



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:13 AM UTC

PDB ID : 8A5I / pdb_00008a5i
EMDB ID : EMD-15175
Title : Cryo-EM structure of Lincomycin bound to the *Listeria monocytogenes* 50S ribosomal subunit.
Authors : Koller, T.O.; Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2022-06-15
Resolution : 2.30 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:

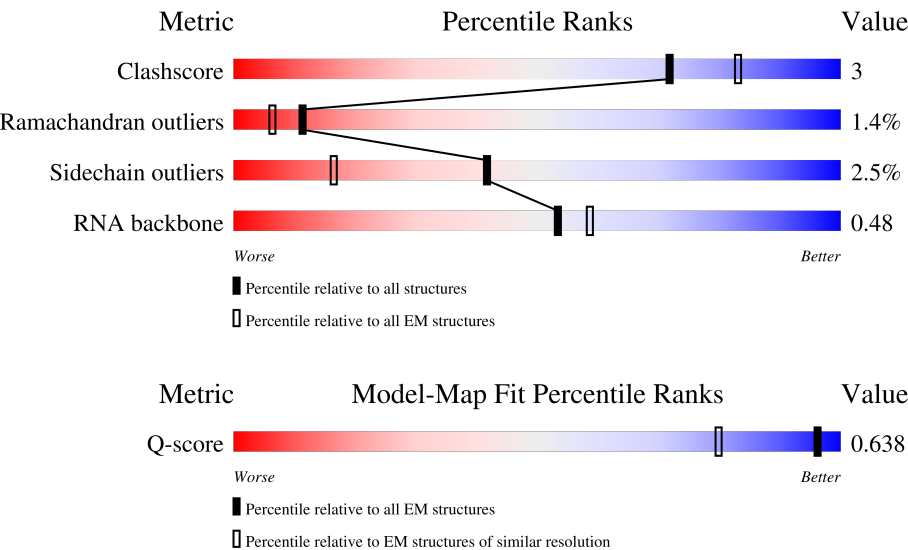
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	1	62	16% 76% 15% • 6%
2	2	63	10% 86% 8% 6%
3	3	59	• 86% 8% 5%

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Mol	Chain	Length	Quality of chain
4	4	81	
5	5	57	
6	6	49	
7	7	44	
8	8	66	
9	9	37	
10	A	2931	
11	B	114	
12	G	277	
13	H	209	
14	I	207	
15	J	179	
16	K	178	
17	M	145	
18	N	122	
19	O	146	
20	P	144	
21	Q	135	
22	R	119	
23	S	114	
24	T	119	
25	U	102	
26	V	118	
27	W	94	
28	X	103	

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Mol	Chain	Length	Quality of chain
29	Z	96	 A horizontal bar chart showing the quality of chain Z. The bar is divided into three segments: a red segment at the beginning, a green segment labeled '70%', a yellow segment labeled '6%', and a grey segment at the end labeled '24%'. A small red dot is visible at the start of the bar.

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 89799 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	58	Total	C	N	O	S	0	0
			457	283	96	76	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	59	Total	C	N	O	S	0	0
			487	298	94	94	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			477	305	75	96	1		

- Molecule 5 is a protein called 50S ribosomal protein L32-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 6 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	47	Total	C	N	O	S	0	0
			400	243	81	73	3		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	42	Total	C	N	O	S	0	0
			357	217	87	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	63	Total	C	N	O	S	0	0
			512	317	113	78	4		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2908	Total	C	N	O	P	0	0
			62459	27874	11544	20133	2908		

- Molecule 11 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	114	Total	C	N	O	P	0	0
			2430	1083	430	803	114		

- Molecule 12 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	206	Total	C	N	O	S	0	0
			1582	995	291	292	4		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	I	203	Total	C	N	O	0	0
			1563	987	286	290		

- Molecule 15 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	J	175	Total	C	N	O	S	0
			1365	865	236	258	6	0

- Molecule 16 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	K	165	Total	C	N	O	S	0
			1271	801	232	237	1	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	142	Total	C	N	O	S	0
			1117	708	201	205	3	0

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	122	Total	C	N	O	S	0
			925	573	175	172	5	0

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	144	Total	C	N	O		0
			1094	675	214	205		0

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	P	133	Total	C	N	O	S	0
			1055	675	205	170	5	0

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	122	Total	C	N	O	S	0	0
			983	619	191	172	1		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	118	Total	C	N	O		0	0
			914	564	176	174			

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	112	Total	C	N	O		0	0
			905	570	181	154			

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	116	Total	C	N	O	S	0	0
			939	596	185	154	4		

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	101	Total	C	N	O	S	0	0
			786	507	134	144	1		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	110	Total	C	N	O		0	0
			848	534	160	154			

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	90	Total	C	N	O	S	0	0
			731	462	129	138	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	95	Total	C	N	O	S	0	0
			723	459	134	127	3		

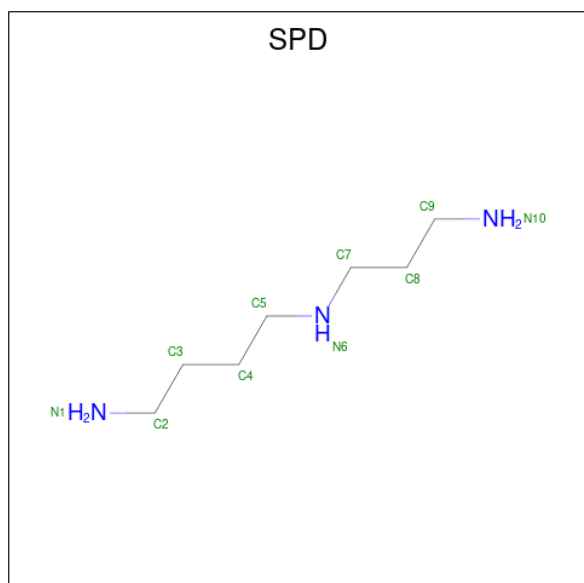
- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	73	Total	C	N	O	S	0	0
			563	345	111	106	1		

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
30	5	1	Total	Zn	0
			1	1	
30	9	1	Total	Zn	0
			1	1	

- Molecule 31 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

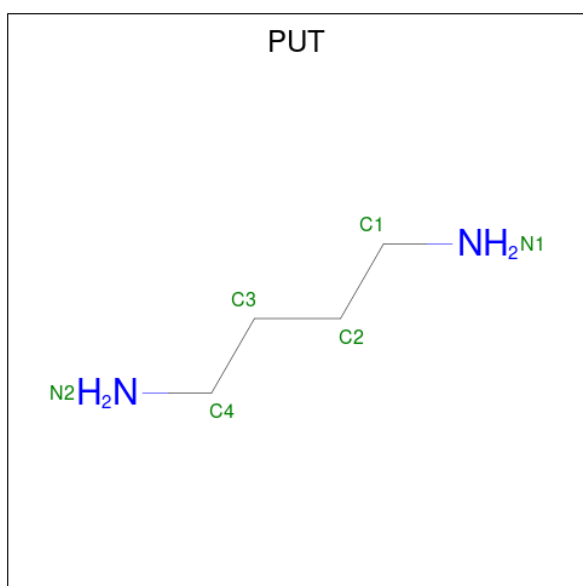


Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	N	0
			10	7	3	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

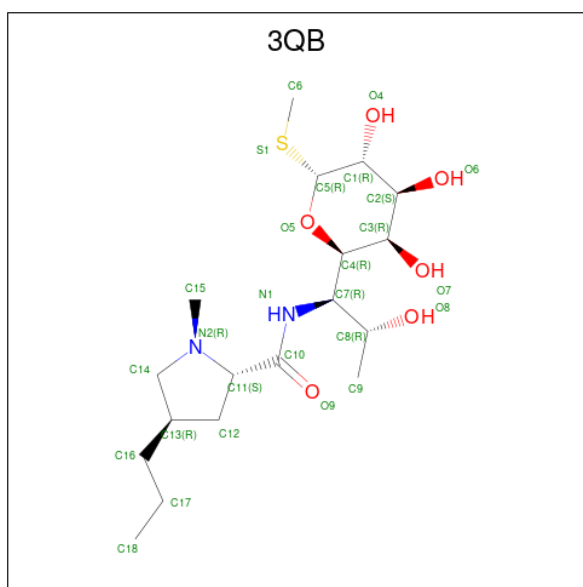
Mol	Chain	Residues	Atoms		AltConf
32	A	162	Total	Mg	0
			162	162	
32	G	1	Total	Mg	0
			1	1	
32	H	1	Total	Mg	0
			1	1	
32	O	1	Total	Mg	0
			1	1	

- Molecule 33 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	N	0
			6	4	2	
33	A	1	Total	C	N	0
			6	4	2	

- Molecule 34 is LINCOMYCIN (CCD ID: 3QB) (formula: $C_{18}H_{34}N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	S	0
			27	18	2	6	1	

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
35	P	1	Total	K	0
			1	1	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	1	1	Total	O	0
			1	1	
36	5	5	Total	O	0
			5	5	
36	7	9	Total	O	0
			9	9	
36	8	7	Total	O	0
			7	7	
36	A	1223	Total	O	0
			1223	1223	
36	B	2	Total	O	0
			2	2	
36	G	40	Total	O	0
			40	40	

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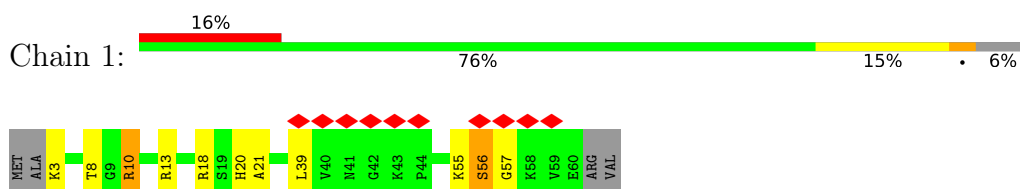
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Mol	Chain	Residues	Atoms		AltConf
36	H	12	Total 12	O 12	0
36	I	15	Total 15	O 15	0
36	M	2	Total 2	O 2	0
36	N	5	Total 5	O 5	0
36	O	24	Total 24	O 24	0
36	P	4	Total 4	O 4	0
36	Q	4	Total 4	O 4	0
36	S	8	Total 8	O 8	0
36	T	8	Total 8	O 8	0
36	U	4	Total 4	O 4	0
36	V	5	Total 5	O 5	0
36	W	1	Total 1	O 1	0
36	Z	2	Total 2	O 2	0

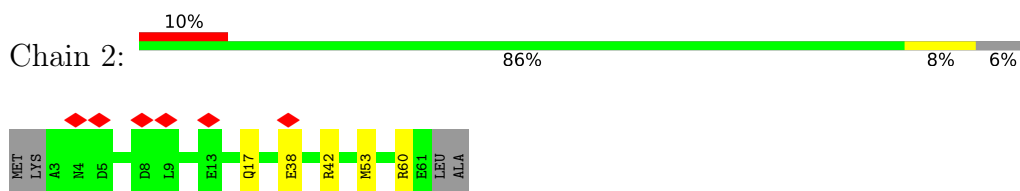
3 Residue-property plots [i](#)

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

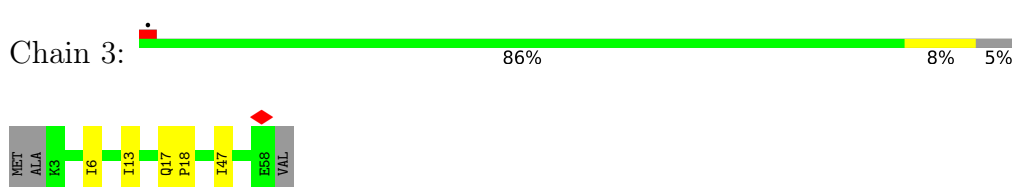
- Molecule 1: 50S ribosomal protein L28



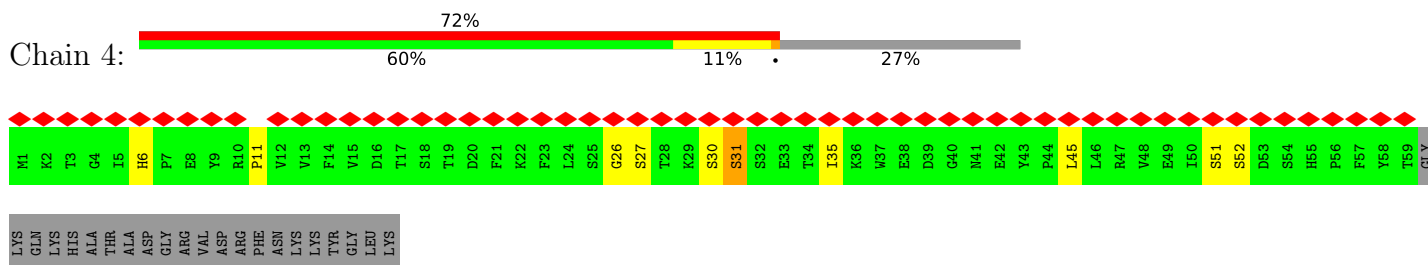
- Molecule 2: 50S ribosomal protein L29



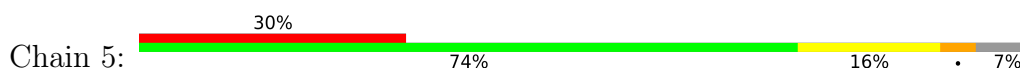
- Molecule 3: 50S ribosomal protein L30

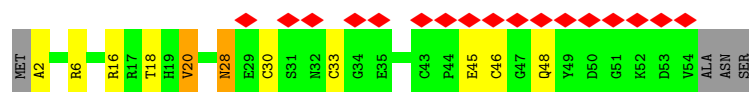


- Molecule 4: 50S ribosomal protein L31 type B

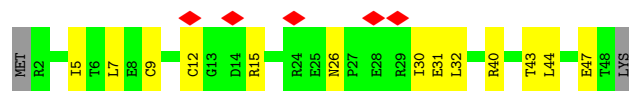


- Molecule 5: 50S ribosomal protein L32-2





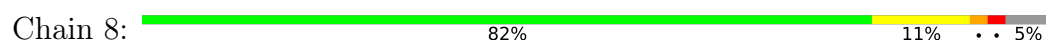
- Molecule 6: 50S ribosomal protein L33 1



- Molecule 7: 50S ribosomal protein L34



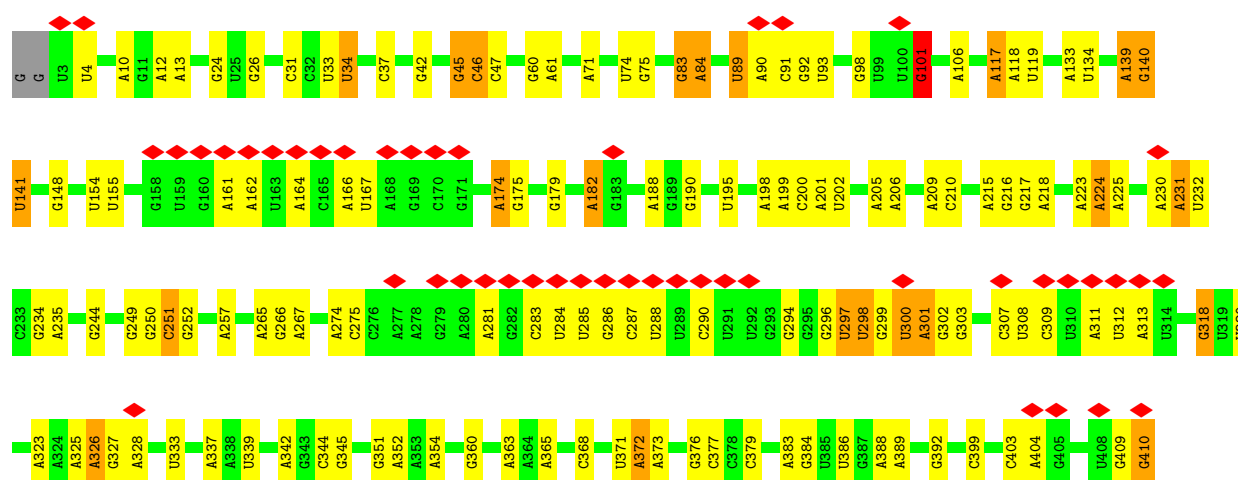
- Molecule 8: 50S ribosomal protein L35

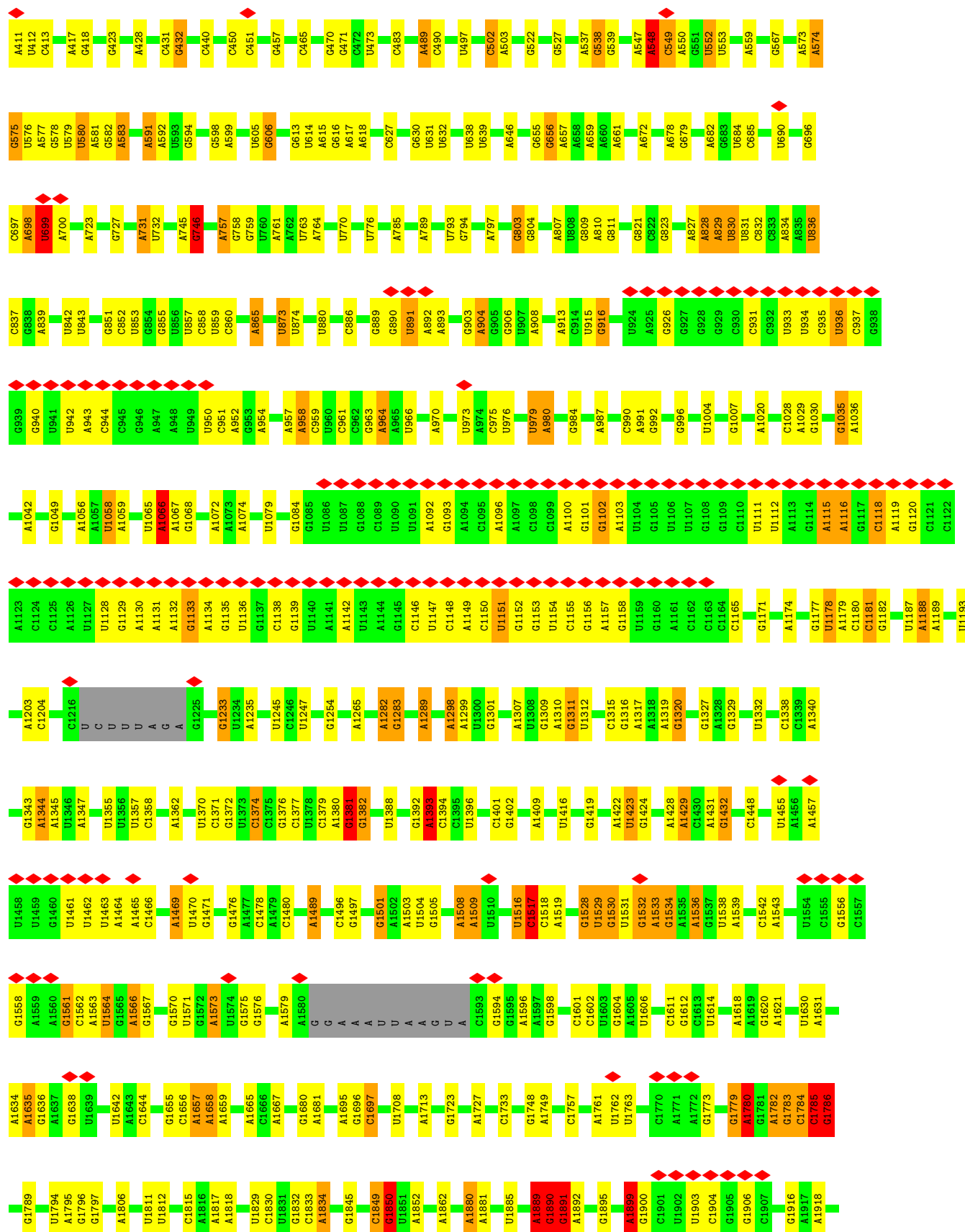


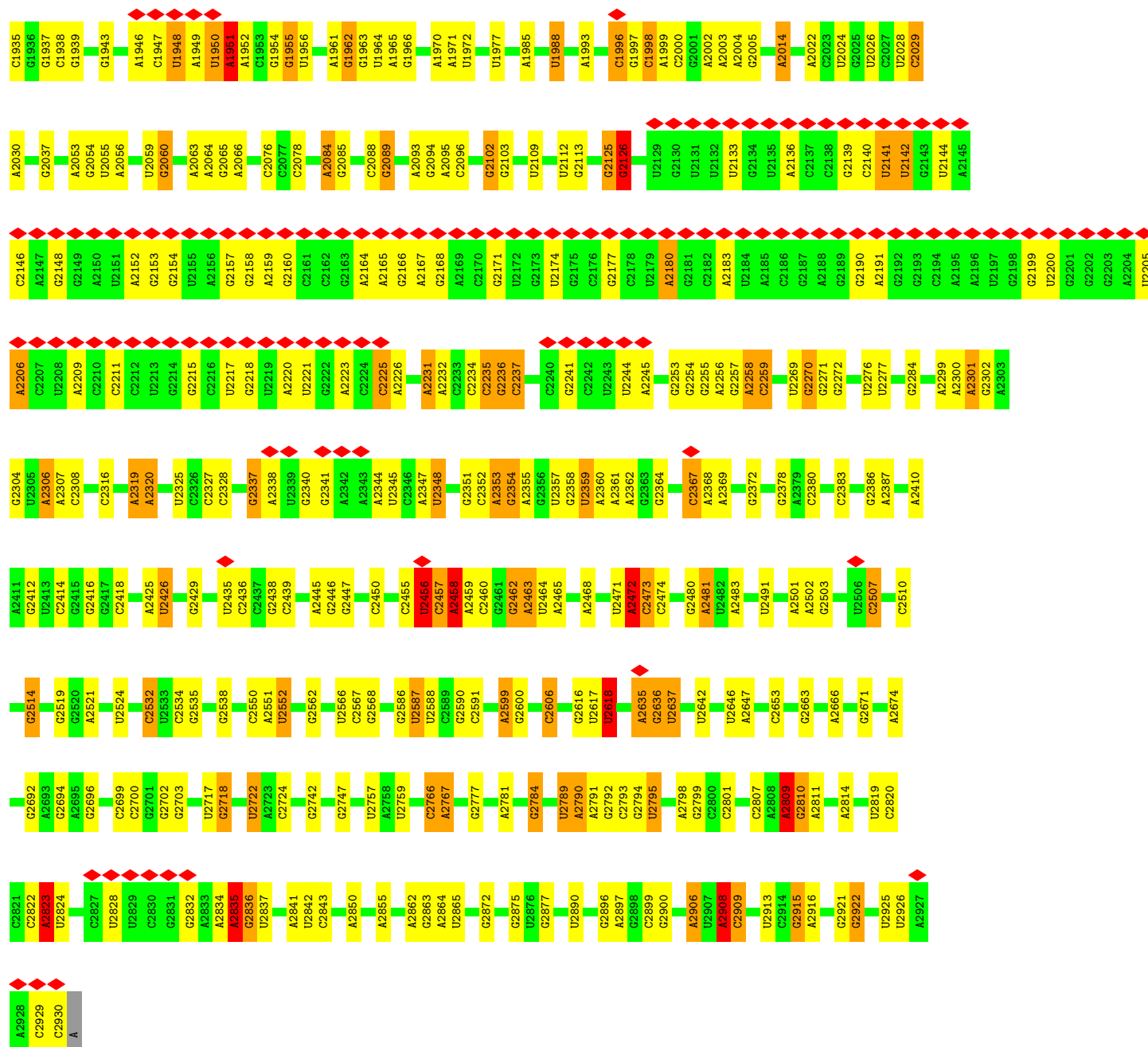
- Molecule 9: 50S ribosomal protein L36



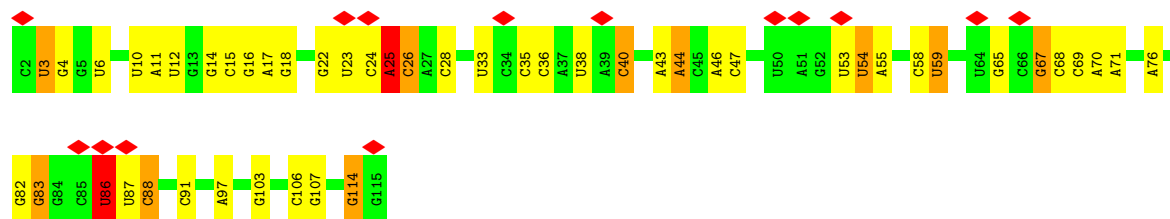
- Molecule 10: 23S ribosomal RNA





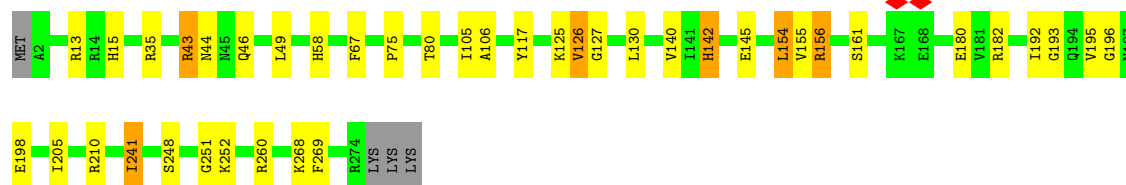


• Molecule 11: 5S ribosomal RNA



• Molecule 12: 50S ribosomal protein L2

Chain G:  84% 13% ..



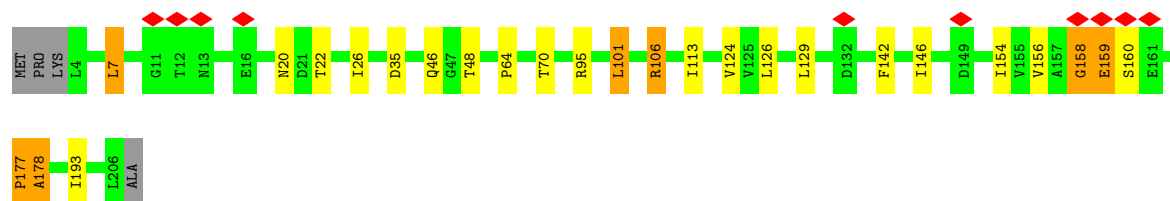
- Molecule 13: 50S ribosomal protein L3

Chain H:  89% 10% .



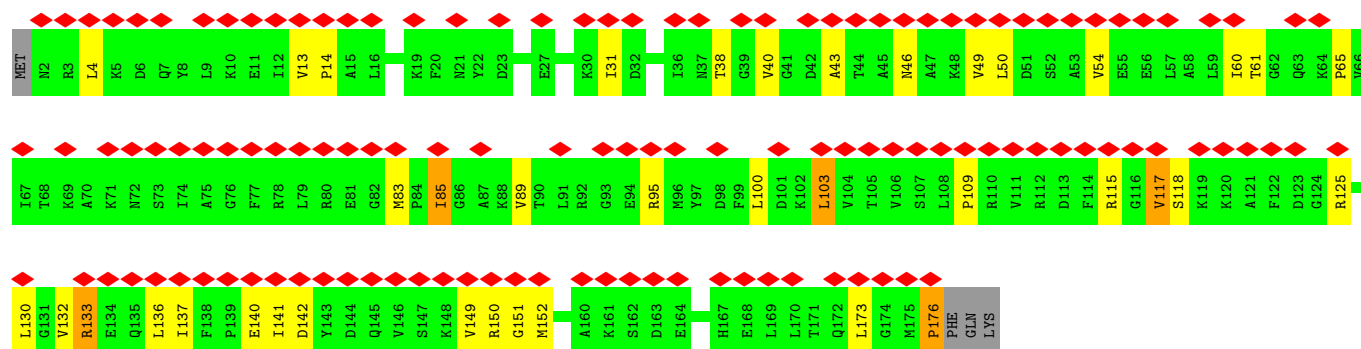
- Molecule 14: 50S ribosomal protein L4

Chain I:  5% 86% 9% ..



- Molecule 15: 50S ribosomal protein L5

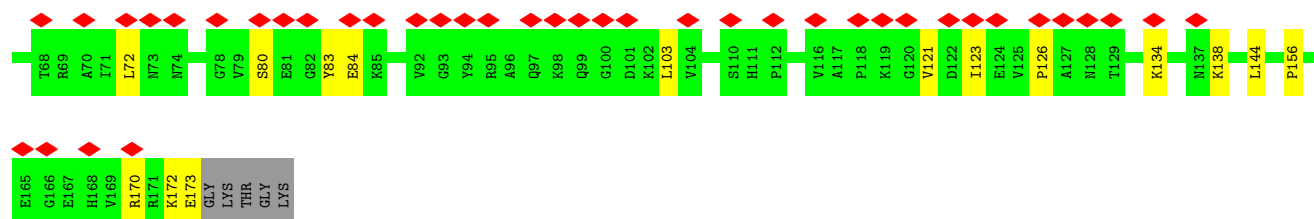
Chain J:  70% 76% 19% ..



- Molecule 16: 50S ribosomal protein L6

Chain K:  50% 80% 13% 7%





- Molecule 17: 50S ribosomal protein L13

Chain M: 79% 17% . .



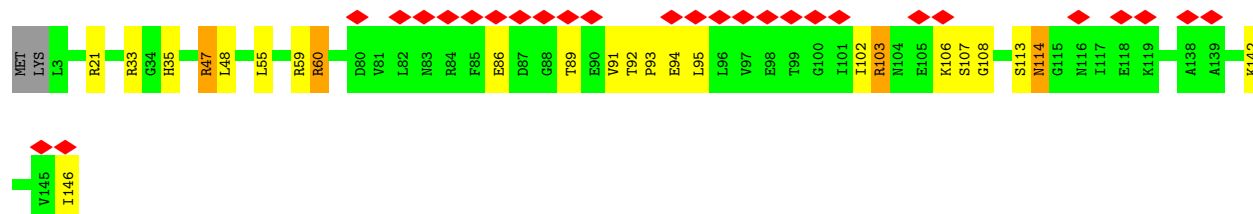
- Molecule 18: 50S ribosomal protein L14

Chain N: 77% 20% .



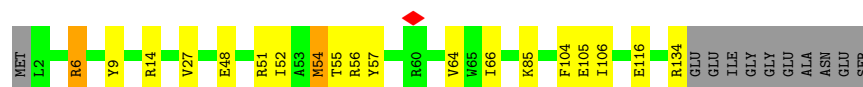
- Molecule 19: 50S ribosomal protein L15

Chain O: 18% 82% 14% . .



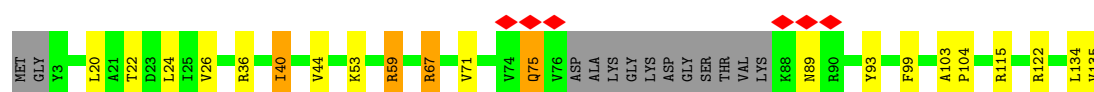
- Molecule 20: 50S ribosomal protein L16

Chain P: 79% 12% 8%

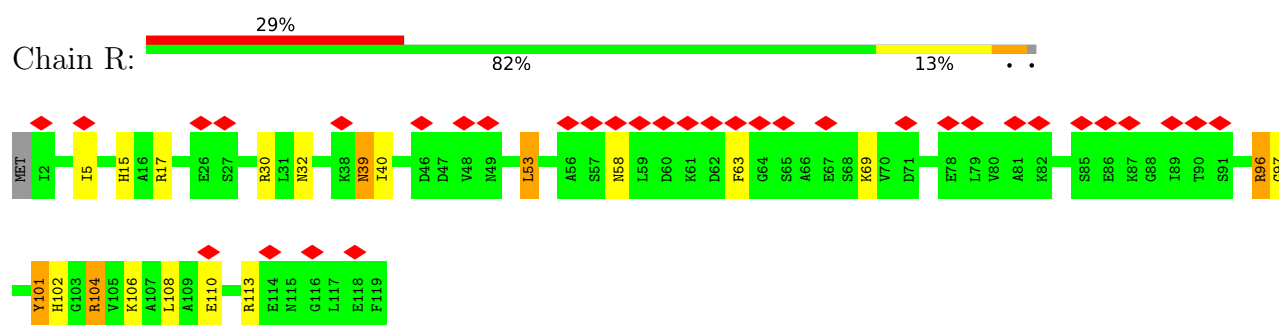


- Molecule 21: 50S ribosomal protein L17

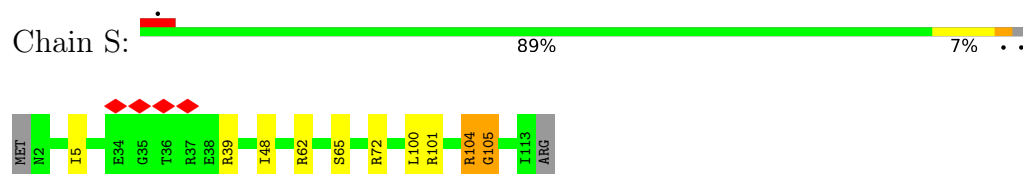
Chain Q: 75% 13% 10%



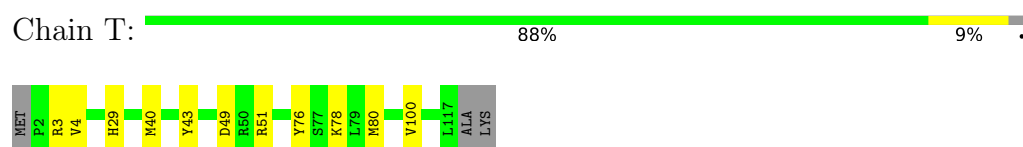
- Molecule 22: 50S ribosomal protein L18



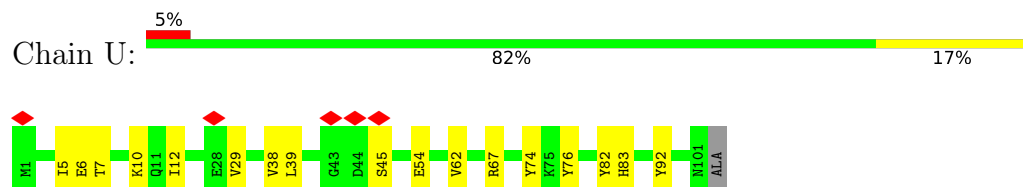
- Molecule 23: 50S ribosomal protein L19



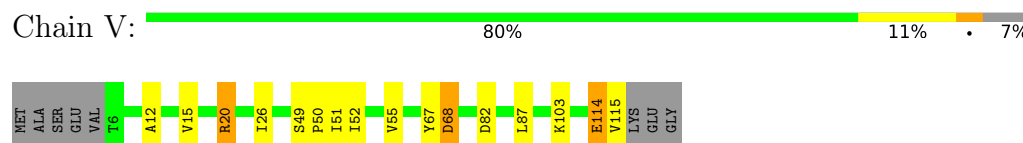
- Molecule 24: 50S ribosomal protein L20



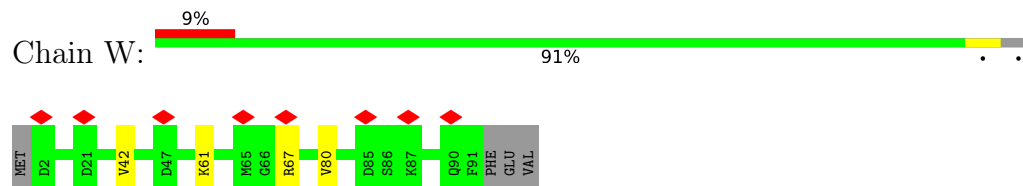
- Molecule 25: 50S ribosomal protein L21



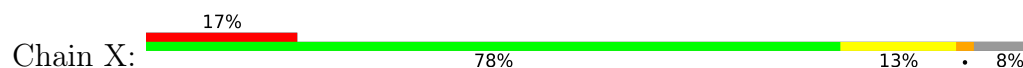
- Molecule 26: 50S ribosomal protein L22

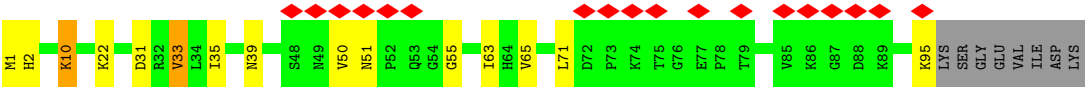


- Molecule 27: 50S ribosomal protein L23

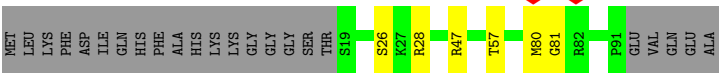


- Molecule 28: 50S ribosomal protein L24





• Molecule 29: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285330	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 ($e^-/\text{\AA}^2$)	40.3	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	270000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.433	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	309.0, 309.0, 309.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7725, 0.7725, 0.7725	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, MG, 3QB, K, ZN, PUT

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	1	0.52	0/462	0.81	0/612
2	2	0.40	0/488	0.80	0/651
3	3	0.50	0/436	0.77	0/585
4	4	0.51	0/491	0.80	0/666
5	5	0.59	0/433	0.86	0/577
6	6	0.44	0/404	0.79	0/541
7	7	0.58	0/360	0.97	1/469 (0.2%)
8	8	0.59	0/519	0.82	0/675
9	9	0.53	0/295	0.89	0/387
10	A	0.59	0/69974	1.11	310/109160 (0.3%)
11	B	0.80	0/2714	1.11	25/4229 (0.6%)
12	G	0.96	3/2144 (0.1%)	1.32	6/2875 (0.2%)
13	H	0.95	0/1604	1.27	0/2156
14	I	0.97	0/1583	1.35	1/2133 (0.0%)
15	J	1.07	0/1383	1.46	0/1863
16	K	1.09	0/1293	1.36	0/1749
17	M	0.94	0/1140	1.26	1/1533 (0.1%)
18	N	0.92	0/932	1.31	0/1248
19	O	0.99	1/1105 (0.1%)	1.36	0/1470
20	P	0.90	0/1077	1.32	0/1439
21	Q	0.91	0/994	1.36	0/1329
22	R	1.03	0/923	1.50	0/1232
23	S	0.93	0/917	1.26	0/1230
24	T	0.89	1/952 (0.1%)	1.36	0/1266
25	U	0.95	1/799 (0.1%)	1.24	0/1072
26	V	0.93	0/858	1.28	0/1160
27	W	0.89	0/739	1.32	0/990
28	X	1.07	0/733	1.34	1/980 (0.1%)
29	Z	0.87	0/570	1.23	0/758
All	All	0.69	6/96322 (0.0%)	1.15	345/145035 (0.2%)

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
1	1	0	3
2	2	0	1
5	5	0	1
6	6	0	1
7	7	0	2
8	8	0	3
12	G	0	6
14	I	0	2
15	J	0	1
16	K	0	1
17	M	0	2
18	N	0	1
19	O	0	4
20	P	0	4
21	Q	0	4
22	R	0	4
23	S	0	3
24	T	0	2
25	U	0	1
26	V	0	1
29	Z	0	2
All	All	0	49

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	15	HIS	CE1-NE2	5.68	1.38	1.32
19	O	35	HIS	CE1-NE2	5.38	1.38	1.32
25	U	83	HIS	CE1-NE2	5.21	1.37	1.32
24	T	29	HIS	CE1-NE2	5.15	1.37	1.32
12	G	142	HIS	CE1-NE2	5.06	1.37	1.32
12	G	58	HIS	CE1-NE2	5.05	1.37	1.32

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	731	A	O3'-P-O5'	-12.50	85.25	104.00
10	A	1849	C	C2'-C3'-O3'	-11.62	96.27	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2809	A	P-O3'-C3'	10.87	136.50	120.20
10	A	2908	A	C2'-C3'-O3'	10.82	125.73	109.50
10	A	2458	A	P-O3'-C3'	10.75	136.32	120.20
10	A	251	C	C2'-C3'-O3'	10.06	124.59	109.50
10	A	224	A	O3'-P-O5'	-10.05	88.92	104.00
10	A	605	U	P-O3'-C3'	-10.05	105.13	120.20
10	A	1849	C	O3'-P-O5'	-9.93	89.10	104.00
10	A	1748	G	O3'-P-O5'	-9.16	90.25	104.00
10	A	574	A	P-O3'-C3'	9.05	133.78	120.20
10	A	2809	A	C2'-C3'-O3'	8.66	122.50	109.50
10	A	2908	A	P-O3'-C3'	8.20	132.50	120.20
10	A	489	A	O3'-P-O5'	-8.15	91.78	104.00
10	A	83	G	O3'-P-O5'	-7.99	92.02	104.00
10	A	2002	A	O3'-P-O5'	7.84	115.76	104.00
10	A	745	A	O3'-P-O5'	-7.77	92.34	104.00
10	A	2618	U	P-O3'-C3'	-7.60	108.80	120.20
10	A	1380	A	O3'-P-O5'	-7.43	92.86	104.00
10	A	548	A	P-O3'-C3'	7.40	131.30	120.20
10	A	2472	A	P-O3'-C3'	7.37	131.26	120.20
10	A	296	G	O3'-P-O5'	-7.30	93.04	104.00
10	A	873	U	C2'-C3'-O3'	-7.16	102.95	113.70
10	A	502	C	P-O3'-C3'	-7.08	109.58	120.20
12	G	154	LEU	CA-C-N	-7.08	116.23	122.96
12	G	154	LEU	C-N-CA	-7.08	116.23	122.96
10	A	539	G	C4'-C3'-O3'	-7.08	102.38	113.00
10	A	2337	G	P-O3'-C3'	-7.06	109.61	120.20
10	A	2606	C	O3'-P-O5'	-7.05	93.42	104.00
10	A	1178	U	P-O3'-C3'	-7.00	109.69	120.20
10	A	2534	C	O3'-P-O5'	-7.00	93.50	104.00
10	A	2109	U	P-O3'-C3'	-6.94	109.78	120.20
10	A	224	A	C2'-C3'-O3'	6.89	119.83	109.50
10	A	574	A	C2'-C3'-O3'	6.86	119.78	109.50
10	A	1602	C	P-O3'-C3'	-6.83	109.95	120.20
10	A	251	C	P-O3'-C3'	6.82	130.43	120.20
10	A	1785	C	P-O5'-C5'	-6.81	110.69	120.90
10	A	2258	A	C2'-C3'-O3'	6.78	119.67	109.50
10	A	980	A	P-O3'-C3'	-6.77	110.04	120.20
10	A	1786	G	P-O5'-C5'	-6.76	110.76	120.90
10	A	431	C	O3'-P-O5'	-6.73	93.90	104.00
10	A	1388	U	P-O3'-C3'	-6.72	110.12	120.20
10	A	1538	U	P-O3'-C3'	-6.64	110.24	120.20
10	A	731	A	C4'-C3'-O3'	6.64	119.36	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	827	A	O3'-P-O5'	-6.62	94.06	104.00
10	A	538	G	O3'-P-O5'	-6.58	94.13	104.00
10	A	2807	C	P-O3'-C3'	-6.56	110.36	120.20
10	A	1620	G	C4'-C3'-O3'	-6.55	103.18	113.00
11	B	86	U	P-O3'-C3'	-6.53	110.40	120.20
10	A	1517	C	C1'-O4'-C4'	-6.48	103.42	109.90
10	A	1529	U	P-O3'-C3'	-6.41	110.58	120.20
10	A	1782	A	P-O3'-C3'	-6.38	110.64	120.20
10	A	1282	A	O3'-P-O5'	-6.36	94.46	104.00
11	B	47	C	P-O3'-C3'	-6.35	110.68	120.20
10	A	1177	G	O3'-P-O5'	-6.29	94.56	104.00
10	A	2462	G	C4'-C3'-O3'	-6.27	103.59	113.00
10	A	1891	G	P-O3'-C3'	-6.26	110.80	120.20
10	A	231	A	C4'-C3'-O3'	6.26	118.78	109.40
10	A	2820	C	P-O3'-C3'	-6.24	110.84	120.20
10	A	1362	A	P-O3'-C3'	-6.24	110.84	120.20
10	A	89	U	P-O3'-C3'	-6.24	110.85	120.20
10	A	1381	G	P-O3'-C3'	-6.21	110.89	120.20
10	A	598	G	P-O3'-C3'	-6.20	110.90	120.20
10	A	298	U	P-O3'-C3'	-6.20	110.91	120.20
10	A	2190	G	P-O3'-C3'	-6.17	110.94	120.20
10	A	1422	A	O3'-P-O5'	-6.17	94.75	104.00
10	A	1315	C	C2'-C3'-O3'	-6.16	104.46	113.70
10	A	1497	G	P-O3'-C3'	-6.16	110.96	120.20
11	B	54	U	P-O3'-C3'	-6.14	110.99	120.20
12	G	43	ARG	CA-C-N	6.14	133.26	121.54
12	G	43	ARG	C-N-CA	6.14	133.26	121.54
10	A	2359	U	P-O3'-C3'	-6.13	111.00	120.20
10	A	2456	U	C2'-C3'-O3'	6.13	118.70	109.50
10	A	224	A	C4'-C3'-O3'	-6.13	100.21	109.40
10	A	1118	C	P-O3'-C3'	-6.13	111.01	120.20
10	A	1880	A	P-O3'-C3'	-6.13	111.01	120.20
10	A	377	C	O3'-P-O5'	-6.12	94.81	104.00
10	A	2458	A	C2'-C3'-O3'	6.12	118.69	109.50
10	A	1999	A	O3'-P-O5'	-6.11	94.84	104.00
10	A	1895	G	P-O3'-C3'	-6.10	111.05	120.20
10	A	2438	G	P-O3'-C3'	-6.09	111.07	120.20
10	A	2550	C	P-O3'-C3'	-6.08	111.08	120.20
10	A	2463	A	P-O3'-C3'	-6.07	111.10	120.20
10	A	1428	A	O3'-P-O5'	-6.06	94.91	104.00
10	A	2103	G	C4'-C3'-O3'	-6.06	103.91	113.00
10	A	1233	G	C4'-C3'-O3'	-6.05	103.93	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	904	A	P-O3'-C3'	-6.03	111.15	120.20
10	A	979	U	P-O3'-C3'	-6.03	111.15	120.20
10	A	2718	G	P-O3'-C3'	-6.02	111.17	120.20
10	A	206	A	O3'-P-O5'	-6.01	94.98	104.00
10	A	1780	A	P-O3'-C3'	-6.01	111.18	120.20
10	A	1181	C	C2'-C3'-O3'	-6.01	104.69	113.70
10	A	2566	U	P-O3'-C3'	-6.00	111.19	120.20
10	A	428	A	P-O3'-C3'	-6.00	111.19	120.20
10	A	591	A	C4'-C3'-O3'	6.00	118.41	109.40
10	A	2126	G	C4'-C3'-C2'	-5.98	96.62	102.60
10	A	2284	G	C3'-C2'-O2'	5.94	119.61	110.70
10	A	2472	A	C2'-C3'-O3'	5.94	118.41	109.50
10	A	2906	A	P-O3'-C3'	-5.93	111.31	120.20
10	A	1299	A	C4'-C3'-O3'	-5.92	104.11	113.00
10	A	2647	A	O3'-P-O5'	-5.92	95.11	104.00
10	A	296	G	C4'-C3'-O3'	-5.92	104.11	113.00
10	A	2793	C	P-O3'-C3'	-5.92	111.33	120.20
10	A	1178	U	O3'-P-O5'	-5.91	95.13	104.00
10	A	1476	G	C4'-C3'-O3'	-5.91	104.13	113.00
10	A	678	A	C2'-C3'-O3'	-5.89	104.86	113.70
10	A	1999	A	P-O3'-C3'	-5.89	111.36	120.20
10	A	1066	A	P-O3'-C3'	5.88	129.03	120.20
10	A	337	A	P-O3'-C3'	-5.88	111.38	120.20
10	A	984	G	P-O3'-C3'	-5.87	111.40	120.20
10	A	46	C	P-O3'-C3'	-5.86	111.41	120.20
10	A	891	U	P-O3'-C3'	-5.86	111.41	120.20
10	A	961	C	P-O3'-C3'	-5.84	111.44	120.20
10	A	699	U	P-O3'-C3'	-5.83	111.45	120.20
10	A	2257	G	C4'-C3'-O3'	-5.83	104.25	113.00
10	A	403	C	P-O3'-C3'	-5.82	111.46	120.20
10	A	2908	A	C4'-C3'-O3'	-5.82	100.67	109.40
10	A	2372	G	P-O3'-C3'	-5.82	111.47	120.20
10	A	2386	G	O3'-P-O5'	-5.82	95.27	104.00
10	A	1564	U	P-O3'-C3'	-5.81	111.48	120.20
10	A	1528	G	C2'-C3'-O3'	5.80	122.41	113.70
10	A	1379	C	O3'-P-O5'	-5.79	95.31	104.00
10	A	1116	A	P-O3'-C3'	-5.77	111.54	120.20
10	A	2241	G	P-O3'-C3'	-5.77	111.54	120.20
10	A	1004	U	P-O3'-C3'	-5.77	111.55	120.20
10	A	2225	C	P-O3'-C3'	-5.75	111.58	120.20
10	A	2255	G	P-O3'-C3'	-5.74	111.59	120.20
10	A	580	U	P-O3'-C3'	-5.72	111.61	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1135	G	P-O3'-C3'	-5.71	111.63	120.20
10	A	1516	U	C2'-C3'-O3'	-5.71	105.14	113.70
10	A	1655	G	C2'-C3'-O3'	-5.69	105.16	113.70
10	A	770	U	P-O3'-C3'	-5.68	111.68	120.20
11	B	14	G	P-O3'-C3'	-5.67	111.69	120.20
17	M	27	GLY	N-CA-C	-5.67	105.28	112.54
10	A	2028	U	C2'-C3'-O3'	-5.67	105.20	113.70
11	B	16	G	P-O3'-C3'	-5.66	111.71	120.20
10	A	1310	A	P-O3'-C3'	-5.66	111.72	120.20
10	A	952	A	P-O3'-C3'	-5.65	111.72	120.20
10	A	1504	U	O3'-P-O5'	-5.65	95.53	104.00
10	A	1065	U	P-O3'-C3'	-5.64	111.74	120.20
10	A	413	C	P-O3'-C3'	-5.64	111.74	120.20
10	A	2635	A	P-O3'-C3'	-5.64	111.74	120.20
11	B	70	A	P-O3'-C3'	-5.64	111.74	120.20
10	A	101	G	P-O3'-C3'	-5.63	111.76	120.20
10	A	2510	C	O3'-P-O5'	-5.63	95.56	104.00
10	A	489	A	C2'-C3'-O3'	-5.62	105.27	113.70
10	A	2534	C	C4'-C3'-O3'	-5.61	104.58	113.00
10	A	1954	G	P-O3'-C3'	-5.61	111.79	120.20
10	A	1889	A	P-O3'-C3'	-5.61	111.79	120.20
10	A	829	A	P-O3'-C3'	-5.60	111.80	120.20
11	B	71	A	P-O3'-C3'	-5.60	111.80	120.20
10	A	1344	A	C2'-C3'-O3'	5.60	117.89	109.50
10	A	2235	C	P-O3'-C3'	-5.60	111.81	120.20
10	A	1298	A	C2'-C3'-O3'	5.59	117.88	109.50
12	G	145	GLU	CB-CA-C	5.59	119.06	109.51
10	A	2232	A	P-O3'-C3'	-5.58	111.82	120.20
10	A	1102	G	P-O3'-C3'	-5.58	111.83	120.20
10	A	1697	C	C4'-C3'-O3'	-5.57	104.64	113.00
10	A	2501	A	P-O3'-C3'	-5.56	111.87	120.20
10	A	2636	G	O3'-P-O5'	-5.55	95.67	104.00
10	A	4	U	P-O3'-C3'	-5.55	111.88	120.20
10	A	606	G	O5'-C5'-C4'	-5.54	103.18	111.50
10	A	966	U	P-O3'-C3'	-5.54	111.88	120.20
10	A	1818	A	C4'-C3'-O3'	-5.54	104.68	113.00
10	A	794	G	C1'-O4'-C4'	-5.54	104.36	109.90
10	A	1428	A	C4'-C3'-O3'	-5.53	104.71	113.00
10	A	2084	A	O3'-P-O5'	-5.53	95.70	104.00
10	A	1620	G	O3'-P-O5'	-5.52	95.71	104.00
10	A	2425	A	P-O3'-C3'	-5.52	111.92	120.20
10	A	2767	A	P-O3'-C3'	-5.52	111.92	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	583	A	P-O3'-C3'	-5.52	111.92	120.20
10	A	372	A	O3'-P-O5'	-5.51	95.74	104.00
10	A	2142	U	P-O3'-C3'	-5.51	111.94	120.20
10	A	471	G	P-O3'-C3'	-5.50	111.94	120.20
10	A	1432	G	P-O3'-C3'	-5.50	111.95	120.20
10	A	1480	C	P-O3'-C3'	-5.50	111.95	120.20
10	A	2552	U	O3'-P-O5'	-5.50	95.75	104.00
10	A	2102	G	O3'-P-O5'	-5.50	95.75	104.00
11	B	46	A	P-O3'-C3'	-5.49	111.97	120.20
10	A	2792	G	P-O3'-C3'	-5.48	111.98	120.20
10	A	975	C	P-O3'-C3'	-5.48	111.98	120.20
10	A	2532	C	C4'-C3'-O3'	-5.47	104.80	113.00
10	A	2455	C	P-O3'-C3'	-5.46	112.01	120.20
10	A	2270	G	P-O3'-C3'	-5.46	112.01	120.20
10	A	368	C	P-O3'-C3'	-5.45	112.02	120.20
10	A	379	C	P-O3'-C3'	-5.45	112.03	120.20
10	A	234	G	P-O3'-C3'	-5.44	112.05	120.20
10	A	2055	U	O3'-P-O5'	-5.42	95.86	104.00
10	A	2234	C	P-O3'-C3'	-5.42	112.07	120.20
11	B	28	C	P-O3'-C3'	-5.42	112.07	120.20
10	A	2256	A	P-O3'-C3'	-5.41	112.09	120.20
10	A	2836	G	P-O3'-C3'	-5.41	112.09	120.20
10	A	1571	U	P-O3'-C3'	-5.40	112.09	120.20
10	A	2053	A	C4'-C3'-O3'	-5.40	104.90	113.00
10	A	2327	C	P-O3'-C3'	-5.40	112.10	120.20
10	A	134	U	P-O3'-C3'	-5.39	112.11	120.20
10	A	2354	G	P-O3'-C3'	-5.39	112.11	120.20
10	A	745	A	C4'-C3'-O3'	-5.39	104.91	113.00
10	A	958	A	O3'-P-O5'	-5.37	95.94	104.00
10	A	1890	G	O3'-P-O5'	-5.37	95.95	104.00
10	A	2037	G	C4'-C3'-C2'	-5.37	97.23	102.60
10	A	371	U	C4'-C3'-O3'	-5.36	104.95	113.00
28	X	55	GLY	CA-C-O	-5.36	118.45	122.37
10	A	1429	A	P-O3'-C3'	-5.36	112.17	120.20
10	A	2141	U	P-O3'-C3'	-5.36	112.17	120.20
11	B	15	C	P-O3'-C3'	-5.35	112.17	120.20
10	A	294	G	P-O3'-C3'	-5.35	112.18	120.20
10	A	148	G	P-O3'-C3'	-5.34	112.19	120.20
10	A	1962	G	P-O3'-C3'	-5.34	112.19	120.20
10	A	1783	G	P-O3'-C3'	-5.33	112.20	120.20
11	B	17	A	P-O3'-C3'	-5.33	112.20	120.20
11	B	58	C	P-O3'-C3'	-5.33	112.21	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1614	U	P-O3'-C3'	-5.33	112.21	120.20
10	A	190	G	C4'-C3'-C2'	-5.33	97.27	102.60
10	A	2835	A	P-O3'-C3'	-5.32	112.22	120.20
10	A	1307	A	P-O3'-C3'	-5.31	112.23	120.20
10	A	2450	C	P-O3'-C3'	-5.31	112.24	120.20
10	A	936	U	P-O3'-C3'	-5.31	112.24	120.20
11	B	26	C	P-O3'-C3'	-5.30	112.24	120.20
10	A	1899	A	P-O3'-C3'	-5.30	112.25	120.20
7	7	4	THR	N-CA-C	-5.30	103.49	110.43
10	A	827	A	C4'-C3'-O3'	-5.30	105.06	113.00
10	A	1371	C	P-O3'-C3'	-5.29	112.26	120.20
11	B	83	G	P-O3'-C3'	-5.29	112.26	120.20
10	A	1431	A	O3'-P-O5'	-5.29	96.06	104.00
11	B	69	C	P-O3'-C3'	-5.28	112.28	120.20
10	A	2514	G	C4'-C3'-O3'	-5.28	105.09	113.00
10	A	465	C	P-O3'-C3'	-5.27	112.29	120.20
10	A	1165	C	P-O3'-C3'	-5.27	112.29	120.20
10	A	133	A	P-O3'-C3'	-5.27	112.29	120.20
10	A	1576	G	P-O3'-C3'	-5.27	112.29	120.20
10	A	1530	G	C4'-C3'-O3'	-5.26	105.11	113.00
10	A	1563	A	P-O3'-C3'	-5.25	112.32	120.20
11	B	18	G	P-O3'-C3'	-5.25	112.32	120.20
10	A	745	A	P-O3'-C3'	-5.25	112.33	120.20
10	A	2014	A	C2'-C3'-O3'	-5.24	105.83	113.70
10	A	2084	A	C3'-C2'-O2'	-5.24	106.73	114.60
10	A	1757	C	P-O3'-C3'	-5.24	112.34	120.20
10	A	746	G	C4'-C3'-O3'	-5.24	105.15	113.00
10	A	2306	A	C4'-C3'-O3'	-5.24	105.15	113.00
10	A	231	A	P-O3'-C3'	5.23	128.05	120.20
10	A	1784	C	O3'-P-O5'	-5.23	96.15	104.00
11	B	59	U	P-O3'-C3'	-5.23	112.36	120.20
10	A	761	A	P-O3'-C3'	-5.22	112.36	120.20
10	A	951	C	P-O3'-C3'	-5.22	112.36	120.20
10	A	1496	C	P-O3'-C3'	-5.22	112.36	120.20
10	A	423	G	P-O3'-C3'	-5.22	112.37	120.20
10	A	2823	A	P-O3'-C3'	-5.22	112.37	120.20
10	A	581	A	P-O3'-C3'	-5.22	112.38	120.20
10	A	1573	A	C1'-O4'-C4'	-5.22	104.48	109.70
10	A	33	U	P-O3'-C3'	-5.21	112.38	120.20
10	A	757	A	P-O3'-C3'	-5.21	112.38	120.20
10	A	2345	U	P-O3'-C3'	-5.21	112.39	120.20
10	A	244	G	C3'-C2'-C1'	-5.20	96.30	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	582	G	C4'-C3'-O3'	-5.20	105.20	113.00
10	A	205	A	P-O3'-C3'	-5.20	112.41	120.20
10	A	697	C	O3'-P-O5'	-5.20	96.21	104.00
11	B	4	G	P-O3'-C3'	-5.20	112.41	120.20
10	A	2357	U	C4'-C3'-O3'	-5.19	105.21	113.00
11	B	40	C	P-O3'-C3'	-5.19	112.41	120.20
10	A	1455	U	P-O3'-C3'	-5.19	112.42	120.20
10	A	2922	G	P-O3'-C3'	-5.19	112.42	120.20
10	A	2702	G	P-O3'-C3'	-5.18	112.43	120.20
10	A	2348	U	P-O3'-C3'	-5.18	112.43	120.20
10	A	1448	C	P-O3'-C3'	-5.17	112.44	120.20
10	A	1115	A	P-O3'-C3'	-5.17	112.44	120.20
10	A	1658	A	P-O3'-C3'	-5.16	112.46	120.20
10	A	591	A	O3'-P-O5'	-5.16	96.27	104.00
10	A	1343	G	C2'-C3'-O3'	-5.16	105.97	113.70
10	A	963	G	P-O3'-C3'	-5.15	112.47	120.20
10	A	339	U	P-O3'-C3'	-5.15	112.48	120.20
10	A	1358	C	C4'-C3'-O3'	-5.14	105.29	113.00
10	A	1885	U	P-O3'-C3'	-5.14	112.49	120.20
10	A	785	A	O3'-P-O5'	-5.13	96.30	104.00
11	B	88	C	P-O3'-C3'	-5.13	112.50	120.20
12	G	196	GLY	CA-C-O	-5.13	118.88	122.22
10	A	266	G	C4'-C3'-O3'	-5.12	105.31	113.00
10	A	2102	G	C4'-C3'-O3'	-5.12	105.32	113.00
10	A	1393	A	P-O5'-C5'	-5.12	113.22	120.90
10	A	1748	G	C2'-C3'-O3'	5.12	117.18	109.50
10	A	1955	G	P-O3'-C3'	-5.12	112.52	120.20
10	A	265	A	P-O3'-C3'	-5.12	112.53	120.20
10	A	1151	U	P-O3'-C3'	-5.11	112.53	120.20
10	A	2521	A	P-O3'-C3'	-5.11	112.53	120.20
10	A	483	C	P-O3'-C3'	-5.11	112.53	120.20
10	A	2801	C	P-O3'-C3'	-5.11	112.53	120.20
10	A	696	G	P-O3'-C3'	-5.11	112.53	120.20
10	A	1996	C	P-O3'-C3'	-5.11	112.54	120.20
10	A	1562	C	P-O3'-C3'	-5.11	112.54	120.20
10	A	1733	C	P-O3'-C3'	-5.10	112.54	120.20
10	A	2254	G	P-O3'-C3'	-5.10	112.54	120.20
10	A	1786	G	C2'-C3'-O3'	5.10	121.35	113.70
10	A	723	A	C4'-C3'-O3'	-5.10	105.35	113.00
10	A	2819	U	P-O3'-C3'	-5.10	112.55	120.20
11	B	91	C	P-O3'-C3'	-5.10	112.55	120.20
10	A	1489	A	P-O3'-C3'	-5.10	112.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1785	C	O3'-P-O5'	-5.10	96.35	104.00
10	A	2325	U	P-O3'-C3'	-5.10	112.56	120.20
10	A	34	U	P-O3'-C3'	-5.09	112.56	120.20
10	A	61	A	P-O3'-C3'	-5.09	112.56	120.20
10	A	1289	A	P-O3'-C3'	-5.09	112.56	120.20
10	A	2666	A	P-O3'-C3'	-5.09	112.56	120.20
11	B	44	A	P-O3'-C3'	-5.09	112.57	120.20
10	A	853	U	C4'-C3'-C2'	-5.09	97.51	102.60
10	A	2671	G	P-O3'-C3'	-5.09	112.57	120.20
10	A	2462	G	O3'-P-O5'	-5.09	96.37	104.00
10	A	1951	A	C4'-C3'-O3'	5.08	117.02	109.40
10	A	915	U	P-O3'-C3'	-5.08	112.58	120.20
10	A	2426	U	C4'-C3'-O3'	-5.08	105.39	113.00
10	A	297	U	P-O3'-C3'	-5.07	112.59	120.20
10	A	809	G	C4'-C3'-O3'	-5.07	105.39	113.00
10	A	2209	A	P-O3'-C3'	-5.07	112.59	120.20
11	B	53	U	P-O3'-C3'	-5.07	112.59	120.20
10	A	386	U	P-O3'-C3'	-5.07	112.60	120.20
10	A	2700	C	P-O3'-C3'	-5.06	112.61	120.20
14	I	64	PRO	CB-CA-C	-5.06	104.31	112.21
10	A	410	G	P-O3'-C3'	-5.06	112.61	120.20
10	A	1561	G	P-O3'-C3'	-5.06	112.61	120.20
10	A	1193	U	P-O3'-C3'	-5.05	112.62	120.20
10	A	2253	G	P-O3'-C3'	-5.05	112.62	120.20
10	A	855	G	C4'-C3'-C2'	-5.05	97.55	102.60
10	A	1850	G	P-O3'-C3'	-5.05	112.63	120.20
10	A	1601	C	P-O3'-C3'	-5.04	112.64	120.20
10	A	1374	C	P-O3'-C3'	-5.04	112.64	120.20
10	A	1631	A	P-O3'-C3'	-5.04	112.64	120.20
10	A	1344	A	P-O3'-C3'	5.03	127.75	120.20
10	A	195	U	P-O3'-C3'	-5.03	112.66	120.20
10	A	1338	C	P-O3'-C3'	-5.03	112.65	120.20
10	A	1556	G	P-O3'-C3'	-5.03	112.66	120.20
10	A	886	C	P-O3'-C3'	-5.03	112.66	120.20
10	A	106	A	P-O3'-C3'	-5.03	112.66	120.20
10	A	2877	G	O3'-P-O5'	-5.03	96.46	104.00
10	A	2921	G	P-O3'-C3'	-5.03	112.66	120.20
11	B	114	G	P-O3'-C3'	-5.03	112.66	120.20
10	A	47	C	P-O3'-C3'	-5.02	112.67	120.20
10	A	1529	U	O3'-P-O5'	-5.02	96.47	104.00
10	A	2757	U	C4'-C3'-O3'	-5.02	105.47	113.00
10	A	823	G	C4'-C3'-O3'	-5.02	105.47	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	880	U	P-O3'-C3'	-5.02	112.67	120.20
10	A	2692	G	P-O3'-C3'	-5.02	112.67	120.20
10	A	797	A	O3'-P-O5'	-5.01	96.49	104.00
10	A	1461	U	P-O3'-C3'	-5.01	112.69	120.20
10	A	1133	G	P-O3'-C3'	-5.01	112.69	120.20
11	B	25	A	P-O3'-C3'	-5.00	112.70	120.20
10	A	1993	A	P-O3'-C3'	-5.00	112.70	120.20

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	10	ARG	Sidechain
1	1	13	ARG	Sidechain
1	1	18	ARG	Sidechain
2	2	60	ARG	Sidechain
5	5	6	ARG	Sidechain
6	6	40	ARG	Sidechain
7	7	10	ARG	Sidechain
7	7	29	ARG	Sidechain
8	8	13	ARG	Sidechain
8	8	45	ARG	Sidechain
8	8	59	ARG	Sidechain
12	G	13	ARG	Sidechain
12	G	156	ARG	Sidechain
12	G	182	ARG	Sidechain
12	G	260	ARG	Sidechain
12	G	35	ARG	Sidechain
12	G	43	ARG	Sidechain
14	I	106	ARG	Sidechain
14	I	95	ARG	Sidechain
15	J	133	ARG	Sidechain
16	K	170	ARG	Sidechain
17	M	14	ARG	Sidechain
17	M	94	ARG	Sidechain
18	N	64	ARG	Sidechain
19	O	33	ARG	Sidechain
19	O	47	ARG	Sidechain
19	O	59	ARG	Sidechain
19	O	60	ARG	Sidechain
20	P	134	ARG	Sidechain
20	P	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	P	56	ARG	Sidechain
20	P	6	ARG	Sidechain
21	Q	122	ARG	Sidechain
21	Q	36	ARG	Sidechain
21	Q	59	ARG	Sidechain
21	Q	67	ARG	Sidechain
22	R	104	ARG	Sidechain
22	R	17	ARG	Sidechain
22	R	30	ARG	Sidechain
22	R	96	ARG	Sidechain
23	S	104	ARG	Sidechain
23	S	39	ARG	Sidechain
23	S	72	ARG	Sidechain
24	T	3	ARG	Sidechain
24	T	51	ARG	Sidechain
25	U	67	ARG	Sidechain
26	V	20	ARG	Sidechain
29	Z	28	ARG	Sidechain
29	Z	47	ARG	Sidechain

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	1	457	0	502	9	0
2	2	487	0	504	1	0
3	3	433	0	479	3	0
4	4	477	0	454	5	0
5	5	425	0	423	14	0
6	6	400	0	410	5	0
7	7	357	0	405	0	0
8	8	512	0	562	5	0
9	9	292	0	334	5	0
10	A	62459	0	31405	250	0
11	B	2430	0	1229	11	0
12	G	2108	0	2184	22	0
13	H	1582	0	1646	14	0
14	I	1563	0	1655	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1365	0	1417	17	0
16	K	1271	0	1308	9	0
17	M	1117	0	1140	17	0
18	N	925	0	982	21	0
19	O	1094	0	1137	12	0
20	P	1055	0	1125	14	0
21	Q	983	0	1045	16	0
22	R	914	0	941	10	0
23	S	905	0	973	6	0
24	T	939	0	1011	6	0
25	U	786	0	825	7	0
26	V	848	0	905	9	0
27	W	731	0	763	3	0
28	X	723	0	794	10	0
29	Z	563	0	568	1	0
30	5	1	0	0	0	0
30	9	1	0	0	0	0
31	A	10	0	19	1	0
32	A	162	0	0	1	0
32	G	1	0	0	0	0
32	H	1	0	0	0	0
32	O	1	0	0	0	0
33	A	12	0	24	1	0
34	A	27	0	34	0	0
35	P	1	0	0	0	0
36	1	1	0	0	1	0
36	5	5	0	0	0	0
36	7	9	0	0	0	0
36	8	7	0	0	0	0
36	A	1223	0	0	26	0
36	B	2	0	0	0	0
36	G	40	0	0	1	0
36	H	12	0	0	0	0
36	I	15	0	0	1	0
36	M	2	0	0	0	0
36	N	5	0	0	0	0
36	O	24	0	0	0	0
36	P	4	0	0	0	0
36	Q	4	0	0	0	0
36	S	8	0	0	0	0
36	T	8	0	0	0	0
36	U	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	5	0	0	0	0
36	W	1	0	0	0	0
36	Z	2	0	0	0	0
All	All	89799	0	57203	479	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 (479) 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)
10:A:83:G:N2	10:A:101:G:O2'	1.96	0.97
10:A:890:G:N2	10:A:980:A:N1	2.15	0.94
10:A:1713:A:H61	10:A:2029:C:H5	1.15	0.94
10:A:1489:A:H2	10:A:1604:G:H21	1.17	0.93
10:A:890:G:H1	10:A:980:A:H61	1.14	0.90
10:A:1416:U:HO2'	10:A:2245:A:H8	1.17	0.90
10:A:1519:A:H62	10:A:1573:A:H2	1.18	0.89
10:A:2481:A:OP1	36:A:3201:HOH:O	1.92	0.86
14:I:156:VAL:O	14:I:177:PRO:O	1.96	0.83
10:A:1890:G:H8	10:A:1918:A:H62	1.27	0.82
10:A:830:U:H5	10:A:839:A:N1	1.77	0.82
10:A:1761:A:N6	10:A:1779:G:O6	2.14	0.81
18:N:102:VAL:HG13	18:N:106:LEU:HD12	1.62	0.81
10:A:1812:U:H5	10:A:1817:A:N7	1.77	0.81
32:A:3035:MG:MG	36:A:3274:HOH:O	1.23	0.81
10:A:1727:A:N1	36:A:3207:HOH:O	2.16	0.79
5:5:2:ALA:HB2	36:A:3948:HOH:O	1.84	0.78
10:A:200:C:OP2	36:A:3202:HOH:O	2.03	0.76
10:A:1891:G:O2'	10:A:1916:G:N2	2.17	0.76
10:A:333:U:H3	10:A:392:G:H1	1.34	0.76
10:A:2022:A:N1	36:A:3207:HOH:O	2.19	0.75
12:G:142:HIS:ND1	12:G:193:GLY:O	2.17	0.75
1:1:20:HIS:O	1:1:21:ALA:HB3	1.87	0.74
10:A:1311:G:H5''	26:V:20:ARG:HH22	1.51	0.74
10:A:2471:U:O3'	10:A:2472:A:H3'	1.86	0.74
10:A:1501:G:N2	10:A:1509:A:H62	1.86	0.73
10:A:613:G:O6	36:A:3201:HOH:O	2.05	0.73
10:A:2789:U:H5	10:A:2791:A:N7	1.85	0.73
18:N:65:THR:OG1	18:N:67:SER:O	2.06	0.73
21:Q:134:LEU:O	21:Q:135:VAL:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1416:U:O2'	10:A:2245:A:H8	1.72	0.72
10:A:199:A:OP1	36:A:3202:HOH:O	2.06	0.71
10:A:1282:A:OP1	36:A:3204:HOH:O	2.09	0.71
10:A:627:C:OP2	36:A:3203:HOH:O	2.08	0.70
13:H:32:GLN:O	13:H:53:PHE:O	2.09	0.70
10:A:1501:G:H21	10:A:1509:A:H62	1.37	0.70
12:G:49:LEU:HD11	36:G:428:HOH:O	1.91	0.70
28:X:31:ASP:O	28:X:65:VAL:HG23	1.91	0.70
21:Q:115:ARG:NH1	21:Q:135:VAL:HG21	2.07	0.70
11:B:86:U:H2'	11:B:86:U:O2	1.92	0.69
14:I:70:THR:OG1	36:I:301:HOH:O	2.09	0.69
10:A:2302:G:OP1	36:A:3205:HOH:O	2.11	0.69
21:Q:115:ARG:NH1	21:Q:135:VAL:CG2	2.56	0.68
10:A:216:G:N7	36:A:3214:HOH:O	2.26	0.68
12:G:106:ALA:O	12:G:195:VAL:O	2.11	0.68
25:U:29:VAL:O	25:U:62:VAL:O	2.11	0.68
10:A:2301:A:OP1	36:A:3205:HOH:O	2.12	0.68
10:A:807:A:OP1	36:A:3206:HOH:O	2.12	0.68
10:A:2722:U:H5	36:A:3992:HOH:O	1.76	0.67
10:A:45:G:H21	10:A:182:A:H62	1.42	0.66
25:U:6:GLU:HG3	25:U:39:LEU:HD21	1.78	0.66
10:A:2456:U:O2'	10:A:2457:C:OP2	2.14	0.65
21:Q:24:LEU:HD23	21:Q:44:VAL:HG21	1.77	0.65
10:A:1332:U:H5	10:A:1370:U:O2	1.79	0.65
28:X:2:HIS:CE1	28:X:65:VAL:HG12	2.31	0.65
10:A:2125:G:N2	10:A:2259:C:OP2	2.29	0.65
18:N:35:ILE:HG21	18:N:103:ALA:HB3	1.79	0.64
26:V:15:VAL:HG11	26:V:51:ILE:HG21	1.79	0.64
15:J:136:LEU:HA	15:J:141:ILE:HG21	1.80	0.64
23:S:104:ARG:O	23:S:105:GLY:O	2.16	0.63
10:A:1850:G:OP2	12:G:156:ARG:NH2	2.31	0.63
1:1:20:HIS:O	1:1:21:ALA:CB	2.46	0.63
10:A:2834:A:O2'	10:A:2835:A:O5'	2.16	0.63
18:N:63:VAL:HB	18:N:102:VAL:HG22	1.80	0.63
10:A:655:G:H21	10:A:661:A:H62	1.47	0.63
10:A:1832:G:O2'	12:G:180:GLU:OE2	2.16	0.63
18:N:68:GLY:HA3	18:N:77:ILE:O	1.99	0.63
16:K:11:ILE:HD11	16:K:50:ILE:HD11	1.81	0.63
1:1:20:HIS:O	10:A:2113:G:OP1	2.16	0.62
8:8:27:GLY:O	8:8:29:THR:N	2.32	0.62
10:A:1784:C:H2'	10:A:1785:C:H5''	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2235:C:O2'	10:A:2237:C:OP1	2.13	0.62
10:A:1852:A:OP2	12:G:154:LEU:O	2.17	0.62
10:A:2029:C:O2	10:A:2029:C:O5'	2.18	0.62
10:A:2699:C:O2	10:A:2699:C:O5'	2.18	0.62
23:S:48:ILE:CD1	23:S:100:LEU:HD12	2.29	0.62
10:A:655:G:N2	10:A:661:A:H62	1.98	0.62
15:J:61:THR:HG21	15:J:89:VAL:HG11	1.82	0.61
28:X:33:VAL:CG1	28:X:35:ILE:HD11	2.30	0.61
10:A:1028:C:O2	10:A:1028:C:O5'	2.18	0.61
10:A:2177:G:H21	10:A:2180:A:H61	1.49	0.61
20:P:64:VAL:HG22	20:P:106:ILE:HG22	1.82	0.60
15:J:60:ILE:HD13	15:J:152:MET:HE1	1.83	0.60
5:5:20:VAL:HG23	5:5:20:VAL:O	2.01	0.60
10:A:1489:A:H2	10:A:1604:G:N2	1.93	0.60
13:H:109:ASP:OD1	13:H:172:GLN:HA	2.02	0.59
28:X:31:ASP:C	28:X:65:VAL:HG23	2.27	0.59
10:A:318:G:H8	10:A:318:G:H5''	1.68	0.59
28:X:1:MET:SD	28:X:65:VAL:HG21	2.42	0.59
10:A:2532:C:OP1	36:A:3201:HOH:O	2.17	0.59
8:8:30:SER:O	8:8:31:HIS:O	2.22	0.58
28:X:10:LYS:HB2	28:X:71:LEU:HD21	1.86	0.58
6:6:7:LEU:HD11	6:6:32:LEU:HD12	1.86	0.58
10:A:2908:A:O2'	10:A:2909:C:OP2	2.19	0.58
8:8:31:HIS:CD2	8:8:32:MET:HG2	2.39	0.58
10:A:1501:G:H21	10:A:1509:A:N6	2.01	0.58
10:A:1680:G:N7	36:A:3222:HOH:O	2.33	0.58
10:A:2875:G:OP2	36:A:3209:HOH:O	2.17	0.57
21:Q:75:GLN:HA	21:Q:89:ASN:HA	1.86	0.57
13:H:122:VAL:HG21	13:H:143:PRO:HA	1.86	0.57
17:M:54:PHE:CE2	17:M:122:LYS:HG2	2.39	0.57
18:N:63:VAL:HG12	18:N:106:LEU:HD11	1.87	0.57
11:B:86:U:O2	11:B:86:U:C2'	2.52	0.57
5:5:2:ALA:HB3	10:A:2089:G:N2	2.20	0.57
10:A:1423:U:OP2	36:A:3208:HOH:O	2.17	0.57
17:M:27:GLY:O	17:M:28:ARG:HB2	2.05	0.57
13:H:8:ARG:NH1	13:H:197:LYS:O	2.37	0.56
10:A:759:G:H21	10:A:764:A:H2	1.53	0.56
10:A:1794:U:H2'	10:A:1795:A:H5''	1.86	0.56
10:A:1889:A:H5''	10:A:1889:A:H8	1.70	0.56
10:A:842:U:H2'	10:A:843:U:C6	2.40	0.56
10:A:2789:U:C5	10:A:2791:A:N7	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:54:VAL:HG13	15:J:65:PRO:HG2	1.86	0.56
6:6:31:GLU:HB3	6:6:44:LEU:HD11	1.88	0.56
10:A:2653:C:OP1	13:H:156:LYS:O	2.22	0.56
10:A:1233:G:H5''	25:U:82:TYR:CE1	2.41	0.56
24:T:76:TYR:CZ	24:T:80:MET:HG3	2.42	0.55
21:Q:134:LEU:O	21:Q:135:VAL:HG13	2.06	0.55
10:A:1786:G:H8	10:A:1786:G:H5''	1.70	0.55
12:G:126:VAL:HG12	12:G:127:GLY:N	2.22	0.55
10:A:698:A:H5''	10:A:699:U:H5''	1.88	0.55
18:N:24:VAL:HG13	18:N:33:ALA:HB2	1.89	0.55
10:A:1392:G:H2'	10:A:1393:A:H5''	1.89	0.54
18:N:98:ILE:HD13	18:N:117:LEU:HB2	1.89	0.54
28:X:2:HIS:HE1	28:X:65:VAL:HG12	1.73	0.54
10:A:661:A:OP1	14:I:106:ARG:HD2	2.07	0.54
10:A:575:G:N3	10:A:575:G:H2'	2.23	0.54
18:N:81:GLU:N	18:N:81:GLU:OE1	2.41	0.54
10:A:579:U:O2'	24:T:49:ASP:OD2	2.19	0.54
10:A:344:C:O4'	10:A:344:C:O2	2.25	0.53
10:A:1899:A:H2'	10:A:1900:G:O4'	2.09	0.53
10:A:2361:A:H2'	10:A:2362:A:C8	2.43	0.53
11:B:12:U:OP2	11:B:68:C:O2'	2.24	0.53
14:I:35:ASP:HB3	14:I:101:LEU:HD11	1.90	0.53
12:G:67:PHE:HE1	12:G:105:ILE:HD11	1.73	0.53
13:H:108:ILE:C	13:H:108:ILE:HD12	2.34	0.53
16:K:83:TYR:CE2	16:K:138:LYS:HB2	2.44	0.53
10:A:2810:G:OP2	10:A:2814:A:O2'	2.17	0.53
26:V:114:GLU:O	26:V:115:VAL:HB	2.08	0.53
21:Q:103:ALA:HB3	21:Q:104:PRO:HD3	1.91	0.53
10:A:631:U:H2'	10:A:632:U:C6	2.44	0.52
10:A:2347:A:H2'	10:A:2348:U:C6	2.43	0.52
10:A:2617:U:H2'	10:A:2618:U:H2'	1.90	0.52
15:J:46:ASN:HD22	15:J:49:VAL:HG23	1.74	0.52
21:Q:115:ARG:NH1	21:Q:135:VAL:HG23	2.24	0.52
5:5:33:CYS:SG	5:5:46:CYS:N	2.81	0.52
10:A:2299:A:H4'	10:A:2300:A:O5'	2.09	0.52
10:A:2472:A:H4'	10:A:2473:C:O5'	2.09	0.52
10:A:1355:U:O2	10:A:1355:U:O5'	2.26	0.52
21:Q:26:VAL:HG22	21:Q:71:VAL:HG22	1.91	0.52
14:I:154:ILE:HD13	14:I:193:ILE:HB	1.90	0.52
18:N:94:ARG:HG3	18:N:94:ARG:HH11	1.74	0.52
9:9:7:VAL:HG13	9:9:25:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1635:A:H1'	10:A:1636:G:O4'	2.10	0.52
14:I:26:ILE:HD12	14:I:26:ILE:C	2.35	0.52
10:A:2507:C:O2	10:A:2507:C:O4'	2.26	0.52
11:B:44:A:H4'	22:R:5:ILE:HD11	1.92	0.52
15:J:13:VAL:HB	15:J:14:PRO:HD3	1.91	0.52
10:A:83:G:H1	10:A:101:G:H2'	1.75	0.52
10:A:2789:U:H1'	10:A:2790:A:H5''	1.92	0.52
18:N:102:VAL:CG1	18:N:106:LEU:HD12	2.37	0.52
10:A:829:A:H2'	10:A:830:U:H4'	1.91	0.52
11:B:22:G:H21	11:B:25:A:H62	1.57	0.52
17:M:25:SER:O	17:M:27:GLY:O	2.28	0.52
10:A:174:A:H8	10:A:174:A:H5''	1.74	0.51
10:A:1319:A:H4'	10:A:1320:G:OP1	2.09	0.51
10:A:613:G:H2'	10:A:2063:A:N7	2.26	0.51
20:P:54:MET:HE2	20:P:64:VAL:HG13	1.92	0.51
17:M:115:LEU:C	17:M:115:LEU:HD23	2.36	0.51
28:X:33:VAL:HG11	28:X:35:ILE:HD11	1.93	0.51
10:A:996:G:N7	36:A:3224:HOH:O	2.34	0.51
10:A:1972:U:OP1	10:A:2637:U:O2'	2.23	0.51
20:P:54:MET:HE1	20:P:104:PHE:HB3	1.93	0.51
10:A:326:A:N1	10:A:399:C:N3	2.58	0.51
10:A:1785:C:H6	10:A:1785:C:C5'	2.24	0.51
18:N:91:LYS:HB3	18:N:111:PHE:CD2	2.46	0.51
12:G:248:SER:OG	12:G:251:GLY:O	2.20	0.51
19:O:102:ILE:HD12	19:O:102:ILE:O	2.11	0.51
10:A:548:A:H4'	10:A:549:C:O5'	2.11	0.50
10:A:1948:U:O2	10:A:1948:U:O4'	2.28	0.50
15:J:40:VAL:HG12	15:J:43:ALA:HB2	1.93	0.50
20:P:54:MET:CE	20:P:64:VAL:HG13	2.41	0.50
10:A:789:A:O2'	10:A:1708:U:OP1	2.23	0.50
10:A:552:U:O3'	10:A:553:U:H6	1.95	0.50
10:A:2458:A:H5''	10:A:2460:C:O4'	2.12	0.50
24:T:43:TYR:HB3	25:U:74:TYR:HB3	1.93	0.50
10:A:2809:A:H3'	10:A:2809:A:OP1	2.11	0.50
17:M:2:ARG:HG3	17:M:3:THR:HG23	1.93	0.50
10:A:2822:C:H2'	10:A:2823:A:C8	2.47	0.50
10:A:2824:U:H3	10:A:2835:A:H61	1.60	0.50
12:G:268:LYS:HE2	12:G:269:PHE:CE2	2.47	0.50
13:H:151:PRO:O	13:H:153:ARG:HG2	2.11	0.50
19:O:113:SER:O	19:O:114:ASN:C	2.55	0.50
4:4:11:PRO:HA	4:4:26:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2835:A:O2'	10:A:2836:G:OP2	2.25	0.49
26:V:87:LEU:HB2	26:V:103:LYS:HB2	1.93	0.49
10:A:1997:G:H4'	10:A:1998:C:OP2	2.12	0.49
10:A:1794:U:C2'	10:A:1795:A:H5''	2.42	0.49
14:I:124:VAL:HG12	14:I:126:LEU:CD2	2.42	0.49
17:M:27:GLY:O	17:M:28:ARG:CB	2.60	0.49
10:A:727:G:N7	36:A:3228:HOH:O	2.35	0.49
10:A:1811:U:H2'	10:A:1817:A:N6	2.28	0.49
10:A:1058:U:O4	17:M:28:ARG:HA	2.12	0.49
28:X:33:VAL:CG1	28:X:35:ILE:CD1	2.91	0.49
10:A:26:G:H1'	10:A:559:A:N6	2.28	0.49
5:5:20:VAL:O	5:5:20:VAL:CG2	2.61	0.49
15:J:54:VAL:HG13	15:J:65:PRO:CG	2.43	0.49
15:J:117:VAL:HG23	15:J:176:PRO:C	2.37	0.49
11:B:35:C:C5	11:B:36:C:C5	3.01	0.49
21:Q:134:LEU:C	21:Q:135:VAL:HG22	2.38	0.48
10:A:2502:A:N6	10:A:2514:G:O2'	2.46	0.48
10:A:1889:A:H5''	10:A:1889:A:C8	2.48	0.48
12:G:75:PRO:HB3	12:G:117:TYR:CE2	2.48	0.48
10:A:579:U:H2'	10:A:580:U:C6	2.48	0.48
10:A:746:G:O2'	10:A:1681:A:N3	2.39	0.48
19:O:93:PRO:HG2	19:O:146:ILE:HD11	1.95	0.48
10:A:2699:C:O2	10:A:2699:C:O4'	2.31	0.48
14:I:158:GLY:O	14:I:160:SER:N	2.47	0.48
1:1:3:LYS:N	36:1:101:HOH:O	2.47	0.48
10:A:890:G:H1	10:A:980:A:N6	1.95	0.48
10:A:1340:A:OP1	10:A:2742:G:O2'	2.27	0.48
17:M:49:ILE:O	17:M:50:ASP:HB3	2.13	0.48
5:5:33:CYS:N	5:5:46:CYS:SG	2.87	0.48
21:Q:20:LEU:HB2	21:Q:40:ILE:HD11	1.95	0.48
10:A:831:U:H2'	10:A:832:C:C6	2.49	0.47
1:1:8:THR:HG21	1:1:10:ARG:NH1	2.30	0.47
22:R:102:HIS:O	22:R:106:LYS:HB3	2.14	0.47
10:A:916:G:O3'	20:P:6:ARG:NH1	2.47	0.47
21:Q:22:THR:HG21	21:Q:67:ARG:HB2	1.95	0.47
10:A:141:U:H5''	10:A:141:U:H6	1.79	0.47
10:A:1779:G:H3'	10:A:1780:A:H5''	1.95	0.47
10:A:2344:A:N3	15:J:85:ILE:HD12	2.30	0.47
10:A:2766:C:H2'	10:A:2767:A:O4'	2.13	0.47
10:A:1501:G:H2'	10:A:1508:A:H62	1.79	0.47
20:P:27:VAL:HG23	20:P:105:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1096:A:C2	10:A:2784:G:C4	3.03	0.47
15:J:132:VAL:HG13	15:J:137:ILE:HD13	1.96	0.47
10:A:2925:U:H2'	10:A:2926:U:C6	2.49	0.47
11:B:11:A:N1	11:B:67:G:O2'	2.43	0.47
20:P:57:TYR:CE2	20:P:116:GLU:HB3	2.50	0.47
5:5:28:ASN:C	5:5:28:ASN:HD22	2.23	0.47
10:A:1784:C:C2'	10:A:1785:C:H5''	2.44	0.47
10:A:2599:A:N1	18:N:28:SER:OG	2.41	0.47
14:I:159:GLU:N	14:I:159:GLU:OE1	2.48	0.47
5:5:2:ALA:HB1	36:A:3658:HOH:O	2.15	0.47
10:A:1074:A:N6	10:A:1171:G:H2'	2.30	0.47
10:A:1834:A:H4'	10:A:2236:G:C2	2.50	0.47
10:A:1489:A:C2	10:A:1604:G:N2	2.66	0.47
19:O:91:VAL:HA	19:O:95:LEU:HD23	1.97	0.47
19:O:106:LYS:C	19:O:108:GLY:H	2.23	0.47
5:5:16:ARG:NH2	10:A:1309:G:OP1	2.46	0.46
10:A:1066:A:C2	10:A:1187:U:C2	3.04	0.46
10:A:1533:A:O2'	10:A:1534:G:OP1	2.30	0.46
10:A:2863:G:H2'	10:A:2908:A:N6	2.29	0.46
21:Q:103:ALA:HB3	21:Q:104:PRO:CD	2.45	0.46
9:9:10:MET:HE3	9:9:34:GLN:CD	2.41	0.46
10:A:1812:U:C5	10:A:1817:A:N7	2.69	0.46
10:A:2157:G:N2	10:A:2206:A:H62	2.13	0.46
4:4:35:ILE:HG22	4:4:45:LEU:HD13	1.96	0.46
10:A:1845:G:N3	12:G:44:ASN:OD1	2.48	0.46
20:P:52:ILE:HA	20:P:55:THR:HG22	1.97	0.46
2:2:17:GLN:HB3	2:2:53:MET:HE3	1.98	0.46
10:A:903:G:H2'	10:A:904:A:C8	2.50	0.46
14:I:142:PHE:CE1	14:I:146:ILE:HG13	2.51	0.46
10:A:2795:U:H5''	10:A:2795:U:H6	1.81	0.46
22:R:53:LEU:N	22:R:53:LEU:HD12	2.30	0.46
6:6:26:ASN:HB3	6:6:30:ILE:HD11	1.98	0.46
10:A:2445:A:H2'	10:A:2446:G:O4'	2.15	0.46
10:A:2834:A:O2'	10:A:2835:A:P	2.74	0.46
12:G:142:HIS:HB2	12:G:155:VAL:O	2.15	0.46
10:A:2899:C:H2'	10:A:2900:G:O4'	2.16	0.46
22:R:40:ILE:HD13	22:R:108:LEU:HD12	1.98	0.46
27:W:42:VAL:HG11	27:W:80:VAL:HG11	1.98	0.46
16:K:83:TYR:CE1	16:K:138:LYS:HD3	2.50	0.46
3:3:13:ILE:HD11	10:A:1035:G:C8	2.51	0.46
10:A:1503:A:C2	21:Q:93:TYR:CD1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:156:PRO:HB2	16:K:172:LYS:HG3	1.98	0.45
20:P:54:MET:HE3	20:P:106:ILE:HG23	1.99	0.45
10:A:2319:A:H4'	10:A:2320:A:O4'	2.16	0.45
10:A:859:U:H2'	10:A:860:C:C6	2.52	0.45
15:J:149:VAL:O	15:J:151:GLY:N	2.47	0.45
16:K:25:THR:HG23	16:K:34:VAL:HG22	1.99	0.45
10:A:803:G:N7	36:A:3230:HOH:O	2.36	0.45
10:A:908:A:C2	10:A:964:A:C4	3.04	0.45
10:A:1785:C:H5''	10:A:1785:C:H6	1.82	0.45
13:H:38:LYS:HG3	13:H:93:ILE:HD11	1.99	0.45
22:R:101:TYR:OH	22:R:113:ARG:NH2	2.49	0.45
1:1:55:LYS:O	1:1:56:SER:CB	2.65	0.45
10:A:2126:G:O2'	10:A:2231:A:N1	2.42	0.45
16:K:45:ILE:HD12	16:K:45:ILE:N	2.30	0.45
1:1:55:LYS:O	1:1:56:SER:OG	2.30	0.45
10:A:342:A:N1	10:A:376:G:O2'	2.46	0.45
10:A:1469:A:H2'	10:A:1471:G:N7	2.32	0.45
14:I:177:PRO:O	14:I:178:ALA:HB2	2.17	0.45
10:A:351:G:H2'	10:A:352:A:C8	2.52	0.45
10:A:1074:A:N3	10:A:2519:G:O2'	2.38	0.45
10:A:1254:G:O2'	10:A:1282:A:N1	2.41	0.45
10:A:1332:U:C5	10:A:1370:U:O2	2.67	0.45
15:J:103:LEU:HD11	15:J:130:LEU:HD23	1.98	0.45
9:9:7:VAL:HG22	9:9:34:GLN:HB3	1.99	0.45
10:A:2586:G:H2'	10:A:2587:U:O4'	2.16	0.45
14:I:101:LEU:N	14:I:101:LEU:HD23	2.31	0.45
23:S:101:ARG:O	23:S:104:ARG:NH2	2.50	0.45
9:9:17:ILE:HD13	9:9:26:ILE:HD13	1.99	0.45
10:A:829:A:C8	10:A:829:A:H3'	2.52	0.45
10:A:1118:C:O4'	10:A:1118:C:O2	2.34	0.45
5:5:30:CYS:HB3	5:5:33:CYS:HB2	1.98	0.44
6:6:5:ILE:HG23	6:6:47:GLU:HG3	1.99	0.44
10:A:1566:A:H5''	10:A:1567:G:OP2	2.16	0.44
1:1:56:SER:OG	1:1:57:GLY:N	2.49	0.44
10:A:117:A:N3	10:A:179:G:H1'	2.33	0.44
10:A:617:A:OP2	31:A:3001:SPD:H22	2.16	0.44
10:A:828:A:H5'	10:A:829:A:C2	2.53	0.44
10:A:1382:G:N7	27:W:61:LYS:NZ	2.66	0.44
17:M:5:TYR:CG	24:T:100:VAL:HG11	2.52	0.44
10:A:1965:A:H2'	10:A:1966:G:O4'	2.16	0.44
10:A:2353:A:H2'	10:A:2353:A:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2587:U:H2'	10:A:2588:U:C6	2.52	0.44
1:1:21:ALA:HA	10:A:2465:A:N1	2.32	0.44
10:A:1424:G:OP2	36:A:3208:HOH:O	2.21	0.44
11:B:3:U:OP1	11:B:59:U:O2'	2.34	0.44
10:A:1372:G:H2'	10:A:1374:C:C5	2.53	0.44
12:G:198:GLU:H	12:G:198:GLU:CD	2.26	0.44
13:H:27:VAL:HG22	13:H:187:LEU:CD2	2.47	0.44
10:A:1977:U:C5	10:A:1988:U:C2	3.06	0.44
22:R:39:ASN:HB2	22:R:58:ASN:HB3	2.00	0.44
10:A:302:G:H2'	10:A:303:G:O4'	2.18	0.44
10:A:655:G:C6	10:A:656:G:C6	3.05	0.44
14:I:159:GLU:HG2	14:I:160:SER:H	1.83	0.44
21:Q:59:ARG:HA	21:Q:99:PHE:CZ	2.53	0.44
10:A:2304:G:OP1	29:Z:26:SER:HB3	2.18	0.43
33:A:3152:PUT:H31	36:A:3563:HOH:O	2.18	0.43
15:J:31:ILE:HD11	15:J:173:LEU:CD1	2.47	0.43
10:A:2269:U:H2'	10:A:2270:G:O4'	2.18	0.43
10:A:2306:A:H2'	10:A:2307:A:C8	2.54	0.43
13:H:146:MET:HE1	13:H:160:LEU:HD11	2.00	0.43
18:N:64:ARG:HB2	18:N:79:PHE:CG	2.53	0.43
25:U:92:TYR:CD1	25:U:92:TYR:C	2.96	0.43
10:A:1245:U:H1'	24:T:4:VAL:HG22	2.00	0.43
10:A:2096:C:O2	10:A:2483:A:N1	2.51	0.43
10:A:2308:C:O2	20:P:85:LYS:HD2	2.18	0.43
5:5:33:CYS:SG	5:5:45:GLU:HB2	2.58	0.43
6:6:9:CYS:SG	6:6:43:THR:HG21	2.59	0.43
18:N:90:ASP:C	18:N:92:SER:H	2.26	0.43
10:A:1357:U:O2	10:A:1357:U:C2'	2.66	0.43
10:A:2276:U:H2'	10:A:2277:U:C6	2.53	0.43
10:A:2590:G:H2'	10:A:2591:C:C6	2.54	0.43
19:O:55:LEU:HD23	19:O:60:ARG:HG2	2.00	0.43
10:A:537:A:H2'	10:A:538:G:O4'	2.18	0.43
10:A:1985:A:C2	18:N:22:ILE:HG23	2.54	0.43
12:G:140:VAL:HG13	12:G:161:SER:HB2	1.99	0.43
18:N:90:ASP:O	18:N:92:SER:N	2.50	0.43
10:A:2367:C:O2	10:A:2367:C:O4'	2.36	0.43
5:5:18:THR:CG2	10:A:2078:C:O2'	2.67	0.43
11:B:76:A:C2	11:B:97:A:C4	3.07	0.43
12:G:44:ASN:HB3	12:G:46:GLN:H	1.83	0.43
17:M:44:GLN:O	17:M:45:PHE:C	2.61	0.43
10:A:2491:U:O5'	10:A:2491:U:O2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2717:U:C4	10:A:2718:G:N7	2.86	0.43
21:Q:40:ILE:HD13	21:Q:40:ILE:HA	1.78	0.43
10:A:489:A:H1'	10:A:1247:U:O4'	2.19	0.42
10:A:638:U:H2'	10:A:639:U:C6	2.54	0.42
10:A:834:A:OP1	10:A:836:U:H5	2.02	0.42
24:T:40:MET:HE2	25:U:76:TYR:CD2	2.54	0.42
10:A:154:U:H2'	10:A:155:U:O4'	2.18	0.42
10:A:1381:G:H5''	10:A:1381:G:H8	1.84	0.42
11:B:26:C:OP1	22:R:39:ASN:OD1	2.37	0.42
13:H:151:PRO:O	13:H:153:ARG:CG	2.66	0.42
14:I:46:GLN:HG2	14:I:48:THR:HG23	2.02	0.42
10:A:1786:G:H5''	10:A:1786:G:C8	2.53	0.42
15:J:31:ILE:HD11	15:J:173:LEU:HD13	2.01	0.42
15:J:60:ILE:CD1	15:J:152:MET:HE1	2.48	0.42
26:V:12:ALA:HB2	26:V:55:VAL:HG22	2.01	0.42
10:A:684:U:H2'	10:A:685:C:C6	2.54	0.42
10:A:1187:U:H4'	10:A:1188:A:O4'	2.20	0.42
10:A:1393:A:H8	10:A:1393:A:C5'	2.32	0.42
22:R:69:LYS:HB3	22:R:104:ARG:HD3	2.01	0.42
5:5:46:CYS:CB	5:5:48:GLN:HE22	2.31	0.42
9:9:15:LYS:HE2	9:9:15:LYS:HA	2.02	0.42
10:A:209:A:H2'	10:A:210:C:O4'	2.19	0.42
10:A:383:A:H2'	10:A:384:G:O4'	2.20	0.42
10:A:1532:G:O2'	10:A:1533:A:OP1	2.31	0.42
20:P:54:MET:HE3	20:P:106:ILE:CG2	2.49	0.42
4:4:51:SER:OG	4:4:52:SER:N	2.52	0.42
10:A:804:G:N3	10:A:2014:A:H2	2.17	0.42
10:A:865:A:C4	10:A:1235:A:C2	3.08	0.42
10:A:2353:A:N3	10:A:2353:A:C2'	2.82	0.42
10:A:2364:G:O2'	10:A:2369:A:N1	2.49	0.42
10:A:2378:G:N3	10:A:2414:C:H2'	2.35	0.42
10:A:1049:G:O2'	10:A:1056:A:N1	2.50	0.42
10:A:1357:U:O2	10:A:1357:U:H2'	2.18	0.42
10:A:1829:U:H2'	10:A:1830:C:C6	2.54	0.42
10:A:1889:A:H2'	10:A:1890:G:H5'	2.00	0.42
28:X:39:ASN:HB2	28:X:63:ILE:HD11	2.02	0.42
10:A:573:A:H5''	10:A:573:A:N3	2.35	0.42
10:A:958:A:H2'	20:P:9:TYR:OH	2.19	0.42
10:A:1713:A:N6	10:A:2029:C:H5	1.98	0.42
18:N:35:ILE:HG21	18:N:103:ALA:CB	2.47	0.42
19:O:106:LYS:O	19:O:108:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:49:SER:HB2	26:V:50:PRO:HD3	2.01	0.42
10:A:249:G:H4'	10:A:432:G:C5	2.55	0.42
11:B:6:U:C5'	22:R:32:ASN:HD21	2.33	0.42
19:O:103:ARG:HH11	19:O:103:ARG:CB	2.33	0.42
10:A:267:A:N1	10:A:473:U:O2'	2.52	0.42
10:A:1327:G:O2'	10:A:1329:G:N7	2.52	0.42
10:A:1536:A:H8	10:A:1536:A:H5''	1.85	0.42
17:M:49:ILE:HD13	17:M:49:ILE:HA	1.88	0.42
17:M:74:ILE:CG2	17:M:87:SER:HB2	2.50	0.42
20:P:48:GLU:OE1	20:P:48:GLU:HA	2.18	0.42
23:S:48:ILE:HG13	23:S:62:ARG:HB2	2.02	0.42
10:A:174:A:H5''	10:A:174:A:C8	2.54	0.41
10:A:300:U:H3'	10:A:301:A:H5'	2.02	0.41
10:A:1937:G:O2'	10:A:1961:A:N1	2.47	0.41
14:I:20:ASN:OD1	14:I:22:THR:OG1	2.38	0.41
16:K:103:LEU:HD22	16:K:123:ILE:HG21	2.02	0.41
17:M:111:PRO:O	17:M:116:GLY:HA3	2.20	0.41
26:V:26:ILE:HD12	26:V:52:ILE:HG21	2.02	0.41
10:A:655:G:H21	10:A:661:A:N6	2.15	0.41
10:A:1517:C:O2'	10:A:1518:C:H6	2.02	0.41
10:A:1519:A:N7	10:A:1573:A:N1	2.68	0.41
14:I:7:LEU:HD12	14:I:146:ILE:HD12	2.02	0.41
19:O:86:GLU:O	19:O:89:THR:OG1	2.33	0.41
4:4:30:SER:O	4:4:31:SER:CB	2.68	0.41
8:8:30:SER:O	8:8:31:HIS:HD2	2.03	0.41
10:A:1501:G:O5'	10:A:1501:G:H8	2.02	0.41
10:A:2865:U:O4	10:A:2908:A:C2	2.73	0.41
12:G:126:VAL:HA	12:G:192:ILE:HG22	2.02	0.41
13:H:27:VAL:HG21	23:S:5:ILE:HG12	2.02	0.41
16:K:123:ILE:HD11	16:K:144:LEU:CD2	2.51	0.41
10:A:1656:C:H4'	10:A:1657:A:O5'	2.21	0.41
12:G:205:ILE:O	12:G:210:ARG:HD3	2.20	0.41
10:A:2059:U:H2'	10:A:2060:G:O4'	2.21	0.41
10:A:522:G:H4'	10:A:547:A:N1	2.36	0.41
10:A:1935:C:O3'	12:G:241:ILE:O	2.38	0.41
10:A:2054:G:H2'	10:A:2054:G:N3	2.35	0.41
13:H:2:THR:HG23	13:H:204:THR:HB	2.02	0.41
26:V:67:TYR:O	26:V:68:ASP:C	2.63	0.41
10:A:24:G:O2'	26:V:82:ASP:HB3	2.21	0.41
17:M:38:ARG:HG2	17:M:38:ARG:HH11	1.84	0.41
17:M:59:ASN:N	17:M:128:GLY:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:84:A:N1	10:A:98:G:O2'	2.49	0.41
10:A:2085:G:N3	13:H:153:ARG:HA	2.36	0.41
12:G:130:LEU:HD12	12:G:130:LEU:N	2.35	0.41
20:P:51:ARG:HD3	20:P:66:ILE:HD11	2.03	0.41
27:W:42:VAL:HG21	27:W:80:VAL:HG21	2.03	0.41
3:3:6:ILE:HD11	3:3:47:ILE:HD11	2.03	0.40
10:A:1381:G:H5''	10:A:1381:G:C8	2.57	0.40
10:A:1579:A:C4	10:A:1596:A:C6	3.09	0.40
10:A:2843:C:N3	10:A:2915:G:O6	2.54	0.40
18:N:94:ARG:HG3	18:N:94:ARG:NH1	2.35	0.40
5:5:18:THR:HG22	10:A:2078:C:O2'	2.22	0.40
10:A:363:A:H4'	10:A:365:A:N7	2.36	0.40
10:A:1532:G:H2'	10:A:1533:A:C8	2.57	0.40
10:A:1950:U:H2'	10:A:1951:A:O5'	2.21	0.40
12:G:126:VAL:O	12:G:192:ILE:O	2.39	0.40
16:K:84:GLU:HG3	16:K:134:LYS:HG2	2.02	0.40
17:M:60:ALA:HB1	17:M:102:LEU:HD12	2.03	0.40
3:3:17:GLN:N	3:3:18:PRO:CD	2.85	0.40
10:A:37:C:H4'	10:A:497:U:OP1	2.21	0.40
10:A:83:G:N1	10:A:101:G:H2'	2.37	0.40
10:A:1794:U:C3'	10:A:1795:A:H5''	2.52	0.40
12:G:130:LEU:HD13	12:G:192:ILE:CD1	2.51	0.40
17:M:73:LYS:HE3	17:M:75:TYR:CZ	2.56	0.40
22:R:15:HIS:CD2	22:R:97:GLY:HA2	2.56	0.40
8:8:27:GLY:O	10:A:2426:U:OP1	2.40	0.40
10:A:139:A:H4'	10:A:140:G:OP1	2.20	0.40
10:A:857:U:H2'	19:O:21:ARG:HA	2.04	0.40
10:A:1401:C:H2'	10:A:1402:G:O4'	2.22	0.40
10:A:2850:A:O2'	10:A:2855:A:N1	2.53	0.40
19:O:103:ARG:HB2	19:O:103:ARG:NH1	2.36	0.40
25:U:5:ILE:HG22	25:U:38:VAL:HG22	2.02	0.40
4:4:27:SER:OG	15:J:140:GLU:CD	2.65	0.40
10:A:31:C:O3'	10:A:1283:G:H5'	2.22	0.40
10:A:829:A:C8	10:A:829:A:C3'	3.05	0.40
10:A:2112:U:H2'	10:A:2113:G:O4'	2.22	0.40
10:A:2616:G:OP2	36:A:3210:HOH:O	2.22	0.40
18:N:13:ASN:ND2	18:N:96:THR:OG1	2.52	0.40
18:N:120:GLU:OE1	23:S:65:SER:OG	2.25	0.40
19:O:48:LEU:HD23	19:O:48:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	56/62 (90%)	49 (88%)	6 (11%)	1 (2%)	6	6
2	2	57/63 (90%)	54 (95%)	2 (4%)	1 (2%)	6	6
3	3	54/59 (92%)	54 (100%)	0	0	100	100
4	4	57/81 (70%)	47 (82%)	9 (16%)	1 (2%)	6	6
5	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
6	6	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
7	7	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
8	8	61/66 (92%)	58 (95%)	1 (2%)	2 (3%)	3	2
9	9	34/37 (92%)	34 (100%)	0	0	100	100
12	G	271/277 (98%)	259 (96%)	9 (3%)	3 (1%)	11	13
13	H	204/209 (98%)	189 (93%)	14 (7%)	1 (0%)	24	31
14	I	201/207 (97%)	187 (93%)	9 (4%)	5 (2%)	4	3
15	J	173/179 (97%)	150 (87%)	17 (10%)	6 (4%)	3	1
16	K	163/178 (92%)	146 (90%)	14 (9%)	3 (2%)	6	6
17	M	140/145 (97%)	134 (96%)	4 (3%)	2 (1%)	9	9
18	N	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	20
19	O	142/146 (97%)	130 (92%)	10 (7%)	2 (1%)	9	9
20	P	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
21	Q	118/135 (87%)	110 (93%)	7 (6%)	1 (1%)	16	20
22	R	116/119 (98%)	104 (90%)	8 (7%)	4 (3%)	3	2
23	S	110/114 (96%)	104 (94%)	5 (4%)	1 (1%)	14	17
24	T	114/119 (96%)	112 (98%)	2 (2%)	0	100	100
25	U	99/102 (97%)	94 (95%)	4 (4%)	1 (1%)	12	15
26	V	108/118 (92%)	103 (95%)	3 (3%)	2 (2%)	6	5
27	W	88/94 (94%)	83 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	X	93/103 (90%)	86 (92%)	5 (5%)	2 (2%)	5	4
29	Z	71/96 (74%)	66 (93%)	4 (6%)	1 (1%)	9	9
All	All	2917/3125 (93%)	2719 (93%)	158 (5%)	40 (1%)	11	9

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	56	SER
8	8	31	HIS
12	G	126	VAL
13	H	152	ASN
14	I	159	GLU
23	S	105	GLY
26	V	114	GLU
28	X	51	ASN
14	I	158	GLY
14	I	178	ALA
15	J	142	ASP
15	J	150	ARG
19	O	114	ASN
28	X	50	VAL
2	2	38	GLU
4	4	31	SER
14	I	129	LEU
15	J	83	MET
15	J	118	SER
16	K	80	SER
18	N	91	LYS
22	R	53	LEU
22	R	96	ARG
25	U	45	SER
26	V	68	ASP
12	G	252	LYS
15	J	109	PRO
17	M	28	ARG
17	M	50	ASP
19	O	107	SER
22	R	63	PHE
15	J	117	VAL
16	K	126	PRO
21	Q	75	GLN

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Mol	Chain	Res	Type
22	R	101	TYR
8	8	27	GLY
14	I	177	PRO
16	K	55	PRO
29	Z	81	GLY
12	G	241	ILE

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	1	50/53 (94%)	49 (98%)	1 (2%)	48	67
2	2	52/55 (94%)	51 (98%)	1 (2%)	50	69
3	3	50/52 (96%)	50 (100%)	0	100	100
4	4	56/73 (77%)	55 (98%)	1 (2%)	51	70
5	5	47/50 (94%)	45 (96%)	2 (4%)	26	39
6	6	46/48 (96%)	44 (96%)	2 (4%)	26	39
7	7	38/39 (97%)	38 (100%)	0	100	100
8	8	53/56 (95%)	51 (96%)	2 (4%)	29	44
9	9	35/35 (100%)	30 (86%)	5 (14%)	3	3
12	G	221/225 (98%)	219 (99%)	2 (1%)	70	84
13	H	169/171 (99%)	169 (100%)	0	100	100
14	I	171/174 (98%)	168 (98%)	3 (2%)	51	70
15	J	151/155 (97%)	140 (93%)	11 (7%)	13	18
16	K	137/147 (93%)	132 (96%)	5 (4%)	31	47
17	M	119/121 (98%)	118 (99%)	1 (1%)	73	86
18	N	101/101 (100%)	97 (96%)	4 (4%)	28	42
19	O	113/115 (98%)	108 (96%)	5 (4%)	25	38
20	P	105/113 (93%)	104 (99%)	1 (1%)	68	82
21	Q	102/111 (92%)	100 (98%)	2 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	R	96/97 (99%)	94 (98%)	2 (2%)	47	66
23	S	98/100 (98%)	98 (100%)	0	100	100
24	T	95/97 (98%)	94 (99%)	1 (1%)	65	81
25	U	82/82 (100%)	78 (95%)	4 (5%)	22	34
26	V	91/97 (94%)	91 (100%)	0	100	100
27	W	80/84 (95%)	79 (99%)	1 (1%)	61	77
28	X	81/88 (92%)	77 (95%)	4 (5%)	22	34
29	Z	58/76 (76%)	56 (97%)	2 (3%)	32	49
All	All	2497/2615 (96%)	2435 (98%)	62 (2%)	42	60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	39	LEU
2	2	42	ARG
4	4	6	HIS
5	5	20	VAL
5	5	28	ASN
6	6	12	CYS
6	6	15	ARG
8	8	15	LYS
8	8	31	HIS
9	9	7	VAL
9	9	8	LYS
9	9	24	MET
9	9	25	VAL
9	9	35	LYS
12	G	80	THR
12	G	125	LYS
14	I	7	LEU
14	I	101	LEU
14	I	113	ILE
15	J	4	LEU
15	J	38	THR
15	J	50	LEU
15	J	85	ILE
15	J	95	ARG
15	J	100	LEU
15	J	103	LEU

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Mol	Chain	Res	Type
15	J	115	ARG
15	J	125	ARG
15	J	133	ARG
15	J	176	PRO
16	K	30	LYS
16	K	43	ILE
16	K	72	LEU
16	K	121	VAL
16	K	173	GLU
17	M	29	LEU
18	N	17	ARG
18	N	81	GLU
18	N	102	VAL
18	N	122	LEU
19	O	47	ARG
19	O	92	THR
19	O	94	GLU
19	O	103	ARG
19	O	142	LYS
20	P	54	MET
21	Q	40	ILE
21	Q	53	LYS
22	R	39	ASN
22	R	110	GLU
24	T	78	LYS
25	U	7	THR
25	U	10	LYS
25	U	12	ILE
25	U	54	GLU
27	W	67	ARG
28	X	10	LYS
28	X	22	LYS
28	X	33	VAL
28	X	95	LYS
29	Z	57	THR
29	Z	80	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	20	HIS
2	2	17	GLN

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Mol	Chain	Res	Type
3	3	17	GLN
3	3	40	ASN
5	5	48	GLN
12	G	194	GLN
13	H	128	GLN
14	I	171	GLN
15	J	37	ASN
15	J	46	ASN
15	J	172	GLN
16	K	38	ASN
16	K	140	HIS
18	N	3	GLN
18	N	109	ASN
22	R	32	ASN
22	R	58	ASN
23	S	12	GLN
27	W	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2905/2931 (99%)	539 (18%)	75 (2%)
11	B	113/114 (99%)	22 (19%)	1 (0%)
All	All	3018/3045 (99%)	561 (18%)	76 (2%)

All (561) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	12	A
10	A	13	A
10	A	34	U
10	A	42	G
10	A	45	G
10	A	46	C
10	A	60	G
10	A	71	A
10	A	74	U
10	A	75	G
10	A	84	A
10	A	89	U

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Mol	Chain	Res	Type
10	A	90	A
10	A	91	C
10	A	92	G
10	A	93	U
10	A	101	G
10	A	117	A
10	A	118	A
10	A	119	U
10	A	140	G
10	A	141	U
10	A	161	A
10	A	162	A
10	A	164	A
10	A	166	A
10	A	167	U
10	A	174	A
10	A	175	G
10	A	182	A
10	A	188	A
10	A	198	A
10	A	201	A
10	A	202	U
10	A	215	A
10	A	217	G
10	A	218	A
10	A	223	A
10	A	224	A
10	A	225	A
10	A	230	A
10	A	232	U
10	A	235	A
10	A	250	G
10	A	251	C
10	A	252	G
10	A	257	A
10	A	274	A
10	A	275	C
10	A	281	A
10	A	283	C
10	A	284	U
10	A	285	U
10	A	286	G

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Mol	Chain	Res	Type
10	A	287	C
10	A	288	U
10	A	290	C
10	A	297	U
10	A	298	U
10	A	299	G
10	A	300	U
10	A	301	A
10	A	307	C
10	A	309	C
10	A	311	A
10	A	312	U
10	A	313	A
10	A	318	G
10	A	320	U
10	A	323	A
10	A	325	A
10	A	326	A
10	A	327	G
10	A	328	A
10	A	345	G
10	A	354	A
10	A	360	G
10	A	372	A
10	A	373	A
10	A	388	A
10	A	389	A
10	A	404	A
10	A	409	G
10	A	410	G
10	A	411	A
10	A	412	U
10	A	417	A
10	A	418	G
10	A	432	G
10	A	440	C
10	A	450	C
10	A	451	C
10	A	457	G
10	A	470	G
10	A	490	C
10	A	502	C

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Mol	Chain	Res	Type
10	A	503	A
10	A	527	G
10	A	549	C
10	A	550	A
10	A	552	U
10	A	567	G
10	A	575	G
10	A	576	U
10	A	577	A
10	A	578	G
10	A	583	A
10	A	591	A
10	A	592	A
10	A	594	G
10	A	599	A
10	A	606	G
10	A	614	U
10	A	615	A
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	656	G
10	A	657	A
10	A	659	A
10	A	672	A
10	A	679	G
10	A	682	A
10	A	690	U
10	A	698	A
10	A	699	U
10	A	700	A
10	A	731	A
10	A	732	U
10	A	746	G
10	A	757	A
10	A	758	G
10	A	763	U
10	A	776	U
10	A	793	U
10	A	803	G
10	A	810	A

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Mol	Chain	Res	Type
10	A	811	G
10	A	821	G
10	A	828	A
10	A	830	U
10	A	836	U
10	A	837	C
10	A	851	G
10	A	852	C
10	A	858	C
10	A	865	A
10	A	873	U
10	A	874	U
10	A	889	G
10	A	891	U
10	A	892	A
10	A	893	A
10	A	906	G
10	A	913	A
10	A	916	G
10	A	926	G
10	A	931	C
10	A	933	U
10	A	934	U
10	A	935	C
10	A	936	U
10	A	937	C
10	A	940	G
10	A	942	U
10	A	943	A
10	A	944	C
10	A	950	U
10	A	954	A
10	A	957	A
10	A	959	C
10	A	964	A
10	A	970	A
10	A	973	U
10	A	976	U
10	A	979	U
10	A	987	A
10	A	990	C
10	A	991	A

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Mol	Chain	Res	Type
10	A	992	G
10	A	1007	G
10	A	1020	A
10	A	1029	A
10	A	1035	G
10	A	1036	A
10	A	1042	A
10	A	1058	U
10	A	1059	A
10	A	1066	A
10	A	1067	A
10	A	1068	G
10	A	1072	A
10	A	1079	U
10	A	1084	G
10	A	1092	A
10	A	1093	G
10	A	1100	A
10	A	1101	G
10	A	1102	G
10	A	1103	A
10	A	1111	U
10	A	1112	U
10	A	1115	A
10	A	1116	A
10	A	1119	A
10	A	1120	G
10	A	1128	U
10	A	1129	G
10	A	1130	A
10	A	1131	A
10	A	1132	A
10	A	1133	G
10	A	1134	A
10	A	1136	U
10	A	1138	C
10	A	1139	G
10	A	1142	A
10	A	1146	C
10	A	1147	U
10	A	1149	A
10	A	1150	C

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Mol	Chain	Res	Type
10	A	1151	U
10	A	1152	G
10	A	1153	G
10	A	1154	U
10	A	1155	C
10	A	1156	G
10	A	1157	A
10	A	1158	G
10	A	1174	A
10	A	1178	U
10	A	1179	A
10	A	1180	C
10	A	1181	C
10	A	1182	G
10	A	1188	A
10	A	1189	A
10	A	1203	A
10	A	1204	C
10	A	1265	A
10	A	1283	G
10	A	1289	A
10	A	1298	A
10	A	1301	G
10	A	1311	G
10	A	1312	U
10	A	1316	G
10	A	1317	A
10	A	1320	G
10	A	1344	A
10	A	1345	A
10	A	1347	A
10	A	1376	G
10	A	1377	C
10	A	1381	G
10	A	1382	G
10	A	1393	A
10	A	1394	C
10	A	1396	U
10	A	1409	A
10	A	1419	G
10	A	1423	U
10	A	1429	A

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Mol	Chain	Res	Type
10	A	1432	G
10	A	1457	A
10	A	1462	U
10	A	1463	U
10	A	1464	A
10	A	1465	A
10	A	1466	C
10	A	1469	A
10	A	1470	U
10	A	1478	C
10	A	1501	G
10	A	1505	G
10	A	1509	A
10	A	1516	U
10	A	1517	C
10	A	1528	G
10	A	1529	U
10	A	1530	G
10	A	1531	U
10	A	1532	G
10	A	1533	A
10	A	1534	G
10	A	1536	A
10	A	1539	A
10	A	1542	C
10	A	1543	A
10	A	1558	G
10	A	1561	G
10	A	1564	U
10	A	1566	A
10	A	1570	G
10	A	1575	G
10	A	1594	G
10	A	1606	U
10	A	1611	C
10	A	1612	G
10	A	1618	A
10	A	1621	A
10	A	1630	U
10	A	1634	A
10	A	1635	A
10	A	1638	G

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Mol	Chain	Res	Type
10	A	1642	U
10	A	1644	C
10	A	1657	A
10	A	1658	A
10	A	1659	A
10	A	1665	A
10	A	1695	A
10	A	1696	G
10	A	1697	C
10	A	1723	G
10	A	1749	A
10	A	1762	U
10	A	1763	U
10	A	1773	G
10	A	1779	G
10	A	1780	A
10	A	1782	A
10	A	1783	G
10	A	1785	C
10	A	1786	G
10	A	1789	G
10	A	1796	G
10	A	1797	G
10	A	1806	A
10	A	1815	C
10	A	1833	C
10	A	1834	A
10	A	1849	C
10	A	1850	G
10	A	1862	A
10	A	1880	A
10	A	1881	A
10	A	1889	A
10	A	1890	G
10	A	1891	G
10	A	1892	A
10	A	1899	A
10	A	1903	U
10	A	1904	C
10	A	1906	G
10	A	1938	C
10	A	1939	G

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Mol	Chain	Res	Type
10	A	1943	G
10	A	1946	A
10	A	1947	C
10	A	1948	U
10	A	1949	A
10	A	1951	A
10	A	1952	A
10	A	1955	G
10	A	1956	U
10	A	1962	G
10	A	1963	G
10	A	1964	U
10	A	1970	A
10	A	1971	A
10	A	1988	U
10	A	1996	C
10	A	1998	C
10	A	2000	C
10	A	2003	A
10	A	2004	A
10	A	2005	G
10	A	2024	U
10	A	2026	U
10	A	2029	C
10	A	2030	A
10	A	2056	A
10	A	2060	G
10	A	2064	A
10	A	2065	G
10	A	2066	A
10	A	2076	C
10	A	2088	C
10	A	2089	G
10	A	2093	A
10	A	2094	G
10	A	2095	A
10	A	2102	G
10	A	2125	G
10	A	2126	G
10	A	2133	U
10	A	2136	A
10	A	2139	G

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Mol	Chain	Res	Type
10	A	2140	C
10	A	2141	U
10	A	2142	U
10	A	2144	U
10	A	2146	C
10	A	2148	G
10	A	2152	A
10	A	2153	G
10	A	2154	G
10	A	2158	G
10	A	2159	A
10	A	2160	G
10	A	2164	A
10	A	2165	A
10	A	2166	G
10	A	2167	A
10	A	2168	G
10	A	2171	G
10	A	2174	U
10	A	2180	A
10	A	2183	A
10	A	2191	A
10	A	2199	G
10	A	2200	U
10	A	2205	U
10	A	2206	A
10	A	2211	C
10	A	2215	G
10	A	2217	U
10	A	2218	G
10	A	2220	A
10	A	2221	U
10	A	2223	A
10	A	2225	C
10	A	2226	A
10	A	2231	A
10	A	2236	G
10	A	2237	C
10	A	2244	U
10	A	2258	A
10	A	2259	C
10	A	2271	G

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Mol	Chain	Res	Type
10	A	2272	G
10	A	2301	A
10	A	2316	C
10	A	2319	A
10	A	2320	A
10	A	2328	C
10	A	2337	G
10	A	2338	A
10	A	2340	G
10	A	2341	G
10	A	2351	G
10	A	2352	C
10	A	2353	A
10	A	2354	G
10	A	2355	A
10	A	2358	G
10	A	2359	U
10	A	2360	A
10	A	2367	C
10	A	2368	A
10	A	2380	C
10	A	2383	C
10	A	2387	A
10	A	2410	A
10	A	2412	G
10	A	2416	G
10	A	2418	C
10	A	2429	G
10	A	2435	U
10	A	2436	C
10	A	2439	C
10	A	2447	G
10	A	2456	U
10	A	2457	C
10	A	2458	A
10	A	2459	A
10	A	2462	G
10	A	2463	A
10	A	2464	U
10	A	2468	A
10	A	2472	A
10	A	2473	C

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Mol	Chain	Res	Type
10	A	2474	C
10	A	2481	A
10	A	2503	G
10	A	2507	C
10	A	2524	U
10	A	2535	G
10	A	2538	G
10	A	2551	A
10	A	2552	U
10	A	2562	G
10	A	2567	C
10	A	2568	G
10	A	2587	U
10	A	2599	A
10	A	2600	G
10	A	2606	C
10	A	2618	U
10	A	2635	A
10	A	2636	G
10	A	2637	U
10	A	2642	U
10	A	2646	U
10	A	2663	G
10	A	2674	A
10	A	2694	G
10	A	2696	G
10	A	2703	G
10	A	2722	U
10	A	2724	C
10	A	2747	G
10	A	2759	U
10	A	2766	C
10	A	2777	G
10	A	2781	A
10	A	2784	G
10	A	2790	A
10	A	2794	G
10	A	2795	U
10	A	2798	A
10	A	2799	G
10	A	2810	G
10	A	2811	A

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Mol	Chain	Res	Type
10	A	2823	A
10	A	2828	U
10	A	2832	G
10	A	2835	A
10	A	2837	U
10	A	2841	A
10	A	2842	U
10	A	2862	A
10	A	2864	A
10	A	2872	G
10	A	2890	U
10	A	2896	G
10	A	2897	A
10	A	2906	A
10	A	2908	A
10	A	2909	C
10	A	2913	U
10	A	2915	G
10	A	2916	A
10	A	2922	G
10	A	2929	C
10	A	2930	C
11	B	3	U
11	B	10	U
11	B	23	U
11	B	24	C
11	B	25	A
11	B	33	U
11	B	38	U
11	B	40	C
11	B	43	A
11	B	54	U
11	B	55	A
11	B	65	G
11	B	67	G
11	B	82	G
11	B	83	G
11	B	86	U
11	B	87	U
11	B	88	C
11	B	103	G
11	B	106	C

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Mol	Chain	Res	Type
11	B	107	G
11	B	114	G

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	12	A
10	A	45	G
10	A	90	A
10	A	92	G
10	A	101	G
10	A	139	A
10	A	174	A
10	A	201	A
10	A	217	G
10	A	231	A
10	A	251	C
10	A	274	A
10	A	297	U
10	A	308	U
10	A	318	G
10	A	388	A
10	A	409	G
10	A	502	C
10	A	548	A
10	A	574	A
10	A	614	U
10	A	630	G
10	A	810	A
10	A	836	U
10	A	851	G
10	A	873	U
10	A	990	C
10	A	1030	G
10	A	1035	G
10	A	1066	A
10	A	1148	C
10	A	1179	A
10	A	1188	A
10	A	1203	A
10	A	1311	G
10	A	1344	A

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Mol	Chain	Res	Type
10	A	1376	G
10	A	1462	U
10	A	1508	A
10	A	1528	G
10	A	1532	G
10	A	1533	A
10	A	1594	G
10	A	1598	G
10	A	1606	U
10	A	1611	C
10	A	1634	A
10	A	1657	A
10	A	1667	A
10	A	1849	C
10	A	1880	A
10	A	1889	A
10	A	1891	G
10	A	1950	U
10	A	1951	A
10	A	1955	G
10	A	2030	A
10	A	2084	A
10	A	2126	G
10	A	2152	A
10	A	2159	A
10	A	2166	G
10	A	2258	A
10	A	2320	A
10	A	2359	U
10	A	2456	U
10	A	2458	A
10	A	2463	A
10	A	2472	A
10	A	2480	G
10	A	2551	A
10	A	2789	U
10	A	2809	A
10	A	2896	G
10	A	2908	A
11	B	106	C

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](#)

Of 172 ligands modelled in this entry, 168 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	PUT	A	3151	-	5,5,5	0.17	0	4,4,4	0.22	0
31	SPD	A	3001	-	9,9,9	0.22	0	8,8,8	0.27	0
33	PUT	A	3152	-	5,5,5	0.17	0	4,4,4	0.21	0
34	3QB	A	3156	-	26,28,28	0.32	0	31,40,40	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PUT	A	3151	-	-	0/3/3/3	-
31	SPD	A	3001	-	-	1/7/7/7	-
33	PUT	A	3152	-	-	1/3/3/3	-
34	3QB	A	3156	-	-	1/21/53/53	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

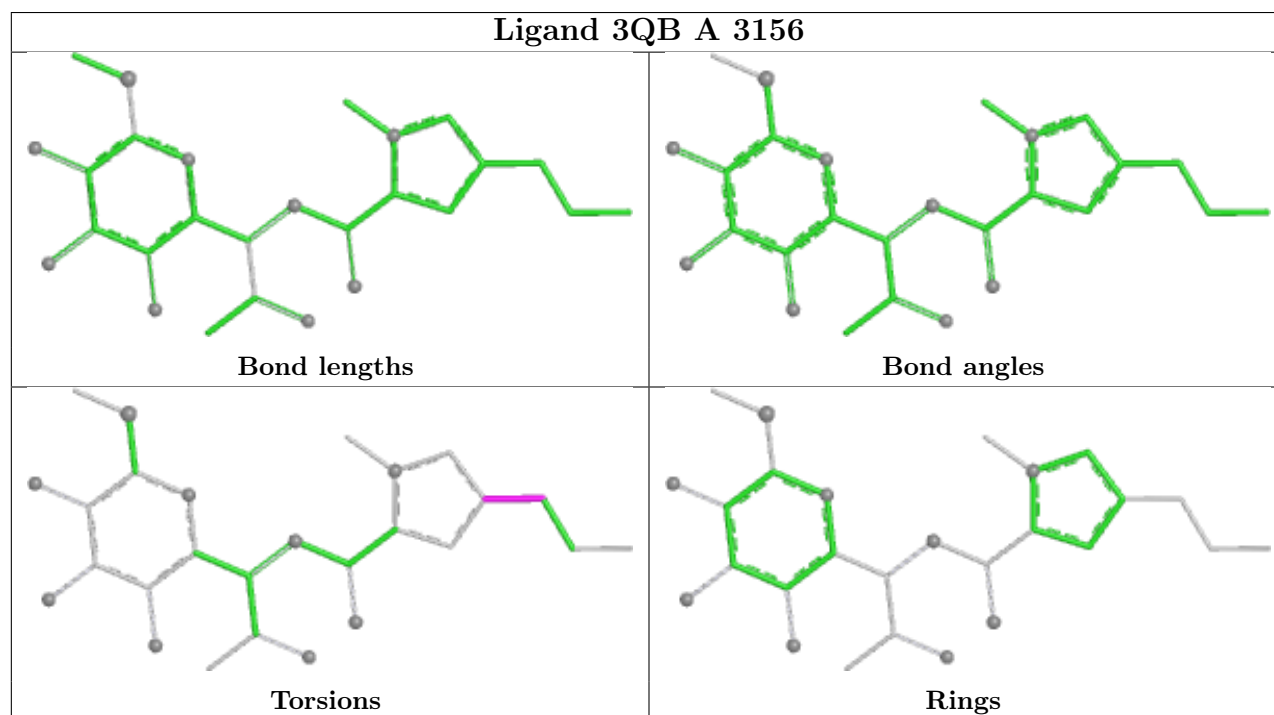
Mol	Chain	Res	Type	Atoms
31	A	3001	SPD	C3-C4-C5-N6
33	A	3152	PUT	C1-C2-C3-C4
34	A	3156	3QB	C12-C13-C16-C17

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3001	SPD	1	0
33	A	3152	PUT	1	0

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



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.

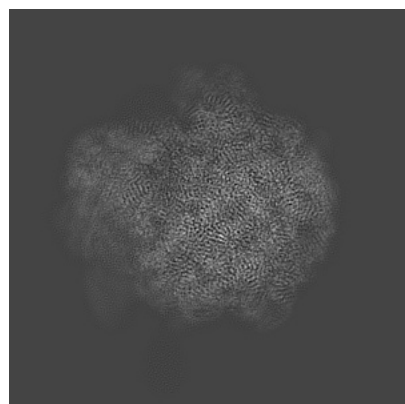
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15175. These allow visual inspection of the internal detail of the map and identification of artifacts.

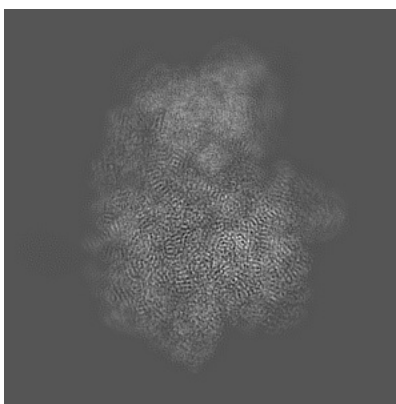
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

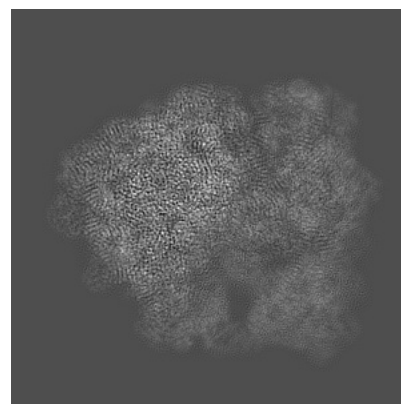
6.1.1 Primary map



X

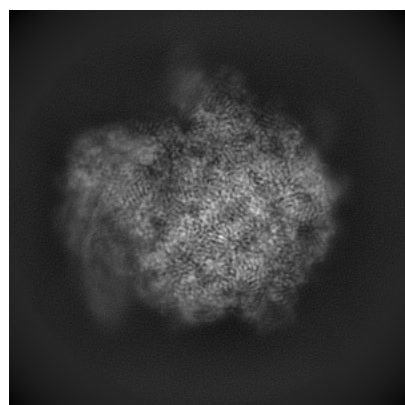


Y

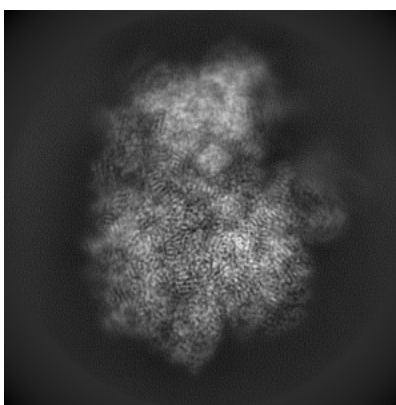


Z

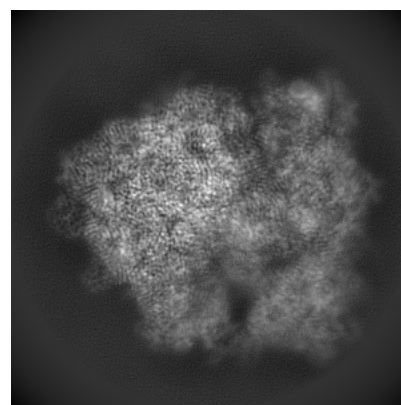
6.1.2 Raw map



X



Y

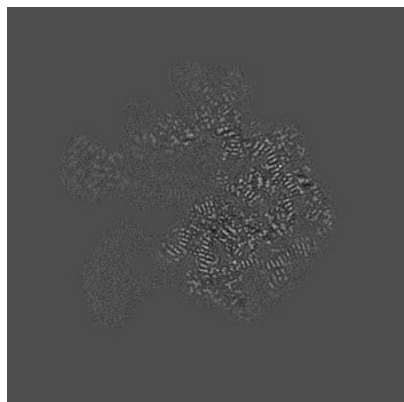


Z

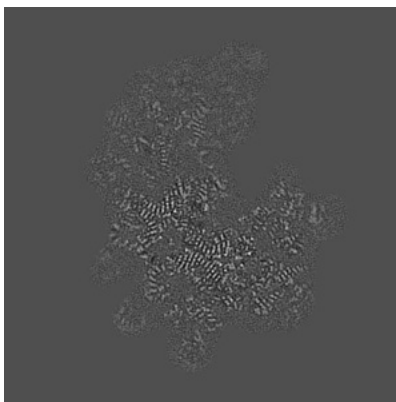
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

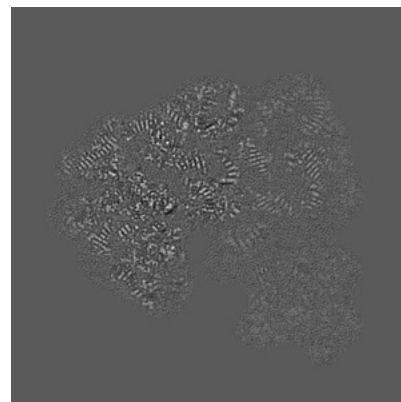
6.2.1 Primary map



X Index: 200

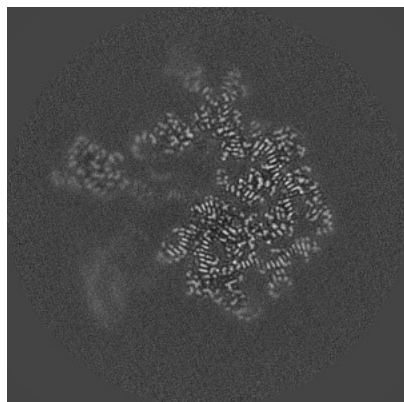


Y Index: 200

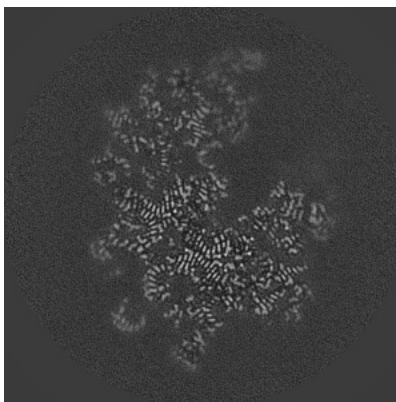


Z Index: 200

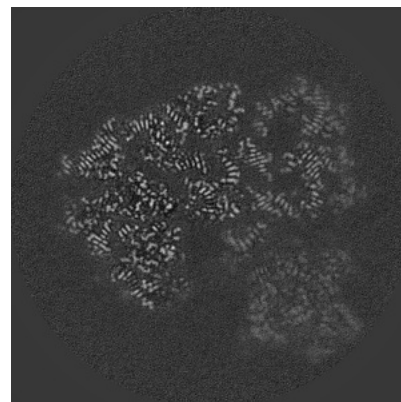
6.2.2 Raw map



X Index: 200



Y Index: 200

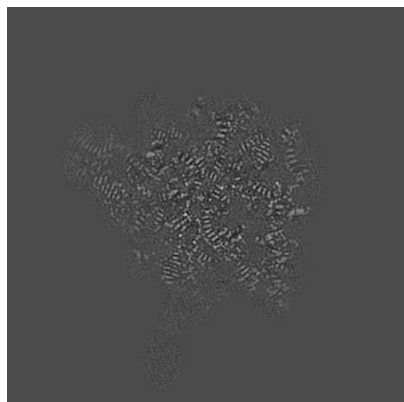


Z Index: 200

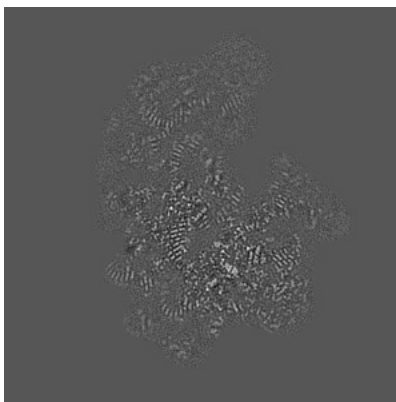
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

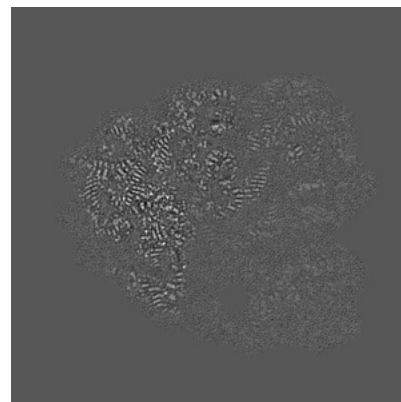
6.3.1 Primary map



X Index: 147

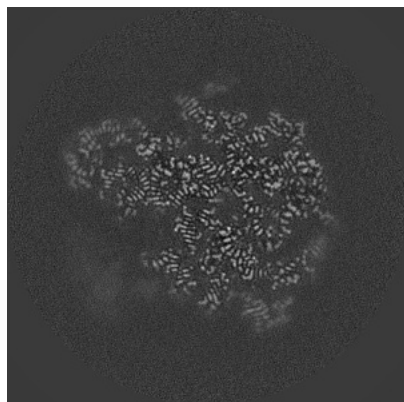


Y Index: 214

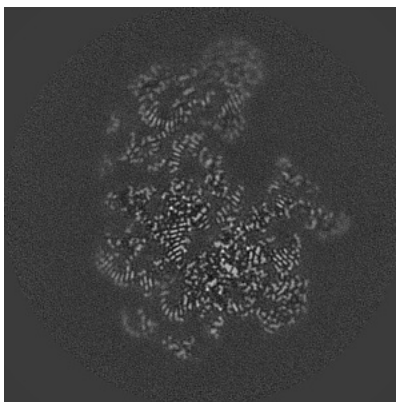


Z Index: 210

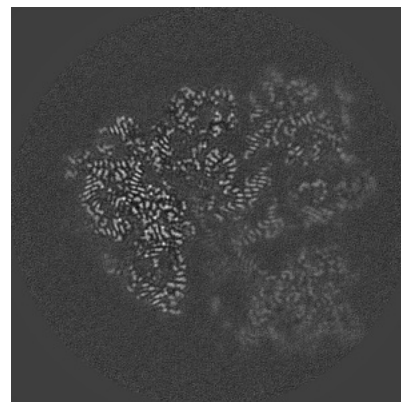
6.3.2 Raw map



X Index: 168



Y Index: 214

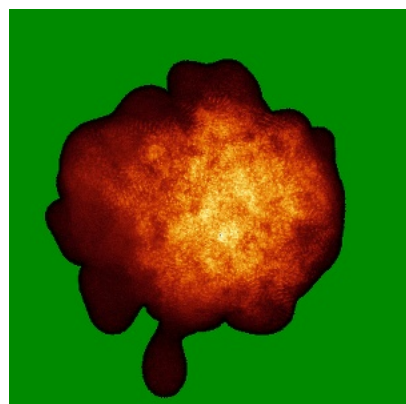


Z Index: 209

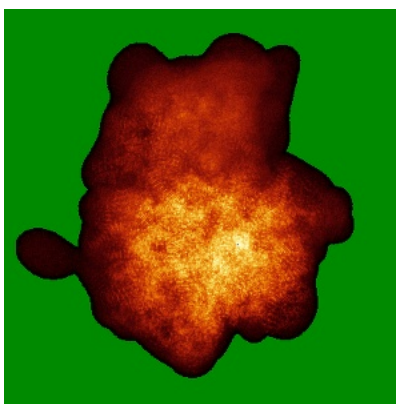
The images above show the largest variance slices of the map in three orthogonal directions.

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

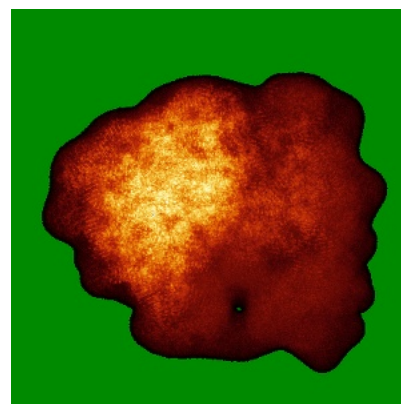
6.4.1 Primary map



X

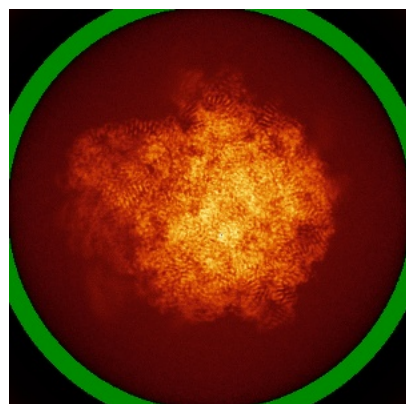


Y

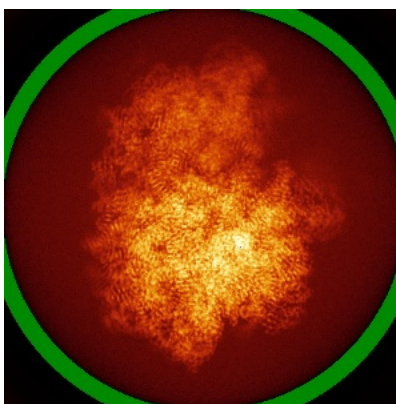


Z

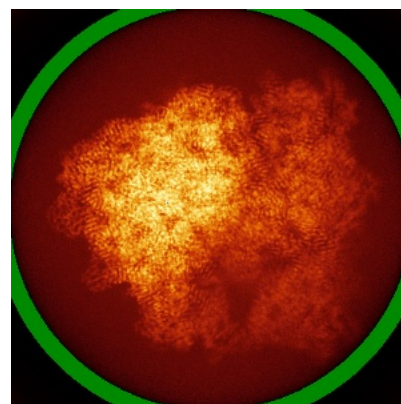
6.4.2 Raw map



X



Y

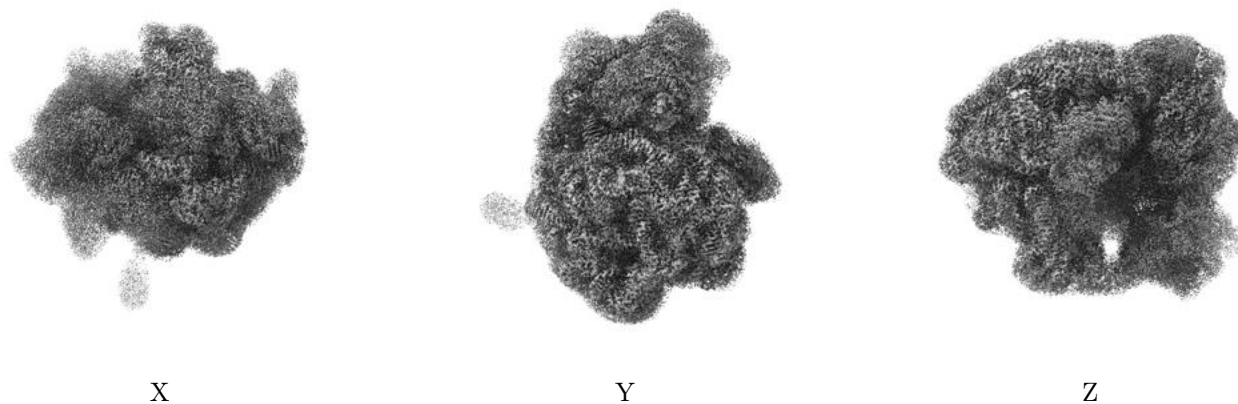


Z

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.

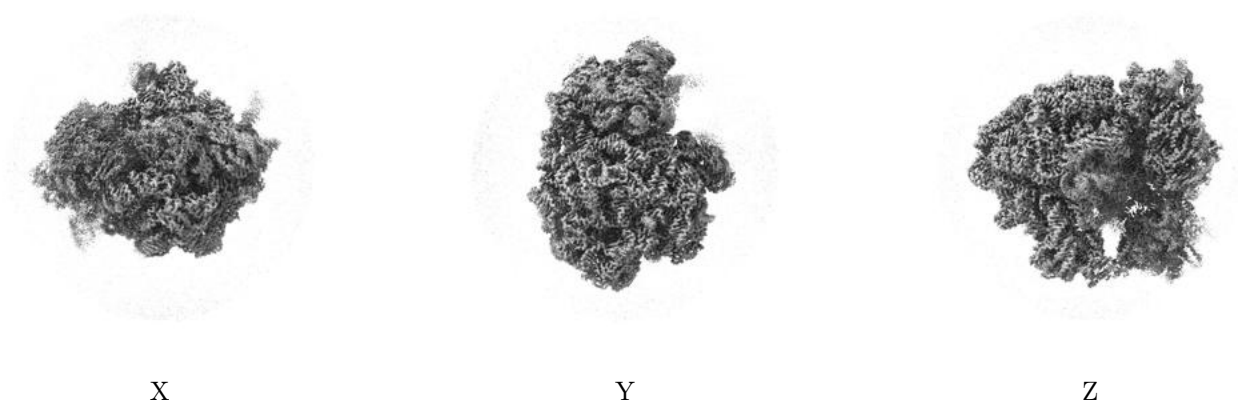
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



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.

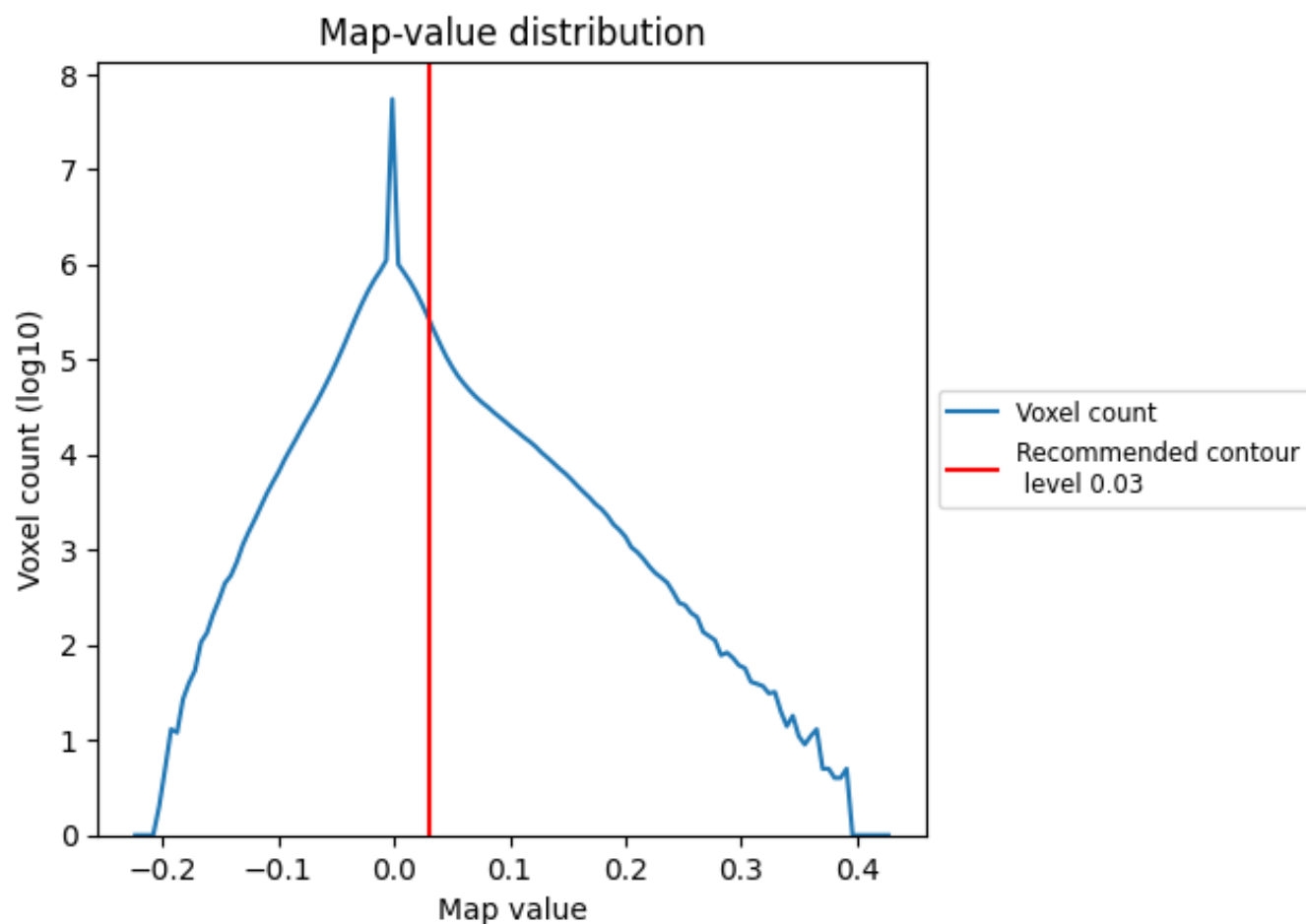
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

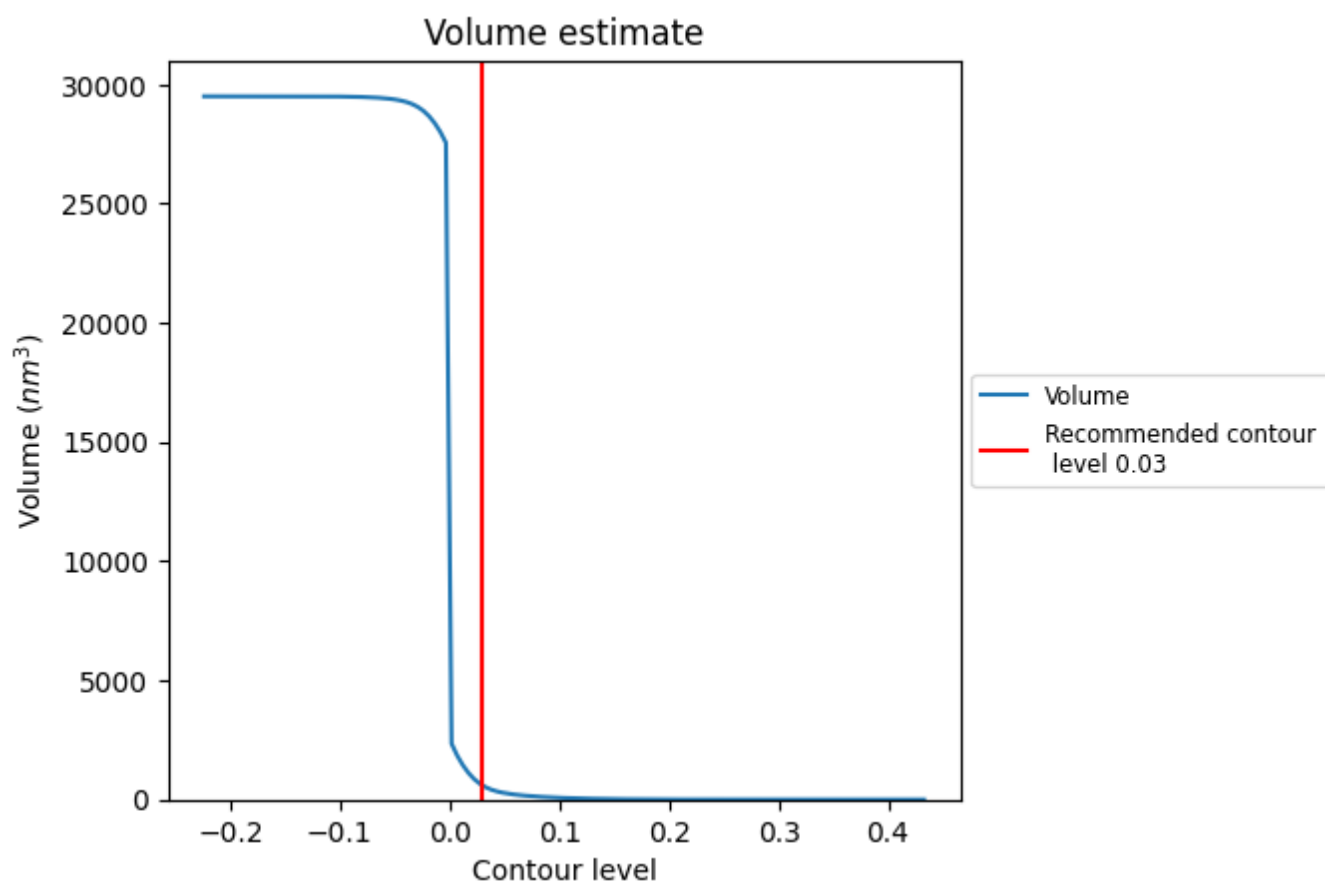
This section contains the results of statistical analysis of the map.

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.

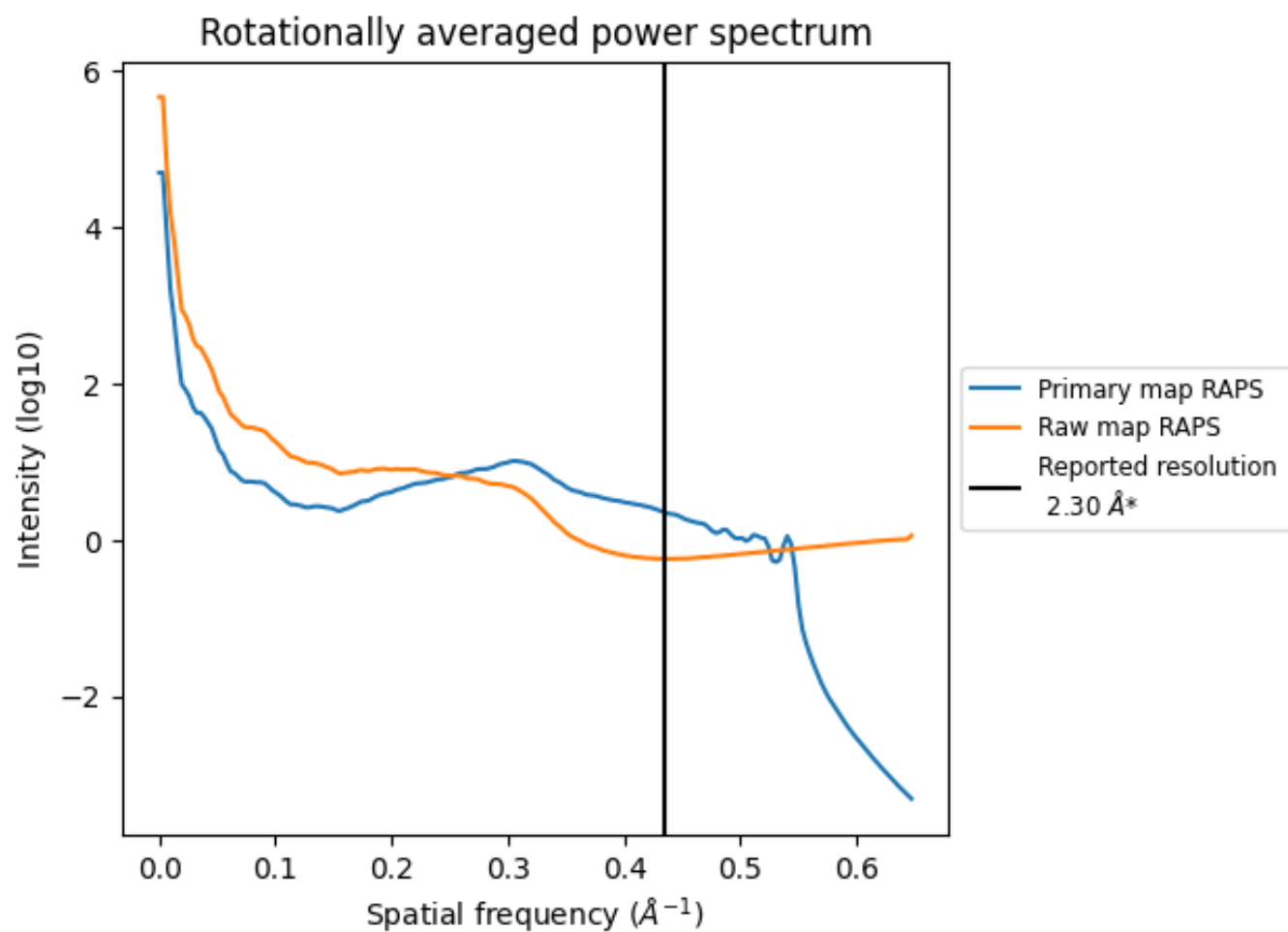
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 600 nm^3 ; this corresponds to an approximate mass of 542 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 ⓘ

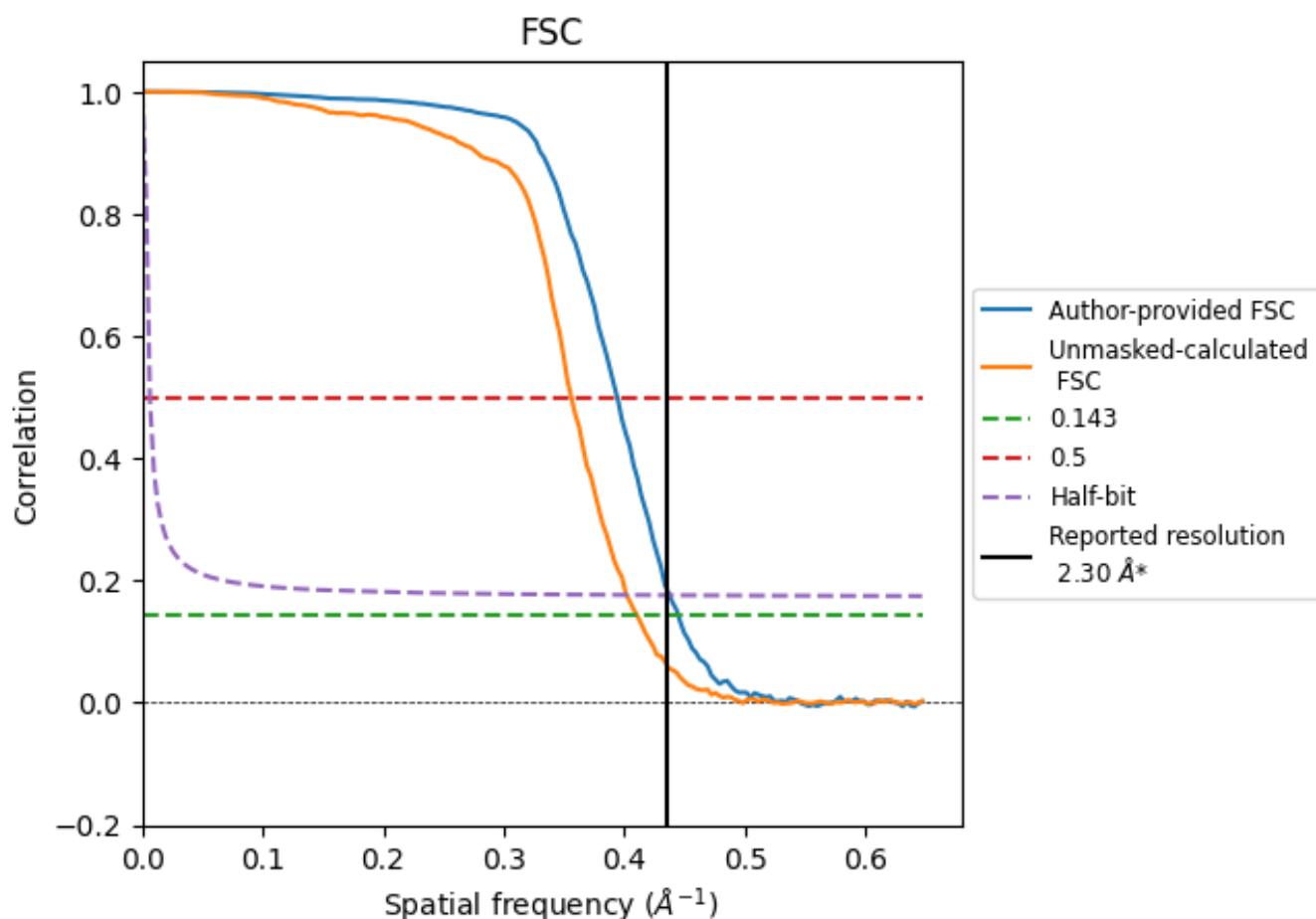


*Reported resolution corresponds to spatial frequency of $0.435 \text{ \AA}^{-1}$

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 $0.435 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

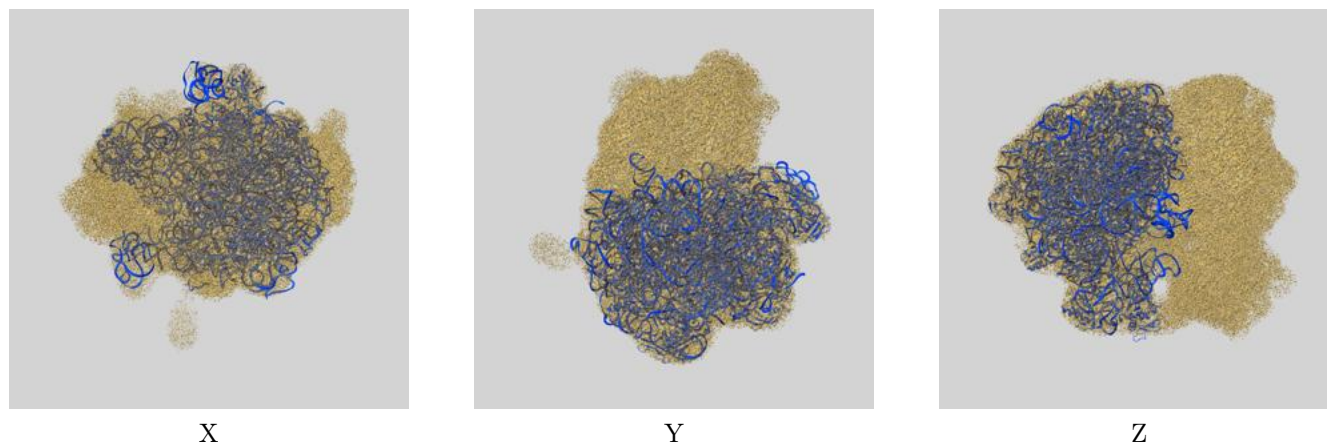
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.25	2.54	2.29
Unmasked-calculated*	2.44	2.81	2.49

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

9 Map-model fit [i](#)

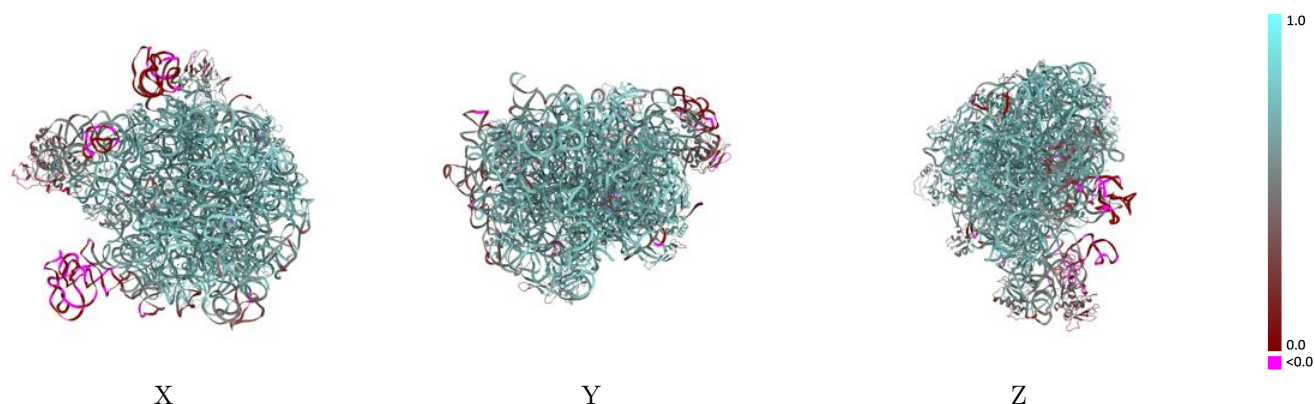
This section contains information regarding the fit between EMDB map EMD-15175 and PDB model 8A5I. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



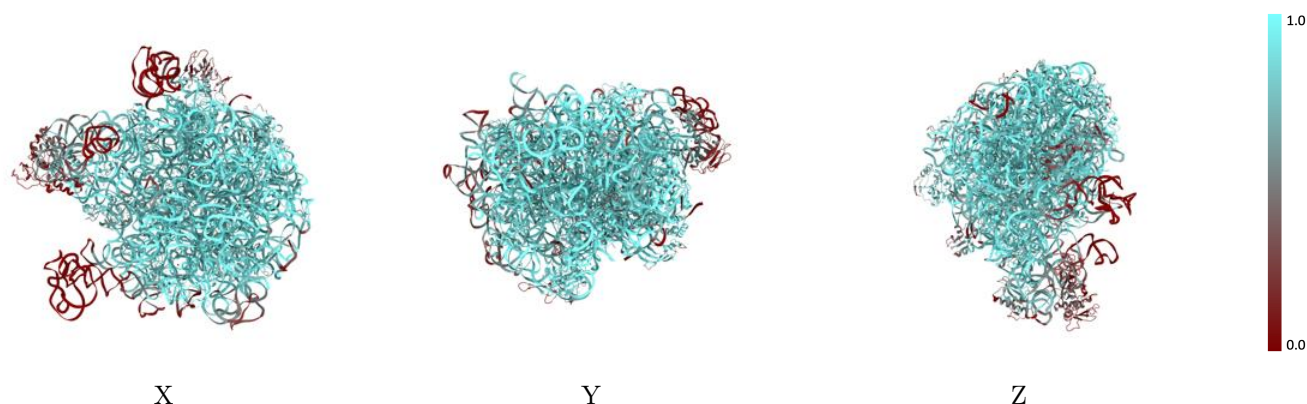
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



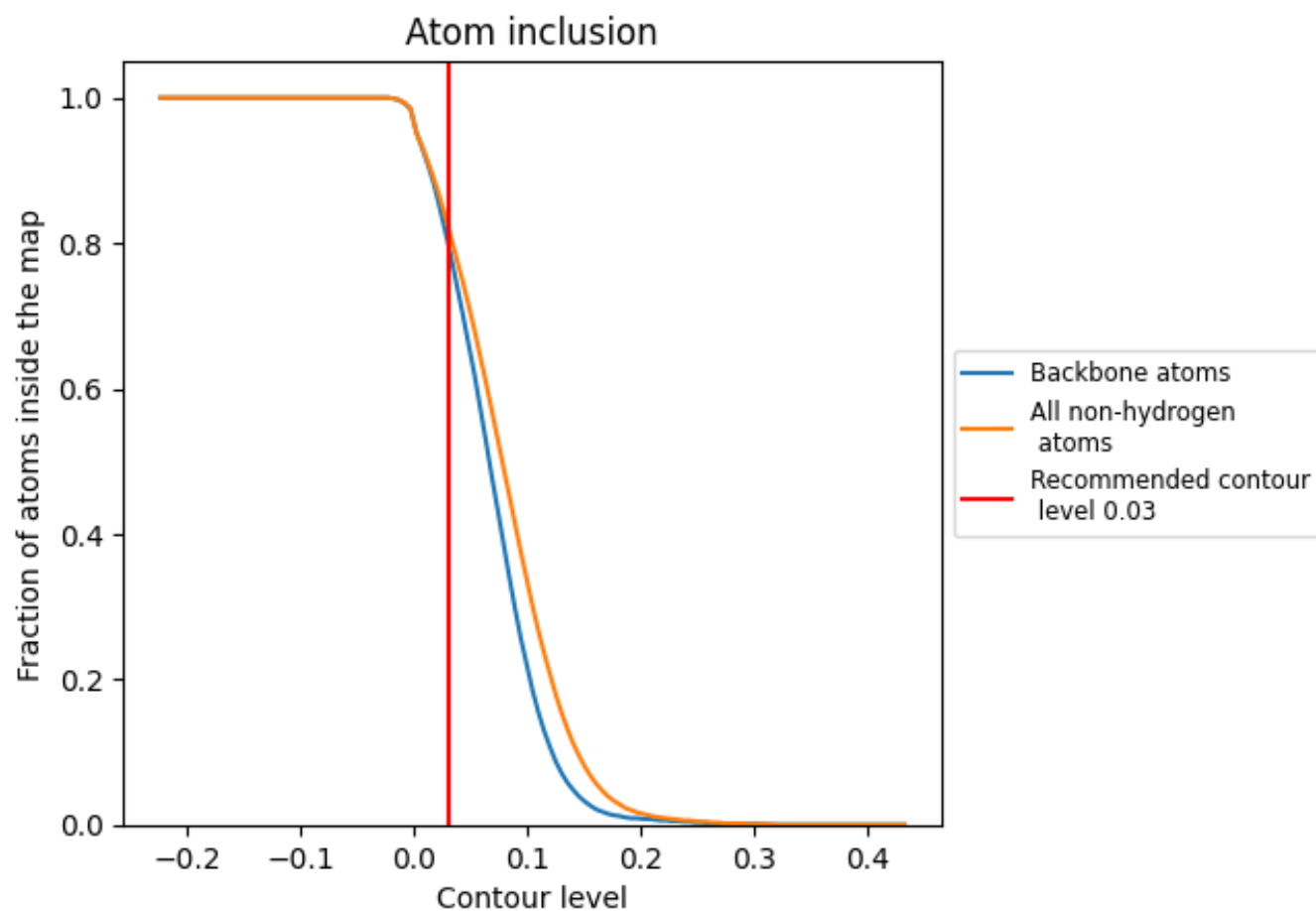
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8230	 0.6380
1	 0.7700	 0.6350
2	 0.7470	 0.5950
3	 0.8800	 0.6950
4	 0.0850	 0.1610
5	 0.6970	 0.5410
6	 0.7300	 0.5880
7	 0.9790	 0.7620
8	 0.9510	 0.7390
9	 0.8880	 0.6750
A	 0.8430	 0.6430
B	 0.6980	 0.5600
G	 0.9330	 0.7310
H	 0.9160	 0.7190
I	 0.8430	 0.6630
J	 0.2780	 0.3340
K	 0.4030	 0.3980
M	 0.9380	 0.7220
N	 0.8960	 0.7050
O	 0.7370	 0.6020
P	 0.8920	 0.6870
Q	 0.8920	 0.7030
R	 0.5700	 0.4900
S	 0.8650	 0.6760
T	 0.9560	 0.7510
U	 0.8750	 0.6770
V	 0.9190	 0.7250
W	 0.8500	 0.6690
X	 0.6660	 0.5530
Z	 0.9320	 0.7300

