



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 09:11 pm BST

PDB ID : 5T7V
EMDB ID : EMD-8369
Title : Methicillin Resistant, Linezolid resistant Staphylococcus aureus 70S ribosome (delta S145 uL3)
Authors : Belousoff, M.J.; Lithgow, T.; Eyal, Z.; Yonath, A.; Radjainia, M.
Deposited on : 2016-09-06
Resolution : 3.60 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:

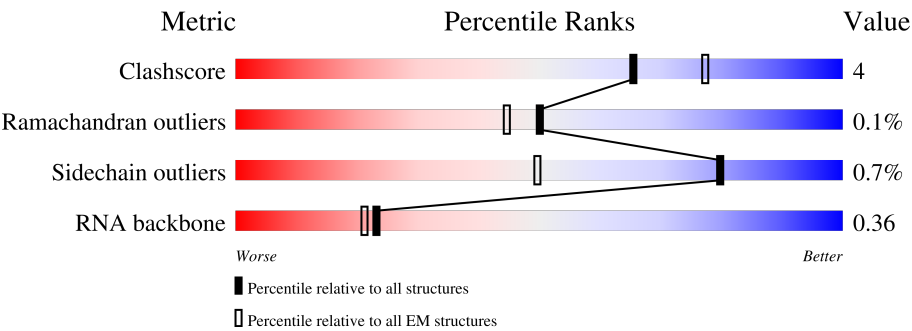
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1547	<div><div>46%</div><div>37%</div><div>9%</div><div>8%</div></div>
2	S1	82	<div><div>38%</div><div>90%</div><div>10%</div></div>
3	S2	115	<div><div>10%</div><div>87%</div><div>13%</div></div>
4	S3	136	<div><div>7%</div><div>78%</div><div>18%</div><div>.</div></div>
5	S6	87	<div><div>5%</div><div>86%</div><div>14%</div></div>
6	S7	76	<div><div>14%</div><div>79%</div><div>21%</div></div>
7	S8	82	<div><div>10%</div><div>87%</div><div>13%</div></div>

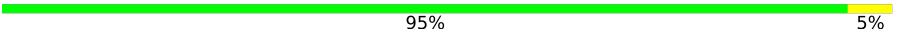









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Mol	Chain	Length	Quality of chain
8	S9	55	
9	SA	76	
10	SC	198	
11	SD	154	
12	SE	92	
13	SF	130	
14	B	2919	
15	C	114	
16	L1	113	
17	L2	275	
18	L3	116	
19	L4	100	
20	L5	111	
21	L6	87	
22	L7	101	
23	L8	93	
24	L9	78	
25	LA	59	
26	LB	61	
27	LC	214	
28	LD	57	
29	LE	53	
30	LF	47	
31	LG	44	
32	LH	64	

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Mol	Chain	Length	Quality of chain
33	LI	37	 95% 5%
34	LJ	204	 91% 9%
35	LL	174	 86% 14%
36	LM	143	 89% 10%
37	LN	121	 90% 10%
38	LO	144	 92% 8%
39	LP	136	 93% 7%
40	LQ	121	 83% 17%
41	LR	116	 84% 15%
42	D	74	 41% 47% 12%

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 126001 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	P	0	0
			30390	13573	5558	9844	1415		

- Molecule 2 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S1	82	Total	C	N	O	S	0	0
			647	405	117	124	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	57	GLY	LYS	conflict	UNP A0A0H2K0A0

- Molecule 3 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	115	Total	C	N	O	S	0	0
			850	525	161	161	3		

- Molecule 4 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S3	136	Total	C	N	O	S	0	0
			1011	622	205	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S3	43	ALA	LYS	conflict	UNP W8U1C6

- Molecule 5 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S6	87	Total	C	N	O	S	0	0
			725	448	149	127	1		

- Molecule 6 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	76	Total	C	N	O		0	0
			594	374	112	108			

- Molecule 7 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	82	Total	C	N	O	S	0	0
			674	427	122	124	1		

- Molecule 8 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S9	55	Total	C	N	O	S	0	0
			456	290	87	77	2		

- Molecule 9 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	SA	76	Total	C	N	O		0
			475	290	96	89		0

- Molecule 10 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	198	Total	C	N	O	S	0	0
			1604	1014	298	290	2		

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SD	154	Total	C	N	O	S	0	0
			1132	711	209	210	2		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SE	92	Total	C	N	O	S	0	0
			763	484	135	142	2		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SF	130	Total	C	N	O	S	0	0
			1012	638	180	190	4		

- Molecule 14 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	2768	Total	C	N	O	P	0	0
			59339	26499	10863	19214	2763		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1866	A	G	conflict	GB 1015534143

- Molecule 15 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	114	Total	C	N	O	P	0	0
			2424	1085	434	792	113		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	A	U	conflict	GB 1043615627
C	?	-	G	deletion	GB 1043615627

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L1	113	Total	C	N	O		0	0
			914	576	184	154			

- Molecule 17 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L2	275	Total	C	N	O	S	0	0
			2086	1301	416	364	5		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L3	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L4	100	Total	C	N	O	S	0	0
			784	499	139	145	1		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L5	111	Total	C	N	O	S	0	0
			852	532	163	154	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L6	87	Total	C	N	O	S	0	0
			684	430	121	130	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L6	87	ASP	ILE	conflict	UNP W8TUB4

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L7	101	Total	C	N	O	S	0	0
			758	479	141	137	1		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L8	93	Total	C	N	O	S	0	0
			726	465	129	131	1		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L9	78	Total	C	N	O		0	0
			590	365	116	109			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LA	59	Total	C	N	O	S	0	0
			462	287	99	75	1		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LB	61	Total	C	N	O	S	0	0
			502	310	95	96	1		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LC	214	Total	C	N	O	S	0	0
			1617	1012	297	303	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LC	?	-	SER	deletion	UNP W8U3W0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	LD	57	Total	C	N	O	0	0
			440	274	83	83		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LE	53	Total	C	N	O	S	0	0
			421	256	86	74	5		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LF	47	Total	C	N	O	S	0	0
			386	232	79	70	5		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	44	Total	C	N	O	S	0	0
			371	228	90	52	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LH	64	Total	C	N	O	S	0	0
			520	324	113	81	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LI	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LJ	204	Total	C	N	O	S	0	0
			1538	965	283	288	2		

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LL	174	Total	C	N	O	S	0	0
			1357	845	248	261	3		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LM	143	Total	C	N	O	S	0	0
			1137	710	209	216	2		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LN	121	Total	C	N	O	S	0	0
			910	566	173	167	4		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LO	144	Total	C	N	O		0	0
			1081	669	213	199			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LP	136	Total	C	N	O	S	0	0
			1088	698	206	180	4		

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LQ	121	Total	C	N	O	S	0	0
			954	586	183	184	1		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LR	116	Total	C	N	O		0	0
			896	559	171	166			

- Molecule 42 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	74	Total	C	N	O	P	0	0
			1577	704	282	518	73		

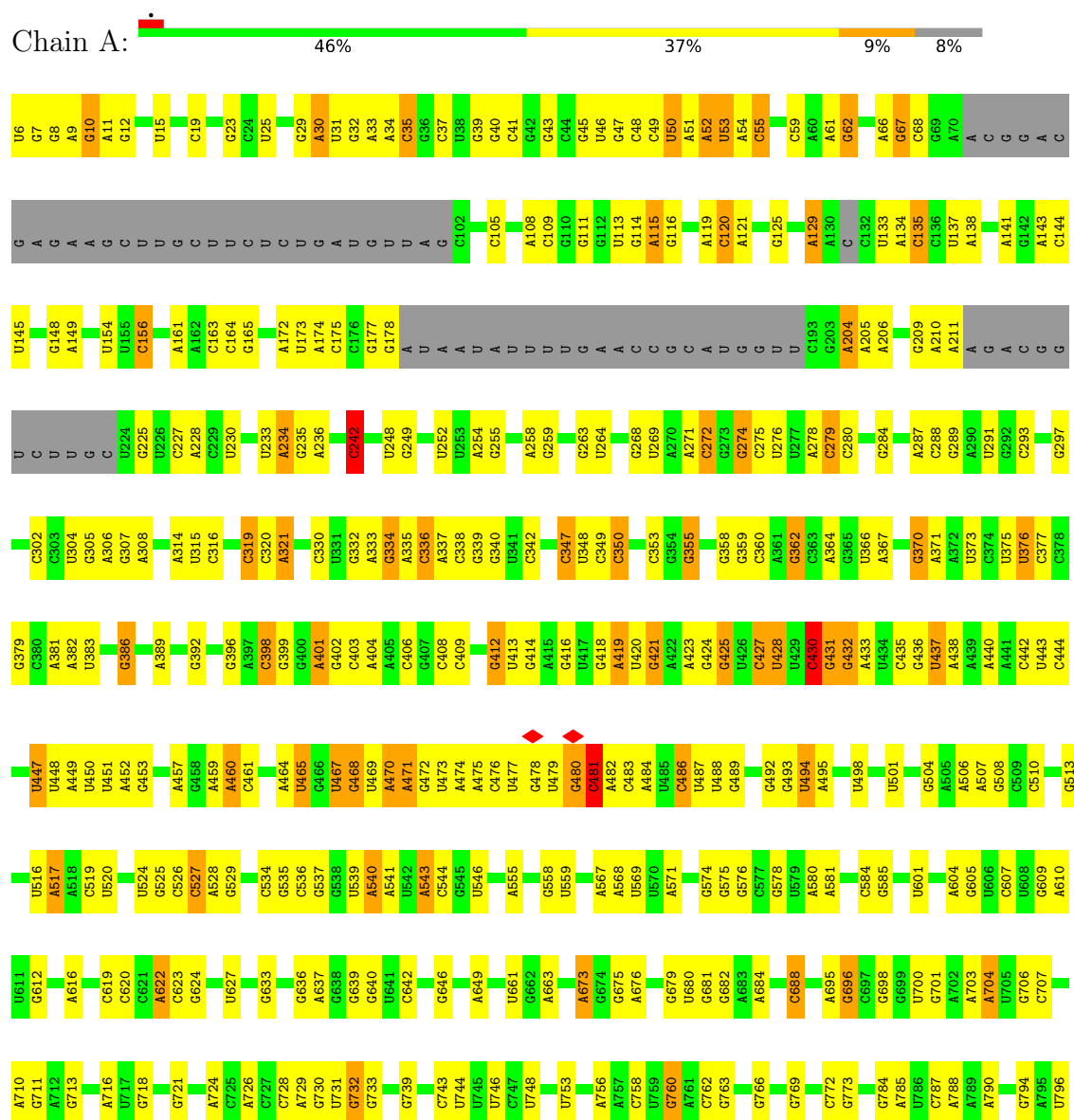
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	A	4	Total 4	Mg 4	0
43	B	13	Total 13	Mg 13	0

3 Residue-property plots

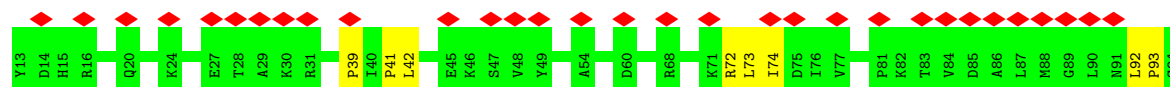
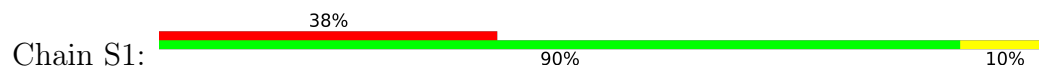
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

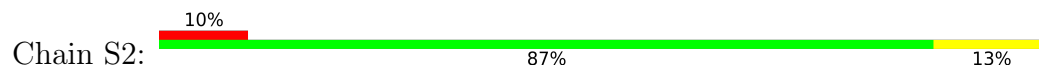


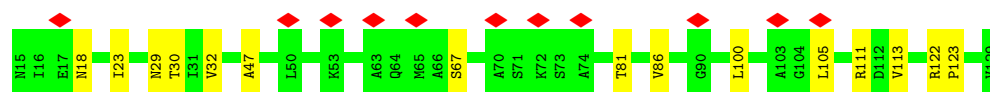


• Molecule 2: 30S ribosomal protein S10

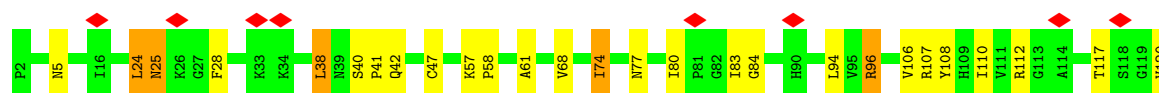
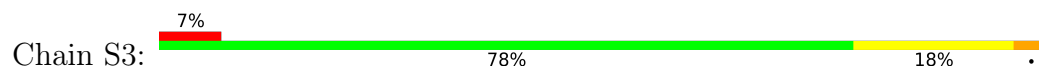


• Molecule 3: 30S ribosomal protein S11

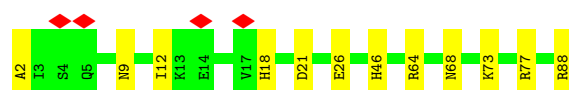
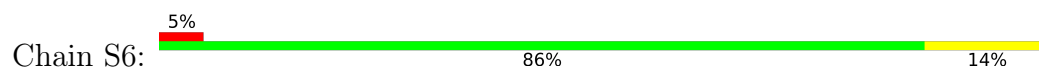




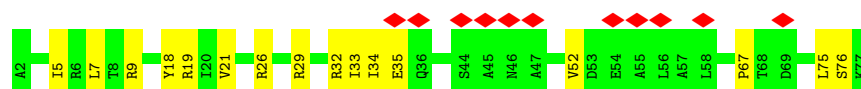
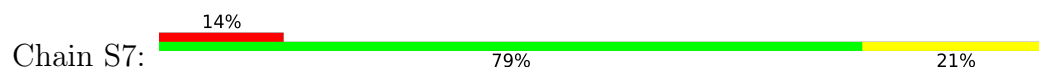
- Molecule 4: 30S ribosomal protein S12



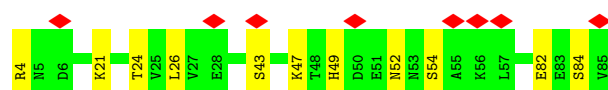
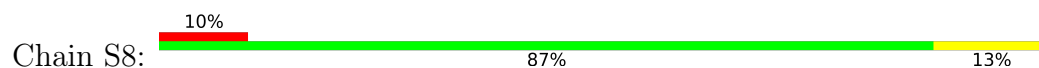
- Molecule 5: 30S ribosomal protein S15



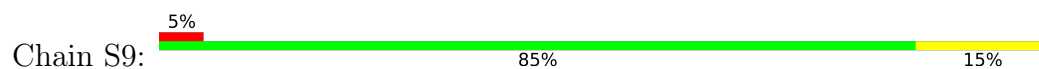
- Molecule 6: 30S ribosomal protein S16



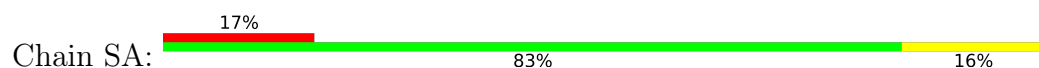
- Molecule 7: 30S ribosomal protein S17

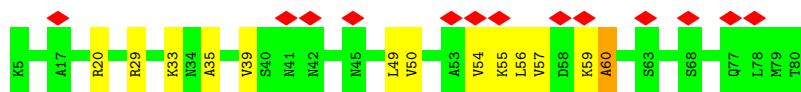


- Molecule 8: 30S ribosomal protein S18

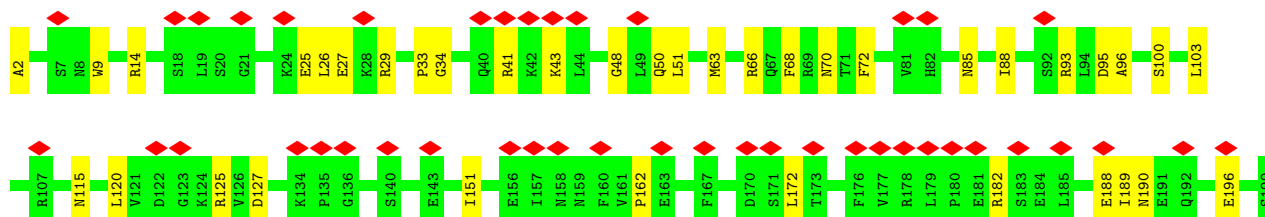
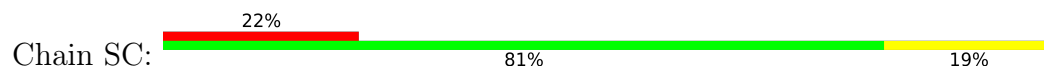


- Molecule 9: 30S ribosomal protein S20

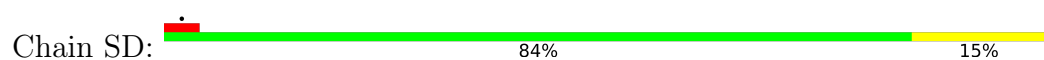




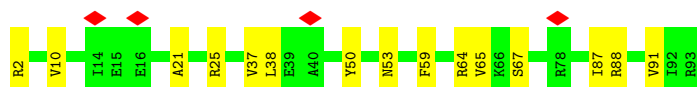
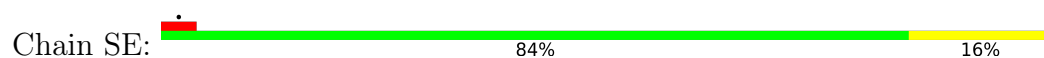
- Molecule 10: 30S ribosomal protein S4



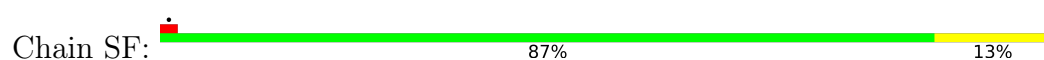
- Molecule 11: 30S ribosomal protein S5



- Molecule 12: 30S ribosomal protein S6



- Molecule 13: 30S ribosomal protein S8

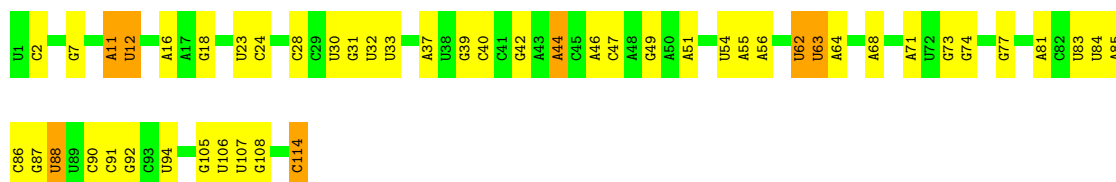


- Molecule 14: 23S ribosomal RNA

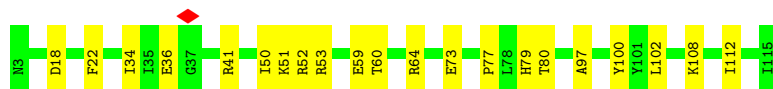
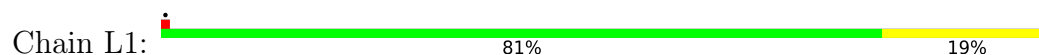




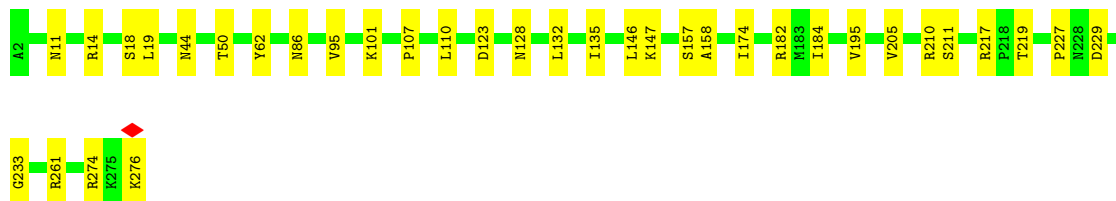




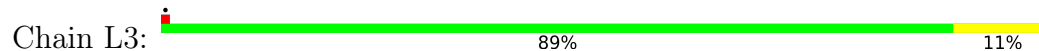
- Molecule 16: 50S ribosomal protein L19



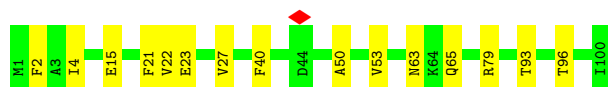
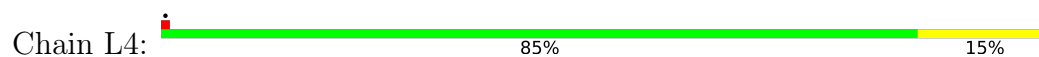
- Molecule 17: 50S ribosomal protein L2



- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21



- Molecule 20: 50S ribosomal protein L22

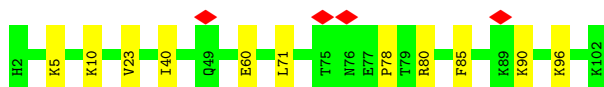
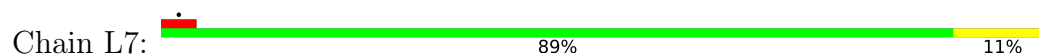


- Molecule 21: 50S ribosomal protein L23

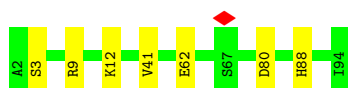




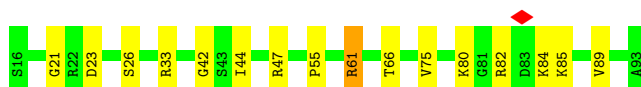
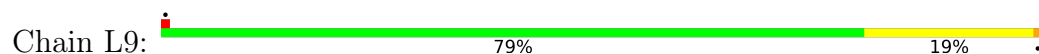
- Molecule 22: 50S ribosomal protein L24



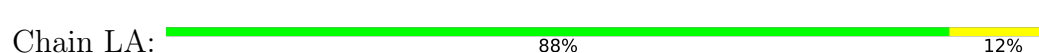
- Molecule 23: 50S ribosomal protein L25



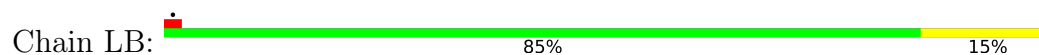
- Molecule 24: 50S ribosomal protein L27



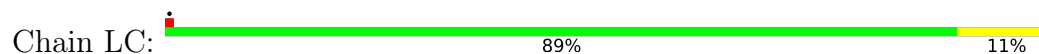
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L3




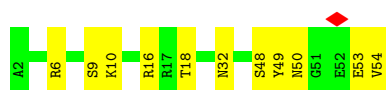
- Molecule 28: 50S ribosomal protein L30

Chain LD:  93% 7%



- Molecule 29: 50S ribosomal protein L32

Chain LE:  79% 21%



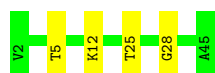
- Molecule 30: 50S ribosomal protein L33

Chain LF:  94% 6%




- Molecule 31: 50S ribosomal protein L34

Chain LG:  91% 9%



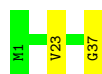
- Molecule 32: 50S ribosomal protein L35

Chain LH:  84% 16%



- Molecule 33: 50S ribosomal protein L36

Chain LI:  95% 5%




- Molecule 34: 50S ribosomal protein L4

Chain LJ:  91% 9%



- Molecule 35: 50S ribosomal protein L6

Chain LL:  86% 14% .



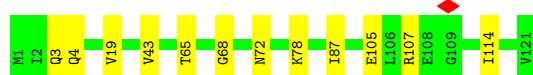
- Molecule 36: 50S ribosomal protein L13

Chain LM:  89% 10% .



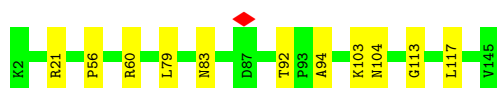
- Molecule 37: 50S ribosomal protein L14

Chain LN:  90% 10% .



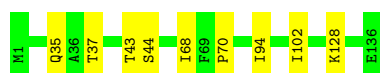
- Molecule 38: 50S ribosomal protein L15

Chain LO:  92% 8% .




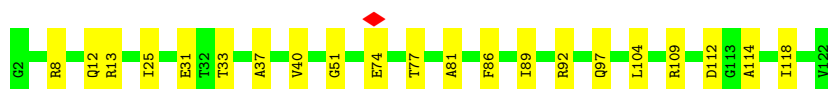
- Molecule 39: 50S ribosomal protein L16

Chain LP:  93% 7% .




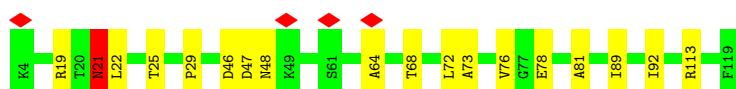
- Molecule 40: 50S ribosomal protein L17

Chain LQ:  83% 17% .

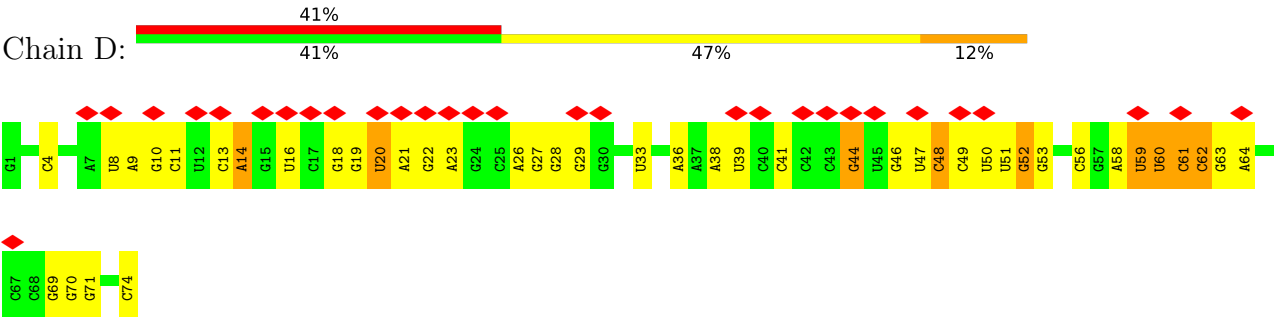


- Molecule 41: 50S ribosomal protein L18

Chain LR:  84% 15% .



● Molecule 42: E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80500	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.740	Depositor
Minimum map value	-0.466	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/34022	1.12	160/53044 (0.3%)
2	S1	0.30	0/659	0.52	0/893
3	S2	0.29	0/865	0.55	0/1170
4	S3	0.34	0/1026	0.77	3/1385 (0.2%)
5	S6	0.32	0/734	0.53	0/981
6	S7	0.29	0/604	0.60	0/819
7	S8	0.34	0/682	0.63	0/912
8	S9	0.31	0/463	0.59	0/619
9	SA	0.28	0/475	0.57	1/645 (0.2%)
10	SC	0.31	0/1634	0.56	0/2196
11	SD	0.35	0/1145	0.62	0/1546
12	SE	0.36	0/774	0.62	0/1039
13	SF	0.31	0/1022	0.56	0/1373
14	B	0.97	5/66453 (0.0%)	1.16	377/103631 (0.4%)
15	C	0.65	0/2710	1.15	20/4221 (0.5%)
16	L1	0.45	0/926	0.63	1/1238 (0.1%)
17	L2	0.53	0/2121	0.66	0/2849
18	L3	0.52	0/954	0.64	0/1264
19	L4	0.45	0/794	0.62	0/1061
20	L5	0.46	0/860	0.66	0/1158
21	L6	0.48	0/691	0.61	0/926
22	L7	0.36	0/765	0.60	0/1021
23	L8	0.36	0/734	0.59	0/985
24	L9	0.52	0/596	0.74	0/792
25	LA	0.43	0/468	0.60	1/624 (0.2%)
26	LB	0.35	0/503	0.63	0/669
27	LC	0.50	0/1641	0.66	1/2203 (0.0%)
28	LD	0.40	0/442	0.64	0/596
29	LE	0.47	0/428	0.63	0/570
30	LF	0.39	0/389	0.55	0/518
31	LG	0.55	0/375	0.60	0/490
32	LH	0.44	0/525	0.61	0/689

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LI	0.45	0/298	0.56	0/392
34	LJ	0.45	0/1561	0.62	0/2110
35	LL	0.36	0/1375	0.58	0/1850
36	LM	0.48	0/1159	0.60	1/1562 (0.1%)
37	LN	0.53	0/917	0.67	0/1231
38	LO	0.47	0/1095	0.63	0/1460
39	LP	0.45	0/1112	0.59	0/1492
40	LQ	0.46	0/958	0.67	0/1281
41	LR	0.38	0/905	0.67	0/1211
42	D	0.41	0/1762	1.06	5/2746 (0.2%)
All	All	0.77	5/137622 (0.0%)	1.05	570/207462 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	S3	0	1
9	SA	0	1
11	SD	0	1
18	L3	0	1
19	L4	0	1
24	L9	0	1
36	LM	0	1
37	LN	0	1
41	LR	0	2
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1289	A	N9-C4	-6.20	1.34	1.37
14	B	1599	G	N3-C4	-5.57	1.31	1.35
14	B	2740	A	N9-C4	-5.20	1.34	1.37
14	B	2625	A	N7-C5	-5.20	1.36	1.39
14	B	1566	G	N9-C4	-5.15	1.33	1.38

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1168	C	N1-C2-O2	12.01	126.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	12	U	C2-N1-C1'	11.85	131.92	117.70
14	B	1350	U	N3-C2-O2	-10.99	114.50	122.20
1	A	373	U	C2-N1-C1'	10.92	130.80	117.70
1	A	1168	C	C2-N1-C1'	10.73	130.61	118.80
14	B	1835	U	C5-C6-N1	10.44	127.92	122.70
14	B	12	U	N1-C2-O2	10.13	129.89	122.80
14	B	1350	U	N1-C2-O2	9.98	129.79	122.80
1	A	376	U	C2-N1-C1'	9.95	129.64	117.70
1	A	758	C	C6-N1-C2	-9.88	116.35	120.30
1	A	373	U	N1-C2-O2	9.84	129.69	122.80
14	B	402	C	C2-N1-C1'	9.47	129.22	118.80
1	A	1168	C	N3-C2-O2	-9.31	115.39	121.90
14	B	12	U	N3-C2-O2	-9.18	115.78	122.20
14	B	1215	U	C2-N1-C1'	9.11	128.64	117.70
4	S3	38	LEU	CA-CB-CG	9.02	136.05	115.30
14	B	402	C	N1-C2-O2	9.01	124.31	118.90
14	B	1835	U	C2-N1-C1'	9.01	128.51	117.70
1	A	135	C	N1-C2-O2	8.94	124.26	118.90
14	B	1514	A	C5-C6-N6	-8.81	116.65	123.70
1	A	376	U	N1-C2-O2	8.79	128.95	122.80
14	B	1215	U	N1-C2-O2	8.51	128.76	122.80
1	A	373	U	N3-C2-O2	-8.49	116.26	122.20
14	B	835	U	N3-C2-O2	-8.38	116.34	122.20
14	B	2017	C	C6-N1-C2	-8.37	116.95	120.30
1	A	135	C	C2-N1-C1'	8.36	128.00	118.80
1	A	288	C	N1-C2-O2	8.33	123.90	118.90
14	B	1370	C	C6-N1-C2	-8.30	116.98	120.30
1	A	376	U	N3-C2-O2	-8.25	116.42	122.20
14	B	2534	C	N1-C2-O2	8.18	123.81	118.90
14	B	1028	G	N3-C4-N9	8.16	130.90	126.00
14	B	999	U	C5-C6-N1	8.15	126.78	122.70
14	B	759	U	C2-N1-C1'	8.06	127.37	117.70
14	B	403	U	C2-N1-C1'	8.02	127.32	117.70
14	B	2035	C	C6-N1-C2	-7.93	117.13	120.30
14	B	1941	C	N1-C2-O2	7.91	123.65	118.90
1	A	758	C	C5-C6-N1	7.90	124.95	121.00
1	A	288	C	C2-N1-C1'	7.87	127.46	118.80
14	B	12	U	C5-C6-N1	7.85	126.62	122.70
15	C	86	C	C2-N1-C1'	7.84	127.43	118.80
1	A	1168	C	C6-N1-C2	-7.78	117.19	120.30
14	B	12	U	C6-N1-C1'	-7.78	110.31	121.20
1	A	319	C	C6-N1-C2	-7.77	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1524	C	C6-N1-C2	-7.76	117.19	120.30
1	A	135	C	N3-C2-O2	-7.76	116.47	121.90
14	B	1514	A	N9-C4-C5	-7.74	102.70	105.80
1	A	1002	G	N3-C4-C5	-7.71	124.75	128.60
14	B	803	C	C6-N1-C2	-7.69	117.22	120.30
1	A	758	C	N1-C2-O2	7.69	123.52	118.90
14	B	1932	C	C2-N1-C1'	7.68	127.25	118.80
14	B	2539	C	C6-N1-C2	-7.67	117.23	120.30
14	B	1961	C	C6-N1-C2	-7.65	117.24	120.30
14	B	2429	U	N1-C2-O2	7.63	128.14	122.80
14	B	1591	G	N3-C4-N9	7.58	130.55	126.00
1	A	6	U	C2-N1-C1'	7.56	126.78	117.70
14	B	1591	G	N3-C4-C5	-7.55	124.83	128.60
14	B	1085	U	N3-C2-O2	-7.55	116.92	122.20
14	B	1778	C	C6-N1-C2	-7.52	117.29	120.30
1	A	476	C	C6-N1-C2	-7.52	117.29	120.30
14	B	2429	U	N3-C2-O2	-7.52	116.94	122.20
14	B	1941	C	C2-N1-C1'	7.51	127.06	118.80
1	A	1002	G	C4-N9-C1'	7.50	136.25	126.50
14	B	2287	C	C6-N1-C2	-7.49	117.30	120.30
14	B	403	U	N3-C2-O2	-7.44	117.00	122.20
1	A	373	U	C6-N1-C1'	-7.43	110.79	121.20
14	B	1350	U	C2-N1-C1'	7.43	126.61	117.70
14	B	1085	U	N1-C2-O2	7.37	127.96	122.80
14	B	1514	A	C4-C5-N7	7.33	114.36	110.70
14	B	402	C	N3-C2-O2	-7.28	116.81	121.90
14	B	1524	C	C5-C6-N1	7.28	124.64	121.00
14	B	320	U	C2-N1-C1'	7.27	126.43	117.70
14	B	1591	G	C4-N9-C1'	7.27	135.95	126.50
14	B	1215	U	N3-C2-O2	-7.25	117.12	122.20
14	B	2621	C	C6-N1-C2	-7.19	117.42	120.30
14	B	835	U	N1-C2-O2	7.18	127.83	122.80
1	A	1168	C	C6-N1-C1'	-7.17	112.20	120.80
4	S3	24	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	336	C	P-O3'-C3'	7.16	128.29	119.70
15	C	63	U	C2-N1-C1'	7.13	126.25	117.70
14	B	249	C	C6-N1-C2	-7.12	117.45	120.30
1	A	1193	U	N1-C2-O2	7.09	127.76	122.80
14	B	1216	U	C2-N1-C1'	7.09	126.21	117.70
14	B	2534	C	N3-C2-O2	-7.09	116.94	121.90
14	B	1503	U	P-O3'-C3'	7.08	128.20	119.70
14	B	781	C	C6-N1-C2	-7.07	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1042	C	C6-N1-C2	-7.07	117.47	120.30
14	B	403	U	N1-C2-O2	7.06	127.74	122.80
14	B	1028	G	N3-C4-C5	-7.06	125.07	128.60
1	A	1219	C	C2-N1-C1'	7.05	126.56	118.80
14	B	515	G	O4'-C1'-N9	7.04	113.83	108.20
1	A	1087	C	C6-N1-C2	-7.02	117.49	120.30
1	A	758	C	N3-C2-O2	-7.02	116.99	121.90
1	A	758	C	C2-N1-C1'	7.01	126.51	118.80
1	A	1219	C	N1-C2-O2	6.99	123.09	118.90
1	A	430	C	N1-C2-O2	6.99	123.09	118.90
14	B	1395	G	C4-C5-N7	6.98	113.59	110.80
14	B	1599	G	C2-N3-C4	-6.97	108.41	111.90
14	B	1835	U	N1-C2-O2	6.92	127.64	122.80
14	B	1289	A	C5-N7-C8	-6.89	100.45	103.90
14	B	2264	G	C8-N9-C4	-6.86	103.66	106.40
15	C	86	C	N1-C2-O2	6.86	123.01	118.90
1	A	851	U	C2-N1-C1'	6.84	125.91	117.70
1	A	1193	U	C2-N1-C1'	6.84	125.91	117.70
14	B	835	U	C2-N1-C1'	6.82	125.88	117.70
14	B	211	C	N1-C2-O2	6.80	122.98	118.90
14	B	2737	C	C6-N1-C2	-6.78	117.59	120.30
15	C	63	U	N1-C2-O2	6.77	127.54	122.80
1	A	510	C	C6-N1-C2	-6.76	117.60	120.30
14	B	811	C	C6-N1-C2	-6.74	117.60	120.30
14	B	1514	A	C5-C6-N1	6.74	121.07	117.70
15	C	86	C	N3-C2-O2	-6.73	117.19	121.90
14	B	1835	U	C6-N1-C2	-6.71	116.97	121.00
14	B	503	A	O4'-C1'-N9	6.71	113.57	108.20
14	B	2386	C	C5-C6-N1	6.70	124.35	121.00
14	B	402	C	C6-N1-C1'	-6.68	112.78	120.80
1	A	820	G	N3-C4-N9	6.67	130.00	126.00
14	B	561	C	C5-C6-N1	6.67	124.33	121.00
1	A	476	C	C5-C6-N1	6.66	124.33	121.00
14	B	1370	C	C5-C6-N1	6.66	124.33	121.00
14	B	1029	C	C5-C6-N1	6.64	124.32	121.00
14	B	2321	C	C6-N1-C2	-6.63	117.65	120.30
14	B	759	U	N1-C2-O2	6.59	127.42	122.80
14	B	1028	G	C4-N9-C1'	6.59	135.07	126.50
14	B	103	U	N3-C2-O2	-6.58	117.59	122.20
14	B	1466	G	C4-N9-C1'	6.58	135.05	126.50
14	B	714	G	N3-C4-N9	6.57	129.94	126.00
15	C	33	U	N1-C2-O2	6.57	127.40	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2035	C	C5-C6-N1	6.55	124.28	121.00
1	A	1211	A	P-O3'-C3'	6.54	127.55	119.70
14	B	680	C	N3-C2-O2	-6.54	117.32	121.90
1	A	1269	C	C6-N1-C2	-6.54	117.69	120.30
1	A	1002	G	N3-C4-N9	6.54	129.92	126.00
14	B	2469	C	C6-N1-C2	-6.54	117.69	120.30
14	B	1566	G	N3-C4-N9	-6.53	122.08	126.00
1	A	851	U	N1-C2-O2	6.52	127.36	122.80
14	B	1599	G	N3-C4-N9	-6.52	122.09	126.00
1	A	851	U	N3-C2-O2	-6.49	117.66	122.20
14	B	695	C	C5-C6-N1	6.49	124.24	121.00
14	B	162	A	OP1-P-OP2	-6.48	109.88	119.60
14	B	1351	C	C2-N1-C1'	6.47	125.92	118.80
14	B	1729	C	C6-N1-C2	-6.47	117.71	120.30
1	A	442	C	N1-C2-O2	6.46	122.78	118.90
14	B	1008	C	C6-N1-C2	-6.46	117.72	120.30
14	B	2609	G	C4-N9-C1'	6.46	134.89	126.50
1	A	288	C	N3-C2-O2	-6.45	117.39	121.90
15	C	33	U	C2-N1-C1'	6.45	125.44	117.70
14	B	518	A	C4-C5-N7	6.44	113.92	110.70
14	B	18	C	C6-N1-C2	-6.43	117.73	120.30
14	B	2881	C	C5-C6-N1	6.43	124.22	121.00
14	B	811	C	C5-C6-N1	6.42	124.21	121.00
14	B	1700	C	C6-N1-C2	-6.41	117.74	120.30
14	B	103	U	N1-C2-O2	6.40	127.28	122.80
1	A	820	G	N3-C4-C5	-6.39	125.40	128.60
14	B	1466	G	N3-C4-N9	6.37	129.82	126.00
14	B	31	C	C5-C6-N1	6.37	124.19	121.00
1	A	376	U	C6-N1-C1'	-6.36	112.29	121.20
14	B	515	G	N1-C6-O6	6.35	123.71	119.90
9	SA	49	LEU	CA-CB-CG	6.34	129.89	115.30
14	B	1865	C	N1-C2-O2	6.34	122.71	118.90
14	B	624	C	C6-N1-C2	-6.33	117.77	120.30
14	B	1409	U	N3-C2-O2	-6.32	117.78	122.20
14	B	2021	C	C6-N1-C2	-6.32	117.77	120.30
14	B	2539	C	C5-C6-N1	6.31	124.16	121.00
14	B	2017	C	C5-C6-N1	6.31	124.15	121.00
1	A	1517	U	N3-C2-O2	-6.31	117.78	122.20
14	B	2469	C	C5-C6-N1	6.28	124.14	121.00
14	B	680	C	N1-C2-O2	6.27	122.66	118.90
14	B	284	C	C2-N1-C1'	6.27	125.69	118.80
1	A	177	G	O4'-C1'-N9	6.26	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	C	C6-N1-C2	-6.26	117.80	120.30
1	A	607	C	C6-N1-C2	-6.26	117.80	120.30
15	C	33	U	C5-C6-N1	6.26	125.83	122.70
14	B	1215	U	C6-N1-C1'	-6.25	112.46	121.20
1	A	373	U	C5-C6-N1	6.24	125.82	122.70
1	A	1007	C	C2-N1-C1'	6.23	125.65	118.80
1	A	1193	U	N3-C2-O2	-6.22	117.85	122.20
14	B	515	G	C4-C5-N7	6.21	113.29	110.80
1	A	1168	C	C5-C6-N1	6.21	124.10	121.00
1	A	15	U	C2-N1-C1'	6.20	125.14	117.70
1	A	1158	U	C2-N1-C1'	6.20	125.14	117.70
14	B	2111	C	C5-C6-N1	6.20	124.10	121.00
14	B	1865	C	C2-N1-C1'	6.19	125.61	118.80
1	A	858	C	N1-C2-O2	6.19	122.61	118.90
14	B	2020	U	C5-C6-N1	6.18	125.79	122.70
14	B	680	C	C6-N1-C2	-6.18	117.83	120.30
15	C	63	U	N3-C2-O2	-6.18	117.88	122.20
1	A	105	C	C6-N1-C2	-6.17	117.83	120.30
14	B	508	C	C6-N1-C2	-6.16	117.83	120.30
14	B	1584	U	N1-C2-O2	6.16	127.11	122.80
42	D	39	U	C2-N1-C1'	6.16	125.09	117.70
14	B	2905	C	C5-C6-N1	6.15	124.08	121.00
14	B	1585	G	N3-C4-C5	-6.15	125.52	128.60
1	A	1374	U	C2-N1-C1'	6.15	125.08	117.70
1	A	272	C	C6-N1-C2	-6.14	117.84	120.30
1	A	442	C	C6-N1-C2	-6.14	117.84	120.30
1	A	969	U	P-O3'-C3'	6.14	127.07	119.70
14	B	2429	U	C2-N1-C1'	6.14	125.07	117.70
14	B	1514	A	N1-C6-N6	6.13	122.28	118.60
1	A	53	U	N1-C2-O2	6.13	127.09	122.80
14	B	698	U	C2-N1-C1'	6.12	125.04	117.70
14	B	1035	C	C5-C6-N1	6.12	124.06	121.00
14	B	256	C	C6-N1-C2	-6.11	117.85	120.30
14	B	1591	G	C8-N9-C1'	-6.11	119.05	127.00
1	A	483	C	C6-N1-C2	-6.10	117.86	120.30
14	B	714	G	N3-C4-C5	-6.10	125.55	128.60
14	B	515	G	C5-N7-C8	-6.09	101.25	104.30
14	B	2483	C	C5-C6-N1	6.09	124.05	121.00
14	B	1395	G	C6-C5-N7	-6.09	126.75	130.40
14	B	603	C	C5-C6-N1	6.09	124.04	121.00
1	A	336	C	N1-C2-O2	6.08	122.55	118.90
1	A	1533	U	C5-C6-N1	6.08	125.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	999	U	C6-N1-C2	-6.08	117.35	121.00
14	B	250	G	N3-C4-N9	6.07	129.64	126.00
14	B	1029	C	C6-N1-C2	-6.07	117.87	120.30
14	B	1035	C	C6-N1-C2	-6.06	117.88	120.30
14	B	1566	G	N3-C4-C5	6.06	131.63	128.60
15	C	114	C	C6-N1-C2	-6.05	117.88	120.30
1	A	227	C	C6-N1-C2	-6.05	117.88	120.30
14	B	1042	C	C5-C6-N1	6.04	124.02	121.00
14	B	733	U	C5-C6-N1	6.03	125.72	122.70
14	B	1153	C	C6-N1-C2	-6.03	117.89	120.30
14	B	1370	C	N1-C2-O2	6.03	122.52	118.90
14	B	1028	G	C8-N9-C1'	-6.02	119.17	127.00
1	A	68	C	C6-N1-C2	-6.01	117.89	120.30
14	B	1466	G	N3-C4-C5	-6.01	125.59	128.60
1	A	442	C	C5-C6-N1	6.01	124.00	121.00
14	B	1487	G	C8-N9-C4	-6.00	104.00	106.40
14	B	698	U	N1-C2-O2	6.00	127.00	122.80
14	B	2621	C	C5-C6-N1	6.00	124.00	121.00
14	B	1591	G	C2-N3-C4	6.00	114.90	111.90
14	B	1585	G	C4-N9-C1'	5.99	134.29	126.50
14	B	842	U	C5-C6-N1	5.99	125.69	122.70
1	A	480	G	P-O3'-C3'	5.98	126.88	119.70
14	B	1985	C	C6-N1-C2	-5.97	117.91	120.30
14	B	1599	G	N1-C2-N3	5.96	127.48	123.90
1	A	376	U	C5-C6-N1	5.96	125.68	122.70
14	B	1773	A	N7-C8-N9	5.96	116.78	113.80
1	A	976	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1200	G	P-O3'-C3'	5.95	126.84	119.70
14	B	1801	C	N3-C2-O2	-5.95	117.73	121.90
14	B	2233	C	C5-C6-N1	5.95	123.97	121.00
14	B	1985	C	C5-C6-N1	5.95	123.97	121.00
14	B	1179	C	N1-C2-O2	5.94	122.46	118.90
1	A	6	U	N1-C2-O2	5.93	126.95	122.80
14	B	803	C	N3-C2-O2	-5.93	117.75	121.90
1	A	481	C	C2-N1-C1'	5.93	125.33	118.80
14	B	593	U	N1-C2-O2	5.93	126.95	122.80
14	B	515	G	C6-C5-N7	-5.92	126.85	130.40
14	B	1599	G	N3-C2-N2	-5.92	115.76	119.90
14	B	2534	C	C2-N1-C1'	5.91	125.30	118.80
14	B	759	U	C6-N1-C1'	-5.90	112.94	121.20
14	B	2020	U	N3-C2-O2	-5.90	118.07	122.20
14	B	1585	G	N3-C4-N9	5.90	129.54	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2386	C	C6-N1-C2	-5.89	117.94	120.30
14	B	1460	U	N1-C2-O2	5.89	126.92	122.80
1	A	1007	C	N1-C2-O2	5.89	122.43	118.90
14	B	1941	C	N3-C2-O2	-5.88	117.78	121.90
14	B	1409	U	N1-C2-O2	5.86	126.90	122.80
1	A	1137	U	N1-C2-O2	5.85	126.89	122.80
14	B	714	G	C4-N9-C1'	5.84	134.10	126.50
14	B	1351	C	C5-C6-N1	5.84	123.92	121.00
14	B	1351	C	C6-N1-C2	-5.84	117.96	120.30
1	A	1292	C	N1-C2-O2	5.83	122.40	118.90
14	B	1030	C	C6-N1-C2	-5.83	117.97	120.30
14	B	831	C	C5-C6-N1	5.82	123.91	121.00
14	B	2070	C	C5-C6-N1	5.82	123.91	121.00
1	A	1218	C	C2-N1-C1'	5.82	125.20	118.80
1	A	1352	C	C6-N1-C2	-5.82	117.97	120.30
1	A	1324	C	C5-C6-N1	5.82	123.91	121.00
14	B	182	C	N3-C2-O2	-5.82	117.83	121.90
14	B	1466	G	OP1-P-O3'	5.82	118.00	105.20
14	B	828	A	C2-N3-C4	5.81	113.51	110.60
14	B	1380	G	C4-N9-C1'	5.81	134.05	126.50
14	B	2233	C	N1-C2-O2	5.81	122.39	118.90
1	A	1374	U	N3-C2-O2	-5.81	118.14	122.20
14	B	182	C	N1-C2-O2	5.81	122.38	118.90
14	B	2905	C	C6-N1-C2	-5.81	117.98	120.30
14	B	739	U	C5-C6-N1	5.80	125.60	122.70
14	B	2239	A	N7-C8-N9	5.80	116.70	113.80
15	C	88	U	N3-C2-O2	-5.80	118.14	122.20
14	B	1778	C	C5-C6-N1	5.79	123.90	121.00
1	A	52	A	P-O3'-C3'	5.79	126.65	119.70
14	B	2324	C	C6-N1-C2	-5.79	117.98	120.30
14	B	1289	A	C4-C5-N7	5.79	113.59	110.70
14	B	1515	G	C8-N9-C1'	-5.79	119.48	127.00
14	B	2070	C	N1-C2-O2	5.78	122.37	118.90
14	B	717	C	C6-N1-C2	-5.78	117.99	120.30
14	B	731	U	N3-C2-O2	-5.78	118.16	122.20
14	B	1370	C	N3-C2-O2	-5.78	117.86	121.90
1	A	1277	C	C2-N1-C1'	5.77	125.15	118.80
15	C	28	C	C5-C6-N1	5.77	123.88	121.00
1	A	272	C	N1-C2-O2	5.77	122.36	118.90
15	C	86	C	C6-N1-C1'	-5.77	113.88	120.80
1	A	1374	U	N1-C2-O2	5.76	126.83	122.80
1	A	941	C	C6-N1-C2	-5.76	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2723	U	C5-C6-N1	5.75	125.58	122.70
14	B	402	C	C6-N1-C2	-5.75	118.00	120.30
14	B	759	U	O4'-C1'-N1	5.75	112.80	108.20
1	A	1372	C	C2-N1-C1'	5.75	125.12	118.80
14	B	31	C	C6-N1-C2	-5.75	118.00	120.30
14	B	1584	U	C2-N1-C1'	5.75	124.60	117.70
1	A	430	C	C2-N1-C1'	5.75	125.12	118.80
14	B	2525	C	N1-C2-O2	5.74	122.34	118.90
1	A	1002	G	C8-N9-C1'	-5.74	119.55	127.00
14	B	2287	C	C5-C6-N1	5.74	123.87	121.00
14	B	561	C	C6-N1-C2	-5.73	118.01	120.30
1	A	849	U	C2-N1-C1'	5.73	124.58	117.70
1	A	1463	U	C2-N1-C1'	5.73	124.57	117.70
14	B	90	A	P-O3'-C3'	5.72	126.57	119.70
14	B	2348	G	N3-C4-N9	5.72	129.44	126.00
1	A	1292	C	N3-C2-O2	-5.72	117.89	121.90
14	B	1036	C	C6-N1-C2	-5.71	118.01	120.30
14	B	1466	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	334	G	C4-N9-C1'	5.71	133.92	126.50
14	B	12	U	C6-N1-C2	-5.70	117.58	121.00
14	B	1351	C	N1-C2-O2	5.70	122.32	118.90
14	B	710	C	N1-C2-O2	5.70	122.32	118.90
14	B	782	C	C5-C6-N1	5.70	123.85	121.00
1	A	1211	A	OP2-P-O3'	5.70	117.73	105.20
14	B	323	C	C6-N1-C2	-5.70	118.02	120.30
14	B	1599	G	C8-N9-C4	-5.69	104.12	106.40
1	A	1213	C	C6-N1-C2	-5.69	118.02	120.30
14	B	2321	C	C5-C6-N1	5.68	123.84	121.00
1	A	59	C	C6-N1-C2	-5.68	118.03	120.30
14	B	1474	C	C6-N1-C2	-5.67	118.03	120.30
14	B	463	C	C5-C6-N1	5.67	123.83	121.00
14	B	1515	G	C4-N9-C1'	5.66	133.86	126.50
14	B	2369	C	C6-N1-C2	-5.65	118.04	120.30
42	D	62	C	C6-N1-C2	-5.65	118.04	120.30
14	B	1983	U	N3-C2-O2	-5.65	118.25	122.20
14	B	1815	C	C5-C6-N1	5.64	123.82	121.00
14	B	2490	C	C6-N1-C2	-5.64	118.04	120.30
1	A	1324	C	C6-N1-C2	-5.63	118.05	120.30
14	B	575	G	N3-C4-C5	-5.62	125.79	128.60
42	D	39	U	N1-C2-O2	5.61	126.73	122.80
14	B	1715	U	C6-N1-C2	-5.60	117.64	121.00
1	A	1219	C	C6-N1-C2	-5.60	118.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2369	C	C5-C6-N1	5.60	123.80	121.00
14	B	1216	U	N1-C2-O2	5.59	126.72	122.80
14	B	2277	G	C8-N9-C4	-5.59	104.16	106.40
14	B	1932	C	C6-N1-C1'	-5.59	114.09	120.80
1	A	607	C	C5-C6-N1	5.59	123.80	121.00
14	B	765	U	N1-C2-O2	5.59	126.71	122.80
1	A	135	C	C6-N1-C1'	-5.59	114.09	120.80
1	A	1002	G	C8-N9-C4	-5.59	104.16	106.40
1	A	1303	G	C4-N9-C1'	5.59	133.76	126.50
14	B	1932	C	N1-C2-O2	5.59	122.25	118.90
14	B	1399	C	C5-C6-N1	5.58	123.79	121.00
14	B	764	C	C5-C6-N1	5.58	123.79	121.00
1	A	1014	C	C6-N1-C2	-5.57	118.07	120.30
14	B	276	C	C2-N1-C1'	5.57	124.93	118.80
1	A	467	U	P-O3'-C3'	5.57	126.38	119.70
1	A	1168	C	C2-N3-C4	5.56	122.68	119.90
1	A	242	C	C6-N1-C2	-5.55	118.08	120.30
1	A	288	C	C6-N1-C2	-5.55	118.08	120.30
15	C	33	U	N3-C2-O2	-5.55	118.31	122.20
14	B	1627	G	P-O3'-C3'	5.55	126.36	119.70
1	A	853	C	N1-C2-O2	5.55	122.23	118.90
14	B	593	U	C2-N1-C1'	5.55	124.36	117.70
14	B	721	A	C5-N7-C8	-5.55	101.13	103.90
14	B	1835	U	N3-C2-O2	-5.55	118.32	122.20
14	B	1441	C	C6-N1-C2	-5.54	118.08	120.30
14	B	1516	C	C6-N1-C2	-5.54	118.08	120.30
15	C	114	C	C2-N1-C1'	5.54	124.90	118.80
1	A	483	C	N1-C2-O2	5.54	122.22	118.90
25	LA	54	LEU	CA-CB-CG	5.54	128.04	115.30
14	B	2487	U	C5-C6-N1	5.53	125.47	122.70
14	B	1296	C	C5-C6-N1	5.53	123.76	121.00
14	B	1363	U	N1-C2-O2	5.52	126.67	122.80
14	B	1865	C	C6-N1-C2	-5.52	118.09	120.30
14	B	249	C	C5-C6-N1	5.52	123.76	121.00
14	B	1007	U	C5-C6-N1	5.52	125.46	122.70
14	B	1305	U	N3-C2-O2	-5.52	118.34	122.20
14	B	2020	U	N1-C2-O2	5.52	126.66	122.80
14	B	385	U	N3-C2-O2	-5.51	118.34	122.20
14	B	1961	C	C5-C6-N1	5.51	123.76	121.00
14	B	2730	C	C6-N1-C2	-5.51	118.09	120.30
14	B	735	C	C5-C6-N1	5.51	123.76	121.00
14	B	764	C	C6-N1-C2	-5.51	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1503	A	P-O3'-C3'	5.51	126.31	119.70
14	B	320	U	N1-C2-O2	5.51	126.65	122.80
14	B	1460	U	C2-N1-C1'	5.51	124.31	117.70
14	B	526	A	C2-N3-C4	5.50	113.35	110.60
14	B	593	U	N3-C2-O2	-5.50	118.35	122.20
14	B	882	C	C6-N1-C2	-5.50	118.10	120.30
14	B	2051	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1002	G	C2-N3-C4	5.49	114.64	111.90
14	B	518	A	C5-N7-C8	-5.48	101.16	103.90
14	B	2794	C	C6-N1-C2	-5.48	118.11	120.30
14	B	1168	C	C6-N1-C2	-5.48	118.11	120.30
1	A	534	C	N1-C2-O2	5.47	122.18	118.90
1	A	1219	C	C5-C6-N1	5.47	123.73	121.00
14	B	1492	G	N3-C4-N9	-5.47	122.72	126.00
1	A	319	C	C5-C6-N1	5.46	123.73	121.00
14	B	1953	U	C2-N1-C1'	5.46	124.25	117.70
1	A	6	U	C6-N1-C1'	-5.45	113.57	121.20
14	B	777	C	N1-C2-O2	5.45	122.17	118.90
14	B	1584	U	N3-C2-O2	-5.45	118.39	122.20
14	B	1941	C	C6-N1-C1'	-5.44	114.27	120.80
14	B	2722	U	C5-C6-N1	5.44	125.42	122.70
14	B	2092	C	C5-C6-N1	5.44	123.72	121.00
1	A	1137	U	C2-N1-C1'	5.43	124.22	117.70
1	A	330	C	C5-C6-N1	5.43	123.72	121.00
14	B	1235	C	C6-N1-C2	-5.43	118.13	120.30
14	B	2070	C	C6-N1-C2	-5.43	118.13	120.30
15	C	12	U	N1-C2-O2	5.43	126.60	122.80
14	B	1898	C	N1-C2-O2	5.42	122.15	118.90
14	B	239	C	C6-N1-C2	-5.42	118.13	120.30
14	B	1676	A	N7-C8-N9	5.42	116.51	113.80
27	LC	81	ASP	CB-CG-OD1	5.42	123.18	118.30
14	B	862	C	C6-N1-C2	-5.41	118.14	120.30
14	B	698	U	N3-C2-O2	-5.40	118.42	122.20
14	B	2595	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2091	C	C6-N1-C2	-5.40	118.14	120.30
1	A	15	U	N3-C2-O2	-5.40	118.42	122.20
14	B	1779	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2488	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2609	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	1219	C	N3-C2-O2	-5.39	118.13	121.90
1	A	35	C	C6-N1-C2	-5.39	118.14	120.30
14	B	1029	C	N1-C2-O2	5.38	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1399	C	C6-N1-C2	-5.37	118.15	120.30
1	A	430	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1372	C	N3-C2-O2	-5.37	118.14	121.90
14	B	1380	G	C8-N9-C1'	-5.37	120.02	127.00
14	B	2348	G	C4-N9-C1'	5.36	133.47	126.50
15	C	28	C	C6-N1-C2	-5.36	118.16	120.30
1	A	1503	A	OP1-P-O3'	5.36	116.99	105.20
14	B	575	G	C4-N9-C1'	5.36	133.46	126.50
14	B	2537	C	C5-C6-N1	5.36	123.68	121.00
1	A	908	C	P-O3'-C3'	5.34	126.11	119.70
14	B	759	U	N3-C2-O2	-5.34	118.46	122.20
14	B	1766	C	N1-C2-O2	5.34	122.10	118.90
14	B	2074	C	C6-N1-C2	-5.34	118.16	120.30
42	D	20	U	C2-N1-C1'	5.34	124.11	117.70
1	A	1474	C	N1-C2-O2	5.34	122.10	118.90
14	B	1492	G	C8-N9-C1'	5.34	133.94	127.00
14	B	1729	C	N1-C2-O2	5.33	122.10	118.90
14	B	1914	C	C6-N1-C2	-5.33	118.17	120.30
14	B	320	U	N3-C2-O2	-5.33	118.47	122.20
14	B	1441	C	C5-C6-N1	5.33	123.66	121.00
1	A	52	A	OP2-P-O3'	5.32	116.90	105.20
14	B	2021	C	C2-N1-C1'	5.32	124.65	118.80
1	A	156	C	C6-N1-C2	-5.32	118.17	120.30
14	B	2264	G	N7-C8-N9	5.31	115.76	113.10
14	B	1865	C	N3-C2-O2	-5.31	118.18	121.90
1	A	773	G	C8-N9-C4	-5.31	104.28	106.40
14	B	1499	U	N3-C2-O2	-5.31	118.49	122.20
1	A	1292	C	C6-N1-C2	-5.30	118.18	120.30
1	A	336	C	N3-C2-O2	-5.30	118.19	121.90
14	B	2894	C	C6-N1-C2	-5.30	118.18	120.30
1	A	820	G	C2-N3-C4	5.30	114.55	111.90
14	B	1801	C	N1-C2-O2	5.30	122.08	118.90
14	B	1460	U	N3-C2-O2	-5.29	118.49	122.20
14	B	1050	C	C6-N1-C2	-5.29	118.18	120.30
1	A	288	C	C6-N1-C1'	-5.28	114.46	120.80
14	B	1492	G	N3-C4-C5	5.28	131.24	128.60
14	B	870	C	C6-N1-C2	-5.28	118.19	120.30
14	B	2547	C	C5-C6-N1	5.27	123.64	121.00
14	B	1729	C	C5-C6-N1	5.27	123.63	121.00
15	C	88	U	C2-N1-C1'	5.26	124.02	117.70
1	A	279	C	P-O3'-C3'	5.26	126.02	119.70
4	S3	94	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2287	C	C6-N1-C1'	5.26	127.11	120.80
14	B	1542	C	C6-N1-C2	-5.26	118.20	120.30
14	B	710	C	C6-N1-C2	-5.25	118.20	120.30
14	B	575	G	N3-C4-N9	5.25	129.15	126.00
14	B	1953	U	N3-C2-O2	-5.25	118.53	122.20
36	LM	143	LEU	CA-CB-CG	5.25	127.37	115.30
14	B	2799	C	C6-N1-C2	-5.24	118.20	120.30
14	B	1515	G	C6-C5-N7	-5.24	127.26	130.40
15	C	114	C	N1-C2-O2	5.24	122.04	118.90
14	B	1773	A	C8-N9-C4	-5.23	103.71	105.80
14	B	2890	C	C6-N1-C2	-5.23	118.21	120.30
14	B	721	A	O4'-C1'-N9	5.23	112.38	108.20
14	B	103	U	C2-N1-C1'	5.22	123.97	117.70
14	B	710	C	N3-C2-O2	-5.22	118.24	121.90
14	B	1942	U	C2-N1-C1'	5.22	123.97	117.70
14	B	2737	C	C5-C6-N1	5.22	123.61	121.00
1	A	1394	C	C6-N1-C2	-5.21	118.21	120.30
14	B	1328	C	C6-N1-C2	-5.21	118.22	120.30
14	B	313	U	C2-N1-C1'	5.20	123.94	117.70
14	B	2623	U	N1-C2-O2	5.20	126.44	122.80
14	B	2071	C	C6-N1-C2	-5.20	118.22	120.30
1	A	762	C	C2-N1-C1'	5.19	124.51	118.80
14	B	152	C	C6-N1-C2	-5.19	118.22	120.30
14	B	2900	C	N1-C2-O2	5.19	122.01	118.90
14	B	2583	C	C5-C6-N1	5.18	123.59	121.00
14	B	660	A	O4'-C1'-N9	-5.18	104.06	108.20
14	B	1515	G	N3-C4-N9	5.18	129.11	126.00
1	A	481	C	N1-C2-O2	5.18	122.01	118.90
1	A	1327	C	N1-C2-O2	5.17	122.00	118.90
14	B	1545	U	N3-C2-O2	-5.17	118.58	122.20
14	B	1510	U	P-O3'-C3'	5.17	125.90	119.70
1	A	1461	U	N1-C2-O2	5.16	126.41	122.80
14	B	515	G	N7-C8-N9	5.16	115.68	113.10
14	B	1845	U	N1-C2-O2	5.16	126.41	122.80
14	B	2006	C	C6-N1-C2	-5.16	118.24	120.30
14	B	2020	U	C2-N1-C1'	5.16	123.89	117.70
14	B	731	U	C2-N1-C1'	5.15	123.88	117.70
1	A	1324	C	N1-C2-O2	5.14	121.99	118.90
1	A	330	C	C6-N1-C2	-5.14	118.24	120.30
14	B	2288	C	C6-N1-C2	-5.14	118.24	120.30
14	B	1715	U	C5-C6-N1	5.14	125.27	122.70
14	B	1998	A	C2-N3-C4	5.14	113.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1004	C	C6-N1-C2	-5.13	118.25	120.30
1	A	272	C	N3-C2-O2	-5.13	118.31	121.90
14	B	518	A	N7-C8-N9	5.13	116.36	113.80
14	B	2051	C	C5-C6-N1	5.12	123.56	121.00
1	A	1218	C	N1-C2-O2	5.12	121.97	118.90
14	B	1676	A	C5-N7-C8	-5.12	101.34	103.90
14	B	144	C	C6-N1-C2	-5.11	118.25	120.30
14	B	163	U	N3-C2-O2	-5.11	118.62	122.20
14	B	1277	C	C5-C6-N1	5.11	123.56	121.00
14	B	421	C	C6-N1-C2	-5.11	118.26	120.30
14	B	90	A	C4-N9-C1'	5.11	135.49	126.30
14	B	1216	U	N3-C2-O2	-5.10	118.63	122.20
14	B	1296	C	C6-N1-C2	-5.10	118.26	120.30
15	C	88	U	N1-C2-O2	5.10	126.37	122.80
14	B	1503	U	OP2-P-O3'	5.10	116.42	105.20
1	A	403	C	C6-N1-C2	-5.10	118.26	120.30
14	B	2723	U	C6-N1-C2	-5.09	117.94	121.00
1	A	46	U	C5-C6-N1	5.09	125.25	122.70
14	B	508	C	C5-C6-N1	5.09	123.55	121.00
14	B	2074	C	C5-C6-N1	5.09	123.55	121.00
1	A	1507	C	C6-N1-C2	-5.09	118.27	120.30
14	B	1704	C	C6-N1-C2	-5.08	118.27	120.30
14	B	385	U	N1-C2-O2	5.08	126.36	122.80
14	B	1785	G	C4-N9-C1'	5.08	133.11	126.50
1	A	1087	C	C5-C6-N1	5.08	123.54	121.00
14	B	2642	U	N1-C2-O2	5.08	126.36	122.80
16	L1	18	ASP	C-N-CA	5.08	134.40	121.70
14	B	2561	C	N1-C2-O2	5.08	121.94	118.90
1	A	1158	U	N3-C2-O2	-5.07	118.65	122.20
14	B	695	C	C6-N1-C2	-5.07	118.27	120.30
14	B	2583	C	N1-C2-O2	5.07	121.94	118.90
1	A	773	G	C4-N9-C1'	5.06	133.08	126.50
1	A	1254	C	C6-N1-C2	-5.06	118.28	120.30
14	B	1215	U	C5-C6-N1	5.06	125.23	122.70
1	A	849	U	N3-C2-O2	-5.06	118.66	122.20
14	B	1628	A	O5'-P-OP2	-5.05	101.15	105.70
14	B	2673	C	N1-C2-O2	5.05	121.93	118.90
1	A	816	C	C6-N1-C2	-5.05	118.28	120.30
14	B	2063	C	C5-C6-N1	5.04	123.52	121.00
14	B	1574	G	C6-C5-N7	-5.04	127.38	130.40
14	B	2347	A	C4-N9-C1'	5.04	135.37	126.30
42	D	36	A	C2-N3-C4	5.04	113.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1372	C	N1-C2-O2	5.04	121.92	118.90
14	B	421	C	C5-C6-N1	5.04	123.52	121.00
14	B	795	A	C4-N9-C1'	5.04	135.37	126.30
14	B	90	A	C2-N3-C4	5.03	113.12	110.60
14	B	1093	C	C6-N1-C2	-5.03	118.29	120.30
14	B	630	G	N3-C4-N9	5.03	129.02	126.00
14	B	518	A	N1-C6-N6	5.03	121.62	118.60
14	B	601	G	O5'-P-OP1	-5.03	101.17	105.70
1	A	1137	U	N3-C2-O2	-5.03	118.68	122.20
1	A	1394	C	C5-C6-N1	5.03	123.51	121.00
1	A	1010	U	C2-N1-C1'	5.03	123.73	117.70
14	B	2529	G	P-O3'-C3'	5.03	125.73	119.70
1	A	116	G	C4-N9-C1'	5.03	133.03	126.50
14	B	402	C	O4'-C1'-N1	5.03	112.22	108.20
14	B	2233	C	C6-N1-C2	-5.02	118.29	120.30
14	B	2566	C	C6-N1-C2	-5.02	118.29	120.30
14	B	403	U	C6-N1-C1'	-5.02	114.17	121.20
14	B	1289	A	C2-N3-C4	-5.02	108.09	110.60
14	B	723	C	C6-N1-C2	-5.01	118.30	120.30
14	B	2020	U	C6-N1-C2	-5.01	118.00	121.00
1	A	1542	A	N7-C8-N9	5.01	116.30	113.80
14	B	2673	C	C6-N1-C2	-5.01	118.30	120.30
14	B	603	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	L3	95	LEU	Peptide
19	L4	23	GLU	Peptide
24	L9	21	GLY	Peptide
36	LM	112	SER	Peptide
37	LN	105	GLU	Peptide
41	LR	21	ASN	Peptide
41	LR	68	THR	Peptide
4	S3	28	PHE	Peptide
9	SA	60	ALA	Peptide
11	SD	108	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30390	0	15318	185	0
2	S1	647	0	657	4	0
3	S2	850	0	860	8	0
4	S3	1011	0	1001	17	0
5	S6	725	0	756	9	0
6	S7	594	0	618	12	0
7	S8	674	0	716	6	0
8	S9	456	0	490	5	0
9	SA	475	0	406	8	0
10	SC	1604	0	1633	24	0
11	SD	1132	0	1188	13	0
12	SE	763	0	766	10	0
13	SF	1012	0	1061	10	0
14	B	59339	0	29847	185	0
15	C	2424	0	1230	11	0
16	L1	914	0	987	13	0
17	L2	2086	0	2194	20	0
18	L3	942	0	1014	9	0
19	L4	784	0	825	7	0
20	L5	852	0	914	7	0
21	L6	684	0	696	3	0
22	L7	758	0	801	7	0
23	L8	726	0	777	5	0
24	L9	590	0	603	11	0
25	LA	462	0	501	4	0
26	LB	502	0	536	5	0
27	LC	1617	0	1651	13	0
28	LD	440	0	478	2	0
29	LE	421	0	430	9	0
30	LF	386	0	394	2	0
31	LG	371	0	420	3	0
32	LH	520	0	586	8	0
33	LI	295	0	340	1	0
34	LJ	1538	0	1561	10	0
35	LL	1357	0	1388	16	0
36	LM	1137	0	1130	8	0
37	LN	910	0	970	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LO	1081	0	1119	6	0
39	LP	1088	0	1155	4	0
40	LQ	954	0	1002	12	0
41	LR	896	0	935	9	0
42	D	1577	0	800	15	0
43	A	4	0	0	0	0
43	B	13	0	0	0	0
All	All	126001	0	80754	625	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 (625) 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)
14:B:2533:U:C6	14:B:2533:U:H5''	2.26	0.71
35:LL:5:GLY:HA2	35:LL:69:ARG:HD3	1.71	0.70
12:SE:10:VAL:HB	12:SE:59:PHE:HB2	1.73	0.70
14:B:262:G:H21	14:B:666:A:H8	1.40	0.69
14:B:2037:G:H5''	20:L5:42:ALA:HB2	1.72	0.68
26:LB:17:GLN:HE22	26:LB:50:ILE:HG23	1.58	0.68
1:A:1368:U:H3	1:A:1373:A:H61	1.40	0.68
14:B:1521:A:H61	14:B:1559:G:H1	1.42	0.68
14:B:540:G:H21	20:L5:61:ASN:HD22	1.40	0.67
1:A:1004:C:H42	1:A:1220:C:H42	1.41	0.67
1:A:1314:G:H21	1:A:1343:A:H62	1.42	0.67
2:S1:42:LEU:HD13	2:S1:73:LEU:H	1.60	0.67
1:A:696:G:H1	1:A:707:C:H42	1.43	0.67
1:A:612:G:H1	1:A:642:C:H42	1.41	0.66
14:B:606:G:H21	18:L3:37:GLN:HE22	1.41	0.66
1:A:519:C:H5'	10:SC:41:ARG:HD2	1.77	0.65
1:A:537:G:H22	4:S3:61:ALA:HB2	1.63	0.64
1:A:979:C:H2'	1:A:1241:G:H1'	1.79	0.64
1:A:263:G:O6	1:A:278:A:N6	2.31	0.64
14:B:2649:U:O2'	14:B:2845:G:N2	2.31	0.63
14:B:132:C:H42	14:B:147:G:H1	1.46	0.63
1:A:1075:G:N2	1:A:1201:A:OP2	2.31	0.63
1:A:10:G:H5'	11:SD:108:GLY:HA2	1.79	0.63
10:SC:9:TRP:NE1	10:SC:25:GLU:O	2.32	0.63
10:SC:120:LEU:HD22	10:SC:125:ARG:HA	1.81	0.63
14:B:826:A:OP1	17:L2:217:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L1:50:ILE:HD11	16:L1:64:ARG:HD2	1.79	0.63
39:LP:44:SER:HB2	39:LP:70:PRO:HG3	1.81	0.63
10:SC:188:GLU:HG2	10:SC:189:ILE:HG13	1.81	0.62
27:LC:186:GLN:HB2	27:LC:195:LEU:HD12	1.82	0.62
14:B:1448:U:H3	14:B:1635:A:H61	1.46	0.62
41:LR:25:THR:HA	41:LR:46:ASP:HB2	1.81	0.62
1:A:1362:C:H42	1:A:1380:G:H22	1.48	0.62
10:SC:100:SER:HB3	10:SC:162:PRO:HG3	1.82	0.62
14:B:1825:U:OP2	17:L2:274:ARG:NH2	2.33	0.62
22:L7:10:LYS:HB2	22:L7:71:LEU:HD23	1.81	0.62
41:LR:29:PRO:HG2	41:LR:89:ILE:HD11	1.81	0.62
6:S7:5:ILE:HD12	6:S7:67:PRO:HG3	1.81	0.61
6:S7:21:VAL:HG11	6:S7:33:ILE:HD12	1.83	0.61
27:LC:185:VAL:HG12	27:LC:186:GLN:HG3	1.81	0.61
1:A:1442:G:O2'	1:A:1478:G:N1	2.34	0.61
14:B:246:U:OP2	32:LH:8:ARG:NH1	2.34	0.61
14:B:349:U:H3	14:B:353:A:H62	1.47	0.61
29:LE:32:ASN:ND2	29:LE:50:ASN:OD1	2.33	0.61
1:A:1407:C:N4	1:A:1412:C:OP1	2.34	0.60
35:LL:28:GLY:H	35:LL:32:GLU:HG2	1.65	0.60
1:A:399:G:OP1	6:S7:9:ARG:NH1	2.34	0.60
41:LR:19:ARG:NH2	41:LR:47:ASP:OD2	2.35	0.60
14:B:1342:C:H42	14:B:1667:G:H1	1.49	0.60
7:S8:24:THR:HG22	7:S8:47:LYS:HG2	1.84	0.60
41:LR:29:PRO:HD2	41:LR:92:ILE:HD12	1.82	0.60
14:B:1651:C:N4	14:B:1666:A:OP2	2.35	0.60
35:LL:38:ASN:HD21	35:LL:72:LEU:HD11	1.66	0.60
14:B:2380:G:N2	24:L9:42:GLY:O	2.35	0.60
1:A:1460:U:H3	1:A:1464:A:H61	1.50	0.60
14:B:2533:U:C6	14:B:2533:U:C5'	2.85	0.60
14:B:2531:U:H2'	14:B:2532:G:H5''	1.84	0.60
1:A:62:G:O2'	1:A:386:G:N2	2.36	0.59
1:A:12:G:N2	1:A:25:U:O2	2.34	0.59
1:A:743:C:H5''	8:S9:62:THR:HG23	1.85	0.59
5:S6:18:HIS:ND1	5:S6:21:ASP:OD2	2.36	0.59
1:A:54:A:N6	1:A:55:C:O2	2.36	0.59
1:A:412:G:N7	10:SC:2:ALA:N	2.51	0.59
1:A:1247:C:O2'	1:A:1344:G:N2	2.36	0.59
14:B:1340:G:HO2'	14:B:1686:G:HO2'	1.44	0.58
25:LA:5:CYS:HB3	25:LA:9:GLY:H	1.68	0.58
1:A:120:C:H41	1:A:242:C:H3'	1.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SD:76:ARG:NH1	11:SD:119:GLY:O	2.36	0.58
14:B:2233:C:H42	14:B:2245:G:H1	1.50	0.58
35:LL:126:GLU:HB2	35:LL:130:VAL:HB	1.85	0.58
1:A:305:G:N2	1:A:308:A:OP2	2.32	0.58
6:S7:34:ILE:HG22	6:S7:35:GLU:HG2	1.86	0.58
10:SC:50:GLN:HG2	10:SC:196:GLU:HB2	1.84	0.58
10:SC:85:ASN:HD22	10:SC:88:ILE:HD12	1.67	0.58
10:SC:14:ARG:NH2	10:SC:33:PRO:O	2.37	0.58
1:A:951:G:N2	1:A:1352:C:O2	2.34	0.58
24:L9:75:VAL:HG12	24:L9:89:VAL:HG22	1.86	0.57
42:D:27:G:N2	42:D:44:G:O2'	2.37	0.57
14:B:2533:U:H2'	14:B:2533:U:O2	2.03	0.57
14:B:1518:G:H1	14:B:1562:C:H42	1.52	0.57
39:LP:35:GLN:HB3	39:LP:102:ILE:HD13	1.86	0.57
11:SD:82:PRO:HD2	11:SD:147:LEU:HD13	1.86	0.57
14:B:1631:G:H21	14:B:1632:A:H1'	1.70	0.57
16:L1:73:GLU:HB2	37:LN:78:LYS:HB2	1.87	0.57
14:B:721:A:H8	14:B:2096:G:H21	1.52	0.57
14:B:2317:G:N1	14:B:2370:U:O2	2.33	0.57
1:A:419:A:N7	1:A:421:G:N2	2.53	0.57
1:A:469:U:O4	1:A:479:U:N3	2.37	0.56
12:SE:50:TYR:OH	12:SE:88:ARG:NH1	2.37	0.56
13:SF:18:ASN:ND2	13:SF:74:ILE:O	2.37	0.56
18:L3:90:ILE:O	18:L3:92:ARG:NH1	2.37	0.56
14:B:1501:G:N2	14:B:2730:C:O2	2.38	0.56
22:L7:10:LYS:HD3	22:L7:78:PRO:HG3	1.87	0.56
1:A:34:A:H61	1:A:559:U:H3	1.53	0.56
1:A:1222:U:O2	1:A:1223:A:N6	2.38	0.56
1:A:1315:G:H2'	1:A:1316:A:H8	1.70	0.56
5:S6:88:ARG:NH2	14:B:759:U:O2	2.38	0.56
14:B:1492:G:HO2'	14:B:1575:A:HO2'	1.47	0.56
1:A:950:G:N2	1:A:1360:A:OP1	2.39	0.56
13:SF:117:GLU:O	13:SF:121:ARG:NH1	2.38	0.56
14:B:1839:G:H21	17:L2:44:ASN:HD22	1.53	0.56
14:B:321:U:O2	14:B:327:G:N2	2.39	0.56
14:B:2298:G:OP1	24:L9:26:SER:OG	2.24	0.56
1:A:834:C:H4'	13:SF:13:ARG:HD3	1.87	0.56
12:SE:21:ALA:O	12:SE:25:ARG:NH1	2.39	0.56
1:A:1000:U:O2	1:A:1223:A:N6	2.38	0.56
14:B:2359:C:OP1	24:L9:84:LYS:NZ	2.38	0.56
15:C:31:G:N2	15:C:47:C:O2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L1:51:LYS:NZ	16:L1:100:TYR:OH	2.38	0.56
1:A:418:G:H21	1:A:440:A:H62	1.51	0.56
14:B:2532:G:H1'	14:B:2533:U:H5	1.71	0.56
1:A:435:C:H5'	10:SC:34:GLY:H	1.70	0.56
36:LM:26:LEU:HD13	36:LM:63:ILE:HD12	1.88	0.56
14:B:675:G:N2	14:B:678:A:OP2	2.38	0.56
1:A:1287:C:O2'	1:A:1289:A:N7	2.39	0.55
14:B:1335:C:H42	14:B:1686:G:H1	1.54	0.55
1:A:470:A:N6	1:A:477:U:O4	2.40	0.55
1:A:799:G:O6	1:A:800:A:N6	2.40	0.55
1:A:959:U:H2'	1:A:960:G:H8	1.70	0.55
17:L2:146:LEU:HD11	17:L2:182:ARG:HH21	1.70	0.55
35:LL:122:THR:HB	35:LL:134:GLU:HB3	1.88	0.55
39:LP:43:THR:HG22	39:LP:94:ILE:HG22	1.87	0.55
1:A:748:U:OP1	5:S6:2:ALA:N	2.39	0.55
14:B:2445:A:OP1	32:LH:45:ARG:NH2	2.39	0.55
40:LQ:8:ARG:HB3	40:LQ:12:GLN:HB2	1.87	0.55
1:A:578:G:O6	1:A:874:A:N6	2.39	0.55
14:B:2007:G:O2'	14:B:2009:U:OP2	2.23	0.55
11:SD:95:PHE:HB3	11:SD:125:SER:HB2	1.89	0.55
1:A:1454:G:O6	1:A:1469:C:N4	2.38	0.55
8:S9:38:ILE:HG22	8:S9:42:GLY:HA2	1.87	0.55
14:B:738:U:O2'	14:B:1390:A:N3	2.35	0.55
1:A:339:G:OP2	1:A:339:G:N2	2.40	0.55
1:A:381:A:H2'	1:A:382:A:H8	1.71	0.55
14:B:28:A:N3	18:L3:11:ARG:NH2	2.55	0.55
14:B:1288:G:OP2	38:LO:21:ARG:NH1	2.40	0.55
1:A:319:C:OP1	6:S7:32:ARG:NH1	2.39	0.54
11:SD:106:ILE:HD11	11:SD:124:LEU:H	1.72	0.54
14:B:640:G:H1	14:B:705:U:H3	1.54	0.54
27:LC:48:ALA:HB2	27:LC:92:ARG:HG2	1.89	0.54
14:B:1487:G:N2	14:B:1598:U:O2	2.39	0.54
37:LN:19:VAL:HG12	37:LN:43:VAL:HA	1.89	0.54
1:A:1366:G:N2	1:A:1376:C:O2	2.41	0.54
1:A:605:G:N2	13:SF:88:TYR:OH	2.41	0.54
14:B:2602:C:H5'	27:LC:156:ALA:HB2	1.89	0.54
14:B:2869:G:N2	14:B:2886:G:O2'	2.40	0.54
35:LL:70:ALA:O	35:LL:74:ASN:ND2	2.41	0.54
42:D:53:G:O6	42:D:61:C:N4	2.40	0.54
11:SD:24:VAL:HG12	11:SD:25:VAL:HG23	1.88	0.54
12:SE:37:VAL:HG12	12:SE:65:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:1967:U:OP2	14:B:2630:G:N2	2.40	0.54
14:B:2046:U:OP2	29:LE:6:ARG:NH1	2.41	0.54
41:LR:72:LEU:O	41:LR:76:VAL:N	2.39	0.54
17:L2:174:ILE:HG13	17:L2:184:ILE:HD12	1.89	0.54
14:B:545:G:N1	14:B:548:A:OP2	2.39	0.54
1:A:141:A:H61	1:A:230:U:H3	1.56	0.54
1:A:1352:C:H2'	1:A:1353:G:H8	1.72	0.54
13:SF:33:LYS:HG2	13:SF:36:ILE:HD12	1.90	0.54
14:B:1488:A:H61	14:B:1595:C:H42	1.55	0.54
18:L3:18:ILE:HD11	18:L3:32:TYR:HA	1.89	0.54
32:LH:58:VAL:HG13	32:LH:61:LEU:HD12	1.90	0.53
1:A:944:A:O2'	1:A:1394:C:N3	2.40	0.53
14:B:2773:U:H5''	35:LL:138:LYS:HE3	1.90	0.53
40:LQ:33:THR:HG23	40:LQ:114:ALA:HB1	1.89	0.53
40:LQ:37:ALA:HA	40:LQ:40:VAL:HG12	1.90	0.53
1:A:401:A:H2'	1:A:402:G:H8	1.73	0.53
1:A:559:U:O2'	4:S3:96:ARG:NH1	2.41	0.53
1:A:1392:C:N4	1:A:1395:G:O6	2.41	0.53
35:LL:59:LYS:HD3	35:LL:62:ARG:HH11	1.74	0.53
1:A:50:U:O2	1:A:370:G:O2'	2.26	0.53
38:LO:83:ASN:ND2	38:LO:117:LEU:O	2.42	0.53
17:L2:132:LEU:HD23	17:L2:135:ILE:HD12	1.90	0.53
34:LJ:182:ASN:ND2	34:LJ:185:ASP:OD2	2.41	0.53
14:B:433:U:H4'	14:B:434:G:H5'	1.89	0.53
15:C:11:A:OP1	24:L9:82:ARG:NH1	2.41	0.53
14:B:540:G:O2'	14:B:541:G:O5'	2.26	0.53
42:D:4:C:H42	42:D:69:G:H1	1.55	0.53
14:B:2650:G:O5'	14:B:2845:G:N2	2.42	0.53
35:LL:115:ILE:HD13	35:LL:148:ILE:HG12	1.91	0.53
1:A:1422:C:O2	1:A:1500:G:N2	2.42	0.52
14:B:1806:U:OP2	14:B:1811:A:N6	2.42	0.52
14:B:2386:C:O2'	32:LH:54:ASP:OD2	2.28	0.52
1:A:947:A:HO2'	1:A:1386:U:HO2'	1.57	0.52
1:A:1316:A:N6	1:A:1341:G:O2'	2.42	0.52
12:SE:2:ARG:N	12:SE:67:SER:O	2.43	0.52
15:C:73:G:O2'	23:L8:88:HIS:NE2	2.36	0.52
26:LB:48:LYS:O	26:LB:52:ARG:NH2	2.42	0.52
1:A:1109:C:O2'	1:A:1177:A:N6	2.39	0.52
1:A:1092:G:OP2	11:SD:52:LYS:NZ	2.42	0.52
18:L3:50:ARG:O	18:L3:54:LYS:NZ	2.39	0.52
1:A:1452:G:H21	1:A:1472:G:H22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:81:A:H61	15:C:90:C:H42	1.58	0.52
41:LR:73:ALA:HA	41:LR:76:VAL:HG12	1.91	0.52
14:B:2033:C:O2'	14:B:2843:A:N3	2.43	0.52
14:B:2082:C:H2'	14:B:2531:U:H5''	1.91	0.52
14:B:2854:A:H2'	14:B:2899:A:H61	1.75	0.52
13:SF:19:MET:O	13:SF:72:ARG:NH1	2.42	0.52
14:B:1302:G:OP1	29:LE:16:ARG:NH1	2.41	0.52
14:B:1823:U:OP2	17:L2:276:LYS:NZ	2.42	0.52
14:B:2127:G:H1	14:B:2216:U:H3	1.58	0.52
27:LC:111:VAL:HG12	27:LC:187:VAL:HG21	1.90	0.52
27:LC:145:HIS:O	27:LC:147:HIS:ND1	2.43	0.52
31:LG:25:THR:HG23	31:LG:28:GLY:H	1.74	0.52
1:A:447:U:OP2	1:A:449:A:N6	2.43	0.52
15:C:18:G:N2	15:C:62:U:O2	2.41	0.52
27:LC:28:VAL:HG11	27:LC:210:ILE:HD11	1.92	0.52
1:A:421:G:N2	1:A:437:U:OP2	2.42	0.52
1:A:1271:A:H62	1:A:1284:A:H2	1.57	0.52
3:S2:23:ILE:HG12	3:S2:32:VAL:HG22	1.91	0.52
13:SF:21:ARG:HE	13:SF:72:ARG:HE	1.56	0.52
17:L2:227:PRO:HB3	17:L2:233:GLY:HA3	1.91	0.52
41:LR:21:ASN:HB3	41:LR:22:LEU:HD12	1.90	0.52
14:B:1599:G:OP1	14:B:1761:G:N2	2.38	0.52
14:B:2389:G:OP1	32:LH:40:GLN:NE2	2.42	0.52
17:L2:157:SER:OG	17:L2:158:ALA:N	2.43	0.52
22:L7:85:PHE:HB3	22:L7:90:LYS:HA	1.92	0.52
1:A:347:C:H42	1:A:358:G:H1	1.56	0.51
14:B:862:C:O2'	14:B:884:U:OP1	2.25	0.51
14:B:1179:C:N4	14:B:1182:G:OP2	2.43	0.51
14:B:1576:A:H61	14:B:1590:C:H42	1.58	0.51
1:A:571:A:HO2'	1:A:574:G:HO2'	1.55	0.51
1:A:1009:U:OP2	1:A:1016:A:N6	2.43	0.51
12:SE:38:LEU:HD12	12:SE:64:ARG:HG2	1.92	0.51
34:LJ:7:LEU:HG	34:LJ:14:SER:HB3	1.92	0.51
1:A:428:U:O2	1:A:432:G:N1	2.44	0.51
1:A:609:G:H2'	1:A:610:A:H8	1.75	0.51
4:S3:107:ARG:HD3	4:S3:108:TYR:HB3	1.91	0.51
14:B:2773:U:H4'	35:LL:138:LYS:HG3	1.92	0.51
16:L1:59:GLU:OE2	16:L1:79:HIS:NE2	2.44	0.51
1:A:1504:A:OP1	14:B:1940:A:N6	2.39	0.51
14:B:1318:G:N2	14:B:1327:C:O2	2.44	0.51
14:B:1398:G:HO2'	14:B:2242:G:HO2'	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LE:9:SER:OG	29:LE:10:LYS:N	2.44	0.51
10:SC:182:ARG:NH2	10:SC:189:ILE:O	2.43	0.51
14:B:629:A:H62	14:B:1289:A:H2	1.57	0.51
24:L9:55:PRO:HG3	24:L9:61:ARG:HB2	1.93	0.51
1:A:682:G:H5'	12:SE:88:ARG:HH22	1.76	0.51
14:B:1083:G:H1	14:B:1160:C:H42	1.59	0.51
14:B:2026:C:O2	14:B:2714:U:O2'	2.29	0.51
33:LI:23:VAL:HB	33:LI:37:GLY:HA3	1.92	0.51
1:A:430:C:O3'	1:A:431:G:N2	2.41	0.51
17:L2:123:ASP:O	17:L2:128:ASN:ND2	2.43	0.51
27:LC:55:ASP:HA	27:LC:85:LYS:HA	1.91	0.51
1:A:494:U:H2'	1:A:495:A:H8	1.75	0.51
1:A:1505:G:H21	14:B:1939:A:H1'	1.74	0.51
14:B:1450:A:N7	14:B:1634:A:N6	2.59	0.50
1:A:248:U:H2'	1:A:249:G:H8	1.77	0.50
14:B:2092:C:O2	14:B:2476:U:N3	2.43	0.50
16:L1:102:LEU:HD11	16:L1:112:ILE:HD11	1.93	0.50
1:A:1134:A:H2	1:A:1160:U:H3	1.59	0.50
13:SF:34:LYS:HD3	13:SF:52:VAL:HG22	1.94	0.50
17:L2:95:VAL:HG22	17:L2:101:LYS:HG2	1.92	0.50
23:L8:9:ARG:NH1	23:L8:41:VAL:O	2.44	0.50
40:LQ:109:ARG:HD2	40:LQ:112:ASP:HB3	1.93	0.50
1:A:481:C:H5'	6:S7:76:SER:HB3	1.93	0.50
1:A:897:G:N2	1:A:917:A:N7	2.60	0.50
14:B:1360:G:OP1	20:L5:84:ARG:NH2	2.36	0.50
42:D:26:A:N1	42:D:44:G:N2	2.58	0.50
1:A:421:G:H22	10:SC:27:GLU:HB3	1.75	0.50
14:B:459:C:HO2'	14:B:1907:U:HO2'	1.58	0.50
1:A:19:C:H4'	1:A:1089:U:H3	1.75	0.50
1:A:1171:C:H42	1:A:1185:G:H22	1.59	0.50
14:B:15:G:H4'	29:LE:18:THR:HG22	1.94	0.50
14:B:864:A:OP2	14:B:1226:G:N2	2.45	0.50
14:B:2106:U:O2'	25:LA:23:ASN:OD1	2.28	0.50
14:B:2381:A:O3'	24:L9:33:ARG:NH2	2.40	0.50
29:LE:54:VAL:HG11	40:LQ:104:LEU:HD13	1.94	0.50
32:LH:9:GLY:O	32:LH:13:ARG:NH2	2.42	0.50
14:B:2766:U:O2	14:B:2793:G:N2	2.44	0.50
21:L6:7:LEU:HD23	21:L6:29:VAL:HG12	1.94	0.50
29:LE:48:SER:HB3	29:LE:53:GLU:HA	1.94	0.50
1:A:67:G:N2	1:A:172:A:O2'	2.45	0.49
1:A:874:A:N3	1:A:927:A:O2'	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LQ:89:ILE:HD13	40:LQ:92:ARG:HH12	1.76	0.49
41:LR:78:GLU:HA	41:LR:81:ALA:HB3	1.94	0.49
14:B:1431:U:H4'	14:B:1647:A:H4'	1.93	0.49
1:A:113:U:H3	1:A:321:A:H61	1.60	0.49
4:S3:25:ASN:ND2	4:S3:40:SER:OG	2.46	0.49
27:LC:115:VAL:HB	27:LC:213:SER:HB2	1.94	0.49
35:LL:13:SER:OG	35:LL:48:ASN:ND2	2.45	0.49
8:S9:42:GLY:O	8:S9:68:ARG:NH2	2.45	0.49
26:LB:36:GLN:HG2	26:LB:38:GLU:H	1.77	0.49
1:A:1258:A:N7	1:A:1300:G:N2	2.60	0.49
6:S7:52:VAL:HG21	6:S7:75:LEU:HD21	1.95	0.49
14:B:2532:G:H1'	14:B:2533:U:C5	2.47	0.49
38:LO:79:LEU:HG	38:LO:113:GLY:HA2	1.94	0.49
14:B:1932:C:HO2'	14:B:1956:G:HO2'	1.52	0.49
14:B:2312:C:OP2	30:LF:2:ARG:NH2	2.37	0.49
14:B:2707:C:H1'	27:LC:199:ASN:HD22	1.77	0.49
15:C:37:A:O2'	15:C:44:A:N1	2.44	0.49
17:L2:18:SER:OG	17:L2:19:LEU:N	2.41	0.49
29:LE:49:TYR:H	29:LE:54:VAL:H	1.61	0.49
40:LQ:74:GLU:HB3	40:LQ:77:THR:HB	1.94	0.49
42:D:52:G:H2'	42:D:53:G:H8	1.78	0.49
1:A:43:G:N2	1:A:409:C:O2	2.46	0.49
1:A:175:C:OP1	9:SA:20:ARG:NH2	2.39	0.49
4:S3:120:VAL:O	4:S3:132:THR:OG1	2.29	0.49
9:SA:29:ARG:O	9:SA:33:LYS:N	2.39	0.49
14:B:86:C:HO2'	14:B:103:U:HO2'	1.54	0.49
22:L7:5:LYS:HA	22:L7:23:VAL:HB	1.94	0.49
1:A:427:C:N4	1:A:432:G:O6	2.46	0.49
1:A:823:A:N7	1:A:1520:C:O2'	2.44	0.49
14:B:902:A:H61	14:B:965:G:H1	1.61	0.49
14:B:1878:U:O2'	42:D:71:G:N3	2.45	0.49
42:D:18:G:O2'	42:D:59:U:OP1	2.30	0.49
1:A:416:G:N2	1:A:443:U:O2'	2.45	0.48
1:A:1075:G:O2'	1:A:1200:G:N2	2.46	0.48
1:A:1262:A:H61	1:A:1295:A:H61	1.59	0.48
10:SC:151:ILE:HG21	10:SC:172:LEU:HD11	1.94	0.48
1:A:35:C:H1'	4:S3:42:GLN:HE22	1.77	0.48
14:B:731:U:O5'	31:LG:12:LYS:NZ	2.44	0.48
14:B:2751:U:OP2	27:LC:125:LYS:NZ	2.43	0.48
17:L2:107:PRO:HA	17:L2:195:VAL:HA	1.95	0.48
21:L6:11:VAL:HG22	21:L6:13:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:A:C6	1:A:437:U:H5''	2.48	0.48
14:B:1711:G:O2'	14:B:2018:U:O4	2.32	0.48
14:B:2740:A:O2'	14:B:2742:C:OP2	2.29	0.48
5:S6:64:ARG:O	5:S6:68:ASN:ND2	2.46	0.48
14:B:1478:A:H61	14:B:1605:A:H61	1.61	0.48
14:B:1569:G:H3'	14:B:1570:G:H8	1.79	0.48
14:B:1894:G:H1	14:B:1901:C:H42	1.61	0.48
42:D:21:A:H5'	42:D:48:C:H41	1.79	0.48
1:A:753:U:H4'	1:A:844:G:H21	1.78	0.48
35:LL:7:LYS:O	35:LL:69:ARG:NH2	2.41	0.48
9:SA:57:VAL:HA	9:SA:60:ALA:HB3	1.96	0.48
15:C:16:A:H61	15:C:105:G:H21	1.60	0.48
5:S6:88:ARG:NH2	14:B:760:A:N7	2.62	0.48
18:L3:64:ARG:HH22	36:LM:46:THR:HG22	1.78	0.48
1:A:274:G:O6	1:A:278:A:N6	2.47	0.48
1:A:412:G:OP1	10:SC:115:ASN:ND2	2.46	0.48
9:SA:55:LYS:O	9:SA:59:LYS:N	2.47	0.48
14:B:616:G:N1	14:B:2058:A:OP1	2.46	0.48
14:B:633:A:OP1	34:LJ:95:ARG:NH2	2.47	0.48
4:S3:84:GLY:H	4:S3:120:VAL:HG13	1.79	0.47
7:S8:82:GLU:HG2	7:S8:84:SER:H	1.78	0.47
22:L7:71:LEU:HA	22:L7:78:PRO:HA	1.96	0.47
14:B:2103:U:OP2	14:B:2265:G:N2	2.47	0.47
14:B:909:G:N2	14:B:958:U:O2	2.48	0.47
14:B:1245:G:N2	14:B:1278:G:N7	2.62	0.47
14:B:2231:C:OP1	17:L2:147:LYS:NZ	2.46	0.47
14:B:2881:C:H2'	14:B:2882:A:H8	1.78	0.47
40:LQ:31:GLU:HG2	40:LQ:118:ILE:HG12	1.96	0.47
1:A:381:A:H62	1:A:399:G:H21	1.63	0.47
14:B:284:C:H3'	14:B:285:U:H4'	1.97	0.47
1:A:453:G:N2	1:A:498:U:O2	2.41	0.47
1:A:1237:A:O2'	1:A:1238:C:O4'	2.33	0.47
40:LQ:25:ILE:HD11	40:LQ:81:ALA:HB1	1.97	0.47
1:A:907:G:N2	1:A:910:A:OP2	2.36	0.47
14:B:687:G:H22	14:B:690:U:H5''	1.79	0.47
1:A:45:G:O6	1:A:404:A:N6	2.48	0.47
10:SC:68:PHE:O	10:SC:72:PHE:N	2.46	0.47
14:B:196:U:N3	14:B:206:U:O2	2.47	0.47
14:B:673:G:O2'	14:B:696:G:O2'	2.27	0.47
14:B:1308:C:H5''	14:B:1309:G:H5'	1.97	0.47
1:A:148:G:H22	1:A:174:A:H61	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:26:LEU:HD11	7:S8:43:SER:HB3	1.95	0.47
14:B:830:U:H4'	14:B:1806:U:H4'	1.97	0.47
14:B:1520:A:O2'	14:B:1521:A:O5'	2.30	0.47
17:L2:62:TYR:HA	17:L2:86:ASN:HD21	1.81	0.46
14:B:2608:G:H2'	14:B:2608:G:N3	2.29	0.46
42:D:18:G:H4'	42:D:60:U:H3	1.80	0.46
1:A:1291:U:OP1	1:A:1293:C:N4	2.48	0.46
1:A:1384:A:H2'	1:A:1385:A:H8	1.80	0.46
14:B:2717:A:OP2	40:LQ:13:ARG:NH2	2.48	0.46
14:B:2776:A:H1'	35:LL:63:THR:HG22	1.96	0.46
17:L2:107:PRO:HD2	17:L2:110:LEU:HD22	1.98	0.46
14:B:1377:U:OP2	21:L6:58:TYR:OH	2.34	0.46
14:B:1491:C:N3	14:B:1492:G:N1	2.64	0.46
30:LF:35:PHE:HA	30:LF:42:GLN:HG2	1.98	0.46
1:A:704:A:O2'	1:A:794:G:O2'	2.33	0.46
1:A:733:G:OP1	1:A:862:G:N2	2.46	0.46
3:S2:23:ILE:HB	3:S2:86:VAL:HG12	1.98	0.46
10:SC:63:MET:HG3	10:SC:93:ARG:HH12	1.80	0.46
27:LC:4:GLY:HA2	27:LC:110:PHE:HZ	1.81	0.46
1:A:536:C:O2	1:A:543:A:O2'	2.30	0.46
1:A:619:C:N4	1:A:637:A:N1	2.63	0.46
1:A:746:U:OP1	12:SE:2:ARG:NH1	2.48	0.46
35:LL:122:THR:N	35:LL:134:GLU:O	2.44	0.46
1:A:129:A:OP1	7:S8:4:ARG:NH1	2.49	0.46
1:A:989:C:N4	1:A:992:A:N1	2.50	0.46
14:B:418:G:O2'	14:B:446:G:O6	2.30	0.46
14:B:624:C:OP2	18:L3:33:LYS:NZ	2.48	0.46
14:B:1517:A:H61	14:B:1563:U:H3	1.62	0.46
34:LJ:51:VAL:HG11	34:LJ:91:GLY:HA3	1.96	0.46
1:A:145:U:O2	1:A:178:G:N1	2.49	0.46
1:A:842:U:H2'	1:A:843:A:C8	2.50	0.46
14:B:352:A:N3	14:B:372:A:O2'	2.49	0.46
14:B:2312:C:H42	14:B:2410:G:H1	1.62	0.46
14:B:2875:U:H2'	14:B:2876:G:H8	1.81	0.46
1:A:744:U:O2'	12:SE:91:VAL:O	2.33	0.46
1:A:952:U:H2'	1:A:953:G:H8	1.81	0.46
1:A:1270:G:H21	1:A:1285:A:H62	1.64	0.46
3:S2:100:LEU:HD22	3:S2:105:LEU:HD23	1.98	0.46
16:L1:51:LYS:HG2	16:L1:52:ARG:H	1.81	0.46
14:B:342:A:N3	14:B:362:C:O2'	2.42	0.46
14:B:1658:A:N6	20:L5:92:ARG:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LJ:157:GLU:O	34:LJ:177:THR:OG1	2.34	0.46
1:A:1504:A:O2'	14:B:1940:A:N7	2.49	0.45
14:B:1713:A:O2'	14:B:2576:G:OP1	2.31	0.45
14:B:2290:C:N4	24:L9:23:ASP:OD1	2.49	0.45
1:A:175:C:H5''	9:SA:20:ARG:HH21	1.82	0.45
17:L2:229:ASP:OD1	17:L2:229:ASP:N	2.48	0.45
7:S8:52:ASN:OD1	7:S8:54:SER:OG	2.32	0.45
14:B:2859:G:N2	40:LQ:97:GLN:O	2.43	0.45
1:A:145:U:H1'	1:A:178:G:H22	1.81	0.45
1:A:633:G:OP1	6:S7:19:ARG:NH2	2.50	0.45
1:A:1265:G:H2'	1:A:1289:A:H61	1.81	0.45
14:B:284:C:O2	14:B:285:U:O2'	2.28	0.45
1:A:1278:G:H8	1:A:1280:G:H22	1.63	0.45
13:SF:5:ASP:OD2	13:SF:79:ARG:NH2	2.50	0.45
14:B:188:C:O2	14:B:215:G:N2	2.49	0.45
14:B:902:A:H5''	24:L9:85:LYS:HE2	1.99	0.45
14:B:2533:U:C5'	14:B:2533:U:N1	2.80	0.45
23:L8:3:SER:OG	23:L8:62:GLU:OE1	2.32	0.45
28:LD:48:ASN:HA	28:LD:51:LYS:HB3	1.97	0.45
1:A:546:U:H4'	4:S3:124:ARG:HH21	1.81	0.45
1:A:844:G:N2	1:A:860:U:O2	2.50	0.45
1:A:957:C:H2'	1:A:958:A:H8	1.81	0.45
1:A:961:U:H2'	1:A:962:G:H8	1.81	0.45
14:B:375:A:O2'	14:B:377:U:OP2	2.29	0.45
14:B:441:C:HO2'	25:LA:13:SER:HG	1.64	0.45
14:B:629:A:N1	14:B:854:G:O2'	2.38	0.45
14:B:1407:C:O2'	14:B:1838:G:O2'	2.34	0.45
14:B:1591:G:N2	14:B:1592:A:H62	2.15	0.45
3:S2:18:ASN:HD22	3:S2:81:THR:H	1.64	0.45
5:S6:9:ASN:HA	5:S6:12:ILE:HD12	1.99	0.45
14:B:1520:A:N6	14:B:1560:A:O2'	2.46	0.45
37:LN:87:ILE:HD11	37:LN:114:ILE:HD11	1.98	0.45
28:LD:12:VAL:HB	28:LD:20:ARG:HG2	1.99	0.45
36:LM:93:LEU:HD23	36:LM:101:LEU:HD13	1.99	0.45
1:A:460:A:H62	1:A:488:U:H3	1.65	0.45
11:SD:99:ALA:HB2	11:SD:123:ILE:HG23	1.99	0.45
4:S3:77:ASN:HB2	4:S3:106:VAL:HA	1.99	0.44
4:S3:112:ARG:HA	4:S3:117:THR:HG22	1.98	0.44
9:SA:35:ALA:O	9:SA:39:VAL:N	2.44	0.44
10:SC:26:LEU:HB2	10:SC:29:ARG:HE	1.82	0.44
15:C:12:U:OP2	15:C:68:A:O2'	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L1:34:ILE:HD12	16:L1:36:GLU:HB2	1.99	0.44
11:SD:108:GLY:O	11:SD:111:VAL:N	2.43	0.44
11:SD:127:SER:HB2	11:SD:130:SER:HB2	1.98	0.44
14:B:2277:G:O2'	14:B:2523:C:OP1	2.26	0.44
1:A:810:A:H3'	1:A:811:G:H8	1.83	0.44
2:S1:41:PRO:HG3	2:S1:72:ARG:HH12	1.82	0.44
4:S3:83:ILE:HD12	4:S3:122:GLY:HA3	2.00	0.44
6:S7:7:LEU:HD22	6:S7:18:TYR:HB3	1.98	0.44
8:S9:31:THR:HA	8:S9:34:LEU:HD13	1.99	0.44
14:B:2869:G:O2'	14:B:2886:G:N2	2.49	0.44
1:A:111:G:H21	1:A:362:G:H4'	1.82	0.44
7:S8:21:LYS:HB3	7:S8:49:HIS:CD2	2.52	0.44
10:SC:182:ARG:HH22	10:SC:190:ASN:HA	1.83	0.44
14:B:2022:U:O2	37:LN:3:GLN:NE2	2.51	0.44
4:S3:80:ILE:HG13	4:S3:110:ILE:HD12	2.00	0.44
12:SE:53:ASN:HB2	12:SE:87:ILE:HD11	1.99	0.44
34:LJ:26:ILE:HD12	34:LJ:111:ARG:HD3	1.99	0.44
1:A:1514:A:OP1	1:A:1542:A:O2'	2.28	0.44
10:SC:66:ARG:O	10:SC:70:ASN:ND2	2.51	0.44
16:L1:77:PRO:HB2	16:L1:80:THR:HG23	2.00	0.44
19:L4:50:ALA:HB3	19:L4:53:VAL:HB	2.00	0.44
1:A:540:A:H2'	1:A:541:A:H2'	1.98	0.44
35:LL:44:LYS:HG2	35:LL:46:GLU:HG3	2.00	0.44
35:LL:89:LEU:HG	35:LL:162:ILE:HG12	1.98	0.44
42:D:9:A:O2'	42:D:11:C:N4	2.37	0.44
1:A:264:U:O4	1:A:274:G:N2	2.51	0.44
5:S6:26:GLU:HB2	5:S6:77:ARG:HH21	1.83	0.44
9:SA:50:VAL:O	9:SA:54:VAL:N	2.43	0.44
11:SD:32:ARG:HE	11:SD:52:LYS:HE2	1.83	0.44
14:B:2532:G:N3	14:B:2532:G:H2'	2.33	0.44
1:A:1009:U:H5''	1:A:1016:A:H62	1.82	0.43
19:L4:63:ASN:ND2	19:L4:96:THR:OG1	2.51	0.43
1:A:425:G:O6	1:A:433:A:N6	2.51	0.43
1:A:796:U:H3	1:A:803:C:H41	1.66	0.43
1:A:961:U:H4'	1:A:973:A:H61	1.82	0.43
1:A:1306:C:H4'	1:A:1312:U:H3	1.82	0.43
1:A:1440:C:O2	1:A:1482:G:N2	2.51	0.43
4:S3:74:ILE:H	4:S3:74:ILE:HG12	1.74	0.43
14:B:647:G:N7	38:LO:103:LYS:NZ	2.57	0.43
16:L1:34:ILE:HD11	16:L1:41:ARG:HE	1.82	0.43
1:A:398:C:H4'	6:S7:29:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:G:N2	1:A:481:C:OP1	2.51	0.43
16:L1:60:THR:HG22	16:L1:77:PRO:HA	2.01	0.43
23:L8:80:ASP:N	23:L8:80:ASP:OD1	2.51	0.43
14:B:593:U:C2	19:L4:21:PHE:HE1	2.36	0.43
20:L5:12:ILE:H	20:L5:12:ILE:HG12	1.69	0.43
1:A:620:C:H42	1:A:636:G:H1	1.66	0.43
1:A:1099:G:H21	1:A:1179:A:H2	1.66	0.43
1:A:1262:A:N6	1:A:1295:A:H61	2.16	0.43
2:S1:92:LEU:HD12	2:S1:93:PRO:HD2	1.99	0.43
14:B:1893:A:N6	14:B:1902:G:O2'	2.51	0.43
14:B:2841:A:O2'	14:B:2846:A:N1	2.47	0.43
17:L2:205:VAL:HG11	17:L2:211:SER:HB2	2.00	0.43
14:B:1465:G:O2'	14:B:1539:A:N6	2.51	0.43
14:B:1962:G:N1	14:B:1989:C:O2'	2.51	0.43
14:B:2873:C:H2'	14:B:2874:A:H8	1.84	0.43
14:B:1293:U:H5''	14:B:1294:G:H5''	2.00	0.43
14:B:2358:G:O2'	14:B:2363:A:N1	2.44	0.43
1:A:1488:C:H2'	1:A:1489:A:C8	2.54	0.43
16:L1:22:PHE:O	16:L1:53:ARG:NH2	2.51	0.43
25:LA:39:LEU:HA	25:LA:44:PRO:HB3	2.00	0.43
34:LJ:4:TYR:OH	34:LJ:203:GLU:OE1	2.37	0.43
1:A:842:U:H2'	1:A:843:A:H8	1.83	0.43
1:A:1323:U:H2'	1:A:1324:C:H6	1.84	0.43
14:B:1091:G:O6	14:B:1154:G:O2'	2.31	0.43
14:B:2040:A:H61	14:B:2640:U:H3	1.67	0.43
1:A:517:A:OP2	10:SC:43:LYS:NZ	2.52	0.42
1:A:673:A:H62	1:A:732:G:H1	1.66	0.42
8:S9:41:ARG:HG3	8:S9:76:VAL:HG13	1.99	0.42
10:SC:95:ASP:OD1	10:SC:96:ALA:N	2.52	0.42
36:LM:19:ILE:HD13	36:LM:143:LEU:HD23	2.00	0.42
1:A:1364:U:H2'	1:A:1365:A:C8	2.54	0.42
14:B:1613:G:OP1	17:L2:210:ARG:NH2	2.52	0.42
14:B:2868:G:C8	16:L1:97:ALA:HB2	2.54	0.42
22:L7:80:ARG:HE	22:L7:96:LYS:HE3	1.84	0.42
1:A:688:C:H42	1:A:718:G:H1	1.68	0.42
1:A:1442:G:OP1	16:L1:108:LYS:N	2.52	0.42
14:B:1027:A:N6	14:B:1028:G:O6	2.51	0.42
14:B:1169:G:O6	14:B:1170:A:N6	2.52	0.42
19:L4:27:VAL:O	19:L4:65:GLN:NE2	2.51	0.42
1:A:680:U:H2'	1:A:681:G:H8	1.84	0.42
1:A:889:C:OP1	4:S3:5:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:U:H2'	1:A:960:G:C8	2.53	0.42
14:B:247:A:OP2	32:LH:8:ARG:NH2	2.52	0.42
14:B:2047:A:H5'	29:LE:9:SER:HB2	2.01	0.42
14:B:2318:U:O2'	14:B:2401:C:O2	2.37	0.42
10:SC:103:LEU:HD22	10:SC:172:LEU:HD23	2.00	0.42
11:SD:64:VAL:HG12	11:SD:68:LYS:HE2	2.01	0.42
14:B:1520:A:O2'	14:B:1521:A:O4'	2.36	0.42
4:S3:24:LEU:HD22	4:S3:107:ARG:HH12	1.84	0.42
4:S3:47:CYS:HA	4:S3:68:VAL:HG12	2.00	0.42
14:B:2103:U:H5''	14:B:2265:G:H22	1.85	0.42
19:L4:22:VAL:O	19:L4:93:THR:N	2.53	0.42
14:B:833:A:OP1	14:B:836:C:N4	2.49	0.42
14:B:1051:C:OP1	36:LM:38:ARG:NH2	2.53	0.42
34:LJ:49:HIS:HD2	34:LJ:92:PRO:HB3	1.84	0.42
13:SF:25:LEU:HD23	13:SF:62:LEU:HD12	2.02	0.42
15:C:74:G:OP2	23:L8:12:LYS:NZ	2.53	0.42
32:LH:31:HIS:CD2	32:LH:32:LEU:HG	2.55	0.42
42:D:51:U:H3	42:D:63:G:H22	1.66	0.42
24:L9:66:THR:O	24:L9:66:THR:OG1	2.32	0.42
1:A:156:C:O2	1:A:165:G:N1	2.47	0.42
10:SC:48:GLY:HA2	10:SC:51:LEU:HB3	2.01	0.42
14:B:86:C:O2'	14:B:103:U:O2'	2.28	0.42
36:LM:70:GLU:HG3	36:LM:71:THR:HG23	2.02	0.42
37:LN:65:THR:HG23	37:LN:68:GLY:H	1.85	0.42
38:LO:92:THR:HG22	38:LO:94:ALA:H	1.85	0.42
1:A:10:G:H2'	1:A:11:A:H8	1.84	0.41
1:A:383:U:O2'	6:S7:7:LEU:O	2.37	0.41
1:A:968:A:O2'	1:A:993:C:O2	2.35	0.41
9:SA:56:LEU:O	9:SA:60:ALA:N	2.52	0.41
14:B:1545:U:O4	14:B:1546:A:N6	2.53	0.41
36:LM:144:ARG:H	36:LM:144:ARG:HG3	1.60	0.41
1:A:1326:G:H2'	1:A:1327:C:H3'	2.02	0.41
20:L5:10:ILE:HG21	20:L5:46:VAL:HG11	2.02	0.41
20:L5:11:ARG:O	20:L5:98:LYS:NZ	2.44	0.41
1:A:115:A:H61	1:A:321:A:H2	1.67	0.41
1:A:471:A:N1	1:A:474:A:O2'	2.53	0.41
1:A:1272:A:N7	1:A:1273:A:N6	2.69	0.41
14:B:1773:A:H8	14:B:1774:A:C8	2.39	0.41
19:L4:4:ILE:HD12	19:L4:40:PHE:HB3	2.02	0.41
40:LQ:51:GLY:HA2	40:LQ:86:PHE:CD1	2.56	0.41
42:D:13:C:H2'	42:D:14:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:O2'	5:S6:46:HIS:ND1	2.48	0.41
2:S1:39:PRO:HB3	2:S1:74:ILE:HG23	2.02	0.41
3:S2:122:ARG:HA	3:S2:123:PRO:HD3	1.87	0.41
14:B:1518:G:H22	14:B:1562:C:H42	1.69	0.41
14:B:2500:U:OP1	14:B:2556:G:N2	2.54	0.41
22:L7:40:ILE:HG22	22:L7:60:GLU:HG3	2.01	0.41
26:LB:16:GLU:HG3	26:LB:19:LYS:HE3	2.03	0.41
1:A:234:A:H2'	1:A:235:G:H8	1.86	0.41
1:A:568:A:H4'	1:A:569:U:H5''	2.02	0.41
1:A:1128:A:H2'	1:A:1189:A:H2	1.85	0.41
1:A:1527:G:N2	1:A:1530:A:OP2	2.53	0.41
1:A:975:G:OP1	1:A:976:C:N4	2.54	0.41
1:A:204:A:H2'	1:A:205:A:H8	1.86	0.41
1:A:760:G:OP1	5:S6:73:LYS:NZ	2.53	0.41
1:A:1416:U:H1'	1:A:1529:A:H4'	2.02	0.41
14:B:735:C:O2'	14:B:825:G:OP1	2.37	0.41
14:B:758:G:H22	14:B:763:A:H8	1.67	0.41
14:B:1540:U:O2	14:B:1624:C:O2'	2.29	0.41
1:A:787:C:H42	1:A:811:G:H1	1.68	0.41
1:A:1178:C:H5''	1:A:1179:A:H2'	2.02	0.41
1:A:1273:A:H61	1:A:1283:C:H42	1.69	0.41
14:B:1726:A:OP1	14:B:1743:G:N1	2.45	0.41
34:LJ:22:ALA:HB1	34:LJ:26:ILE:HD11	2.03	0.41
34:LJ:57:VAL:HG21	34:LJ:79:ARG:HB3	2.03	0.41
36:LM:75:TYR:HB2	36:LM:88:ILE:HG23	2.02	0.41
1:A:30:A:N6	1:A:31:U:O4	2.54	0.41
1:A:796:U:H3	1:A:803:C:N4	2.19	0.41
3:S2:30:THR:HB	3:S2:47:ALA:HB2	2.02	0.41
3:S2:32:VAL:HG21	3:S2:67:SER:HA	2.02	0.41
11:SD:36:LEU:HD22	11:SD:134:ILE:HG12	2.02	0.41
14:B:1063:U:OP1	14:B:1079:U:O2'	2.30	0.41
26:LB:14:ILE:HA	26:LB:17:GLN:HB3	2.02	0.41
41:LR:64:ALA:HA	41:LR:72:LEU:HD21	2.03	0.41
1:A:271:A:H2'	1:A:272:C:H6	1.86	0.41
1:A:527:C:H42	1:A:541:A:N6	2.19	0.41
1:A:622:A:N6	1:A:633:G:O6	2.54	0.41
14:B:23:G:H1	14:B:562:C:H42	1.67	0.41
14:B:1250:G:H2'	14:B:1274:G:H22	1.86	0.41
14:B:1290:G:OP2	18:L3:14:ARG:NH2	2.44	0.41
14:B:2850:G:H5'	27:LC:67:LYS:HE3	2.03	0.41
14:B:504:G:O2'	14:B:515:G:O6	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:971:U:H2'	14:B:972:A:C8	2.57	0.40
19:L4:2:PHE:HB3	19:L4:15:GLU:HG2	2.02	0.40
4:S3:83:ILE:H	4:S3:120:VAL:HG11	1.87	0.40
15:C:91:C:H2'	15:C:92:G:C8	2.56	0.40
37:LN:3:GLN:HG2	37:LN:4:GLN:H	1.86	0.40
42:D:13:C:H2'	42:D:14:A:C8	2.56	0.40
1:A:350:C:N4	1:A:355:G:O6	2.49	0.40
14:B:732:C:H1'	31:LG:5:THR:HG22	2.02	0.40
14:B:994:A:H5''	15:C:85:A:H61	1.85	0.40
14:B:2050:A:H5'	14:B:2644:C:H4'	2.02	0.40
24:L9:44:ILE:HG21	24:L9:47:ARG:HD3	2.02	0.40
38:LO:56:PRO:O	38:LO:60:ARG:NH1	2.54	0.40
1:A:29:G:H21	1:A:304:U:H5'	1.86	0.40
1:A:109:C:O2'	6:S7:26:ARG:O	2.36	0.40
1:A:1198:A:N6	1:A:1199:U:O2	2.54	0.40
1:A:1449:G:H1	1:A:1473:C:H42	1.70	0.40
10:SC:125:ARG:NE	10:SC:127:ASP:OD2	2.55	0.40
39:LP:37:THR:OG1	39:LP:128:LYS:O	2.29	0.40
1:A:465:U:H3	1:A:486:C:H41	1.67	0.40
3:S2:111:ARG:HG2	3:S2:113:VAL:HG23	2.02	0.40
14:B:2682:G:O2'	14:B:2691:G:O6	2.32	0.40
17:L2:11:ASN:ND2	17:L2:14:ARG:HH21	2.19	0.40
18:L3:53:ARG:HH11	18:L3:53:ARG:HD3	1.76	0.40
42:D:51:U:H3	42:D:63:G:H1	1.69	0.40
42:D:63:G:H2'	42:D:64:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S1	80/82 (98%)	70 (88%)	10 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S2	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
4	S3	134/136 (98%)	109 (81%)	22 (16%)	3 (2%)	5	32
5	S6	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
6	S7	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	S8	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
8	S9	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
9	SA	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
10	SC	196/198 (99%)	180 (92%)	16 (8%)	0	100	100
11	SD	152/154 (99%)	136 (90%)	16 (10%)	0	100	100
12	SE	90/92 (98%)	80 (89%)	10 (11%)	0	100	100
13	SF	128/130 (98%)	109 (85%)	19 (15%)	0	100	100
16	L1	111/113 (98%)	94 (85%)	17 (15%)	0	100	100
17	L2	273/275 (99%)	233 (85%)	39 (14%)	1 (0%)	30	63
18	L3	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
19	L4	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
20	L5	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
21	L6	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
22	L7	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
23	L8	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
24	L9	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
25	LA	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
26	LB	59/61 (97%)	53 (90%)	6 (10%)	0	100	100
27	LC	212/214 (99%)	176 (83%)	36 (17%)	0	100	100
28	LD	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
29	LE	51/53 (96%)	43 (84%)	8 (16%)	0	100	100
30	LF	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
31	LG	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
32	LH	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
33	LI	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
34	LJ	202/204 (99%)	173 (86%)	29 (14%)	0	100	100
35	LL	172/174 (99%)	147 (86%)	24 (14%)	1 (1%)	22	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	LM	141/143 (99%)	122 (86%)	19 (14%)	0	100	100
37	LN	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
38	LO	142/144 (99%)	121 (85%)	21 (15%)	0	100	100
39	LP	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
40	LQ	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
41	LR	114/116 (98%)	99 (87%)	15 (13%)	0	100	100
All	All	4076/4152 (98%)	3590 (88%)	481 (12%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	LL	59	LYS
17	L2	50	THR
4	S3	57	LYS
4	S3	58	PRO
4	S3	41	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S1	73/73 (100%)	73 (100%)	0	100	100
3	S2	91/91 (100%)	90 (99%)	1 (1%)	70	83
4	S3	103/117 (88%)	99 (96%)	4 (4%)	27	57
5	S6	79/79 (100%)	79 (100%)	0	100	100
6	S7	64/64 (100%)	64 (100%)	0	100	100
7	S8	77/77 (100%)	77 (100%)	0	100	100
8	S9	50/50 (100%)	50 (100%)	0	100	100
9	SA	29/64 (45%)	29 (100%)	0	100	100
10	SC	173/173 (100%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	SD	118/120 (98%)	116 (98%)	2 (2%)	56	75
12	SE	80/80 (100%)	80 (100%)	0	100	100
13	SF	110/111 (99%)	110 (100%)	0	100	100
16	L1	99/99 (100%)	99 (100%)	0	100	100
17	L2	217/222 (98%)	215 (99%)	2 (1%)	75	87
18	L3	96/96 (100%)	96 (100%)	0	100	100
19	L4	85/85 (100%)	84 (99%)	1 (1%)	67	82
20	L5	90/90 (100%)	89 (99%)	1 (1%)	70	83
21	L6	74/79 (94%)	73 (99%)	1 (1%)	62	79
22	L7	79/86 (92%)	79 (100%)	0	100	100
23	L8	81/81 (100%)	81 (100%)	0	100	100
24	L9	59/61 (97%)	57 (97%)	2 (3%)	32	60
25	LA	49/49 (100%)	49 (100%)	0	100	100
26	LB	55/55 (100%)	55 (100%)	0	100	100
27	LC	171/172 (99%)	169 (99%)	2 (1%)	67	82
28	LD	51/51 (100%)	51 (100%)	0	100	100
29	LE	48/48 (100%)	48 (100%)	0	100	100
30	LF	44/45 (98%)	44 (100%)	0	100	100
31	LG	39/39 (100%)	39 (100%)	0	100	100
32	LH	55/55 (100%)	55 (100%)	0	100	100
33	LI	35/35 (100%)	35 (100%)	0	100	100
34	LJ	160/167 (96%)	160 (100%)	0	100	100
35	LL	151/152 (99%)	151 (100%)	0	100	100
36	LM	122/122 (100%)	120 (98%)	2 (2%)	58	76
37	LN	99/99 (100%)	97 (98%)	2 (2%)	50	72
38	LO	110/110 (100%)	109 (99%)	1 (1%)	75	87
39	LP	113/113 (100%)	112 (99%)	1 (1%)	75	87
40	LQ	101/101 (100%)	101 (100%)	0	100	100
41	LR	91/92 (99%)	88 (97%)	3 (3%)	33	61
All	All	3421/3503 (98%)	3396 (99%)	25 (1%)	80	90

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S2	29	ASN
4	S3	25	ASN
4	S3	38	LEU
4	S3	74	ILE
4	S3	96	ARG
11	SD	23	LYS
11	SD	26	LYS
17	L2	219	THR
17	L2	261	ARG
19	L4	79	ARG
20	L5	84	ARG
21	L6	6	ILE
24	L9	61	ARG
24	L9	80	LYS
27	LC	66	ASN
27	LC	138	ARG
36	LM	11	ASN
36	LM	85	ILE
37	LN	72	ASN
37	LN	107	ARG
38	LO	104	ASN
39	LP	68	ILE
41	LR	21	ASN
41	LR	48	ASN
41	LR	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	S2	18	ASN
3	S2	29	ASN
4	S3	25	ASN
4	S3	72	ASN
4	S3	77	ASN
6	S7	62	ASN
10	SC	8	ASN
10	SC	67	GLN
10	SC	85	ASN
13	SF	31	ASN
17	L2	11	ASN
17	L2	86	ASN
17	L2	232	HIS
18	L3	44	GLN

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Mol	Chain	Res	Type
20	L5	60	HIS
20	L5	61	ASN
20	L5	77	ASN
22	L7	2	HIS
24	L9	37	GLN
26	LB	17	GLN
27	LC	66	ASN
29	LE	32	ASN
29	LE	50	ASN
32	LH	31	HIS
35	LL	38	ASN
35	LL	48	ASN
36	LM	11	ASN
37	LN	72	ASN
38	LO	83	ASN
38	LO	104	ASN
41	LR	21	ASN
41	LR	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1411/1547 (91%)	486 (34%)	14 (0%)
14	B	2759/2919 (94%)	765 (27%)	9 (0%)
15	C	113/114 (99%)	31 (27%)	1 (0%)
42	D	73/74 (98%)	28 (38%)	0
All	All	4356/4654 (93%)	1310 (30%)	24 (0%)

All (1310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	G
1	A	9	A
1	A	10	G
1	A	23	G
1	A	30	A
1	A	32	G
1	A	33	A
1	A	37	C
1	A	39	G

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Mol	Chain	Res	Type
1	A	40	G
1	A	41	C
1	A	47	G
1	A	48	C
1	A	49	C
1	A	50	U
1	A	51	A
1	A	52	A
1	A	53	U
1	A	55	C
1	A	61	A
1	A	62	G
1	A	66	A
1	A	67	G
1	A	108	A
1	A	114	G
1	A	115	A
1	A	119	A
1	A	120	C
1	A	121	A
1	A	125	G
1	A	129	A
1	A	133	U
1	A	134	A
1	A	135	C
1	A	137	U
1	A	138	A
1	A	143	A
1	A	144	C
1	A	149	A
1	A	154	U
1	A	161	A
1	A	163	C
1	A	164	C
1	A	173	U
1	A	204	A
1	A	206	A
1	A	209	G
1	A	210	A
1	A	211	A
1	A	225	G
1	A	228	A

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Mol	Chain	Res	Type
1	A	233	U
1	A	234	A
1	A	236	A
1	A	242	C
1	A	252	U
1	A	254	A
1	A	255	G
1	A	258	A
1	A	259	G
1	A	268	G
1	A	269	U
1	A	274	G
1	A	275	C
1	A	276	U
1	A	280	C
1	A	284	G
1	A	287	A
1	A	289	G
1	A	291	U
1	A	293	C
1	A	297	G
1	A	302	C
1	A	306	A
1	A	307	G
1	A	314	A
1	A	315	U
1	A	316	C
1	A	320	C
1	A	321	A
1	A	332	G
1	A	333	A
1	A	334	G
1	A	335	A
1	A	336	C
1	A	337	A
1	A	338	C
1	A	340	G
1	A	342	C
1	A	347	C
1	A	348	U
1	A	349	C
1	A	350	C

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Mol	Chain	Res	Type
1	A	353	C
1	A	355	G
1	A	359	G
1	A	360	C
1	A	362	G
1	A	364	A
1	A	366	U
1	A	367	A
1	A	370	G
1	A	371	A
1	A	375	U
1	A	376	U
1	A	377	C
1	A	379	G
1	A	386	G
1	A	389	A
1	A	392	G
1	A	396	G
1	A	398	C
1	A	401	A
1	A	406	C
1	A	408	C
1	A	412	G
1	A	413	U
1	A	414	G
1	A	419	A
1	A	420	U
1	A	421	G
1	A	423	A
1	A	424	G
1	A	425	G
1	A	427	C
1	A	428	U
1	A	430	C
1	A	431	G
1	A	432	G
1	A	436	G
1	A	437	U
1	A	438	A
1	A	444	C
1	A	447	U
1	A	448	U

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Mol	Chain	Res	Type
1	A	450	U
1	A	451	U
1	A	452	A
1	A	457	A
1	A	459	A
1	A	460	A
1	A	461	C
1	A	464	A
1	A	465	U
1	A	467	U
1	A	468	G
1	A	470	A
1	A	471	A
1	A	472	G
1	A	473	U
1	A	475	A
1	A	478	G
1	A	481	C
1	A	482	A
1	A	484	A
1	A	486	C
1	A	487	U
1	A	489	G
1	A	492	G
1	A	493	G
1	A	494	U
1	A	501	U
1	A	504	G
1	A	506	A
1	A	507	A
1	A	508	G
1	A	513	G
1	A	516	U
1	A	517	A
1	A	520	U
1	A	524	U
1	A	525	G
1	A	526	C
1	A	527	C
1	A	528	A
1	A	529	G
1	A	535	G

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Mol	Chain	Res	Type
1	A	539	U
1	A	540	A
1	A	543	A
1	A	544	C
1	A	555	A
1	A	558	G
1	A	567	A
1	A	575	G
1	A	576	G
1	A	580	A
1	A	581	A
1	A	584	C
1	A	585	G
1	A	601	U
1	A	604	A
1	A	616	A
1	A	622	A
1	A	623	C
1	A	624	G
1	A	627	U
1	A	639	G
1	A	640	G
1	A	646	G
1	A	649	A
1	A	661	U
1	A	663	A
1	A	673	A
1	A	675	G
1	A	679	G
1	A	684	A
1	A	688	C
1	A	695	A
1	A	696	G
1	A	698	G
1	A	700	U
1	A	701	G
1	A	703	A
1	A	704	A
1	A	706	G
1	A	710	A
1	A	711	G
1	A	713	G

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Mol	Chain	Res	Type
1	A	716	A
1	A	721	G
1	A	724	A
1	A	726	A
1	A	728	C
1	A	729	A
1	A	730	G
1	A	731	U
1	A	732	G
1	A	739	G
1	A	756	A
1	A	760	G
1	A	763	G
1	A	766	G
1	A	769	G
1	A	772	C
1	A	784	G
1	A	785	A
1	A	788	A
1	A	790	A
1	A	802	A
1	A	803	C
1	A	804	C
1	A	807	G
1	A	820	G
1	A	821	U
1	A	823	A
1	A	825	C
1	A	829	G
1	A	835	U
1	A	836	A
1	A	849	U
1	A	850	U
1	A	851	U
1	A	853	C
1	A	858	C
1	A	862	G
1	A	864	G
1	A	873	A
1	A	876	G
1	A	879	U
1	A	880	U

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Mol	Chain	Res	Type
1	A	881	A
1	A	885	A
1	A	894	G
1	A	896	G
1	A	898	A
1	A	906	C
1	A	909	A
1	A	919	C
1	A	928	A
1	A	931	G
1	A	935	G
1	A	936	G
1	A	939	C
1	A	940	C
1	A	943	C
1	A	944	A
1	A	945	C
1	A	946	A
1	A	948	G
1	A	950	G
1	A	954	G
1	A	955	A
1	A	969	U
1	A	970	U
1	A	971	C
1	A	975	G
1	A	978	A
1	A	980	G
1	A	984	A
1	A	985	G
1	A	986	A
1	A	989	C
1	A	990	U
1	A	992	A
1	A	993	C
1	A	994	C
1	A	1002	G
1	A	1003	A
1	A	1006	U
1	A	1009	U
1	A	1010	U
1	A	1012	G

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Mol	Chain	Res	Type
1	A	1013	A
1	A	1014	C
1	A	1016	A
1	A	1065	C
1	A	1067	U
1	A	1068	G
1	A	1075	G
1	A	1076	U
1	A	1081	U
1	A	1090	G
1	A	1093	A
1	A	1096	U
1	A	1100	G
1	A	1103	A
1	A	1104	A
1	A	1105	G
1	A	1106	U
1	A	1109	C
1	A	1111	C
1	A	1112	A
1	A	1115	G
1	A	1121	A
1	A	1122	A
1	A	1124	C
1	A	1125	C
1	A	1126	U
1	A	1130	G
1	A	1134	A
1	A	1135	G
1	A	1136	U
1	A	1138	G
1	A	1140	C
1	A	1141	A
1	A	1143	C
1	A	1144	A
1	A	1145	U
1	A	1162	A
1	A	1164	U
1	A	1168	C
1	A	1169	U
1	A	1170	G
1	A	1173	G

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Mol	Chain	Res	Type
1	A	1177	A
1	A	1179	A
1	A	1180	A
1	A	1184	G
1	A	1185	G
1	A	1186	A
1	A	1187	G
1	A	1188	G
1	A	1189	A
1	A	1191	G
1	A	1192	G
1	A	1197	G
1	A	1198	A
1	A	1199	U
1	A	1200	G
1	A	1201	A
1	A	1206	A
1	A	1207	A
1	A	1208	A
1	A	1210	C
1	A	1212	U
1	A	1213	C
1	A	1217	C
1	A	1218	C
1	A	1219	C
1	A	1220	C
1	A	1222	U
1	A	1223	A
1	A	1224	U
1	A	1225	G
1	A	1228	U
1	A	1235	A
1	A	1236	C
1	A	1238	C
1	A	1243	G
1	A	1246	A
1	A	1247	C
1	A	1248	A
1	A	1251	G
1	A	1254	C
1	A	1255	A
1	A	1257	U

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Mol	Chain	Res	Type
1	A	1264	G
1	A	1266	C
1	A	1267	A
1	A	1268	G
1	A	1271	A
1	A	1273	A
1	A	1275	C
1	A	1279	A
1	A	1280	G
1	A	1281	G
1	A	1288	A
1	A	1289	A
1	A	1290	A
1	A	1291	U
1	A	1292	C
1	A	1296	U
1	A	1297	A
1	A	1299	A
1	A	1304	U
1	A	1305	U
1	A	1308	C
1	A	1309	A
1	A	1310	G
1	A	1311	U
1	A	1315	G
1	A	1332	C
1	A	1333	G
1	A	1335	C
1	A	1336	U
1	A	1342	A
1	A	1343	A
1	A	1347	G
1	A	1350	A
1	A	1355	U
1	A	1357	G
1	A	1358	U
1	A	1361	U
1	A	1362	C
1	A	1364	U
1	A	1374	U
1	A	1380	G
1	A	1381	G

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Mol	Chain	Res	Type
1	A	1388	C
1	A	1389	G
1	A	1392	C
1	A	1394	C
1	A	1395	G
1	A	1397	G
1	A	1404	A
1	A	1407	C
1	A	1408	A
1	A	1410	C
1	A	1411	G
1	A	1416	U
1	A	1429	G
1	A	1442	G
1	A	1444	A
1	A	1446	C
1	A	1451	G
1	A	1452	G
1	A	1453	A
1	A	1456	A
1	A	1458	C
1	A	1461	U
1	A	1462	U
1	A	1463	U
1	A	1464	A
1	A	1465	G
1	A	1469	C
1	A	1479	A
1	A	1485	G
1	A	1486	G
1	A	1495	U
1	A	1498	G
1	A	1501	U
1	A	1502	G
1	A	1503	A
1	A	1504	A
1	A	1505	G
1	A	1508	G
1	A	1510	A
1	A	1514	A
1	A	1516	G
1	A	1517	U

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Mol	Chain	Res	Type
1	A	1518	A
1	A	1519	G
1	A	1522	G
1	A	1524	A
1	A	1528	G
1	A	1530	A
1	A	1531	G
1	A	1540	G
1	A	1541	G
1	A	1542	A
1	A	1544	C
1	A	1545	A
1	A	1546	C
1	A	1547	C
14	B	2	A
14	B	3	U
14	B	4	U
14	B	8	U
14	B	12	U
14	B	13	A
14	B	25	U
14	B	32	C
14	B	34	U
14	B	42	G
14	B	43	A
14	B	49	A
14	B	51	G
14	B	54	G
14	B	56	A
14	B	60	U
14	B	64	A
14	B	71	A
14	B	75	G
14	B	88	G
14	B	89	U
14	B	90	A
14	B	91	A
14	B	93	U
14	B	96	G
14	B	99	U
14	B	102	A
14	B	103	U

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Mol	Chain	Res	Type
14	B	109	G
14	B	114	C
14	B	117	A
14	B	118	A
14	B	119	U
14	B	124	A
14	B	130	A
14	B	148	U
14	B	152	C
14	B	153	G
14	B	154	A
14	B	156	A
14	B	157	U
14	B	160	G
14	B	161	A
14	B	162	A
14	B	163	U
14	B	169	G
14	B	174	U
14	B	176	A
14	B	182	C
14	B	183	A
14	B	184	C
14	B	185	A
14	B	189	G
14	B	191	A
14	B	194	A
14	B	199	A
14	B	202	A
14	B	218	G
14	B	219	A
14	B	224	A
14	B	225	A
14	B	229	A
14	B	233	U
14	B	235	G
14	B	236	A
14	B	244	A
14	B	246	U
14	B	248	G
14	B	251	G
14	B	253	G

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Mol	Chain	Res	Type
14	B	255	G
14	B	264	G
14	B	267	G
14	B	268	A
14	B	269	G
14	B	276	C
14	B	277	C
14	B	278	A
14	B	283	G
14	B	284	C
14	B	285	U
14	B	286	U
14	B	287	G
14	B	288	C
14	B	289	U
14	B	290	U
14	B	291	G
14	B	294	G
14	B	298	U
14	B	300	G
14	B	301	U
14	B	302	A
14	B	303	G
14	B	310	C
14	B	319	G
14	B	320	U
14	B	321	U
14	B	322	A
14	B	327	G
14	B	328	G
14	B	332	A
14	B	337	A
14	B	338	G
14	B	344	U
14	B	353	A
14	B	354	A
14	B	359	A
14	B	366	G
14	B	372	A
14	B	373	A
14	B	375	A
14	B	378	C

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Mol	Chain	Res	Type
14	B	385	U
14	B	389	A
14	B	395	U
14	B	396	G
14	B	397	U
14	B	398	C
14	B	399	U
14	B	404	U
14	B	405	G
14	B	410	G
14	B	411	A
14	B	416	G
14	B	432	G
14	B	433	U
14	B	434	G
14	B	435	A
14	B	444	C
14	B	445	G
14	B	446	G
14	B	447	A
14	B	452	G
14	B	457	G
14	B	458	A
14	B	459	C
14	B	462	U
14	B	463	C
14	B	482	U
14	B	489	A
14	B	494	U
14	B	496	G
14	B	502	C
14	B	503	A
14	B	504	G
14	B	510	U
14	B	513	G
14	B	518	A
14	B	519	G
14	B	526	A
14	B	527	G
14	B	535	G
14	B	541	G
14	B	548	A

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Mol	Chain	Res	Type
14	B	549	U
14	B	550	A
14	B	552	A
14	B	553	A
14	B	554	C
14	B	565	G
14	B	566	U
14	B	567	G
14	B	572	C
14	B	575	G
14	B	576	U
14	B	577	A
14	B	578	G
14	B	583	A
14	B	587	C
14	B	589	U
14	B	590	U
14	B	591	A
14	B	592	A
14	B	593	U
14	B	594	G
14	B	606	G
14	B	616	G
14	B	618	A
14	B	626	G
14	B	629	A
14	B	630	G
14	B	638	U
14	B	644	C
14	B	646	A
14	B	647	G
14	B	648	G
14	B	658	A
14	B	659	A
14	B	660	A
14	B	661	U
14	B	662	G
14	B	667	G
14	B	673	G
14	B	679	G
14	B	681	G
14	B	682	A

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Mol	Chain	Res	Type
14	B	683	G
14	B	691	A
14	B	696	G
14	B	698	U
14	B	702	U
14	B	705	U
14	B	715	A
14	B	716	C
14	B	722	A
14	B	731	U
14	B	735	C
14	B	745	G
14	B	748	U
14	B	751	A
14	B	752	G
14	B	759	U
14	B	761	A
14	B	762	C
14	B	763	A
14	B	764	C
14	B	768	A
14	B	773	G
14	B	775	A
14	B	793	G
14	B	794	A
14	B	795	A
14	B	799	U
14	B	802	G
14	B	809	A
14	B	820	G
14	B	822	G
14	B	823	G
14	B	827	A
14	B	828	A
14	B	829	U
14	B	837	G
14	B	838	A
14	B	842	U
14	B	850	G
14	B	851	C
14	B	857	C
14	B	859	C

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Mol	Chain	Res	Type
14	B	864	A
14	B	870	C
14	B	872	U
14	B	874	A
14	B	879	U
14	B	883	C
14	B	890	G
14	B	891	A
14	B	896	U
14	B	904	G
14	B	908	A
14	B	910	C
14	B	911	A
14	B	951	G
14	B	952	A
14	B	955	A
14	B	960	C
14	B	964	U
14	B	970	U
14	B	971	U
14	B	977	A
14	B	979	C
14	B	981	U
14	B	985	A
14	B	989	A
14	B	990	G
14	B	997	G
14	B	1005	G
14	B	1014	U
14	B	1017	A
14	B	1018	A
14	B	1024	A
14	B	1027	A
14	B	1033	G
14	B	1040	A
14	B	1045	A
14	B	1048	U
14	B	1049	C
14	B	1052	A
14	B	1053	A
14	B	1055	A
14	B	1056	U

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Mol	Chain	Res	Type
14	B	1057	A
14	B	1061	G
14	B	1066	G
14	B	1067	U
14	B	1069	G
14	B	1070	A
14	B	1074	G
14	B	1077	U
14	B	1081	G
14	B	1082	C
14	B	1083	G
14	B	1086	G
14	B	1090	A
14	B	1091	G
14	B	1092	A
14	B	1093	C
14	B	1095	A
14	B	1132	A
14	B	1134	U
14	B	1136	C
14	B	1138	U
14	B	1139	A
14	B	1140	A
14	B	1141	U
14	B	1142	A
14	B	1143	G
14	B	1147	A
14	B	1148	C
14	B	1151	G
14	B	1154	G
14	B	1155	A
14	B	1156	G
14	B	1158	G
14	B	1160	C
14	B	1162	C
14	B	1163	U
14	B	1170	A
14	B	1173	A
14	B	1174	U
14	B	1176	U
14	B	1178	C
14	B	1183	G

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Mol	Chain	Res	Type
14	B	1185	U
14	B	1186	A
14	B	1187	A
14	B	1189	C
14	B	1210	U
14	B	1213	C
14	B	1215	U
14	B	1217	U
14	B	1223	A
14	B	1229	G
14	B	1250	G
14	B	1258	A
14	B	1270	U
14	B	1273	G
14	B	1274	G
14	B	1276	G
14	B	1278	G
14	B	1285	A
14	B	1288	G
14	B	1291	A
14	B	1293	U
14	B	1294	G
14	B	1296	C
14	B	1300	G
14	B	1309	G
14	B	1310	A
14	B	1312	A
14	B	1313	G
14	B	1315	C
14	B	1318	G
14	B	1322	G
14	B	1333	A
14	B	1337	A
14	B	1338	U
14	B	1339	U
14	B	1350	U
14	B	1355	A
14	B	1364	C
14	B	1366	U
14	B	1378	U
14	B	1382	C
14	B	1383	G

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Mol	Chain	Res	Type
14	B	1389	U
14	B	1390	A
14	B	1402	A
14	B	1403	C
14	B	1405	G
14	B	1410	A
14	B	1412	G
14	B	1416	U
14	B	1417	G
14	B	1421	A
14	B	1424	A
14	B	1432	A
14	B	1437	U
14	B	1439	U
14	B	1447	A
14	B	1448	U
14	B	1449	A
14	B	1451	U
14	B	1452	C
14	B	1453	G
14	B	1454	U
14	B	1460	U
14	B	1462	G
14	B	1464	U
14	B	1466	G
14	B	1467	G
14	B	1471	A
14	B	1472	C
14	B	1473	G
14	B	1482	U
14	B	1484	G
14	B	1489	A
14	B	1490	G
14	B	1491	C
14	B	1494	G
14	B	1495	C
14	B	1496	G
14	B	1503	U
14	B	1504	U
14	B	1505	G
14	B	1507	A
14	B	1508	C

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Mol	Chain	Res	Type
14	B	1509	G
14	B	1510	U
14	B	1511	C
14	B	1515	G
14	B	1517	A
14	B	1518	G
14	B	1519	U
14	B	1520	A
14	B	1521	A
14	B	1524	C
14	B	1526	G
14	B	1527	A
14	B	1528	G
14	B	1530	A
14	B	1540	U
14	B	1541	C
14	B	1542	C
14	B	1544	G
14	B	1546	A
14	B	1548	U
14	B	1550	G
14	B	1556	G
14	B	1557	C
14	B	1559	G
14	B	1561	G
14	B	1568	U
14	B	1570	G
14	B	1572	G
14	B	1575	A
14	B	1578	A
14	B	1581	U
14	B	1582	U
14	B	1583	G
14	B	1584	U
14	B	1586	U
14	B	1590	C
14	B	1592	A
14	B	1598	U
14	B	1599	G
14	B	1605	A
14	B	1613	G
14	B	1614	A

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Mol	Chain	Res	Type
14	B	1616	A
14	B	1618	A
14	B	1625	U
14	B	1627	G
14	B	1628	A
14	B	1629	U
14	B	1630	A
14	B	1631	G
14	B	1633	A
14	B	1646	U
14	B	1647	A
14	B	1652	A
14	B	1653	A
14	B	1654	A
14	B	1656	C
14	B	1660	A
14	B	1676	A
14	B	1687	G
14	B	1690	A
14	B	1691	G
14	B	1692	C
14	B	1697	G
14	B	1698	A
14	B	1712	A
14	B	1718	G
14	B	1719	C
14	B	1721	A
14	B	1735	C
14	B	1736	U
14	B	1737	U
14	B	1738	C
14	B	1739	G
14	B	1740	G
14	B	1742	A
14	B	1743	G
14	B	1745	A
14	B	1747	G
14	B	1748	G
14	B	1751	G
14	B	1756	U
14	B	1759	G
14	B	1765	A

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Mol	Chain	Res	Type
14	B	1766	C
14	B	1772	G
14	B	1783	G
14	B	1785	G
14	B	1790	G
14	B	1791	G
14	B	1796	A
14	B	1800	A
14	B	1803	G
14	B	1808	U
14	B	1809	C
14	B	1811	A
14	B	1812	A
14	B	1813	A
14	B	1821	U
14	B	1826	G
14	B	1827	C
14	B	1828	U
14	B	1835	U
14	B	1836	A
14	B	1838	G
14	B	1839	G
14	B	1842	A
14	B	1843	U
14	B	1844	G
14	B	1845	U
14	B	1851	G
14	B	1853	C
14	B	1855	G
14	B	1856	A
14	B	1863	C
14	B	1866	A
14	B	1867	G
14	B	1873	G
14	B	1875	A
14	B	1878	U
14	B	1881	A
14	B	1884	G
14	B	1893	A
14	B	1896	U
14	B	1899	U
14	B	1900	G

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Mol	Chain	Res	Type
14	B	1902	G
14	B	1905	G
14	B	1911	A
14	B	1912	A
14	B	1915	G
14	B	1926	A
14	B	1933	G
14	B	1940	A
14	B	1941	C
14	B	1943	A
14	B	1944	U
14	B	1945	A
14	B	1946	A
14	B	1947	C
14	B	1957	G
14	B	1961	C
14	B	1965	A
14	B	1967	U
14	B	1982	U
14	B	1990	C
14	B	1991	G
14	B	1992	C
14	B	1994	C
14	B	1997	A
14	B	1998	A
14	B	1999	G
14	B	2002	G
14	B	2009	U
14	B	2012	G
14	B	2015	C
14	B	2018	U
14	B	2019	G
14	B	2020	U
14	B	2023	C
14	B	2024	A
14	B	2032	A
14	B	2034	U
14	B	2044	C
14	B	2048	G
14	B	2050	A
14	B	2058	A
14	B	2059	G

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Mol	Chain	Res	Type
14	B	2060	A
14	B	2063	C
14	B	2068	U
14	B	2070	C
14	B	2073	G
14	B	2079	G
14	B	2081	A
14	B	2082	C
14	B	2083	G
14	B	2086	A
14	B	2087	A
14	B	2088	G
14	B	2089	A
14	B	2090	C
14	B	2096	G
14	B	2102	U
14	B	2111	C
14	B	2114	G
14	B	2116	U
14	B	2119	U
14	B	2121	A
14	B	2123	A
14	B	2129	C
14	B	2131	C
14	B	2132	A
14	B	2133	G
14	B	2210	C
14	B	2214	G
14	B	2215	U
14	B	2218	G
14	B	2220	U
14	B	2225	A
14	B	2226	A
14	B	2230	G
14	B	2231	C
14	B	2232	A
14	B	2233	C
14	B	2237	U
14	B	2238	U
14	B	2240	U
14	B	2241	C
14	B	2242	G

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Mol	Chain	Res	Type
14	B	2246	U
14	B	2252	A
14	B	2253	C
14	B	2261	G
14	B	2265	G
14	B	2270	U
14	B	2278	G
14	B	2293	A
14	B	2296	A
14	B	2297	G
14	B	2307	G
14	B	2310	C
14	B	2312	C
14	B	2314	A
14	B	2315	A
14	B	2321	C
14	B	2330	G
14	B	2331	G
14	B	2333	U
14	B	2335	G
14	B	2337	A
14	B	2338	A
14	B	2339	U
14	B	2341	A
14	B	2346	U
14	B	2349	A
14	B	2352	G
14	B	2353	U
14	B	2354	A
14	B	2360	A
14	B	2362	A
14	B	2367	A
14	B	2370	U
14	B	2371	U
14	B	2374	C
14	B	2375	U
14	B	2377	C
14	B	2380	G
14	B	2381	A
14	B	2384	U
14	B	2385	A
14	B	2396	A

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Mol	Chain	Res	Type
14	B	2397	G
14	B	2398	G
14	B	2406	G
14	B	2409	G
14	B	2410	G
14	B	2411	A
14	B	2412	C
14	B	2414	U
14	B	2419	A
14	B	2429	U
14	B	2432	G
14	B	2433	C
14	B	2438	A
14	B	2440	G
14	B	2441	G
14	B	2452	A
14	B	2453	A
14	B	2456	G
14	B	2457	A
14	B	2458	U
14	B	2463	G
14	B	2467	C
14	B	2468	C
14	B	2470	C
14	B	2475	A
14	B	2490	C
14	B	2492	C
14	B	2497	G
14	B	2499	G
14	B	2502	C
14	B	2505	A
14	B	2521	G
14	B	2528	C
14	B	2529	G
14	B	2530	A
14	B	2531	U
14	B	2532	G
14	B	2533	U
14	B	2534	C
14	B	2545	A
14	B	2546	U
14	B	2547	C

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Mol	Chain	Res	Type
14	B	2554	C
14	B	2556	G
14	B	2557	U
14	B	2561	C
14	B	2562	G
14	B	2564	U
14	B	2567	C
14	B	2581	U
14	B	2583	C
14	B	2584	G
14	B	2591	A
14	B	2593	A
14	B	2594	G
14	B	2600	C
14	B	2610	G
14	B	2611	U
14	B	2613	C
14	B	2624	G
14	B	2631	U
14	B	2636	U
14	B	2640	U
14	B	2642	U
14	B	2656	A
14	B	2657	G
14	B	2661	A
14	B	2666	A
14	B	2673	C
14	B	2689	A
14	B	2690	G
14	B	2695	G
14	B	2712	G
14	B	2715	G
14	B	2716	U
14	B	2717	A
14	B	2741	G
14	B	2753	U
14	B	2760	A
14	B	2771	G
14	B	2775	A
14	B	2777	A
14	B	2784	A
14	B	2792	A

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Mol	Chain	Res	Type
14	B	2793	G
14	B	2796	C
14	B	2805	A
14	B	2807	G
14	B	2808	A
14	B	2809	G
14	B	2819	C
14	B	2821	U
14	B	2823	G
14	B	2824	G
14	B	2832	A
14	B	2841	A
14	B	2844	U
14	B	2845	G
14	B	2853	U
14	B	2854	A
14	B	2855	A
14	B	2881	C
14	B	2892	G
14	B	2906	G
14	B	2907	A
14	B	2913	G
14	B	2918	A
15	C	2	C
15	C	7	G
15	C	11	A
15	C	23	U
15	C	24	C
15	C	30	U
15	C	32	U
15	C	39	G
15	C	40	C
15	C	42	G
15	C	44	A
15	C	46	A
15	C	49	G
15	C	51	A
15	C	54	U
15	C	55	A
15	C	56	A
15	C	62	U
15	C	63	U

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Mol	Chain	Res	Type
15	C	64	A
15	C	71	A
15	C	77	G
15	C	83	U
15	C	84	U
15	C	87	G
15	C	88	U
15	C	94	U
15	C	106	U
15	C	107	U
15	C	108	G
15	C	114	C
42	D	8	U
42	D	10	G
42	D	14	A
42	D	16	U
42	D	19	G
42	D	20	U
42	D	22	G
42	D	23	A
42	D	28	G
42	D	29	G
42	D	33	U
42	D	38	A
42	D	41	C
42	D	44	G
42	D	46	G
42	D	47	U
42	D	48	C
42	D	49	C
42	D	50	U
42	D	52	G
42	D	56	C
42	D	58	A
42	D	59	U
42	D	60	U
42	D	61	C
42	D	62	C
42	D	70	G
42	D	74	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	52	A
1	A	279	C
1	A	336	C
1	A	467	U
1	A	480	G
1	A	908	C
1	A	935	G
1	A	969	U
1	A	970	U
1	A	1089	U
1	A	1200	G
1	A	1211	A
1	A	1354	C
1	A	1503	A
14	B	90	A
14	B	660	A
14	B	1503	U
14	B	1510	U
14	B	1940	A
14	B	2530	A
14	B	2533	U
14	B	2608	G
14	B	2783	U
15	C	55	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](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	193:C	O3'	203:G	P	30.87

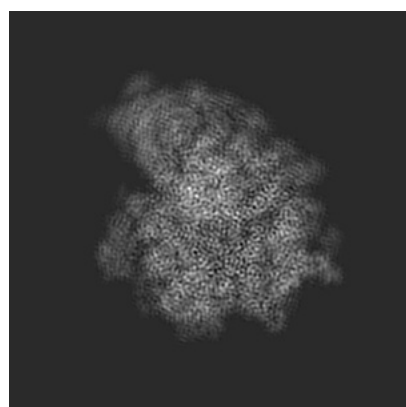
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8369. These allow visual inspection of the internal detail of the map and identification of artifacts.

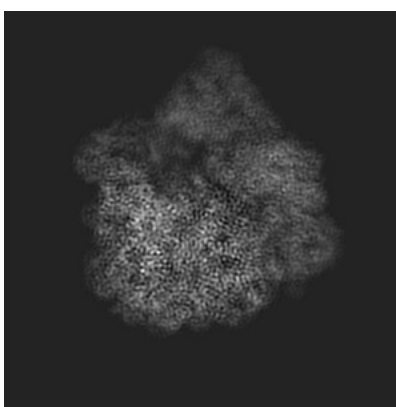
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

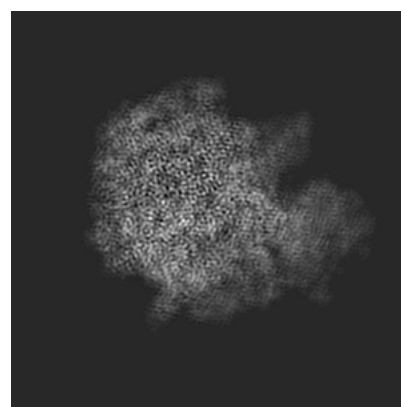
6.1.1 Primary map



X



Y

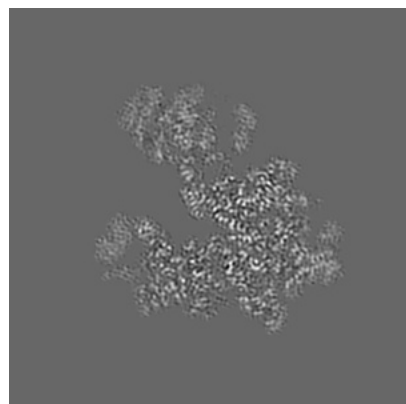


Z

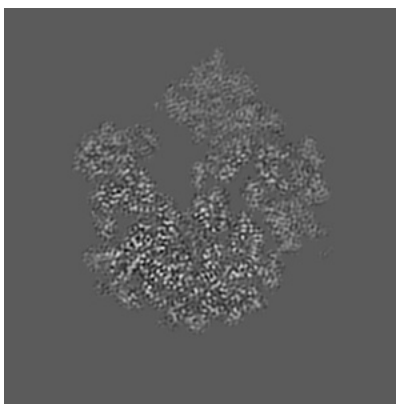
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

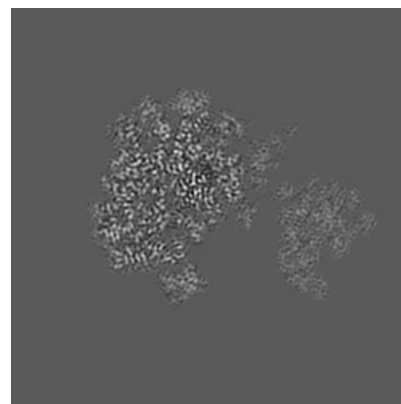
6.2.1 Primary map



X Index: 160



Y Index: 160

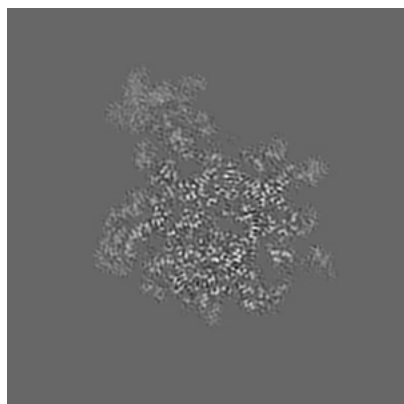


Z Index: 160

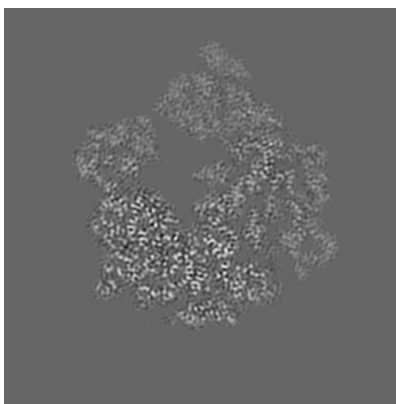
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

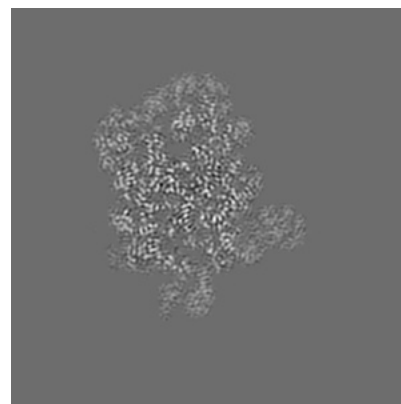
6.3.1 Primary map



X Index: 126



Y Index: 149

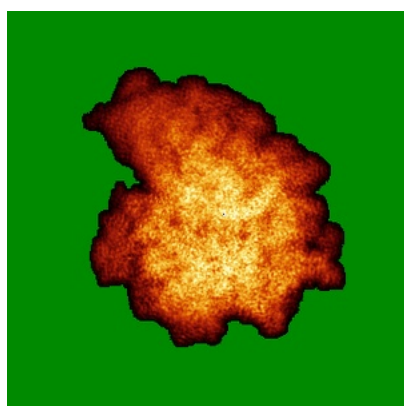


Z Index: 110

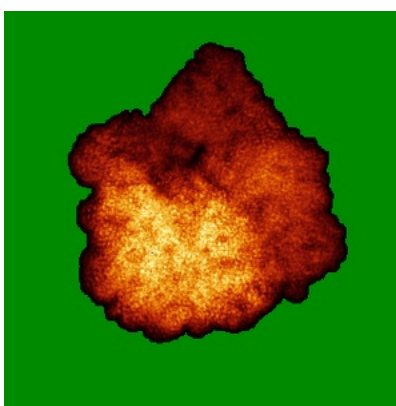
The images above show the largest variance slices of the map in three orthogonal directions.

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

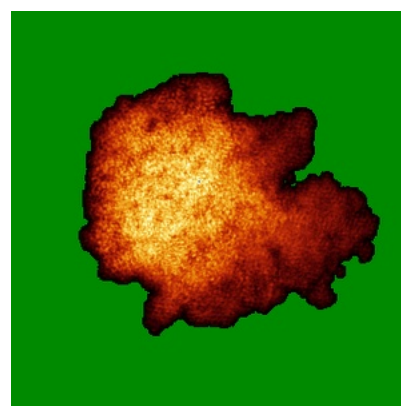
6.4.1 Primary map



X



Y

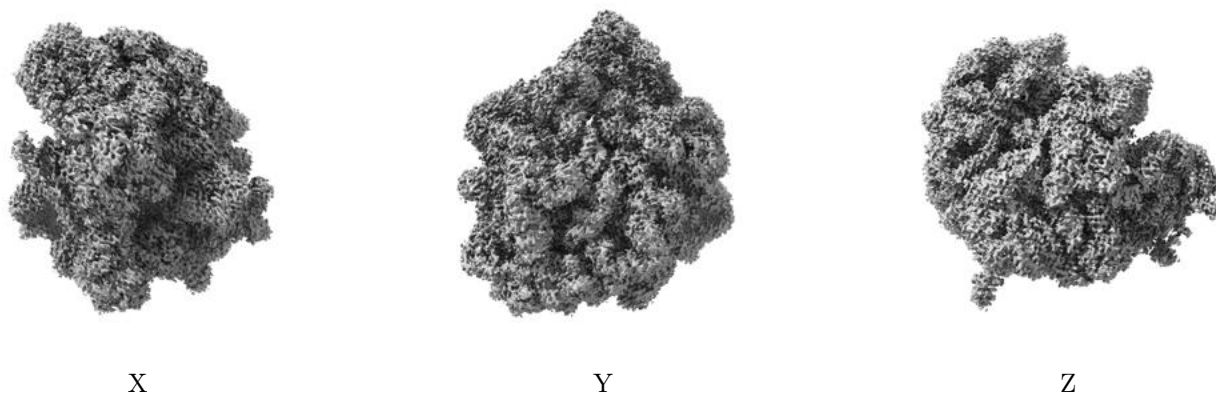


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

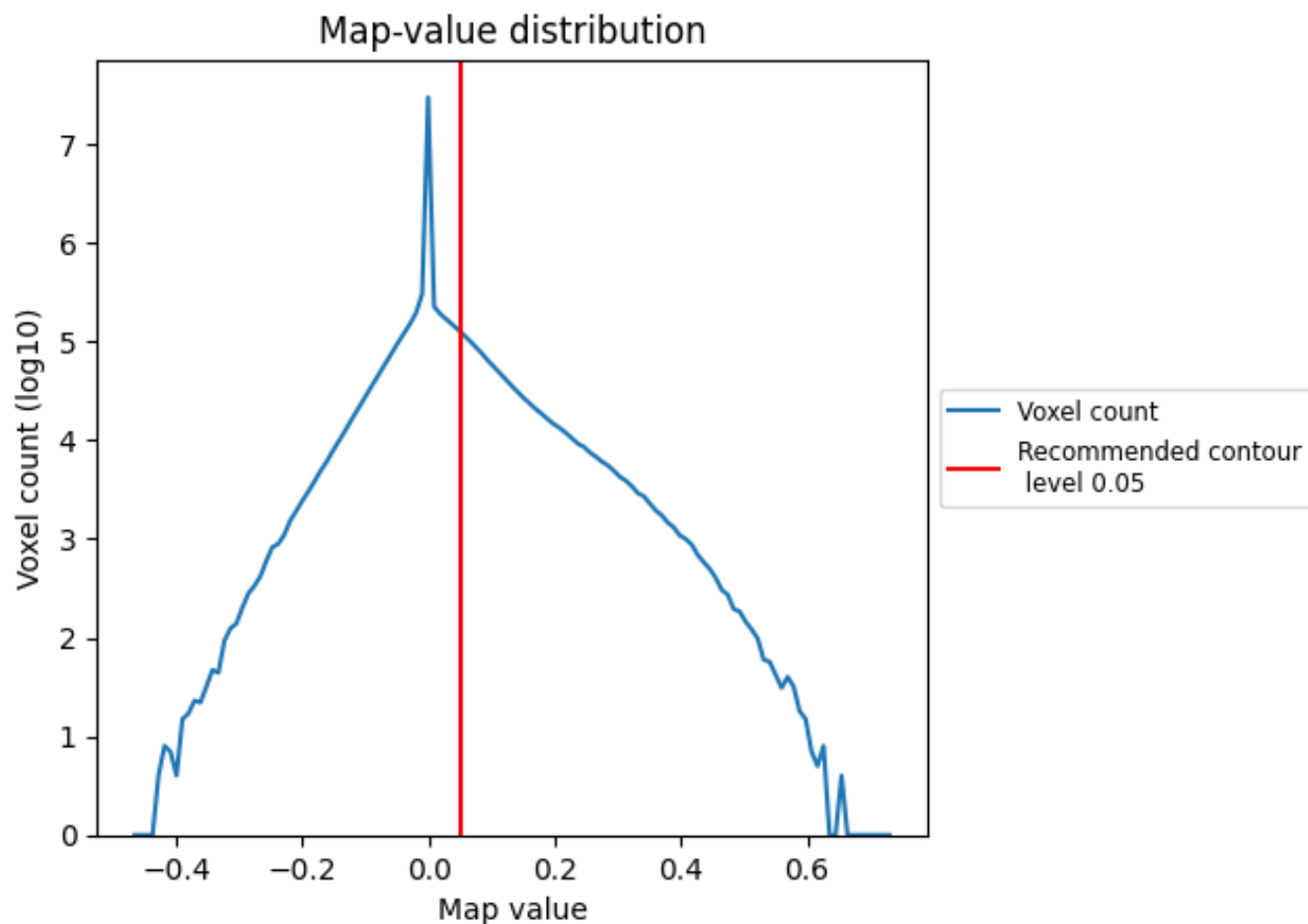
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

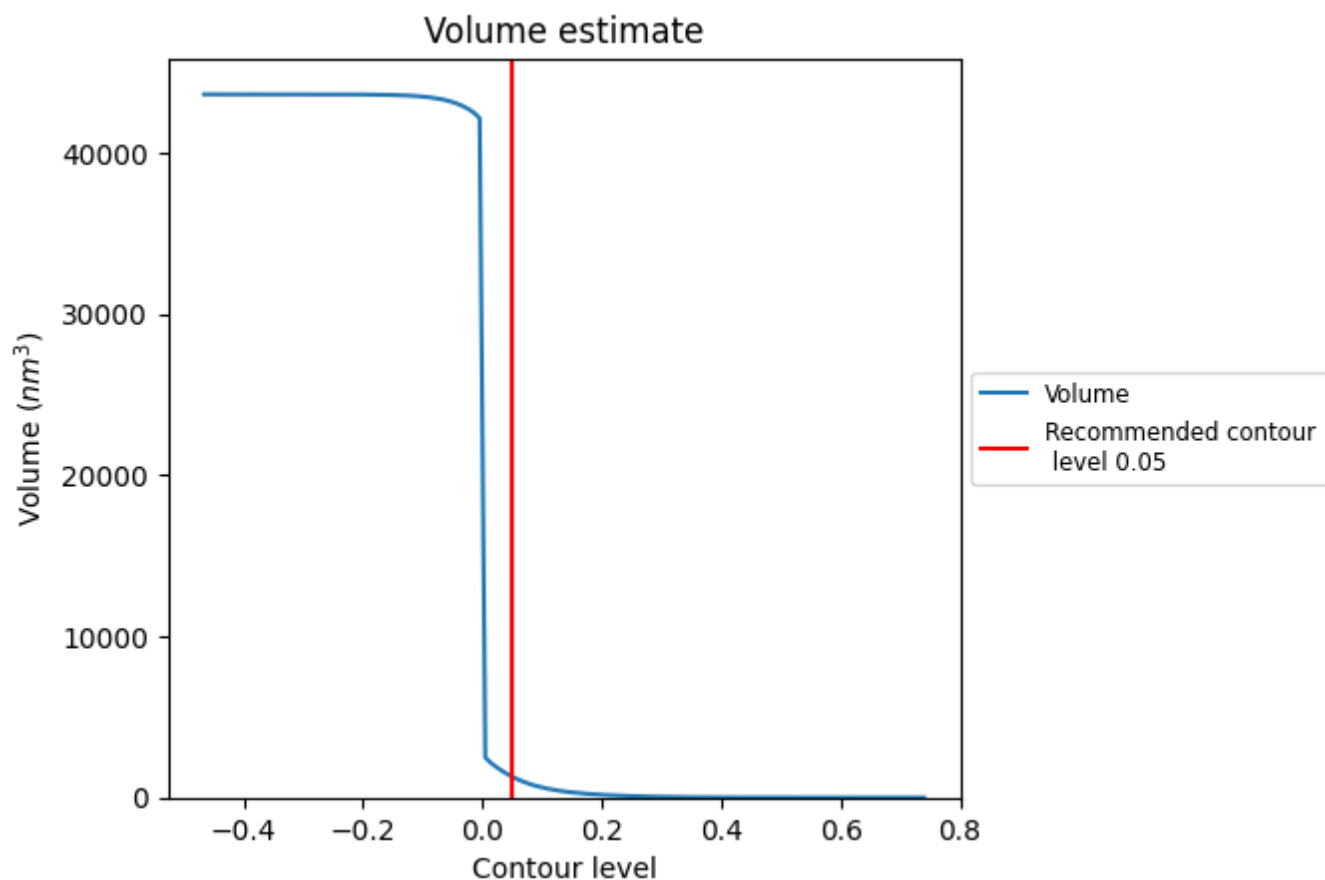
This section contains the results of statistical analysis of the map.

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.

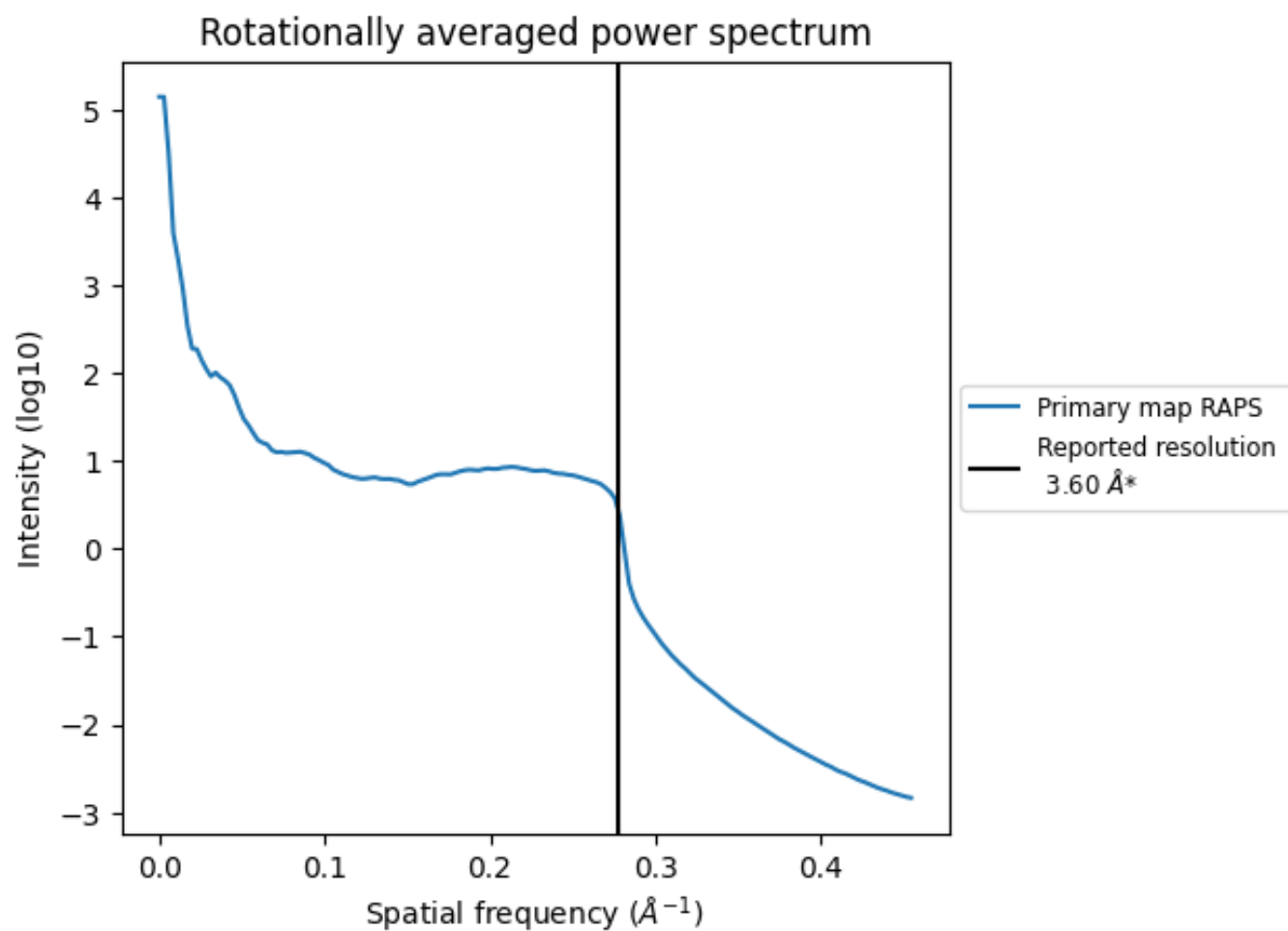
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm³; this corresponds to an approximate mass of 1173 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 0.278 Å⁻¹

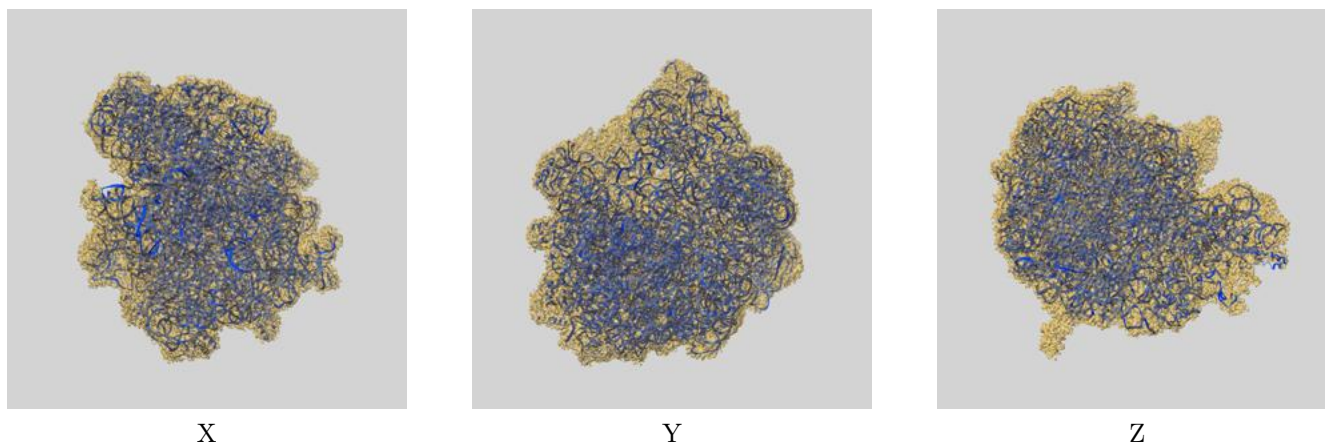
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

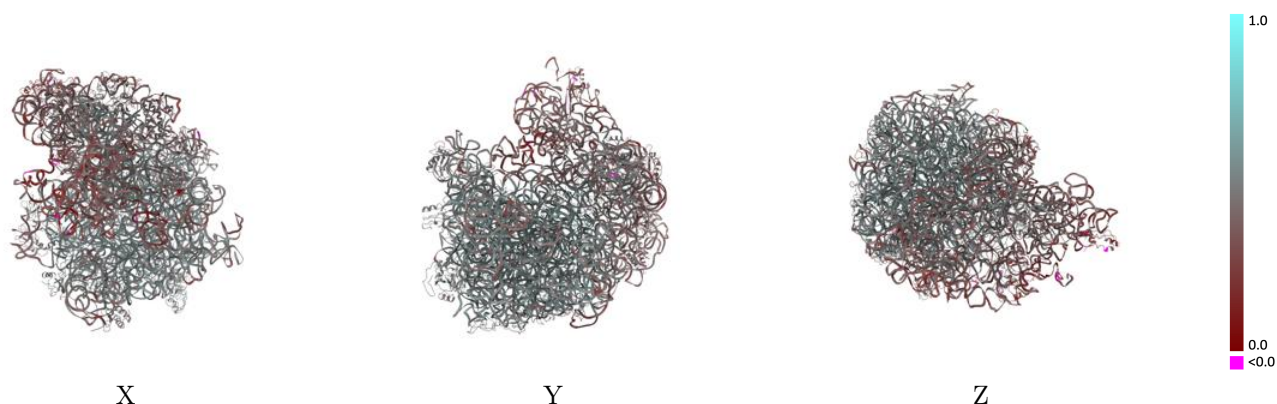
This section contains information regarding the fit between EMDB map EMD-8369 and PDB model 5T7V. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



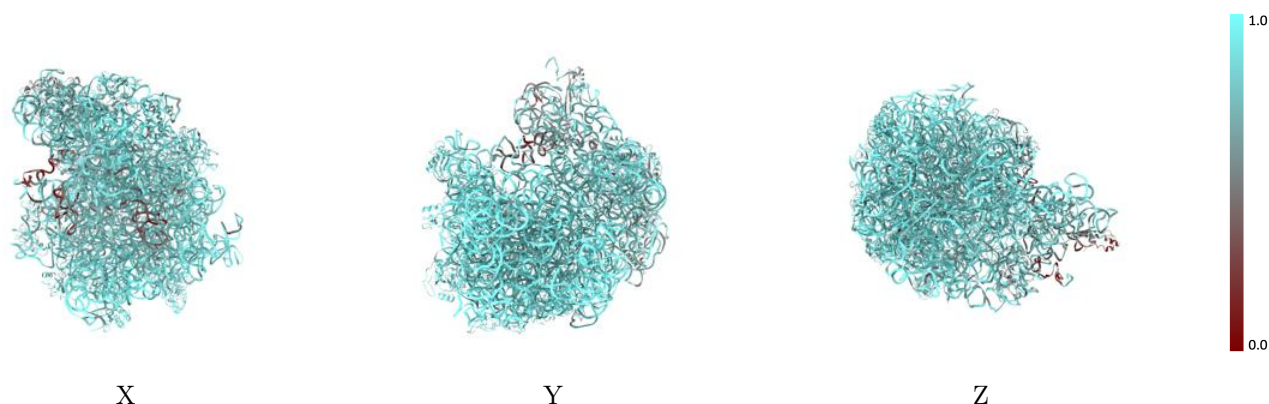
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



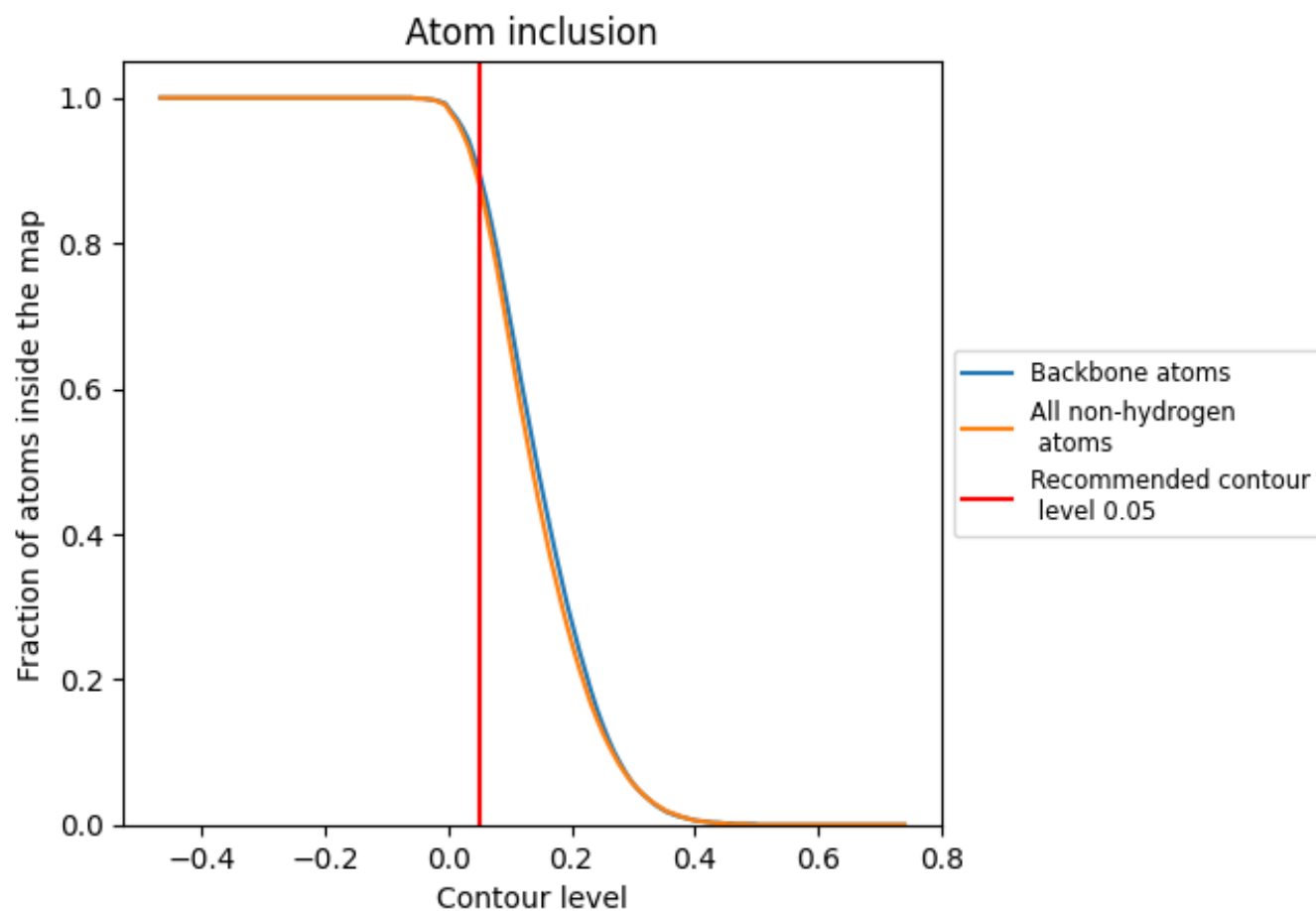
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.4620
A	 0.8280	 0.3890
B	 0.9520	 0.5050
C	 0.9310	 0.4460
D	 0.4760	 0.2820
L1	 0.8750	 0.5030
L2	 0.8990	 0.5290
L3	 0.9040	 0.5200
L4	 0.8940	 0.5000
L5	 0.8960	 0.5190
L6	 0.8850	 0.5020
L7	 0.8430	 0.4710
L8	 0.8350	 0.4670
L9	 0.9210	 0.5180
LA	 0.8880	 0.5120
LB	 0.8520	 0.4710
LC	 0.8860	 0.5010
LD	 0.8890	 0.5070
LE	 0.8750	 0.5170
LF	 0.8580	 0.4890
LG	 0.9310	 0.5550
LH	 0.9400	 0.5550
LI	 0.9000	 0.5220
LJ	 0.8700	 0.4980
LL	 0.8230	 0.4310
LM	 0.9030	 0.5200
LN	 0.8740	 0.5120
LO	 0.8920	 0.5050
LP	 0.9050	 0.5280
LQ	 0.8910	 0.5150
LR	 0.8420	 0.4420
S1	 0.4980	 0.2880
S2	 0.7070	 0.3820
S3	 0.7540	 0.4010
S6	 0.7910	 0.4220



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Chain	Atom inclusion	Q-score
S7	 0.6550	 0.3500
S8	 0.7110	 0.3770
S9	 0.7340	 0.3880
SA	 0.6870	 0.3610
SC	 0.5980	 0.3170
SD	 0.8050	 0.4330
SE	 0.7640	 0.3930
SF	 0.7840	 0.4070