HB3	26:1:418:G:C8	2.43	0.53
26:1:421:C:H2'	26:1:422:G:H8	1.74	0.53
26:1:2876:G:O6	26:1:2882:A:N6	2.41	0.53
24:Z:89:ILE:HG13	24:Z:92:ARG:HH21	1.74	0.52
26:1:1518:G:H1	26:1:1562:C:H42	1.56	0.52
26:1:1943:A:H5"	26:1:1944:U:H5	1.74	0.52
18:R:1:MET:HG2	18:R:33:LYS:HE3	1.90	0.52
2:B:7:LYS:NZ	26:1:751:A:OP1	2.32	0.52
3:C:105:ALA:HB2	4:D:47:LYS:HE2	1.89	0.52
26:1:1063:U:OP1	26:1:1079:U:O2'	2.21	0.52
26:1:1500:G:N7	26:1:1501:G:N2	2.58	0.52
16:P:25:THR:HG23	16:P:28:GLY:H	1.74	0.52
26:1:2058:A:N3	26:1:2482:G:O2'	2.41	0.52
27:2:11:A:O2'	27:2:13:A:OP2	2.27	0.52
26:1:509:G:N2	26:1:512:A:OP2	2.38	0.52
26:1:917:U:H2'	26:1:918:G:C8	2.45	0.52
26:1:1487:G:N2	26:1:1596:G:H22	2.07	0.52
26:1:917:U:H2'	26:1:918:G:H8	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:632:U:H2'	26:1:633:A:C8	2.44	0.51
26:1:787:U:H2'	26:1:788:A:H8	1.75	0.51
18:R:16:VAL:HG12	18:R:25:VAL:HG22	1.93	0.51
26:1:1981:G:O2'	26:1:1983:U:O4	2.19	0.51
27:2:92:C:H2'	27:2:93:G:O4'	2.11	0.51
8:H:33:GLY:O	8:H:36:THR:HG22	2.10	0.51
26:1:744:A:H8	26:1:1677:G:HO2'	1.58	0.51
26:1:1065:A:H61	26:1:1186:A:H61	1.57	0.51
26:1:116:G:OP2	26:1:118:A:O2'	2.29	0.51
26:1:683:G:H2'	26:1:684:U:C6	2.45	0.51
26:1:556:U:H4'	26:1:1273:G:H4'	1.93	0.51
27:2:12:U:OP2	27:2:68:U:O2'	2.29	0.51
7:G:6:GLY:HA2	7:G:22:LYS:HE2	1.92	0.51
19:S:139:PHE:HA	19:S:142:VAL:HG22	1.92	0.51
20:V:19:ILE:HG12	20:V:141:TYR:HB3	1.92	0.51
26:1:83:G:H21	26:1:102:A:H2	1.58	0.51
26:1:1516:C:H2'	26:1:1517:A:C8	2.46	0.51
26:1:460:C:H2'	26:1:461:A:H8	1.75	0.51
26:1:1423:C:H2'	26:1:1424:A:H8	1.76	0.51
26:1:66:C:H2'	26:1:67:G:H8	1.75	0.51
26:1:615:A:H61	26:1:2056:G:H8	1.57	0.51
26:1:896:U:H2'	26:1:897:A:H8	1.77	0.50
26:1:955:A:N3	26:1:2291:C:O2'	2.42	0.50
26:1:2056:G:OP2	26:1:2056:G:N2	2.29	0.50
2:B:13:ARG:HD2	26:1:773:G:H4'	1.93	0.50
5:E:11:ARG:NH2	5:E:98:LYS:HD2	2.26	0.50
7:G:10:LYS:HE2	7:G:18:GLY:HA2	1.93	0.50
2:B:227:PRO:HA	2:B:233:GLY:HA2	1.94	0.50
6:F:39:LYS:HG3	6:F:50:VAL:HG21	1.93	0.50
24:Z:96:ARG:NH1	26:1:2900:C:O2'	2.44	0.50
26:1:268:A:N6	26:1:474:A:N7	2.59	0.50
26:1:310:C:N4	26:1:407:G:H1	2.09	0.50
26:1:637:U:H2'	26:1:638:U:C6	2.47	0.50
26:1:2402:G:N2	26:1:2405:A:OP2	2.34	0.50
26:1:2618:C:H2'	26:1:2619:G:C8	2.46	0.50
23:Y:44:SER:HB3	23:Y:70:PRO:HG2	1.93	0.50
26:1:2574:U:H2'	26:1:2575:G:H8	1.76	0.50
23:Y:51:ARG:HD3	23:Y:66:ILE:HD11	1.94	0.50
26:1:2098:A:H2'	26:1:2099:G:C8	2.46	0.50
26:1:2052:C:H2'	26:1:2053:U:C6	2.47	0.50
26:1:2839:A:O2'	26:1:2841:A:N7	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1083:G:H1	26:1:1160:C:H42	1.59	0.49
26:1:1185:U:H4'	26:1:1186:A:O4'	2.12	0.49
26:1:2574:U:H2'	26:1:2575:G:C8	2.47	0.49
26:1:872:U:O2'	26:1:2095:U:N3	2.45	0.49
26:1:1390:A:H3'	26:1:1391:A:H8	1.77	0.49
15:O:22:ASN:HB3	15:O:25:ASN:HB2	1.93	0.49
26:1:702:U:H2'	26:1:703:A:C8	2.48	0.49
26:1:1460:U:H3	26:1:1628:A:H61	1.60	0.49
26:1:460:C:H2'	26:1:461:A:C8	2.47	0.49
26:1:755:C:H2'	26:1:756:A:H8	1.78	0.49
2:B:140:VAL:HG13	2:B:161:SER:HB2	1.95	0.49
26:1:59:U:O2'	26:1:74:U:OP2	2.26	0.49
22:X:18:ARG:NH2	26:1:1288:G:N7	2.60	0.49
26:1:901:G:H2'	26:1:902:A:C8	2.48	0.49
26:1:1943:A:H5"	26:1:1944:U:C5	2.47	0.49
26:1:2359:C:O2'	26:1:2362:A:O2'	2.27	0.49
26:1:150:A:H61	26:1:179:A:H2	1.60	0.49
26:1:1487:G:H1	26:1:1596:G:H1	1.59	0.49
26:1:1836:A:H2'	26:1:1837:A:C8	2.47	0.49
26:1:2051:C:H2'	26:1:2052:C:C6	2.48	0.49
2:B:135:ILE:O	2:B:167:LYS:NZ	2.46	0.49
19:S:157:GLU:OE2	19:S:201:LYS:NZ	2.41	0.49
22:X:50:PHE:HE2	22:X:53:GLY:HA3	1.78	0.49
26:1:140:A:H2'	26:1:141:U:C6	2.48	0.49
26:1:1521:A:N6	26:1:1559:G:H22	2.11	0.49
2:B:43:ARG:HH11	2:B:49:LEU:HD13	1.78	0.48
19:S:123:LEU:HD12	19:S:192:LEU:HD23	1.95	0.48
26:1:1442:C:H2'	26:1:1443:A:C8	2.48	0.48
26:1:1487:G:H22	26:1:1596:G:H1	1.61	0.48
26:1:1891:U:OP1	26:1:2437:G:O2'	2.28	0.48
26:1:2431:C:H2'	26:1:2432:G:O4'	2.13	0.48
1:A:64:ARG:HB2	1:A:73:GLU:HG2	1.95	0.48
26:1:1442:C:H2'	26:1:1443:A:H8	1.77	0.48
26:1:1672:G:H2'	26:1:1673:A:H8	1.78	0.48
5:E:82:LEU:HB2	5:E:98:LYS:HB2	1.96	0.48
22:X:74:TYR:CZ	22:X:127:LYS:HD2	2.49	0.48
26:1:1025:A:OP2	26:1:1026:C:N4	2.41	0.48
26:1:1449:A:N1	26:1:1632:A:N6	2.61	0.48
10:J:3:LYS:HE2	10:J:33:LEU:HD12	1.96	0.48
26:1:2705:U:H2'	26:1:2706:A:H8	1.78	0.48
19:S:66:LYS:HE3	19:S:69:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:SER:OG	4:D:46:VAL:N	2.46	0.48
26:1:2881:C:H2'	26:1:2882:A:C8	2.49	0.47
3:C:33:LYS:HG2	26:1:1290:G:C2	2.49	0.47
26:1:1563:U:H2'	26:1:1564:G:H8	1.78	0.47
23:Y:28:THR:HG23	23:Y:29:PHE:CD1	2.49	0.47
26:1:194:A:H2'	26:1:195:C:H6	1.79	0.47
26:1:229:A:O2'	26:1:230:A:OP1	2.28	0.47
2:B:141:VAL:HG23	2:B:144:ILE:HD11	1.97	0.47
23:Y:78:PRO:HG2	23:Y:81:VAL:HG11	1.97	0.47
26:1:2041:A:H2'	26:1:2042:A:C8	2.49	0.47
26:1:422:G:H2'	26:1:423:A:C8	2.50	0.47
26:1:1506:C:H2'	26:1:1507:A:H8	1.77	0.47
3:C:33:LYS:HG2	26:1:1290:G:N3	2.30	0.47
26:1:84:A:N1	26:1:98:U:O2'	2.43	0.47
26:1:348:C:H2'	26:1:349:U:C6	2.49	0.47
26:1:1521:A:H61	26:1:1559:G:H22	1.62	0.47
5:E:66:THR:HA	5:E:69:LEU:HG	1.97	0.47
5:E:92:ARG:NH2	26:1:792:U:O2'	2.48	0.47
19:S:115:SER:HA	19:S:118:VAL:HG12	1.97	0.47
19:S:155:VAL:HG22	19:S:194:ILE:HG22	1.97	0.47
26:1:908:A:O2'	27:2:95:U:O2	2.26	0.47
26:1:1756:U:H3	26:1:1773:A:N6	2.13	0.47
26:1:1514:A:N6	26:1:1566:G:H1	2.11	0.47
5:E:28:ASN:HB3	5:E:31:GLU:HB2	1.97	0.47
20:V:70:GLU:OE1	20:V:94:ARG:NH2	2.47	0.47
26:1:1486:C:H2'	26:1:1487:G:C8	2.50	0.47
26:1:2360:A:H5"	26:1:2362:A:H1'	1.97	0.47
2:B:72:ASP:OD1	2:B:72:ASP:N	2.48	0.46
26:1:1353:A:H2'	26:1:1354:G:H8	1.80	0.46
1:A:29:ARG:HB2	1:A:87:GLU:HB2	1.98	0.46
4:D:50:ALA:HB1	4:D:51:PRO:HA	1.97	0.46
12:L:133:ARG:HG3	12:L:173:MET:HB3	1.98	0.46
27:2:52:G:H2'	27:2:53:U:C6	2.50	0.46
4:D:10:LYS:NZ	4:D:23:GLU:OE2	2.48	0.46
12:L:142:SER:OG	12:L:143:HIS:N	2.48	0.46
19:S:115:SER:O	19:S:119:GLN:HG3	2.15	0.46
23:Y:35:GLN:HE21	23:Y:100:GLY:HA2	1.80	0.46
26:1:106:A:H2'	26:1:107:G:C8	2.49	0.46
26:1:1063:U:HO2'	26:1:1065:A:H2	1.62	0.46
27:2:75:U:H3	27:2:94:C:H5	1.61	0.46
9:I:19:LYS:O	9:I:22:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1873:G:H2'	26:1:1874:A:C8	2.50	0.46
26:1:1951:C:H2'	26:1:1952:C:C6	2.49	0.46
7:G:69:GLN:OE1	7:G:78:PRO:HB2	2.16	0.46
8:H:55:VAL:HG12	8:H:59:GLY:HA3	1.97	0.46
12:L:80:ALA:HB2	12:L:101:VAL:HG12	1.98	0.46
21:W:111:PHE:HB3	21:W:114:ILE:HD12	1.97	0.46
26:1:1501:G:H3'	26:1:1502:A:C8	2.51	0.46
13:M:29:LYS:HB3	13:M:29:LYS:HE3	1.70	0.46
24:Z:33:THR:HB	24:Z:36:ARG:HG3	1.96	0.46
26:1:2098:A:H2'	26:1:2099:G:H8	1.81	0.46
26:1:2342:U:H2'	26:1:2343:U:C6	2.51	0.46
15:O:31:GLU:OE2	15:O:46:ARG:NH1	2.49	0.46
26:1:135:G:H2'	26:1:136:A:H8	1.81	0.46
26:1:766:G:H2'	26:1:767:A:C8	2.51	0.46
26:1:1818:A:C2	26:1:1856:A:H4'	2.50	0.46
26:1:579:U:H2'	26:1:580:C:C6	2.51	0.46
26:1:873:U:H4'	26:1:876:G:N1	2.31	0.46
26:1:1708:A:N6	26:1:2023:C:H42	2.13	0.46
2:B:108:LYS:HD2	2:B:198:LEU:HD11	1.97	0.46
26:1:1315:C:H2'	26:1:1316:G:H8	1.81	0.46
12:L:127:PHE:CE2	26:1:1699:A:H1'	2.51	0.46
13:M:2:ALA:O	13:M:3:LYS:NZ	2.35	0.46
24:Z:39:GLU:OE1	26:1:2717:A:N6	2.41	0.46
26:1:886:A:H2'	26:1:887:A:H8	1.82	0.46
26:1:1508:C:H2'	26:1:1593:G:H22	1.80	0.46
14:N:40:HIS:HD1	26:1:2835:C:HO2'	1.64	0.45
21:W:9:LYS:HD2	21:W:81:GLU:OE2	2.16	0.45
21:W:52:VAL:HG22	21:W:94:ARG:HH11	1.81	0.45
26:1:105:C:H2'	26:1:106:A:H8	1.82	0.45
26:1:1453:G:H4'	26:1:1453:G:OP1	2.16	0.45
26:1:2606:C:H2'	26:1:2607:U:O2	2.16	0.45
26:1:754:U:H2'	26:1:755:C:C6	2.51	0.45
26:1:793:G:N3	26:1:793:G:H2'	2.31	0.45
26:1:1629:U:H3	26:1:1630:A:H62	1.62	0.45
26:1:1942:U:H5"	26:1:1943:A:H2	1.82	0.45
26:1:2649:U:O3'	26:1:2845:G:N2	2.49	0.45
12:L:127:PHE:HE2	26:1:1699:A:H1'	1.81	0.45
26:1:830:U:H4'	26:1:1806:U:H4'	1.98	0.45
27:2:4:G:N2	27:2:109:G:H1	2.10	0.45
26:1:2758:G:H2'	26:1:2759:G:C8	2.51	0.45
26:1:631:U:H2'	26:1:632:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1087:C:H42	26:1:1156:G:H1	1.64	0.45
26:1:1240:U:H2'	26:1:1241:A:H8	1.81	0.45
26:1:1509:G:O4'	26:1:1593:G:N2	2.49	0.45
2:B:43:ARG:NH1	2:B:49:LEU:HD13	2.31	0.45
7:G:66:SER:OG	26:1:378:C:O2	2.35	0.45
26:1:1423:C:H2'	26:1:1424:A:C8	2.52	0.45
26:1:2235:A:H2'	26:1:2236:C:C6	2.51	0.45
26:1:2457:A:N3	26:1:2457:A:H2'	2.32	0.45
21:W:88:ARG:N	21:W:92:GLY:O	2.39	0.45
26:1:268:A:N6	26:1:473:U:O2'	2.49	0.45
26:1:440:C:H2'	26:1:441:C:C6	2.51	0.45
24:Z:34:GLU:O	24:Z:38:LYS:HG2	2.16	0.45
26:1:390:A:H2'	26:1:391:A:C8	2.52	0.45
22:X:120:LYS:HE2	22:X:140:GLY:HA3	1.98	0.45
26:1:363:A:H4'	26:1:365:A:N7	2.32	0.45
26:1:422:G:H2'	26:1:423:A:H8	1.81	0.45
26:1:969:A:OP1	26:1:970:U:N3	2.50	0.45
26:1:1755:U:H2'	26:1:1756:U:C6	2.52	0.45
26:1:2060:A:O2'	26:1:2062:G:OP2	2.26	0.45
26:1:2318:U:H2'	26:1:2319:U:C6	2.52	0.45
3:C:66:ASN:O	3:C:70:ARG:HG2	2.17	0.45
26:1:909:G:H21	26:1:911:A:H61	1.62	0.45
26:1:1353:A:H2'	26:1:1354:G:C8	2.52	0.45
26:1:2318:U:OP1	26:1:2407:A:O2'	2.34	0.45
26:1:342:A:H2'	26:1:343:A:C8	2.52	0.44
26:1:1696:C:H2'	26:1:1697:G:O4'	2.18	0.44
1:A:105:LEU:HD12	1:A:109:ALA:HB1	2.00	0.44
26:1:2844:U:H2'	26:1:2845:G:O4'	2.18	0.44
26:1:659:A:H2'	26:1:659:A:N3	2.33	0.44
27:2:28:C:O2	27:2:52:G:N2	2.50	0.44
26:1:625:G:H2'	26:1:626:G:H8	1.81	0.44
26:1:702:U:H2'	26:1:703:A:H8	1.83	0.44
26:1:793:G:H22	26:1:796:A:H5'	1.82	0.44
26:1:1482:U:H2'	26:1:1483:A:C8	2.50	0.44
26:1:1821:U:H2'	26:1:1822:C:C6	2.53	0.44
22:X:121:LEU:HD23	22:X:121:LEU:H	1.83	0.44
26:1:5:A:H2'	26:1:6:A:C8	2.53	0.44
26:1:625:G:H2'	26:1:626:G:C8	2.52	0.44
26:1:955:A:H2'	26:1:956:A:C8	2.53	0.44
26:1:1636:U:H2'	26:1:1637:A:C8	2.51	0.44
26:1:2343:U:H2'	26:1:2344:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2359:C:HO2'	26:1:2362:A:HO2'	1.57	0.44
26:1:2857:A:H2'	26:1:2858:G:H8	1.83	0.44
26:1:2821:U:O2'	26:1:2823:G:N2	2.48	0.44
26:1:222:A:N3	26:1:237:U:O2'	2.39	0.44
26:1:747:U:H2'	26:1:748:U:C6	2.53	0.44
26:1:2336:A:H4'	26:1:2337:A:O5'	2.18	0.44
26:1:2340:C:H2'	26:1:2341:A:C8	2.52	0.44
5:E:10:ILE:HD13	5:E:103:ILE:HD12	2.00	0.44
26:1:685:C:H2'	26:1:686:U:C6	2.53	0.44
26:1:2343:U:H2'	26:1:2344:C:H6	1.83	0.44
26:1:2817:A:HO2'	26:1:2818:A:H8	1.61	0.44
22:X:79:LEU:HG	22:X:113:GLY:HA2	2.00	0.43
26:1:130:A:H2'	26:1:131:G:H8	1.83	0.43
26:1:745:G:O2'	26:1:1676:A:H8	2.01	0.43
26:1:991:A:H2'	26:1:992:A:C8	2.52	0.43
26:1:1966:U:OP1	26:1:2631:U:O2'	2.36	0.43
26:1:2883:U:H2'	26:1:2884:G:C8	2.53	0.43
7:G:8:ASN:HB3	7:G:71:LEU:HD12	1.99	0.43
11:K:35:GLY:O	11:K:36:GLN:NE2	2.51	0.43
13:M:18:THR:OG1	13:M:49:LYS:NZ	2.51	0.43
26:1:259:A:H2'	26:1:260:A:C8	2.53	0.43
26:1:1395:G:N1	26:1:1408:G:N7	2.66	0.43
26:1:2856:U:H2'	26:1:2857:A:C8	2.53	0.43
2:B:243:ARG:NH2	2:B:247:MET:SD	2.90	0.43
9:I:26:SER:OG	26:1:2298:G:OP1	2.36	0.43
26:1:1314:A:H2'	26:1:1315:C:C6	2.53	0.43
26:1:1806:U:O2	26:1:1810:A:N6	2.52	0.43
26:1:2051:C:H2'	26:1:2052:C:H6	1.81	0.43
26:1:306:C:H2'	26:1:307:A:C8	2.53	0.43
26:1:805:G:H2'	26:1:806:A:O4'	2.18	0.43
26:1:1235:C:C2	26:1:1236:G:C8	3.07	0.43
26:1:2747:U:C2	26:1:2748:A:C8	3.07	0.43
26:1:2901:U:H2'	26:1:2902:A:C8	2.54	0.43
21:W:7:ARG:NE	21:W:20:LEU:HD12	2.34	0.43
26:1:506:A:N1	26:1:515:G:C2	2.87	0.43
26:1:734:A:H2'	26:1:735:C:C6	2.54	0.43
20:V:66:THR:HG21	26:1:1185:U:H2'	2.00	0.43
26:1:487:U:H2'	26:1:488:G:C8	2.53	0.43
26:1:2260:A:H2'	26:1:2261:G:H8	1.84	0.43
26:1:2649:U:O2'	26:1:2845:G:N2	2.52	0.43
26:1:1221:C:H2'	26:1:1222:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1352:C:H2'	26:1:1353:A:C8	2.50	0.43
26:1:505:U:C5	26:1:515:G:N2	2.86	0.43
26:1:902:A:H61	26:1:965:G:H1	1.67	0.43
26:1:1424:A:H5'	26:1:1512:U:H1'	2.00	0.43
26:1:1636:U:H2'	26:1:1637:A:H8	1.82	0.43
26:1:1753:U:H2'	26:1:1754:C:C6	2.53	0.43
26:1:2377:C:H2'	26:1:2378:G:O4'	2.19	0.43
15:O:39:GLU:HB3	15:O:41:LYS:HG2	2.00	0.43
26:1:1481:A:O2'	26:1:1562:C:H4'	2.19	0.43
26:1:1806:U:H5	26:1:1811:A:N7	2.17	0.43
26:1:1865:C:H5	26:1:1928:A:H62	1.67	0.43
26:1:2050:A:H2'	26:1:2051:C:C6	2.54	0.43
26:1:2260:A:H2'	26:1:2261:G:C8	2.54	0.43
26:1:841:C:H2'	26:1:842:U:C6	2.54	0.43
26:1:2539:C:H2'	26:1:2540:A:O4'	2.19	0.43
2:B:135:ILE:HD13	2:B:141:VAL:HG11	2.00	0.42
26:1:47:C:C2	26:1:181:G:N2	2.87	0.42
26:1:684:U:H2'	26:1:685:C:C6	2.54	0.42
27:2:58:C:C2	27:2:59:U:C5	3.07	0.42
4:D:7:THR:O	4:D:7:THR:HG22	2.19	0.42
12:L:56:LYS:N	12:L:84:PRO:O	2.33	0.42
26:1:1070:A:N1	26:1:1178:C:N4	2.63	0.42
26:1:1856:A:H3'	26:1:1857:C:H6	1.85	0.42
26:1:1901:C:H3'	26:1:1902:G:H8	1.84	0.42
26:1:2270:U:H2'	26:1:2271:U:C6	2.55	0.42
5:E:6:VAL:HG22	5:E:104:THR:HG23	2.01	0.42
26:1:624:C:H2'	26:1:625:G:H8	1.84	0.42
27:2:76:A:H62	27:2:93:G:H21	1.67	0.42
26:1:753:U:H2'	26:1:754:U:C6	2.53	0.42
26:1:1579:C:HO2'	26:1:1588:U:H3	1.68	0.42
26:1:2050:A:H2'	26:1:2051:C:H6	1.84	0.42
13:M:20:ARG:HE	13:M:20:ARG:HB3	1.71	0.42
26:1:879:U:H2'	26:1:880:A:H8	1.84	0.42
26:1:1053:A:N3	26:1:1197:C:O2'	2.49	0.42
26:1:2313:A:H4'	26:1:2314:A:O4'	2.20	0.42
26:1:2856:U:H2'	26:1:2857:A:H8	1.84	0.42
27:2:15:C:N4	27:2:103:A:H2	2.16	0.42
2:B:84:ASP:OD2	2:B:87:ARG:HD3	2.19	0.42
20:V:25:THR:HB	20:V:28:ARG:HG3	2.02	0.42
24:Z:36:ARG:O	24:Z:40:VAL:HG23	2.20	0.42
26:1:167:U:H2'	26:1:168:A:H5"	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:181:G:H2'	26:1:182:C:O4'	2.19	0.42
26:1:1453:G:N2	26:1:1631:G:O4'	2.50	0.42
20:V:79:SER:HB2	26:1:2668:A:H5"	2.02	0.42
26:1:2064:A:H2'	26:1:2065:G:C8	2.55	0.42
3:C:4:VAL:HG22	26:1:1238:U:H1'	2.01	0.42
26:1:636:A:H2'	26:1:637:U:C6	2.55	0.42
26:1:1241:A:H2'	26:1:1242:A:C8	2.55	0.42
26:1:1311:A:N7	26:1:1690:A:O2'	2.44	0.42
26:1:2535:G:H1	26:1:2607:U:H5	1.65	0.42
2:B:53:HIS:HA	2:B:217:ARG:HB2	2.01	0.42
21:W:88:ARG:HG2	21:W:89:ASP:N	2.32	0.42
26:1:1083:G:H2'	26:1:1084:U:C6	2.55	0.42
26:1:2293:A:H4'	26:1:2294:A:N3	2.34	0.42
27:2:30:U:H2'	27:2:31:G:C8	2.55	0.42
26:1:1476:G:H2'	26:1:1477:U:C6	2.55	0.42
26:1:1573:A:N6	26:1:1592:A:N1	2.68	0.42
23:Y:48:GLU:OE2	23:Y:51:ARG:NH2	2.45	0.41
24:Z:22:THR:O	24:Z:26:ILE:HG12	2.20	0.41
26:1:2113:U:H2'	26:1:2114:G:C8	2.55	0.41
2:B:8:PRO:HB3	2:B:14:ARG:HA	2.01	0.41
20:V:16:TRP:CE2	20:V:136:GLN:HG2	2.55	0.41
22:X:118:ASP:HA	22:X:139:LYS:HE2	2.03	0.41
26:1:1087:C:N4	26:1:1156:G:H1	2.19	0.41
26:1:2406:G:H2'	26:1:2407:A:C8	2.55	0.41
27:2:17:A:H2'	27:2:18:G:H8	1.84	0.41
21:W:1:MET:SD	21:W:65:THR:HG22	2.61	0.41
26:1:638:U:H2'	26:1:639:U:C6	2.55	0.41
26:1:1013:U:H2'	26:1:1014:U:C6	2.55	0.41
26:1:1711:G:O2'	26:1:2018:U:O4	2.30	0.41
26:1:2842:G:O2'	26:1:2844:U:OP2	2.39	0.41
20:V:40:LYS:HE2	20:V:40:LYS:HB3	1.91	0.41
26:1:838:A:OP2	26:1:2098:A:O2'	2.38	0.41
26:1:2372:G:N3	26:1:2408:C:H2'	2.34	0.41
8:H:81:PRO:O	23:Y:35:GLN:NE2	2.39	0.41
22:X:87:ASP:N	22:X:87:ASP:OD1	2.53	0.41
26:1:29:U:C2	26:1:30:G:C8	3.09	0.41
26:1:441:C:H2'	26:1:442:G:H8	1.86	0.41
26:1:713:A:H2'	26:1:715:A:H62	1.86	0.41
26:1:744:A:H8	26:1:1677:G:O2'	2.03	0.41
26:1:1880:A:H2'	26:1:1881:A:C8	2.55	0.41
26:1:2860:U:H2'	26:1:2861:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2906:G:H2'	26:1:2907:A:H8	1.85	0.41
15:O:2:ARG:HG3	26:1:2311:U:OP2	2.21	0.41
15:O:5:VAL:HG11	15:O:21:LYS:HE3	2.02	0.41
26:1:332:A:H2'	26:1:333:C:C6	2.55	0.41
26:1:2767:A:H2'	26:1:2768:A:C8	2.56	0.41
26:1:613:G:H2'	26:1:2057:A:N7	2.36	0.41
26:1:1066:G:N2	26:1:1067:U:O4	2.47	0.41
14:N:50:ASN:OD1	14:N:51:GLY:N	2.53	0.41
21:W:10:VAL:HG11	21:W:86:ILE:HD11	2.03	0.41
26:1:566:U:H2'	26:1:567:G:C8	2.56	0.41
26:1:788:A:O2'	26:1:1703:U:OP1	2.39	0.41
26:1:886:A:H2'	26:1:887:A:C8	2.56	0.41
26:1:1598:U:H2'	26:1:1599:G:C8	2.56	0.41
26:1:1680:U:H2'	26:1:1681:U:C6	2.55	0.41
26:1:2083:G:H1	26:1:2639:C:H5	1.66	0.41
26:1:2268:A:H2'	26:1:2269:G:C8	2.56	0.41
2:B:260:ARG:NH1	26:1:1826:G:OP1	2.41	0.41
13:M:15:ARG:HD3	13:M:15:ARG:HA	1.87	0.41
23:Y:59:LYS:HG3	23:Y:61:GLY:H	1.86	0.41
24:Z:24:LEU:HD13	24:Z:30:ILE:HG12	2.02	0.41
26:1:464:U:H2'	26:1:465:C:C6	2.56	0.41
26:1:1674:U:H2'	26:1:1675:G:O4'	2.21	0.41
26:1:1939:A:O2'	26:1:1941:C:OP2	2.39	0.41
26:1:2676:U:H2'	26:1:2677:C:C6	2.55	0.41
9:I:80:LYS:O	9:I:84:LYS:HB2	2.21	0.41
12:L:71:LYS:HB3	12:L:72:PRO:HD3	2.03	0.41
17:Q:45:ARG:HD3	26:1:2445:A:OP1	2.20	0.41
26:1:569:U:H2'	26:1:570:U:C6	2.56	0.41
26:1:1086:G:HO2'	26:1:1087:C:H6	1.67	0.41
26:1:2348:G:H5'	26:1:2349:A:OP2	2.21	0.41
26:1:2705:U:H2'	26:1:2706:A:C8	2.55	0.41
27:2:11:A:H4'	27:2:13:A:H2'	2.03	0.41
26:1:557:G:OP1	26:1:1272:U:O2'	2.39	0.40
26:1:1328:C:H2'	26:1:1329:G:H8	1.86	0.40
26:1:2404:A:H2'	26:1:2405:A:C8	2.55	0.40
26:1:2858:G:H1	26:1:2900:C:H41	1.69	0.40
27:2:49:G:O2'	27:2:50:A:OP1	2.36	0.40
10:J:39:LEU:HB3	10:J:59:VAL:HG21	2.03	0.40
26:1:1203:U:H2'	26:1:1204:G:H8	1.87	0.40
26:1:1400:C:O2'	26:1:1836:A:N3	2.51	0.40
6:F:83:LYS:HE2	6:F:83:LYS:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:THR:OG1	11:K:36:GLN:OE1	2.36	0.40
12:L:56:LYS:HE3	12:L:69:ALA:HB2	2.04	0.40
26:1:774:G:H5'	26:1:775:A:H5"	2.04	0.40
26:1:830:U:H2'	26:1:831:C:C6	2.57	0.40
26:1:1031:C:H2'	26:1:1032:A:O4'	2.22	0.40
26:1:1823:U:H2'	26:1:1824:C:C6	2.56	0.40
16:P:4:ARG:HA	16:P:4:ARG:HD3	1.90	0.40
26:1:525:A:H1'	26:1:526:A:H5"	2.02	0.40
26:1:923:A:H2	26:1:946:A:C5	2.40	0.40
26:1:1725:G:O2'	26:1:1789:A:O2'	2.18	0.40
5:E:88:ARG:NH2	26:1:793:G:OP1	2.39	0.40
11:K:28:LEU:HD13	11:K:43:ILE:HD13	2.03	0.40
23:Y:69:PHE:HA	23:Y:70:PRO:HD3	1.85	0.40
26:1:651:A:H2'	26:1:652:A:C8	2.56	0.40
26:1:1072:A:N6	26:1:1169:G:H2'	2.36	0.40
26:1:2395:C:H2'	26:1:2396:A:H8	1.87	0.40
26:1:2698:A:H2'	26:1:2699:U:O4'	2.22	0.40

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	A	111/116 (96%)	106 (96%)	5 (4%)	0	100	100
2	B	271/277 (98%)	264 (97%)	7 (3%)	0	100	100
3	C	114/118 (97%)	114 (100%)	0	0	100	100
4	D	98/102 (96%)	93 (95%)	5 (5%)	0	100	100
5	E	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
6	F	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
7	G	86/105 (82%)	79 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	91/217 (42%)	87 (96%)	4 (4%)	0	100	100
9	I	76/94 (81%)	71 (93%)	5 (7%)	0	100	100
10	J	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
11	K	59/73 (81%)	56 (95%)	3 (5%)	0	100	100
12	L	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
13	M	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
14	N	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
15	O	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
16	P	42/45 (93%)	42 (100%)	0	0	100	100
17	Q	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
18	R	35/37 (95%)	35 (100%)	0	0	100	100
19	S	190/207 (92%)	180 (95%)	10 (5%)	0	100	100
20	V	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
21	W	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
22	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
23	Y	134/144 (93%)	132 (98%)	2 (2%)	0	100	100
24	Z	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
25	a	106/119 (89%)	102 (96%)	4 (4%)	0	100	100
All	All	2607/2904 (90%)	2513 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	99/102 (97%)	99 (100%)	0	100	100
2	B	220/224 (98%)	220 (100%)	0	100	100
3	C	96/98 (98%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	85/86 (99%)	85 (100%)	0	100	100
5	E	90/94 (96%)	90 (100%)	0	100	100
6	F	79/79 (100%)	79 (100%)	0	100	100
7	G	77/90 (86%)	77 (100%)	0	100	100
8	H	81/190 (43%)	81 (100%)	0	100	100
9	I	61/75 (81%)	61 (100%)	0	100	100
10	J	49/51 (96%)	49 (100%)	0	100	100
11	K	55/66 (83%)	55 (100%)	0	100	100
12	L	173/177 (98%)	173 (100%)	0	100	100
13	M	50/53 (94%)	50 (100%)	0	100	100
14	N	45/50 (90%)	45 (100%)	0	100	100
15	O	45/47 (96%)	45 (100%)	0	100	100
16	P	39/40 (98%)	39 (100%)	0	100	100
17	Q	55/56 (98%)	55 (100%)	0	100	100
18	R	35/35 (100%)	35 (100%)	0	100	100
19	S	158/170 (93%)	158 (100%)	0	100	100
20	V	122/123 (99%)	122 (100%)	0	100	100
21	W	99/100 (99%)	99 (100%)	0	100	100
22	X	110/112 (98%)	110 (100%)	0	100	100
23	Y	113/119 (95%)	113 (100%)	0	100	100
24	Z	101/102 (99%)	101 (100%)	0	100	100
25	a	87/95 (92%)	87 (100%)	0	100	100
All	All	2224/2434 (91%)	2224 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2673/2923 (91%)	388 (14%)	5 (0%)
27	2	110/115 (95%)	21 (19%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2783/3038 (91%)	409 (14%)	6 (0%)

All (409) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	35	G
26	1	36	G
26	1	51	G
26	1	60	U
26	1	69	C
26	1	71	A
26	1	74	U
26	1	75	G
26	1	89	U
26	1	90	A
26	1	91	A
26	1	117	A
26	1	119	U
26	1	137	G
26	1	139	U
26	1	140	A
26	1	156	A
26	1	160	G
26	1	161	A
26	1	168	A
26	1	176	A
26	1	180	G
26	1	183	A
26	1	199	A
26	1	202	A
26	1	218	G
26	1	219	A
26	1	225	A
26	1	230	A
26	1	233	U
26	1	248	G
26	1	251	G
26	1	253	G
26	1	255	G
26	1	258	A
26	1	259	A
26	1	268	A

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Mol	Chain	Res	Type
26	1	278	A
26	1	279	A
26	1	298	U
26	1	301	U
26	1	302	A
26	1	306	C
26	1	309	U
26	1	311	U
26	1	320	U
26	1	321	U
26	1	322	A
26	1	330	C
26	1	332	A
26	1	333	C
26	1	354	A
26	1	358	G
26	1	372	A
26	1	373	A
26	1	381	G
26	1	396	G
26	1	397	U
26	1	406	A
26	1	407	G
26	1	408	U
26	1	410	G
26	1	411	A
26	1	432	G
26	1	433	U
26	1	440	C
26	1	447	A
26	1	450	C
26	1	452	G
26	1	457	G
26	1	463	C
26	1	489	A
26	1	501	C
26	1	502	C
26	1	503	A
26	1	526	A
26	1	527	G
26	1	535	G
26	1	536	A

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Mol	Chain	Res	Type
26	1	537	A
26	1	545	G
26	1	546	A
26	1	550	A
26	1	553	A
26	1	554	C
26	1	575	G
26	1	576	U
26	1	577	A
26	1	578	G
26	1	583	A
26	1	593	U
26	1	594	G
26	1	606	G
26	1	616	G
26	1	617	A
26	1	618	A
26	1	646	A
26	1	647	G
26	1	650	U
26	1	659	A
26	1	660	A
26	1	661	U
26	1	662	G
26	1	667	G
26	1	682	A
26	1	683	G
26	1	690	U
26	1	691	A
26	1	698	U
26	1	699	U
26	1	700	A
26	1	731	U
26	1	744	A
26	1	758	G
26	1	761	A
26	1	763	A
26	1	775	A
26	1	785	C
26	1	792	U
26	1	809	A
26	1	810	A

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Mol	Chain	Res	Type
26	1	819	A
26	1	820	G
26	1	822	G
26	1	827	A
26	1	829	U
26	1	835	U
26	1	837	G
26	1	850	G
26	1	857	C
26	1	872	U
26	1	875	G
26	1	891	A
26	1	921	C
26	1	923	A
26	1	924	G
26	1	944	G
26	1	955	A
26	1	970	U
26	1	972	A
26	1	977	A
26	1	985	A
26	1	989	A
26	1	990	G
26	1	1005	G
26	1	1018	A
26	1	1027	A
26	1	1040	A
26	1	1046	G
26	1	1056	U
26	1	1057	A
26	1	1066	G
26	1	1070	A
26	1	1077	U
26	1	1087	C
26	1	1093	C
26	1	1094	A
26	1	1156	G
26	1	1160	C
26	1	1173	A
26	1	1176	U
26	1	1177	A
26	1	1179	C

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Mol	Chain	Res	Type
26	1	1186	A
26	1	1187	A
26	1	1220	A
26	1	1250	G
26	1	1258	A
26	1	1274	G
26	1	1278	G
26	1	1288	G
26	1	1291	A
26	1	1294	G
26	1	1309	G
26	1	1310	A
26	1	1313	G
26	1	1321	A
26	1	1327	C
26	1	1337	A
26	1	1338	U
26	1	1358	A
26	1	1362	C
26	1	1366	U
26	1	1374	G
26	1	1387	C
26	1	1389	U
26	1	1395	G
26	1	1402	A
26	1	1416	U
26	1	1421	A
26	1	1429	G
26	1	1432	A
26	1	1433	U
26	1	1451	U
26	1	1452	C
26	1	1453	G
26	1	1454	U
26	1	1463	A
26	1	1471	A
26	1	1472	C
26	1	1489	A
26	1	1490	G
26	1	1491	C
26	1	1497	A
26	1	1503	U

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Mol	Chain	Res	Type
26	1	1504	U
26	1	1516	C
26	1	1519	U
26	1	1557	C
26	1	1561	G
26	1	1566	G
26	1	1570	G
26	1	1578	A
26	1	1588	U
26	1	1593	G
26	1	1605	A
26	1	1606	C
26	1	1616	A
26	1	1628	A
26	1	1629	U
26	1	1634	A
26	1	1639	G
26	1	1651	C
26	1	1652	A
26	1	1654	A
26	1	1663	G
26	1	1683	U
26	1	1690	A
26	1	1691	G
26	1	1692	C
26	1	1711	G
26	1	1718	G
26	1	1740	G
26	1	1744	A
26	1	1758	A
26	1	1759	G
26	1	1773	A
26	1	1790	G
26	1	1791	G
26	1	1800	A
26	1	1811	A
26	1	1827	C
26	1	1828	U
26	1	1829	A
26	1	1836	A
26	1	1843	U
26	1	1854	U

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Mol	Chain	Res	Type
26	1	1856	A
26	1	1860	C
26	1	1897	U
26	1	1898	C
26	1	1901	C
26	1	1910	G
26	1	1933	G
26	1	1940	A
26	1	1941	C
26	1	1942	U
26	1	1943	A
26	1	1944	U
26	1	1946	A
26	1	1957	G
26	1	1965	A
26	1	1982	U
26	1	1994	C
26	1	1997	A
26	1	1998	A
26	1	1999	G
26	1	2004	A
26	1	2009	U
26	1	2018	U
26	1	2020	U
26	1	2021	C
26	1	2050	A
26	1	2058	A
26	1	2059	G
26	1	2060	A
26	1	2070	C
26	1	2082	C
26	1	2083	G
26	1	2087	A
26	1	2088	G
26	1	2089	A
26	1	2090	C
26	1	2096	G
26	1	2120	G
26	1	2124	U
26	1	2126	C
26	1	2226	A
26	1	2231	C

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Mol	Chain	Res	Type
26	1	2232	A
26	1	2238	U
26	1	2252	A
26	1	2265	G
26	1	2266	G
26	1	2295	A
26	1	2302	C
26	1	2306	G
26	1	2307	G
26	1	2310	C
26	1	2333	U
26	1	2335	G
26	1	2336	A
26	1	2337	A
26	1	2338	A
26	1	2339	U
26	1	2346	U
26	1	2348	G
26	1	2349	A
26	1	2350	G
26	1	2352	G
26	1	2361	U
26	1	2362	A
26	1	2363	A
26	1	2372	G
26	1	2374	C
26	1	2377	C
26	1	2398	G
26	1	2399	G
26	1	2410	G
26	1	2412	C
26	1	2429	U
26	1	2430	C
26	1	2450	U
26	1	2452	A
26	1	2456	G
26	1	2457	A
26	1	2468	C
26	1	2475	A
26	1	2497	G
26	1	2503	A
26	1	2505	A

Continued on next page...

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Mol	Chain	Res	Type
26	1	2521	G
26	1	2525	C
26	1	2529	G
26	1	2530	A
26	1	2545	A
26	1	2547	C
26	1	2556	G
26	1	2561	C
26	1	2593	A
26	1	2594	G
26	1	2599	A
26	1	2600	C
26	1	2609	G
26	1	2612	U
26	1	2613	C
26	1	2629	A
26	1	2636	U
26	1	2637	C
26	1	2640	U
26	1	2641	A
26	1	2657	G
26	1	2663	U
26	1	2673	C
26	1	2677	C
26	1	2690	G
26	1	2712	G
26	1	2716	U
26	1	2717	A
26	1	2732	A
26	1	2741	G
26	1	2749	G
26	1	2753	U
26	1	2760	A
26	1	2771	G
26	1	2775	A
26	1	2778	G
26	1	2784	A
26	1	2791	A
26	1	2792	A
26	1	2793	G
26	1	2805	A
26	1	2807	G

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Mol	Chain	Res	Type
26	1	2820	U
26	1	2821	U
26	1	2822	C
26	1	2823	G
26	1	2824	G
26	1	2827	A
26	1	2828	U
26	1	2840	A
26	1	2853	U
26	1	2887	G
26	1	2892	G
26	1	2893	A
26	1	2900	C
26	1	2911	A
26	1	2913	G
27	2	4	G
27	2	10	U
27	2	12	U
27	2	13	A
27	2	23	U
27	2	39	G
27	2	40	C
27	2	42	G
27	2	43	A
27	2	45	C
27	2	49	G
27	2	50	A
27	2	71	A
27	2	84	U
27	2	86	A
27	2	94	C
27	2	100	U
27	2	104	A
27	2	105	C
27	2	106	G
27	2	109	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	229	A
26	1	525	A

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Mol	Chain	Res	Type
26	1	2336	A
26	1	2783	U
26	1	2827	A
27	2	49	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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-26124. 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
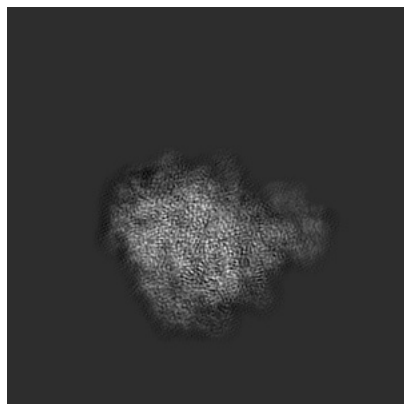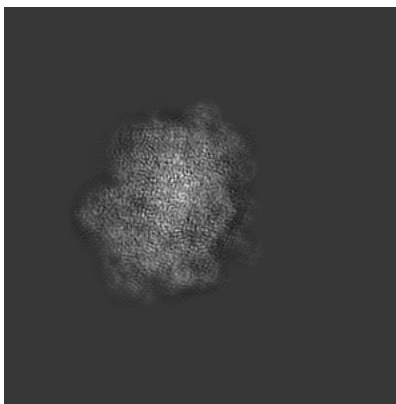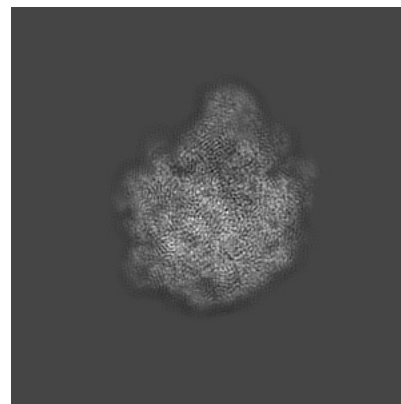
| X | Y | Z |

6.1.2 Raw map

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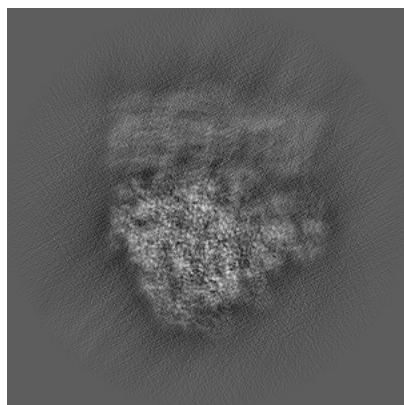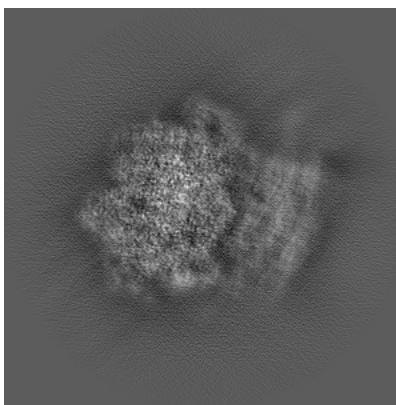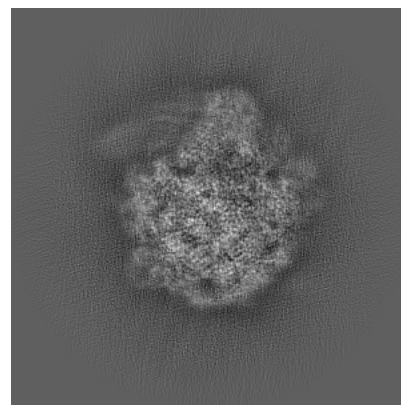
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
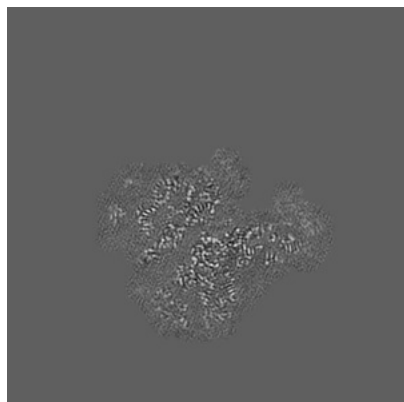
6.2.1   Primary map
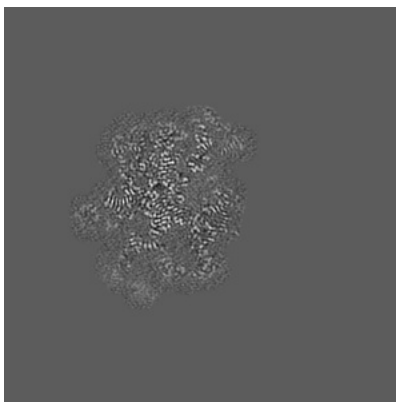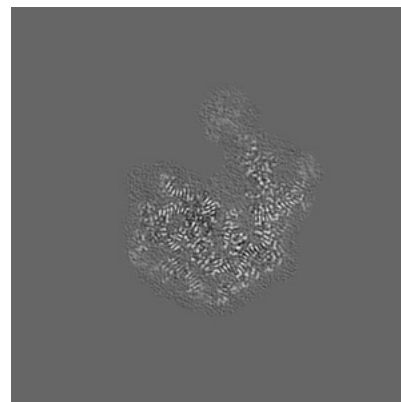
X Index: 224   Y Index: 224   Z Index: 224

6.2.2   Raw map
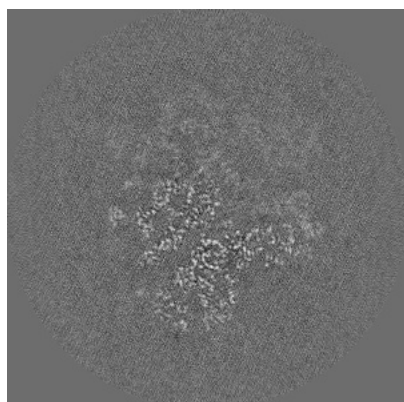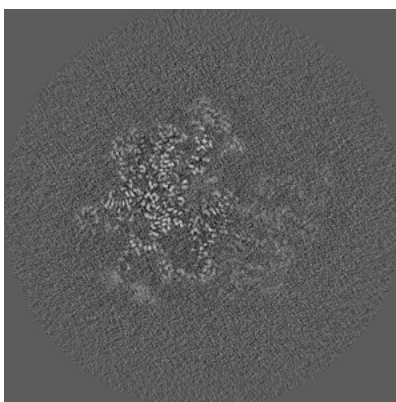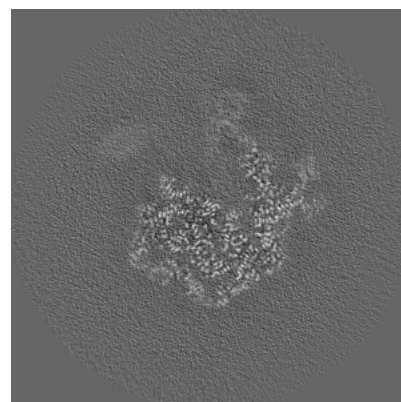
X Index: 224   Y Index: 224   Z Index: 224

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

6.3 Largest variance slices ⓘ
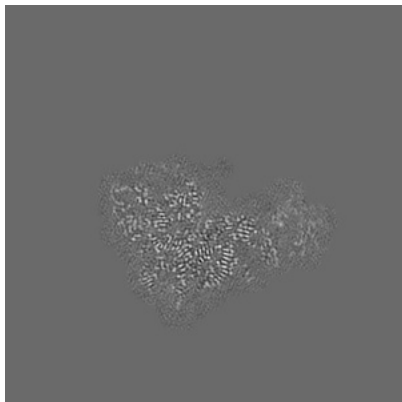
6.3.1 Primary map

X Index: 247
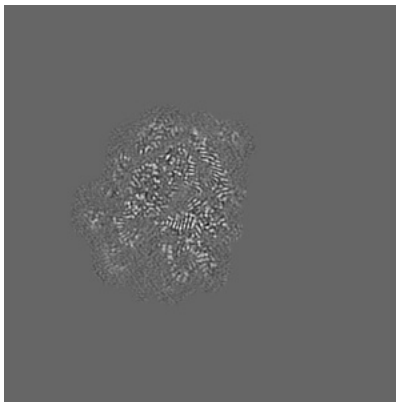
Y Index: 210
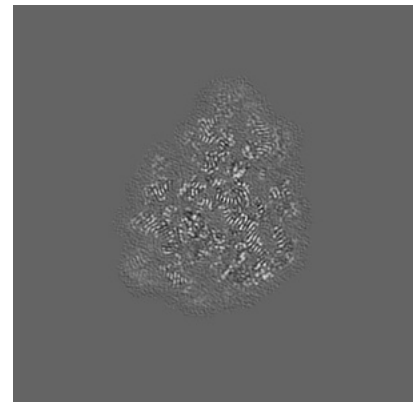
Z Index: 191

6.3.2 Raw map
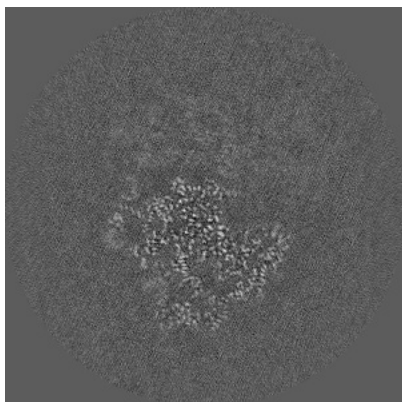
X Index: 209
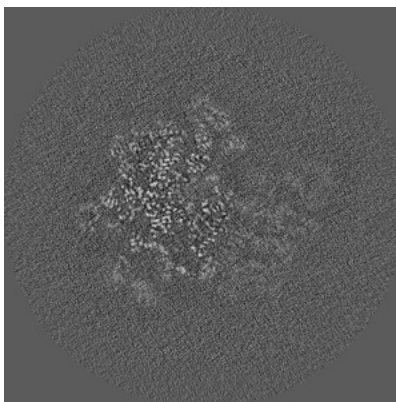
Y Index: 223
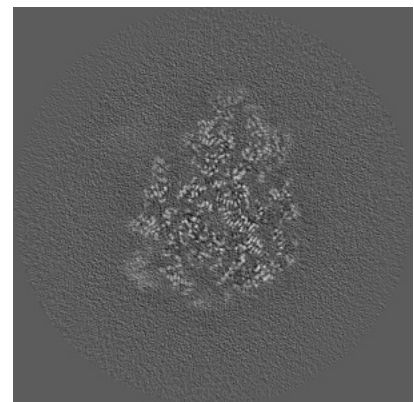
Z Index: 191

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
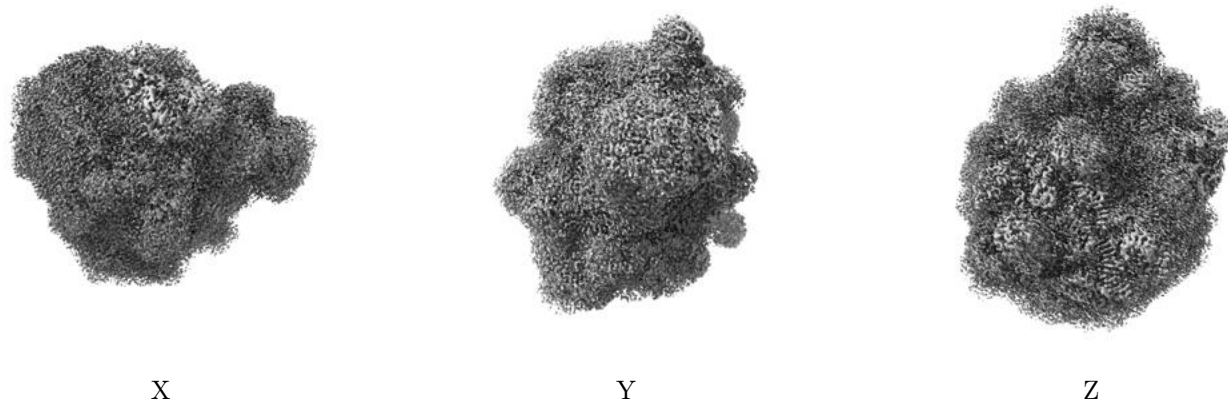
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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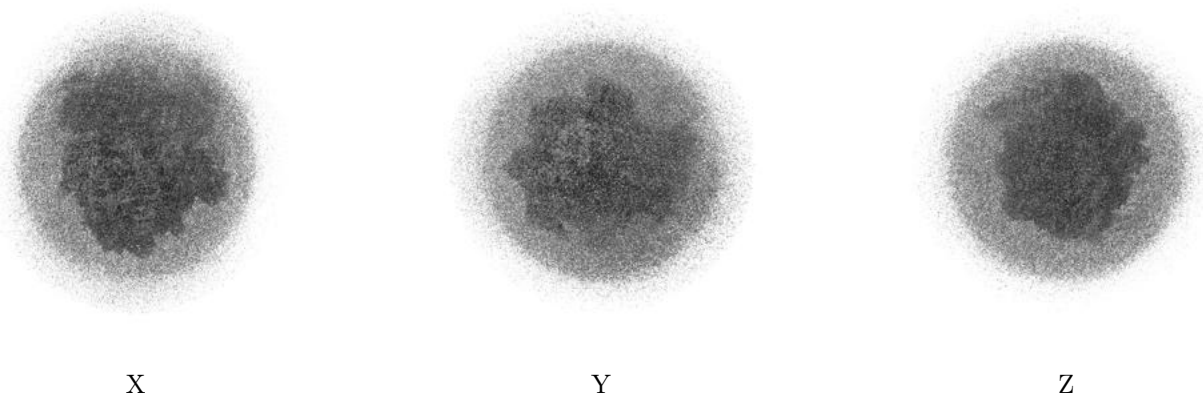
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

6.5.1 emd_26124_msk_1.map ⓘ

X   Y   Z
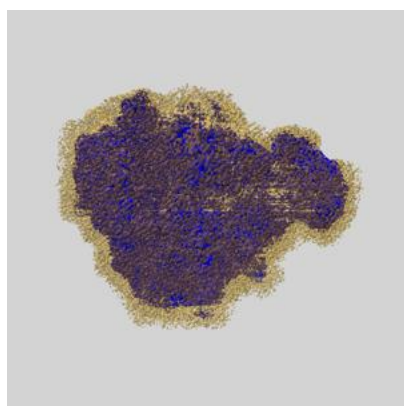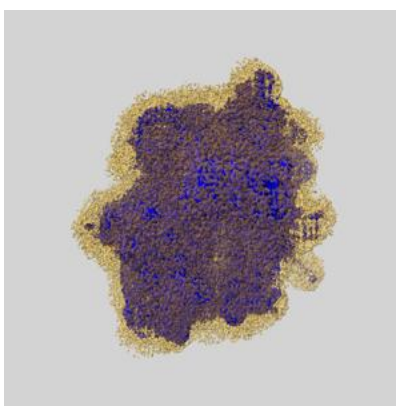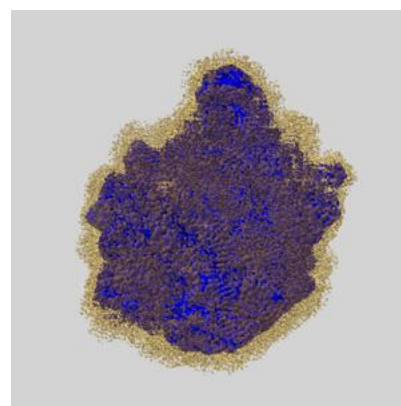
7 Map analysis ⓘ

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 ⓘ
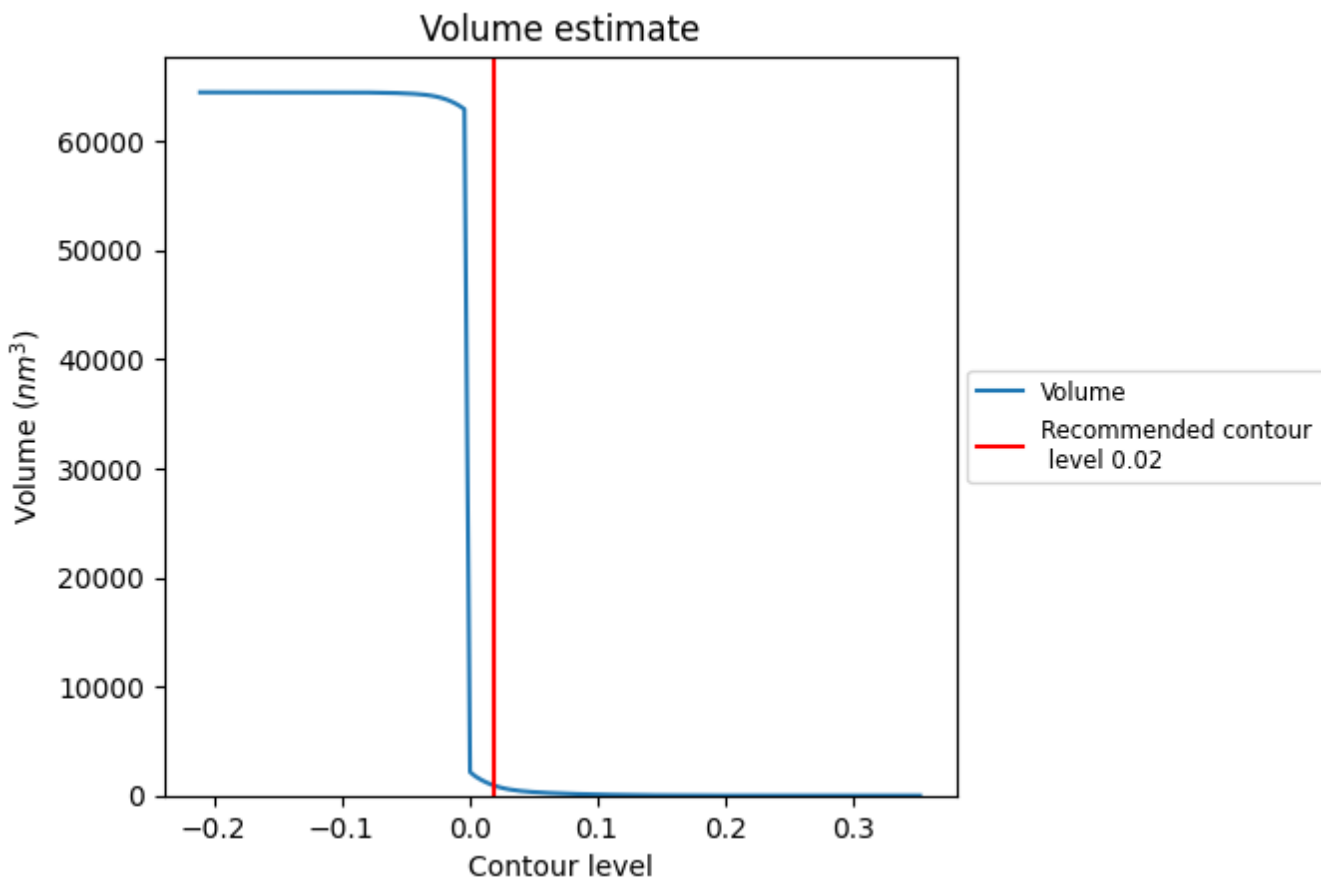
The volume at the recommended contour level is 903 nm^3; this corresponds to an approximate mass of 816 kDa.

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

7.3　Rotationally averaged power spectrum (i)
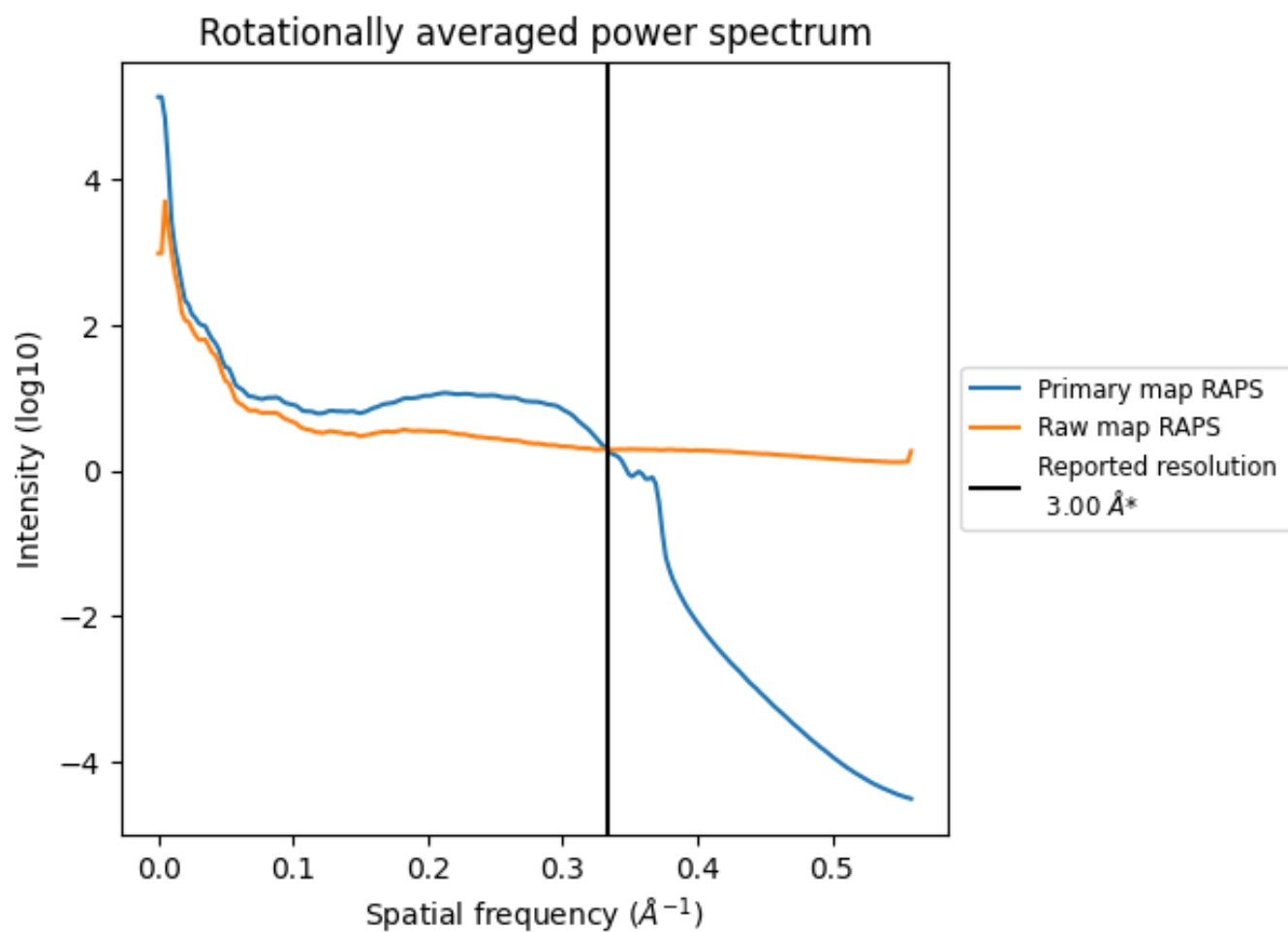
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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)
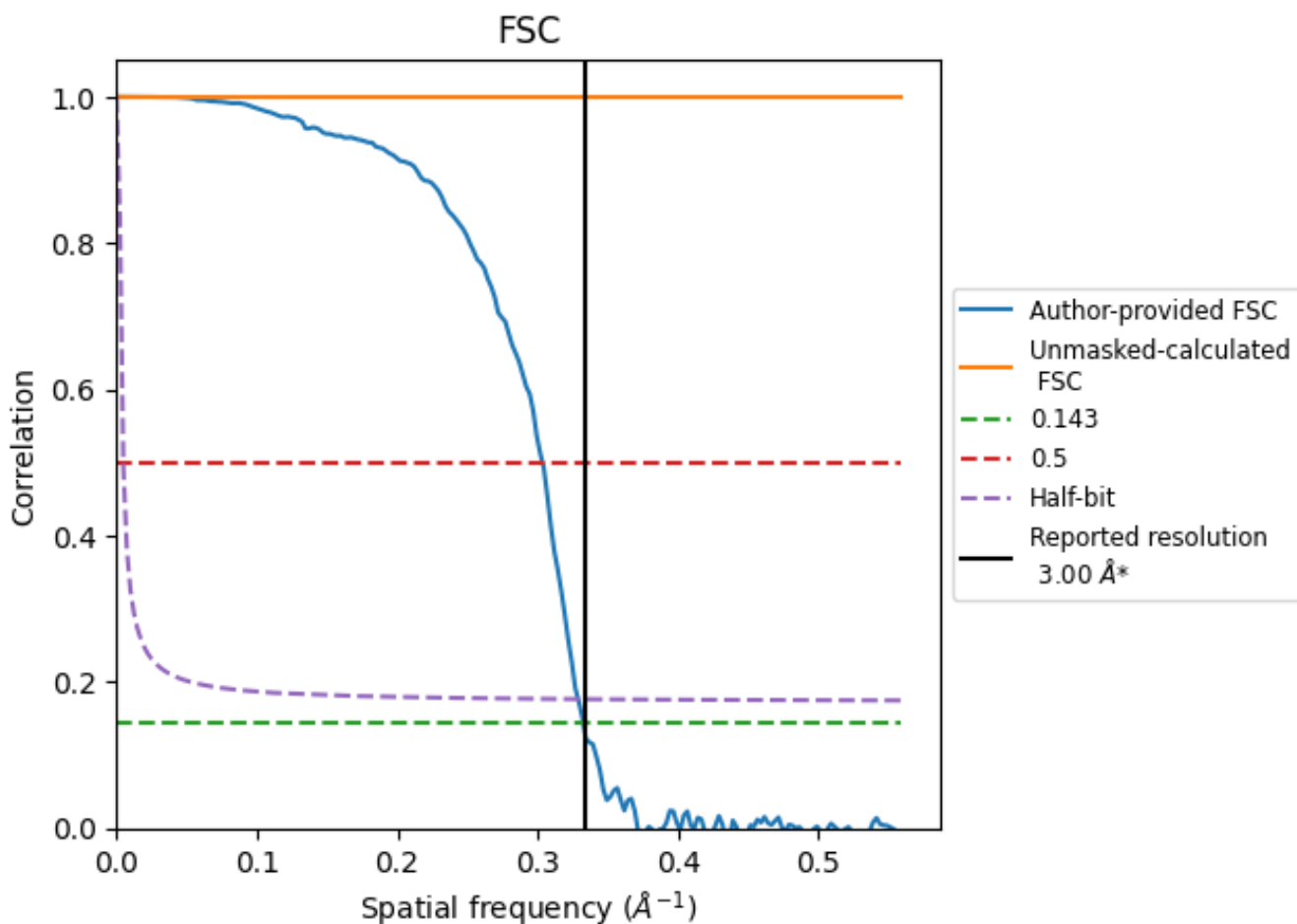
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.30	3.04
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-26124 and PDB model 7TTU. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay ⓘ

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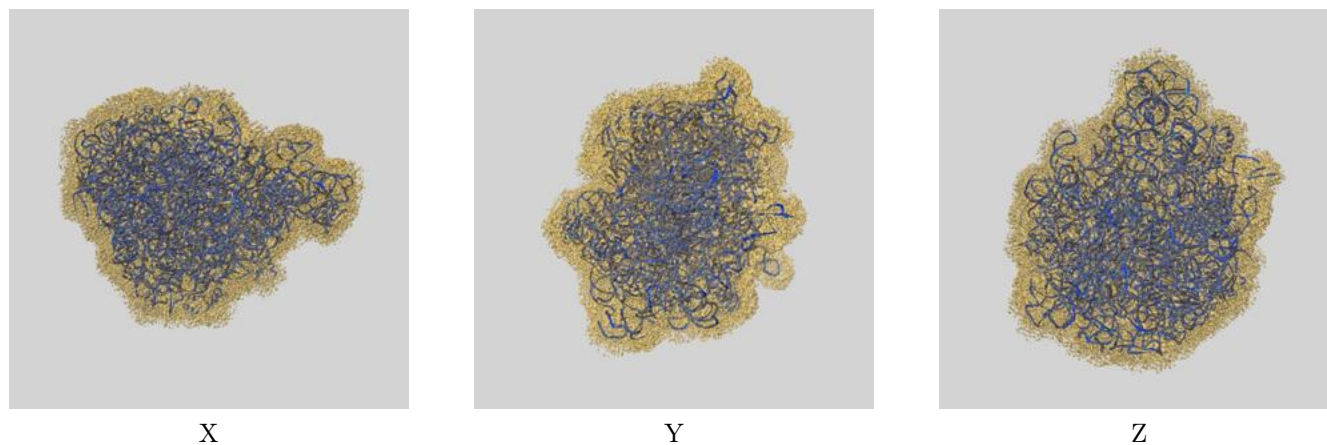
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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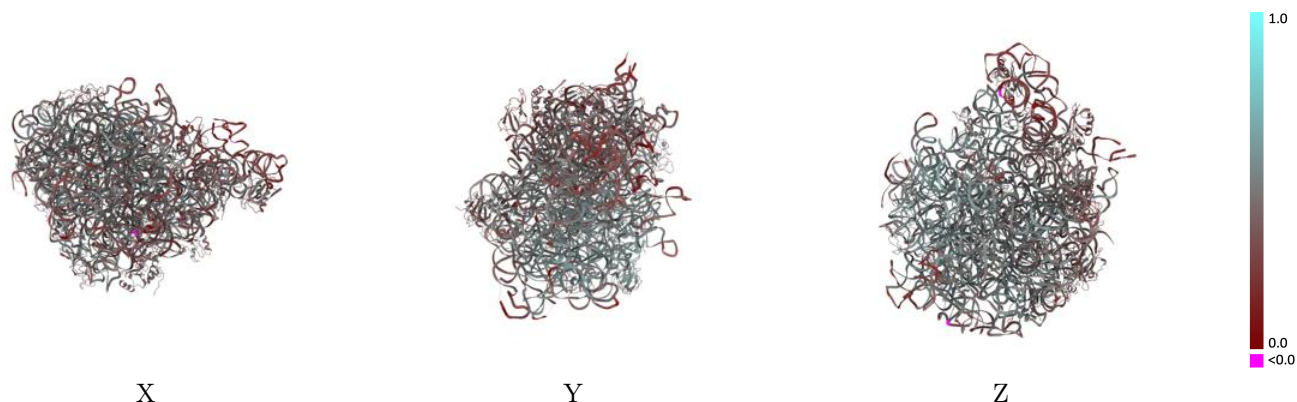
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
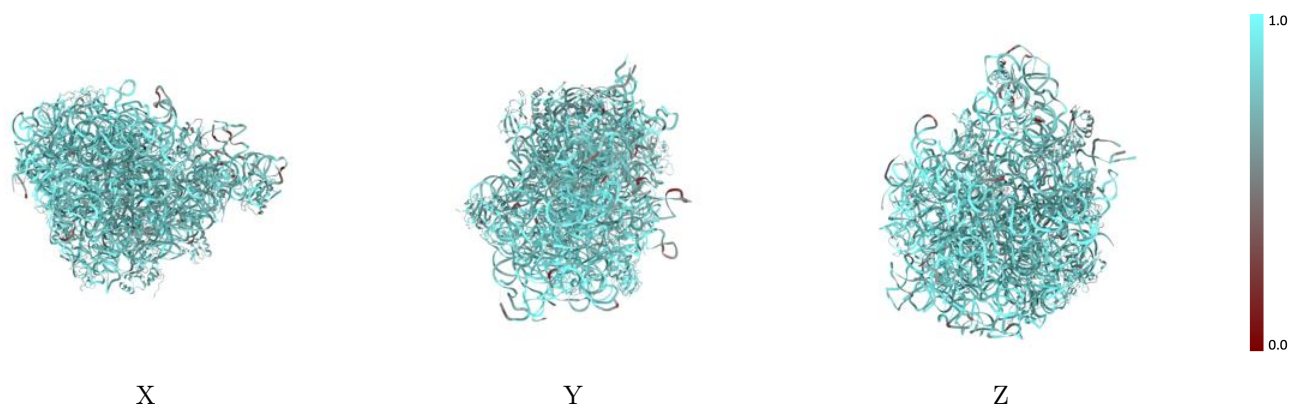
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ
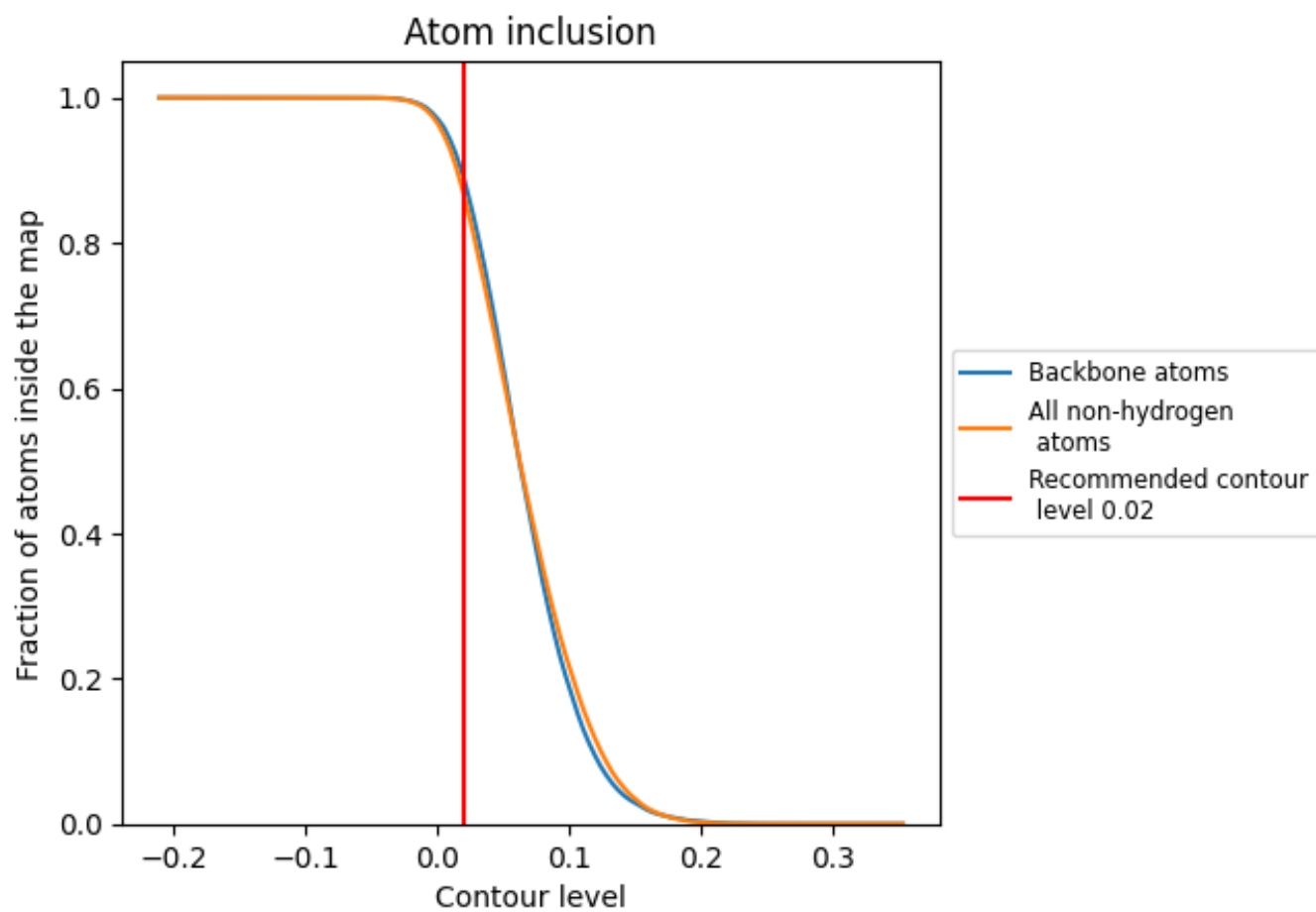
At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.8678	0.4470
1	0.8873	0.4580
2	0.7759	0.3340
A	0.8077	0.4420
B	0.8945	0.5270
C	0.8231	0.3960
D	0.7568	0.3500
E	0.8652	0.4600
F	0.8672	0.4760
G	0.7612	0.3820
H	0.6443	0.3270
I	0.8114	0.4230
J	0.8837	0.4930
K	0.8501	0.4090
L	0.8335	0.4280
M	0.7877	0.3850
N	0.8956	0.4520
O	0.7905	0.4180
P	0.9544	0.5620
Q	0.8884	0.5010
R	0.7655	0.3730
S	0.8315	0.4380
V	0.8027	0.3880
W	0.8041	0.4160
X	0.8347	0.4430
Y	0.7913	0.4120
Z	0.8644	0.4690
a	0.7305	0.3610

1.0

0.0
<0.0