



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:15 AM UTC

PDB ID : 8RPY / pdb_00008rpy
EMDB ID : EMD-19426
Title : Escherichia coli 50S subunit in complex with the antimicrobial peptide Api137
Authors : Lauer, S.; Nikolay, R.; Spahn, C.
Deposited on : 2024-01-17
Resolution : 2.64 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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

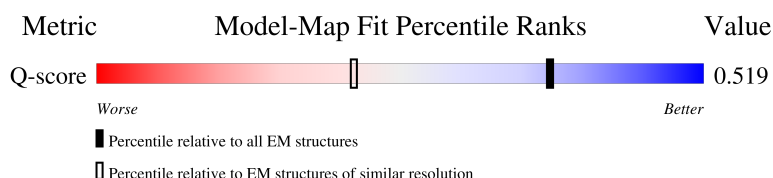
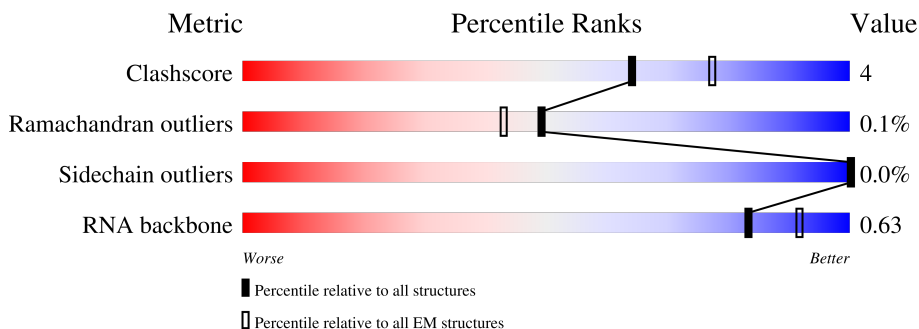
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



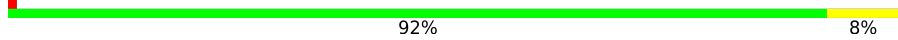
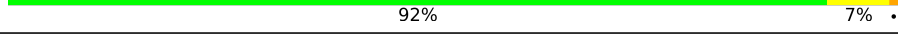
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8968 (2.14 - 3.14)

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	50	
3	2	46	

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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	38	
6	6	66	
7	A	2903	
8	B	120	
9	C	271	
10	D	209	
11	E	201	
12	F	177	
13	G	176	
14	H	149	
15	J	142	
16	K	122	
17	L	143	
18	M	136	
19	N	120	
20	O	116	
21	P	114	
22	Q	117	
23	R	103	
24	S	110	
25	T	93	
26	U	102	
27	V	94	
28	W	75	

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Mol	Chain	Length	Quality of chain
29	X	77	90%10%
30	Y	63	5% 94%6%
31	Z	58	84%16%
32	y	17	24% 47%47%6%
32	z	17	24% 59%41%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 90576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	43	Total	C	N	O	S	0	0
			333	206	59	62	6		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2900	Total	C	N	O	P	1	0
			62282	27783	11462	20136	2901		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 14 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 18 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	110	Total	C	N	O	S	1	0
			868	538	170	157	3		

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL30.

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

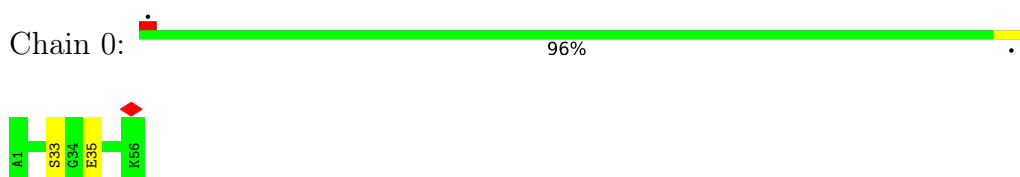
- Molecule 32 is a protein called Apidaecins type 137.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	y	17	Total	C	N	O	0	0
			148	94	33	21		
32	z	17	Total	C	N	O	0	0
			148	94	33	21		

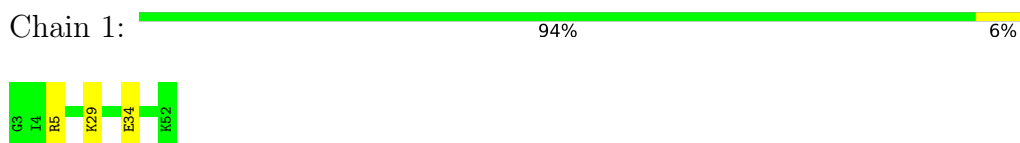
3 Residue-property plots [i](#)

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

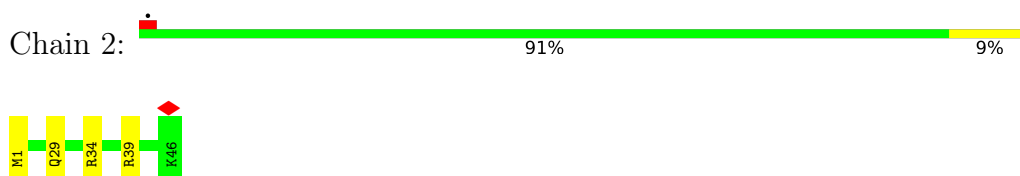
- Molecule 1: Large ribosomal subunit protein bL32



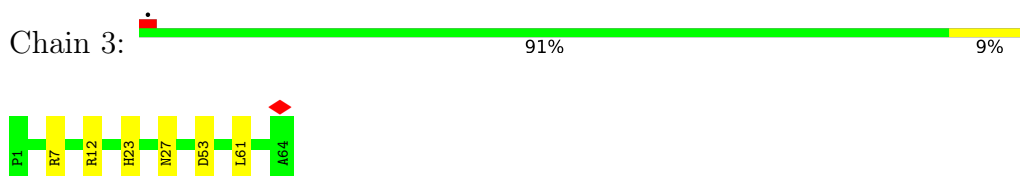
- Molecule 2: Large ribosomal subunit protein bL33



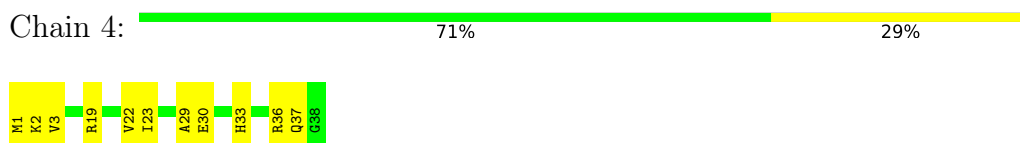
- Molecule 3: Large ribosomal subunit protein bL34



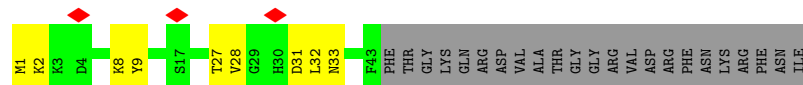
- Molecule 4: Large ribosomal subunit protein bL35



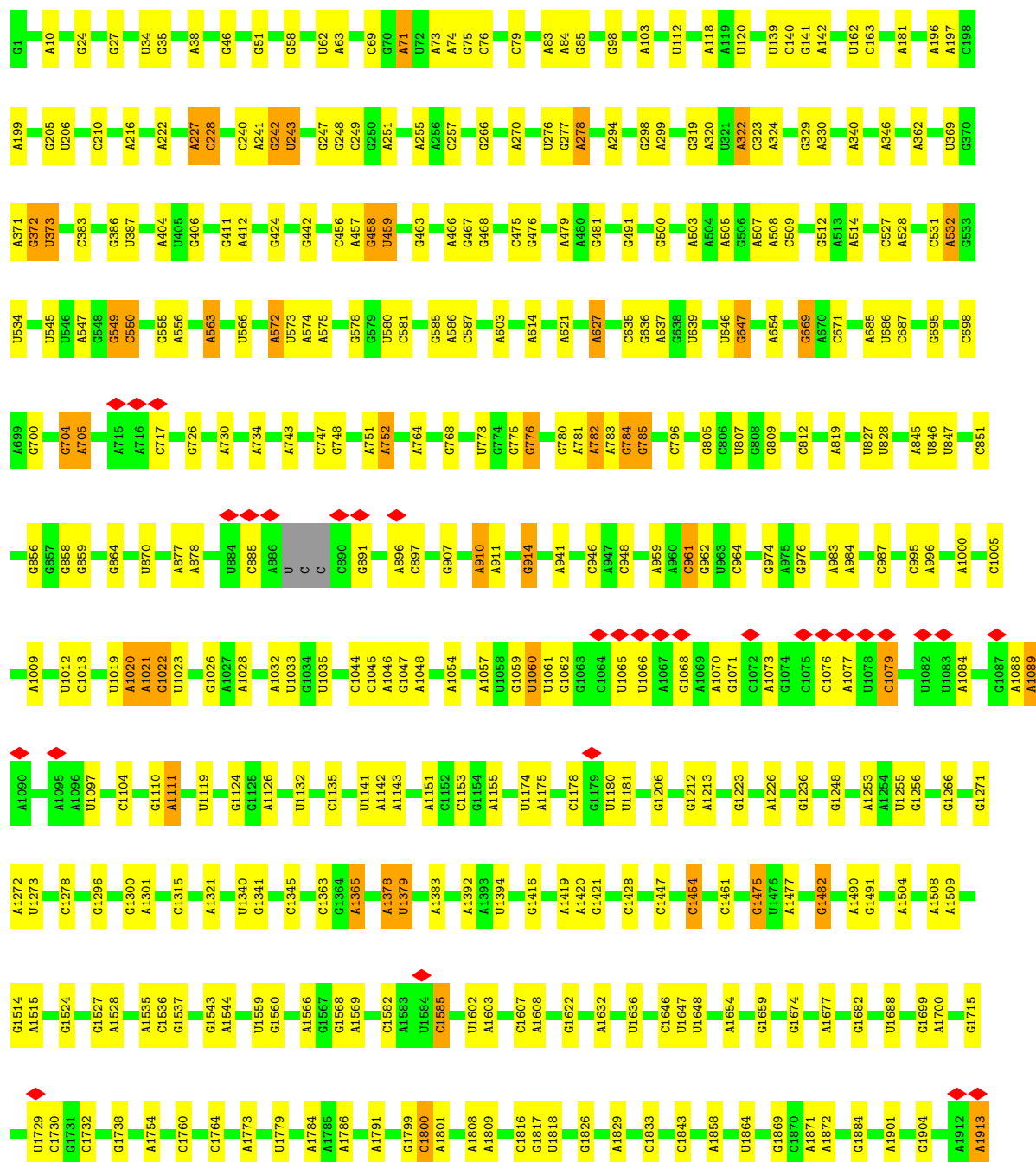
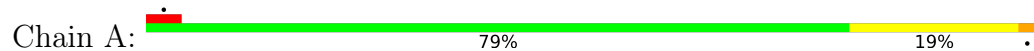
- Molecule 5: Large ribosomal subunit protein bL36A

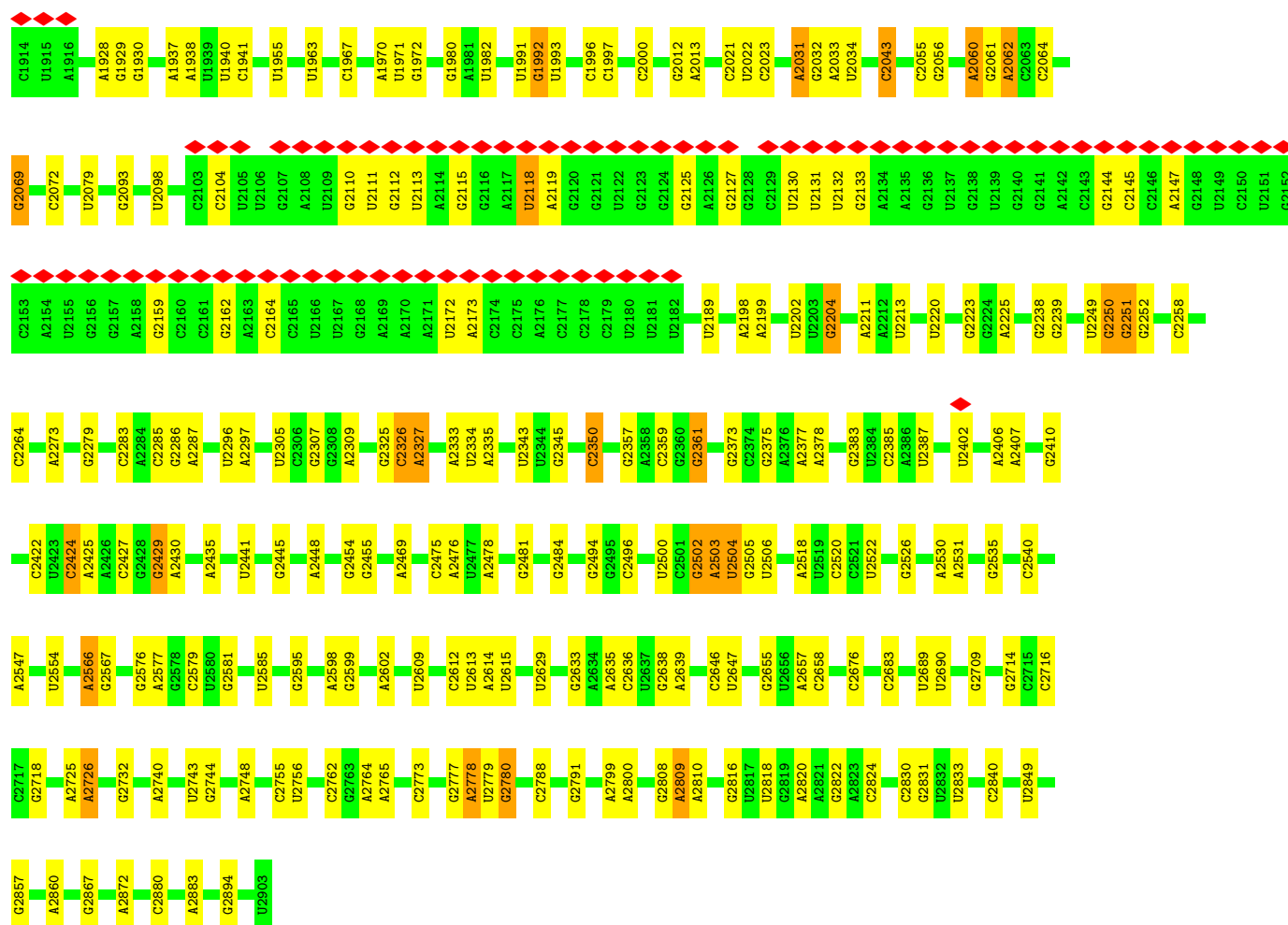


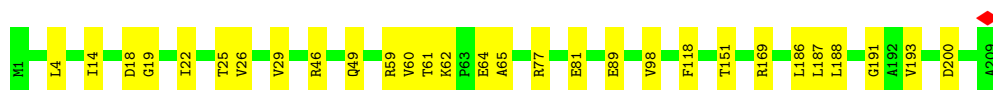
- Molecule 6: Large ribosomal subunit protein bL31



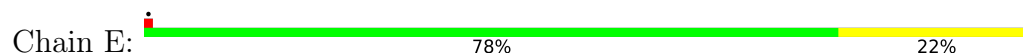
• Molecule 7: 23S ribosomal RNA



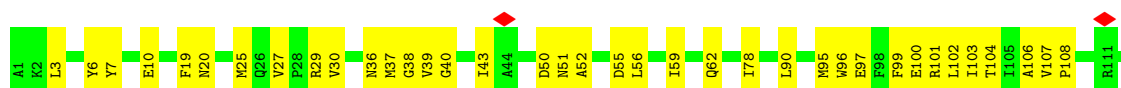




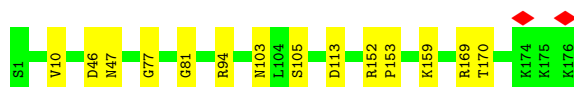
- Molecule 11: Large ribosomal subunit protein uL4



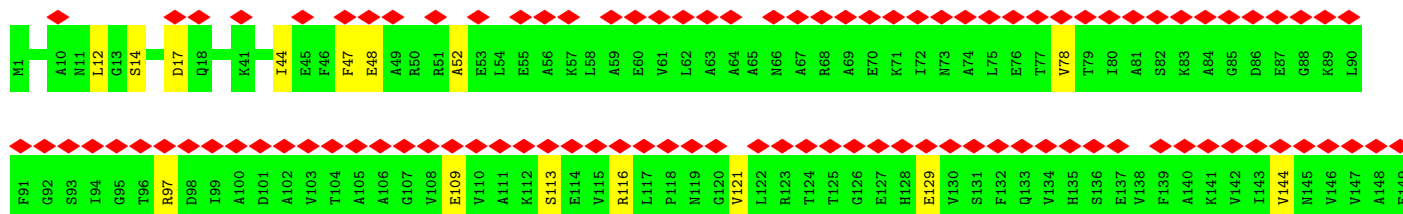
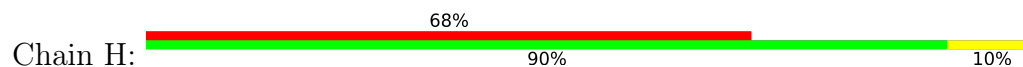
- Molecule 12: Large ribosomal subunit protein uL5



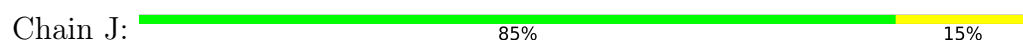
- Molecule 13: Large ribosomal subunit protein uL6



- Molecule 14: Large ribosomal subunit protein bL9

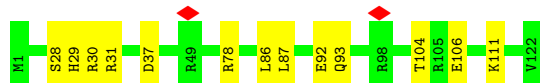
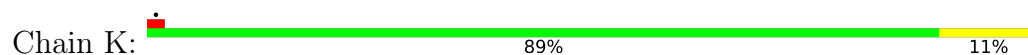


- Molecule 15: Large ribosomal subunit protein uL13

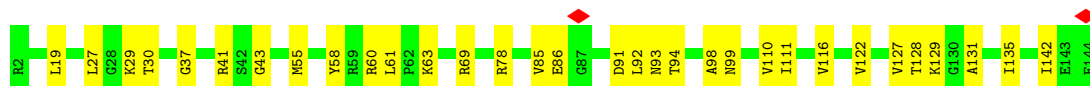
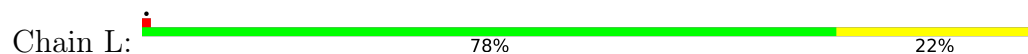




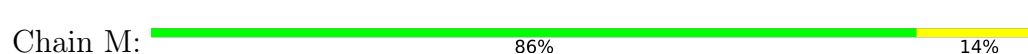
- Molecule 16: Large ribosomal subunit protein uL14



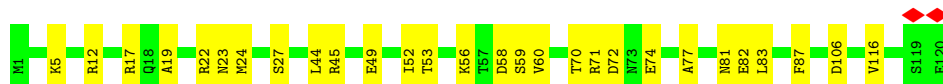
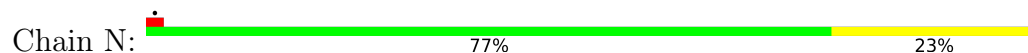
- Molecule 17: Large ribosomal subunit protein uL15



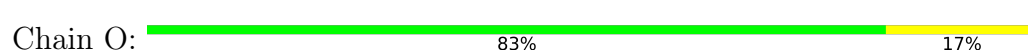
- Molecule 18: Large ribosomal subunit protein uL16



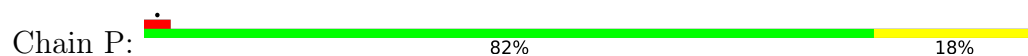
- Molecule 19: Large ribosomal subunit protein bL17



- Molecule 20: Large ribosomal subunit protein uL18



- Molecule 21: Large ribosomal subunit protein bL19



- Molecule 22: Large ribosomal subunit protein bL20

Chain Q:  89% 11%



- Molecule 23: Large ribosomal subunit protein bL21

Chain R:  92% 7%



- Molecule 24: Large ribosomal subunit protein uL22

Chain S:  81% 19%



- Molecule 25: Large ribosomal subunit protein uL23

Chain T:  77% 23%



- Molecule 26: Large ribosomal subunit protein uL24

Chain U:  79% 21%



- Molecule 27: Large ribosomal subunit protein bL25

Chain V:  68% 32%



- Molecule 28: Large ribosomal subunit protein bL27

Chain W:  84% 16%



- Molecule 29: Large ribosomal subunit protein bL28

Chain X:  90% 10%



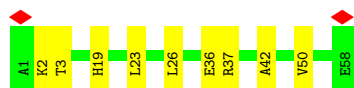
- Molecule 30: Large ribosomal subunit protein uL29

Chain Y:  5% 94% 6%



- Molecule 31: Large ribosomal subunit protein uL30

Chain Z:  84% 16%



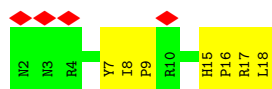
- Molecule 32: Apidaecins type 137

Chain y:  24% 47% 47% 6%



- Molecule 32: Apidaecins type 137

Chain z:  24% 59% 41%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	424506	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.538	Depositor
Minimum map value	-0.573	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.124	Depositor
Map size (Å)	353.99997, 353.99997, 353.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	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	0	0.16	0/450	0.28	0/599
2	1	0.12	0/416	0.25	0/554
3	2	0.17	0/380	0.23	0/498
4	3	0.13	0/513	0.26	0/676
5	4	0.17	0/303	0.27	0/397
6	6	0.15	0/339	0.30	0/454
7	A	0.13	0/69756	0.17	2/108822 (0.0%)
8	B	0.10	0/2876	0.16	0/4483
9	C	0.15	0/2121	0.29	0/2852
10	D	0.15	0/1586	0.27	0/2134
11	E	0.15	0/1571	0.29	0/2113
12	F	0.11	0/1434	0.33	0/1926
13	G	0.13	0/1343	0.32	0/1816
14	H	0.11	0/1122	0.26	0/1515
15	J	0.15	0/1152	0.24	0/1551
16	K	0.14	0/947	0.29	0/1268
17	L	0.15	0/1054	0.34	0/1403
18	M	0.14	0/1093	0.27	0/1460
19	N	0.16	0/973	0.32	0/1301
20	O	0.10	0/902	0.23	0/1209
21	P	0.15	0/929	0.27	0/1242
22	Q	0.16	0/960	0.26	0/1278
23	R	0.15	0/829	0.27	0/1107
24	S	0.15	0/875	0.30	0/1170
25	T	0.15	0/744	0.27	0/994
26	U	0.14	0/787	0.29	0/1051
27	V	0.17	0/766	0.37	0/1025
28	W	0.15	0/582	0.29	0/769
29	X	0.15	0/635	0.25	0/848
30	Y	0.15	0/510	0.30	0/677
31	Z	0.22	0/453	0.29	0/605
32	y	0.67	0/155	0.96	0/212
32	z	0.17	0/155	0.33	0/212
All	All	0.14	0/98711	0.21	2/148221 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1913	A	OP1-P-O3'	-8.85	81.45	108.00
7	A	1913	A	OP2-P-O3'	-8.45	82.66	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	1	0
2	1	409	0	440	3	0
3	2	377	0	418	4	0
4	3	504	0	574	7	0
5	4	302	0	343	10	0
6	6	333	0	332	8	0
7	A	62282	0	31324	260	0
8	B	2572	0	1302	15	0
9	C	2082	0	2157	31	0
10	D	1565	0	1616	28	0
11	E	1552	0	1619	29	0
12	F	1410	0	1447	38	0
13	G	1323	0	1374	10	0
14	H	1111	0	1148	10	0
15	J	1129	0	1162	14	0
16	K	938	0	1012	13	0
17	L	1045	0	1117	34	0
18	M	1074	0	1157	15	0
19	N	960	0	1000	19	0
20	O	892	0	923	16	0
21	P	917	0	965	18	0
22	Q	947	0	1022	11	0
23	R	816	0	839	7	0
24	S	868	0	934	14	0
25	T	738	0	807	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	U	779	0	834	16	0
27	V	753	0	780	24	0
28	W	575	0	592	8	0
29	X	625	0	655	5	0
30	Y	509	0	543	3	0
31	Z	449	0	491	6	0
32	y	148	0	152	16	0
32	z	148	0	152	7	0
All	All	90576	0	59692	580	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 (580) 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)
25:T:72:GLN:HB3	32:y:12:ARG:HH21	1.16	1.05
27:V:62:THR:OG1	27:V:69:GLU:OE2	1.83	0.97
31:Z:26:LEU:O	31:Z:37:ARG:NH1	2.02	0.92
7:A:2326:C:O2'	7:A:2327:A:OP1	1.89	0.91
14:H:113:SER:O	14:H:116:ARG:NH1	2.03	0.91
30:Y:34:SER:OG	30:Y:36:GLN:OE1	1.87	0.90
7:A:585:G:N7	22:Q:5:ARG:NH2	2.21	0.89
4:3:7:ARG:NH1	7:A:243:U:OP1	2.07	0.88
7:A:948:C:O2	7:A:984:A:O2'	1.92	0.86
7:A:1843:C:O2'	9:C:253:GLY:O	1.92	0.86
7:A:1392:A:N6	25:T:18:GLU:OE2	2.09	0.86
7:A:240:C:O2	7:A:257:C:N4	2.08	0.85
25:T:72:GLN:HB3	32:y:12:ARG:NH2	1.93	0.84
7:A:24:G:O2'	24:S:77:ASP:OD1	1.96	0.83
27:V:58:SER:OG	27:V:59:GLU:OE1	1.96	0.83
13:G:103:ASN:ND2	13:G:113:ASP:OD1	2.11	0.82
7:A:1779:U:OP2	7:A:1784:A:N6	2.13	0.81
7:A:2013:A:O2'	24:S:94:ASP:OD2	1.97	0.81
7:A:320:A:N3	11:E:163:ASN:ND2	2.28	0.81
17:L:128:THR:HG23	17:L:129:LYS:H	1.44	0.80
20:O:31:THR:OG1	20:O:33:ARG:O	1.99	0.80
9:C:77:VAL:HG21	9:C:109:LEU:HD11	1.63	0.80
7:A:2144:G:O2'	7:A:2147:A:N1	2.15	0.79
7:A:2469:A:N6	7:A:2481:G:O2'	2.15	0.79
28:W:14:ALA:O	28:W:16:ARG:NH1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2202:U:O2'	7:A:2204:G:OP1	2.01	0.79
7:A:1869:G:N2	7:A:1872:A:OP2	2.15	0.78
7:A:1607:C:N4	7:A:1622:G:OP2	2.16	0.78
18:M:47:GLU:OE2	18:M:51:ARG:NH1	2.15	0.78
7:A:227:A:O2'	7:A:228:C:O5'	2.00	0.78
7:A:621:A:OP2	17:L:99:ASN:ND2	2.17	0.77
9:C:78:GLU:OE2	9:C:100:ARG:NE	2.18	0.77
7:A:1475:G:O2'	7:A:1732:C:N4	2.18	0.77
5:4:19:ARG:NE	7:A:2756:U:OP2	2.19	0.76
7:A:2469:A:O2'	18:M:55:ARG:NH1	2.17	0.76
7:A:1528:A:OP2	7:A:1543:G:N2	2.19	0.76
7:A:1826:G:O2'	7:A:1971:U:OP2	2.04	0.75
27:V:42:LEU:HD13	27:V:47:VAL:HG21	1.67	0.75
14:H:129:GLU:N	14:H:129:GLU:OE1	2.20	0.75
7:A:2115:G:N2	7:A:2118:U:OP2	2.19	0.75
7:A:2377:A:O2'	20:O:117:PHE:O	2.05	0.74
12:F:25:MET:O	12:F:29:ARG:NH1	2.20	0.74
7:A:566:U:OP1	17:L:29:LYS:NZ	2.20	0.74
7:A:1022:G:O6	15:J:68:LYS:NZ	2.18	0.74
23:R:6:GLN:OE1	23:R:10:LYS:N	2.21	0.73
7:A:2576:G:O2'	7:A:2579:C:OP2	2.07	0.73
10:D:61:THR:OG1	10:D:64:GLU:OE1	2.06	0.73
7:A:864:G:O2'	7:A:914:G:O6	2.05	0.72
12:F:161:SER:N	12:F:164:GLU:OE2	2.22	0.72
17:L:29:LYS:O	17:L:30:THR:OG1	2.05	0.72
7:A:858:G:OP1	28:W:74:LYS:NZ	2.21	0.72
7:A:2581:G:N2	7:A:2581:G:OP2	2.21	0.72
27:V:35:GLU:OE2	27:V:93:ARG:NH1	2.22	0.72
7:A:807:U:OP2	17:L:41:ARG:NH2	2.22	0.72
12:F:10:GLU:N	12:F:10:GLU:OE1	2.21	0.72
24:S:78:GLU:OE1	24:S:78:GLU:N	2.22	0.72
7:A:796:C:OP1	11:E:57:LYS:NZ	2.21	0.72
15:J:88:THR:OG1	15:J:91:GLU:OE2	2.07	0.71
19:N:77:ALA:O	19:N:81:ASN:ND2	2.24	0.71
27:V:45:ASP:OD1	27:V:46:LYS:N	2.23	0.71
7:A:1315:C:O2'	7:A:1392:A:N3	2.22	0.70
12:F:143:ASP:OD1	12:F:144:LYS:N	2.24	0.70
7:A:84:A:N1	7:A:98:G:O2'	2.21	0.70
16:K:78:ARG:NH1	21:P:70:GLU:OE1	2.25	0.70
7:A:1508:A:O2'	7:A:1509:A:O4'	2.09	0.69
12:F:125:GLY:O	12:F:157:THR:OG1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1296:G:OP1	7:A:2709:G:O2'	2.10	0.69
7:A:2484:G:OP2	18:M:44:ARG:NH2	2.26	0.69
20:O:8:ILE:O	20:O:12:THR:OG1	2.11	0.69
7:A:514:A:N3	7:A:581:C:O2'	2.23	0.69
9:C:250:GLN:NE2	9:C:251:THR:O	2.27	0.68
7:A:563:A:OP2	23:R:79:ARG:NH1	2.26	0.68
7:A:2566:A:N1	16:K:28:SER:OG	2.27	0.68
25:T:6:ARG:NH2	25:T:37:ASP:OD2	2.27	0.68
7:A:1799:G:OP1	9:C:257:ARG:NH1	2.27	0.68
6:6:9:TYR:OH	12:F:97:GLU:OE1	2.10	0.67
12:F:122:ASP:OD1	12:F:123:GLY:N	2.27	0.67
11:E:189:THR:OG1	11:E:191:ASP:OD1	2.07	0.67
17:L:93:ASN:O	17:L:94:THR:OG1	2.13	0.66
7:A:227:A:HO2'	7:A:228:C:P	2.17	0.66
7:A:500:G:N1	7:A:503:A:OP2	2.29	0.66
7:A:2633:G:O2'	10:D:64:GLU:OE2	2.10	0.66
7:A:2725:A:O2'	7:A:2726:A:O5'	2.12	0.65
7:A:2683:C:OP1	21:P:50:ARG:NH2	2.29	0.65
21:P:63:ILE:HG23	21:P:63:ILE:O	1.97	0.65
7:A:1864:U:OP1	7:A:2410:G:O2'	2.14	0.65
11:E:97:ASN:ND2	11:E:100:MET:SD	2.70	0.65
7:A:2522:U:O2'	7:A:2647:U:OP1	2.11	0.65
21:P:7:LEU:O	21:P:7:LEU:HD23	1.96	0.65
7:A:1447:C:O2'	7:A:1544:A:N3	2.29	0.65
7:A:276:U:O2'	7:A:278:A:N7	2.30	0.65
7:A:62:U:H1'	32:y:3:ASN:OD1	1.96	0.64
7:A:1365:A:OP1	29:X:2:ARG:NH1	2.31	0.64
31:Z:3:THR:OG1	31:Z:36:GLU:OE2	2.06	0.64
5:4:22:VAL:HG11	5:4:36:ARG:NH1	2.12	0.64
7:A:2506[A]:U:O4	32:z:17:ARG:C	2.40	0.64
12:F:148:VAL:HG12	12:F:148:VAL:O	1.96	0.64
16:K:92:GLU:OE2	16:K:111:LYS:NZ	2.30	0.64
6:6:27:THR:HG22	6:6:27:THR:O	1.97	0.64
7:A:270:A:N1	7:A:369:U:O2'	2.31	0.64
20:O:50:ALA:O	20:O:81:ARG:NH1	2.31	0.64
7:A:2343:U:HO2'	7:A:2373:G:HO2'	1.42	0.64
7:A:1321:A:C5	32:y:16:PRO:HA	2.32	0.64
26:U:48:VAL:O	26:U:53:GLN:NE2	2.31	0.64
26:U:24:VAL:HA	26:U:35:VAL:HG12	1.80	0.64
7:A:62:U:O4'	32:y:3:ASN:CG	2.40	0.64
7:A:627:A:OP1	17:L:78:ARG:NH2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1568:G:N7	9:C:27:LYS:NZ	2.46	0.63
26:U:85:ARG:NH2	26:U:101:THR:OG1	2.30	0.63
25:T:72:GLN:OE1	32:y:12:ARG:NH2	2.31	0.63
10:D:25:THR:OG1	10:D:191:GLY:O	2.16	0.63
7:A:2831:G:OP2	10:D:59:ARG:NH2	2.32	0.63
7:A:463:G:N2	7:A:466:A:OP2	2.26	0.63
7:A:2646:C:OP2	7:A:2732:G:O2'	2.15	0.63
12:F:51:ASN:OD1	12:F:149:ARG:NH1	2.31	0.62
17:L:55:MET:O	17:L:60:ARG:NH1	2.33	0.62
7:A:534:U:O2'	22:Q:48:ASP:OD1	2.09	0.62
7:A:2130:U:O2'	7:A:2159:G:N1	2.32	0.62
7:A:647:G:N2	7:A:2350:C:O2'	2.32	0.62
7:A:2375:G:N2	7:A:2378:A:OP2	2.28	0.62
7:A:1363:C:O2'	7:A:1809:A:N3	2.29	0.62
5:4:30:GLU:OE1	5:4:33:HIS:ND1	2.32	0.62
5:4:23:ILE:HD13	7:A:1032:A:H1'	1.82	0.62
6:6:8:LYS:O	6:6:27:THR:OG1	2.18	0.62
24:S:67:ASP:OD1	24:S:68:ASP:N	2.32	0.62
8:B:27:C:OP1	20:O:34:HIS:NE2	2.33	0.61
7:A:910:A:N3	7:A:2264:C:O2'	2.30	0.61
11:E:191:ASP:OD1	11:E:192:ALA:N	2.33	0.61
12:F:55:ASP:OD1	12:F:56:LEU:N	2.34	0.61
24:S:20:VAL:HG21	24:S:43:ALA:HB3	1.81	0.61
15:J:92:MET:SD	15:J:95:ARG:NH2	2.74	0.61
7:A:636:G:P	17:L:128:THR:OG1	2.59	0.61
7:A:83:A:O2'	7:A:103:A:N6	2.33	0.60
18:M:40:ARG:HD3	18:M:93:VAL:HG21	1.83	0.60
7:A:2788:C:O2'	7:A:2809:A:N3	2.30	0.60
7:A:1009:A:N3	7:A:1153:C:O2'	2.33	0.60
7:A:2595:G:N2	7:A:2598:A:OP2	2.32	0.60
17:L:128:THR:HG23	17:L:129:LYS:N	2.15	0.59
5:4:3:VAL:HG12	5:4:3:VAL:O	2.01	0.59
7:A:1019:U:OP1	7:A:1035:U:O2'	2.10	0.59
7:A:1044:C:O2'	7:A:1111:A:N1	2.32	0.59
8:B:47:C:OP2	20:O:3:LYS:NZ	2.35	0.59
6:6:1:MET:N	8:B:40:U:O4	2.21	0.59
7:A:964:C:O2'	7:A:2273:A:N3	2.33	0.59
26:U:5:ARG:N	26:U:8:ASP:OD2	2.35	0.59
12:F:102:LEU:O	12:F:106:ALA:HB3	2.02	0.59
26:U:6:ARG:NH1	26:U:25:LYS:O	2.36	0.59
7:A:1266:G:O2'	7:A:2012:G:O6	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:4:ILE:HG22	24:S:106:VAL:HG22	1.85	0.59
7:A:62:U:H4'	32:y:3:ASN:HB2	1.84	0.58
7:A:2064:C:O2'	7:A:2251:G:N2	2.36	0.58
24:S:71:VAL:O	24:S:71:VAL:HG23	2.02	0.58
7:A:910:A:H62	18:M:12:MET:HA	1.68	0.57
7:A:340:A:O2'	11:E:162:ARG:NH2	2.37	0.57
7:A:249:C:O2'	17:L:63:LYS:NZ	2.21	0.57
9:C:123:ILE:O	9:C:123:ILE:HG22	2.04	0.57
7:A:2585:U:C2	32:z:18:LEU:HD12	2.39	0.57
17:L:91:ASP:OD1	17:L:92:LEU:N	2.37	0.57
7:A:781:A:OP1	9:C:216:ARG:NH2	2.34	0.57
19:N:72:ASP:OD1	19:N:74:GLU:N	2.36	0.57
12:F:3:LEU:O	12:F:7:TYR:N	2.33	0.57
7:A:2326:C:HO2'	7:A:2327:A:P	2.25	0.56
13:G:46:ASP:O	13:G:47:ASN:OD1	2.23	0.56
7:A:476:G:N1	7:A:479:A:OP2	2.36	0.56
7:A:1248:G:OP1	11:E:44:ARG:NH1	2.38	0.56
31:Z:50:VAL:HG12	31:Z:50:VAL:O	2.05	0.56
7:A:299:A:N6	7:A:322:A:O2'	2.39	0.56
8:B:57:A:C5	12:F:25:MET:HE1	2.41	0.56
7:A:685:A:O2'	7:A:773:U:O4	2.14	0.56
16:K:106:GLU:OE1	16:K:106:GLU:N	2.39	0.56
17:L:127:VAL:HG13	17:L:131:ALA:HB3	1.87	0.56
25:T:37:ASP:OD1	25:T:38:ALA:N	2.32	0.56
6:6:31:ASP:C	6:6:32:LEU:HD22	2.31	0.56
7:A:1223:G:N2	7:A:1226:A:OP2	2.34	0.56
24:S:109:ASP:OD1	24:S:110:ARG:N	2.38	0.56
11:E:115:GLN:O	11:E:116:ASP:OD1	2.24	0.56
19:N:116:VAL:HG23	19:N:116:VAL:O	2.06	0.56
11:E:199:MET:SD	11:E:200:LEU:HD22	2.46	0.55
11:E:171:ASP:OD1	11:E:172:ALA:N	2.39	0.55
32:y:4:ARG:N	32:y:5:PRO:HD2	2.20	0.55
4:3:53:ASP:OD2	7:A:2359:C:O2'	2.24	0.55
22:Q:96:ASP:OD2	23:R:13:ARG:NH1	2.39	0.55
7:A:2816:G:N3	7:A:2883:A:O2'	2.36	0.55
12:F:27:VAL:O	12:F:29:ARG:NH1	2.36	0.55
10:D:77:ARG:NH2	10:D:200:ASP:OD1	2.39	0.55
7:A:1048:A:OP2	7:A:1110:G:N2	2.33	0.55
14:H:109:GLU:N	14:H:109:GLU:OE1	2.40	0.55
14:H:121:VAL:HG12	14:H:121:VAL:O	2.07	0.55
8:B:52:A:O2'	8:B:53:A:O5'	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:W:37:ARG:O	28:W:53:HIS:ND1	2.39	0.54
7:A:298:G:O2'	7:A:322:A:N1	2.38	0.54
7:A:962:G:O2'	7:A:2496:C:O2'	2.24	0.54
11:E:15:SER:HG	11:E:18:THR:HG1	1.48	0.54
12:F:50:ASP:OD1	12:F:51:ASN:N	2.38	0.54
16:K:86:LEU:O	16:K:87:LEU:HD23	2.06	0.54
7:A:1654:A:O2'	10:D:118:PHE:O	2.23	0.54
18:M:106:ASP:OD1	18:M:107:GLY:N	2.38	0.54
7:A:1071:G:N2	7:A:1089:A:N3	2.56	0.54
7:A:2249:U:O2'	7:A:2252:G:OP2	2.26	0.54
7:A:2822:G:O2'	7:A:2824:C:OP2	2.22	0.54
12:F:59:ILE:O	12:F:101:ARG:NH2	2.41	0.54
15:J:17:VAL:HG23	15:J:137:PRO:HB2	1.90	0.54
7:A:2585:U:C2	32:z:18:LEU:CD1	2.91	0.54
18:M:69:PRO:O	18:M:70:ASP:OD1	2.26	0.54
3:2:29:GLN:NE2	7:A:210:C:OP1	2.40	0.54
7:A:1005:C:O2'	15:J:30:THR:HG21	2.08	0.54
7:A:2635:A:O2'	10:D:81:GLU:OE2	2.26	0.54
10:D:4:LEU:CD2	10:D:29:VAL:HG11	2.38	0.53
15:J:125:TYR:OH	15:J:132:HIS:NE2	2.39	0.53
18:M:53:MET:HE1	18:M:103:TYR:CB	2.38	0.53
11:E:149:ILE:HG23	11:E:149:ILE:O	2.07	0.53
25:T:28:ASN:ND2	25:T:88:LYS:O	2.42	0.53
7:A:743:A:O2'	7:A:1659:G:OP1	2.26	0.53
17:L:135:ILE:HD11	17:L:142:ILE:HD11	1.89	0.53
26:U:38:ILE:HG13	26:U:39:ASN:N	2.22	0.53
7:A:71:A:OP1	7:A:112:U:O2'	2.21	0.53
18:M:135:VAL:O	18:M:135:VAL:HG23	2.09	0.53
24:S:34:ASP:OD1	24:S:35:ILE:N	2.41	0.53
7:A:2000:C:OP1	19:N:5:LYS:NZ	2.42	0.53
7:A:2079:U:O2'	29:X:22:ASN:OD1	2.26	0.53
7:A:2840:C:H5''	19:N:53:THR:HG21	1.90	0.53
11:E:90:GLN:OE1	11:E:90:GLN:N	2.42	0.53
12:F:95:MET:SD	12:F:96:TRP:N	2.82	0.53
24:S:35:ILE:O	24:S:39:THR:OG1	2.20	0.52
27:V:77:VAL:CG2	27:V:86:LEU:HD22	2.39	0.52
7:A:549:G:O2'	7:A:550:C:P	2.67	0.52
7:A:2676:C:OP1	16:K:31:ARG:NH2	2.42	0.52
9:C:15:VAL:HG22	9:C:205:GLY:HA3	1.90	0.52
10:D:18:ASP:OD1	10:D:19:GLY:N	2.43	0.52
7:A:475:C:O2	7:A:479:A:N6	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:5:U:OP1	8:B:61:G:O2'	2.25	0.52
9:C:220:ARG:NH1	9:C:222:THR:OG1	2.42	0.52
9:C:235:GLU:N	9:C:235:GLU:OE1	2.43	0.52
28:W:29:ALA:N	28:W:60:ASP:OD2	2.42	0.52
5:4:37:GLN:OE1	7:A:1124:G:O2'	2.08	0.52
7:A:507:A:H2'	32:y:10:ARG:HE	1.75	0.52
7:A:776:G:H22	7:A:2072:C:H5'	1.73	0.52
11:E:140:ASP:OD1	11:E:141:MET:N	2.43	0.52
17:L:85:VAL:HG13	17:L:86:GLU:N	2.25	0.52
21:P:7:LEU:HD23	21:P:7:LEU:C	2.35	0.52
2:1:34:GLU:OE1	2:1:34:GLU:N	2.43	0.52
5:4:2:LYS:NZ	7:A:2478:A:OP2	2.37	0.52
7:A:987:C:O2'	7:A:1000:A:N3	2.35	0.52
27:V:26:PHE:CZ	27:V:42:LEU:HD11	2.44	0.51
7:A:372:G:O2'	7:A:373:U:P	2.68	0.51
7:A:574:A:N6	7:A:2034:U:OP1	2.42	0.51
7:A:961:C:O2	7:A:2031:A:N6	2.43	0.51
20:O:4:LYS:O	20:O:8:ILE:HD12	2.09	0.51
7:A:870:U:OP1	18:M:6:ARG:NH1	2.42	0.51
7:A:2307:G:N1	12:F:38:GLY:O	2.43	0.51
7:A:1151:A:O2'	22:Q:80:ASN:ND2	2.38	0.51
7:A:1454:C:O2'	19:N:60:VAL:HG13	2.10	0.51
22:Q:103:VAL:O	22:Q:106:THR:OG1	2.22	0.51
32:y:17:ARG:O	32:y:18:LEU:HB3	2.10	0.51
7:A:62:U:O4'	32:y:3:ASN:ND2	2.43	0.51
7:A:1754:A:N1	7:A:2716:C:O2'	2.41	0.51
7:A:2062:A:N1	32:z:16:PRO:HA	2.26	0.51
19:N:12:ARG:O	19:N:17:ARG:NH1	2.43	0.51
7:A:2130:U:HO2'	7:A:2159:G:H1	1.57	0.51
20:O:94:ARG:NH1	20:O:97:PHE:O	2.44	0.51
7:A:2387:U:O4'	28:W:37:ARG:NH1	2.44	0.51
9:C:44:ASN:OD1	9:C:45:ASN:N	2.43	0.51
6:6:33:ASN:OD1	6:6:33:ASN:O	2.27	0.50
7:A:2540:C:O2'	7:A:2740:A:N3	2.43	0.50
21:P:33:GLU:O	21:P:33:GLU:HG2	2.11	0.50
6:6:28:VAL:HG21	6:6:32:LEU:HD21	1.93	0.50
7:A:1688:U:O2'	7:A:1700:A:N7	2.42	0.50
18:M:53:MET:HE1	18:M:103:TYR:CG	2.46	0.50
27:V:65:VAL:O	27:V:66:ASP:OD1	2.30	0.50
19:N:56:LYS:NZ	19:N:87:PHE:O	2.43	0.50
7:A:76:C:O2'	30:Y:55:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:53:MET:HE1	18:M:103:TYR:HB3	1.94	0.50
18:M:59:ARG:HD2	18:M:59:ARG:O	2.12	0.50
13:G:77:GLY:O	13:G:81:GLY:N	2.45	0.50
21:P:112:ARG:C	21:P:113:LEU:HD23	2.36	0.50
7:A:700:G:O2'	7:A:1632:A:N3	2.39	0.49
23:R:49:ILE:CG2	23:R:54:VAL:HG12	2.42	0.49
7:A:1582:C:O2'	7:A:1585:C:N3	2.33	0.49
24:S:80:PRO:O	24:S:100:THR:OG1	2.26	0.49
7:A:580:U:O3'	22:Q:30:VAL:HG13	2.11	0.49
8:B:8:C:O3'	20:O:25:ARG:NH2	2.46	0.49
10:D:26:VAL:HG11	21:P:4:ILE:CD1	2.42	0.49
16:K:29:HIS:O	16:K:29:HIS:ND1	2.45	0.49
11:E:148:ILE:HG21	11:E:157:LEU:HD21	1.93	0.49
7:A:2424:C:O2	7:A:2429:G:O2'	2.28	0.49
7:A:2780:G:OP2	15:J:120:ARG:NH1	2.46	0.49
22:Q:90:ASP:OD1	22:Q:90:ASP:C	2.56	0.49
6:6:2:LYS:NZ	8:B:42:C:OP2	2.46	0.49
7:A:976:G:O2'	7:A:1155:A:O2'	2.30	0.49
10:D:14:ILE:HD11	10:D:188:LEU:HD23	1.94	0.48
20:O:43:ASN:OD1	20:O:44:GLY:N	2.46	0.48
7:A:299:A:N3	7:A:319:G:O2'	2.45	0.48
7:A:1980:G:O2'	7:A:1982:U:OP2	2.29	0.48
25:T:65:GLY:N	25:T:79:ASP:OD2	2.40	0.48
7:A:247:G:OP2	7:A:249:C:N4	2.46	0.48
7:A:1858:A:N6	7:A:1884:G:O2'	2.45	0.48
10:D:62:LYS:HA	10:D:65:ALA:HB3	1.96	0.48
11:E:65:THR:HG21	11:E:67:ARG:HE	1.79	0.48
12:F:3:LEU:HB3	12:F:100:GLU:OE2	2.13	0.48
7:A:458:G:O2'	7:A:459:U:P	2.72	0.48
7:A:2638:G:HO2'	7:A:2639:A:C5'	2.26	0.48
17:L:85:VAL:HG13	17:L:86:GLU:H	1.79	0.48
27:V:30:ILE:HD12	27:V:40:ILE:HD11	1.94	0.48
12:F:19:PHE:O	12:F:20:ASN:OD1	2.31	0.48
12:F:134:GLN:HB3	12:F:140:ILE:HD13	1.96	0.48
25:T:10:VAL:HG23	25:T:11:LEU:HD12	1.95	0.48
9:C:173:LEU:HD12	9:C:183:VAL:HG21	1.96	0.48
15:J:109:LEU:HD13	15:J:118:MET:HG3	1.96	0.48
27:V:20:LEU:HD11	27:V:41:GLU:OE1	2.14	0.48
7:A:1213:A:H62	7:A:1236:G:H1'	1.78	0.47
7:A:2857:G:N2	7:A:2860:A:OP2	2.37	0.47
14:H:14:SER:OG	14:H:17:ASP:OD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:64:SER:OG	21:P:65:ASN:N	2.47	0.47
27:V:76:ASP:OD1	27:V:77:VAL:N	2.46	0.47
21:P:26:GLU:OE2	21:P:41:ALA:HB1	2.14	0.47
25:T:61:LEU:HD11	25:T:82:LYS:HD3	1.97	0.47
20:O:2:ASP:OD1	20:O:3:LYS:N	2.47	0.47
26:U:5:ARG:O	26:U:24:VAL:HG21	2.13	0.47
7:A:1527:G:N1	7:A:1544:A:OP2	2.43	0.47
7:A:1682:G:OP2	7:A:1699:G:N2	2.44	0.47
7:A:85:G:OP1	26:U:6:ARG:N	2.48	0.47
7:A:2296:U:OP2	20:O:9:ARG:NH2	2.47	0.47
7:A:2500:U:O2'	7:A:2504:U:OP1	2.33	0.47
19:N:106:ASP:N	19:N:106:ASP:OD1	2.48	0.47
7:A:240:C:OP2	7:A:241:A:O2'	2.24	0.47
7:A:586:A:N1	7:A:809:G:O2'	2.46	0.47
10:D:25:THR:HG21	10:D:193:VAL:HG22	1.95	0.47
22:Q:85:ALA:O	22:Q:86:SER:OG	2.29	0.47
7:A:319:G:OP1	11:E:132:LYS:NZ	2.48	0.47
12:F:30:VAL:HG22	12:F:157:THR:HG22	1.96	0.47
7:A:2032:G:N2	10:D:151:THR:OG1	2.47	0.47
7:A:2773:C:OP1	10:D:169:ARG:NH1	2.48	0.47
7:A:578:G:OP1	7:A:1255:U:O2'	2.28	0.46
7:A:1071:G:N3	7:A:1089:A:O2'	2.46	0.46
11:E:58:LYS:HE2	11:E:62:GLN:HB2	1.97	0.46
3:2:39:ARG:NH2	7:A:468:G:O6	2.48	0.46
9:C:128:THR:C	9:C:129:LEU:HD22	2.40	0.46
12:F:3:LEU:HD11	12:F:96:TRP:HE3	1.81	0.46
25:T:13:ALA:O	25:T:33:LYS:N	2.48	0.46
26:U:33:VAL:HG13	26:U:66:VAL:HG22	1.97	0.46
16:K:30:ARG:NH2	16:K:37:ASP:OD2	2.49	0.46
7:A:372:G:HO2'	7:A:373:U:P	2.38	0.46
10:D:26:VAL:HG11	21:P:4:ILE:HD11	1.97	0.46
13:G:46:ASP:O	13:G:47:ASN:CG	2.59	0.46
21:P:2:ASN:OD1	21:P:3:ILE:HD12	2.15	0.46
26:U:97:SER:O	26:U:98:ASN:CG	2.57	0.46
10:D:26:VAL:O	10:D:26:VAL:HG13	2.16	0.46
14:H:44:ILE:HG22	14:H:48:GLU:OE1	2.16	0.46
32:z:15:HIS:HB2	32:z:17:ARG:HE	1.81	0.46
4:3:27:ASN:ND2	7:A:2361:G:O3'	2.49	0.46
4:3:61:LEU:HG	4:3:61:LEU:O	2.15	0.46
7:A:587:C:O2'	17:L:19:LEU:HD12	2.16	0.45
26:U:3:LYS:O	26:U:93:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:6:VAL:HG23	29:X:50:VAL:HG12	1.98	0.45
7:A:2743:U:OP2	7:A:2755:C:N4	2.49	0.45
12:F:148:VAL:O	12:F:148:VAL:CG1	2.63	0.45
7:A:1021:A:N6	7:A:1142:A:H61	2.14	0.45
7:A:2406:A:N3	17:L:69:ARG:NH1	2.52	0.45
9:C:90:ILE:HD12	9:C:102:TYR:CD1	2.52	0.45
13:G:169:ARG:HE	13:G:170:THR:H	1.64	0.45
20:O:108:ASP:OD2	20:O:108:ASP:N	2.49	0.45
7:A:532:A:N7	7:A:2021:C:O2'	2.39	0.45
7:A:636:G:OP1	17:L:129:LYS:NZ	2.49	0.45
12:F:3:LEU:HD22	12:F:100:GLU:HG2	1.97	0.45
13:G:46:ASP:OD1	13:G:46:ASP:N	2.48	0.45
15:J:84:ILE:O	15:J:84:ILE:HG23	2.16	0.45
26:U:98:ASN:OD1	26:U:98:ASN:O	2.34	0.45
7:A:636:G:C2	17:L:111:ILE:HD12	2.52	0.45
8:B:80:U:O4	27:V:14:LYS:NZ	2.49	0.45
10:D:60:VAL:HG13	10:D:60:VAL:O	2.15	0.45
11:E:117:ARG:NH2	11:E:183:PHE:O	2.50	0.45
7:A:780:G:O2'	7:A:783:A:N6	2.40	0.45
7:A:1477:A:N6	7:A:1514:G:O2'	2.49	0.45
7:A:2031:A:N3	7:A:2455:G:O2'	2.47	0.45
10:D:26:VAL:HG22	10:D:186:LEU:HD11	1.97	0.45
13:G:10:VAL:O	13:G:10:VAL:HG13	2.16	0.45
16:K:104:THR:OG1	16:K:106:GLU:OE1	2.26	0.45
21:P:96:LEU:HB3	21:P:99:LEU:HD13	1.99	0.45
7:A:796:C:P	11:E:57:LYS:HZ3	2.37	0.45
7:A:807:U:O2'	7:A:2060:A:N1	2.47	0.45
7:A:1378:A:C4'	7:A:1379:U:OP1	2.64	0.45
9:C:110:LYS:N	9:C:113:ASP:OD1	2.47	0.45
8:B:13:G:H1	8:B:69:G:HO2'	1.65	0.45
9:C:71:ASP:OD2	9:C:188:ARG:NH2	2.50	0.45
9:C:179:GLU:OE2	9:C:266:ILE:HG23	2.17	0.45
10:D:46:ARG:NH2	10:D:89:GLU:OE2	2.50	0.45
32:y:17:ARG:HA	32:y:17:ARG:HH11	1.82	0.45
7:A:58:G:O2'	7:A:73:A:N1	2.38	0.45
7:A:372:G:O2'	7:A:373:U:O5'	2.33	0.45
7:A:671:C:OP1	17:L:43:GLY:N	2.36	0.45
7:A:1060:U:O4	7:A:1079:C:N4	2.48	0.45
7:A:1996:C:OP1	16:K:31:ARG:NH1	2.50	0.45
10:D:187:LEU:C	10:D:188:LEU:HD12	2.42	0.45
7:A:1817:G:OP1	9:C:86:ARG:NH1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1904:G:O2'	7:A:1928:A:N1	2.34	0.44
7:A:2032:G:OP2	7:A:2454:G:O2'	2.18	0.44
19:N:82:GLU:HG2	19:N:83:LEU:HD12	1.99	0.44
26:U:17:ASP:OD1	26:U:17:ASP:N	2.48	0.44
7:A:751:A:C2	32:z:7:TYR:CZ	3.05	0.44
2:1:5:ARG:NH1	7:A:2285:C:OP2	2.46	0.44
7:A:2258:C:O2'	7:A:2427:C:OP2	2.29	0.44
21:P:112:ARG:O	21:P:113:LEU:HD23	2.18	0.44
27:V:20:LEU:HD21	27:V:41:GLU:OE2	2.17	0.44
3:2:1:MET:CE	7:A:752:A:H3'	2.48	0.44
7:A:2676:C:P	16:K:31:ARG:HH21	2.39	0.44
15:J:19:ASP:OD2	15:J:21:THR:N	2.48	0.44
19:N:70:THR:O	19:N:71:ARG:C	2.59	0.44
20:O:8:ILE:HD12	20:O:8:ILE:H	1.83	0.44
21:P:27:VAL:CG2	21:P:80:VAL:HG23	2.47	0.44
22:Q:111:LYS:NZ	23:R:50:GLY:HA2	2.32	0.44
2:1:29:LYS:NZ	7:A:2286:G:OP1	2.41	0.44
7:A:458:G:C2'	7:A:459:U:OP2	2.65	0.44
7:A:2810:A:H5''	10:D:62:LYS:HZ1	1.83	0.44
10:D:22:ILE:O	10:D:22:ILE:HG13	2.16	0.44
24:S:20:VAL:HG21	24:S:43:ALA:CB	2.46	0.44
7:A:242:G:H4'	7:A:243:U:O5'	2.16	0.44
7:A:1141:U:H4'	7:A:1142:A:O4'	2.18	0.44
27:V:21:ARG:HA	27:V:25:LYS:O	2.18	0.44
27:V:70:ILE:HG22	27:V:72:VAL:HG13	2.00	0.44
9:C:20:ASN:OD1	9:C:22:GLU:HG2	2.18	0.44
11:E:61:ARG:NH1	11:E:64:GLY:HA3	2.33	0.44
11:E:187:VAL:HG23	11:E:187:VAL:O	2.17	0.44
4:3:12:ARG:NH1	17:L:58:TYR:O	2.51	0.44
7:A:549:G:O2'	7:A:550:C:OP1	2.32	0.44
7:A:549:G:H2'	7:A:550:C:C6	2.53	0.44
13:G:152:ARG:HD3	13:G:153:PRO:HD2	1.99	0.44
19:N:24:MET:HG2	19:N:44:LEU:HD13	2.00	0.44
21:P:63:ILE:O	21:P:63:ILE:CG2	2.65	0.44
27:V:64:VAL:O	27:V:64:VAL:HG13	2.17	0.44
32:z:8:ILE:HD12	32:z:9:PRO:HD2	2.00	0.44
7:A:62:U:C1'	32:y:3:ASN:OD1	2.64	0.43
12:F:37:MET:CE	12:F:56:LEU:HD13	2.48	0.43
27:V:20:LEU:HD23	27:V:25:LYS:O	2.17	0.43
29:X:64:ASP:OD1	29:X:65:THR:N	2.51	0.43
7:A:442:G:O4'	11:E:41:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:12:LEU:HD12	14:H:12:LEU:O	2.18	0.43
7:A:2502:G:H3'	7:A:2503:A:C5'	2.48	0.43
31:Z:19:HIS:O	31:Z:23:LEU:HD23	2.18	0.43
7:A:62:U:C1'	32:y:3:ASN:CG	2.91	0.43
7:A:1020:A:H4'	7:A:1021:A:O5'	2.18	0.43
9:C:144:GLU:OE2	9:C:150:GLY:N	2.48	0.43
12:F:43:ILE:HD11	12:F:78:ILE:HG22	2.00	0.43
14:H:47:PHE:O	14:H:52:ALA:N	2.51	0.43
27:V:42:LEU:HD12	27:V:42:LEU:C	2.42	0.43
7:A:698:C:O2'	7:A:734:A:N6	2.51	0.43
12:F:39:VAL:HG23	12:F:40:GLY:N	2.33	0.43
27:V:77:VAL:HG22	27:V:86:LEU:HD22	2.01	0.43
7:A:2249:U:H3'	7:A:2250:G:H5'	2.01	0.43
12:F:36:ASN:OD1	12:F:37:MET:N	2.51	0.43
15:J:81:ILE:HG23	15:J:82:GLY:N	2.34	0.43
15:J:81:ILE:HG23	15:J:82:GLY:H	1.83	0.43
16:K:92:GLU:O	16:K:93:GLN:C	2.61	0.43
20:O:14:ALA:O	20:O:18:LEU:HD23	2.18	0.43
26:U:80:ASP:OD1	26:U:81:ARG:N	2.52	0.43
28:W:33:ILE:HG22	28:W:34:VAL:HG23	2.01	0.43
4:3:12:ARG:NH1	17:L:61:LEU:O	2.52	0.43
12:F:37:MET:HE1	12:F:56:LEU:HD22	2.00	0.43
28:W:7:ARG:O	28:W:10:ARG:NH1	2.42	0.43
9:C:208:GLY:O	9:C:212:TRP:CE3	2.72	0.43
3:2:34:ARG:HD3	7:A:467:G:OP2	2.19	0.43
9:C:228:ASP:OD1	9:C:229:HIS:N	2.52	0.43
12:F:3:LEU:HA	12:F:6:TYR:HB3	2.01	0.43
27:V:20:LEU:HD11	27:V:41:GLU:CD	2.43	0.43
7:A:205:G:HO2'	7:A:206:U:P	2.42	0.42
7:A:549:G:HO2'	7:A:550:C:P	2.39	0.42
7:A:1340:U:OP1	25:T:19:LYS:NZ	2.48	0.42
12:F:3:LEU:HD22	12:F:100:GLU:CG	2.49	0.42
8:B:52:A:HO2'	8:B:53:A:P	2.42	0.42
23:R:49:ILE:HG22	23:R:54:VAL:HG12	2.00	0.42
8:B:57:A:C8	12:F:25:MET:HE1	2.54	0.42
11:E:142:ALA:C	11:E:143:LEU:HD22	2.44	0.42
27:V:61:LEU:HD12	27:V:61:LEU:N	2.35	0.42
7:A:2830:C:OP2	10:D:59:ARG:NH1	2.52	0.42
14:H:78:VAL:HB	14:H:144:VAL:HG12	2.01	0.42
15:J:13:ARG:NH2	15:J:49:ASP:O	2.51	0.42
26:U:98:ASN:OD1	26:U:98:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:35:GLU:N	27:V:35:GLU:OE1	2.52	0.42
7:A:566:U:O2'	7:A:809:G:OP2	2.32	0.42
7:A:851:C:O2'	31:Z:42:ALA:O	2.36	0.42
10:D:98:VAL:HG22	10:D:98:VAL:O	2.19	0.42
22:Q:13:HIS:O	22:Q:17:LEU:HD23	2.20	0.42
7:A:507:A:H2'	32:y:10:ARG:NE	2.34	0.42
7:A:1566:A:O4'	9:C:212:TRP:CD1	2.73	0.42
7:A:2223:G:OP1	9:C:170:TYR:OH	2.23	0.42
7:A:2387:U:OP1	28:W:51:ARG:NH2	2.52	0.42
7:A:2530:A:OP2	7:A:2535:G:N2	2.52	0.42
17:L:27:LEU:O	17:L:27:LEU:HG	2.20	0.42
17:L:37:GLY:O	17:L:41:ARG:HG2	2.19	0.42
26:U:35:VAL:CG2	26:U:38:ILE:HD11	2.49	0.42
7:A:38:A:H4'	11:E:45:ALA:HB3	2.02	0.42
7:A:784:G:H5'	7:A:785:G:OP1	2.20	0.42
7:A:1602:U:OP2	25:T:64:LYS:NZ	2.45	0.42
17:L:122:VAL:HG22	17:L:142:ILE:HD13	2.02	0.42
7:A:2657:A:O3'	13:G:159:LYS:NZ	2.53	0.42
7:A:2725:A:O2'	7:A:2726:A:C8	2.73	0.42
11:E:105:LEU:O	11:E:109:LEU:HD23	2.20	0.42
12:F:99:PHE:CE2	12:F:103:ILE:HD13	2.54	0.42
25:T:56:GLU:OE1	25:T:57:VAL:HG12	2.18	0.42
7:A:27:G:N2	7:A:512:G:H1'	2.35	0.42
4:3:23:HIS:CG	17:L:61:LEU:HD13	2.55	0.41
5:4:29:ALA:HB3	5:4:30:GLU:OE2	2.20	0.41
7:A:372:G:C2'	7:A:373:U:OP2	2.68	0.41
7:A:1278:C:O2'	19:N:27:SER:OG	2.32	0.41
7:A:508:A:C4	32:y:13:PRO:HB3	2.55	0.41
12:F:51:ASN:OD1	12:F:52:ALA:N	2.53	0.41
7:A:704:G:O2'	7:A:705:A:O5'	2.33	0.41
7:A:2220:U:O2'	14:H:97:ARG:NH2	2.53	0.41
7:A:2599:G:OP2	9:C:234:GLY:N	2.42	0.41
12:F:100:GLU:O	12:F:104:THR:OG1	2.26	0.41
17:L:116:VAL:O	17:L:116:VAL:HG13	2.20	0.41
7:A:1379:U:OP1	7:A:1379:U:C6	2.73	0.41
7:A:2531:A:N3	7:A:2658:C:O2'	2.48	0.41
19:N:52:ILE:HD12	19:N:52:ILE:H	1.86	0.41
24:S:72:THR:HG21	24:S:108:SER:HB3	2.03	0.41
30:Y:52:ARG:O	30:Y:55:THR:HG22	2.20	0.41
7:A:704:G:H2'	7:A:726:G:H22	1.86	0.41
7:A:1800:C:OP2	9:C:181:ARG:NH2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:62:GLN:HE22	12:F:90:LEU:HD13	1.85	0.41
12:F:107:VAL:N	12:F:108:PRO:CD	2.83	0.41
21:P:70:GLU:OE2	21:P:100:ARG:NE	2.53	0.41
27:V:89:ILE:HG21	27:V:91:PHE:CZ	2.56	0.41
7:A:251:A:OP1	17:L:58:TYR:OH	2.23	0.41
7:A:782:A:H2	9:C:228:ASP:OD2	2.03	0.41
7:A:911:A:N6	18:M:11:LYS:O	2.51	0.41
7:A:2638:G:H1'	7:A:2778:A:H61	1.86	0.41
9:C:131:MET:HE1	9:C:187:CYS:SG	2.60	0.41
18:M:111:GLU:O	18:M:115:GLU:OE1	2.38	0.41
5:4:1:MET:HB2	7:A:2526:G:O2'	2.20	0.41
7:A:527:C:N4	7:A:2777:G:O2'	2.48	0.41
7:A:1151:A:O3'	22:Q:80:ASN:OD1	2.39	0.41
7:A:1992:G:N2	7:A:1996:C:O2'	2.53	0.41
7:A:2639:A:O2'	15:J:96:ARG:NH1	2.53	0.41
8:B:31:C:O2'	8:B:53:A:N6	2.41	0.41
11:E:91:ASP:OD1	11:E:91:ASP:O	2.39	0.41
11:E:155:GLU:HG2	11:E:156:ASN:N	2.36	0.41
17:L:110:VAL:HB	17:L:127:VAL:HG22	2.02	0.41
29:X:54:GLY:O	29:X:57:VAL:HG22	2.20	0.41
7:A:768:G:N2	7:A:1379:U:O2'	2.53	0.41
7:A:784:G:C5'	7:A:785:G:OP1	2.68	0.41
7:A:1077:A:N6	7:A:1089:A:OP2	2.54	0.41
7:A:1800:C:N4	7:A:1818:U:O2'	2.54	0.41
7:A:1996:C:P	16:K:31:ARG:HH12	2.44	0.41
10:D:81:GLU:N	10:D:81:GLU:OE1	2.54	0.41
19:N:58:ASP:OD2	19:N:59:SER:N	2.53	0.41
1:0:33:SER:CB	1:0:35:GLU:OE1	2.69	0.41
7:A:69:C:O2	7:A:73:A:O2'	2.38	0.41
7:A:1636:U:HO2'	7:A:1760:C:HO2'	1.55	0.41
7:A:1786:A:H1'	7:A:1938:A:N6	2.36	0.41
10:D:49:GLN:HA	10:D:81:GLU:HB3	2.03	0.41
17:L:85:VAL:HG23	17:L:98:ALA:HB2	2.01	0.41
19:N:19:ALA:O	19:N:23:ASN:ND2	2.46	0.41
25:T:1:MET:SD	25:T:3:ARG:N	2.94	0.41
7:A:197:A:H4'	7:A:2069:G:OP1	2.20	0.41
7:A:572:A:OP2	23:R:80:ARG:NH1	2.53	0.41
7:A:627:A:C5	17:L:111:ILE:HD11	2.56	0.41
8:B:93:C:OP2	27:V:18:ARG:NH1	2.51	0.41
7:A:1213:A:N6	7:A:1236:G:O2'	2.54	0.40
9:C:132:ARG:NH2	9:C:186:ASP:OD1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:128:THR:CG2	17:L:129:LYS:H	2.24	0.40
31:Z:2:LYS:HE2	31:Z:2:LYS:HA	2.03	0.40
5:4:30:GLU:OE2	5:4:30:GLU:N	2.54	0.40
7:A:79:C:O2'	7:A:346:A:N3	2.52	0.40
7:A:635:C:O2'	7:A:639:U:H5''	2.21	0.40
7:A:1482:G:O2'	7:A:1509:A:N1	2.48	0.40
10:D:26:VAL:CG2	10:D:186:LEU:HD11	2.52	0.40
19:N:49:GLU:O	19:N:53:THR:HG23	2.21	0.40
7:A:669:G:N3	7:A:669:G:H2'	2.35	0.40
7:A:1028:A:OP2	7:A:1126:A:N6	2.54	0.40
7:A:1394:U:H4'	7:A:1603:A:H4'	2.03	0.40
8:B:52:A:N7	20:O:33:ARG:NH1	2.69	0.40
9:C:6:LYS:O	9:C:8:THR:N	2.50	0.40
13:G:94:ARG:HB2	13:G:105:SER:OG	2.21	0.40
19:N:45:ARG:O	19:N:49:GLU:OE1	2.39	0.40
7:A:2445:G:OP1	11:E:69:ARG:NH1	2.44	0.40
7:A:2577:A:O4'	7:A:2612:C:N4	2.55	0.40
17:L:27:LEU:HD23	17:L:27:LEU:H	1.86	0.40
21:P:26:GLU:OE1	21:P:43:GLU:OE1	2.39	0.40
7:A:528:A:C2	7:A:2043:C:H4'	2.57	0.40
19:N:22:ARG:CG	19:N:70:THR:HA	2.51	0.40
24:S:6:LYS:HG2	24:S:104:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
2	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
6	6	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
9	C	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
10	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
11	E	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	36
12	F	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
13	G	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
14	H	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
15	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
16	K	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
17	L	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
18	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
19	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
20	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
21	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
22	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
23	R	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12	18
24	S	109/110 (99%)	105 (96%)	4 (4%)	0	100	100
25	T	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
26	U	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
27	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
28	W	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
29	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
30	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
31	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
32	y	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
32	z	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	3238/3322 (98%)	3093 (96%)	143 (4%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	R	54	VAL
11	E	83	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	45/45 (100%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/51 (100%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
6	6	40/59 (68%)	40 (100%)	0	100	100
9	C	216/216 (100%)	216 (100%)	0	100	100
10	D	164/164 (100%)	164 (100%)	0	100	100
11	E	165/165 (100%)	165 (100%)	0	100	100
12	F	148/148 (100%)	148 (100%)	0	100	100
13	G	137/137 (100%)	137 (100%)	0	100	100
14	H	114/114 (100%)	114 (100%)	0	100	100
15	J	116/116 (100%)	116 (100%)	0	100	100
16	K	103/103 (100%)	103 (100%)	0	100	100
17	L	102/102 (100%)	102 (100%)	0	100	100
18	M	109/109 (100%)	109 (100%)	0	100	100
19	N	100/100 (100%)	100 (100%)	0	100	100
20	O	86/86 (100%)	86 (100%)	0	100	100
21	P	99/99 (100%)	99 (100%)	0	100	100
22	Q	89/89 (100%)	89 (100%)	0	100	100
23	R	84/84 (100%)	84 (100%)	0	100	100
24	S	94/93 (101%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	T	80/80 (100%)	80 (100%)	0	100	100
26	U	83/83 (100%)	83 (100%)	0	100	100
27	V	78/78 (100%)	78 (100%)	0	100	100
28	W	57/57 (100%)	57 (100%)	0	100	100
29	X	67/67 (100%)	67 (100%)	0	100	100
30	Y	55/55 (100%)	55 (100%)	0	100	100
31	Z	48/48 (100%)	48 (100%)	0	100	100
32	y	17/17 (100%)	16 (94%)	1 (6%)	18	29
32	z	17/17 (100%)	17 (100%)	0	100	100
All	All	2683/2701 (99%)	2682 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
32	y	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
9	C	24	HIS
9	C	250	GLN
10	D	164	GLN
10	D	173	GLN
11	E	115	GLN
11	E	165	HIS
13	G	63	GLN
13	G	103	ASN
13	G	114	HIS
15	J	80	HIS
17	L	54	GLN
18	M	13	HIS
19	N	9	GLN
21	P	55	HIS
24	S	9	HIS
24	S	60	HIS
24	S	61	ASN
25	T	70	HIS
27	V	44	HIS

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Mol	Chain	Res	Type
28	W	72	ASN
29	X	35	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	2897/2903 (99%)	339 (11%)	14 (0%)
8	B	119/120 (99%)	11 (9%)	3 (2%)
All	All	3016/3023 (99%)	350 (11%)	17 (0%)

All (350) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	10	A
7	A	34	U
7	A	35	G
7	A	46	G
7	A	51	G
7	A	63	A
7	A	71	A
7	A	74	A
7	A	75	G
7	A	118	A
7	A	120	U
7	A	139	U
7	A	140	C
7	A	141	G
7	A	142	A
7	A	162	U
7	A	163	C
7	A	181	A
7	A	196	A
7	A	199	A
7	A	216	A
7	A	222	A
7	A	228	C
7	A	242	G
7	A	243	U
7	A	248	G
7	A	255	A
7	A	266	G

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Mol	Chain	Res	Type
7	A	277	G
7	A	278	A
7	A	294	A
7	A	322	A
7	A	323	C
7	A	324	A
7	A	329	G
7	A	330	A
7	A	362	A
7	A	371	A
7	A	372	G
7	A	373	U
7	A	383	C
7	A	386	G
7	A	387	U
7	A	404	A
7	A	406	G
7	A	411	G
7	A	412	A
7	A	424	G
7	A	456	C
7	A	457	A
7	A	458	G
7	A	459	U
7	A	481	G
7	A	491	G
7	A	505	A
7	A	509	C
7	A	531	C
7	A	532	A
7	A	545	U
7	A	547	A
7	A	550	C
7	A	556	A
7	A	563	A
7	A	572	A
7	A	573	U
7	A	575	A
7	A	603	A
7	A	614	A
7	A	627	A
7	A	637	A

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Mol	Chain	Res	Type
7	A	646	U
7	A	647	G
7	A	654	A
7	A	669	G
7	A	686	U
7	A	687	C
7	A	695	G
7	A	705	A
7	A	717	C
7	A	730	A
7	A	747	C
7	A	748	G
7	A	752	A
7	A	764	A
7	A	775	G
7	A	776	G
7	A	782	A
7	A	784	G
7	A	785	G
7	A	805	G
7	A	812	C
7	A	819	A
7	A	827	U
7	A	828	U
7	A	845	A
7	A	846	U
7	A	847	U
7	A	856	G
7	A	859	G
7	A	877	A
7	A	878	A
7	A	885	C
7	A	891	G
7	A	896	A
7	A	897	C
7	A	907	G
7	A	910	A
7	A	914	G
7	A	941	A
7	A	946	C
7	A	959	A
7	A	961	C

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Mol	Chain	Res	Type
7	A	974	G
7	A	983	A
7	A	995	C
7	A	996	A
7	A	1012	U
7	A	1013	C
7	A	1021	A
7	A	1023	U
7	A	1026	G
7	A	1033	U
7	A	1045	C
7	A	1046	A
7	A	1047	G
7	A	1054	A
7	A	1057	A
7	A	1059	G
7	A	1060	U
7	A	1061	U
7	A	1062	G
7	A	1065	U
7	A	1066	U
7	A	1068	G
7	A	1070	A
7	A	1073	A
7	A	1076	C
7	A	1079	C
7	A	1084	A
7	A	1088	A
7	A	1089	A
7	A	1097	U
7	A	1104	C
7	A	1111	A
7	A	1119	U
7	A	1132	U
7	A	1135	C
7	A	1143	A
7	A	1174	U
7	A	1175	A
7	A	1178	C
7	A	1180	U
7	A	1181	U
7	A	1206	G

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Mol	Chain	Res	Type
7	A	1212	G
7	A	1253	A
7	A	1256	G
7	A	1271	G
7	A	1272	A
7	A	1273	U
7	A	1300	G
7	A	1301	A
7	A	1341	G
7	A	1345	C
7	A	1365	A
7	A	1378	A
7	A	1379	U
7	A	1383	A
7	A	1416	G
7	A	1419	A
7	A	1420	A
7	A	1421	G
7	A	1428	C
7	A	1454	C
7	A	1461	C
7	A	1475	G
7	A	1482	G
7	A	1490	A
7	A	1491	G
7	A	1504	A
7	A	1515	A
7	A	1524	G
7	A	1535	A
7	A	1536	C
7	A	1537	G
7	A	1559	U
7	A	1560	G
7	A	1569	A
7	A	1585	C
7	A	1608	A
7	A	1646	C
7	A	1647	U
7	A	1648	U
7	A	1674	G
7	A	1677	A
7	A	1715	G

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Mol	Chain	Res	Type
7	A	1729	U
7	A	1730	C
7	A	1738	G
7	A	1764	C
7	A	1773	A
7	A	1791	A
7	A	1800	C
7	A	1801	A
7	A	1808	A
7	A	1816	C
7	A	1829	A
7	A	1833	C
7	A	1871	A
7	A	1901	A
7	A	1913	A
7	A	1929	G
7	A	1930	G
7	A	1937	A
7	A	1940	U
7	A	1941	C
7	A	1955	U
7	A	1963	U
7	A	1967	C
7	A	1970	A
7	A	1972	G
7	A	1991	U
7	A	1992	G
7	A	1993	U
7	A	1997	C
7	A	2022	U
7	A	2023	C
7	A	2031	A
7	A	2033	A
7	A	2043	C
7	A	2055	C
7	A	2056	G
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2069	G
7	A	2093	G
7	A	2098	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	2104	C
7	A	2110	G
7	A	2111	U
7	A	2112	G
7	A	2113	U
7	A	2118	U
7	A	2119	A
7	A	2125	G
7	A	2127	G
7	A	2131	U
7	A	2132	U
7	A	2133	G
7	A	2145	C
7	A	2162	G
7	A	2164	C
7	A	2172	U
7	A	2173	A
7	A	2189	U
7	A	2198	A
7	A	2199	A
7	A	2204	G
7	A	2211	A
7	A	2213	U
7	A	2225	A
7	A	2238	G
7	A	2239	G
7	A	2250	G
7	A	2251	G
7	A	2279	G
7	A	2283	C
7	A	2287	A
7	A	2297	A
7	A	2305	U
7	A	2309	A
7	A	2325	G
7	A	2327	A
7	A	2333	A
7	A	2334	U
7	A	2335	A
7	A	2345	G
7	A	2350	C
7	A	2357	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	2361	G
7	A	2383	G
7	A	2385	C
7	A	2402	U
7	A	2407	A
7	A	2422	C
7	A	2424	C
7	A	2425	A
7	A	2429	G
7	A	2430	A
7	A	2435	A
7	A	2441	U
7	A	2448	A
7	A	2475	C
7	A	2476	A
7	A	2494	G
7	A	2502	G
7	A	2503	A
7	A	2504	U
7	A	2505	G
7	A	2518	A
7	A	2520	C
7	A	2547	A
7	A	2554	U
7	A	2566	A
7	A	2567	G
7	A	2602	A
7	A	2609	U
7	A	2613	U
7	A	2614	A
7	A	2615	U
7	A	2629	U
7	A	2636	C
7	A	2655	G
7	A	2689	U
7	A	2690	U
7	A	2714	G
7	A	2718	G
7	A	2726	A
7	A	2744	G
7	A	2748	A
7	A	2762	C

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Mol	Chain	Res	Type
7	A	2764	A
7	A	2765	A
7	A	2778	A
7	A	2779	U
7	A	2780	G
7	A	2791	G
7	A	2799	A
7	A	2800	A
7	A	2809	A
7	A	2818	U
7	A	2820	A
7	A	2833	U
7	A	2849	U
7	A	2867	G
7	A	2872	A
7	A	2880	C
7	A	2894	G
8	B	4	C
8	B	13	G
8	B	35	C
8	B	42	C
8	B	44	G
8	B	45	A
8	B	53	A
8	B	67	G
8	B	88	C
8	B	89	U
8	B	109	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	227	A
7	A	242	G
7	A	372	G
7	A	458	G
7	A	549	G
7	A	555	G
7	A	704	G
7	A	784	G
7	A	1020	A
7	A	1022	G

Continued on next page...

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Mol	Chain	Res	Type
7	A	1378	A
7	A	1940	U
7	A	2326	C
7	A	2808	G
8	B	44	G
8	B	52	A
8	B	66	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

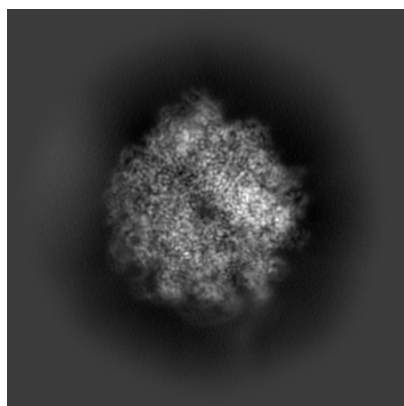
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19426. These allow visual inspection of the internal detail of the map and identification of artifacts.

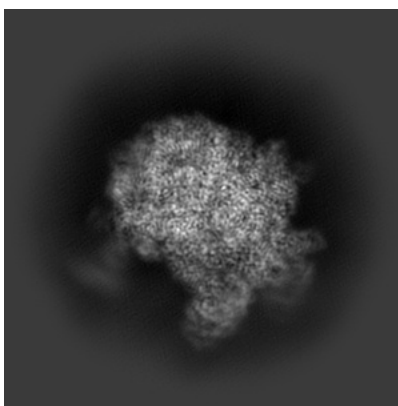
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

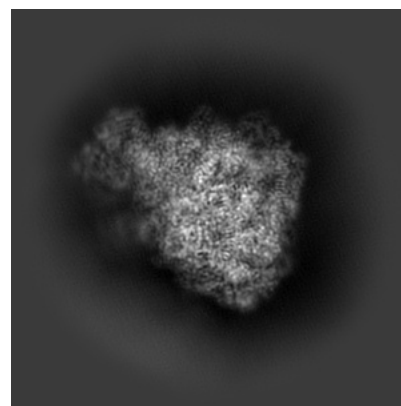
6.1.1 Primary map



X

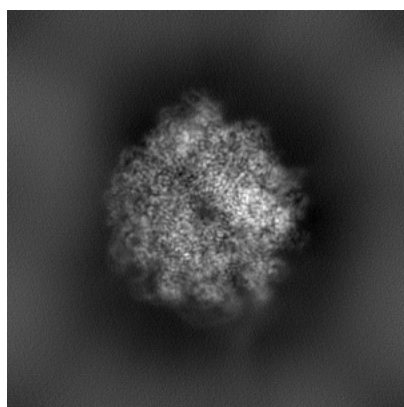


Y

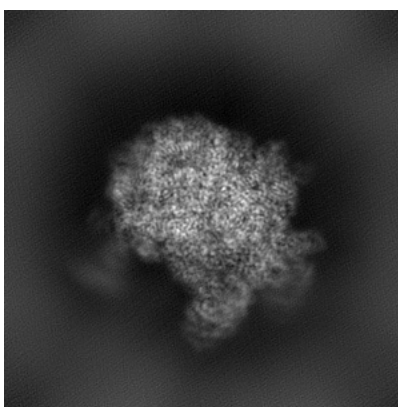


Z

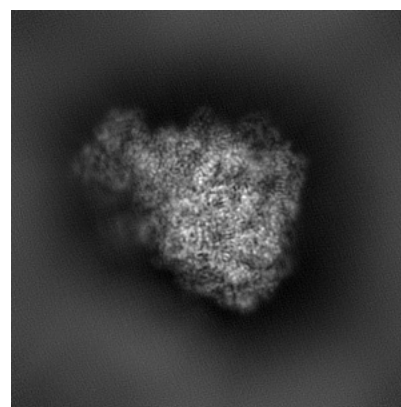
6.1.2 Raw map



X



Y

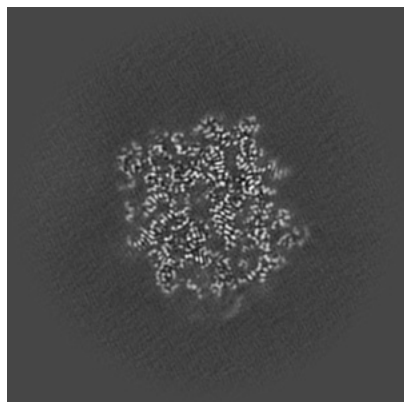


Z

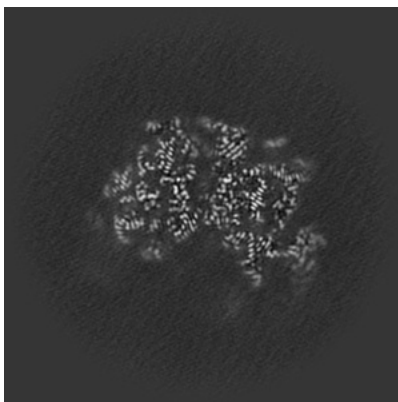
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

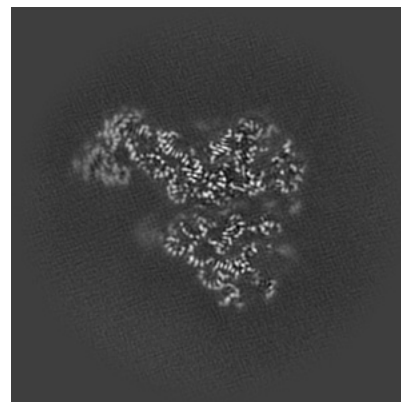
6.2.1 Primary map



X Index: 150

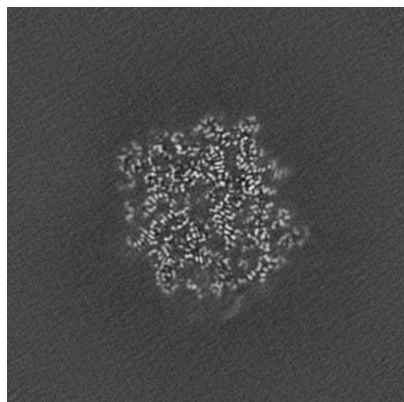


Y Index: 150

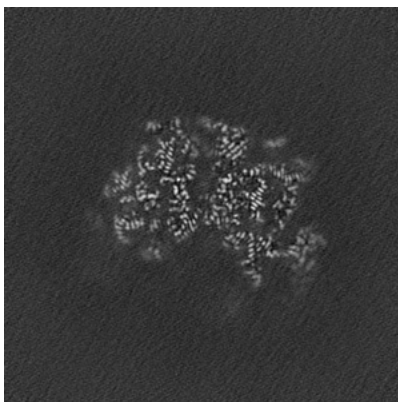


Z Index: 150

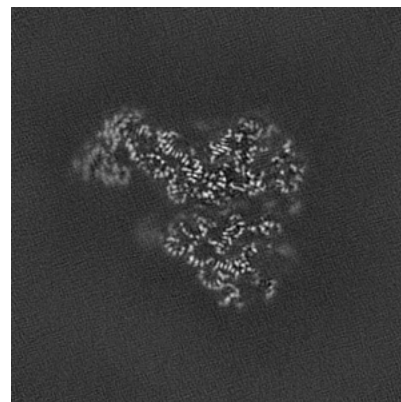
6.2.2 Raw map



X Index: 150



Y Index: 150

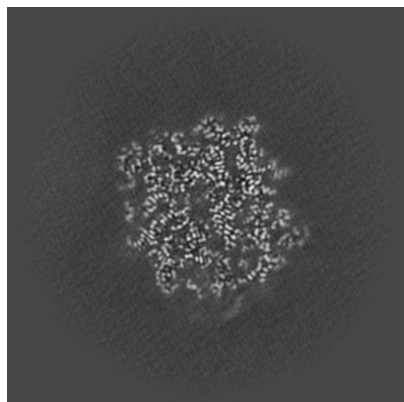


Z Index: 150

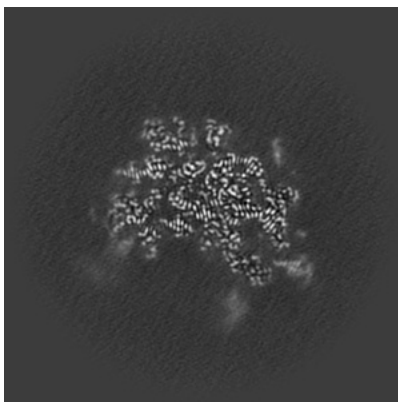
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

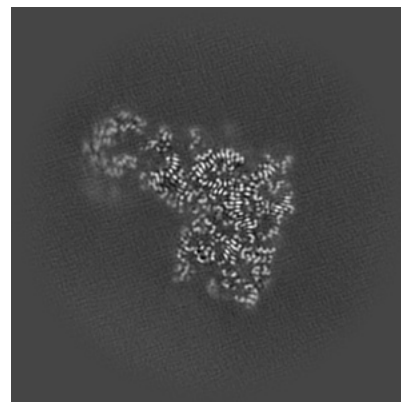
6.3.1 Primary map



X Index: 150

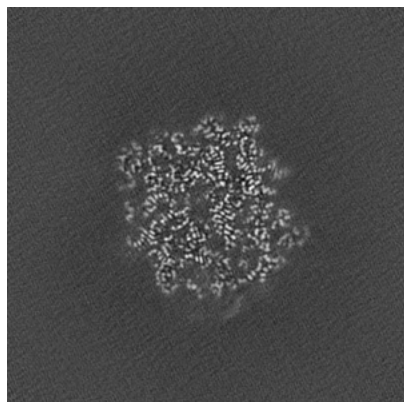


Y Index: 159

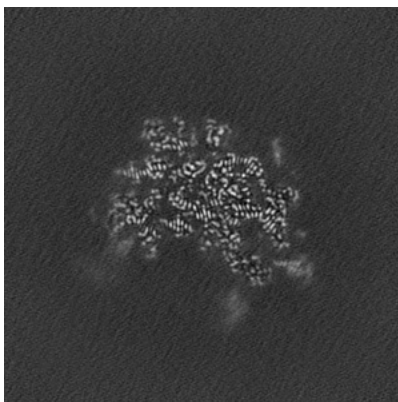


Z Index: 165

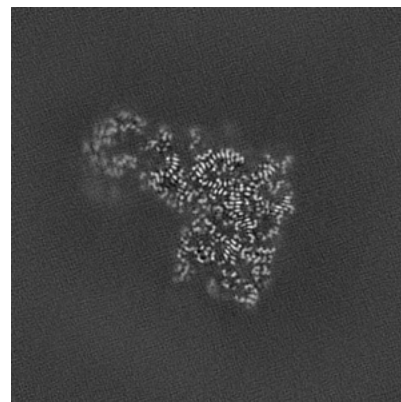
6.3.2 Raw map



X Index: 150



Y Index: 159

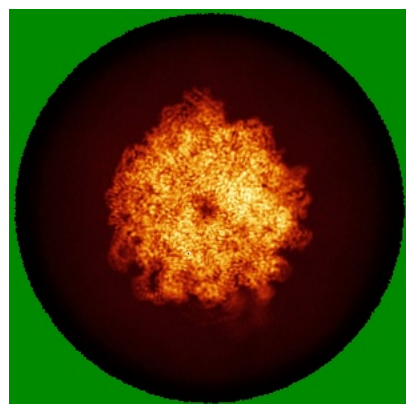


Z Index: 165

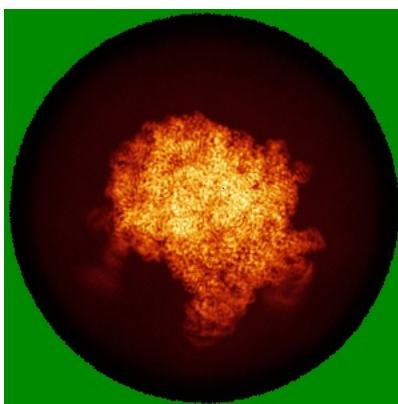
The images above show the largest variance slices of the map in three orthogonal directions.

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

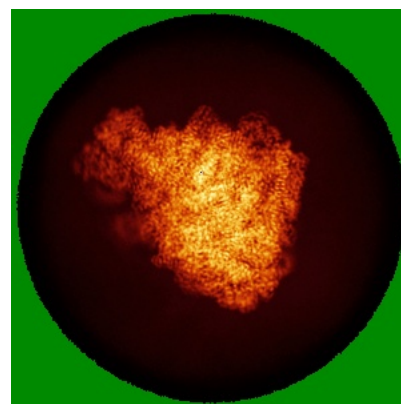
6.4.1 Primary map



X

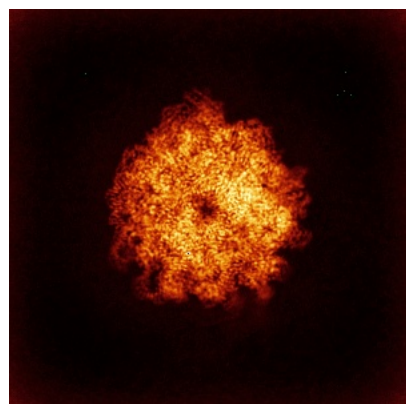


Y

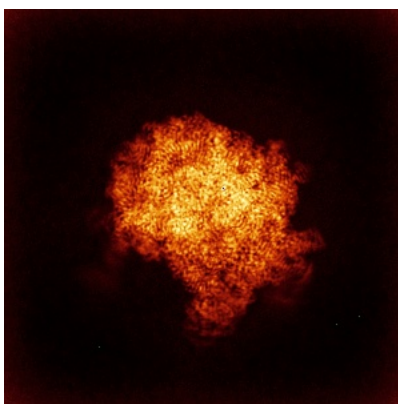


Z

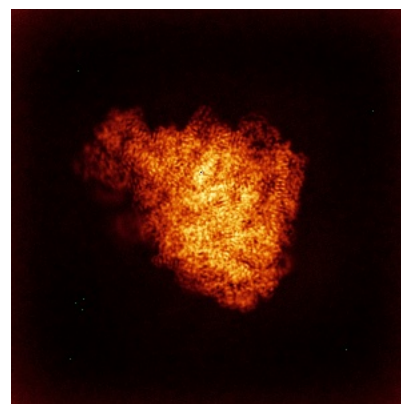
6.4.2 Raw map



X



Y



Z

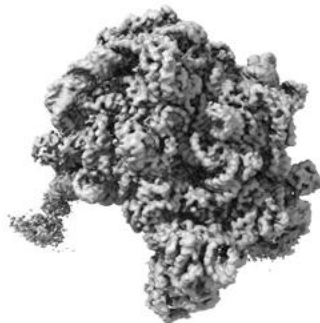
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

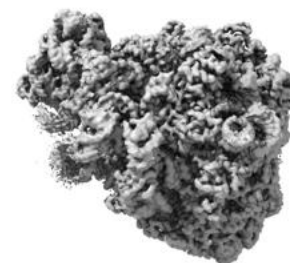
6.5.1 Primary map



X



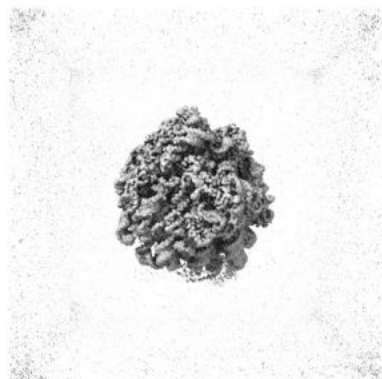
Y



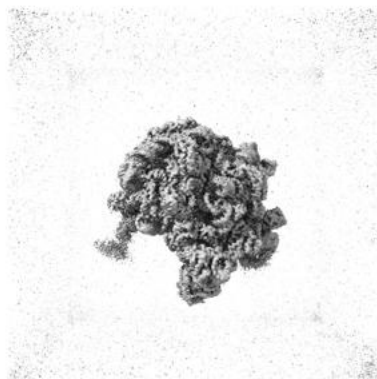
Z

The images above show the 3D surface view of the map at the recommended contour level 0.124. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

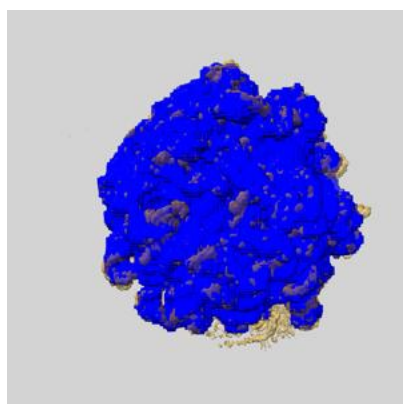
6.6 Mask visualisation [i](#)

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

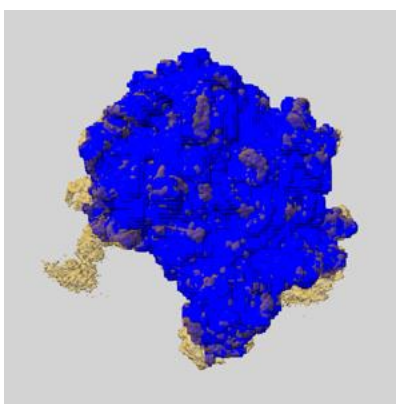
A mask typically either:

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

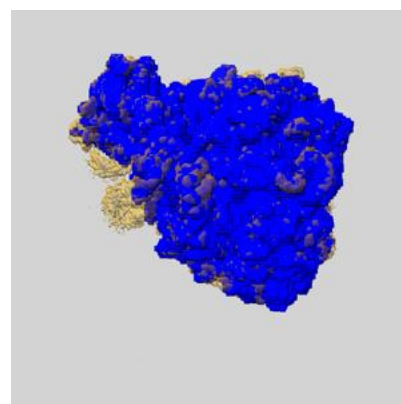
6.6.1 emd_19426_msk_1.map [i](#)



X



Y

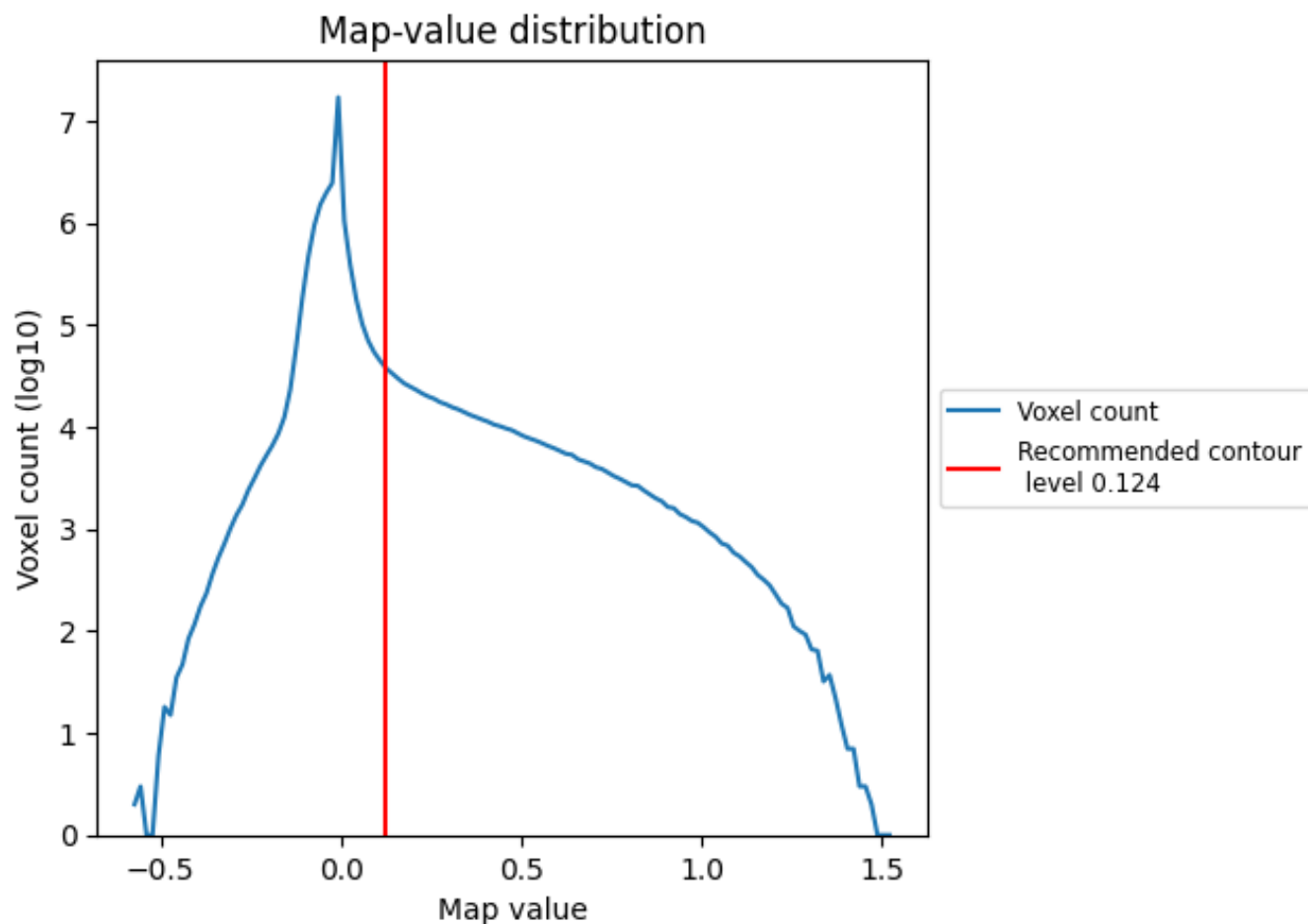


Z

7 Map analysis [i](#)

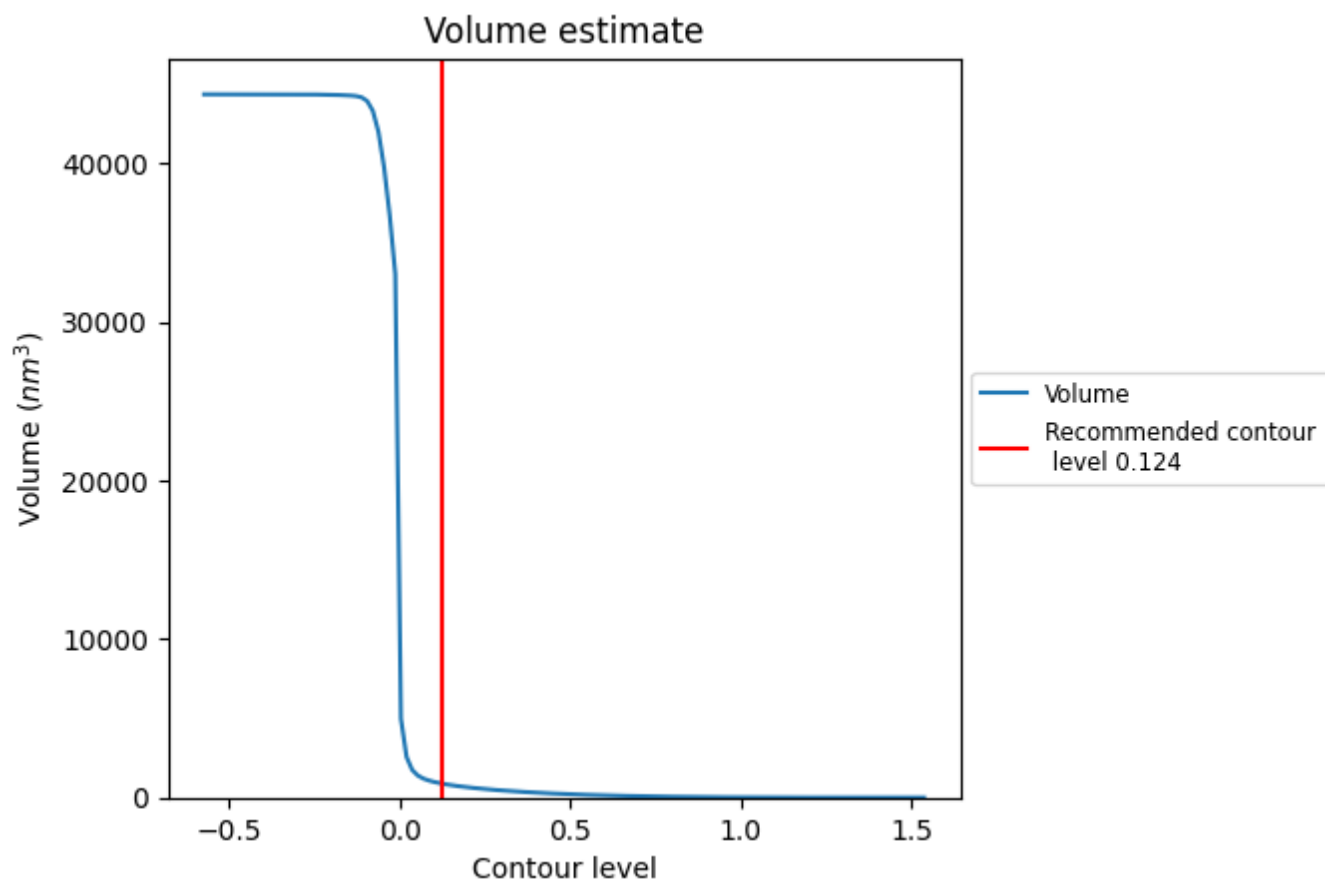
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

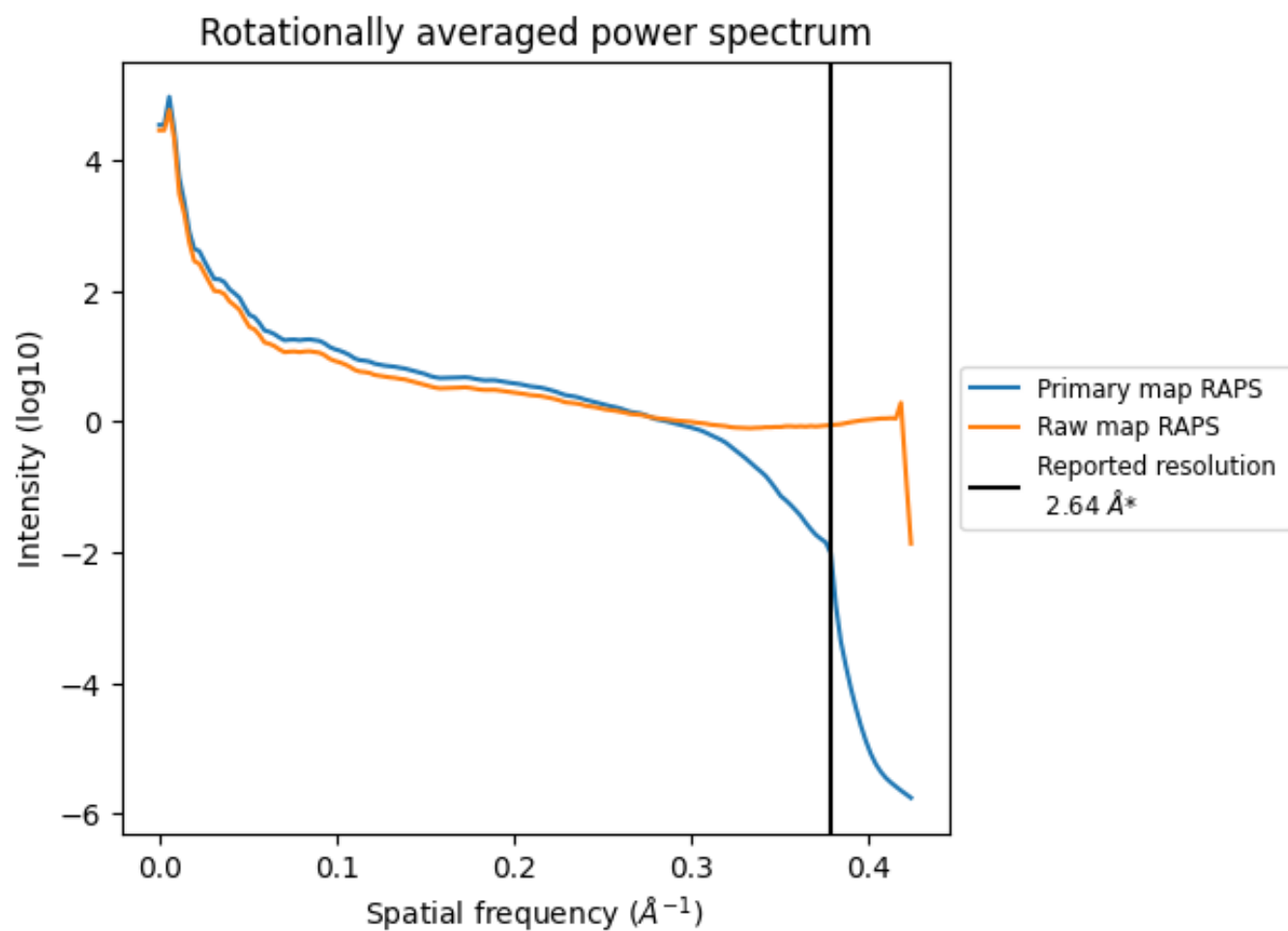
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 884 nm³; this corresponds to an approximate mass of 798 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](#)

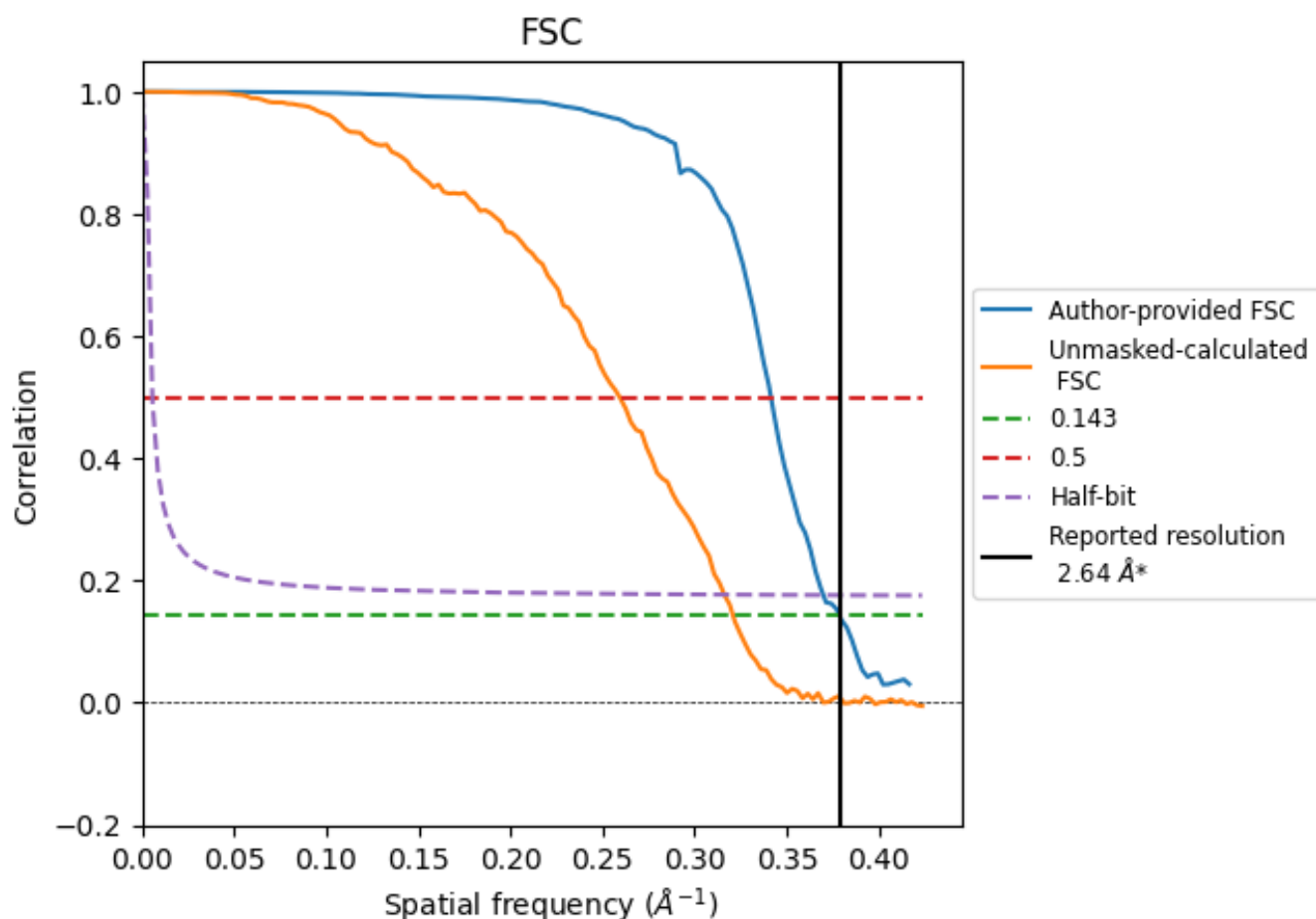


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 Å⁻¹

8.2 Resolution estimates [i](#)

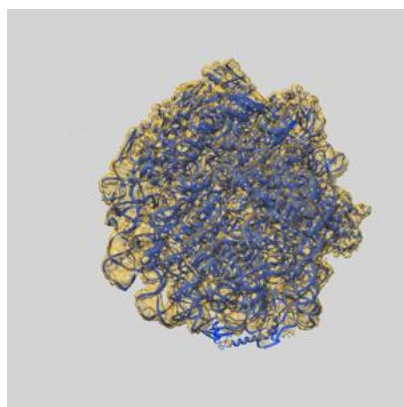
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	2.93	2.70
Unmasked-calculated*	3.12	3.86	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.64 by more than 10 %

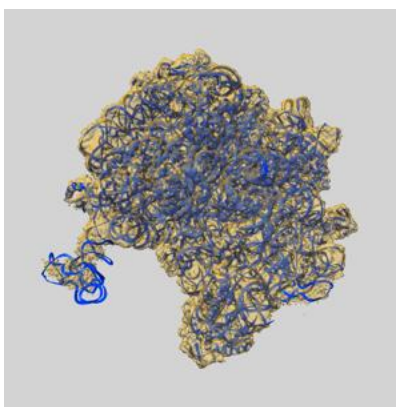
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19426 and PDB model 8RPY. Per-residue inclusion information can be found in section 3 on page 10.

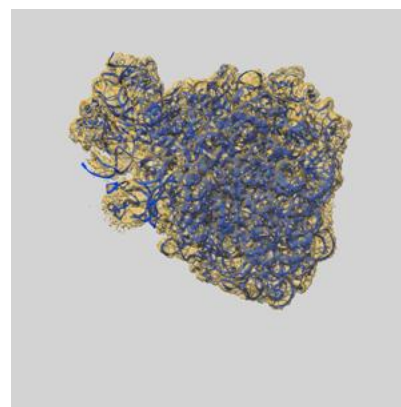
9.1 Map-model overlay [i](#)



X



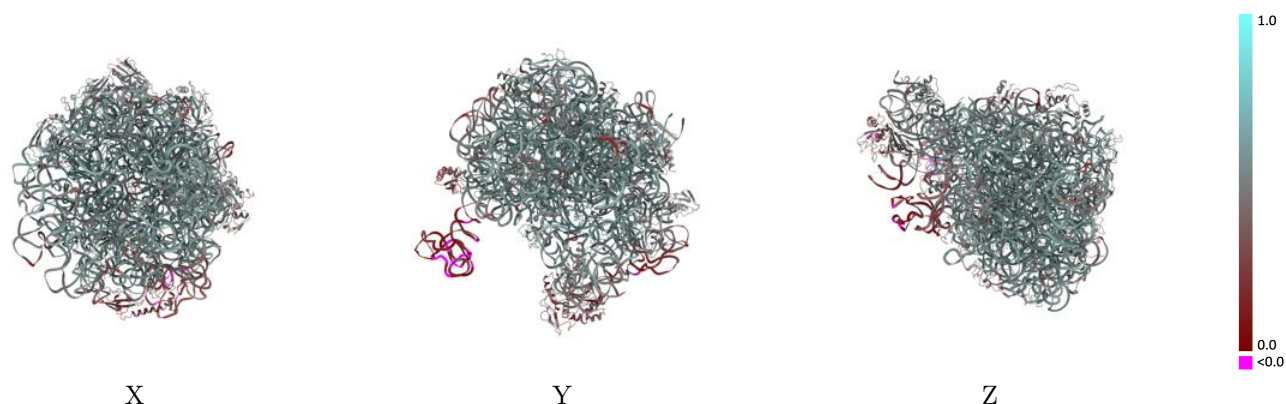
Y



Z

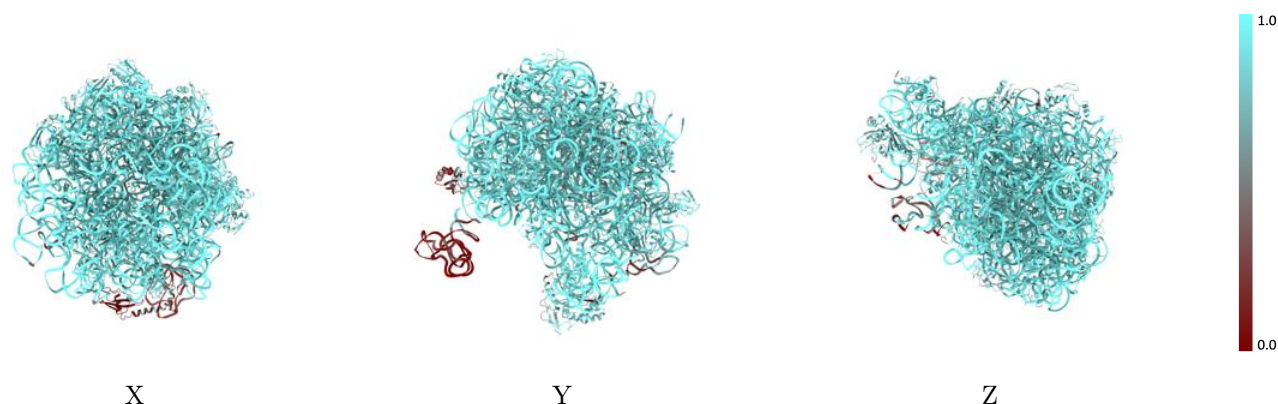
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



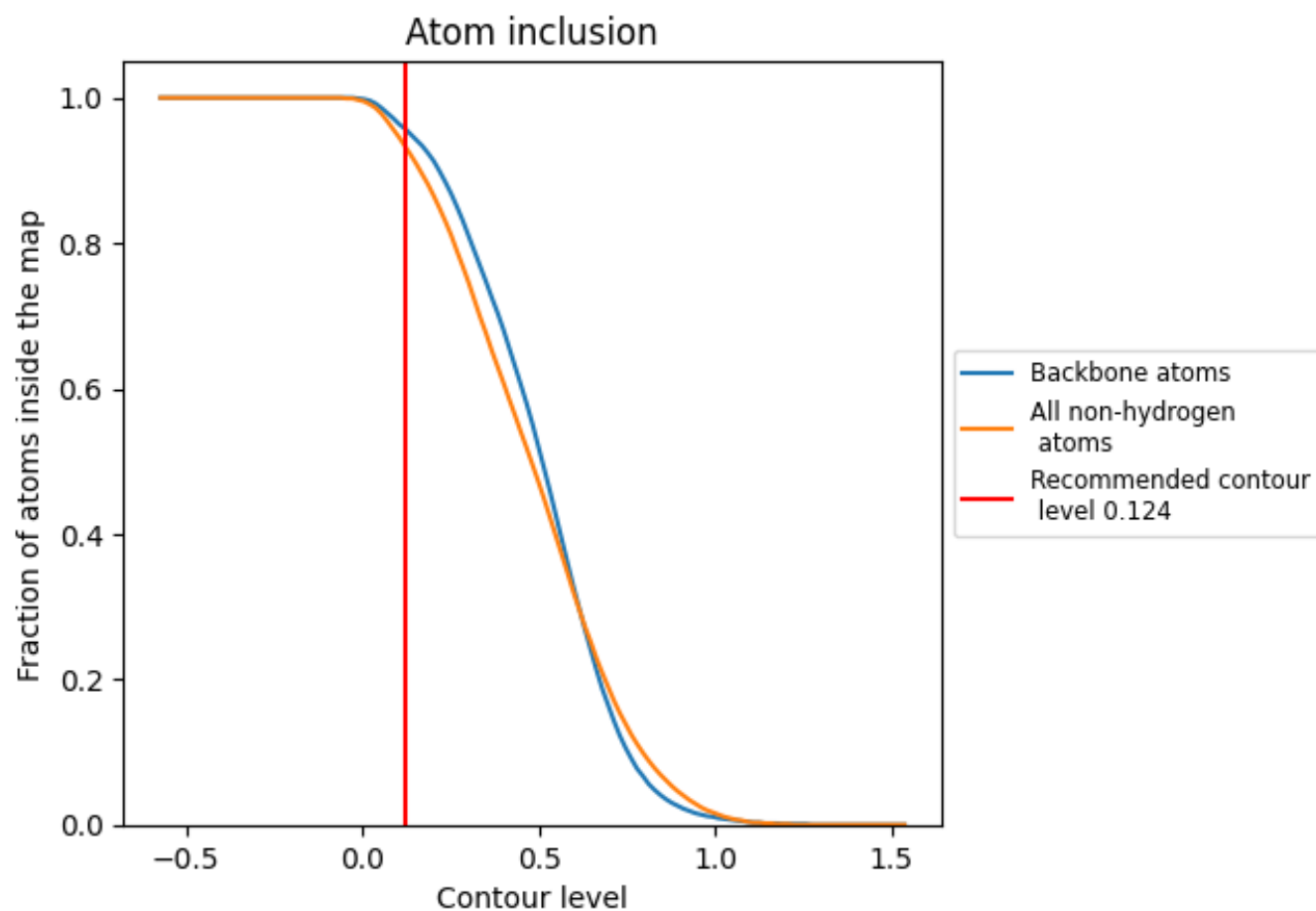
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.124).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.5190
0	 0.9320	 0.5340
1	 0.9180	 0.5130
2	 0.9440	 0.5650
3	 0.9450	 0.5590
4	 0.9310	 0.5180
6	 0.7490	 0.3360
A	 0.9500	 0.5320
B	 0.9810	 0.4960
C	 0.9470	 0.5460
D	 0.9260	 0.5300
E	 0.9080	 0.4970
F	 0.8020	 0.3510
G	 0.8710	 0.4590
H	 0.3200	 0.2940
J	 0.9410	 0.5350
K	 0.8630	 0.4980
L	 0.8930	 0.4920
M	 0.9200	 0.5290
N	 0.9410	 0.5400
O	 0.9040	 0.4650
P	 0.8840	 0.5040
Q	 0.9570	 0.5530
R	 0.8960	 0.5010
S	 0.9100	 0.5200
T	 0.9040	 0.4950
U	 0.9270	 0.4970
V	 0.9010	 0.4940
W	 0.9320	 0.5530
X	 0.9400	 0.5280
Y	 0.8890	 0.4560
Z	 0.9150	 0.5070
y	 0.5610	 0.3980
z	 0.5470	 0.4590

