WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 02:20 PM EST

PDB ID	:	7SAE
EMDB ID	:	EMD-24950
Title	:	44SR70P Class1 ribosomal particle
Authors	:	Ortega, J.; Seffouh, A.
Deposited on	:	2021-09-22
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:

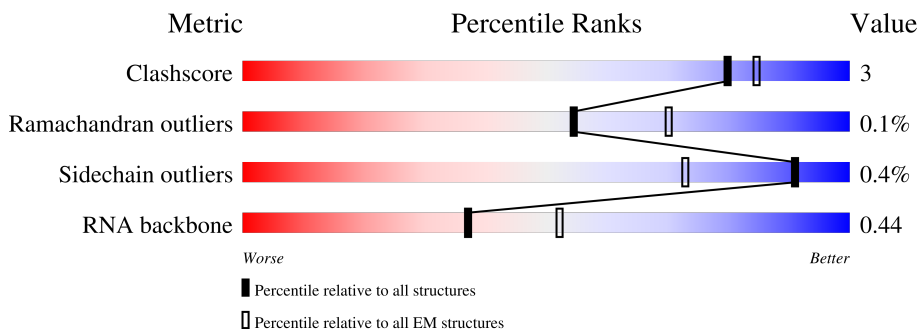|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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.
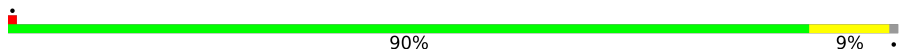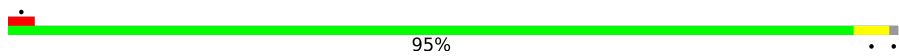
Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		0.4%
RNA backbone		0.44

Worse .... *Better*

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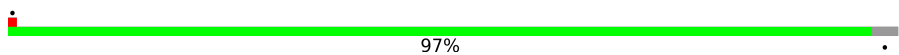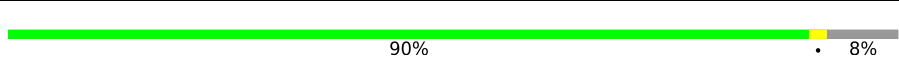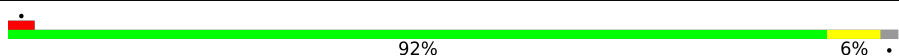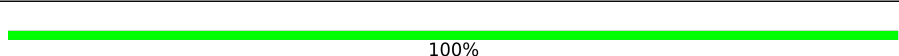
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2928	5% 52% 25% 6% · 17%
2	C	277	17% 87% 9% ·
3	D	209	· 75% 11% 14%
4	E	207	· 93% 6% ·
5	J	145	· 92% 6% ·
6	K	122	14% 89% 11%
7	L	146	10% 81% 8% 11%

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Mol	Chain	Length	Quality of chain
8	N	120	90%　9%
9	P	115	13%　88%　11%
10	Q	119	89%　9%
11	R	102	95%
12	S	113	85%　12%
13	T	95	97%
14	U	103	8%　85%　12%
15	V	94	13%　67%　10%　23%
16	Z	59	5%　86%　12%
17	b	59	90%　8%
18	Y	66	92%　6%
19	d	44	100%

2 Entry composition ⓘ

There are 19 unique types of molecules in this entry. The entry contains 68571 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 RNA chain called RNA (2434-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2434	Total 52303	C 23336	N 9696	O 16837	P 2434	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 1864548803

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	267	Total 2052	C 1277	N 402	O 367	S 6	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	179	Total 1354	C 854	N 241	O 256	S 3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	205	Total 1561	C 980	N 289	O 290	S 2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	142	Total 1123	C 710	N 206	O 202	S 5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	122	Total 920	C 571	N 173	O 172	S 4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	130	Total 973	C 608	N 183	O 180	S 2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	119	Total 953	C 583	N 186	O 180	S 4	0	0

- Molecule 9 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	114	Total 936	C 595	N 184	O 157	0	0

- Molecule 10 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	117	Total 940	C 591	N 189	O 156	S 4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	101	Total 780	C 495	N 139	O 146	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	74	HIS	PHE	conflict	UNP P26908
R	83	ALA	HIS	conflict	UNP P26908

- Molecule 12 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	109	Total 842	C 525	N 164	O 150	S 3	0	0

- Molecule 13 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	92	Total 741	C 463	N 136	O 138	S 4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	100	Total 754	C 473	N 141	O 137	S 3	0	0

- Molecule 15 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	72	Total 561	C 349	N 109	O 103	0	0

- Molecule 16 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	58	Total 455	C 281	N 89	O 84	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	54	Total 426	C 262	N 86	O 71	S 7	0	0

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	65	Total 530	C 328	N 102	O 98	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	d	44	367	222	89	54	2	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: RNA (2434-MER)
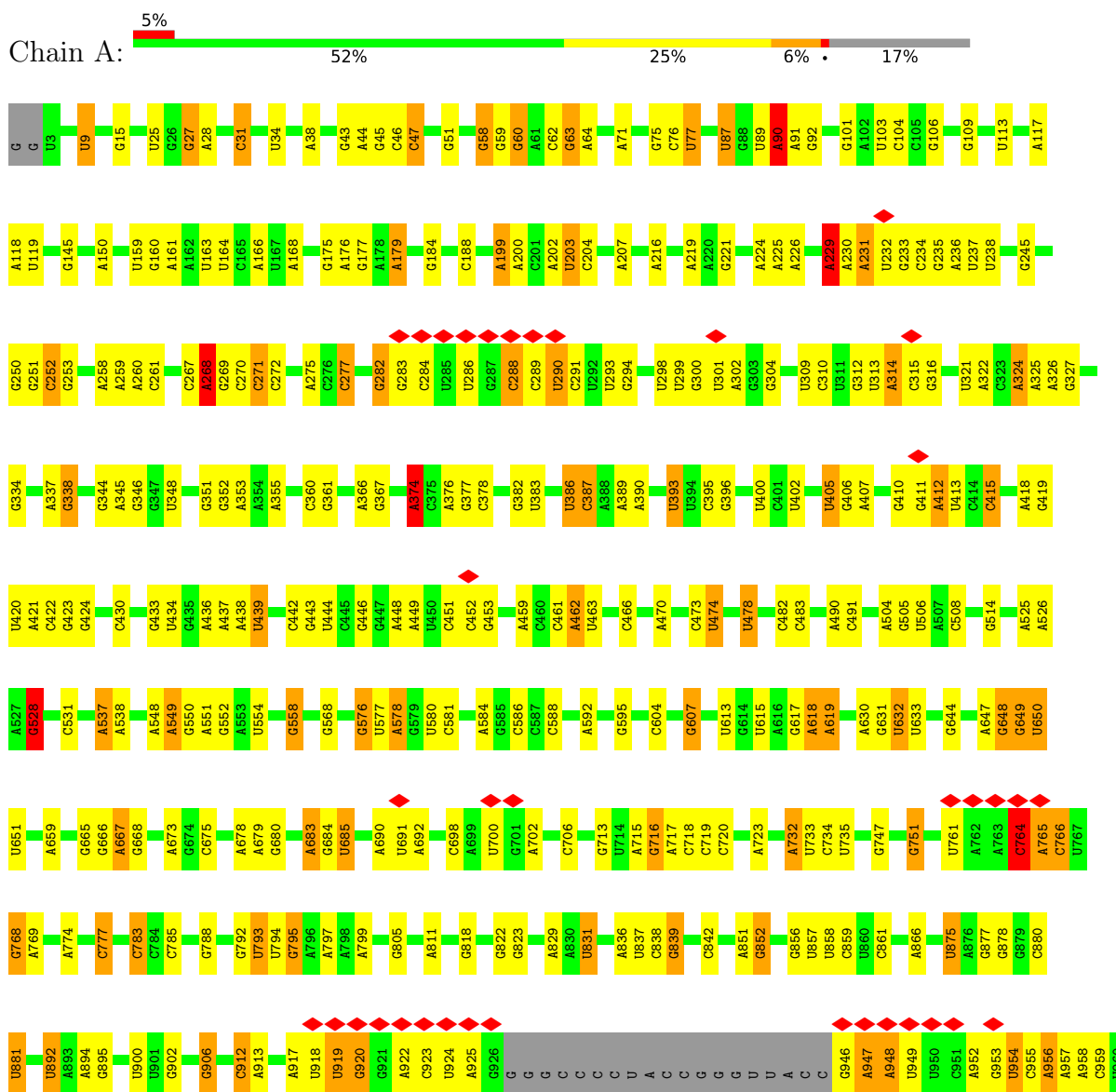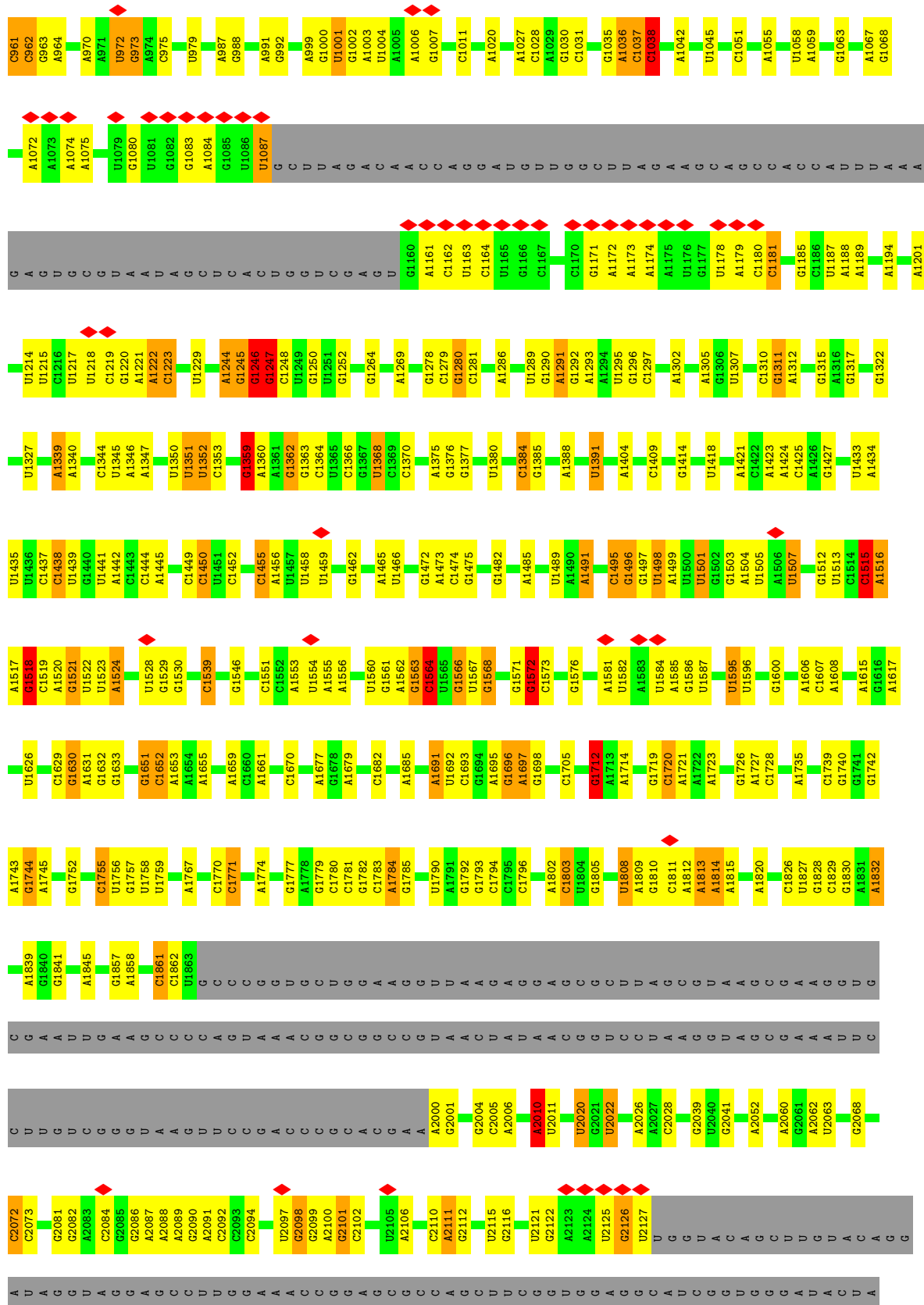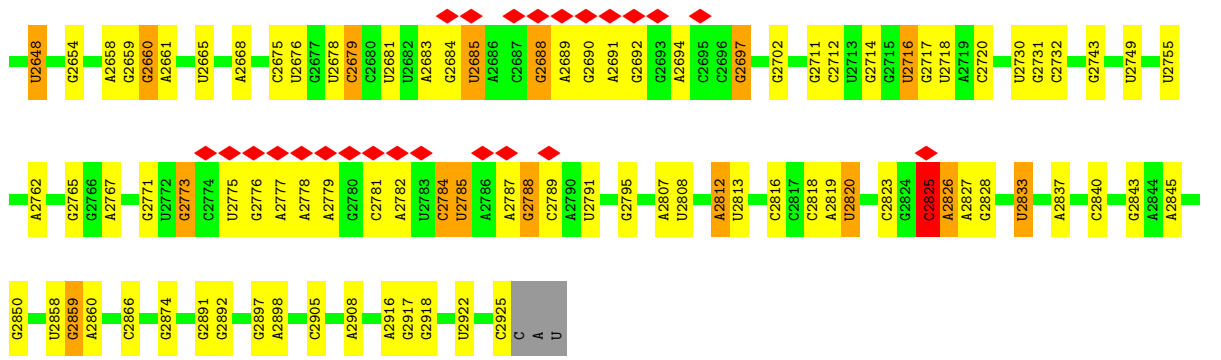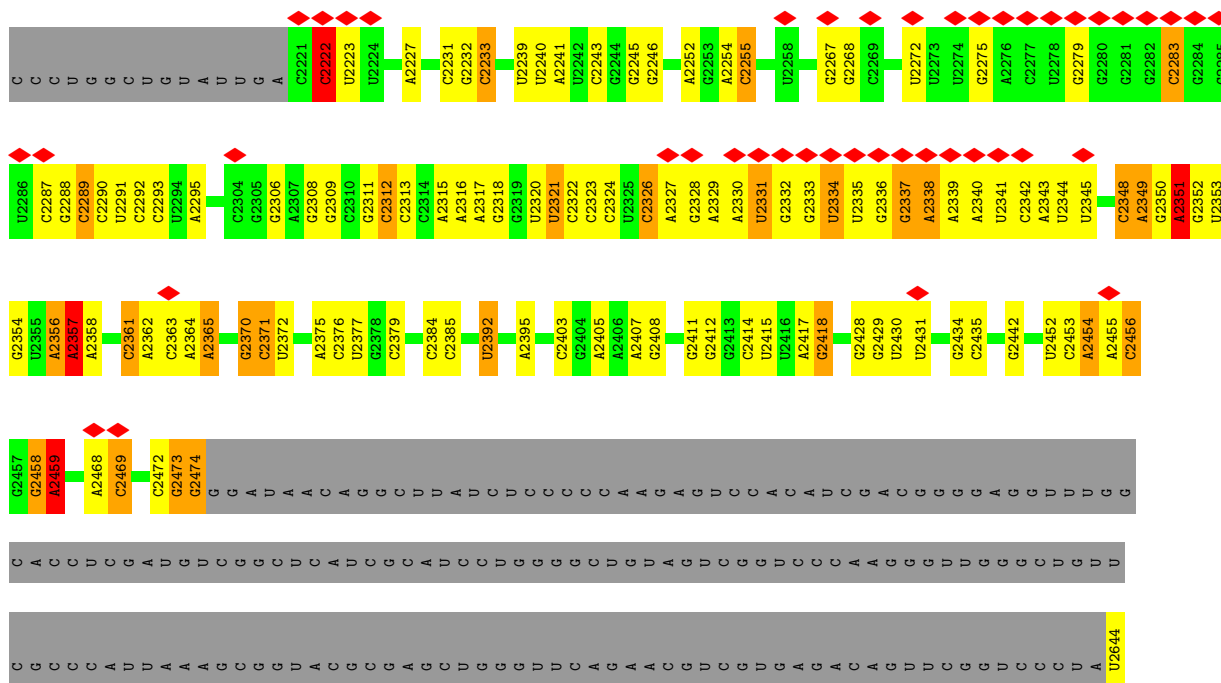
• Molecule 2: 50S ribosomal protein L2

Chain C:

17%

87%   9%   ·

• Molecule 3: 50S ribosomal protein L3

Chain D:

75%   11%   14%

ASP PRO ASN ARG VAL PHE LYS G157 K158 L159 L160 P161 R183 G190 S208 LYS
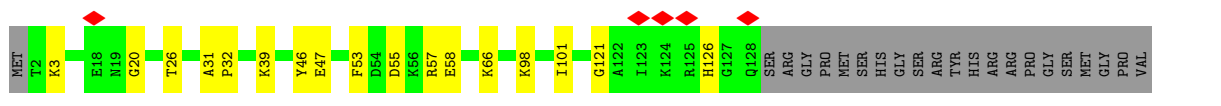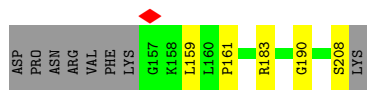
• Molecule 4: 50S ribosomal protein L4

Chain E:

93%   6%

MET P2 L6 A14 I17 R54 R66 G69 T70 G71 R72 A73 R74 P81 V89 D128 D132 V155 D158 N182 I194 L206 ALA
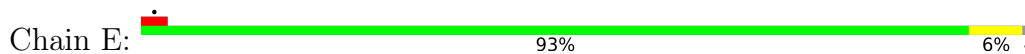
• Molecule 5: 50S ribosomal protein L13

Chain J:

92%   6%

MET ARG THR T4 P5 M6 T44 K68 D72 H78 T79 Q80 H81 P82 K86 A135 R144 G145
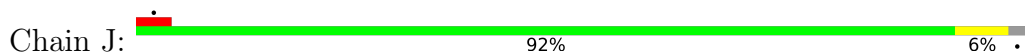
• Molecule 6: 50S ribosomal protein L14

Chain K:

14%   89%   11%

M1 L8 D12 G15 A16 R17 T42 Q45 A46 T47 P48 G49 G50 K53 K54 V57 R64 C84 R88 D89 D90 K91 S92 R97 P101 R107 N110 K113 I114 V115 I122
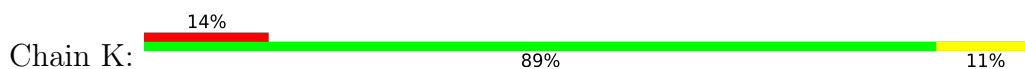
• Molecule 7: 50S ribosomal protein L15

Chain L:

10%   81%   8%   11%

M1 H4 V19 N27 G28 K29 T30 Q38 ASN ALA ARG SER GLY GLY GLY VAL ARG PRO GLY PHE GLU GLY GLY GLN M55 P56 L57 R71 K72 G84 F85 A86 E87 G88 T89 E90 V91 L105 K116 L117 E118 V123 E137 A138 A139 G140 G141 T142 A143

I146
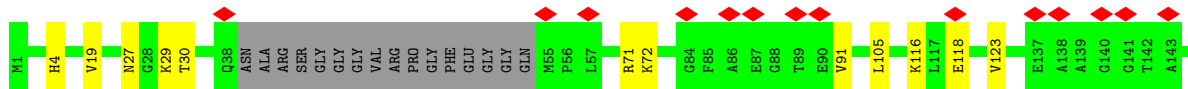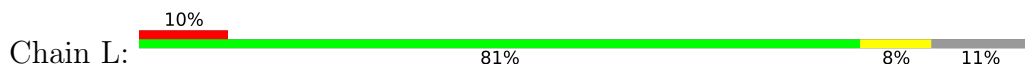
• Molecule 8: 50S ribosomal protein L17

Chain N:

90%   9%

MET S2 Y3 L24 I30 T35 R41 V44 E45 N72 E73 E74 N75 T99 V120
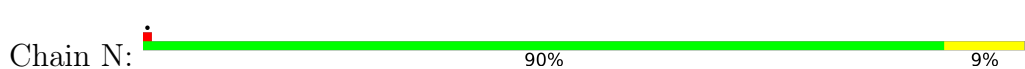
• Molecule 9: 50S ribosomal protein L19

Chain P:

13%   88%   11%
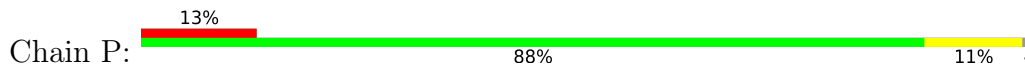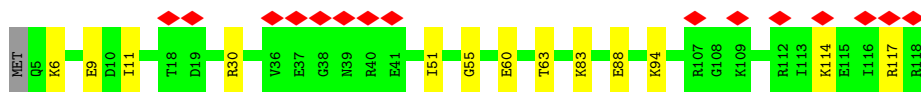
• Molecule 10: 50S ribosomal protein L20

Chain Q:
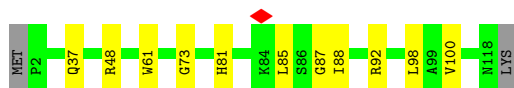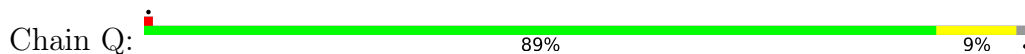
• Molecule 11: 50S ribosomal protein L21

Chain R:
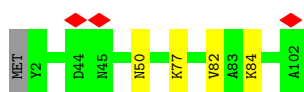
• Molecule 12: 50S ribosomal protein L22

Chain S:
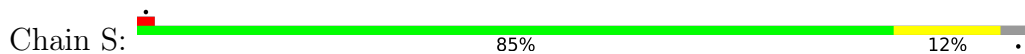
• Molecule 13: 50S ribosomal protein L23

Chain T:
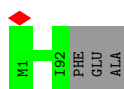
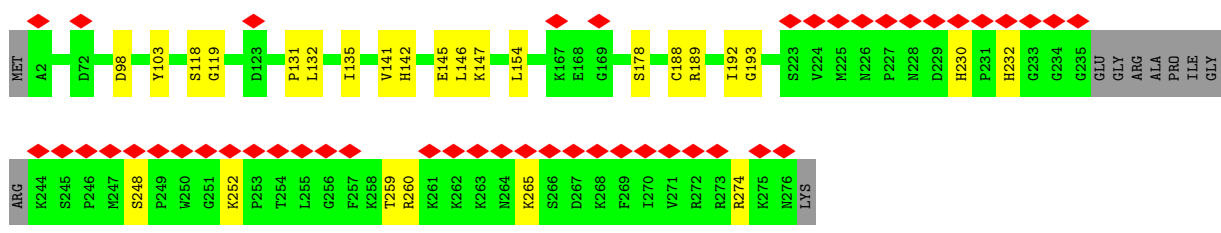• Molecule 14: 50S ribosomal protein L24

Chain U:
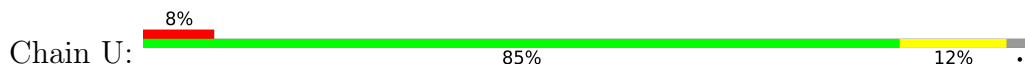
• Molecule 15: 50S ribosomal protein L27

Chain V:

• Molecule 16: 50S ribosomal protein L30
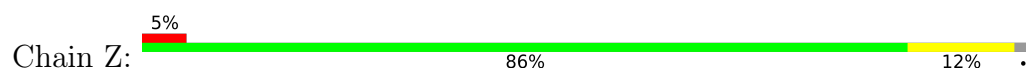
Chain Z:

- Molecule 17: 50S ribosomal protein L32
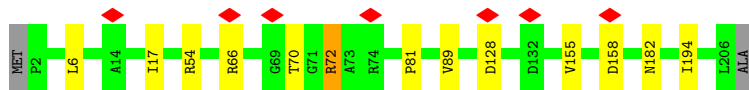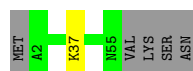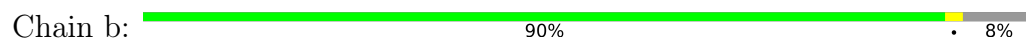
Chain b:

- Molecule 18: 50S ribosomal protein L29

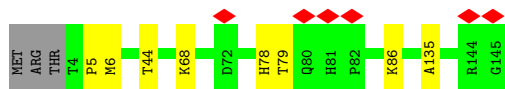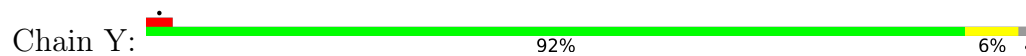Chain Y:

- Molecule 19: 50S ribosomal protein L34

Chain d:

There are no outlier residues recorded for this chain.

4　Experimental information　ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168942	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 $(e^-/\text{Å}^2)$	74	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0131	Depositor
Map size (Å)	362.52002, 362.52002, 362.52002	wwPDB
Map dimensions	424, 424, 424	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5   Model quality   ⓘ

5.1   Standard geometry   ⓘ

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	0.90	4/58595 (0.0%)	1.18	500/91408 (0.5%)
2	C	0.34	0/2087	0.53	0/2798
3	D	0.44	0/1367	0.55	0/1830
4	E	0.45	0/1580	0.57	0/2132
5	J	0.43	0/1146	0.58	0/1542
6	K	0.35	0/927	0.54	0/1245
7	L	0.37	0/982	0.58	1/1308 (0.1%)
8	N	0.50	0/960	0.56	0/1284
9	P	0.40	0/949	0.58	0/1269
10	Q	0.58	0/952	0.63	0/1266
11	R	0.48	0/790	0.65	0/1061
12	S	0.43	0/851	0.55	0/1146
13	T	0.45	0/747	0.53	0/995
14	U	0.42	0/764	0.59	0/1022
15	V	0.32	0/569	0.53	0/757
16	Z	0.39	0/457	0.52	0/613
17	b	0.46	0/433	0.52	0/574
18	Y	0.38	0/531	0.52	0/707
19	d	0.45	0/370	0.52	0/483
All	All	0.82	4/75057 (0.0%)	1.09	501/113440 (0.4%)

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
2	C	0	1
10	Q	0	1
11	R	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	A	N9-C4	-5.52	1.34	1.37
1	A	1697	A	N9-C8	-5.43	1.33	1.37
1	A	1832	A	N9-C8	-5.24	1.33	1.37
1	A	179	A	N9-C4	-5.19	1.34	1.37

All (501) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	881	U	O5'-P-OP1	-13.75	93.33	105.70
1	A	1433	U	C2-N1-C1'	11.47	131.47	117.70
1	A	1368	U	N3-C2-O2	-11.09	114.44	122.20
1	A	881	U	C5-C6-N1	11.08	128.24	122.70
1	A	1281	C	N3-C2-O2	-10.54	114.53	121.90
1	A	1433	U	N1-C2-O2	10.13	129.89	122.80
1	A	857	U	N3-C2-O2	-9.72	115.39	122.20
1	A	1368	U	C2-N1-C1'	9.65	129.28	117.70
1	A	1327	U	N3-C2-O2	-9.43	115.60	122.20
1	A	1433	U	N3-C2-O2	-9.39	115.63	122.20
1	A	478	U	N3-C2-O2	-9.34	115.66	122.20
1	A	1368	U	N1-C2-O2	9.29	129.30	122.80
1	A	1281	C	C6-N1-C2	-9.24	116.60	120.30
1	A	1246	G	O4'-C1'-N9	9.20	115.56	108.20
1	A	2825	C	N1-C2-O2	9.15	124.39	118.90
1	A	1352	U	C2-N1-C1'	9.14	128.67	117.70
1	A	1523	U	N3-C2-O2	-9.10	115.83	122.20
1	A	858	U	N3-C2-O2	-9.00	115.90	122.20
1	A	1247	G	O4'-C1'-N9	8.99	115.39	108.20
1	A	720	C	C2-N1-C1'	8.96	128.66	118.80
1	A	1245	G	O4'-C1'-N9	8.91	115.33	108.20
1	A	1281	C	C2-N1-C1'	8.85	128.53	118.80
1	A	2255	C	N1-C2-O2	8.81	124.19	118.90
1	A	2685	U	N1-C2-O2	8.79	128.95	122.80
1	A	2283	C	N1-C2-O2	8.73	124.14	118.90
1	A	633	U	N3-C2-O2	-8.71	116.10	122.20
1	A	478	U	C2-N1-C1'	8.66	128.09	117.70
1	A	1028	C	N3-C2-O2	-8.60	115.88	121.90
1	A	1523	U	C2-N1-C1'	8.59	128.01	117.70
1	A	2685	U	C2-N1-C1'	8.57	127.98	117.70
1	A	1281	C	N1-C2-O2	8.51	124.00	118.90
1	A	1433	U	C6-N1-C1'	-8.48	109.32	121.20
1	A	1359	G	N3-C4-N9	-8.47	120.92	126.00
1	A	1353	C	C2-N1-C1'	8.47	128.12	118.80
1	A	2825	C	C2-N1-C1'	8.44	128.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	U	C5-C6-N1	8.38	126.89	122.70
1	A	1515	C	C2-N1-C1'	8.33	127.96	118.80
1	A	1327	U	N1-C2-O2	8.29	128.60	122.80
1	A	720	C	N3-C2-O2	-8.28	116.11	121.90
1	A	478	U	N1-C2-O2	8.25	128.57	122.80
1	A	1028	C	N1-C2-O2	8.17	123.80	118.90
1	A	633	U	C2-N1-C1'	8.05	127.36	117.70
1	A	2685	U	N3-C2-O2	-7.99	116.61	122.20
1	A	1352	U	N1-C2-O2	7.97	128.38	122.80
1	A	2781	C	N1-C2-O2	7.96	123.67	118.90
1	A	261	C	N1-C2-O2	7.94	123.66	118.90
1	A	1515	C	C6-N1-C2	-7.90	117.14	120.30
1	A	1523	U	N1-C2-O2	7.90	128.33	122.80
1	A	1832	A	N7-C8-N9	7.88	117.74	113.80
1	A	881	U	C6-N1-C2	-7.85	116.29	121.00
1	A	277	C	N1-C2-O2	7.84	123.61	118.90
1	A	1181	C	N1-C2-O2	7.83	123.60	118.90
1	A	1037	C	C6-N1-C2	-7.79	117.18	120.30
1	A	732	A	N7-C8-N9	7.77	117.69	113.80
1	A	764	C	N1-C2-O2	7.76	123.56	118.90
1	A	483	C	C2-N1-C1'	7.74	127.31	118.80
1	A	2679	C	C2-N1-C1'	7.73	127.30	118.80
1	A	1352	U	N3-C2-O2	-7.67	116.83	122.20
1	A	720	C	N1-C2-O2	7.62	123.47	118.90
1	A	2825	C	C6-N1-C2	-7.61	117.25	120.30
1	A	716	G	C4-N9-C1'	7.60	136.38	126.50
1	A	2283	C	C2-N1-C1'	7.45	127.00	118.80
1	A	1770	C	C2-N1-C1'	7.42	126.96	118.80
1	A	857	U	C2-N1-C1'	7.37	126.54	117.70
1	A	732	A	C8-N9-C4	-7.36	102.85	105.80
1	A	1028	C	C6-N1-C2	-7.35	117.36	120.30
1	A	268	A	O4'-C1'-N9	7.32	114.06	108.20
1	A	1491	A	N1-C6-N6	-7.30	114.22	118.60
1	A	881	U	OP1-P-OP2	7.29	130.54	119.60
1	A	1244	A	N7-C8-N9	7.28	117.44	113.80
1	A	2222	C	C2-N1-C1'	7.28	126.81	118.80
1	A	63	G	O4'-C1'-N9	7.21	113.96	108.20
1	A	2028	C	C6-N1-C2	-7.20	117.42	120.30
1	A	881	U	C2-N1-C1'	7.18	126.31	117.70
1	A	1728	C	N1-C2-O2	7.15	123.19	118.90
1	A	2781	C	C6-N1-C2	-7.12	117.45	120.30
1	A	1564	C	N1-C2-O2	7.11	123.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1045	U	N3-C2-O2	-7.10	117.23	122.20
1	A	2255	C	N3-C2-O2	-7.08	116.95	121.90
1	A	2283	C	N3-C2-O2	-7.06	116.96	121.90
1	A	31	C	C6-N1-C2	-7.04	117.48	120.30
1	A	1518	G	N3-C2-N2	-7.04	114.97	119.90
1	A	1522	U	N3-C2-O2	-7.02	117.29	122.20
1	A	2825	C	N3-C2-O2	-7.02	116.99	121.90
1	A	2384	C	C2-N1-C1'	7.00	126.50	118.80
1	A	1712	G	O4'-C1'-N9	7.00	113.80	108.20
1	A	2825	C	C5-C6-N1	7.00	124.50	121.00
1	A	422	C	N1-C2-O2	6.99	123.09	118.90
1	A	558	G	O4'-C1'-N9	6.98	113.79	108.20
1	A	482	C	C2-N1-C1'	6.97	126.47	118.80
1	A	104	C	C2-N1-C1'	6.96	126.46	118.80
1	A	31	C	C2-N1-C1'	6.94	126.44	118.80
1	A	27	G	N3-C2-N2	-6.94	115.04	119.90
1	A	261	C	N3-C2-O2	-6.93	117.05	121.90
1	A	1572	G	O4'-C1'-N9	6.91	113.73	108.20
1	A	237	U	N3-C2-O2	-6.91	117.37	122.20
1	A	2469	C	N1-C2-O2	6.89	123.03	118.90
1	A	1244	A	C5-N7-C8	-6.88	100.46	103.90
1	A	2022	U	N3-C2-O2	-6.87	117.39	122.20
1	A	1495	C	N1-C2-O2	6.87	123.02	118.90
1	A	439	U	N1-C2-O2	6.86	127.60	122.80
1	A	1280	G	N7-C8-N9	6.86	116.53	113.10
1	A	1652	C	P-O3'-C3'	6.85	127.92	119.70
1	A	706	C	C6-N1-C2	-6.84	117.56	120.30
1	A	2716	U	P-O3'-C3'	6.81	127.87	119.70
1	A	1028	C	C2-N1-C1'	6.77	126.24	118.80
1	A	2283	C	C6-N1-C2	-6.77	117.59	120.30
1	A	1728	C	C6-N1-C2	-6.74	117.61	120.30
1	A	2644	U	N1-C2-O2	6.74	127.52	122.80
1	A	506	U	N1-C2-O2	6.73	127.51	122.80
1	A	649	G	P-O3'-C3'	6.73	127.78	119.70
1	A	1327	U	C2-N1-C1'	6.73	125.77	117.70
1	A	648	G	C4-C5-N7	6.72	113.49	110.80
1	A	1245	G	P-O3'-C3'	6.72	127.76	119.70
1	A	1515	C	N1-C2-O2	6.71	122.93	118.90
1	A	1291	A	C5-N7-C8	-6.70	100.55	103.90
1	A	1728	C	C2-N1-C1'	6.68	126.15	118.80
1	A	683	A	P-O3'-C3'	6.65	127.68	119.70
1	A	2255	C	C6-N1-C2	-6.62	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1036	A	N7-C8-N9	6.62	117.11	113.80
1	A	1629	C	C2-N1-C1'	6.62	126.08	118.80
1	A	439	U	C2-N1-C1'	6.61	125.63	117.70
1	A	716	G	C8-N9-C1'	-6.60	118.42	127.00
1	A	1280	G	C5-N7-C8	-6.60	101.00	104.30
1	A	720	C	C6-N1-C2	-6.59	117.66	120.30
1	A	1291	A	N7-C8-N9	6.59	117.09	113.80
1	A	506	U	N3-C2-O2	-6.58	117.59	122.20
1	A	237	U	C2-N1-C1'	6.58	125.59	117.70
1	A	1455	C	N1-C2-O2	6.55	122.83	118.90
1	A	2101	G	C4-N9-C1'	6.55	135.01	126.50
1	A	785	C	C2-N1-C1'	6.54	126.00	118.80
1	A	104	C	C6-N1-C2	-6.54	117.68	120.30
1	A	1036	A	C5-N7-C8	-6.53	100.64	103.90
1	A	2781	C	C5-C6-N1	6.53	124.26	121.00
1	A	2823	C	N1-C2-O2	6.51	122.81	118.90
1	A	1162	C	N1-C2-O2	6.51	122.81	118.90
1	A	1515	C	C5-C6-N1	6.49	124.24	121.00
1	A	203	U	N1-C2-O2	6.48	127.34	122.80
1	A	31	C	C5-C6-N1	6.47	124.24	121.00
1	A	2469	C	C2-N1-C1'	6.47	125.91	118.80
1	A	62	C	C2-N1-C1'	6.45	125.89	118.80
1	A	439	U	N3-C2-O2	-6.44	117.69	122.20
1	A	2371	C	C6-N1-C2	-6.43	117.73	120.30
1	A	90	A	P-O3'-C3'	6.43	127.41	119.70
1	A	113	U	C2-N1-C1'	6.42	125.41	117.70
1	A	2255	C	C2-N1-C1'	6.40	125.84	118.80
1	A	387	C	C2-N1-C1'	6.38	125.82	118.80
1	A	1771	C	C2-N1-C1'	6.38	125.81	118.80
1	A	1280	G	C4-C5-N7	6.37	113.35	110.80
1	A	857	U	N1-C2-O2	6.37	127.26	122.80
1	A	588	C	C2-N1-C1'	6.36	125.79	118.80
1	A	1351	U	P-O3'-C3'	6.36	127.33	119.70
1	A	1771	C	C6-N1-C2	-6.36	117.76	120.30
1	A	442	C	C2-N1-C1'	6.34	125.77	118.80
1	A	2072	C	C6-N1-C2	-6.34	117.77	120.30
1	A	1491	A	C2-N3-C4	6.31	113.75	110.60
1	A	1498	U	C2-N1-C1'	6.30	125.26	117.70
1	A	104	C	N1-C2-O2	6.29	122.67	118.90
1	A	483	C	N1-C2-O2	6.29	122.67	118.90
1	A	62	C	N1-C2-O2	6.28	122.67	118.90
1	A	483	C	C6-N1-C2	-6.27	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2073	C	C6-N1-C2	-6.26	117.80	120.30
1	A	1495	C	N3-C2-O2	-6.26	117.52	121.90
1	A	482	C	N3-C2-O2	-6.25	117.52	121.90
1	A	2749	U	N3-C2-O2	-6.25	117.83	122.20
1	A	1359	G	C8-N9-C1'	6.24	135.11	127.00
1	A	422	C	C2-N1-C1'	6.24	125.66	118.80
1	A	1564	C	C2-N1-C1'	6.23	125.65	118.80
1	A	2840	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2648	U	C2-N1-C1'	6.22	125.17	117.70
1	A	1203	G	N3-C4-N9	6.22	129.73	126.00
1	A	2781	C	N3-C2-O2	-6.21	117.56	121.90
1	A	1181	C	N3-C2-O2	-6.20	117.56	121.90
1	A	2781	C	C2-N1-C1'	6.19	125.61	118.80
1	A	2816	C	C6-N1-C2	-6.19	117.82	120.30
1	A	1771	C	C5-C6-N1	6.18	124.09	121.00
1	A	203	U	N3-C2-O2	-6.18	117.87	122.20
1	A	2820	U	C2-N1-C1'	6.18	125.11	117.70
1	A	393	U	C2-N1-C1'	6.18	125.11	117.70
1	A	1030	G	N3-C4-C5	-6.17	125.51	128.60
1	A	1728	C	N3-C2-O2	-6.17	117.58	121.90
1	A	734	C	N1-C2-O2	6.16	122.60	118.90
1	A	2313	C	C2-N1-C1'	6.16	125.58	118.80
1	A	632	U	C2-N1-C1'	6.15	125.08	117.70
1	A	63	G	P-O3'-C3'	6.15	127.08	119.70
1	A	1359	G	N3-C4-C5	6.14	131.67	128.60
1	A	537	A	P-O3'-C3'	6.13	127.06	119.70
1	A	1031	C	C2-N1-C1'	6.13	125.54	118.80
1	A	1359	G	N3-C2-N2	-6.13	115.61	119.90
1	A	1796	C	C2-N1-C1'	6.13	125.54	118.80
1	A	415	C	N1-C2-O2	6.12	122.57	118.90
1	A	271	C	C6-N1-C2	-6.12	117.85	120.30
1	A	1353	C	N1-C2-O2	6.11	122.57	118.90
1	A	1515	C	N3-C2-O2	-6.11	117.62	121.90
1	A	648	G	N9-C4-C5	-6.10	102.96	105.40
1	A	2222	C	N1-C2-O2	6.10	122.56	118.90
1	A	237	U	N1-C2-O2	6.10	127.07	122.80
1	A	785	C	N1-C2-O2	6.09	122.56	118.90
1	A	880	C	N3-C2-O2	-6.08	117.64	121.90
1	A	1339	A	P-O3'-C3'	6.08	127.00	119.70
1	A	482	C	N1-C2-O2	6.08	122.55	118.90
1	A	2644	U	N3-C2-O2	-6.07	117.95	122.20
1	A	1352	U	C6-N1-C1'	-6.06	112.72	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	U	C6-N1-C2	-6.05	117.37	121.00
1	A	648	G	O4'-C1'-N9	6.05	113.04	108.20
1	A	1353	C	C6-N1-C1'	-6.05	113.54	120.80
1	A	1696	G	O4'-C1'-N9	6.05	113.04	108.20
1	A	1051	C	C2-N1-C1'	6.05	125.45	118.80
1	A	2454	A	P-O3'-C3'	6.04	126.95	119.70
1	A	204	C	C2-N1-C1'	6.04	125.44	118.80
1	A	1037	C	C5-C6-N1	6.04	124.02	121.00
1	A	764	C	N3-C2-O2	-6.04	117.68	121.90
1	A	1495	C	C2-N1-C1'	6.03	125.43	118.80
1	A	880	C	N1-C2-O2	6.02	122.51	118.90
1	A	667	A	N1-C6-N6	-6.02	114.99	118.60
1	A	1861	C	P-O3'-C3'	6.01	126.92	119.70
1	A	2905	C	C6-N1-C2	-6.01	117.90	120.30
1	A	1455	C	N3-C2-O2	-6.00	117.70	121.90
1	A	1720	C	N1-C2-O2	6.00	122.50	118.90
1	A	1523	U	C6-N1-C2	-6.00	117.40	121.00
1	A	277	C	C2-N1-C1'	5.99	125.39	118.80
1	A	478	U	C6-N1-C1'	-5.99	112.81	121.20
1	A	954	U	N1-C2-O2	5.99	126.99	122.80
1	A	234	C	C2-N1-C1'	5.99	125.38	118.80
1	A	1521	G	N3-C2-N2	-5.97	115.72	119.90
1	A	649	G	C8-N9-C4	-5.96	104.02	106.40
1	A	1670	C	C2-N1-C1'	5.95	125.35	118.80
1	A	1691	A	C2-N3-C4	5.95	113.58	110.60
1	A	720	C	C6-N1-C1'	-5.93	113.68	120.80
1	A	1808	U	C2-N1-C1'	5.93	124.81	117.70
1	A	528	G	O4'-C1'-N9	5.93	112.94	108.20
1	A	1162	C	N3-C2-O2	-5.92	117.76	121.90
1	A	2289	C	C2-N1-C1'	5.91	125.30	118.80
1	A	2816	C	C2-N1-C1'	5.91	125.30	118.80
1	A	1450	C	C2-N1-C1'	5.90	125.29	118.80
1	A	1808	U	N1-C2-O2	5.89	126.92	122.80
1	A	1421	A	O4'-C1'-N9	5.89	112.91	108.20
1	A	1368	U	C6-N1-C1'	-5.89	112.96	121.20
1	A	374	A	C2-N3-C4	-5.88	107.66	110.60
1	A	1568	G	C6-C5-N7	-5.87	126.88	130.40
1	A	2866	C	C2-N1-C1'	5.87	125.25	118.80
1	A	288	C	P-O3'-C3'	5.87	126.74	119.70
1	A	508	C	C2-N1-C1'	5.87	125.25	118.80
1	A	1246	G	C4-C5-N7	5.87	113.15	110.80
1	A	1566	G	N3-C2-N2	-5.86	115.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2676	U	N1-C2-O2	5.86	126.90	122.80
1	A	47	C	C6-N1-C2	-5.85	117.96	120.30
1	A	2313	C	N1-C2-O2	5.85	122.41	118.90
1	A	27	G	N3-C4-N9	-5.84	122.50	126.00
1	A	387	C	C5-C6-N1	5.82	123.91	121.00
1	A	777	C	C6-N1-C2	-5.82	117.97	120.30
1	A	261	C	C6-N1-C2	-5.79	117.98	120.30
1	A	858	U	C2-N1-C1'	5.79	124.65	117.70
1	A	1164	C	C6-N1-C2	-5.79	117.98	120.30
1	A	1437	C	C2-N1-C1'	5.78	125.16	118.80
1	A	2000	A	C2-N3-C4	5.78	113.49	110.60
1	A	2338	A	C2-N3-C4	5.77	113.49	110.60
1	A	62	C	N3-C2-O2	-5.77	117.86	121.90
1	A	1181	C	C2-N1-C1'	5.77	125.14	118.80
1	A	785	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1280	G	C6-C5-N7	-5.76	126.94	130.40
1	A	2099	G	N3-C4-N9	-5.76	122.55	126.00
1	A	718	C	O4'-C1'-N1	5.75	112.80	108.20
1	A	1438	C	C6-N1-C2	-5.74	118.00	120.30
1	A	2898	A	O4'-C1'-N9	5.74	112.79	108.20
1	A	783	C	C2-N1-C1'	5.74	125.11	118.80
1	A	2648	U	N3-C2-O2	-5.74	118.18	122.20
1	A	1011	C	N1-C2-O2	5.73	122.34	118.90
1	A	1564	C	N3-C2-O2	-5.73	117.89	121.90
1	A	648	G	C6-C5-N7	-5.71	126.98	130.40
1	A	2685	U	C5-C6-N1	5.70	125.55	122.70
1	A	2679	C	N1-C2-O2	5.70	122.32	118.90
1	A	2072	C	C2-N1-C1'	5.68	125.05	118.80
1	A	549	A	P-O3'-C3'	5.66	126.50	119.70
1	A	2101	G	N3-C4-N9	5.66	129.40	126.00
1	A	2283	C	C5-C6-N1	5.66	123.83	121.00
1	A	491	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2459	A	C2-N3-C4	5.65	113.42	110.60
1	A	277	C	N3-C2-O2	-5.64	117.95	121.90
1	A	1568	G	N7-C8-N9	5.64	115.92	113.10
1	A	2072	C	C5-C6-N1	5.64	123.82	121.00
1	A	1250	G	C5-N7-C8	-5.64	101.48	104.30
1	A	58	G	P-O3'-C3'	5.63	126.45	119.70
1	A	1244	A	O4'-C1'-N9	5.62	112.70	108.20
1	A	954	U	C2-N1-C1'	5.62	124.44	117.70
1	A	1223	C	C2-N1-C1'	5.62	124.98	118.80
1	A	2676	U	N3-C2-O2	-5.62	118.27	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1045	U	N1-C2-O2	5.61	126.73	122.80
1	A	1203	G	C4-N9-C1'	5.61	133.79	126.50
1	A	60	G	O4'-C1'-N9	5.60	112.68	108.20
1	A	2644	U	C2-N1-C1'	5.60	124.42	117.70
1	A	633	U	N1-C2-O2	5.59	126.72	122.80
1	A	1164	C	C6-N1-C1'	5.59	127.51	120.80
1	A	962	C	N1-C2-O2	5.59	122.25	118.90
1	A	892	U	N3-C2-O2	-5.59	118.29	122.20
1	A	764	C	C2-N1-C1'	5.59	124.95	118.80
1	A	1455	C	C6-N1-C2	-5.58	118.07	120.30
1	A	1651	G	N7-C8-N9	5.57	115.89	113.10
1	A	1600	G	O4'-C1'-N9	5.57	112.66	108.20
1	A	900	U	N1-C2-O2	5.57	126.70	122.80
1	A	586	C	C6-N1-C2	-5.57	118.07	120.30
1	A	2730	U	C5-C6-N1	5.56	125.48	122.70
1	A	1691	A	N3-C4-N9	5.56	131.85	127.40
1	A	1246	G	C5-N7-C8	-5.56	101.52	104.30
1	A	732	A	C5-N7-C8	-5.56	101.12	103.90
1	A	87	U	C5-C6-N1	5.55	125.47	122.70
1	A	880	C	O3'-P-O5'	5.55	114.55	104.00
1	A	1452	C	C2-N1-C1'	5.55	124.90	118.80
1	A	31	C	N1-C2-O2	5.54	122.22	118.90
1	A	113	U	C5-C6-N1	5.54	125.47	122.70
1	A	1246	G	N7-C8-N9	5.53	115.87	113.10
1	A	1682	C	C6-N1-C2	-5.53	118.09	120.30
1	A	648	G	C8-N9-C1'	-5.53	119.81	127.00
1	A	2866	C	C6-N1-C2	-5.52	118.09	120.30
1	A	1600	G	C5-N7-C8	-5.52	101.54	104.30
1	A	261	C	C2-N1-C1'	5.51	124.86	118.80
1	A	2712	C	N1-C2-O2	5.51	122.21	118.90
1	A	1229	U	N1-C2-O2	5.51	126.66	122.80
1	A	393	U	N1-C2-O2	5.50	126.65	122.80
1	A	1498	U	N1-C2-O2	5.50	126.65	122.80
1	A	1564	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1600	G	N7-C8-N9	5.50	115.85	113.10
1	A	1037	C	P-O3'-C3'	5.50	126.30	119.70
1	A	1438	C	P-O3'-C3'	5.50	126.30	119.70
1	A	785	C	N3-C2-O2	-5.50	118.05	121.90
1	A	1501	U	N3-C2-O2	-5.49	118.36	122.20
1	A	1720	C	C2-N1-C1'	5.49	124.84	118.80
1	A	1697	A	N7-C8-N9	5.49	116.54	113.80
1	A	2469	C	N3-C2-O2	-5.49	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1214	U	C2-N1-C1'	5.48	124.28	117.70
1	A	2338	A	C4-N9-C1'	5.48	136.17	126.30
1	A	1670	C	C6-N1-C2	-5.48	118.11	120.30
1	A	880	C	OP2-P-O3'	5.48	117.26	105.20
1	A	387	C	C6-N1-C2	-5.48	118.11	120.30
1	A	25	U	N3-C2-O2	-5.47	118.37	122.20
1	A	383	U	N3-C2-O2	-5.46	118.38	122.20
1	A	1307	U	N3-C2-O2	-5.46	118.38	122.20
1	A	1803	C	N3-C2-O2	-5.46	118.08	121.90
1	A	1784	A	P-O3'-C3'	5.45	126.24	119.70
1	A	393	U	N3-C2-O2	-5.45	118.38	122.20
1	A	2073	C	C5-C6-N1	5.45	123.72	121.00
1	A	1770	C	C5-C6-N1	5.45	123.72	121.00
1	A	1705	C	C6-N1-C2	-5.45	118.12	120.30
1	A	531	C	C5-C6-N1	5.44	123.72	121.00
1	A	1223	C	C6-N1-C2	-5.44	118.12	120.30
1	A	2292	C	C2-N1-C1'	5.44	124.78	118.80
1	A	483	C	C5-C6-N1	5.43	123.72	121.00
1	A	954	U	N3-C2-O2	-5.43	118.40	122.20
1	A	1391	U	N3-C2-O2	-5.43	118.40	122.20
1	A	25	U	N1-C2-O2	5.43	126.60	122.80
1	A	1861	C	C2-N1-C1'	5.43	124.77	118.80
1	A	2255	C	C5-C6-N1	5.43	123.71	121.00
1	A	1203	G	C8-N9-C1'	-5.42	119.95	127.00
1	A	2679	C	C6-N1-C2	-5.42	118.13	120.30
1	A	9	U	C2-N1-C1'	5.42	124.20	117.70
1	A	1246	G	C4-N9-C1'	5.41	133.53	126.50
1	A	1368	U	C6-N1-C2	-5.41	117.76	121.00
1	A	1031	C	N1-C2-O2	5.40	122.14	118.90
1	A	1712	G	C4-C5-N7	5.39	112.96	110.80
1	A	1307	U	C2-N1-C1'	5.39	124.17	117.70
1	A	1755	C	P-O3'-C3'	5.39	126.16	119.70
1	A	2101	G	C8-N9-C1'	-5.38	120.00	127.00
1	A	1307	U	N1-C2-O2	5.38	126.56	122.80
1	A	732	A	C4-N9-C1'	5.37	135.96	126.30
1	A	188	C	C6-N1-C2	-5.36	118.16	120.30
1	A	9	U	N1-C2-O2	5.36	126.55	122.80
1	A	1720	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2115	U	N1-C2-O2	5.35	126.54	122.80
1	A	2222	C	C6-N1-C1'	-5.34	114.39	120.80
1	A	2020	U	N3-C2-O2	-5.34	118.46	122.20
1	A	880	C	P-O3'-C3'	-5.32	113.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2101	G	N3-C4-C5	-5.32	125.94	128.60
1	A	506	U	C2-N1-C1'	5.31	124.07	117.70
1	A	1038	C	C6-N1-C2	-5.31	118.18	120.30
1	A	2685	U	C6-N1-C1'	-5.31	113.77	121.20
1	A	9	U	N3-C2-O2	-5.31	118.48	122.20
1	A	900	U	N3-C2-O2	-5.31	118.48	122.20
1	A	104	C	N3-C2-O2	-5.31	118.19	121.90
1	A	405	U	P-O3'-C3'	5.30	126.06	119.70
1	A	1568	G	C4-N9-C1'	5.30	133.39	126.50
1	A	2644	U	C5-C6-N1	5.30	125.35	122.70
1	A	1518	G	C8-N9-C4	-5.30	104.28	106.40
1	A	1803	C	N1-C2-O2	5.30	122.08	118.90
1	A	720	C	O4'-C1'-N1	5.29	112.44	108.20
1	A	1832	A	C5-N7-C8	-5.29	101.25	103.90
1	A	1485	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	1491	A	C5-C6-N1	5.29	120.34	117.70
1	A	1539	C	N1-C2-O2	5.29	122.07	118.90
1	A	1568	G	O4'-C1'-N9	5.29	112.43	108.20
7	L	105	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	1291	A	C2-N3-C4	-5.28	107.96	110.60
1	A	77	U	N1-C2-O2	5.27	126.49	122.80
1	A	2679	C	C6-N1-C1'	-5.27	114.48	120.80
1	A	648	G	N3-C4-N9	5.26	129.16	126.00
1	A	734	C	N3-C2-O2	-5.26	118.22	121.90
1	A	2351	A	P-O3'-C3'	5.26	126.02	119.70
1	A	2350	G	C4-N9-C1'	5.26	133.34	126.50
1	A	783	C	C6-N1-C2	-5.26	118.20	120.30
1	A	1036	A	C8-N9-C4	-5.26	103.70	105.80
1	A	2679	C	C5-C6-N1	5.25	123.62	121.00
1	A	393	U	C5-C6-N1	5.25	125.32	122.70
1	A	2010	A	C2-N3-C4	5.25	113.22	110.60
1	A	1808	U	N3-C2-O2	-5.24	118.53	122.20
1	A	1223	C	C5-C6-N1	5.23	123.62	121.00
1	A	2730	U	C6-N1-C2	-5.23	117.86	121.00
1	A	2825	C	C6-N1-C1'	-5.23	114.53	120.80
1	A	1630	G	P-O3'-C3'	5.22	125.97	119.70
1	A	422	C	N3-C2-O2	-5.22	118.25	121.90
1	A	1353	C	C6-N1-C2	-5.22	118.21	120.30
1	A	1515	C	O4'-C1'-N1	5.22	112.38	108.20
1	A	2833	U	N3-C2-O2	-5.22	118.55	122.20
1	A	2749	U	N1-C2-O2	5.21	126.45	122.80
1	A	2289	C	N1-C2-O2	5.21	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	U	C2-N1-C1'	5.21	123.95	117.70
1	A	777	C	C2-N1-C1'	5.21	124.53	118.80
1	A	1691	A	C4-N9-C1'	5.21	135.68	126.30
1	A	2289	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1350	U	N3-C2-O2	-5.20	118.56	122.20
1	A	2905	C	C2-N1-C1'	5.20	124.52	118.80
1	A	288	C	N1-C2-O2	5.20	122.02	118.90
1	A	632	U	N1-C2-O2	5.20	126.44	122.80
1	A	2245	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	2392	U	N1-C2-O2	5.20	126.44	122.80
1	A	1359	G	C4-N9-C1'	-5.19	119.75	126.50
1	A	2331	U	N1-C2-O2	5.19	126.44	122.80
1	A	1518	G	N3-C4-N9	-5.18	122.89	126.00
1	A	1770	C	C6-N1-C2	-5.18	118.23	120.30
1	A	2331	U	N3-C2-O2	-5.18	118.57	122.20
1	A	204	C	N1-C2-O2	5.18	122.01	118.90
1	A	1352	U	C5-C6-N1	5.18	125.29	122.70
1	A	1861	C	N1-C2-O2	5.17	122.00	118.90
1	A	857	U	C6-N1-C2	-5.17	117.90	121.00
1	A	1600	G	C4-C5-N7	5.17	112.87	110.80
1	A	1803	C	C6-N1-C2	-5.17	118.23	120.30
1	A	77	U	N3-C2-O2	-5.16	118.59	122.20
1	A	400	U	N3-C2-O2	-5.16	118.59	122.20
1	A	1030	G	C4-N9-C1'	5.16	133.20	126.50
1	A	1832	A	C8-N9-C4	-5.16	103.74	105.80
1	A	2384	C	N1-C2-O2	5.16	121.99	118.90
1	A	104	C	C5-C6-N1	5.15	123.58	121.00
1	A	271	C	P-O3'-C3'	5.15	125.88	119.70
1	A	1498	U	N3-C2-O2	-5.15	118.59	122.20
1	A	2820	U	N1-C2-O2	5.15	126.41	122.80
1	A	1720	C	N3-C2-O2	-5.15	118.30	121.90
1	A	1031	C	C6-N1-C2	-5.14	118.24	120.30
1	A	2289	C	C5-C6-N1	5.14	123.57	121.00
1	A	2712	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1651	G	C5-N7-C8	-5.14	101.73	104.30
1	A	2000	A	N3-C4-N9	5.14	131.51	127.40
1	A	2337	G	N3-C4-C5	-5.13	126.03	128.60
1	A	880	C	OP1-P-O3'	-5.13	93.92	105.20
1	A	685	U	N1-C2-O2	5.12	126.39	122.80
1	A	1489	U	N3-C2-O2	-5.12	118.61	122.20
1	A	1651	G	O4'-C1'-N9	5.12	112.30	108.20
1	A	777	C	C5-C6-N1	5.12	123.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1770	C	C6-N1-C1'	-5.12	114.66	120.80
1	A	1794	C	C6-N1-C2	-5.12	118.25	120.30
1	A	2850	G	C4-N9-C1'	5.11	133.15	126.50
1	A	113	U	N1-C2-O2	5.11	126.38	122.80
1	A	858	U	N1-C2-O2	5.10	126.37	122.80
1	A	2812	A	P-O3'-C3'	5.09	125.81	119.70
1	A	386	U	C5-C6-N1	5.09	125.25	122.70
1	A	179	A	C5-N7-C8	-5.08	101.36	103.90
1	A	229	A	P-O3'-C3'	5.08	125.80	119.70
1	A	1794	C	C2-N1-C1'	5.08	124.39	118.80
1	A	473	C	C2-N1-C1'	5.08	124.38	118.80
1	A	2357	A	N7-C8-N9	5.08	116.34	113.80
1	A	505	G	O4'-C1'-N9	5.07	112.26	108.20
1	A	1229	U	N3-C2-O2	-5.07	118.65	122.20
1	A	1728	C	C5-C6-N1	5.07	123.54	121.00
1	A	204	C	C6-N1-C2	-5.07	118.27	120.30
1	A	2022	U	N1-C2-O2	5.06	126.34	122.80
1	A	2392	U	N3-C2-O2	-5.06	118.66	122.20
1	A	1450	C	C6-N1-C2	-5.06	118.28	120.30
1	A	400	U	N1-C2-O2	5.05	126.34	122.80
1	A	1291	A	C4-C5-N7	5.05	113.23	110.70
1	A	1523	U	C5-C6-N1	5.05	125.23	122.70
1	A	2917	G	C5-N7-C8	-5.05	101.77	104.30
1	A	395	C	C2-N1-C1'	5.05	124.36	118.80
1	A	764	C	C6-N1-C2	-5.05	118.28	120.30
1	A	103	U	N3-C2-O2	-5.05	118.67	122.20
1	A	632	U	N3-C2-O2	-5.05	118.67	122.20
1	A	858	U	C6-N1-C2	-5.05	117.97	121.00
1	A	1244	A	C8-N9-C4	-5.05	103.78	105.80
1	A	1384	C	C6-N1-C2	-5.05	118.28	120.30
1	A	473	C	N1-C2-O2	5.04	121.93	118.90
1	A	1437	C	N1-C2-O2	5.04	121.93	118.90
1	A	2678	U	C2-N1-C1'	5.04	123.75	117.70
1	A	1362	G	P-O3'-C3'	5.04	125.74	119.70
1	A	2732	C	C2-N1-C1'	5.04	124.34	118.80
1	A	482	C	C6-N1-C2	-5.03	118.29	120.30
1	A	387	C	N1-C2-O2	5.03	121.92	118.90
1	A	1359	G	N9-C4-C5	5.02	107.41	105.40
1	A	271	C	C5-C6-N1	5.02	123.51	121.00
1	A	1595	U	P-O3'-C3'	5.02	125.72	119.70
1	A	1001	U	C5-C6-N1	5.01	125.21	122.70
1	A	1712	G	C5-N7-C8	-5.01	101.79	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1568	G	C5-N7-C8	-5.01	101.79	104.30
1	A	1031	C	C5-C6-N1	5.01	123.50	121.00
1	A	1214	U	N1-C2-O2	5.01	126.31	122.80
1	A	2000	A	C4-N9-C1'	5.01	135.31	126.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	154	LEU	Peptide
10	Q	87	GLY	Peptide
11	R	50	ASN	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	A	52303	0	26314	183	0
2	C	2052	0	2138	16	0
3	D	1354	0	1425	14	0
4	E	1561	0	1647	9	0
5	J	1123	0	1162	7	0
6	K	920	0	977	7	0
7	L	973	0	1032	6	0
8	N	953	0	983	7	0
9	P	936	0	1008	7	0
10	Q	940	0	1005	7	0
11	R	780	0	822	2	0
12	S	842	0	899	9	0
13	T	741	0	793	0	0
14	U	754	0	809	6	0
15	V	561	0	567	8	0
16	Z	455	0	491	4	0
17	b	426	0	445	0	0
18	Y	530	0	568	2	0
19	d	367	0	410	0	0
All	All	68571	0	43495	263	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.

All (263) 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)
1:A:2778:A:H62	1:A:2782:A:H61	1.05	1.00
1:A:2771:G:H1	1:A:2791:U:H3	0.94	0.91
1:A:2778:A:H62	1:A:2782:A:N6	1.70	0.90
1:A:912:C:H42	1:A:956:A:H62	1.35	0.74
1:A:2785:U:C4	1:A:2788:G:C6	2.75	0.73
1:A:1496:G:H1	1:A:1507:U:H3	1.38	0.72
1:A:2778:A:N6	1:A:2782:A:H61	1.86	0.69
1:A:1521:G:H22	1:A:1563:G:H1	1.39	0.69
1:A:1244:A:H8	7:L:4:HIS:HB3	1.58	0.68
1:A:1524:A:H61	1:A:1560:U:H3	1.41	0.68
1:A:732:A:H8	1:A:735:U:H3	1.42	0.66
1:A:2685:U:C2	1:A:2694:A:N7	2.63	0.66
1:A:630:A:H62	1:A:1291:A:H2	1.44	0.66
1:A:2126:G:N1	1:A:2222:C:C2	2.64	0.65
1:A:644:G:N2	1:A:650:U:OP1	2.29	0.64
1:A:27:G:N2	1:A:558:G:O2’	2.32	0.63
1:A:792:G:H21	1:A:797:A:H61	1.47	0.63
1:A:2685:U:O2	1:A:2694:A:C5	2.52	0.63
3:D:121:GLY:HA2	3:D:161:PRO:HB3	1.79	0.63
1:A:1516:A:H62	1:A:1568:G:H8	1.47	0.62
1:A:894:A:H62	1:A:979:U:H3	1.46	0.62
5:J:6:MET:SD	5:J:6:MET:N	2.73	0.61
1:A:792:G:HO2’	1:A:795:G:HO2’	1.48	0.60
1:A:1246:G:H1’	1:A:1247:G:H5’	1.84	0.60
1:A:1292:G:H1	10:Q:37:GLN:HE21	1.48	0.60
1:A:912:C:N4	1:A:956:A:H62	1.98	0.60
1:A:1002:G:N2	1:A:1006:A:OP2	2.33	0.60
1:A:1002:G:H21	1:A:1006:A:H2	1.50	0.59
1:A:1359:G:H1	1:A:1370:C:H41	1.51	0.59
1:A:2100:A:H2’	1:A:2101:G:H8	1.68	0.59
7:L:19:VAL:HG23	7:L:27:ASN:HB3	1.84	0.58
1:A:410:G:H21	1:A:412:A:H62	1.50	0.58
3:D:32:PRO:HB3	3:D:98:LYS:HG2	1.85	0.58
1:A:1087:U:H1’	1:A:1161:A:H61	1.67	0.58
14:U:2:HIS:O	14:U:92:ARG:NH1	2.36	0.58
1:A:792:G:H21	1:A:797:A:N6	2.02	0.57
18:Y:42:ARG:NH1	18:Y:45:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:G:O2'	1:A:168:A:N6	2.37	0.57
1:A:2316:A:H8	1:A:2375:A:H62	1.52	0.57
7:L:116:LYS:NZ	7:L:118:GLU:OE2	2.36	0.57
1:A:221:G:H22	1:A:238:U:H4'	1.69	0.57
1:A:2326:C:O2'	1:A:2351:A:N3	2.37	0.57
1:A:913:A:C6	1:A:961:C:C4	2.92	0.57
9:P:94:LYS:HB3	9:P:114:LYS:HG3	1.87	0.57
1:A:925:A:H61	1:A:947:A:H5"	1.70	0.56
1:A:2685:U:O2	1:A:2694:A:N7	2.38	0.56
1:A:1659:A:N6	12:S:88:ARG:O	2.38	0.56
1:A:1482:G:H21	1:A:1562:A:H8	1.54	0.56
1:A:528:G:O2'	1:A:552:G:N2	2.39	0.56
1:A:1497:G:H22	1:A:1505:U:H3	1.54	0.56
1:A:2773:G:OP2	1:A:2784:C:N4	2.39	0.56
1:A:282:G:H22	1:A:290:U:H3	1.53	0.56
4:E:182:ASN:OD1	4:E:182:ASN:N	2.38	0.55
1:A:1820:A:N6	1:A:1857:G:O2'	2.37	0.55
1:A:1310:C:H5"	1:A:1311:G:H5'	1.88	0.55
9:P:30:ARG:NH1	9:P:88:GLU:OE2	2.40	0.55
1:A:1808:U:O4	1:A:1814:A:N6	2.40	0.55
12:S:18:ARG:NH1	12:S:76:VAL:O	2.40	0.55
1:A:923:C:C2	1:A:948:A:N6	2.75	0.55
1:A:1513:U:H3	1:A:1572:G:H1	1.53	0.55
1:A:618:A:N6	1:A:2063:U:OP1	2.38	0.55
14:U:84:LYS:NZ	14:U:86:GLU:OE1	2.39	0.55
6:K:64:ARG:NH1	6:K:101:PRO:O	2.39	0.54
8:N:2:SER:OG	8:N:3:TYR:N	2.40	0.54
6:K:90:ASP:OD1	6:K:113:LYS:NZ	2.40	0.54
1:A:751:G:O2'	1:A:774:A:N6	2.40	0.54
1:A:2332:G:N2	1:A:2334:U:O4	2.40	0.54
6:K:45:GLN:HA	6:K:54:LYS:HE3	1.88	0.54
1:A:268:A:N6	1:A:474:U:O2'	2.40	0.54
1:A:250:G:OP2	1:A:252:C:N4	2.35	0.54
1:A:607:G:H21	10:Q:37:GLN:HE22	1.54	0.53
1:A:2685:U:N3	1:A:2694:A:C8	2.76	0.53
1:A:2365:A:H61	15:V:51:THR:HG21	1.73	0.53
1:A:229:A:O2'	1:A:231:A:N1	2.38	0.53
3:D:55:ASP:OD1	3:D:55:ASP:N	2.42	0.53
1:A:1517:A:H61	1:A:1567:U:H3	1.56	0.53
6:K:42:THR:HG22	6:K:57:VAL:HG22	1.91	0.53
1:A:2684:G:N2	1:A:2685:U:O4	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:A:N6	1:A:2459:A:O2'	2.39	0.52
1:A:2688:G:N2	1:A:2691:A:OP2	2.43	0.52
2:C:118:SER:OG	2:C:119:GLY:N	2.41	0.52
8:N:72:ASN:ND2	8:N:75:ASN:OD1	2.42	0.52
1:A:1497:G:H1	1:A:1505:U:H3	1.57	0.52
1:A:1712:G:O2'	1:A:1714:A:N7	2.43	0.52
1:A:912:C:H42	1:A:956:A:N6	2.07	0.52
14:U:39:ASN:HD22	14:U:63:ILE:HG22	1.75	0.52
1:A:604:C:O2'	10:Q:48:ARG:NH1	2.43	0.52
1:A:161:A:OP2	1:A:166:A:N6	2.41	0.51
1:A:1743:A:H4'	1:A:1744:G:H5'	1.91	0.51
12:S:25:ARG:NH1	12:S:74:ALA:O	2.41	0.51
1:A:1735:A:H62	1:A:1742:G:H21	1.58	0.51
2:C:145:GLU:HB2	2:C:188:CYS:HB3	1.92	0.51
1:A:1067:A:H62	1:A:1187:U:H3	1.59	0.51
1:A:2126:G:C2	1:A:2222:C:N3	2.79	0.51
2:C:230:HIS:HD2	2:C:232:HIS:HB2	1.76	0.51
6:K:8:LEU:HD22	6:K:84:CYS:HB3	1.93	0.51
16:Z:18:ASP:N	16:Z:18:ASP:OD1	2.44	0.51
16:Z:39:ASP:OD2	16:Z:44:ARG:NH2	2.43	0.51
1:A:337:A:O2'	1:A:338:G:O4'	2.29	0.51
1:A:1038:C:OP1	11:R:84:LYS:NZ	2.43	0.50
1:A:1727:A:OP2	1:A:1744:G:N2	2.43	0.50
3:D:20:GLY:HA3	9:P:83:LYS:HE2	1.92	0.50
1:A:2111:A:H3'	1:A:2112:G:H8	1.75	0.50
9:P:55:GLY:HA2	9:P:60:GLU:HG2	1.93	0.50
2:C:132:LEU:HD23	2:C:135:ILE:HD12	1.93	0.50
1:A:792:G:N2	1:A:797:A:H61	2.09	0.50
1:A:1828:G:OP1	2:C:260:ARG:NE	2.45	0.49
1:A:2252:A:O2'	2:C:265:LYS:NZ	2.45	0.49
1:A:1491:A:H62	1:A:1512:G:H1	1.60	0.49
1:A:1696:G:OP1	8:N:35:THR:OG1	2.29	0.49
1:A:2660:G:H4'	1:A:2916:A:H5'	1.94	0.49
1:A:805:G:H21	1:A:2010:A:H62	1.58	0.49
1:A:2320:U:H3	1:A:2370:G:H1	1.60	0.49
11:R:77:LYS:HB2	11:R:82:VAL:HB	1.93	0.49
1:A:2321:U:H5'	1:A:2407:A:H61	1.76	0.49
1:A:861:C:O2'	1:A:1264:G:N2	2.45	0.49
16:Z:12:VAL:O	16:Z:20:ARG:NH1	2.45	0.49
1:A:2287:C:O2'	1:A:2456:C:OP2	2.31	0.49
4:E:155:VAL:HB	4:E:194:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:44:THR:HG22	10:Q:100:VAL:HG13	1.95	0.49
1:A:576:G:O2'	1:A:578:A:N7	2.46	0.48
1:A:765:A:H5"	1:A:766:C:H5	1.79	0.48
16:Z:24:ARG:O	16:Z:24:ARG:NH1	2.40	0.48
1:A:351:G:H21	1:A:374:A:H62	1.62	0.48
3:D:208:SER:O	3:D:208:SER:OG	2.26	0.48
8:N:24:LEU:HD23	8:N:44:VAL:HG21	1.96	0.48
1:A:304:G:N2	1:A:415:C:N3	2.62	0.48
1:A:324:A:H3'	1:A:325:A:H8	1.78	0.48
1:A:461:C:H2'	1:A:462:A:H8	1.78	0.48
1:A:924:U:H5"	1:A:946:G:H1	1.79	0.48
1:A:1462:G:HO2'	1:A:1633:G:HO2'	1.61	0.48
5:J:78:HIS:ND1	5:J:79:THR:O	2.40	0.48
1:A:259:A:H2'	1:A:260:A:H8	1.78	0.47
1:A:2771:G:O6	1:A:2791:U:O4	2.32	0.47
1:A:150:A:H61	1:A:179:A:H2	1.62	0.47
1:A:1171:G:O6	1:A:1172:A:N6	2.47	0.47
1:A:2456:C:H5"	1:A:2458:G:H5'	1.95	0.47
1:A:2434:G:N2	1:A:2442:G:O6	2.47	0.47
1:A:2785:U:O4	1:A:2788:G:C6	2.67	0.47
3:D:58:GLU:OE1	3:D:66:LYS:NZ	2.48	0.47
1:A:1491:A:H62	1:A:1512:G:H22	1.61	0.47
1:A:2415:U:O2'	15:V:49:ARG:NH1	2.47	0.47
5:J:5:PRO:HG3	10:Q:61:TRP:HE1	1.80	0.47
1:A:2039:G:H5"	12:S:42:ALA:HB2	1.97	0.47
1:A:2233:C:OP2	2:C:147:LYS:NZ	2.46	0.47
1:A:106:G:H4'	1:A:337:A:H5"	1.96	0.47
1:A:411:G:O2'	1:A:413:U:O4	2.33	0.47
1:A:617:G:O2'	1:A:619:A:OP1	2.33	0.47
1:A:1347:A:H62	1:A:1651:G:H8	1.62	0.47
1:A:1359:G:H22	1:A:1370:C:N4	2.13	0.47
1:A:1726:G:N2	1:A:1792:G:OP2	2.42	0.47
1:A:2098:G:N2	1:A:2472:C:O2	2.47	0.47
1:A:2428:G:H2'	1:A:2429:G:H8	1.79	0.47
7:L:29:LYS:HE3	7:L:30:THR:HG23	1.97	0.47
1:A:923:C:N3	1:A:948:A:N1	2.63	0.46
1:A:2785:U:C4	1:A:2788:G:O6	2.68	0.46
1:A:199:A:H62	1:A:878:G:H21	1.62	0.46
1:A:2041:G:OP1	12:S:11:ARG:NH2	2.47	0.46
4:E:54:ARG:HD2	4:E:81:PRO:HD3	1.97	0.46
1:A:2318:G:H1	1:A:2372:U:H3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:U:OP2	2:C:274:ARG:NH1	2.48	0.46
8:N:41:ARG:HE	8:N:41:ARG:HB3	1.54	0.46
1:A:2126:G:C2	1:A:2222:C:C2	3.04	0.46
1:A:2357:A:H2'	1:A:2358:A:C8	2.52	0.45
1:A:313:U:H5'	1:A:314:A:H5'	1.99	0.45
1:A:2859:G:OP1	3:D:57:ARG:NH1	2.49	0.45
1:A:420:U:O2'	1:A:470:A:N3	2.49	0.45
1:A:793:U:H1'	1:A:795:G:H21	1.81	0.45
2:C:248:SER:HB3	2:C:252:LYS:H	1.81	0.45
3:D:31:ALA:HB3	3:D:53:PHE:HE1	1.82	0.45
1:A:906:G:O2'	1:A:963:G:O6	2.26	0.45
1:A:423:G:H2'	1:A:424:G:H8	1.81	0.45
1:A:1518:G:H1	1:A:1566:G:H1	1.64	0.45
1:A:259:A:H2'	1:A:260:A:C8	2.52	0.45
1:A:678:A:H2'	1:A:679:A:C8	2.51	0.45
1:A:875:U:H4'	1:A:878:G:C6	2.52	0.44
2:C:141:VAL:HG23	2:C:192:ILE:HD13	2.00	0.44
4:E:66:ARG:HA	4:E:66:ARG:HD2	1.83	0.44
9:P:6:LYS:HA	9:P:9:GLU:HG2	1.98	0.44
1:A:2126:G:C6	1:A:2222:C:O2	2.70	0.44
1:A:630:A:H5'	4:E:89:VAL:HG21	1.99	0.44
4:E:6:LEU:HD12	4:E:17:ILE:HB	1.97	0.44
1:A:913:A:C5	1:A:961:C:N3	2.86	0.44
1:A:2357:A:H2'	1:A:2358:A:H8	1.81	0.44
1:A:2126:G:N2	1:A:2222:C:C4	2.86	0.44
9:P:51:ILE:HG22	9:P:63:THR:HB	1.99	0.44
1:A:1221:A:H2'	1:A:1222:A:C8	2.53	0.44
1:A:1515:C:H2'	1:A:1516:A:C8	2.52	0.44
1:A:2922:U:O2'	5:J:135:ALA:O	2.35	0.44
12:S:88:ARG:HB2	12:S:92:ARG:HB2	2.00	0.44
1:A:902:G:O2'	15:V:35:ASP:OD1	2.33	0.44
1:A:2385:C:H4'	15:V:28:ARG:HD3	1.99	0.44
1:A:1002:G:H2'	1:A:1003:A:H2'	1.99	0.44
2:C:131:PRO:HA	2:C:189:ARG:HA	2.00	0.43
3:D:126:HIS:CG	3:D:159:LEU:HB3	2.53	0.43
1:A:615:U:O2'	1:A:617:G:OP2	2.25	0.43
1:A:1322:G:H1'	1:A:1368:U:H5	1.83	0.43
3:D:183:ARG:HD2	9:P:11:ILE:HD11	2.01	0.43
3:D:3:LYS:NZ	3:D:101:ILE:O	2.41	0.43
4:E:70:THR:OG1	4:E:72:ARG:NH1	2.52	0.43
1:A:293:U:H2'	1:A:294:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1520:A:H61	1:A:1564:C:H42	1.65	0.43
1:A:2348:C:H4'	1:A:2349:A:C4	2.53	0.43
12:S:65:ASP:OD2	12:S:65:ASP:N	2.52	0.43
1:A:2312:C:OP2	1:A:2418:G:O2'	2.36	0.43
2:C:178:SER:O	2:C:178:SER:OG	2.31	0.43
1:A:2415:U:H4'	15:V:64:ASP:HA	2.00	0.43
1:A:831:U:O4	1:A:839:G:N2	2.52	0.43
1:A:2825:C:H3'	1:A:2826:A:H8	1.84	0.43
5:J:86:LYS:HB2	5:J:86:LYS:HE2	1.81	0.43
1:A:1518:G:N2	1:A:1566:G:H22	2.17	0.43
2:C:142:HIS:ND1	2:C:193:GLY:O	2.47	0.43
12:S:86:ARG:HA	12:S:87:PRO:HD3	1.91	0.43
1:A:89:U:H5"	1:A:90:A:H3'	2.01	0.43
1:A:761:U:N3	1:A:764:C:OP2	2.52	0.42
4:E:158:ASP:N	4:E:158:ASP:OD1	2.52	0.42
1:A:2874:G:O2'	1:A:2891:G:N2	2.53	0.42
2:C:146:LEU:HD23	2:C:146:LEU:HA	1.92	0.42
12:S:73:GLN:HB2	12:S:106:VAL:HB	2.01	0.42
1:A:1317:G:H4'	8:N:30:ILE:HD11	2.00	0.42
7:L:71:ARG:NH1	7:L:72:LYS:O	2.53	0.42
3:D:39:LYS:O	3:D:47:GLU:HA	2.19	0.42
5:J:68:LYS:HD3	5:J:68:LYS:HA	1.85	0.42
14:U:8:LYS:HG3	14:U:71:LEU:HD12	2.01	0.42
1:A:1813:A:H1'	1:A:1814:A:C8	2.55	0.42
1:A:2361:C:OP1	15:V:84:ARG:NH2	2.39	0.42
1:A:1444:C:H2'	1:A:1445:A:C8	2.55	0.41
1:A:2371:C:O2'	1:A:2403:C:OP1	2.36	0.41
4:E:128:ASP:OD2	4:E:128:ASP:N	2.53	0.41
1:A:448:A:H2'	1:A:449:A:C8	2.55	0.41
1:A:1826:C:O2'	2:C:259:THR:OG1	2.38	0.41
6:K:92:SER:HA	6:K:113:LYS:HD2	2.01	0.41
18:Y:4:ASN:HB2	18:Y:7:ARG:HH21	1.84	0.41
1:A:747:G:O2'	1:A:1677:A:N3	2.46	0.41
1:A:1518:G:H22	1:A:1566:G:H1	1.68	0.41
1:A:2356:A:N7	1:A:2417:A:N6	2.68	0.41
3:D:26:THR:OG1	3:D:190:GLY:O	2.31	0.41
1:A:675:C:O2	1:A:685:U:O2'	2.39	0.41
1:A:919:U:N3	1:A:920:G:N7	2.68	0.41
1:A:2293:C:N4	15:V:23:ASP:OD2	2.52	0.41
1:A:1491:A:N6	1:A:1512:G:H1	2.18	0.41
8:N:45:GLU:OE2	8:N:99:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:48:THR:H	14:U:52:PRO:HG2	1.86	0.41
1:A:923:C:N3	1:A:948:A:C6	2.89	0.41
14:U:75:THR:OG1	14:U:76:GLY:N	2.53	0.41
1:A:768:G:H2'	1:A:769:A:H8	1.85	0.41
1:A:972:U:H1'	1:A:973:G:C8	2.56	0.41
1:A:1521:G:H22	1:A:1563:G:H22	1.67	0.41
1:A:2086:G:H2'	1:A:2087:A:C8	2.55	0.41
1:A:2665:U:HO2'	3:D:46:TYR:HH	1.68	0.41
15:V:27:LYS:HA	15:V:27:LYS:HD3	1.92	0.41
1:A:1546:G:N2	2:C:98:ASP:O	2.49	0.40
1:A:2681:U:H3	1:A:2697:G:H1	1.68	0.40
10:Q:81:HIS:HD2	10:Q:85:LEU:HD12	1.87	0.40
1:A:352:G:H2'	1:A:353:A:C8	2.56	0.40
1:A:2094:C:H42	1:A:2474:G:H1	1.68	0.40
1:A:1491:A:H62	1:A:1512:G:N2	2.20	0.40
6:K:107:ARG:HB3	6:K:115:VAL:HG11	2.02	0.40
7:L:91:VAL:HB	7:L:123:VAL:HA	2.03	0.40
1:A:580:U:H2'	1:A:581:C:C6	2.56	0.40
10:Q:98:LEU:HD23	10:Q:98:LEU:HA	1.93	0.40
1:A:852:G:H22	1:A:2473:G:H2'	1.84	0.40
1:A:1497:G:O2'	1:A:1504:A:N1	2.42	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	
2	C	263/277 (95%)	243 (92%)	20 (8%)	0	100	100
3	D	175/209 (84%)	166 (95%)	9 (5%)	0	100	100
4	E	203/207 (98%)	184 (91%)	19 (9%)	0	100	100
5	J	140/145 (97%)	135 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	120/122 (98%)	102 (85%)	18 (15%)	0	100	100
7	L	126/146 (86%)	116 (92%)	10 (8%)	0	100	100
8	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
9	P	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
10	Q	115/119 (97%)	104 (90%)	9 (8%)	2 (2%)	9	39
11	R	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
12	S	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
13	T	90/95 (95%)	80 (89%)	10 (11%)	0	100	100
14	U	98/103 (95%)	83 (85%)	15 (15%)	0	100	100
15	V	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
16	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
17	b	52/59 (88%)	49 (94%)	3 (6%)	0	100	100
18	Y	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
19	d	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
All	All	2048/2195 (93%)	1886 (92%)	160 (8%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Q	88	ILE
10	Q	73	GLY

5.3.2   Protein sidechains   ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	218/225 (97%)	217 (100%)	1 (0%)	88	96
3	D	144/170 (85%)	144 (100%)	0	100	100
4	E	169/170 (99%)	168 (99%)	1 (1%)	86	95
5	J	120/123 (98%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	101/101 (100%)	101 (100%)	0	100	100
7	L	101/110 (92%)	101 (100%)	0	100	100
8	N	99/100 (99%)	99 (100%)	0	100	100
9	P	99/100 (99%)	98 (99%)	1 (1%)	76	91
10	Q	96/98 (98%)	95 (99%)	1 (1%)	76	91
11	R	82/83 (99%)	82 (100%)	0	100	100
12	S	90/93 (97%)	90 (100%)	0	100	100
13	T	83/85 (98%)	83 (100%)	0	100	100
14	U	84/87 (97%)	84 (100%)	0	100	100
15	V	56/74 (76%)	55 (98%)	1 (2%)	59	85
16	Z	52/53 (98%)	51 (98%)	1 (2%)	57	84
17	b	48/53 (91%)	47 (98%)	1 (2%)	53	82
18	Y	56/57 (98%)	56 (100%)	0	100	100
19	d	39/39 (100%)	39 (100%)	0	100	100
All	All	1737/1821 (95%)	1730 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	103	TYR
4	E	72	ARG
9	P	117	ARG
10	Q	92	ARG
15	V	22	ARG
16	Z	54	VAL
17	b	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	230	HIS
2	C	232	HIS
3	D	33	ASN
4	E	49	HIS
4	E	75	GLN
4	E	121	ASN

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Mol	Chain	Res	Type
5	J	131	HIS
7	L	38	GLN
7	L	78	ASN
10	Q	37	GLN
10	Q	72	ASN
10	Q	81	HIS
10	Q	107	ASN
11	R	81	ASN
11	R	86	GLN
14	U	39	ASN
14	U	64	HIS
15	V	37	GLN
15	V	58	ASN
17	b	40	HIS
18	Y	31	GLN
19	d	9	ASN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2428/2928 (82%)	640 (26%)	38 (1%)

All (640) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	28	A
1	A	31	C
1	A	34	U
1	A	38	A
1	A	43	G
1	A	44	A
1	A	45	G
1	A	46	C
1	A	47	C
1	A	51	G
1	A	59	G
1	A	60	G
1	A	64	A
1	A	71	A

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Mol	Chain	Res	Type
1	A	75	G
1	A	76	C
1	A	77	U
1	A	87	U
1	A	90	A
1	A	91	A
1	A	92	G
1	A	101	G
1	A	109	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	145	G
1	A	159	U
1	A	163	U
1	A	164	U
1	A	175	G
1	A	176	A
1	A	177	G
1	A	184	G
1	A	199	A
1	A	202	A
1	A	203	U
1	A	207	A
1	A	216	A
1	A	219	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	229	A
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	235	G
1	A	236	A
1	A	245	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	258	A
1	A	268	A

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Mol	Chain	Res	Type
1	A	269	G
1	A	270	C
1	A	272	C
1	A	275	A
1	A	277	C
1	A	282	G
1	A	283	G
1	A	284	C
1	A	286	U
1	A	288	C
1	A	289	C
1	A	290	U
1	A	291	C
1	A	298	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	309	U
1	A	310	C
1	A	312	G
1	A	314	A
1	A	315	C
1	A	316	G
1	A	321	U
1	A	322	A
1	A	324	A
1	A	326	A
1	A	327	G
1	A	334	G
1	A	338	G
1	A	344	G
1	A	345	A
1	A	346	G
1	A	348	U
1	A	355	A
1	A	360	C
1	A	361	G
1	A	366	A
1	A	367	G
1	A	374	A
1	A	376	A

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Mol	Chain	Res	Type
1	A	378	C
1	A	382	G
1	A	386	U
1	A	387	C
1	A	389	A
1	A	390	A
1	A	393	U
1	A	396	G
1	A	402	U
1	A	405	U
1	A	406	G
1	A	407	A
1	A	412	A
1	A	418	A
1	A	419	G
1	A	421	A
1	A	430	C
1	A	433	G
1	A	434	U
1	A	436	A
1	A	437	A
1	A	438	A
1	A	439	U
1	A	443	G
1	A	444	U
1	A	446	G
1	A	451	C
1	A	452	C
1	A	453	G
1	A	459	A
1	A	462	A
1	A	463	U
1	A	466	C
1	A	474	U
1	A	478	U
1	A	490	A
1	A	504	A
1	A	514	G
1	A	525	A
1	A	526	A
1	A	528	G
1	A	537	A

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Mol	Chain	Res	Type
1	A	538	A
1	A	548	A
1	A	550	G
1	A	551	A
1	A	554	U
1	A	568	G
1	A	576	G
1	A	577	U
1	A	578	A
1	A	584	A
1	A	592	A
1	A	595	G
1	A	607	G
1	A	613	U
1	A	618	A
1	A	619	A
1	A	631	G
1	A	632	U
1	A	647	A
1	A	648	G
1	A	649	G
1	A	650	U
1	A	651	U
1	A	659	A
1	A	665	G
1	A	666	G
1	A	667	A
1	A	668	G
1	A	673	A
1	A	680	G
1	A	683	A
1	A	684	G
1	A	690	A
1	A	691	U
1	A	692	A
1	A	698	C
1	A	700	U
1	A	702	A
1	A	713	G
1	A	715	A
1	A	716	G
1	A	717	A

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Mol	Chain	Res	Type
1	A	719	C
1	A	723	A
1	A	733	U
1	A	751	G
1	A	764	C
1	A	765	A
1	A	766	C
1	A	768	G
1	A	777	C
1	A	783	C
1	A	788	G
1	A	793	U
1	A	794	U
1	A	795	G
1	A	799	A
1	A	811	A
1	A	818	G
1	A	822	G
1	A	823	G
1	A	829	A
1	A	831	U
1	A	836	A
1	A	837	U
1	A	838	C
1	A	839	G
1	A	842	C
1	A	852	G
1	A	856	G
1	A	859	C
1	A	866	A
1	A	875	U
1	A	877	G
1	A	881	U
1	A	892	U
1	A	895	G
1	A	906	G
1	A	912	C
1	A	917	A
1	A	918	U
1	A	919	U
1	A	920	G
1	A	922	A

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Mol	Chain	Res	Type
1	A	947	A
1	A	948	A
1	A	949	U
1	A	952	A
1	A	953	G
1	A	954	U
1	A	955	C
1	A	956	A
1	A	957	A
1	A	958	A
1	A	959	C
1	A	961	C
1	A	962	C
1	A	964	A
1	A	970	A
1	A	972	U
1	A	973	G
1	A	975	C
1	A	987	A
1	A	988	G
1	A	991	A
1	A	992	G
1	A	999	A
1	A	1000	G
1	A	1001	U
1	A	1004	U
1	A	1007	G
1	A	1020	A
1	A	1027	A
1	A	1035	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1042	A
1	A	1055	A
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1068	G
1	A	1072	A
1	A	1074	A
1	A	1075	A

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Mol	Chain	Res	Type
1	A	1080	G
1	A	1083	G
1	A	1084	A
1	A	1087	U
1	A	1163	U
1	A	1173	A
1	A	1174	A
1	A	1178	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1185	G
1	A	1188	A
1	A	1189	A
1	A	1194	A
1	A	1201	A
1	A	1202	A
1	A	1215	U
1	A	1217	U
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1222	A
1	A	1223	C
1	A	1246	G
1	A	1247	G
1	A	1248	C
1	A	1252	G
1	A	1269	A
1	A	1278	G
1	A	1279	C
1	A	1280	G
1	A	1286	A
1	A	1289	U
1	A	1290	G
1	A	1293	A
1	A	1295	U
1	A	1296	G
1	A	1297	C
1	A	1302	A
1	A	1305	A
1	A	1311	G

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Mol	Chain	Res	Type
1	A	1312	A
1	A	1315	G
1	A	1339	A
1	A	1340	A
1	A	1344	C
1	A	1345	U
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1359	G
1	A	1360	A
1	A	1363	G
1	A	1364	C
1	A	1366	C
1	A	1375	A
1	A	1376	G
1	A	1377	G
1	A	1380	U
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1391	U
1	A	1404	A
1	A	1409	C
1	A	1414	G
1	A	1418	U
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1427	G
1	A	1434	A
1	A	1435	U
1	A	1439	U
1	A	1441	U
1	A	1442	A
1	A	1449	C
1	A	1450	C
1	A	1456	A
1	A	1458	U
1	A	1459	U
1	A	1465	A
1	A	1466	U

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Mol	Chain	Res	Type
1	A	1472	G
1	A	1473	A
1	A	1474	C
1	A	1475	G
1	A	1495	C
1	A	1496	G
1	A	1498	U
1	A	1499	A
1	A	1501	U
1	A	1503	G
1	A	1507	U
1	A	1515	C
1	A	1516	A
1	A	1519	C
1	A	1524	A
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1539	C
1	A	1551	C
1	A	1553	A
1	A	1554	U
1	A	1555	A
1	A	1556	A
1	A	1561	G
1	A	1563	G
1	A	1564	C
1	A	1571	G
1	A	1572	G
1	A	1573	C
1	A	1576	G
1	A	1581	A
1	A	1582	U
1	A	1584	U
1	A	1585	A
1	A	1586	G
1	A	1587	U
1	A	1596	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1615	A

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Mol	Chain	Res	Type
1	A	1617	A
1	A	1626	U
1	A	1631	A
1	A	1632	G
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1661	A
1	A	1679	A
1	A	1685	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1695	A
1	A	1697	A
1	A	1698	G
1	A	1712	G
1	A	1719	G
1	A	1720	C
1	A	1721	A
1	A	1723	A
1	A	1739	C
1	A	1740	G
1	A	1744	G
1	A	1745	A
1	A	1752	G
1	A	1756	U
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1767	A
1	A	1771	C
1	A	1774	A
1	A	1777	G
1	A	1779	G
1	A	1780	C
1	A	1781	C
1	A	1782	G
1	A	1783	C
1	A	1785	G
1	A	1790	U
1	A	1793	G

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Mol	Chain	Res	Type
1	A	1802	A
1	A	1803	C
1	A	1805	G
1	A	1809	A
1	A	1810	G
1	A	1811	C
1	A	1812	A
1	A	1813	A
1	A	1814	A
1	A	1815	A
1	A	1829	C
1	A	1830	G
1	A	1832	A
1	A	1839	A
1	A	1841	G
1	A	1845	A
1	A	1858	A
1	A	1862	C
1	A	2001	G
1	A	2004	G
1	A	2005	C
1	A	2006	A
1	A	2010	A
1	A	2011	U
1	A	2020	U
1	A	2022	U
1	A	2026	A
1	A	2052	A
1	A	2060	A
1	A	2062	A
1	A	2068	G
1	A	2072	C
1	A	2081	G
1	A	2082	G
1	A	2084	C
1	A	2088	A
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2092	C
1	A	2097	U
1	A	2098	G

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Mol	Chain	Res	Type
1	A	2102	C
1	A	2106	A
1	A	2110	C
1	A	2111	A
1	A	2116	G
1	A	2121	U
1	A	2122	G
1	A	2125	U
1	A	2126	G
1	A	2127	U
1	A	2222	C
1	A	2223	U
1	A	2227	A
1	A	2231	C
1	A	2232	G
1	A	2233	C
1	A	2239	U
1	A	2240	U
1	A	2241	A
1	A	2243	C
1	A	2246	G
1	A	2254	A
1	A	2255	C
1	A	2267	G
1	A	2268	G
1	A	2272	U
1	A	2275	G
1	A	2279	G
1	A	2283	C
1	A	2288	G
1	A	2289	C
1	A	2290	C
1	A	2291	U
1	A	2295	A
1	A	2306	G
1	A	2308	G
1	A	2309	G
1	A	2311	G
1	A	2312	C
1	A	2315	A
1	A	2317	A
1	A	2321	U

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Mol	Chain	Res	Type
1	A	2322	C
1	A	2323	C
1	A	2324	C
1	A	2326	C
1	A	2327	A
1	A	2328	G
1	A	2329	A
1	A	2330	A
1	A	2331	U
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2337	G
1	A	2338	A
1	A	2339	A
1	A	2340	A
1	A	2341	U
1	A	2342	C
1	A	2343	A
1	A	2344	U
1	A	2345	U
1	A	2348	C
1	A	2349	A
1	A	2351	A
1	A	2352	G
1	A	2353	U
1	A	2354	G
1	A	2356	A
1	A	2357	A
1	A	2362	A
1	A	2363	C
1	A	2364	A
1	A	2365	A
1	A	2370	G
1	A	2376	C
1	A	2377	U
1	A	2379	C
1	A	2392	U
1	A	2395	A
1	A	2405	A
1	A	2408	G

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Mol	Chain	Res	Type
1	A	2411	G
1	A	2412	G
1	A	2414	C
1	A	2418	G
1	A	2430	U
1	A	2431	U
1	A	2435	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2456	C
1	A	2458	G
1	A	2459	A
1	A	2468	A
1	A	2469	C
1	A	2473	G
1	A	2474	G
1	A	2648	U
1	A	2654	G
1	A	2658	A
1	A	2659	G
1	A	2660	G
1	A	2661	A
1	A	2668	A
1	A	2675	C
1	A	2679	C
1	A	2683	A
1	A	2688	G
1	A	2689	A
1	A	2690	G
1	A	2692	G
1	A	2697	G
1	A	2702	G
1	A	2711	G
1	A	2714	G
1	A	2717	G
1	A	2718	U
1	A	2720	C
1	A	2731	G
1	A	2743	G
1	A	2755	U

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Mol	Chain	Res	Type
1	A	2762	A
1	A	2765	G
1	A	2767	A
1	A	2773	G
1	A	2775	U
1	A	2776	G
1	A	2777	A
1	A	2779	A
1	A	2784	C
1	A	2785	U
1	A	2787	A
1	A	2788	G
1	A	2789	C
1	A	2795	G
1	A	2807	A
1	A	2808	U
1	A	2813	U
1	A	2818	C
1	A	2819	A
1	A	2820	U
1	A	2825	C
1	A	2826	A
1	A	2827	A
1	A	2828	G
1	A	2833	U
1	A	2837	A
1	A	2843	G
1	A	2845	A
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2892	G
1	A	2897	G
1	A	2908	A
1	A	2918	G
1	A	2925	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	43	G
1	A	58	G

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Mol	Chain	Res	Type
1	A	63	G
1	A	90	A
1	A	229	A
1	A	267	C
1	A	271	C
1	A	288	C
1	A	377	G
1	A	405	U
1	A	537	A
1	A	549	A
1	A	649	G
1	A	683	A
1	A	837	U
1	A	851	A
1	A	1037	C
1	A	1245	G
1	A	1339	A
1	A	1351	U
1	A	1362	G
1	A	1438	C
1	A	1455	C
1	A	1518	G
1	A	1595	U
1	A	1630	G
1	A	1652	C
1	A	1755	C
1	A	1779	G
1	A	1784	A
1	A	1861	C
1	A	2334	U
1	A	2351	A
1	A	2361	C
1	A	2454	A
1	A	2716	U
1	A	2784	C
1	A	2812	A

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

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 ⓘ

This section contains visualisations of the EMDB entry EMD-24950. 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 |
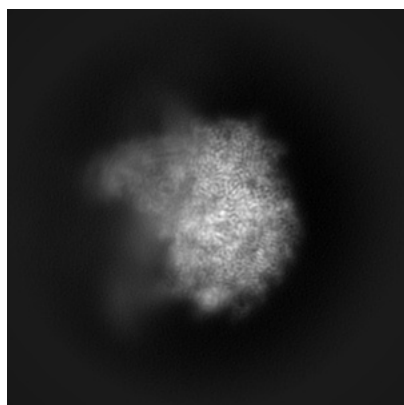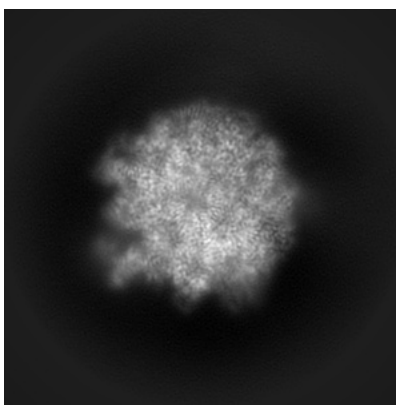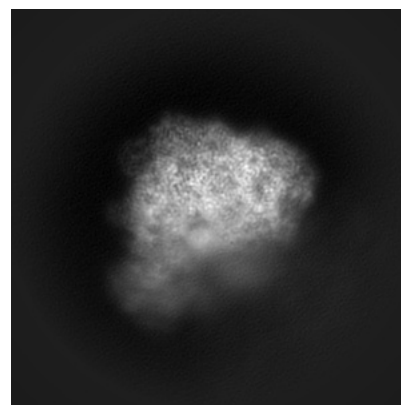
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
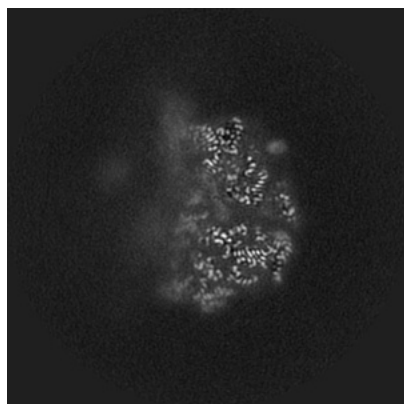
6.2.1 Primary map
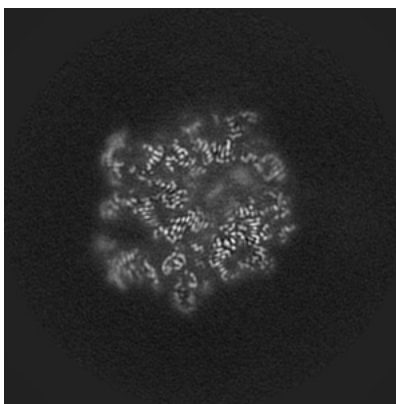
| X Index: 212 | Y Index: 212 | Z Index: 212 |
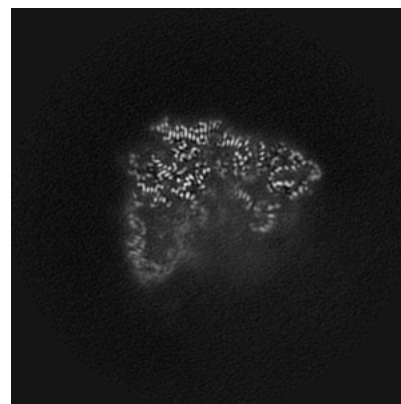
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
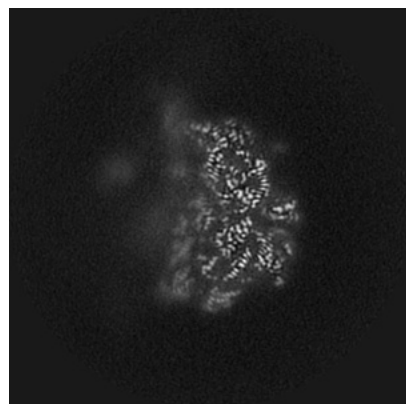
6.3.1 Primary map
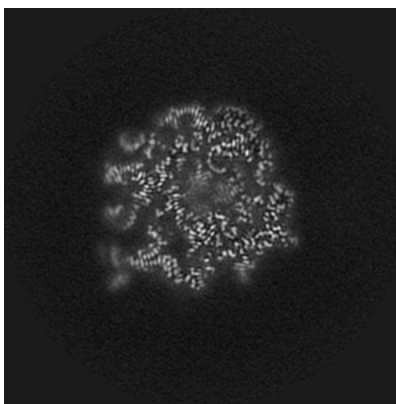
| X Index: 206 | Y Index: 227 | Z Index: 217 |
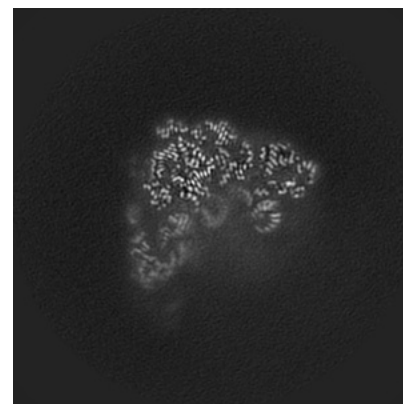
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ
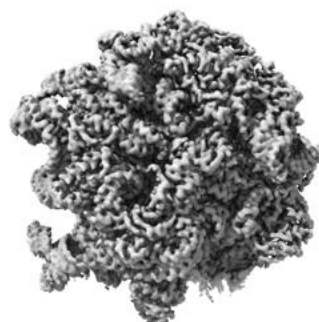
6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0131. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 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 ⓘ
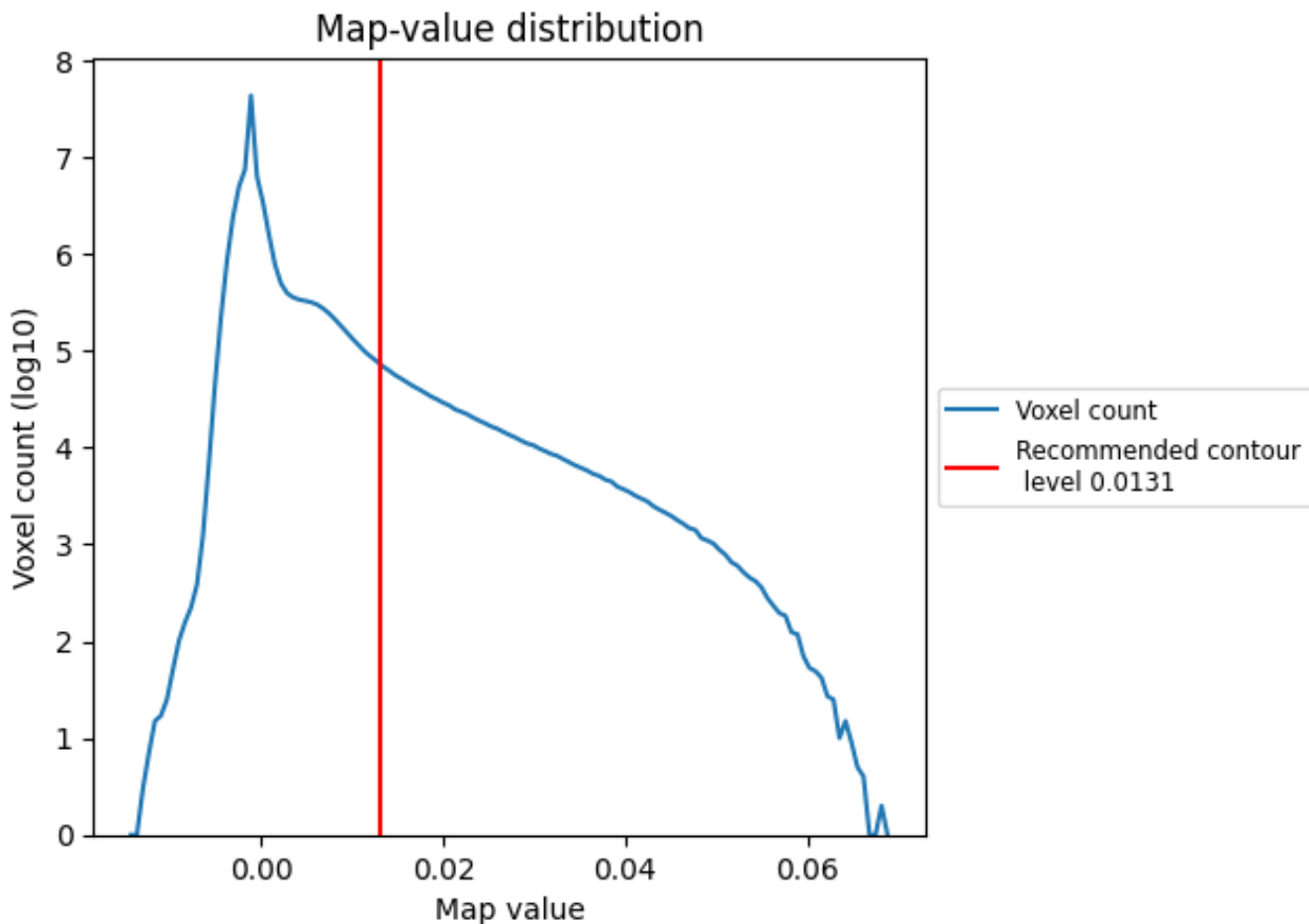
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
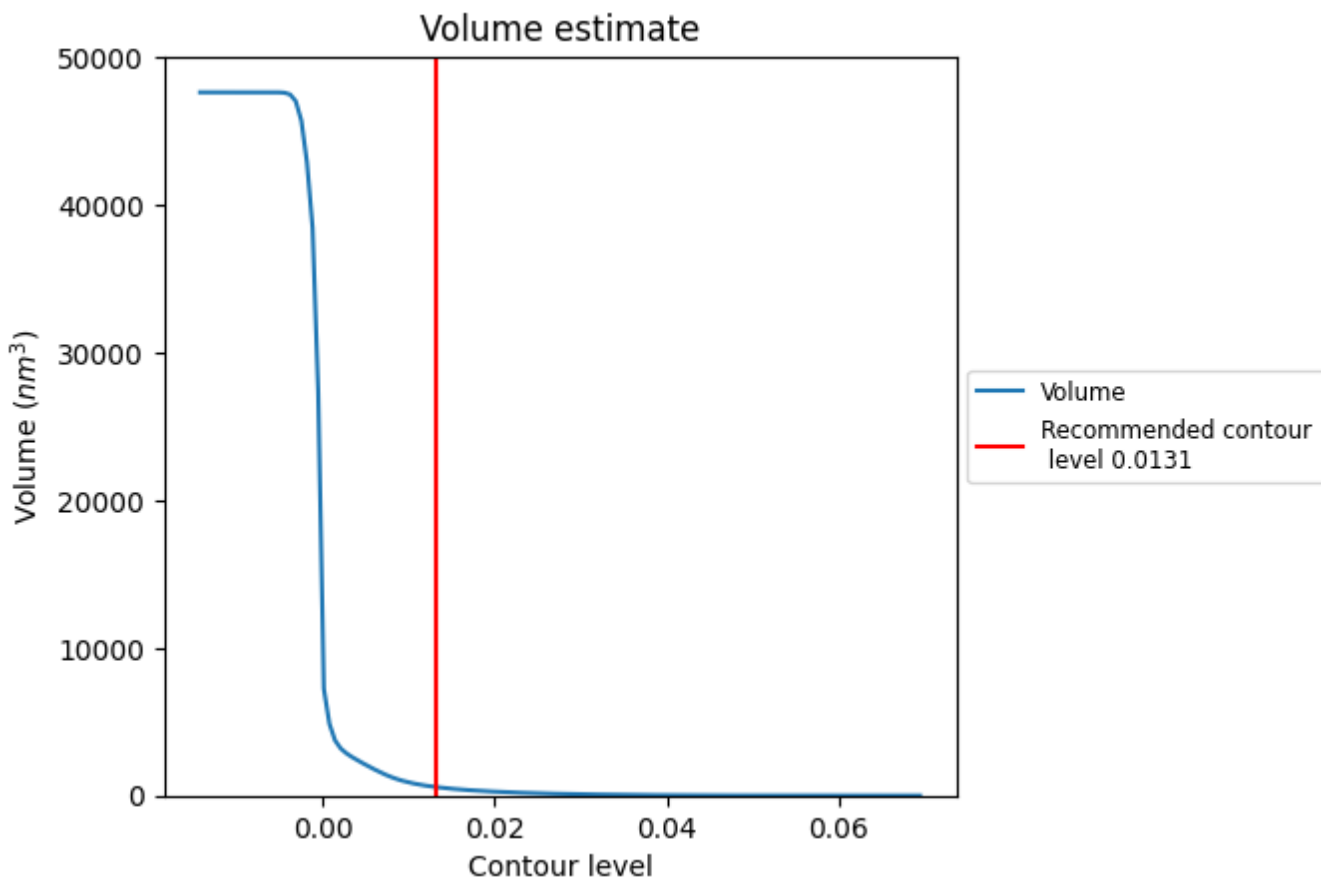
The volume at the recommended contour level is 582 nm^3; this corresponds to an approximate mass of 526 kDa.

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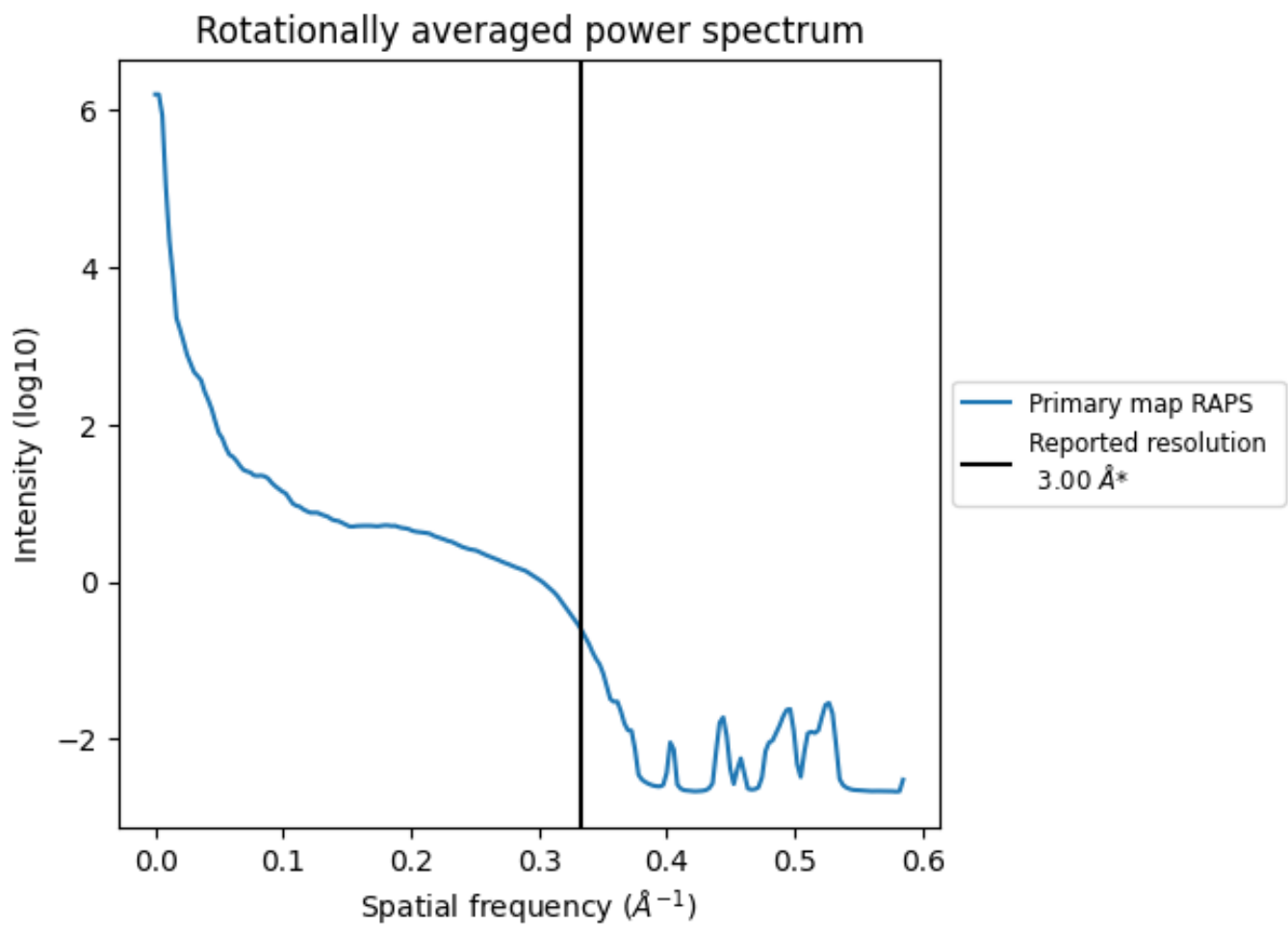
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8   Fourier-Shell correlation ⓘ

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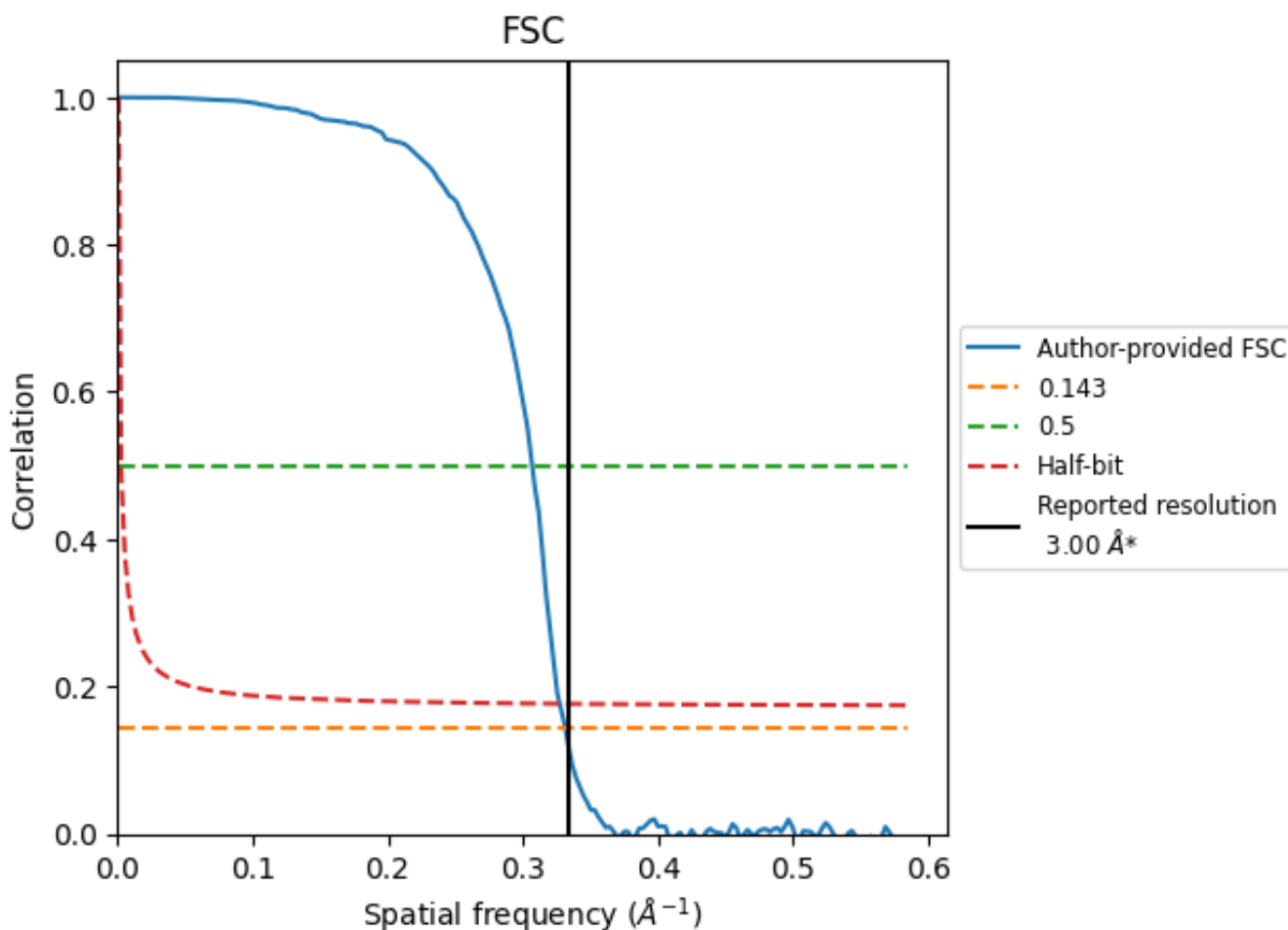
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.26	3.06
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-24950 and PDB model 7SAE. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ
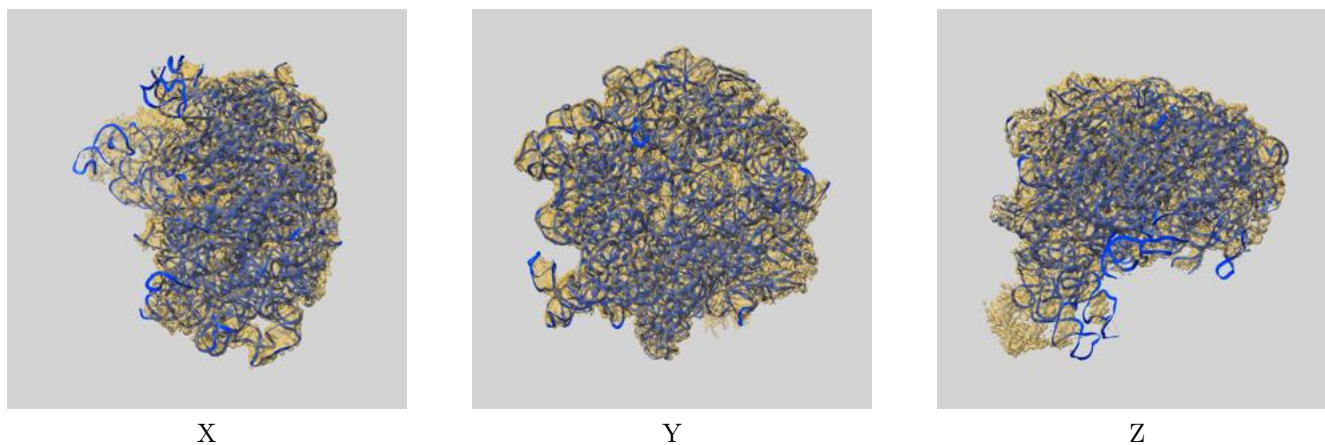
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0131 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
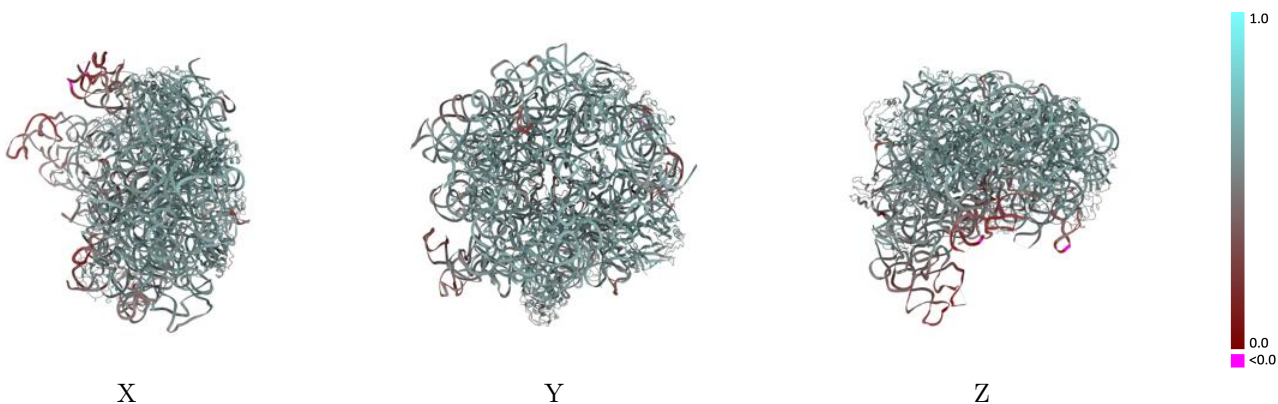
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
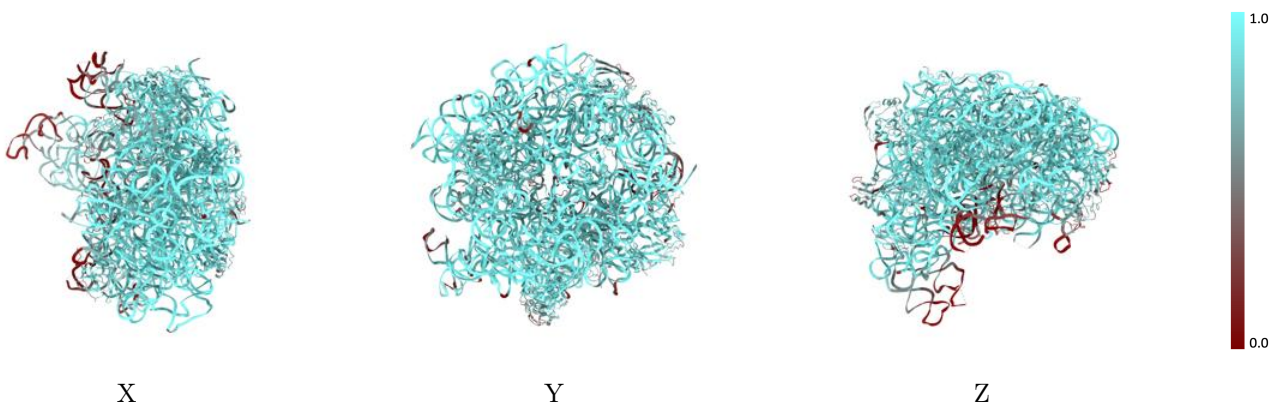
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0131).

9.4 Atom inclusion ⓘ
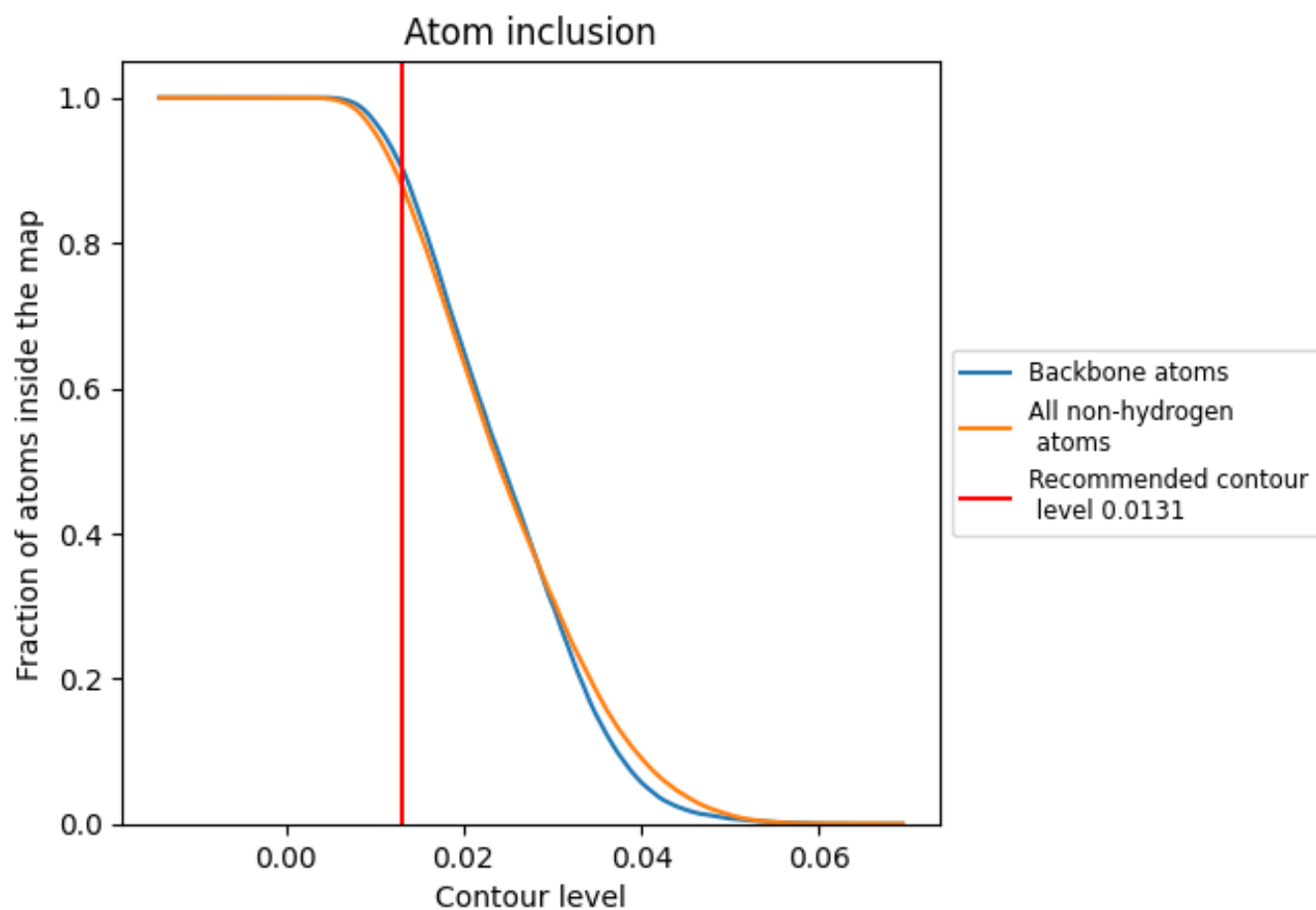
At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8778	0.5430
A	0.8990	0.5380
C	0.6975	0.5450
D	0.8580	0.5760
E	0.8272	0.5490
J	0.8780	0.5610
K	0.6444	0.5350
L	0.7150	0.5240
N	0.9258	0.5900
P	0.6982	0.5460
Q	0.9175	0.5780
R	0.8494	0.5710
S	0.9158	0.5840
T	0.8778	0.5620
U	0.7845	0.5590
V	0.6370	0.5210
Y	0.8093	0.5390
Z	0.8472	0.5620
b	0.9225	0.5830
d	0.9565	0.6020

1.0

0.0
<0.0