



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 30, 2020 – 01:37 PM EST

PDB ID : 6V3D
EMDB ID: : EMD-21033
Title : Cryo-EM structure of the *Acinetobacter baumannii* Ribosome: 50S subunit
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2019-11-25
Resolution : 2.95 Å(reported)
Based on PDB ID : 5AFI

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

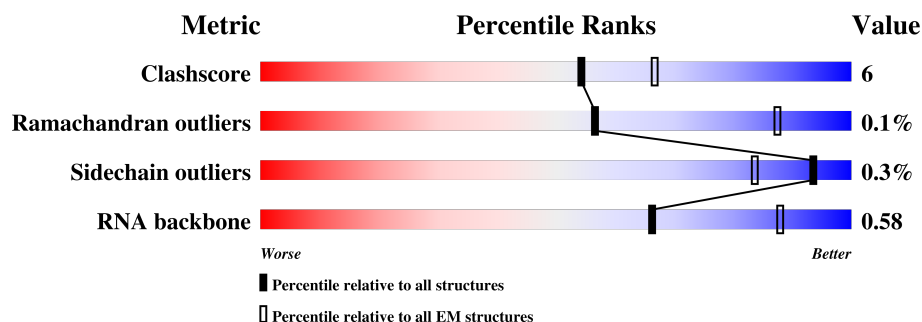
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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.















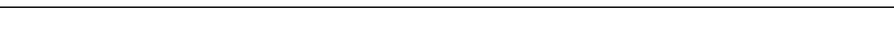

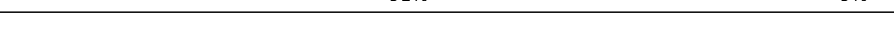

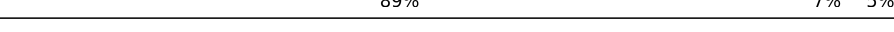




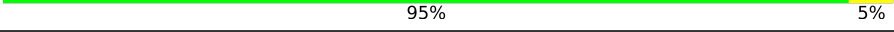
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	51	94% 6%
2	1	44	84% 16%
3	2	64	75% 20% . .
4	3	38	63% 34% .
5	AN1	2918	63% 32% 5% .
6	B	115	52% 39% 9%
7	C	274	86% 13% .
8	D	212	88% 11%

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Mol	Chain	Length	Quality of chain
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 89040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN1	2892	Total	C	N	O	P	0	0
			62023	27689	11345	20098	2891		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	270	Total	C	N	O	S	0	0
			2096	1291	434	363	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1419	893	265	257	4		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1381	877	247	249	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	146	Total	C	N	O	S	0	0
			1089	673	215	200	1		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	117	Total	C	N	O	0	0
			919	578	177	164		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	90	Total	C	N	O		0	0
			702	447	127	128			

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	100	Total	C	N	O		0	0
			749	465	139	145			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	80	Total	C	N	O	S	0	0
			598	370	115	111	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	62	Total	C	N	O	S	0	0
			498	308	96	93	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	58	Total	C	N	O	S	0	0
			463	286	88	85	4		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	3	1	Total	Zn	0
			1	1	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	AN1	105	Total	Mg	0
			105	105	
32	C	1	Total	Mg	0
			1	1	

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
33	AN1	1	Total	Na	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	1	1	Total	O	0
			1	1	
34	AN1	218	Total	O	0
			218	218	

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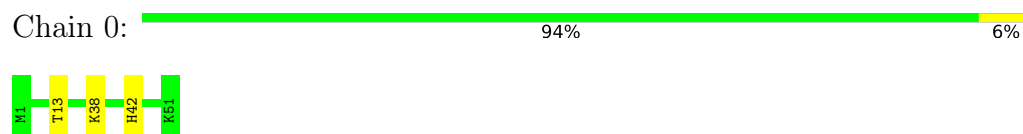
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Mol	Chain	Residues	Atoms		AltConf
34	B	3	Total 3	O 3	0
34	C	1	Total 1	O 1	0
34	D	1	Total 1	O 1	0
34	E	1	Total 1	O 1	0
34	K	1	Total 1	O 1	0
34	N	1	Total 1	O 1	0
34	R	1	Total 1	O 1	0
34	V	1	Total 1	O 1	0
34	W	1	Total 1	O 1	0
34	Z	1	Total 1	O 1	0

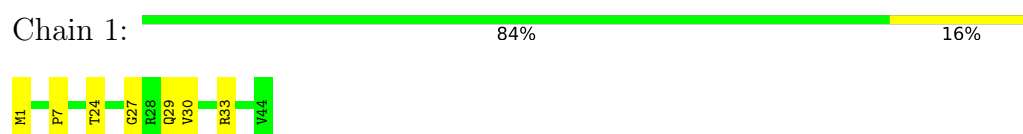
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

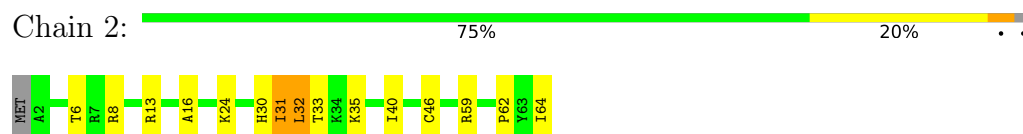
- Molecule 1: 50S ribosomal protein L33



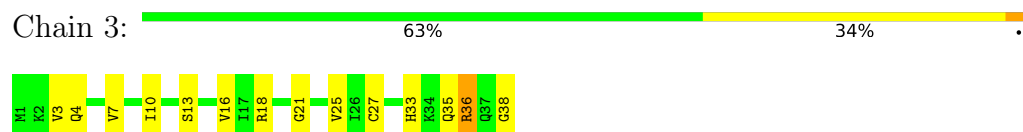
- Molecule 2: 50S ribosomal protein L34



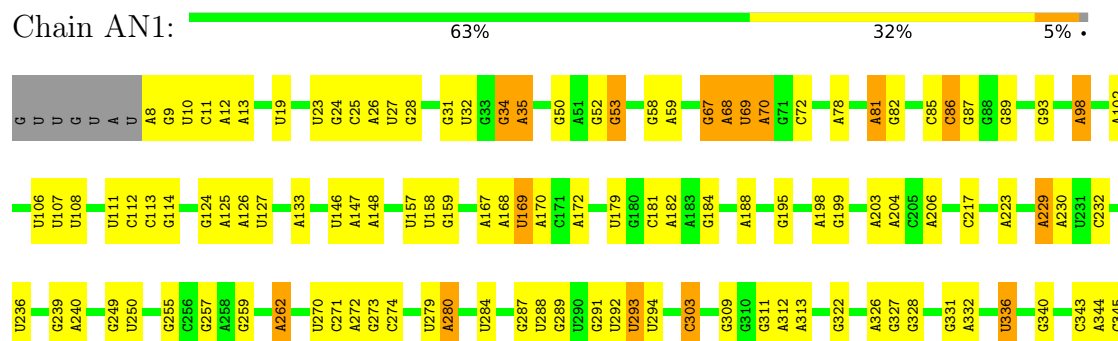
- Molecule 3: 50S ribosomal protein L35



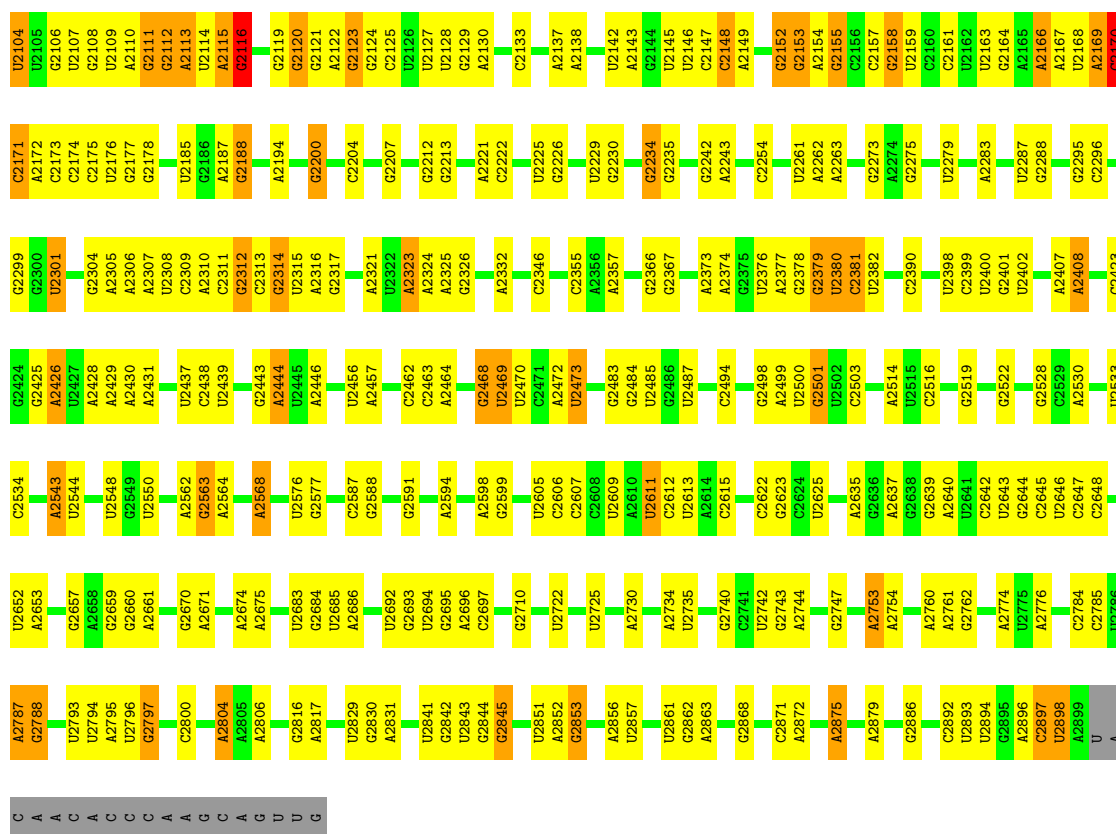
- Molecule 4: 50S ribosomal protein L36



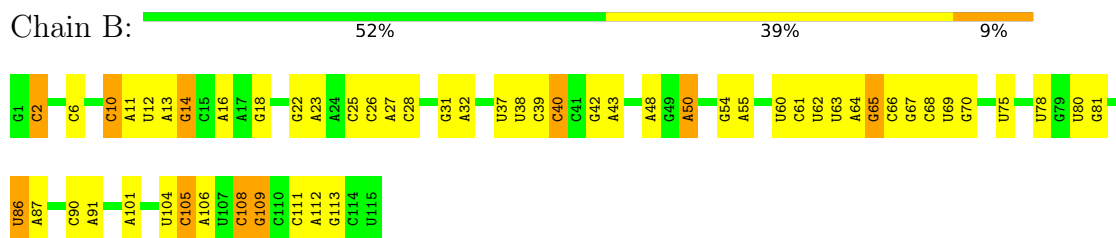
- Molecule 5: 23S ribosomal RNA



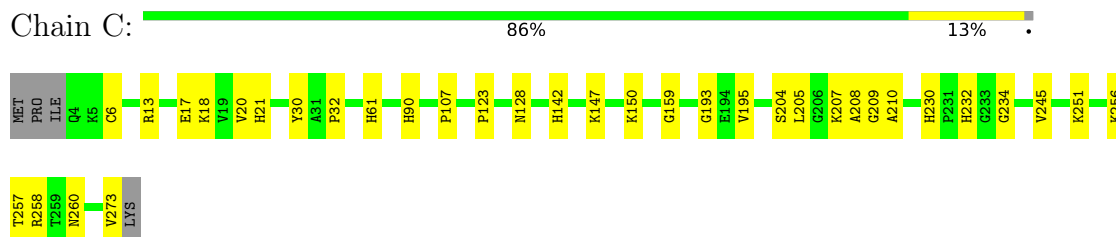


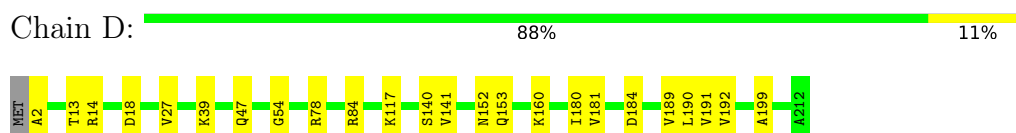
• Molecule 6: 5s ribosomal RNA




• Molecule 7: 50S ribosomal protein L2

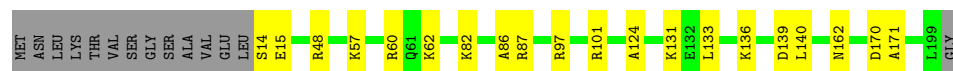


• Molecule 8: 50S ribosomal protein L3



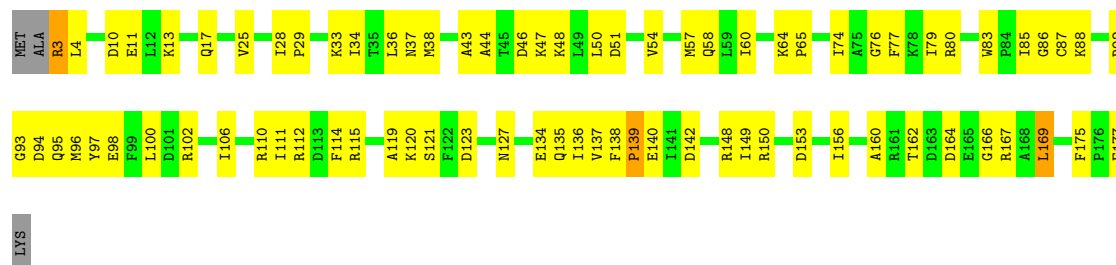
- Molecule 9: 50S ribosomal protein L4

Chain E:  83% 10% 7%



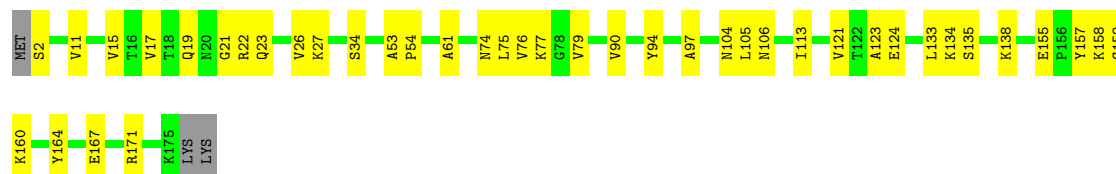
- Molecule 10: 50S ribosomal protein L5

Chain F: 54% 42% .



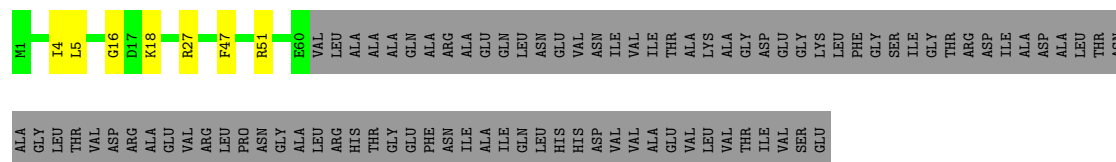
- Molecule 11: 50S ribosomal protein L6

Chain G: 75% 23%



- Molecule 12: 50S ribosomal protein L9

Chain H: 36% 5% 59%



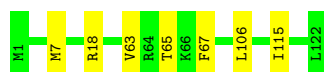
- Molecule 13: 50S ribosomal protein L13

Chain I: 88% 12%



- Molecule 14: 50S ribosomal protein L14

Chain J: 94% 6%



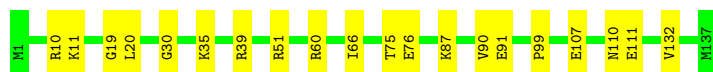
- Molecule 15: 50S ribosomal protein L15

Chain K: 84% 16%



- Molecule 16: 50S ribosomal protein L16

Chain L: 85% 15%



- Molecule 17: 50S ribosomal protein L17

Chain M: 93% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 89% 9%



- Molecule 19: 50S ribosomal protein L19

Chain O: 80% 16%



- Molecule 20: 50S ribosomal protein L20

Chain P: 93% 5%



- Molecule 21: 50S ribosomal protein L21

Chain Q: 85% 15%



- Molecule 22: 50S ribosomal protein L22

Chain R:  91% 9%




- Molecule 23: 50S ribosomal protein L23

Chain S:  72% 13% 15%



- Molecule 24: 50S ribosomal protein L24

Chain T:  89% 7% 5%




- Molecule 25: 50S ribosomal protein L25

Chain U:  90% 9% .




- Molecule 26: 50S ribosomal protein L27

Chain V:  85% 9% 6%




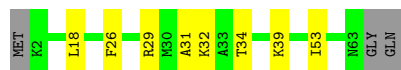
- Molecule 27: 50S ribosomal protein L28

Chain W:  87% 12% .



- Molecule 28: 50S ribosomal protein L29

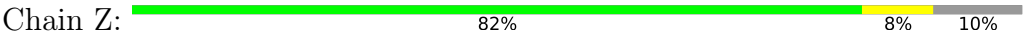
Chain X:  83% 12% 5%



- Molecule 29: 50S ribosomal protein L30



- Molecule 30: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MU, ZN, OMG, NA, MG, 2MA, 6MZ, 2MG, OMU, 7MG, PSU

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 >2	RMSZ	# Z >2
1	0	0.24	0/434	0.43	0/573
10	F	0.26	0/1401	0.52	0/1877
11	G	0.24	0/1337	0.43	0/1807
12	H	0.25	0/461	0.49	0/616
13	I	0.24	0/1151	0.40	0/1551
14	J	0.24	0/956	0.44	0/1286
15	K	0.24	0/1097	0.43	0/1461
16	L	0.24	0/1104	0.44	0/1475
17	M	0.23	0/956	0.40	0/1282
18	N	0.23	0/865	0.42	0/1156
19	O	0.24	0/931	0.42	0/1249
2	1	0.23	0/367	0.39	0/481
20	P	0.24	0/947	0.34	0/1262
21	Q	0.23	0/818	0.45	0/1094
22	R	0.23	0/831	0.40	0/1113
23	S	0.25	0/708	0.43	0/947
24	T	0.24	0/753	0.47	0/1010
25	U	0.24	0/770	0.40	0/1036
26	V	0.25	0/606	0.44	0/810
27	W	0.22	0/642	0.40	0/856
28	X	0.23	0/499	0.38	0/662
29	Y	0.22	0/468	0.41	0/624
3	2	0.23	0/515	0.44	0/678
30	Z	0.22	0/462	0.41	0/615
4	3	0.22	0/296	0.45	0/389
5	AN1	0.19	0/69101	0.76	20/107780 (0.0%)
6	B	0.17	0/2739	0.77	2/4266 (0.0%)
7	C	0.24	0/2136	0.43	0/2869
8	D	0.24	0/1590	0.45	0/2142
9	E	0.24	0/1440	0.40	0/1944
All	All	0.20	0/96381	0.70	22/144911 (0.0%)

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	3	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	503	U	C2-N1-C1'	7.29	126.44	117.70
5	AN1	1308	U	C2-N1-C1'	6.88	125.95	117.70
5	AN1	503	U	N1-C2-O2	6.69	127.48	122.80
5	AN1	788	U	C2-N1-C1'	6.41	125.39	117.70
5	AN1	2170	C	N1-C2-O2	6.38	122.73	118.90
5	AN1	1308	U	N1-C2-O2	6.21	127.15	122.80
5	AN1	503	U	N3-C2-O2	-6.05	117.96	122.20
5	AN1	2116	G	N1-C6-O6	-5.86	116.38	119.90
5	AN1	1308	U	N3-C2-O2	-5.75	118.17	122.20
5	AN1	2170	C	N3-C2-O2	-5.70	117.91	121.90
5	AN1	788	U	N1-C2-O2	5.62	126.73	122.80
5	AN1	715	C	C2-N1-C1'	5.53	124.88	118.80
5	AN1	912	C	C2-N1-C1'	5.52	124.87	118.80
5	AN1	1889	C	N3-C2-O2	-5.44	118.09	121.90
6	B	10	C	N1-C2-O2	5.40	122.14	118.90
5	AN1	715	C	N1-C2-O2	5.38	122.13	118.90
5	AN1	2175	C	C2-N1-C1'	5.38	124.72	118.80
5	AN1	368	C	OP2-P-O3'	5.21	116.67	105.20
5	AN1	2313	C	N3-C2-O2	-5.17	118.28	121.90
5	AN1	2473	U	C2-N1-C1'	5.16	123.89	117.70
5	AN1	788	U	N3-C2-O2	-5.12	118.61	122.20
6	B	10	C	C2-N1-C1'	5.10	124.41	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	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	0	427	0	462	3	0
2	1	363	0	401	5	0
3	2	509	0	566	12	0
4	3	295	0	327	7	0
5	AN1	62023	0	31192	550	0
6	B	2450	0	1241	44	0
7	C	2096	0	2157	28	0
8	D	1572	0	1610	18	0
9	E	1419	0	1464	15	0
10	F	1381	0	1433	59	0
11	G	1318	0	1373	25	0
12	H	458	0	480	4	0
13	I	1125	0	1148	11	0
14	J	946	0	1007	4	0
15	K	1089	0	1159	15	0
16	L	1087	0	1162	9	0
17	M	942	0	987	3	0
18	N	857	0	899	7	0
19	O	919	0	973	10	0
20	P	934	0	997	5	0
21	Q	807	0	842	10	0
22	R	826	0	894	7	0
23	S	702	0	756	10	0
24	T	749	0	797	4	0
25	U	760	0	783	6	0
26	V	598	0	600	6	0
27	W	632	0	667	7	0
28	X	498	0	537	7	0
29	Y	463	0	488	2	0
30	Z	456	0	448	5	0
31	3	1	0	0	0	0
32	AN1	105	0	0	0	0
32	C	1	0	0	0	0
33	AN1	1	0	0	0	0
34	1	1	0	0	0	0
34	AN1	218	0	0	4	0
34	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	E	1	0	0	0	0
34	K	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	V	1	0	0	0	0
34	W	1	0	0	1	0
34	Z	1	0	0	0	0
All	All	89040	0	57850	819	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 6.

All (819) 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)
5:AN1:1462:G:H1	5:AN1:1520:A:N6	1.49	1.10
6:B:70:G:N2	6:B:101:A:H62	1.59	1.00
6:B:70:G:H21	6:B:101:A:N6	1.64	0.96
5:AN1:2096:G:H1	5:AN1:2185:U:H3	0.91	0.89
6:B:2:C:O2	6:B:113:G:N2	2.06	0.88
29:Y:19:HIS:HD1	29:Y:52:TYR:HH	1.21	0.88
6:B:70:G:H21	6:B:101:A:H62	0.88	0.82
5:AN1:1846:G:N2	5:AN1:1888:C:O2	2.12	0.81
5:AN1:1595:A:H5''	5:AN1:1596:A:H5'	1.63	0.81
5:AN1:873:G:N2	5:AN1:900:C:O2	2.15	0.79
5:AN1:52:G:H5''	5:AN1:53:G:H5'	1.65	0.79
25:U:34:ILE:O	25:U:41:PRO:HA	1.83	0.78
6:B:2:C:N3	6:B:113:G:N1	2.31	0.78
5:AN1:293:U:H3	5:AN1:351:G:H1	1.32	0.78
10:F:106:ILE:HD12	10:F:136:ILE:HD11	1.66	0.77
6:B:18:G:N1	6:B:61:C:N3	2.30	0.77
5:AN1:873:G:N1	5:AN1:900:C:N3	2.33	0.76
5:AN1:1862:A:H61	5:AN1:1871:G:H2'	1.49	0.76
5:AN1:1036:A:H61	5:AN1:1113:G:H1	1.33	0.74
5:AN1:862:G:H21	5:AN1:864:A:H61	1.37	0.72
10:F:13:LYS:HD3	10:F:28:ILE:HG21	1.71	0.72
21:Q:1:MET:HA	21:Q:42:VAL:O	1.91	0.71
5:AN1:69:U:H2'	5:AN1:70:A:H8	1.56	0.71
5:AN1:2112:G:O6	5:AN1:2166:A:N6	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:198:A:H3'	5:AN1:199:G:H21	1.56	0.70
6:B:18:G:N2	6:B:61:C:O2	2.19	0.70
11:G:94:TYR:HA	11:G:106:ASN:O	1.91	0.70
10:F:10:ASP:OD1	10:F:11:GLU:N	2.26	0.69
5:AN1:2311:C:HO2'	5:AN1:2312:G:H8	1.41	0.69
5:AN1:2159:U:OP1	5:AN1:2161:C:N4	2.25	0.69
5:AN1:843:G:O2'	5:AN1:845:A:N7	2.25	0.69
5:AN1:1775:U:OP2	5:AN1:1780:A:N6	2.25	0.69
5:AN1:711:G:H8	5:AN1:716:A:H62	1.39	0.69
8:D:39:LYS:O	8:D:47:GLN:HA	1.94	0.68
5:AN1:2743:G:H21	5:AN1:2753:A:H62	1.41	0.68
5:AN1:184:G:N2	5:AN1:184:G:OP2	2.22	0.68
5:AN1:1846:G:N1	5:AN1:1888:C:N3	2.32	0.68
5:AN1:846:U:H2'	5:AN1:847:A:H8	1.59	0.68
5:AN1:829:G:O2'	15:K:40:GLN:NE2	2.26	0.68
5:AN1:2111:G:H4'	5:AN1:2113:A:H62	1.59	0.67
5:AN1:2522:G:H1	5:AN1:2533:U:H3	1.41	0.67
5:AN1:2804:A:O2'	5:AN1:2886:G:O6	2.12	0.67
5:AN1:879:G:O6	5:AN1:893:U:O2	2.13	0.66
5:AN1:1528:G:O2'	5:AN1:1536:A:N1	2.28	0.66
5:AN1:1865:G:O2'	5:AN1:1868:A:N6	2.29	0.66
6:B:18:G:O6	6:B:61:C:N4	2.28	0.66
4:3:4:GLN:NE2	4:3:35:GLN:OE1	2.29	0.66
5:AN1:1413:G:N2	5:AN1:1577:A:OP2	2.29	0.66
5:AN1:862:G:N2	5:AN1:864:A:H61	1.94	0.65
5:AN1:2130:A:H62	5:AN1:2153:G:H4'	1.62	0.65
5:AN1:474:C:O2	5:AN1:478:A:N6	2.29	0.65
5:AN1:2787:A:HO2'	5:AN1:2788:G:H8	1.42	0.65
5:AN1:2332:A:H61	26:V:43:THR:HG21	1.61	0.65
5:AN1:499:G:N1	5:AN1:502:A:OP2	2.28	0.65
3:2:8:ARG:NH1	5:AN1:250:U:OP2	2.31	0.65
5:AN1:1749:G:N2	5:AN1:1752:G:OP2	2.29	0.65
5:AN1:1041:A:O2'	5:AN1:1108:A:N6	2.31	0.64
5:AN1:862:G:H21	5:AN1:864:A:N6	1.95	0.64
5:AN1:2111:G:O2'	5:AN1:2113:A:N7	2.28	0.64
5:AN1:878:G:H2'	5:AN1:879:G:H8	1.62	0.64
5:AN1:1052:G:H1'	5:AN1:1082:A:H2	1.63	0.64
5:AN1:875:U:O2	5:AN1:898:A:N7	2.31	0.64
5:AN1:877:G:H2'	5:AN1:878:G:H8	1.63	0.64
5:AN1:973:G:HO2'	5:AN1:1153:A:HO2'	1.45	0.63
5:AN1:2309:C:H5''	10:F:88:LYS:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:162:THR:HG22	10:F:164:ASP:H	1.63	0.63
5:AN1:879:G:H2'	5:AN1:880:G:H8	1.63	0.63
5:AN1:2077:C:H2'	5:AN1:2078:A:H8	1.63	0.63
5:AN1:1258:U:O2	30:Z:4:GLN:NE2	2.32	0.63
2:1:7:PRO:HB2	5:AN1:1304:G:H4'	1.80	0.63
4:3:10:ILE:HD12	4:3:33:HIS:HD2	1.63	0.63
5:AN1:718:U:HO2'	5:AN1:719:A:H8	1.45	0.62
10:F:120:LYS:HG3	10:F:121:SER:H	1.63	0.62
5:AN1:2591:G:N2	5:AN1:2594:A:OP2	2.25	0.62
9:E:97:ARG:HD3	9:E:101:ARG:HH21	1.64	0.62
5:AN1:364:A:OP2	5:AN1:424:G:O2'	2.18	0.61
3:2:30:HIS:O	3:2:32:LEU:N	2.33	0.61
5:AN1:1462:G:H1	5:AN1:1520:A:H61	0.72	0.61
11:G:21:GLY:O	11:G:22:ARG:NH2	2.34	0.61
9:E:14:SER:OG	9:E:15:GLU:OE1	2.19	0.61
5:AN1:2879:A:OP2	30:Z:49:ARG:NH1	2.34	0.61
11:G:23:GLN:NE2	11:G:34:SER:OG	2.31	0.61
6:B:22:G:O6	6:B:54:G:O2'	2.19	0.61
5:AN1:877:G:H2'	5:AN1:878:G:C8	2.36	0.60
5:AN1:462:G:N2	5:AN1:465:A:OP2	2.26	0.60
3:2:32:LEU:HD23	3:2:35:LYS:HD2	1.83	0.60
5:AN1:93:G:HO2'	5:AN1:111:U:HO2'	1.45	0.60
7:C:6:CYS:SG	7:C:18:LYS:NZ	2.75	0.60
6:B:75:U:OP1	25:U:25:ARG:NH1	2.34	0.60
5:AN1:1524:A:H62	5:AN1:1539:G:H21	1.50	0.59
5:AN1:1533:U:N3	5:AN1:1534:G:N3	2.47	0.59
6:B:31:G:N1	6:B:48:A:C6	2.71	0.59
5:AN1:2615:C:OP1	8:D:160:LYS:NZ	2.31	0.59
10:F:74:ILE:HG22	10:F:76:GLY:H	1.67	0.59
5:AN1:2123:G:H2'	5:AN1:2124:G:C8	2.38	0.59
5:AN1:2225:U:H2'	5:AN1:2226:G:H8	1.67	0.59
5:AN1:1029:A:O2'	5:AN1:1030:U:O4'	2.13	0.59
23:S:14:VAL:HG12	23:S:32:LYS:HG3	1.85	0.59
5:AN1:67:G:C2	5:AN1:68:A:N6	2.71	0.59
5:AN1:31:G:O2'	22:R:78:GLU:O	2.21	0.59
2:1:30:VAL:HG22	2:1:33:ARG:HH11	1.68	0.58
26:V:37:ILE:HG22	26:V:38:VAL:HG23	1.85	0.58
5:AN1:2072:U:OP2	5:AN1:2234:G:N2	2.33	0.58
5:AN1:1717:G:N2	5:AN1:1734:G:O2'	2.36	0.58
5:AN1:2390:C:H42	5:AN1:2428:A:H61	1.51	0.58
22:R:11:ALA:H	22:R:100:THR:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2747:G:N2	5:AN1:2747:G:OP1	2.33	0.58
5:AN1:1844:A:H4'	5:AN1:1845:G:H8	1.69	0.58
8:D:54:GLY:HA3	8:D:78:ARG:HG2	1.84	0.58
5:AN1:167:A:N3	5:AN1:2204:C:O2'	2.35	0.58
5:AN1:582:C:N4	5:AN1:583:G:O6	2.37	0.58
7:C:20:VAL:HG13	7:C:21:HIS:H	1.67	0.58
5:AN1:1010:C:H2'	5:AN1:1011:A:H8	1.68	0.58
5:AN1:848:C:O2'	29:Y:22:CYS:SG	2.62	0.58
5:AN1:1587:U:H2'	5:AN1:1588:A:H8	1.69	0.58
5:AN1:2123:G:N2	5:AN1:2158:G:O6	2.37	0.58
5:AN1:70:A:H61	5:AN1:98:A:H61	1.49	0.57
5:AN1:322:G:N3	9:E:162:ASN:ND2	2.52	0.57
5:AN1:510:U:H4'	5:AN1:1230:G:H4'	1.86	0.57
10:F:17:GLN:HE22	10:F:25:VAL:HA	1.68	0.57
24:T:12:VAL:HG22	24:T:68:VAL:HG12	1.86	0.57
5:AN1:527:A:H5'	13:I:113:PRO:HG3	1.86	0.57
5:AN1:294:U:H3	5:AN1:350:G:H22	1.52	0.57
7:C:258:ARG:NH2	7:C:260:ASN:O	2.38	0.57
8:D:2:ALA:N	8:D:84:ARG:O	2.38	0.57
5:AN1:2315:U:H2'	5:AN1:2317:G:H1	1.70	0.57
10:F:37:ASN:OD1	10:F:153:ASP:HB3	2.04	0.57
6:B:12:U:OP2	6:B:68:C:O2'	2.22	0.57
25:U:84:HIS:HD2	25:U:87:LYS:H	1.52	0.57
5:AN1:2104:U:O2	5:AN1:2177:G:N2	2.36	0.56
5:AN1:280:A:H2	5:AN1:364:A:H62	1.52	0.56
5:AN1:553:G:HO2'	5:AN1:554:A:H8	1.52	0.56
5:AN1:86:C:H2'	5:AN1:87:G:H8	1.69	0.56
10:F:58:GLN:HB2	10:F:65:PRO:HD3	1.87	0.56
13:I:23:LYS:HG2	13:I:142:ILE:HD11	1.85	0.56
5:AN1:195:G:H5'	27:W:14:VAL:HG11	1.86	0.56
5:AN1:168:A:H3'	5:AN1:169:U:H5''	1.87	0.56
5:AN1:1713:U:H3	5:AN1:1739:G:H1	1.54	0.56
5:AN1:1923:A:H2'	5:AN1:1924:A:C8	2.41	0.56
6:B:111:C:H2'	6:B:112:A:H8	1.71	0.56
11:G:105:LEU:HB2	11:G:113:ILE:HG23	1.88	0.56
6:B:108:C:H2'	6:B:109:G:H8	1.70	0.56
10:F:97:TYR:O	10:F:100:LEU:HG	2.06	0.56
10:F:80:ARG:H	10:F:83:TRP:HD1	1.54	0.56
5:AN1:1108:A:H8	5:AN1:1109:G:H4'	1.70	0.56
18:N:63:THR:OG1	18:N:66:ASN:ND2	2.39	0.56
22:R:72:SER:OG	22:R:106:LYS:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:26:SER:HB3	24:T:33:LYS:HB2	1.87	0.56
5:AN1:2287:U:H2'	5:AN1:2288:G:C8	2.41	0.56
9:E:86:ALA:O	9:E:87:ARG:NH1	2.39	0.55
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.87	0.55
3:2:30:HIS:ND1	3:2:31:ILE:HG13	2.22	0.55
5:AN1:2896:A:H2'	5:AN1:2897:C:C6	2.42	0.55
5:AN1:878:G:H2'	5:AN1:879:G:C8	2.40	0.55
6:B:90:C:H2'	6:B:91:A:H8	1.71	0.55
11:G:17:VAL:HG12	11:G:26:VAL:HG22	1.89	0.55
11:G:74:ASN:HA	11:G:77:LYS:HG2	1.88	0.55
2:1:24:THR:HG23	2:1:27:GLY:H	1.71	0.55
5:AN1:1310:C:O2'	5:AN1:1387:A:N3	2.32	0.55
5:AN1:1870:C:H3'	5:AN1:1871:G:H4'	1.87	0.55
5:AN1:844:A:N6	5:AN1:929:C:O2'	2.40	0.55
23:S:53:GLU:HG2	23:S:87:LYS:HD3	1.89	0.55
3:2:31:ILE:O	3:2:33:THR:N	2.40	0.55
5:AN1:1111:C:H2'	5:AN1:1112:G:H8	1.70	0.55
5:AN1:1523:A:N7	5:AN1:1539:G:N2	2.55	0.55
5:AN1:2483:G:H2'	5:AN1:2484:G:H8	1.72	0.55
5:AN1:2576:PSU:OP1	8:D:140:SER:OG	2.24	0.55
5:AN1:673:A:OP1	9:E:57:LYS:NZ	2.40	0.55
5:AN1:1016:U:OP1	5:AN1:1032:U:O2'	2.22	0.55
5:AN1:2130:A:OP2	5:AN1:2152:G:N1	2.40	0.55
8:D:27:VAL:HG22	8:D:191:VAL:HG12	1.87	0.55
3:2:6:THR:HG22	3:2:62:PRO:HD2	1.89	0.54
5:AN1:2324:A:H2'	5:AN1:2325:A:C8	2.42	0.54
5:AN1:2734:A:N1	5:AN1:2762:G:O6	2.40	0.54
14:J:65:THR:HG22	14:J:67:PHE:H	1.73	0.54
15:K:134:LYS:HE3	15:K:144:VAL:HG11	1.89	0.54
5:AN1:628:G:N2	5:AN1:631:A:OP2	2.27	0.54
5:AN1:520:U:H2'	5:AN1:521:G:H8	1.72	0.54
5:AN1:805:U:OP2	15:K:43:ARG:NH2	2.38	0.54
5:AN1:1919:U:H2'	5:AN1:1920:C:C6	2.42	0.54
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.90	0.54
30:Z:25:ASN:OD1	30:Z:38:ARG:NH2	2.41	0.54
5:AN1:1500:A:O2'	5:AN1:1502:U:O4'	2.24	0.54
5:AN1:2587:C:H2'	5:AN1:2588:G:H8	1.72	0.54
10:F:17:GLN:NE2	10:F:25:VAL:HA	2.23	0.54
28:X:32:LYS:HB2	28:X:39:LYS:HD2	1.90	0.54
5:AN1:1483:U:O2	5:AN1:1496:G:N2	2.32	0.54
5:AN1:2577:G:OP2	5:AN1:2577:G:N2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:91:ARG:HH21	19:O:115:GLU:HB2	1.73	0.54
11:G:155:GLU:HG2	11:G:159:GLY:H	1.73	0.53
14:J:106:LEU:HB2	14:J:115:ILE:HD11	1.89	0.53
5:AN1:1589:C:H2'	5:AN1:1590:A:H8	1.73	0.53
5:AN1:579:C:H2'	5:AN1:580:A:H8	1.73	0.53
5:AN1:876:A:H3'	5:AN1:877:G:H8	1.72	0.53
10:F:112:ARG:HD2	10:F:134:GLU:HG3	1.89	0.53
5:AN1:372:U:H2'	5:AN1:373:A:H8	1.73	0.53
10:F:135:GLN:HE21	10:F:149:ILE:HG12	1.73	0.53
10:F:138:PHE:O	10:F:140:GLU:N	2.42	0.53
10:F:95:GLN:O	10:F:98:GLU:HG3	2.09	0.53
4:3:7:VAL:HG13	4:3:38:GLY:HA3	1.89	0.53
5:AN1:1310:C:H2'	5:AN1:1311:A:H8	1.74	0.53
5:AN1:2637:A:H5''	13:I:78:THR:HG21	1.90	0.53
5:AN1:293:U:O4	5:AN1:351:G:O6	2.27	0.53
5:AN1:627:A:N3	5:AN1:637:U:O2'	2.41	0.53
10:F:123:ASP:HB2	10:F:127:ASN:HD22	1.74	0.53
5:AN1:1717:G:H21	5:AN1:1735:A:H62	1.56	0.53
5:AN1:2254:C:O2'	5:AN1:2423:C:OP2	2.24	0.53
27:W:42:SER:OG	27:W:43:GLU:OE1	2.26	0.53
15:K:77:ALA:HB2	15:K:107:GLN:HE21	1.74	0.53
23:S:7:TYR:O	28:X:29:ARG:NH1	2.38	0.53
5:AN1:1872:A:H3'	5:AN1:1873:A:H8	1.74	0.53
5:AN1:2563:G:H2'	5:AN1:2564:A:C8	2.44	0.53
5:AN1:413:C:H2'	5:AN1:414:A:H8	1.74	0.53
5:AN1:631:A:O2'	5:AN1:2400:U:OP1	2.26	0.53
3:2:24:LYS:NZ	3:2:46:CYS:SG	2.82	0.52
5:AN1:1920:C:H2'	5:AN1:1921:C:C6	2.45	0.52
11:G:26:VAL:HG11	11:G:76:VAL:HG12	1.91	0.52
28:X:31:ALA:HB3	28:X:39:LYS:HE3	1.90	0.52
5:AN1:1430:G:H2'	5:AN1:1431:G:H8	1.73	0.52
5:AN1:229:A:H61	5:AN1:239:G:H1'	1.75	0.52
11:G:164:TYR:HB2	11:G:167:GLU:HB2	1.92	0.52
5:AN1:2055:A:H2'	5:AN1:2499:2MA:HM23	1.91	0.52
5:AN1:413:C:H2'	5:AN1:414:A:C8	2.44	0.52
5:AN1:579:C:H2'	5:AN1:580:A:C8	2.45	0.52
10:F:148:ARG:O	10:F:150:ARG:NH2	2.43	0.52
5:AN1:1911:3TD:N1	5:AN1:1938:C:O2	2.42	0.52
5:AN1:916:A:N3	6:B:78:U:O2'	2.35	0.52
5:AN1:1387:A:N6	23:S:17:GLU:OE1	2.42	0.52
5:AN1:2137:A:H2	5:AN1:2138:A:H62	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:696:C:O2'	5:AN1:732:A:N6	2.40	0.52
7:C:142:HIS:ND1	7:C:193:GLY:O	2.34	0.52
10:F:38:MET:O	10:F:86:GLY:HA3	2.10	0.52
21:Q:61:ALA:HA	21:Q:99:THR:HG23	1.92	0.52
5:AN1:1535:U:H2'	5:AN1:1536:A:H8	1.75	0.52
5:AN1:229:A:N1	5:AN1:240:A:H5''	2.25	0.52
5:AN1:1111:C:H2'	5:AN1:1112:G:C8	2.43	0.52
5:AN1:1442:C:O2'	5:AN1:1542:A:N3	2.38	0.52
5:AN1:719:A:H2'	5:AN1:720:A:C8	2.45	0.52
6:B:108:C:H2'	6:B:109:G:C8	2.45	0.52
15:K:93:SER:HB2	15:K:125:GLN:HE21	1.75	0.52
19:O:17:LYS:HD3	19:O:80:HIS:HA	1.92	0.52
5:AN1:2568:A:H2'	8:D:152:ASN:HD21	1.75	0.51
5:AN1:1255:A:OP1	22:R:83:LYS:NZ	2.43	0.51
5:AN1:1525:G:H2'	5:AN1:1526:C:O4'	2.10	0.51
5:AN1:1273:C:H2'	5:AN1:1274:G:H8	1.75	0.51
5:AN1:2309:C:H2'	5:AN1:2310:A:H8	1.75	0.51
5:AN1:2311:C:O2'	5:AN1:2312:G:H8	1.91	0.51
10:F:115:ARG:O	10:F:115:ARG:HG2	2.09	0.51
5:AN1:148:A:N6	5:AN1:1593:G:O2'	2.32	0.51
6:B:64:A:H61	6:B:105:C:H2'	1.74	0.51
5:AN1:1787:A:H5''	7:C:205:LEU:HD12	1.93	0.51
5:AN1:1730:U:H2'	5:AN1:1731:C:C6	2.46	0.51
5:AN1:552:U:H2'	5:AN1:553:G:O4'	2.10	0.51
5:AN1:873:G:O6	5:AN1:900:C:N4	2.39	0.51
5:AN1:1306:G:OP2	5:AN1:1306:G:N2	2.43	0.51
5:AN1:1535:U:H2'	5:AN1:1536:A:C8	2.46	0.51
5:AN1:2299:G:H4'	10:F:121:SER:HA	1.93	0.51
26:V:65:GLY:HA3	26:V:83:GLU:O	2.11	0.51
5:AN1:1437:U:H2'	5:AN1:1438:C:H6	1.76	0.51
5:AN1:1506:U:H2'	5:AN1:1507:G:H8	1.76	0.51
5:AN1:2066:A:H2'	5:AN1:2067:A:H8	1.76	0.51
10:F:94:ASP:O	10:F:97:TYR:HB2	2.11	0.51
22:R:2:GLU:OE1	22:R:72:SER:OG	2.29	0.51
3:2:16:ALA:HB2	3:2:64:ILE:HG13	1.93	0.51
5:AN1:1095:A:H2'	5:AN1:1096:G:H8	1.75	0.51
5:AN1:1528:G:N2	5:AN1:1535:U:O4	2.44	0.51
5:AN1:2119:G:N2	5:AN1:2120:G:O6	2.43	0.51
5:AN1:587:U:H2'	5:AN1:588:A:H8	1.76	0.51
11:G:121:VAL:HG23	11:G:135:SER:HB2	1.92	0.51
5:AN1:2499:2MA:O2'	5:AN1:2501:G:OP2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:119:ALA:HB1	10:F:167:ARG:HH12	1.75	0.50
5:AN1:1412:C:H3'	5:AN1:1413:G:H8	1.76	0.50
5:AN1:181:C:H2'	5:AN1:182:A:H8	1.76	0.50
5:AN1:1961:C:H5''	5:AN1:1962:A:H2'	1.93	0.50
10:F:57:MET:HA	10:F:60:ILE:HG12	1.93	0.50
5:AN1:2861:U:OP2	5:AN1:2862:G:O2'	2.22	0.50
21:Q:59:VAL:HG22	21:Q:101:ILE:HG23	1.93	0.50
5:AN1:12:A:H2'	5:AN1:13:A:C8	2.46	0.50
5:AN1:1311:A:H2'	5:AN1:1312:G:H8	1.77	0.50
5:AN1:1844:A:H4'	5:AN1:1845:G:C8	2.45	0.50
5:AN1:2096:G:O6	5:AN1:2185:U:O4	2.29	0.50
3:2:13:ARG:HD2	15:K:65:LYS:HG2	1.93	0.50
5:AN1:34:G:H22	5:AN1:511:G:H2'	1.76	0.50
5:AN1:570:A:OP2	21:Q:80:ARG:NH2	2.43	0.50
5:AN1:2325:A:H2'	5:AN1:2326:G:C8	2.47	0.50
5:AN1:2639:G:H2'	5:AN1:2640:A:H8	1.76	0.50
5:AN1:719:A:H2'	5:AN1:720:A:H8	1.76	0.50
11:G:158:LYS:HD2	11:G:160:LYS:HD2	1.92	0.50
5:AN1:204:A:N6	5:AN1:2426:A:O2'	2.45	0.50
5:AN1:876:A:H3'	5:AN1:877:G:C8	2.46	0.50
5:AN1:881:G:H2'	5:AN1:882:U:H6	1.77	0.50
5:AN1:270:U:O2'	5:AN1:428:A:N3	2.38	0.49
7:C:230:HIS:HD2	7:C:232:HIS:H	1.60	0.49
5:AN1:322:G:N7	9:E:131:LYS:NZ	2.60	0.49
5:AN1:1016:U:O2'	5:AN1:1018:A:N7	2.37	0.49
7:C:107:PRO:HA	7:C:195:VAL:HA	1.93	0.49
10:F:43:ALA:HB3	10:F:85:ILE:HG22	1.94	0.49
6:B:6:C:O3'	18:N:26:ARG:NH2	2.45	0.49
5:AN1:1348:A:H2'	5:AN1:1349:A:H8	1.77	0.49
5:AN1:1259:G:OP1	30:Z:16:ARG:NH1	2.37	0.49
5:AN1:1826:U:H2'	5:AN1:1827:G:H8	1.76	0.49
5:AN1:2639:G:H2'	5:AN1:2640:A:C8	2.47	0.49
5:AN1:410:G:OP2	5:AN1:2402:U:O2'	2.22	0.49
6:B:109:G:O2'	18:N:47:LYS:NZ	2.45	0.49
3:2:30:HIS:C	3:2:32:LEU:H	2.16	0.49
5:AN1:1383:G:H2'	5:AN1:1384:G:C8	2.48	0.49
5:AN1:667:G:N2	5:AN1:670:C:OP1	2.45	0.49
5:AN1:70:A:H61	5:AN1:98:A:N6	2.10	0.49
5:AN1:12:A:H2'	5:AN1:13:A:H8	1.77	0.49
5:AN1:35:A:H61	5:AN1:511:G:H1'	1.78	0.49
5:AN1:663:U:H2'	5:AN1:664:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:762:A:H5'	7:C:209:GLY:HA2	1.94	0.49
13:I:125:TYR:OH	13:I:132:HIS:NE2	2.38	0.49
5:AN1:1430:G:H2'	5:AN1:1431:G:C8	2.47	0.49
5:AN1:2229:U:H2'	5:AN1:2230:G:H8	1.78	0.49
5:AN1:2309:C:H2'	5:AN1:2310:A:C8	2.48	0.49
5:AN1:2309:C:O3'	10:F:88:LYS:NZ	2.45	0.49
5:AN1:2830:G:H2'	5:AN1:2875:A:H61	1.78	0.49
5:AN1:879:G:N2	5:AN1:893:U:O2'	2.37	0.49
6:B:90:C:OP1	25:U:26:ARG:NH2	2.45	0.49
5:AN1:1383:G:H2'	5:AN1:1384:G:H8	1.78	0.49
5:AN1:1591:C:H2'	5:AN1:1592:A:C8	2.48	0.49
5:AN1:1679:G:P	5:AN1:1753:A:H61	2.36	0.49
5:AN1:879:G:H2'	5:AN1:880:G:C8	2.47	0.49
5:AN1:1719:U:O4	5:AN1:1734:G:N2	2.46	0.49
5:AN1:1862:A:H2	5:AN1:1872:A:H8	1.59	0.49
5:AN1:303:C:H5''	5:AN1:336:U:H2'	1.94	0.48
9:E:124:ALA:O	9:E:136:LYS:NZ	2.46	0.48
10:F:102:ARG:O	10:F:106:ILE:HG12	2.13	0.48
25:U:23:ARG:HG2	25:U:26:ARG:HH12	1.78	0.48
1:O:42:HIS:HD1	5:AN1:2367:G:HO2'	1.57	0.48
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.95	0.48
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.94	0.48
18:N:82:LYS:HE2	18:N:113:GLY:HA3	1.95	0.48
20:P:81:ASP:OD1	20:P:85:LYS:NZ	2.44	0.48
5:AN1:1078:U:H2'	5:AN1:1079:U:H5	1.78	0.48
5:AN1:2242:G:H2'	5:AN1:2243:A:H8	1.78	0.48
5:AN1:395:G:OP2	27:W:10:LYS:NZ	2.43	0.48
9:E:60:ARG:NH2	9:E:62:LYS:O	2.46	0.48
5:AN1:2622:C:H2'	5:AN1:2623:G:C8	2.48	0.48
16:L:19:GLY:O	16:L:39:ARG:NH1	2.36	0.48
5:AN1:1681:U:H2'	5:AN1:1682:A:C8	2.48	0.48
5:AN1:1681:U:H2'	5:AN1:1682:A:H8	1.78	0.48
5:AN1:309:G:N1	5:AN1:312:A:OP2	2.34	0.48
5:AN1:898:A:H3'	5:AN1:899:A:H8	1.78	0.48
5:AN1:1437:U:H2'	5:AN1:1438:C:C6	2.49	0.48
5:AN1:2787:A:O2'	5:AN1:2788:G:H8	1.95	0.48
5:AN1:25:C:O2'	5:AN1:552:U:OP1	2.31	0.48
10:F:29:PRO:HB3	10:F:160:ALA:HB2	1.95	0.48
5:AN1:1591:C:H2'	5:AN1:1592:A:H8	1.78	0.48
5:AN1:2169:A:H2'	5:AN1:2170:C:C5	2.49	0.48
5:AN1:394:U:O2'	5:AN1:395:G:N7	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:86:C:H2'	5:AN1:87:G:C8	2.48	0.48
6:B:111:C:H2'	6:B:112:A:C8	2.48	0.48
5:AN1:1524:A:H62	5:AN1:1539:G:N2	2.11	0.48
5:AN1:1662:A:H61	5:AN1:1992:C:H42	1.60	0.48
5:AN1:2067:A:H2'	5:AN1:2068:C:C6	2.48	0.48
5:AN1:72:C:O2'	5:AN1:455:C:N3	2.41	0.48
5:AN1:879:G:C6	5:AN1:893:U:O2	2.66	0.48
7:C:256:LYS:HE2	7:C:273:VAL:HG13	1.96	0.48
12:H:47:PHE:HA	12:H:51:ARG:HH11	1.79	0.48
5:AN1:1750:C:H5	19:O:97:ARG:HH11	1.60	0.48
5:AN1:1276:G:H2'	5:AN1:1277:U:C6	2.49	0.48
5:AN1:437:G:H2'	5:AN1:438:A:C8	2.49	0.48
19:O:60:SER:OG	19:O:79:THR:OG1	2.24	0.48
5:AN1:580:A:H2'	5:AN1:581:G:H8	1.78	0.48
15:K:31:LYS:HE3	15:K:32:THR:HG23	1.96	0.48
6:B:50:A:N7	18:N:34:ARG:NH2	2.61	0.48
5:AN1:2743:G:N2	5:AN1:2753:A:H62	2.10	0.47
8:D:13:THR:HG22	8:D:14:ARG:H	1.79	0.47
9:E:139:ASP:OD2	9:E:140:LEU:N	2.47	0.47
16:L:35:LYS:HE3	16:L:132:VAL:HG11	1.96	0.47
19:O:94:ASP:HB2	19:O:116:LYS:HB2	1.96	0.47
27:W:33:LEU:HD22	27:W:50:ARG:HG2	1.94	0.47
5:AN1:1024:A:N6	5:AN1:1123:A:N3	2.63	0.47
5:AN1:2622:C:H2'	5:AN1:2623:G:H8	1.79	0.47
5:AN1:727:G:OP1	7:C:13:ARG:HG2	2.14	0.47
8:D:152:ASN:OD1	8:D:153:GLN:N	2.40	0.47
5:AN1:390:A:N7	34:AN1:3235:HOH:O	2.36	0.47
16:L:75:THR:HG22	16:L:90:VAL:HG22	1.96	0.47
5:AN1:1356:G:H2'	5:AN1:1357:C:C6	2.50	0.47
5:AN1:1786:U:H2'	5:AN1:1787:A:C8	2.50	0.47
5:AN1:2563:G:H2'	5:AN1:2564:A:H8	1.79	0.47
5:AN1:580:A:H2'	5:AN1:581:G:C8	2.50	0.47
5:AN1:587:U:H2'	5:AN1:588:A:C8	2.49	0.47
23:S:37:ALA:O	23:S:80:LYS:NZ	2.44	0.47
7:C:17:GLU:HB2	7:C:204:SER:N	2.29	0.47
10:F:111:ILE:HG21	10:F:114:PHE:CE1	2.49	0.47
10:F:136:ILE:HG13	10:F:138:PHE:HD1	1.78	0.47
5:AN1:1053:G:H21	5:AN1:1101:C:H41	1.63	0.47
5:AN1:1478:G:H2'	5:AN1:1479:U:C6	2.50	0.47
5:AN1:2176:U:H2'	5:AN1:2177:G:C8	2.49	0.47
5:AN1:2742:U:H5''	11:G:138:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:35:LYS:HB2	3:2:40:ILE:HD11	1.95	0.47
5:AN1:753:C:H2'	5:AN1:754:A:H8	1.80	0.47
7:C:230:HIS:CD2	7:C:232:HIS:H	2.33	0.47
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.96	0.47
23:S:49:LEU:HD13	28:X:26:PHE:CZ	2.49	0.47
26:V:65:GLY:HA2	26:V:85:VAL:HG23	1.95	0.47
5:AN1:1427:G:H2'	5:AN1:1428:A:C8	2.50	0.47
5:AN1:2674:A:H2'	5:AN1:2675:A:C8	2.50	0.47
5:AN1:597:A:H2'	5:AN1:598:G:H8	1.80	0.47
17:M:106:ASP:N	17:M:106:ASP:OD1	2.48	0.47
5:AN1:1561:U:H2'	5:AN1:1562:C:C6	2.50	0.47
5:AN1:605:U:H2'	5:AN1:606:A:H8	1.79	0.47
5:AN1:876:A:H62	5:AN1:897:A:H2	1.62	0.47
6:B:60:U:H2'	6:B:61:C:C6	2.50	0.47
5:AN1:2894:U:O2'	13:I:134:ALA:O	2.32	0.47
12:H:27:ARG:NH1	27:W:60:ASP:OD2	2.48	0.47
5:AN1:1462:G:N2	5:AN1:1520:A:N1	2.45	0.46
5:AN1:966:G:H2'	5:AN1:967:U:C6	2.50	0.46
5:AN1:181:C:H2'	5:AN1:182:A:C8	2.50	0.46
5:AN1:2229:U:H2'	5:AN1:2230:G:C8	2.51	0.46
11:G:11:VAL:HG13	11:G:15:VAL:HG23	1.97	0.46
5:AN1:1164:G:N7	34:AN1:3237:HOH:O	2.36	0.46
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.96	0.46
5:AN1:1103:A:N6	5:AN1:1104:G:O6	2.48	0.46
5:AN1:812:C:H1'	5:AN1:1220:G:H21	1.81	0.46
5:AN1:1356:G:H2'	5:AN1:1357:C:H6	1.80	0.46
5:AN1:875:U:H2'	5:AN1:876:A:H8	1.81	0.46
5:AN1:568:G:O4'	5:AN1:980:A:N6	2.48	0.46
10:F:166:GLY:O	10:F:169:LEU:HD23	2.16	0.46
5:AN1:1199:A:H4'	5:AN1:1200:A:H5'	1.97	0.46
5:AN1:1413:G:O2'	5:AN1:1577:A:N6	2.49	0.46
5:AN1:1921:C:H2'	5:AN1:1922:U:C6	2.50	0.46
5:AN1:498:U:H2'	5:AN1:499:G:O4'	2.16	0.46
5:AN1:856:G:H3'	5:AN1:857:G:C8	2.50	0.46
10:F:93:GLY:O	10:F:96:MET:HG2	2.14	0.46
5:AN1:1108:A:H2'	5:AN1:1109:G:H4'	1.97	0.46
5:AN1:1962:A:N3	5:AN1:2588:G:O2'	2.32	0.46
5:AN1:2049:G:H5'	8:D:152:ASN:O	2.15	0.46
11:G:124:GLU:OE1	11:G:134:LYS:NZ	2.46	0.46
5:AN1:2212:G:H2'	5:AN1:2213:G:H8	1.80	0.46
5:AN1:2295:G:H2'	5:AN1:2296:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:25:C:H2'	5:AN1:26:A:C8	2.51	0.46
5:AN1:678:A:H2'	5:AN1:679:G:C8	2.51	0.46
10:F:47:LYS:HZ1	10:F:83:TRP:HE3	1.60	0.46
5:AN1:2242:G:H2'	5:AN1:2243:A:C8	2.51	0.46
5:AN1:665:U:H2'	5:AN1:666:A:O4'	2.15	0.46
10:F:54:VAL:HG12	10:F:87:CYS:SG	2.56	0.46
11:G:74:ASN:OD1	11:G:75:LEU:N	2.49	0.46
14:J:63:VAL:HG12	14:J:106:LEU:HD11	1.98	0.46
5:AN1:1025:A:H2'	5:AN1:1026:A:C8	2.51	0.46
5:AN1:1151:C:OP1	20:P:92:ARG:NH2	2.46	0.46
5:AN1:1793:C:O2'	7:C:257:THR:OG1	2.34	0.46
5:AN1:23:U:H2'	5:AN1:24:G:H8	1.81	0.46
5:AN1:955:U:O2'	6:B:86:U:O4	2.34	0.46
9:E:170:ASP:OD2	9:E:171:ALA:N	2.44	0.46
5:AN1:1424:G:H2'	5:AN1:1425:G:H8	1.81	0.46
5:AN1:1850:A:H4'	5:AN1:2229:U:H4'	1.98	0.46
5:AN1:1860:U:H2'	5:AN1:1861:U:C6	2.51	0.46
5:AN1:1665:G:O2'	5:AN1:1987:U:O4	2.30	0.46
5:AN1:475:G:N1	5:AN1:478:A:OP2	2.45	0.46
5:AN1:591:U:H2'	5:AN1:592:U:C6	2.51	0.46
5:AN1:2301:U:H5	10:F:153:ASP:HB2	1.81	0.46
21:Q:37:ASP:N	21:Q:37:ASP:OD1	2.49	0.46
5:AN1:1010:C:H2'	5:AN1:1011:A:C8	2.49	0.45
5:AN1:1515:C:H2'	5:AN1:1516:U:C6	2.50	0.45
5:AN1:2119:G:H1	5:AN1:2169:A:N6	2.14	0.45
5:AN1:249:G:N2	5:AN1:262:A:OP2	2.42	0.45
5:AN1:596:U:H2'	5:AN1:597:A:C8	2.51	0.45
5:AN1:720:A:H2'	5:AN1:721:C:H6	1.81	0.45
11:G:76:VAL:HA	11:G:79:VAL:HG12	1.98	0.45
5:AN1:1441:C:H2'	5:AN1:1442:C:H6	1.81	0.45
5:AN1:2187:A:H2'	5:AN1:2188:G:C8	2.51	0.45
5:AN1:2533:U:H2'	5:AN1:2534:C:H6	1.82	0.45
6:B:26:C:H2'	6:B:27:A:C8	2.50	0.45
1:O:13:THR:HB	1:O:38:LYS:HD3	1.98	0.45
5:AN1:113:C:H2'	5:AN1:114:G:C8	2.51	0.45
5:AN1:1467:G:O6	5:AN1:1468:A:N6	2.49	0.45
5:AN1:2066:A:H2'	5:AN1:2067:A:C8	2.51	0.45
5:AN1:2096:G:N2	5:AN1:2185:U:O2	2.35	0.45
5:AN1:575:G:H2'	5:AN1:576:G:C8	2.52	0.45
5:AN1:578:U:H2'	5:AN1:579:C:C6	2.51	0.45
11:G:19:GLN:HG2	11:G:21:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1798:A:H2'	5:AN1:1799:A:C8	2.52	0.45
5:AN1:2021:C:H2'	5:AN1:2022:U:C6	2.52	0.45
5:AN1:2683:U:H2'	5:AN1:2684:G:O4'	2.17	0.45
5:AN1:625:A:N6	15:K:114:LEU:O	2.43	0.45
23:S:15:PHE:HE2	28:X:34:THR:HA	1.81	0.45
2:1:29:GLN:NE2	5:AN1:217:C:OP1	2.50	0.45
5:AN1:1589:C:H2'	5:AN1:1590:A:C8	2.50	0.45
5:AN1:287:G:O6	5:AN1:358:A:N6	2.50	0.45
6:B:37:U:H2'	6:B:38:U:C6	2.51	0.45
5:AN1:2324:A:H2'	5:AN1:2325:A:H8	1.82	0.45
5:AN1:2456:U:C2	5:AN1:2457:A:C8	3.05	0.45
7:C:205:LEU:HB3	7:C:210:ALA:HB3	1.97	0.45
10:F:175:PHE:HB3	10:F:177:PHE:HD1	1.82	0.45
10:F:33:LYS:HD3	10:F:92:ARG:NH1	2.32	0.45
13:I:70:LEU:HA	13:I:88:ASN:HD21	1.81	0.45
15:K:37:ILE:HG22	15:K:38:LYS:H	1.81	0.45
5:AN1:113:C:H2'	5:AN1:114:G:H8	1.81	0.45
5:AN1:1787:A:C2	5:AN1:1825:A:H4'	2.52	0.45
5:AN1:1394:C:H2'	5:AN1:1395:A:H8	1.81	0.45
5:AN1:1408:A:H2'	5:AN1:1409:A:C8	2.51	0.45
5:AN1:1436:A:H2'	5:AN1:1437:U:C6	2.52	0.45
5:AN1:1833:C:O2'	5:AN1:1923:A:HI'	2.16	0.45
5:AN1:2647:C:H2'	5:AN1:2648:C:C6	2.52	0.45
5:AN1:568:G:H2'	5:AN1:2026:6MZ:N7	2.32	0.45
5:AN1:925:A:H2'	5:AN1:926:G:C8	2.52	0.45
16:L:76:GLU:HG2	16:L:91:GLU:HG3	1.99	0.45
5:AN1:1359:G:N7	27:W:2:SER:N	2.64	0.45
5:AN1:1432:C:HO2'	5:AN1:1512:G:HO2'	1.64	0.45
5:AN1:2119:G:HI'	5:AN1:2172:A:C2	2.52	0.45
5:AN1:2323:A:H2'	5:AN1:2324:A:C8	2.52	0.45
8:D:13:THR:HG22	8:D:14:ARG:N	2.32	0.45
10:F:34:ILE:HG13	10:F:156:ILE:HG22	1.98	0.45
5:AN1:1321:U:H2'	5:AN1:1322:A:C8	2.52	0.45
6:B:22:G:O2'	6:B:25:C:N4	2.49	0.45
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.99	0.45
26:V:20:MET:SD	26:V:20:MET:N	2.90	0.45
5:AN1:2852:A:H2'	5:AN1:2853:G:O4'	2.17	0.44
5:AN1:862:G:H2'	5:AN1:863:C:C6	2.52	0.44
5:AN1:1483:U:H3	5:AN1:1496:G:H1	1.65	0.44
5:AN1:1583:C:H3'	5:AN1:1584:A:H8	1.83	0.44
5:AN1:1943:C:H2'	5:AN1:1944:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:21:THR:HA	13:I:61:GLN:HB3	1.98	0.44
25:U:8:ALA:HB1	25:U:44:VAL:HB	1.99	0.44
4:3:13:SER:OG	4:3:27:CYS:SG	2.70	0.44
5:AN1:2147:C:O2	5:AN1:2148:C:N4	2.50	0.44
5:AN1:2694:U:H2'	5:AN1:2695:G:C8	2.52	0.44
5:AN1:25:C:H2'	5:AN1:26:A:H8	1.82	0.44
8:D:117:LYS:HE2	8:D:199:ALA:HB2	1.98	0.44
5:AN1:920:C:O2'	26:V:29:GLN:NE2	2.48	0.44
5:AN1:11:C:H2'	5:AN1:12:A:H8	1.83	0.44
5:AN1:1487:G:H5''	5:AN1:1488:C:H5''	1.98	0.44
5:AN1:1503:C:H3'	5:AN1:1504:U:H4'	1.99	0.44
5:AN1:2104:U:H3	5:AN1:2177:G:H1	1.65	0.44
5:AN1:513:A:N3	5:AN1:579:C:O2'	2.44	0.44
5:AN1:720:A:H2'	5:AN1:721:C:C6	2.52	0.44
5:AN1:891:C:N4	5:AN1:892:U:O2	2.50	0.44
5:AN1:124:G:OP2	5:AN1:126:A:O2'	2.28	0.44
5:AN1:1521:G:H2'	5:AN1:1522:C:C6	2.53	0.44
5:AN1:158:U:H2'	5:AN1:159:G:H8	1.82	0.44
5:AN1:292:U:H2'	5:AN1:293:U:C6	2.52	0.44
5:AN1:35:A:N6	5:AN1:511:G:O2'	2.51	0.44
2:1:1:MET:HE1	5:AN1:750:A:H3'	2.00	0.44
5:AN1:1053:G:N2	5:AN1:1099:C:OP2	2.44	0.44
5:AN1:1846:G:H2'	5:AN1:1847:U:C6	2.52	0.44
5:AN1:2376:U:H2'	5:AN1:2377:A:C8	2.53	0.44
5:AN1:664:A:H2'	5:AN1:665:U:C6	2.53	0.44
5:AN1:718:U:O2'	5:AN1:719:A:H8	1.97	0.44
5:AN1:2381:C:H2'	5:AN1:2382:U:C6	2.52	0.44
5:AN1:968:C:H2'	5:AN1:969:A:O4'	2.17	0.44
6:B:16:A:H1'	6:B:65:G:N2	2.33	0.44
10:F:77:PHE:CD2	10:F:79:ILE:HG12	2.53	0.44
12:H:4:ILE:HG22	12:H:18:LYS:HB3	1.98	0.44
5:AN1:1052:G:H1'	5:AN1:1082:A:C2	2.49	0.44
5:AN1:2674:A:H2'	5:AN1:2675:A:H8	1.83	0.44
5:AN1:663:U:H2'	5:AN1:664:A:C8	2.52	0.44
5:AN1:849:C:H2'	5:AN1:850:A:H8	1.83	0.44
5:AN1:971:G:OP1	5:AN1:1182:G:O2'	2.27	0.44
23:S:3:ASN:HD21	23:S:48:LYS:HE2	1.81	0.44
6:B:12:U:O3'	6:B:104:U:O2'	2.32	0.44
7:C:17:GLU:HB2	7:C:204:SER:H	1.83	0.44
10:F:120:LYS:HG3	10:F:121:SER:N	2.30	0.44
6:B:40:C:H4'	10:F:64:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2659:G:H2'	5:AN1:2660:G:O4'	2.18	0.43
5:AN1:1797:A:OP2	7:C:150:LYS:NZ	2.51	0.43
10:F:50:LEU:O	10:F:54:VAL:HG13	2.18	0.43
11:G:97:ALA:HB3	11:G:104:ASN:HD21	1.82	0.43
5:AN1:1436:A:H2'	5:AN1:1437:U:H6	1.83	0.43
5:AN1:2093:U:H2'	5:AN1:2094:U:C6	2.53	0.43
5:AN1:2171:C:H2'	5:AN1:2172:A:N7	2.33	0.43
5:AN1:2444:A:OP1	34:AN1:3201:HOH:O	2.21	0.43
10:F:51:ASP:O	10:F:54:VAL:HG22	2.18	0.43
13:I:17:VAL:HG23	13:I:137:PRO:HB2	2.00	0.43
5:AN1:1273:C:H2'	5:AN1:1274:G:C8	2.54	0.43
5:AN1:1842:G:H2'	5:AN1:1843:A:C8	2.53	0.43
5:AN1:229:A:N6	5:AN1:239:G:H1'	2.34	0.43
5:AN1:2484:G:H2'	5:AN1:2485:U:C6	2.53	0.43
5:AN1:287:G:H2'	5:AN1:288:U:C6	2.53	0.43
5:AN1:636:G:H2'	5:AN1:637:U:C6	2.54	0.43
6:B:61:C:H2'	6:B:62:U:C6	2.53	0.43
6:B:81:G:O6	6:B:91:A:N6	2.52	0.43
8:D:180:ILE:HD12	8:D:190:LEU:HD22	2.00	0.43
10:F:3:ARG:NH1	10:F:4:LEU:O	2.50	0.43
11:G:123:ALA:HB2	11:G:133:LEU:HD13	1.99	0.43
5:AN1:1464:A:H2'	5:AN1:1465:A:C8	2.54	0.43
5:AN1:1854:A:C2	5:AN1:1881:A:H1'	2.54	0.43
5:AN1:2643:U:H2'	5:AN1:2644:G:H8	1.84	0.43
5:AN1:27:U:H2'	5:AN1:28:G:H8	1.83	0.43
5:AN1:727:G:C8	7:C:207:LYS:HD2	2.53	0.43
6:B:68:C:H2'	6:B:69:U:H6	1.83	0.43
8:D:184:ASP:HB3	8:D:189:VAL:HG22	2.00	0.43
5:AN1:816:G:N1	5:AN1:1183:U:OP2	2.38	0.43
5:AN1:11:C:H2'	5:AN1:12:A:C8	2.54	0.43
5:AN1:2113:A:H2	5:AN1:2166:A:N6	2.15	0.43
5:AN1:2594:A:H5''	7:C:234:GLY:HA3	2.00	0.43
5:AN1:520:U:H2'	5:AN1:521:G:C8	2.53	0.43
7:C:21:HIS:ND1	7:C:90:HIS:HE1	2.16	0.43
10:F:36:LEU:HD23	10:F:36:LEU:H	1.82	0.43
5:AN1:1466:G:O6	5:AN1:1517:G:N2	2.52	0.43
6:B:64:A:N6	6:B:105:C:H2'	2.33	0.43
5:AN1:1647:G:O2'	17:M:106:ASP:OD2	2.22	0.43
21:Q:2:TYR:HB3	21:Q:15:VAL:HG22	1.99	0.43
5:AN1:1506:U:H2'	5:AN1:1507:G:C8	2.54	0.43
5:AN1:1588:A:H2'	5:AN1:1589:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2115:A:N3	5:AN1:2166:A:H1'	2.33	0.43
5:AN1:2314:G:C5	5:AN1:2315:U:H1'	2.54	0.43
5:AN1:2463:C:H2'	5:AN1:2464:A:O4'	2.19	0.43
5:AN1:671:C:OP1	9:E:48:ARG:NH2	2.52	0.43
10:F:175:PHE:HD2	10:F:177:PHE:HB3	1.84	0.43
5:AN1:1472:A:N6	5:AN1:1510:G:O2'	2.52	0.43
5:AN1:1470:G:N1	5:AN1:1510:G:N7	2.67	0.43
5:AN1:1817:A:H2'	5:AN1:1818:G:H8	1.84	0.43
5:AN1:2670:G:H2'	5:AN1:2671:A:C8	2.54	0.43
5:AN1:327:G:H2'	5:AN1:328:G:H8	1.84	0.43
5:AN1:482:A:O4'	24:T:43:HIS:HB3	2.19	0.43
5:AN1:593:C:H2'	5:AN1:594:A:H8	1.84	0.43
10:F:137:VAL:HG12	10:F:142:ASP:HB2	2.00	0.43
16:L:20:LEU:HD23	16:L:99:PRO:HG2	2.01	0.43
5:AN1:1087:A:H2'	5:AN1:1088:G:C8	2.54	0.43
5:AN1:1856:G:H1	5:AN1:1878:U:H3	1.66	0.43
5:AN1:1878:U:H2'	5:AN1:1879:U:C6	2.54	0.43
5:AN1:2125:C:H2'	5:AN1:2155:G:H22	1.84	0.43
5:AN1:2306:A:H2'	5:AN1:2307:A:H5''	2.00	0.43
6:B:31:G:C2	6:B:48:A:C6	3.06	0.43
9:E:82:LYS:HE2	9:E:82:LYS:HB3	1.78	0.43
15:K:31:LYS:HE2	15:K:31:LYS:HB3	1.77	0.43
5:AN1:2652:U:H2'	5:AN1:2653:A:H8	1.83	0.43
9:E:133:LEU:HA	9:E:136:LYS:HG2	2.01	0.43
13:I:141:ASP:OD1	13:I:142:ILE:N	2.43	0.43
5:AN1:1655:U:H5''	8:D:141:VAL:O	2.19	0.42
15:K:57:THR:O	15:K:62:ARG:NH1	2.52	0.42
24:T:5:LYS:HE2	24:T:5:LYS:HB3	1.91	0.42
5:AN1:1411:G:H2'	5:AN1:1412:C:C6	2.54	0.42
5:AN1:1984:C:N4	5:AN1:1985:G:O6	2.52	0.42
5:AN1:2098:C:H2'	5:AN1:2099:C:O4'	2.19	0.42
5:AN1:67:G:O6	5:AN1:81:A:N6	2.52	0.42
10:F:54:VAL:O	10:F:65:PRO:HG3	2.19	0.42
11:G:90:VAL:HG13	11:G:160:LYS:HA	2.02	0.42
5:AN1:1348:A:H2'	5:AN1:1349:A:C8	2.54	0.42
5:AN1:1549:U:H2'	5:AN1:1550:G:O4'	2.18	0.42
5:AN1:2519:G:O2'	5:AN1:2760:A:O2'	2.29	0.42
5:AN1:326:A:H61	5:AN1:340:G:H2'	1.85	0.42
5:AN1:861:A:H2'	5:AN1:862:G:C8	2.54	0.42
5:AN1:2309:C:H1'	10:F:37:ASN:ND2	2.35	0.42
11:G:157:TYR:O	11:G:171:ARG:NH1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1004:C:OP1	13:I:37:ARG:NH1	2.51	0.42
5:AN1:1862:A:H2'	5:AN1:1863:G:C8	2.55	0.42
5:AN1:2612:C:N4	34:AN1:3247:HOH:O	2.40	0.42
5:AN1:2696:A:H2'	5:AN1:2697:C:C6	2.54	0.42
5:AN1:400:A:H2'	5:AN1:401:A:C8	2.54	0.42
5:AN1:521:G:H2'	5:AN1:522:C:C6	2.55	0.42
5:AN1:67:G:O6	5:AN1:81:A:C6	2.73	0.42
5:AN1:873:G:H2'	5:AN1:874:C:C6	2.54	0.42
8:D:180:ILE:HD13	8:D:192:VAL:HB	2.01	0.42
5:AN1:2123:G:H2'	5:AN1:2124:G:H8	1.84	0.42
5:AN1:2795:A:H2'	5:AN1:2797:G:OP2	2.20	0.42
5:AN1:994:G:OP2	20:P:58:ARG:NH1	2.52	0.42
16:L:11:LYS:HD3	16:L:87:LYS:HD3	2.00	0.42
5:AN1:1420:G:H2'	5:AN1:1421:G:C8	2.55	0.42
5:AN1:2287:U:H2'	5:AN1:2288:G:H8	1.82	0.42
5:AN1:2543:A:H2'	5:AN1:2544:U:C6	2.55	0.42
5:AN1:591:U:H2'	5:AN1:592:U:H6	1.85	0.42
5:AN1:677:C:H2'	5:AN1:678:A:H8	1.85	0.42
8:D:181:VAL:HG12	8:D:191:VAL:O	2.19	0.42
10:F:46:ASP:C	10:F:48:LYS:H	2.23	0.42
13:I:11:VAL:HG11	13:I:50:THR:HA	2.02	0.42
5:AN1:1193:U:H2'	5:AN1:1194:U:C6	2.54	0.42
5:AN1:2060:C:H2'	5:AN1:2061:C:C6	2.54	0.42
5:AN1:2695:G:H2'	5:AN1:2696:A:C8	2.55	0.42
5:AN1:2845:G:H1'	5:AN1:2862:G:H21	1.84	0.42
5:AN1:89:G:H22	5:AN1:112:C:N4	2.18	0.42
5:AN1:946:U:H2'	5:AN1:947:G:H8	1.85	0.42
7:C:20:VAL:HG13	7:C:21:HIS:N	2.33	0.42
10:F:44:ALA:O	10:F:47:LYS:HE2	2.20	0.42
5:AN1:1081:A:O3'	5:AN1:1102:U:O2'	2.33	0.42
5:AN1:1053:G:N2	5:AN1:1101:C:H41	2.18	0.42
5:AN1:1567:A:OP1	7:C:61:HIS:NE2	2.44	0.42
5:AN1:2366:G:H2'	5:AN1:2367:G:C8	2.54	0.42
5:AN1:701:U:H2'	5:AN1:702:G:O4'	2.20	0.42
5:AN1:825:U:O2'	5:AN1:2064:U:N3	2.53	0.42
5:AN1:1240:G:OP1	15:K:15:LYS:NZ	2.51	0.42
5:AN1:1457:C:H2'	5:AN1:1458:A:H8	1.85	0.42
5:AN1:1685:G:H21	5:AN1:1699:A:H62	1.67	0.42
5:AN1:1743:A:H2'	5:AN1:1744:C:C6	2.55	0.42
5:AN1:2692:U:H2'	5:AN1:2693:G:H8	1.85	0.42
5:AN1:2784:C:H2'	5:AN1:2785:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:31:G:H2'	5:AN1:32:U:C6	2.54	0.42
5:AN1:932:U:H2'	5:AN1:933:C:C6	2.55	0.42
5:AN1:9:G:H2'	5:AN1:10:U:H6	1.84	0.42
8:D:18:ASP:OD1	8:D:18:ASP:N	2.52	0.42
10:F:162:THR:HG22	10:F:164:ASP:N	2.33	0.42
5:AN1:1028:G:C5	5:AN1:1029:A:C2	3.08	0.42
5:AN1:1412:C:H3'	5:AN1:1413:G:C8	2.54	0.42
5:AN1:157:U:H2'	5:AN1:158:U:C6	2.55	0.42
5:AN1:1861:U:H2'	5:AN1:1862:A:C8	2.55	0.42
5:AN1:2373:A:H2'	5:AN1:2374:A:C8	2.55	0.42
5:AN1:592:U:H2'	5:AN1:593:C:C6	2.54	0.42
5:AN1:970:A:H5'	5:AN1:1183:U:H1'	2.01	0.42
7:C:6:CYS:SG	7:C:13:ARG:NH2	2.93	0.42
21:Q:75:ILE:HG12	21:Q:86:GLN:HG2	2.02	0.42
5:AN1:19:U:O2	5:AN1:2622:C:H4'	2.20	0.41
5:AN1:2110:A:H3'	5:AN1:2111:G:H8	1.84	0.41
5:AN1:2379:G:O2'	5:AN1:2380:U:OP1	2.33	0.41
5:AN1:2063:G:H1	5:AN1:2439:U:H3	1.67	0.41
5:AN1:2645:C:H2'	5:AN1:2646:U:H6	1.84	0.41
5:AN1:358:A:HO2'	5:AN1:359:U:H6	1.68	0.41
5:AN1:590:A:H2'	5:AN1:591:U:C6	2.54	0.41
5:AN1:981:A:N3	5:AN1:981:A:H2'	2.35	0.41
6:B:108:C:O2'	6:B:109:G:OP1	2.30	0.41
5:AN1:1816:U:C4	7:C:159:GLY:HA3	2.55	0.41
10:F:114:PHE:O	10:F:115:ARG:HB3	2.20	0.41
16:L:30:GLY:HA2	16:L:107:GLU:HB2	2.02	0.41
5:AN1:493:G:H21	22:R:57:ASN:HD21	1.67	0.41
1:O:42:HIS:ND1	5:AN1:2367:G:O2'	2.51	0.41
5:AN1:1441:C:H2'	5:AN1:1442:C:C6	2.56	0.41
5:AN1:2051:C:H2'	5:AN1:2500:PSU:H4'	2.02	0.41
5:AN1:2109:U:O4	5:AN1:2163:U:O2'	2.38	0.41
9:E:97:ARG:HG2	9:E:101:ARG:HE	1.85	0.41
10:F:110:ARG:HD2	10:F:110:ARG:HA	1.83	0.41
20:P:78:ARG:HD3	20:P:78:ARG:HA	1.81	0.41
5:AN1:1407:U:O4	5:AN1:1408:A:N6	2.52	0.41
5:AN1:2262:A:H4'	5:AN1:2263:A:N3	2.34	0.41
5:AN1:522:C:H2'	5:AN1:523:A:H8	1.84	0.41
5:AN1:68:A:H2'	5:AN1:69:U:C6	2.55	0.41
5:AN1:714:A:C5	5:AN1:715:C:H1'	2.54	0.41
5:AN1:1296:A:H2	5:AN1:1624:A:H2	1.68	0.41
5:AN1:1471:U:H2'	5:AN1:1472:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2695:G:H2'	5:AN1:2696:A:H8	1.86	0.41
5:AN1:850:A:H2'	5:AN1:851:U:C6	2.56	0.41
5:AN1:2611:U:C2	30:Z:4:GLN:HA	2.56	0.41
5:AN1:2892:C:H2'	5:AN1:2893:U:C6	2.55	0.41
6:B:63:U:H2'	6:B:64:A:O4'	2.20	0.41
17:M:13:THR:HG23	17:M:16:HIS:H	1.86	0.41
5:AN1:2116:G:H5''	5:AN1:2164:G:H22	1.84	0.41
5:AN1:2200:G:OP2	7:C:147:LYS:NZ	2.40	0.41
5:AN1:2325:A:H2'	5:AN1:2326:G:H8	1.86	0.41
5:AN1:2401:G:O2'	5:AN1:2407:A:N6	2.53	0.41
5:AN1:1311:A:H2'	5:AN1:1312:G:C8	2.55	0.41
5:AN1:1358:C:O2'	5:AN1:1805:A:N3	2.41	0.41
5:AN1:2172:A:H2'	5:AN1:2173:C:C6	2.55	0.41
5:AN1:2462:C:H2'	5:AN1:2463:C:C6	2.56	0.41
5:AN1:2871:C:H2'	5:AN1:2872:A:C8	2.55	0.41
3:2:59:ARG:NH2	5:AN1:663:U:O3'	2.47	0.41
5:AN1:673:A:N3	5:AN1:2439:U:O2'	2.48	0.41
5:AN1:849:C:H2'	5:AN1:850:A:C8	2.56	0.41
19:O:30:VAL:HG22	19:O:47:GLU:HG2	2.02	0.41
20:P:105:ALA:HA	21:Q:47:ILE:HD13	2.02	0.41
27:W:56:MET:SD	34:W:101:HOH:O	2.63	0.41
5:AN1:1306:G:HO2'	5:AN1:1307:U:H5	1.66	0.41
5:AN1:1321:U:H2'	5:AN1:1322:A:H8	1.86	0.41
5:AN1:1471:U:H2'	5:AN1:1472:A:H8	1.86	0.41
5:AN1:1588:A:H2'	5:AN1:1589:C:C6	2.56	0.41
5:AN1:413:C:H1'	5:AN1:1860:U:H1'	2.02	0.41
5:AN1:2207:G:H2'	5:AN1:2207:G:N3	2.36	0.41
5:AN1:2407:A:H2'	5:AN1:2408:A:C8	2.56	0.41
5:AN1:355:C:O2'	5:AN1:356:A:H2'	2.21	0.41
5:AN1:831:A:H2'	5:AN1:832:G:C8	2.56	0.41
5:AN1:1401:U:H3	5:AN1:1594:G:H1	1.66	0.41
5:AN1:909:A:H8	5:AN1:2273:G:H21	1.68	0.41
5:AN1:621:C:H2'	5:AN1:622:C:H6	1.86	0.41
5:AN1:741:U:O2'	5:AN1:1657:U:OP1	2.39	0.41
5:AN1:843:G:H2'	5:AN1:844:A:H5''	2.02	0.41
6:B:13:A:H3'	6:B:14:G:H8	1.86	0.41
6:B:43:A:H5'	10:F:92:ARG:HD3	2.03	0.41
7:C:245:VAL:HG12	7:C:251:LYS:HD3	2.03	0.41
4:3:3:VAL:HG22	4:3:36:ARG:HB3	2.03	0.41
5:AN1:1835:G:C5	5:AN1:1923:A:C6	3.09	0.41
5:AN1:2070:U:H2'	5:AN1:2071:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2468:G:N2	5:AN1:2469:U:O2'	2.54	0.41
5:AN1:2842:G:H2'	5:AN1:2843:U:C6	2.56	0.41
5:AN1:2843:U:H2'	5:AN1:2844:G:O4'	2.21	0.41
5:AN1:343:C:H2'	5:AN1:344:A:H8	1.86	0.41
16:L:110:ASN:OD1	16:L:111:GLU:N	2.54	0.41
4:3:18:ARG:HE	4:3:21:GLY:HA2	1.85	0.41
5:AN1:1165:U:H2'	5:AN1:1166:A:C8	2.56	0.41
5:AN1:2170:C:H2'	5:AN1:2171:C:O4'	2.21	0.41
5:AN1:730:C:H2'	5:AN1:731:G:O4'	2.21	0.41
9:E:136:LYS:HE3	9:E:136:LYS:HB2	1.85	0.41
11:G:2:SER:OG	11:G:2:SER:O	2.36	0.41
18:N:3:GLU:HB2	18:N:6:GLN:HG2	2.02	0.41
23:S:15:PHE:CE2	28:X:34:THR:HA	2.56	0.41
5:AN1:674:A:HO2'	5:AN1:2438:C:HO2'	1.67	0.40
5:AN1:2018:U:O2'	5:AN1:2613:U:H5'	2.21	0.40
5:AN1:414:A:H2'	5:AN1:415:U:C6	2.56	0.40
5:AN1:86:C:C2	5:AN1:87:G:C8	3.09	0.40
5:AN1:9:G:H2'	5:AN1:10:U:C6	2.56	0.40
6:B:60:U:H2'	6:B:61:C:H6	1.86	0.40
7:C:123:PRO:O	7:C:128:ASN:ND2	2.51	0.40
10:F:57:MET:SD	10:F:87:CYS:HB2	2.60	0.40
15:K:111:ARG:HG2	15:K:128:ALA:HB3	2.03	0.40
18:N:69:ALA:O	18:N:73:VAL:HG23	2.21	0.40
5:AN1:1464:A:H2'	5:AN1:1465:A:H8	1.85	0.40
5:AN1:1835:G:C2	5:AN1:1836:G:C8	3.09	0.40
5:AN1:8:A:H61	5:AN1:2898:U:H3	1.67	0.40
5:AN1:611:U:H5''	5:AN1:612:A:C8	2.56	0.40
5:AN1:85:C:C2	5:AN1:86:C:C5	3.09	0.40
6:B:66:C:H2'	6:B:67:G:O4'	2.22	0.40
11:G:27:LYS:HB2	11:G:27:LYS:HE2	1.95	0.40
12:H:5:LEU:HB2	12:H:16:GLY:HA2	2.03	0.40
19:O:95:VAL:HG11	19:O:100:LEU:HD21	2.02	0.40
5:AN1:1193:U:H2'	5:AN1:1194:U:H6	1.86	0.40
5:AN1:1784:C:C2	5:AN1:1785:A:C8	3.10	0.40
5:AN1:2110:A:H61	5:AN1:2115:A:N6	2.18	0.40
5:AN1:2533:U:H2'	5:AN1:2534:C:C6	2.56	0.40
5:AN1:2841:U:H5''	19:O:55:ASN:O	2.20	0.40
5:AN1:2853:G:N2	5:AN1:2856:A:OP2	2.52	0.40
6:B:28:C:H1'	6:B:55:A:H61	1.86	0.40
10:F:138:PHE:HB2	10:F:139:PRO:HD2	2.02	0.40
10:F:38:MET:O	10:F:86:GLY:CA	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:7:MET:HB3	14:J:18:ARG:HH11	1.86	0.40
15:K:63:LEU:HA	15:K:64:PRO:HD3	1.94	0.40
19:O:103:LEU:HD22	19:O:111:ALA:HB1	2.02	0.40
19:O:34:LYS:HE2	19:O:41:GLU:HB3	2.03	0.40
5:AN1:569:U:H3'	21:Q:80:ARG:NH2	2.36	0.40
5:AN1:1394:C:H2'	5:AN1:1395:A:C8	2.55	0.40
5:AN1:1786:U:O2'	7:C:208:ALA:HB2	2.22	0.40
5:AN1:1876:U:H2'	5:AN1:1877:C:C6	2.57	0.40
5:AN1:2528:G:N2	5:AN1:2659:G:O2'	2.55	0.40
5:AN1:2806:A:H62	5:AN1:2886:G:H21	1.69	0.40
7:C:30:TYR:CD2	7:C:32:PRO:HD2	2.56	0.40
11:G:53:ALA:HA	11:G:54:PRO:HD3	1.94	0.40
5:AN1:309:G:N2	5:AN1:311:G:H3'	2.37	0.40
5:AN1:943:G:H2'	5:AN1:944:A:H8	1.86	0.40
6:B:80:U:H2'	6:B:81:G:H8	1.86	0.40
23:S:27:GLY:HA2	23:S:90:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	57 (93%)	2 (3%)	2 (3%)	4	20
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	268/274 (98%)	258 (96%)	10 (4%)	0	100	100
8	D	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
9	E	184/200 (92%)	184 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	F	173/178 (97%)	149 (86%)	23 (13%)	1 (1%)	27	64
11	G	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
15	K	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
16	L	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
19	O	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
24	T	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
25	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
26	V	78/85 (92%)	77 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
28	X	60/65 (92%)	60 (100%)	0	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100	100
All	All	3061/3283 (93%)	2972 (97%)	86 (3%)	3 (0%)	56	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	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	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	216/220 (98%)	216 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	144/155 (93%)	144 (100%)	0	100	100
10	F	145/147 (99%)	143 (99%)	2 (1%)	69	89
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	108/108 (100%)	107 (99%)	1 (1%)	81	93
16	L	113/113 (100%)	111 (98%)	2 (2%)	62	86
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	99/102 (97%)	98 (99%)	1 (1%)	78	92
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	82/85 (96%)	81 (99%)	1 (1%)	74	90
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	54/56 (96%)	54 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
All	All	2521/2646 (95%)	2514 (100%)	7 (0%)	93	98

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

Mol	Chain	Res	Type
10	F	3	ARG
10	F	169	LEU
15	K	44	LYS
16	L	10	ARG
16	L	60	ARG
19	O	112	ARG
24	T	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	48	HIS
7	C	58	HIS
7	C	60	GLN
7	C	90	HIS
7	C	117	GLN
7	C	230	HIS
7	C	243	GLN
7	C	250	GLN
8	D	50	GLN
8	D	108	GLN
8	D	139	ASN
8	D	143	HIS
9	E	96	ASN
9	E	114	GLN
10	F	17	GLN
10	F	127	ASN
10	F	135	GLN
11	G	13	ASN
11	G	23	GLN
13	I	40	HIS
13	I	135	GLN
15	K	40	GLN
15	K	107	GLN
15	K	125	GLN
16	L	3	GLN
17	M	72	ASN
18	N	39	GLN
18	N	66	ASN
19	O	13	ASN
19	O	15	GLN

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Mol	Chain	Res	Type
19	O	59	ASN
19	O	78	GLN
20	P	11	HIS
21	Q	82	HIS
21	Q	87	GLN
22	R	37	ASN
22	R	57	ASN
22	R	60	HIS
23	S	29	GLN
24	T	59	GLN
25	U	16	GLN
25	U	75	ASN
25	U	84	HIS
26	V	29	GLN
27	W	6	GLN
28	X	61	GLN
30	Z	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	AN1	2888/2918 (98%)	485 (16%)	8 (0%)
6	B	114/115 (99%)	17 (14%)	1 (0%)
All	All	3002/3033 (98%)	502 (16%)	9 (0%)

All (502) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	34	G
5	AN1	35	A
5	AN1	50	G
5	AN1	53	G
5	AN1	58	G
5	AN1	59	A
5	AN1	67	G
5	AN1	68	A
5	AN1	69	U
5	AN1	70	A
5	AN1	78	A
5	AN1	81	A
5	AN1	82	G

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Mol	Chain	Res	Type
5	AN1	86	C
5	AN1	98	A
5	AN1	102	A
5	AN1	106	U
5	AN1	107	U
5	AN1	108	U
5	AN1	125	A
5	AN1	127	U
5	AN1	133	A
5	AN1	146	U
5	AN1	147	A
5	AN1	169	U
5	AN1	170	A
5	AN1	172	A
5	AN1	179	U
5	AN1	188	A
5	AN1	203	A
5	AN1	206	A
5	AN1	223	A
5	AN1	229	A
5	AN1	230	A
5	AN1	232	C
5	AN1	236	U
5	AN1	255	G
5	AN1	257	G
5	AN1	259	G
5	AN1	262	A
5	AN1	271	C
5	AN1	272	A
5	AN1	273	G
5	AN1	274	C
5	AN1	279	U
5	AN1	280	A
5	AN1	284	U
5	AN1	289	G
5	AN1	291	G
5	AN1	293	U
5	AN1	303	C
5	AN1	313	A
5	AN1	331	G
5	AN1	332	A
5	AN1	336	U

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Mol	Chain	Res	Type
5	AN1	345	C
5	AN1	351	G
5	AN1	356	A
5	AN1	357	C
5	AN1	359	U
5	AN1	366	G
5	AN1	369	G
5	AN1	371	G
5	AN1	385	G
5	AN1	386	U
5	AN1	395	G
5	AN1	403	A
5	AN1	410	G
5	AN1	416	C
5	AN1	423	G
5	AN1	434	C
5	AN1	455	C
5	AN1	479	A
5	AN1	480	G
5	AN1	504	A
5	AN1	508	C
5	AN1	509	C
5	AN1	526	C
5	AN1	529	G
5	AN1	530	C
5	AN1	531	A
5	AN1	541	C
5	AN1	543	U
5	AN1	544	U
5	AN1	545	C
5	AN1	547	U
5	AN1	554	A
5	AN1	561	A
5	AN1	564	U
5	AN1	571	U
5	AN1	573	A
5	AN1	595	G
5	AN1	601	A
5	AN1	612	A
5	AN1	613	U
5	AN1	625	A
5	AN1	635	A

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Mol	Chain	Res	Type
5	AN1	637	U
5	AN1	643	U
5	AN1	644	A
5	AN1	651	U
5	AN1	652	U
5	AN1	654	G
5	AN1	657	G
5	AN1	666	A
5	AN1	667	G
5	AN1	668	A
5	AN1	684	U
5	AN1	692	U
5	AN1	703	A
5	AN1	711	G
5	AN1	712	U
5	AN1	713	A
5	AN1	714	A
5	AN1	719	A
5	AN1	724	G
5	AN1	727	G
5	AN1	728	A
5	AN1	745	U
5	AN1	762	A
5	AN1	763	C
5	AN1	773	G
5	AN1	774	G
5	AN1	780	A
5	AN1	782	G
5	AN1	783	G
5	AN1	803	G
5	AN1	810	C
5	AN1	817	A
5	AN1	825	U
5	AN1	828	G
5	AN1	843	G
5	AN1	851	U
5	AN1	855	G
5	AN1	857	G
5	AN1	880	G
5	AN1	883	C
5	AN1	884	A
5	AN1	888	C

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Mol	Chain	Res	Type
5	AN1	889	G
5	AN1	890	A
5	AN1	894	A
5	AN1	895	C
5	AN1	904	U
5	AN1	908	A
5	AN1	929	C
5	AN1	930	U
5	AN1	938	A
5	AN1	942	A
5	AN1	943	G
5	AN1	950	G
5	AN1	955	U
5	AN1	958	C
5	AN1	971	G
5	AN1	977	A
5	AN1	980	A
5	AN1	993	A
5	AN1	1006	A
5	AN1	1009	U
5	AN1	1010	C
5	AN1	1017	A
5	AN1	1023	G
5	AN1	1028	G
5	AN1	1031	G
5	AN1	1032	U
5	AN1	1036	A
5	AN1	1037	A
5	AN1	1039	G
5	AN1	1040	C
5	AN1	1041	A
5	AN1	1042	U
5	AN1	1043	A
5	AN1	1044	G
5	AN1	1054	A
5	AN1	1057	U
5	AN1	1058	U
5	AN1	1059	G
5	AN1	1061	C
5	AN1	1063	U
5	AN1	1067	A
5	AN1	1070	A

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Mol	Chain	Res	Type
5	AN1	1076	C
5	AN1	1078	U
5	AN1	1079	U
5	AN1	1081	A
5	AN1	1082	A
5	AN1	1085	A
5	AN1	1086	A
5	AN1	1091	U
5	AN1	1101	C
5	AN1	1108	A
5	AN1	1109	G
5	AN1	1110	U
5	AN1	1121	G
5	AN1	1129	U
5	AN1	1130	A
5	AN1	1131	A
5	AN1	1132	C
5	AN1	1140	A
5	AN1	1149	G
5	AN1	1167	U
5	AN1	1170	U
5	AN1	1171	U
5	AN1	1172	U
5	AN1	1173	G
5	AN1	1179	G
5	AN1	1200	A
5	AN1	1201	G
5	AN1	1231	G
5	AN1	1242	A
5	AN1	1245	G
5	AN1	1248	A
5	AN1	1251	G
5	AN1	1267	A
5	AN1	1296	A
5	AN1	1309	C
5	AN1	1324	U
5	AN1	1336	G
5	AN1	1340	C
5	AN1	1360	A
5	AN1	1363	G
5	AN1	1373	A
5	AN1	1374	U

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Mol	Chain	Res	Type
5	AN1	1378	A
5	AN1	1383	G
5	AN1	1390	A
5	AN1	1393	C
5	AN1	1407	U
5	AN1	1408	A
5	AN1	1411	G
5	AN1	1414	A
5	AN1	1415	U
5	AN1	1423	C
5	AN1	1428	A
5	AN1	1432	C
5	AN1	1433	U
5	AN1	1447	G
5	AN1	1448	U
5	AN1	1453	U
5	AN1	1455	U
5	AN1	1456	C
5	AN1	1470	G
5	AN1	1473	G
5	AN1	1477	U
5	AN1	1485	A
5	AN1	1501	C
5	AN1	1502	U
5	AN1	1504	U
5	AN1	1505	A
5	AN1	1520	A
5	AN1	1530	A
5	AN1	1531	C
5	AN1	1533	U
5	AN1	1534	G
5	AN1	1539	G
5	AN1	1540	C
5	AN1	1541	G
5	AN1	1542	A
5	AN1	1545	U
5	AN1	1564	A
5	AN1	1567	A
5	AN1	1574	U
5	AN1	1583	C
5	AN1	1605	G
5	AN1	1606	A

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Mol	Chain	Res	Type
5	AN1	1642	C
5	AN1	1645	U
5	AN1	1646	U
5	AN1	1672	G
5	AN1	1691	U
5	AN1	1712	U
5	AN1	1713	U
5	AN1	1714	G
5	AN1	1717	G
5	AN1	1718	A
5	AN1	1725	U
5	AN1	1726	C
5	AN1	1731	C
5	AN1	1742	G
5	AN1	1746	G
5	AN1	1760	G
5	AN1	1769	A
5	AN1	1776	A
5	AN1	1780	A
5	AN1	1796	C
5	AN1	1797	A
5	AN1	1798	A
5	AN1	1805	A
5	AN1	1812	C
5	AN1	1825	A
5	AN1	1829	C
5	AN1	1830	U
5	AN1	1831	G
5	AN1	1844	A
5	AN1	1855	U
5	AN1	1861	U
5	AN1	1866	U
5	AN1	1871	G
5	AN1	1872	A
5	AN1	1875	C
5	AN1	1885	A
5	AN1	1895	A
5	AN1	1897	A
5	AN1	1899	G
5	AN1	1902	G
5	AN1	1905	C
5	AN1	1907	PSU

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Mol	Chain	Res	Type
5	AN1	1909	A
5	AN1	1910	C
5	AN1	1915	A
5	AN1	1917	G
5	AN1	1925	G
5	AN1	1926	G
5	AN1	1933	A
5	AN1	1934	A
5	AN1	1936	U
5	AN1	1940	U
5	AN1	1950	G
5	AN1	1951	U
5	AN1	1960	G
5	AN1	1963	C
5	AN1	1966	A
5	AN1	1967	U
5	AN1	1968	G
5	AN1	1978	U
5	AN1	1987	U
5	AN1	1989	U
5	AN1	1993	C
5	AN1	2018	U
5	AN1	2019	C
5	AN1	2025	G
5	AN1	2027	A
5	AN1	2029	A
5	AN1	2030	U
5	AN1	2039	C
5	AN1	2051	C
5	AN1	2052	G
5	AN1	2056	A
5	AN1	2057	G
5	AN1	2058	A
5	AN1	2065	7MG
5	AN1	2091	A
5	AN1	2092	C
5	AN1	2104	U
5	AN1	2106	G
5	AN1	2107	U
5	AN1	2108	G
5	AN1	2111	G
5	AN1	2112	G

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Mol	Chain	Res	Type
5	AN1	2113	A
5	AN1	2114	U
5	AN1	2115	A
5	AN1	2116	G
5	AN1	2120	G
5	AN1	2121	G
5	AN1	2122	A
5	AN1	2123	G
5	AN1	2127	U
5	AN1	2128	U
5	AN1	2129	G
5	AN1	2133	C
5	AN1	2142	U
5	AN1	2143	A
5	AN1	2145	U
5	AN1	2146	U
5	AN1	2148	C
5	AN1	2149	A
5	AN1	2152	G
5	AN1	2153	G
5	AN1	2154	A
5	AN1	2155	G
5	AN1	2157	C
5	AN1	2158	G
5	AN1	2166	A
5	AN1	2167	A
5	AN1	2168	U
5	AN1	2169	A
5	AN1	2171	C
5	AN1	2174	C
5	AN1	2178	G
5	AN1	2188	G
5	AN1	2194	A
5	AN1	2200	G
5	AN1	2221	A
5	AN1	2222	C
5	AN1	2234	G
5	AN1	2235	G
5	AN1	2261	U
5	AN1	2275	G
5	AN1	2279	U
5	AN1	2283	A

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Mol	Chain	Res	Type
5	AN1	2301	U
5	AN1	2304	G
5	AN1	2305	A
5	AN1	2308	U
5	AN1	2312	G
5	AN1	2314	G
5	AN1	2316	A
5	AN1	2321	A
5	AN1	2323	A
5	AN1	2346	C
5	AN1	2355	C
5	AN1	2357	A
5	AN1	2378	G
5	AN1	2379	G
5	AN1	2380	U
5	AN1	2381	C
5	AN1	2398	U
5	AN1	2399	C
5	AN1	2408	A
5	AN1	2425	G
5	AN1	2426	A
5	AN1	2429	A
5	AN1	2430	A
5	AN1	2431	A
5	AN1	2437	U
5	AN1	2443	G
5	AN1	2444	A
5	AN1	2446	A
5	AN1	2468	G
5	AN1	2469	U
5	AN1	2470	U
5	AN1	2472	A
5	AN1	2473	U
5	AN1	2487	U
5	AN1	2494	C
5	AN1	2498	G
5	AN1	2501	G
5	AN1	2503	C
5	AN1	2514	A
5	AN1	2516	C
5	AN1	2530	A
5	AN1	2543	A

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Mol	Chain	Res	Type
5	AN1	2548	OMU
5	AN1	2550	U
5	AN1	2562	A
5	AN1	2563	G
5	AN1	2568	A
5	AN1	2598	A
5	AN1	2599	G
5	AN1	2605	U
5	AN1	2606	C
5	AN1	2607	C
5	AN1	2609	U
5	AN1	2611	U
5	AN1	2625	U
5	AN1	2635	A
5	AN1	2642	C
5	AN1	2657	G
5	AN1	2661	A
5	AN1	2685	U
5	AN1	2686	A
5	AN1	2710	G
5	AN1	2722	U
5	AN1	2725	U
5	AN1	2730	A
5	AN1	2735	U
5	AN1	2740	G
5	AN1	2744	A
5	AN1	2753	A
5	AN1	2754	A
5	AN1	2761	A
5	AN1	2774	A
5	AN1	2776	A
5	AN1	2787	A
5	AN1	2788	G
5	AN1	2793	U
5	AN1	2794	U
5	AN1	2796	U
5	AN1	2797	G
5	AN1	2800	C
5	AN1	2804	A
5	AN1	2816	G
5	AN1	2817	A
5	AN1	2829	U

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Mol	Chain	Res	Type
5	AN1	2831	A
5	AN1	2845	G
5	AN1	2851	U
5	AN1	2853	G
5	AN1	2857	U
5	AN1	2863	A
5	AN1	2868	G
5	AN1	2875	A
5	AN1	2897	C
5	AN1	2898	U
6	B	2	C
6	B	10	C
6	B	11	A
6	B	14	G
6	B	23	A
6	B	32	A
6	B	39	C
6	B	40	C
6	B	42	G
6	B	50	A
6	B	65	G
6	B	86	U
6	B	87	A
6	B	105	C
6	B	106	A
6	B	108	C
6	B	109	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AN1	355	C
5	AN1	356	A
5	AN1	368	C
5	AN1	478	A
5	AN1	782	G
5	AN1	1538	A
5	AN1	2170	C
5	AN1	2379	G
6	B	108	C

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	PSU	AN1	1907	5	16,21,22	1.14	1 (6%)	20,30,33	3.13	6 (30%)
5	3TD	AN1	1911	5	16,22,23	3.24	6 (37%)	19,32,35	1.49	3 (15%)
5	PSU	AN1	1913	5	16,21,22	1.06	1 (6%)	20,30,33	3.20	7 (35%)
5	5MU	AN1	1935	5	13,22,23	1.60	2 (15%)	14,32,35	3.01	2 (14%)
5	6MZ	AN1	2026	5	17,25,26	2.00	3 (17%)	15,36,39	4.36	5 (33%)
5	7MG	AN1	2065	5	20,26,27	4.49	10 (50%)	24,39,42	1.77	6 (25%)
5	OMG	AN1	2247	5	18,26,27	3.51	7 (38%)	22,38,41	1.81	5 (22%)
5	2MG	AN1	2441	5	18,26,27	4.61	7 (38%)	19,38,41	2.23	8 (42%)
5	PSU	AN1	2453	5	16,21,22	1.15	2 (12%)	20,30,33	3.10	6 (30%)
5	2MA	AN1	2499	5	16,25,26	4.14	5 (31%)	17,37,40	2.50	5 (29%)
5	PSU	AN1	2500	5	16,21,22	1.15	1 (6%)	20,30,33	3.14	6 (30%)
5	OMU	AN1	2548	5	14,22,23	3.53	5 (35%)	17,31,34	0.64	0
5	PSU	AN1	2576	5	16,21,22	1.14	2 (12%)	20,30,33	3.09	5 (25%)
5	PSU	AN1	2601	5	16,21,22	1.13	1 (6%)	20,30,33	3.14	6 (30%)
5	PSU	AN1	952	5	16,21,22	1.14	1 (6%)	20,30,33	3.13	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	AN1	1907	5	-	1/7/25/26	0/2/2/2
5	3TD	AN1	1911	5	-	3/7/25/26	0/2/2/2
5	PSU	AN1	1913	5	-	4/7/25/26	0/2/2/2
5	5MU	AN1	1935	5	-	0/3/25/26	0/2/2/2
5	6MZ	AN1	2026	5	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7MG	AN1	2065	5	-	2/7/37/38	0/3/3/3
5	OMG	AN1	2247	5	-	0/5/27/28	0/3/3/3
5	2MG	AN1	2441	5	-	0/5/27/28	0/3/3/3
5	PSU	AN1	2453	5	-	0/7/25/26	0/2/2/2
5	2MA	AN1	2499	5	-	1/3/25/26	0/3/3/3
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2
5	OMU	AN1	2548	5	-	2/5/27/28	0/2/2/2
5	PSU	AN1	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	2601	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	952	5	-	0/7/25/26	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2441	2MG	C2-N2	13.64	1.45	1.34
5	AN1	2065	7MG	C4-N3	10.51	1.47	1.34
5	AN1	2065	7MG	C6-C5	9.37	1.52	1.41
5	AN1	2499	2MA	C4-N3	9.09	1.50	1.35
5	AN1	2441	2MG	C4-N3	8.80	1.49	1.35
5	AN1	2247	OMG	C4-N3	8.54	1.49	1.35
5	AN1	2499	2MA	C6-C5	8.05	1.54	1.41
5	AN1	2548	OMU	C4-N3	7.56	1.46	1.33
5	AN1	2499	2MA	C2-N3	7.54	1.47	1.34
5	AN1	1911	3TD	C6-C5	7.39	1.49	1.38
5	AN1	2548	OMU	C6-N1	7.11	1.45	1.35
5	AN1	2441	2MG	C6-C5	6.99	1.53	1.41
5	AN1	2247	OMG	C6-C5	6.86	1.53	1.41
5	AN1	2065	7MG	C6-N1	6.85	1.45	1.33
5	AN1	2026	6MZ	C6-N6	6.77	1.45	1.35
5	AN1	2065	7MG	C2-N3	6.77	1.47	1.35
5	AN1	2065	7MG	C2-N1	6.56	1.47	1.35
5	AN1	2499	2MA	C2-N1	6.06	1.44	1.34
5	AN1	2247	OMG	C6-N1	6.06	1.43	1.33
5	AN1	2548	OMU	C2-N3	6.06	1.50	1.38
5	AN1	2065	7MG	C2-N2	5.94	1.45	1.33
5	AN1	2441	2MG	C6-N1	5.90	1.43	1.33
5	AN1	1911	3TD	C2-N1	5.76	1.49	1.38
5	AN1	1911	3TD	C4-N3	5.55	1.46	1.38
5	AN1	1911	3TD	C6-N1	5.49	1.46	1.34
5	AN1	2247	OMG	C2-N2	4.91	1.43	1.33
5	AN1	2499	2MA	C6-N1	4.90	1.44	1.34
5	AN1	2247	OMG	C2-N1	4.79	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2548	OMU	C6-C5	4.66	1.48	1.38
5	AN1	1935	5MU	C4-N3	-4.37	1.25	1.33
5	AN1	2441	2MG	C2-N3	3.80	1.46	1.34
5	AN1	2065	7MG	C4-N9	3.50	1.44	1.38
5	AN1	1913	PSU	C4-N3	3.10	1.38	1.33
5	AN1	2441	2MG	C2-N1	3.08	1.44	1.34
5	AN1	1907	PSU	C4-N3	3.06	1.38	1.33
5	AN1	2500	PSU	C4-N3	3.03	1.38	1.33
5	AN1	952	PSU	C4-N3	3.00	1.38	1.33
5	AN1	2601	PSU	C4-N3	2.97	1.38	1.33
5	AN1	2453	PSU	C4-N3	2.97	1.38	1.33
5	AN1	2576	PSU	C4-N3	2.96	1.38	1.33
5	AN1	2026	6MZ	C5-C4	-2.93	1.33	1.40
5	AN1	2065	7MG	C5-C4	2.70	1.43	1.38
5	AN1	1911	3TD	C5-C1'	-2.65	1.50	1.52
5	AN1	2247	OMG	C2-N3	2.55	1.46	1.35
5	AN1	1935	5MU	O4-C4	-2.51	1.18	1.24
5	AN1	2247	OMG	O6-C6	-2.46	1.18	1.24
5	AN1	2065	7MG	C8-N9	2.35	1.51	1.45
5	AN1	2065	7MG	O6-C6	-2.32	1.18	1.24
5	AN1	1911	3TD	O4-C4	-2.24	1.19	1.24
5	AN1	2026	6MZ	C2-N3	2.24	1.35	1.32
5	AN1	2441	2MG	O6-C6	-2.24	1.18	1.24
5	AN1	2548	OMU	O4-C4	-2.23	1.18	1.24
5	AN1	2453	PSU	C5-C1'	-2.07	1.50	1.52
5	AN1	2576	PSU	O4'-C1'	-2.01	1.41	1.44

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	2026	6MZ	C1'-N9-C4	-13.54	103.25	126.64
5	AN1	1913	PSU	N1-C2-N3	-10.64	119.97	128.43
5	AN1	2601	PSU	N1-C2-N3	-10.41	120.15	128.43
5	AN1	2576	PSU	N1-C2-N3	-10.41	120.16	128.43
5	AN1	2453	PSU	N1-C2-N3	-10.39	120.17	128.43
5	AN1	1907	PSU	N1-C2-N3	-10.39	120.17	128.43
5	AN1	952	PSU	N1-C2-N3	-10.38	120.18	128.43
5	AN1	2500	PSU	N1-C2-N3	-10.27	120.26	128.43
5	AN1	1935	5MU	C5-C6-N1	-8.60	112.84	122.15
5	AN1	2026	6MZ	C5-C6-N6	7.71	133.12	120.37
5	AN1	2499	2MA	C1'-N9-C4	7.23	139.13	126.64
5	AN1	1935	5MU	C4-N3-C2	7.05	121.09	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	1913	PSU	C4-N3-C2	5.98	120.19	115.14
5	AN1	1907	PSU	C4-N3-C2	5.58	119.85	115.14
5	AN1	952	PSU	C4-N3-C2	5.54	119.82	115.14
5	AN1	2576	PSU	C4-N3-C2	5.53	119.81	115.14
5	AN1	2500	PSU	C4-N3-C2	5.47	119.76	115.14
5	AN1	2601	PSU	C4-N3-C2	5.39	119.69	115.14
5	AN1	2453	PSU	C4-N3-C2	5.33	119.64	115.14
5	AN1	2247	OMG	N3-C2-N1	-5.28	120.10	127.25
5	AN1	2499	2MA	C2-N3-C4	5.14	119.73	115.53
5	AN1	2026	6MZ	N3-C2-N1	-5.04	120.56	128.68
5	AN1	1913	PSU	C5-C4-N3	-4.53	119.52	125.36
5	AN1	1907	PSU	C5-C4-N3	-4.44	119.64	125.36
5	AN1	2500	PSU	C5-C4-N3	-4.44	119.64	125.36
5	AN1	2576	PSU	C5-C4-N3	-4.44	119.64	125.36
5	AN1	952	PSU	C5-C4-N3	-4.40	119.69	125.36
5	AN1	2453	PSU	C5-C4-N3	-4.33	119.79	125.36
5	AN1	2441	2MG	C2-N3-C4	4.29	120.15	115.28
5	AN1	2601	PSU	C5-C4-N3	-4.28	119.84	125.36
5	AN1	2247	OMG	C2-N3-C4	4.20	120.15	115.36
5	AN1	2065	7MG	C6-C5-C4	4.03	119.53	115.20
5	AN1	2441	2MG	C1'-N9-C4	-3.97	119.77	126.64
5	AN1	2441	2MG	N3-C2-N1	-3.91	120.13	126.22
5	AN1	2065	7MG	C5-C4-N3	-3.65	120.37	126.47
5	AN1	1911	3TD	C5-C6-N1	-3.55	119.99	124.44
5	AN1	2453	PSU	C5-C6-N1	-3.47	120.10	124.44
5	AN1	2500	PSU	C5-C1'-C2'	-3.38	109.29	115.32
5	AN1	2500	PSU	C5-C6-N1	-3.34	120.25	124.44
5	AN1	2065	7MG	N1-C2-N3	-3.34	120.13	125.42
5	AN1	2601	PSU	C5-C6-N1	-3.34	120.26	124.44
5	AN1	2453	PSU	C6-N1-C2	3.30	120.58	115.32
5	AN1	2576	PSU	C5-C6-N1	-3.30	120.31	124.44
5	AN1	2601	PSU	C6-N1-C2	3.28	120.55	115.32
5	AN1	1907	PSU	C5-C6-N1	-3.27	120.34	124.44
5	AN1	952	PSU	C5-C6-N1	-3.25	120.36	124.44
5	AN1	2576	PSU	C6-N1-C2	3.23	120.47	115.32
5	AN1	1907	PSU	C6-N1-C2	3.23	120.46	115.32
5	AN1	2601	PSU	C5-C1'-C2'	-3.22	109.57	115.32
5	AN1	2500	PSU	C6-N1-C2	3.20	120.42	115.32
5	AN1	952	PSU	C6-N1-C2	3.20	120.42	115.32
5	AN1	2441	2MG	CM2-N2-C2	-3.17	119.77	123.59
5	AN1	1913	PSU	C6-N1-C2	3.13	120.31	115.32
5	AN1	2441	2MG	N2-C2-N3	3.13	119.97	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	1911	3TD	C6-N1-C2	3.12	120.30	115.32
5	AN1	2499	2MA	N3-C2-N1	-3.08	119.95	125.70
5	AN1	952	PSU	C5-C1'-C2'	-3.06	109.85	115.32
5	AN1	2441	2MG	N2-C2-N1	3.06	119.90	116.96
5	AN1	2026	6MZ	C2-N1-C6	2.82	119.12	116.62
5	AN1	2065	7MG	C6-N1-C2	2.81	120.06	116.06
5	AN1	2065	7MG	C5-C4-N9	2.80	110.23	106.29
5	AN1	1907	PSU	C5-C1'-C2'	-2.79	110.35	115.32
5	AN1	1913	PSU	C5-C6-N1	-2.76	120.99	124.44
5	AN1	2499	2MA	C5-C6-N1	-2.75	120.09	123.10
5	AN1	1911	3TD	C5-C1'-C2'	-2.71	110.49	115.32
5	AN1	2441	2MG	C5-C6-N1	-2.45	120.06	123.47
5	AN1	2247	OMG	C6-N1-C2	2.44	119.53	116.06
5	AN1	2441	2MG	C6-N1-C2	2.44	119.54	115.18
5	AN1	2026	6MZ	C9-N6-C6	-2.43	120.78	122.87
5	AN1	2247	OMG	C5-C6-N1	-2.41	120.11	123.47
5	AN1	1913	PSU	O4'-C1'-C5	2.30	113.49	109.93
5	AN1	2453	PSU	C5-C1'-C2'	-2.30	111.22	115.32
5	AN1	2065	7MG	C2-N3-C4	2.22	120.16	113.94
5	AN1	1913	PSU	O4'-C1'-C2'	2.09	108.05	104.66
5	AN1	2247	OMG	C1'-N9-C4	2.09	130.24	126.64
5	AN1	2499	2MA	CM2-C2-N1	2.02	120.31	117.16

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AN1	1913	PSU	O4'-C1'-C5-C4
5	AN1	1913	PSU	O4'-C1'-C5-C6
5	AN1	2548	OMU	C3'-C4'-C5'-O5'
5	AN1	2548	OMU	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	O4'-C4'-C5'-O5'
5	AN1	1911	3TD	C4'-C5'-O5'-P
5	AN1	1907	PSU	C4'-C5'-O5'-P
5	AN1	2499	2MA	O4'-C4'-C5'-O5'
5	AN1	1913	PSU	O4'-C4'-C5'-O5'
5	AN1	2065	7MG	O4'-C4'-C5'-O5'
5	AN1	2065	7MG	C3'-C4'-C5'-O5'
5	AN1	1913	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AN1	1911	3TD	1	0
5	AN1	2026	6MZ	1	0
5	AN1	2499	2MA	2	0
5	AN1	2500	PSU	1	0
5	AN1	2576	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 108 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.