



wwPDB EM Map/Model Validation Report ⓘ

May 12, 2016 – 11:27 AM EDT

PDB ID : 5IT9
EMDB ID: : EMD-8124
Title : Structure of the yeast *Kluyveromyces lactis* small ribosomal subunit in complex with the cricket paralysis virus IRES.
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on : 2016-03-16
Resolution : 3.80 Å(reported)
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

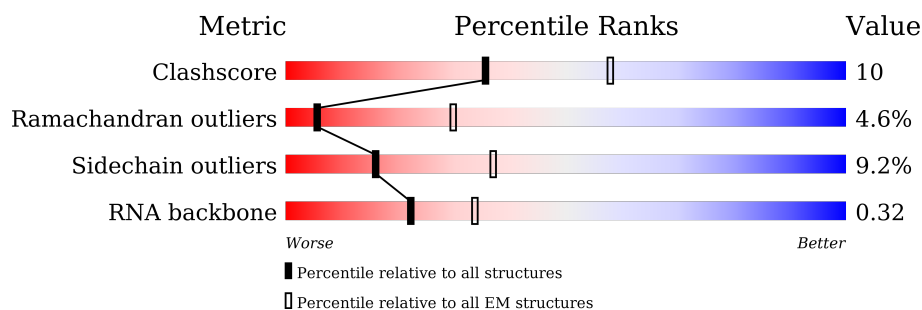
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.
























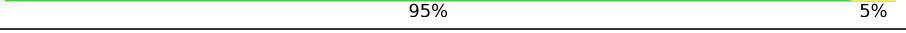



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	206	76% 22% .
2	B	214	89% 10% .
3	C	217	83% 15% .
4	D	223	87% 13%
5	E	260	88% 11% .
6	F	206	78% 20% .
7	G	226	80% 16% . .
8	H	184	82% 17% .

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Mol	Chain	Length	Quality of chain
9	I	200	 71%19%••6%
10	J	182	 73%19%8%
11	K	96	 80%20%
12	L	155	 88%10%•
13	M	122	 82%16%•
14	N	150	 86%13%•
15	O	127	 86%13%••
16	P	123	 77%19%••
17	Q	141	 84%13%•
18	R	129	 82%16%•
19	S	145	 76%21%••
20	T	143	 86%12%•
21	U	106	 85%14%•
22	V	87	 85%15%
23	W	129	 72%24%•
24	X	145	 78%19%••
25	Y	134	 75%19%5%•
26	Z	70	 56%31%11%•
27	a	100	 80%16%•
28	b	82	 90%10%
29	c	63	 95%5%
30	d	53	 92%8%
31	e	55	 87%13%
32	f	69	 80%17%•
33	g	324	 92%6%•

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Mol	Chain	Length	Quality of chain
34	2	1780	<div><div></div><div>36%</div><div>47%</div><div>16%</div><div></div></div>
35	i	192	<div><div></div><div>44%</div><div>55%</div><div></div></div>

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 80144 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 Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 2 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 3 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 4 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 5 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 7 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 8 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 9 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 10 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 11 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 12 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 13 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			922	575	167	180			

- Molecule 14 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 15 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 16 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 17 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 18 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	129	Total	C	N	O	S	0	0
			1031	641	193	194	3		

- Molecule 19 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 20 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 21 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 22 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 23 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 24 is a protein called Ribosomal protein uS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	145	Total	C	N	O	S	0	0
			1127	713	219	192	3		

- Molecule 25 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 26 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 27 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	100	Total	C	N	O	S	0	0
			798	491	170	131	6		

- Molecule 28 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	82	Total	C	N	O	S	0	0
			617	384	113	114	6		

- Molecule 29 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 30 is a protein called Ribosomal protein eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 31 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	55	Total	C	N	O	S	0	0
			443	276	90	76	1		

- Molecule 32 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 33 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 35 is a RNA chain called Cricket paralysis virus IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	192	Total	C	N	O	P	0	0
			3968	1774	669	1333	192		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	6176	C	U	conflict	GB 8895506

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	X	1	Total	Mg	0
			1	1	
36	G	1	Total	Mg	0
			1	1	
36	2	76	Total	Mg	0
			76	76	
36	T	1	Total	Mg	0
			1	1	
36	N	1	Total	Mg	0
			1	1	

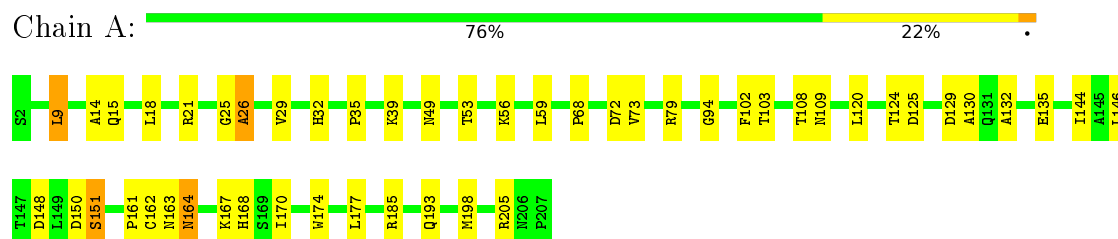
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	b	1	Total	Zn	0
			1	1	
37	a	1	Total	Zn	0
			1	1	
37	f	1	Total	Zn	0
			1	1	

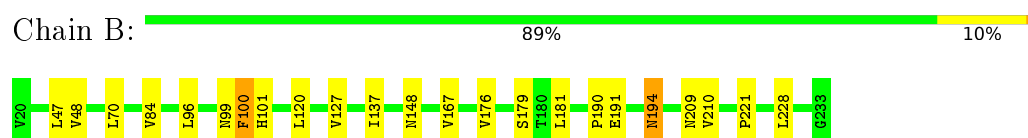
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

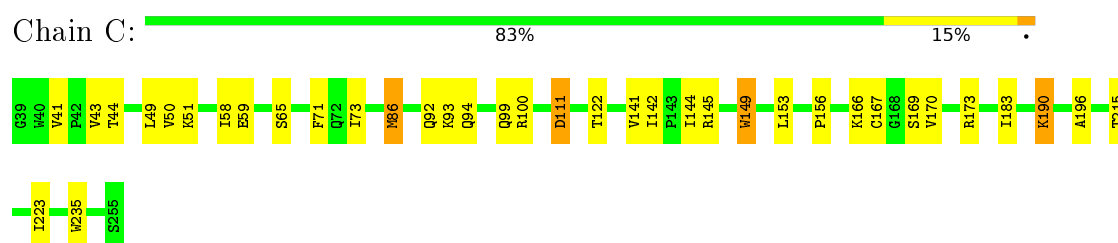
• Molecule 1: Ribosomal protein uS2



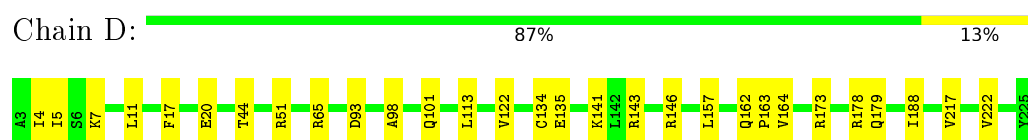
• Molecule 2: Ribosomal protein eS1



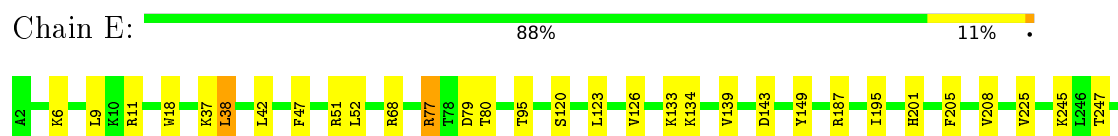
• Molecule 3: Ribosomal protein uS5



• Molecule 4: Ribosomal protein uS3


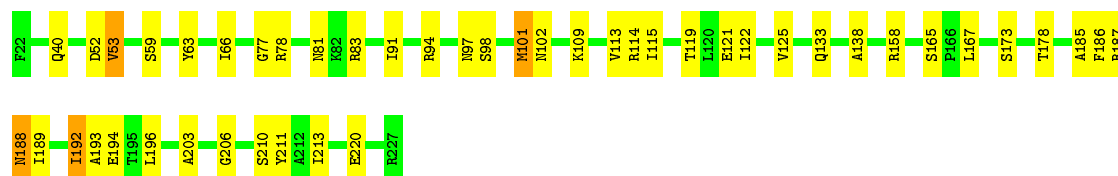


• Molecule 5: Ribosomal protein eS4


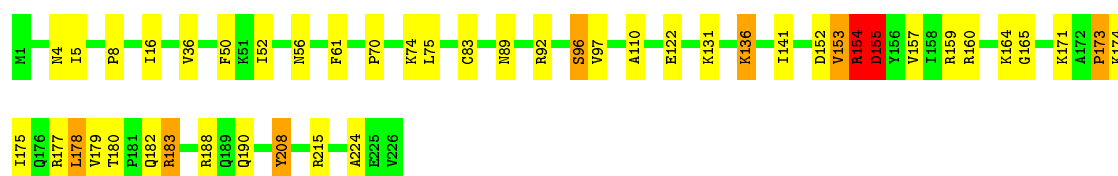


L261


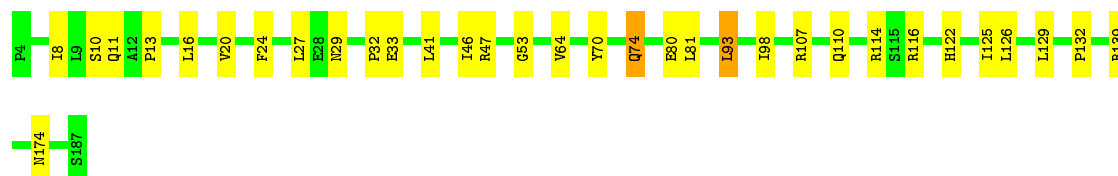
- Molecule 6: Ribosomal protein uS7

Chain F:  78% 20%

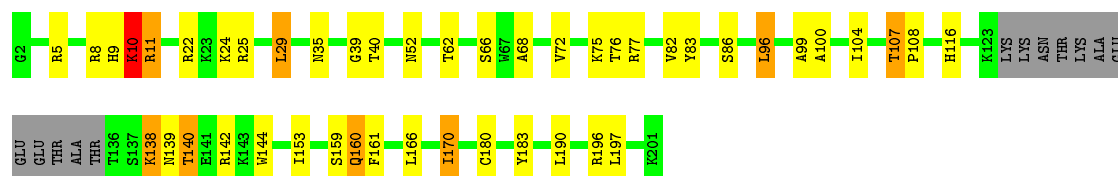
- Molecule 7: Ribosomal protein eS6

Chain G:  80% 16%

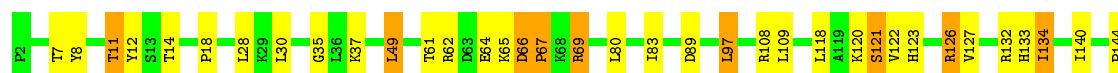
- Molecule 8: Ribosomal protein eS7

Chain H:  82% 17%

- Molecule 9: Ribosomal protein eS8

Chain I:  71% 19% 6%

- Molecule 10: Ribosomal protein uS4

Chain J:  73% 19% 8%



- Molecule 11: Ribosomal protein eS10

Chain K: 80% 20%



- Molecule 12: Ribosomal protein uS17

Chain L: 88% 10%



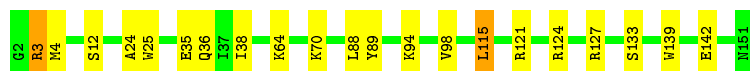
- Molecule 13: Ribosomal protein eS12

Chain M: 82% 16%



- Molecule 14: Ribosomal protein uS15

Chain N: 86% 13%



- Molecule 15: Ribosomal protein uS14

Chain O: 86% 13%



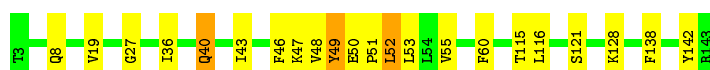
- Molecule 16: Ribosomal protein uS19

Chain P: 77% 19%

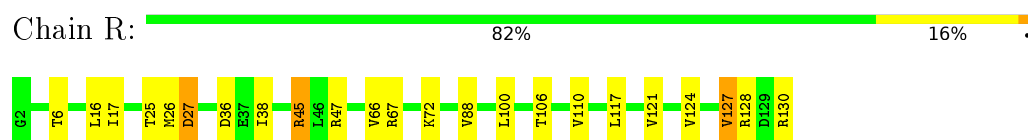


- Molecule 17: Ribosomal protein uS9

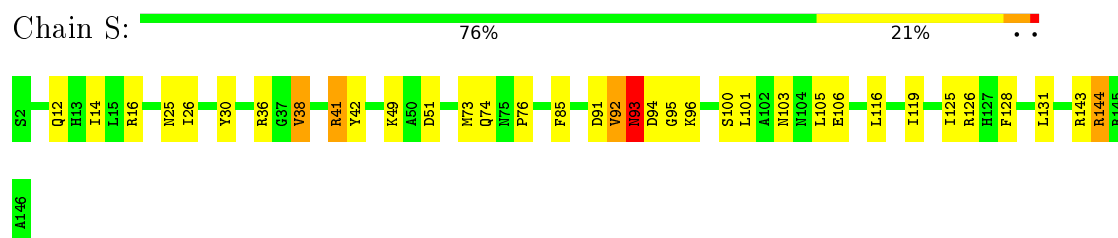
Chain Q: 84% 13%



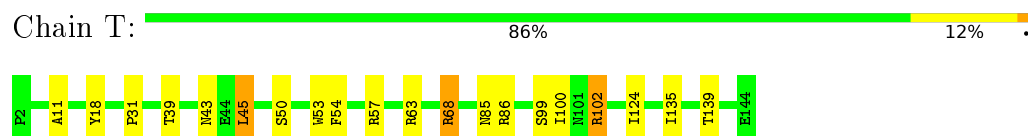
- Molecule 18: Ribosomal protein eS17



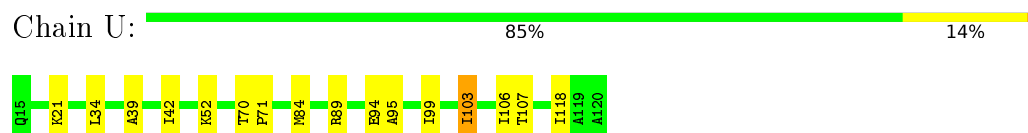
- Molecule 19: Ribosomal protein uS13



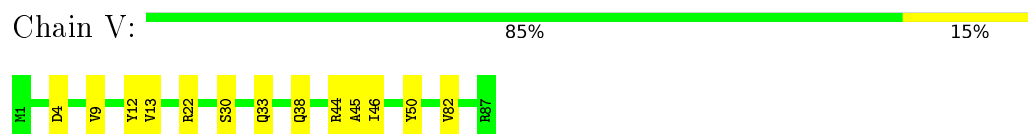
- Molecule 20: Ribosomal protein eS19



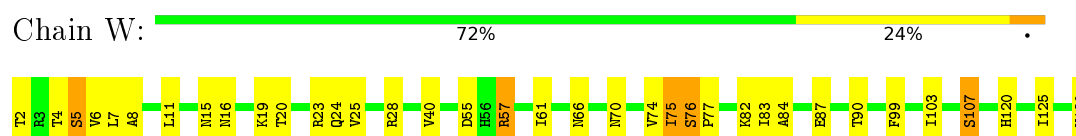
- Molecule 21: Ribosomal protein uS10



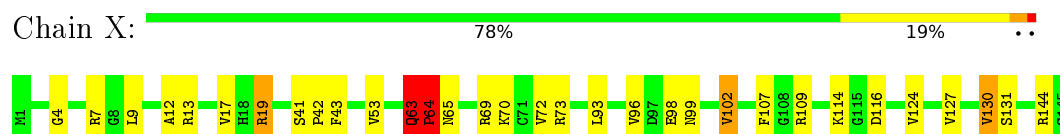
- Molecule 22: Ribosomal protein eS21




- Molecule 23: Ribosomal protein uS8

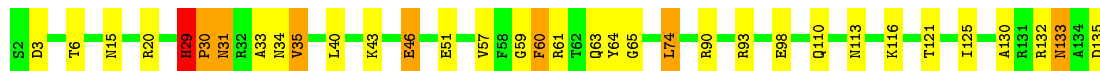


- Molecule 24: Ribosomal protein uS21



- Molecule 25: Ribosomal protein eS24

Chain Y:  75% 19% 5% .




- Molecule 26: Ribosomal protein eS25

Chain Z:  56% 31% 11% .




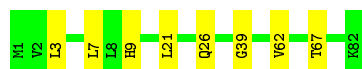
- Molecule 27: Ribosomal protein eS26

Chain a:  80% 16% .



- Molecule 28: Ribosomal protein eS27

Chain b:  90% 10%



- Molecule 29: Ribosomal protein eS28

Chain c:  95% 5%




- Molecule 30: Ribosomal protein eS29

Chain d:  92% 8%




- Molecule 31: Ribosomal protein eS30

Chain e:  87% 13%



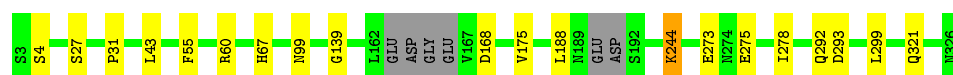
- Molecule 32: Ribosomal protein eS31

Chain f:  80% 17% .



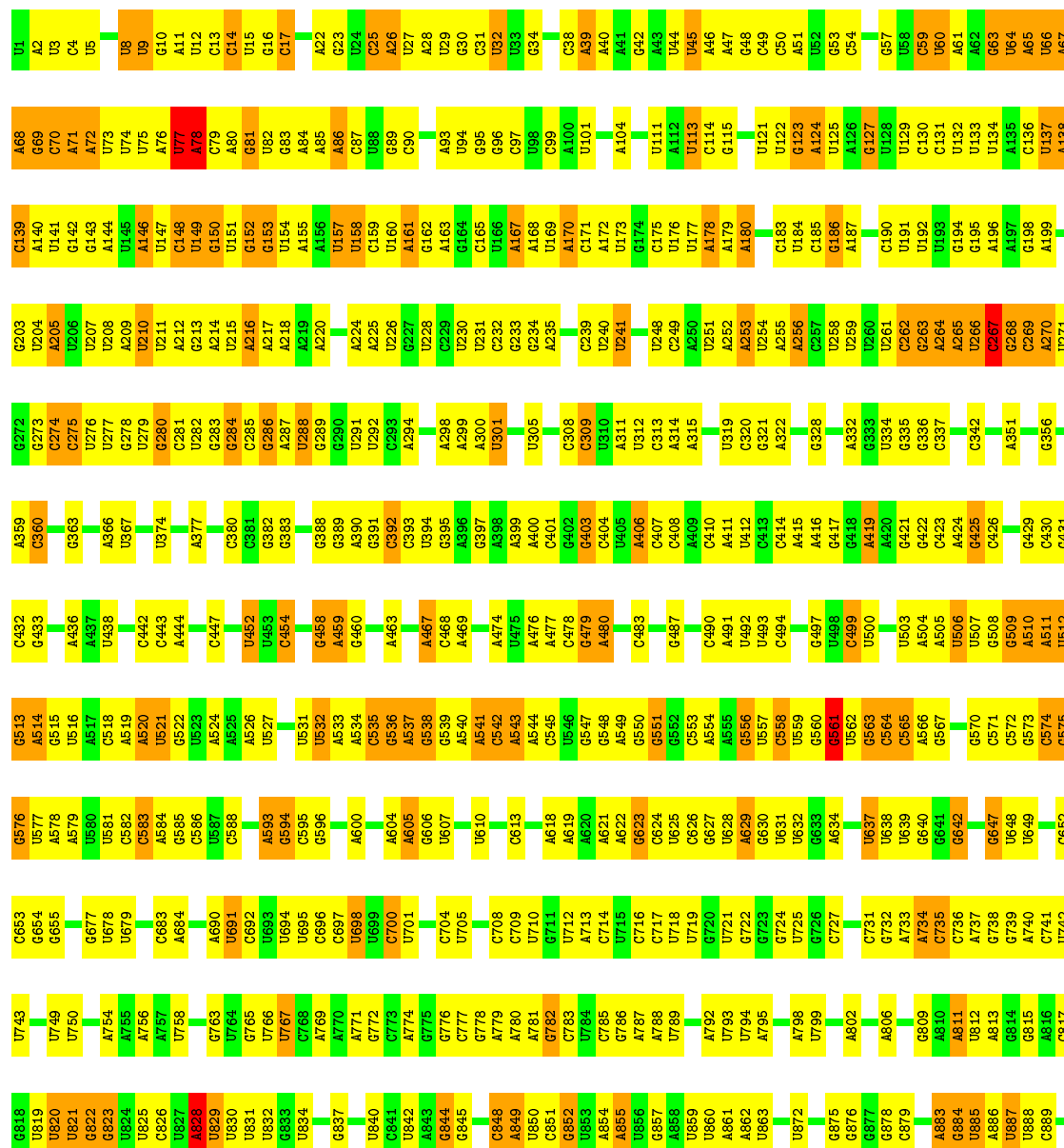
• Molecule 33: Ribosomal protein RACK1

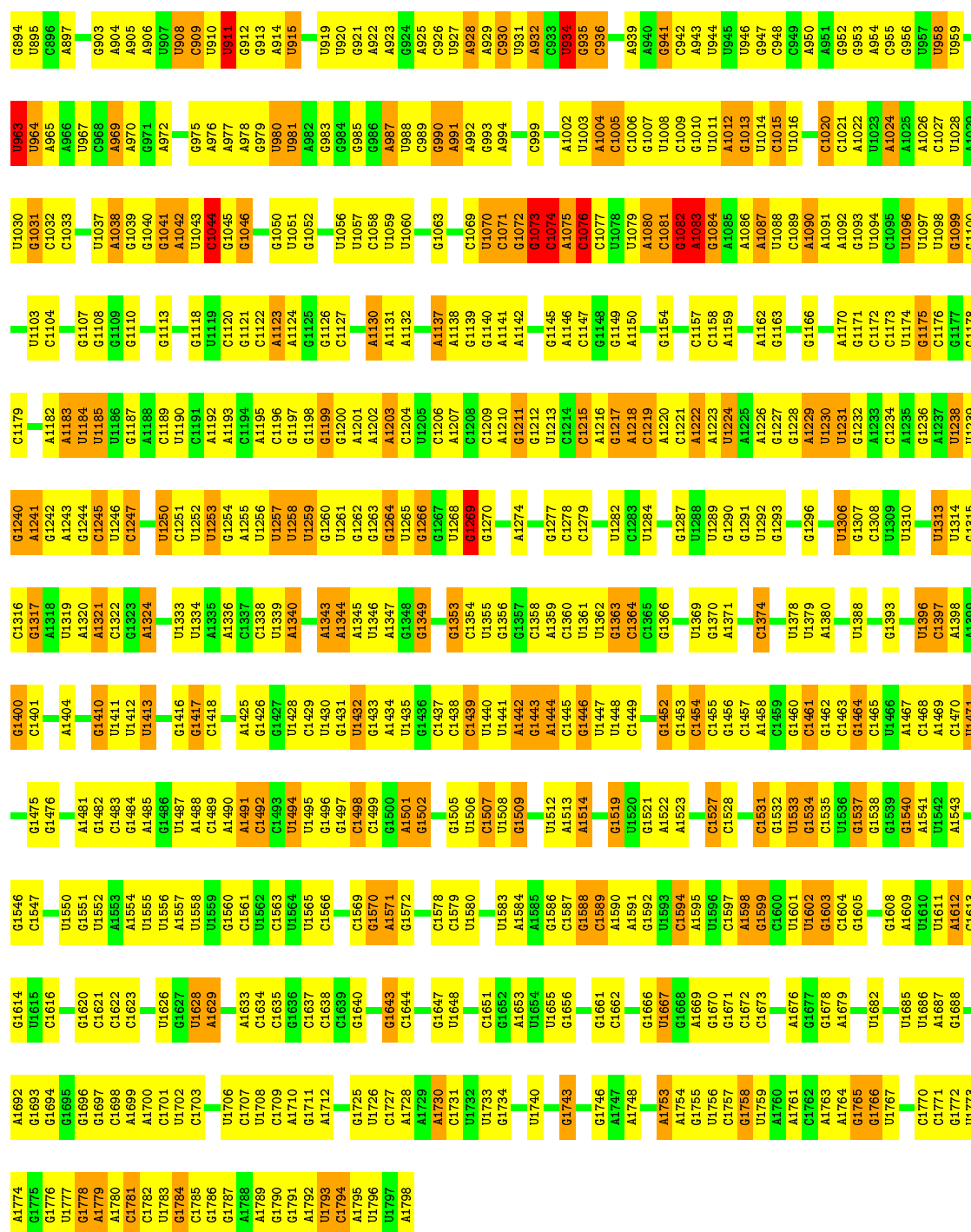
Chain g:  92% 6% .



• Molecule 34: 18S ribosomal RNA

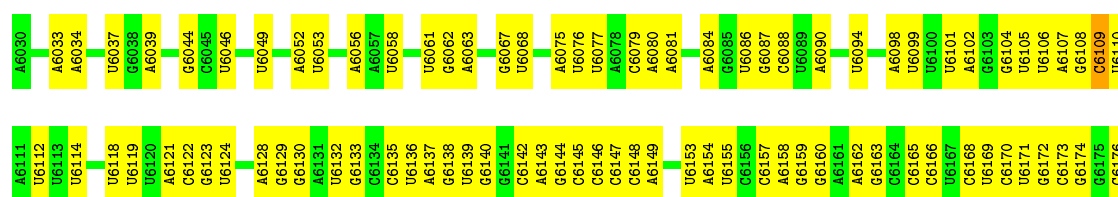
Chain 2:  36% 47% 16% .





• Molecule 35: Cricket paralysis virus IRES RNA

Chain i:



U6177	U6178	U6179	U6180	U6181	A6182	G6183	A6184	U6185	U6186	A6187	G6192	A6197	A6198	A6199	A6200	C6201	C6202	U6210	U6211	U6212	A6213	C6218	U6219	A6220	C6221
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	54481	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.39	0/1656	0.77	0/2264
10	J	0.44	1/1495 (0.1%)	0.90	3/2001 (0.1%)
11	K	0.40	0/831	0.68	0/1123
12	L	0.36	0/1276	0.67	0/1718
13	M	0.40	0/929	0.76	0/1255
14	N	0.40	0/1210	0.84	0/1628
15	O	0.40	0/953	0.77	0/1279
16	P	0.53	1/1000 (0.1%)	0.80	1/1343 (0.1%)
17	Q	0.38	0/1125	0.75	1/1510 (0.1%)
18	R	0.40	0/1042	0.84	0/1399
19	S	0.45	1/1212 (0.1%)	0.81	2/1629 (0.1%)
2	B	0.38	0/1747	0.71	0/2353
20	T	0.36	0/1129	0.75	0/1520
21	U	0.35	0/857	0.69	0/1158
22	V	0.37	0/696	0.69	0/938
23	W	0.40	0/1039	0.81	0/1399
24	X	0.39	0/1145	0.81	1/1526 (0.1%)
25	Y	0.39	0/1075	0.77	0/1433
26	Z	0.42	0/567	0.81	1/762 (0.1%)
27	a	0.40	0/810	0.82	0/1084
28	b	0.34	0/627	0.67	0/847
29	c	0.37	0/496	0.73	0/666
3	C	0.37	0/1659	0.71	0/2252
30	d	0.38	0/457	0.64	0/607
31	e	0.36	0/450	0.68	0/599
32	f	0.42	0/562	0.67	0/751
33	g	0.35	0/2521	0.58	0/3431
34	2	0.34	14/42269 (0.0%)	0.78	26/65862 (0.0%)
35	i	0.34	1/4425 (0.0%)	0.72	1/6875 (0.0%)
4	D	0.36	0/1769	0.70	0/2378
5	E	0.36	0/2122	0.67	0/2861
6	F	0.38	0/1628	0.79	0/2198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	G	0.46	2/1835 (0.1%)	0.80	2/2451 (0.1%)
8	H	0.38	0/1507	0.73	0/2028
9	I	0.40	0/1519	0.79	0/2033
All	All	0.37	20/85640 (0.0%)	0.76	38/125161 (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
1	A	0	2
10	J	0	1
15	O	0	1
17	Q	0	2
22	V	0	1
23	W	0	1
26	Z	0	1
27	a	0	1
34	2	0	7
7	G	0	1
All	All	0	18

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	1073	G	C2-N2	-13.62	1.21	1.34
34	2	1074	C	C4-N4	11.59	1.44	1.33
34	2	1072	G	C2-N2	10.69	1.45	1.34
34	2	1073	G	N1-C2	-10.45	1.29	1.37
34	2	1073	G	C6-O6	-10.32	1.14	1.24
34	2	934	U	O3'-P	-10.18	1.49	1.61
35	i	6109	C	O3'-P	-9.66	1.49	1.61
34	2	1044	C	C2-O2	7.30	1.31	1.24
7	G	154	ARG	CA-C	7.19	1.71	1.52
34	2	1073	G	C6-N1	-7.07	1.34	1.39
34	2	8	U	O3'-P	-7.04	1.52	1.61
34	2	520	A	O3'-P	-6.29	1.53	1.61
34	2	77	U	O3'-P	6.25	1.68	1.61
34	2	1069	C	O3'-P	-6.04	1.53	1.61
16	P	19	GLY	N-CA	5.95	1.54	1.46
7	G	154	ARG	N-CA	5.81	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	883	A	O3'-P	-5.39	1.54	1.61
34	2	1044	C	N1-C2	5.21	1.45	1.40
10	J	170	GLY	CA-C	5.07	1.59	1.51
19	S	93	ASN	N-CA	5.00	1.56	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1073	G	N1-C2-N2	-16.67	101.20	116.20
34	2	1074	C	C2'-C3'-O3'	11.15	134.03	109.50
34	2	1074	C	N1-C1'-C2'	-9.84	101.17	112.00
26	Z	68	ARG	N-CA-C	-8.17	88.93	111.00
34	2	78	A	C4'-C3'-O3'	7.94	128.88	113.00
34	2	1044	C	N1-C2-O2	7.40	123.34	118.90
34	2	1044	C	C2-N1-C1'	7.22	126.74	118.80
34	2	78	A	C5'-C4'-C3'	7.09	127.34	116.00
34	2	1073	G	N1-C6-O6	-7.08	115.65	119.90
34	2	1082	G	P-O3'-C3'	-6.52	111.88	119.70
34	2	911	U	N1-C1'-C2'	6.41	122.34	114.00
34	2	1076	C	N1-C1'-C2'	-6.38	104.98	112.00
34	2	1074	C	C3'-C2'-C1'	6.34	106.58	101.50
34	2	1044	C	C6-N1-C1'	-6.13	113.44	120.80
34	2	511	A	O5'-P-OP1	6.07	117.98	110.70
34	2	1534	G	C2'-C3'-O3'	6.04	123.36	113.70
34	2	78	A	P-O5'-C5'	6.00	130.51	120.90
34	2	1083	A	O5'-P-OP2	-5.93	100.37	105.70
24	X	64	PRO	CA-N-CD	-5.82	103.36	111.50
34	2	267	C	N1-C1'-C2'	-5.81	105.61	112.00
34	2	113	U	C2'-C3'-O3'	5.76	122.92	113.70
7	G	155	ASP	CB-CA-C	-5.71	98.99	110.40
35	i	6212	U	N1-C1'-C2'	-5.47	105.98	112.00
34	2	930	C	O4'-C1'-N1	5.46	112.57	108.20
19	S	30	TYR	CB-CA-C	5.43	121.26	110.40
17	Q	52	LEU	CA-CB-CG	5.35	127.61	115.30
34	2	828	A	C2'-C3'-O3'	5.29	122.17	113.70
19	S	93	ASN	N-CA-C	5.20	125.04	111.00
10	J	176	ARG	N-CA-CB	5.18	119.92	110.60
34	2	78	A	O4'-C4'-C3'	-5.12	98.88	104.00
10	J	170	GLY	N-CA-C	5.09	125.81	113.10
10	J	49	LEU	CA-CB-CG	5.08	126.98	115.30
34	2	1628	U	C4'-C3'-O3'	5.08	123.16	113.00
34	2	963	U	C2'-C3'-O3'	5.07	121.82	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	20	VAL	N-CA-C	5.05	124.63	111.00
34	2	1073	G	N3-C2-N2	5.05	123.43	119.90
34	2	511	A	P-O5'-C5'	5.02	128.93	120.90
7	G	208	TYR	CA-CB-CG	-5.01	103.87	113.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	2	1044	C	Sidechain
34	2	1073	G	Sidechain
34	2	1074	C	Sidechain
34	2	1269	G	Sidechain
34	2	1439	C	Sidechain
34	2	561	G	Sidechain
34	2	583	C	Sidechain
1	A	164	ASN	Peptide
1	A	168	HIS	Peptide
7	G	155	ASP	Peptide
10	J	66	ASP	Peptide
15	O	122	PRO	Peptide
17	Q	40	GLN	Peptide
17	Q	49	TYR	Peptide
22	V	13	VAL	Peptide
23	W	75	ILE	Peptide
26	Z	68	ARG	Sidechain
27	a	83	ILE	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	1616	0	1636	18	0
2	B	1722	0	1795	3	0
3	C	1629	0	1710	8	0
4	D	1744	0	1825	2	0
5	E	2078	0	2157	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1609	0	1679	25	0
7	G	1812	0	1911	56	0
8	H	1483	0	1579	6	0
9	I	1493	0	1515	19	0
10	J	1471	0	1554	37	0
11	K	809	0	810	4	0
12	L	1248	0	1311	5	0
13	M	922	0	953	7	0
14	N	1187	0	1251	5	0
15	O	942	0	979	8	0
16	P	980	0	1026	22	0
17	Q	1105	0	1170	6	0
18	R	1031	0	1082	6	0
19	S	1193	0	1217	21	0
20	T	1110	0	1124	4	0
21	U	845	0	913	5	0
22	V	687	0	682	2	0
23	W	1021	0	1056	12	0
24	X	1127	0	1210	22	0
25	Y	1061	0	1111	14	0
26	Z	558	0	585	74	0
27	a	798	0	855	0	0
28	b	617	0	642	0	0
29	c	494	0	534	0	0
30	d	446	0	436	0	0
31	e	443	0	481	0	0
32	f	549	0	564	0	0
33	g	2466	0	2406	0	0
34	2	37797	0	19010	942	0
35	i	3968	0	1986	0	0
36	2	76	0	0	0	0
36	G	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	X	1	0	0	0	0
37	a	1	0	0	0	0
37	b	1	0	0	0	0
37	f	1	0	0	0	0
All	All	80144	0	60755	1189	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 10.

All (1189) 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)
26:Z:52:LYS:HA	26:Z:53:GLU:CG	1.47	1.43
34:2:513:G:H1	34:2:542:C:N4	1.27	1.31
24:X:63:GLN:NE2	34:2:1753:A:OP1	1.64	1.29
34:2:480:A:N1	34:2:506:U:C4	2.04	1.26
26:Z:51:MET:O	26:Z:53:GLU:HA	1.13	1.26
34:2:1072:G:N2	34:2:1073:G:N7	1.84	1.24
34:2:480:A:N1	34:2:506:U:O4	1.72	1.22
26:Z:58:ARG:NH1	26:Z:103:ARG:HH22	1.40	1.20
10:J:170:GLY:O	34:2:511:A:H5'	1.39	1.18
34:2:1044:C:N3	34:2:1072:G:N2	1.90	1.18
34:2:1292:U:O4	34:2:1321:A:N1	1.77	1.17
34:2:1044:C:N4	34:2:1072:G:H1	1.44	1.15
10:J:170:GLY:O	34:2:511:A:P	2.05	1.15
10:J:170:GLY:O	34:2:511:A:C5'	1.93	1.14
34:2:1221:C:O2	34:2:1261:U:O2	1.67	1.13
7:G:155:ASP:N	34:2:78:A:O5'	1.83	1.11
26:Z:53:GLU:HB3	26:Z:55:PRO:HD2	1.34	1.10
26:Z:51:MET:O	26:Z:53:GLU:CA	2.02	1.08
7:G:136:LYS:NZ	34:2:65:A:OP1	1.87	1.08
34:2:955:C:O2'	34:2:1046:G:O2'	1.71	1.08
26:Z:52:LYS:HA	26:Z:53:GLU:HG3	1.08	1.07
24:X:63:GLN:HE21	34:2:1753:A:P	1.77	1.07
7:G:154:ARG:N	34:2:78:A:O5'	1.87	1.07
10:J:170:GLY:HA3	34:2:511:A:H5'	1.36	1.07
7:G:155:ASP:H	34:2:78:A:C5'	1.68	1.07
26:Z:63:SER:O	26:Z:66:VAL:O	1.70	1.06
26:Z:58:ARG:NH1	26:Z:103:ARG:NH2	2.02	1.06
34:2:1292:U:C4	34:2:1321:A:N1	2.23	1.06
26:Z:52:LYS:CA	26:Z:53:GLU:HG3	1.87	1.05
26:Z:54:ALA:HB2	26:Z:83:LEU:HD22	1.39	1.05
10:J:170:GLY:C	34:2:511:A:P	2.36	1.04
26:Z:52:LYS:HA	26:Z:53:GLU:HG2	1.37	1.04
34:2:138:A:N7	34:2:265:A:H2	1.55	1.03
34:2:1072:G:C2	34:2:1073:G:N7	2.24	1.03
34:2:511:A:H2'	34:2:512:U:H5'	1.42	1.01
34:2:513:G:N2	34:2:542:C:C5	2.28	1.01
34:2:883:A:H2'	34:2:884:G:H5'	1.41	1.01
26:Z:58:ARG:O	26:Z:102:THR:HG23	1.60	1.01
10:J:170:GLY:HA3	34:2:511:A:C5'	1.91	0.99
34:2:935:G:OP2	34:2:1074:C:N3	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:51:MET:C	26:Z:53:GLU:HA	1.83	0.98
10:J:170:GLY:C	34:2:511:A:OP1	2.03	0.97
34:2:537:A:C8	34:2:542:C:N3	2.33	0.96
26:Z:60:VAL:HG12	26:Z:80:LEU:HD21	1.44	0.96
34:2:513:G:C2	34:2:542:C:H5	1.82	0.96
34:2:1084:G:N2	34:2:1088:U:C2	2.34	0.96
34:2:1044:C:N4	34:2:1072:G:N1	2.14	0.95
26:Z:52:LYS:CA	26:Z:53:GLU:CG	2.42	0.95
34:2:1218:A:N6	34:2:1263:G:O2'	2.00	0.94
34:2:264:A:N1	34:2:288:U:O4	1.98	0.94
34:2:1082:G:O2'	34:2:1093:G:O2'	1.84	0.94
34:2:1082:G:H2'	34:2:1083:A:H5''	1.49	0.94
26:Z:49:ARG:HG2	26:Z:49:ARG:HH11	1.32	0.92
34:2:1012:A:H2'	34:2:1013:G:O4'	1.70	0.92
34:2:513:G:N2	34:2:542:C:H5	1.68	0.91
34:2:1040:G:C2	34:2:1076:C:N3	2.39	0.91
34:2:480:A:C2	34:2:506:U:O4	2.25	0.90
10:J:170:GLY:CA	34:2:511:A:H5'	2.02	0.90
34:2:143:G:O6	34:2:170:A:N6	2.05	0.90
26:Z:104:ALA:HB1	26:Z:105:THR:HA	1.52	0.90
34:2:267:C:N4	34:2:286:G:H1	1.69	0.89
7:G:154:ARG:CA	34:2:78:A:O5'	2.19	0.89
34:2:1072:G:N2	34:2:1073:G:C5	2.39	0.89
34:2:269:C:H2'	34:2:270:A:H8	1.35	0.89
34:2:1258:U:C5	34:2:1259:U:O4	2.25	0.89
34:2:1040:G:C6	34:2:1076:C:N4	2.41	0.88
34:2:935:G:OP1	34:2:1044:C:C1'	2.21	0.88
34:2:884:G:H8	34:2:884:G:H5'	1.36	0.88
7:G:154:ARG:HA	34:2:78:A:H3'	1.56	0.88
34:2:511:A:C2'	34:2:512:U:H5'	2.04	0.87
34:2:1229:A:N3	34:2:1257:U:C5	2.43	0.86
34:2:560:G:HO2'	34:2:561:G:H8	1.23	0.86
34:2:1258:U:O2'	34:2:1259:U:C5	2.29	0.86
7:G:155:ASP:N	34:2:78:A:C5'	2.39	0.85
34:2:1044:C:C2	34:2:1072:G:N2	2.35	0.85
34:2:1040:G:C2	34:2:1076:C:C4	2.63	0.85
34:2:1229:A:C2	34:2:1257:U:C6	2.64	0.85
34:2:1292:U:O4	34:2:1321:A:C6	2.29	0.85
34:2:513:G:C2	34:2:542:C:C5	2.64	0.85
34:2:1042:A:N1	34:2:1075:A:C2	2.44	0.85
10:J:170:GLY:CA	34:2:511:A:OP1	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1292:U:O4	34:2:1321:A:C2	2.30	0.84
34:2:513:G:N1	34:2:542:C:N4	2.07	0.84
7:G:171:LYS:HE3	34:2:71:A:H61	1.41	0.84
34:2:1082:G:C2'	34:2:1083:A:H5''	2.07	0.83
10:J:170:GLY:C	34:2:511:A:C5'	2.46	0.83
34:2:884:G:C8	34:2:884:G:H5'	2.13	0.83
34:2:8:U:C3'	34:2:9:U:H5'	2.09	0.83
7:G:155:ASP:H	34:2:78:A:P	2.02	0.83
34:2:1222:A:C6	34:2:1260:G:C6	2.67	0.82
34:2:1258:U:O2'	34:2:1259:U:C6	2.32	0.82
34:2:566:A:H2'	34:2:567:G:O4'	1.80	0.82
34:2:1292:U:C4	34:2:1321:A:C2	2.68	0.82
34:2:65:A:H2'	34:2:83:G:H1	1.45	0.82
34:2:1040:G:N2	34:2:1076:C:C2	2.48	0.81
34:2:513:G:H1	34:2:542:C:H41	0.85	0.81
26:Z:54:ALA:HB3	26:Z:88:ILE:CG2	2.10	0.81
34:2:883:A:C2'	34:2:884:G:H5'	2.09	0.81
10:J:170:GLY:CA	34:2:511:A:C5'	2.57	0.81
7:G:155:ASP:N	34:2:78:A:P	2.53	0.81
34:2:935:G:OP1	34:2:1044:C:H1'	1.80	0.80
34:2:480:A:C6	34:2:506:U:O4	2.33	0.80
26:Z:54:ALA:CB	26:Z:83:LEU:HD22	2.10	0.80
34:2:1230:U:O3'	34:2:1257:U:O2'	1.99	0.80
34:2:1040:G:N1	34:2:1076:C:C4	2.50	0.80
26:Z:54:ALA:HB2	26:Z:83:LEU:CD2	2.11	0.80
34:2:560:G:C2'	34:2:561:G:H8	1.95	0.80
34:2:511:A:H2'	34:2:512:U:C5'	2.13	0.79
34:2:513:G:N1	34:2:542:C:C5	2.50	0.79
34:2:138:A:N7	34:2:265:A:C2	2.46	0.79
34:2:537:A:H4'	34:2:538:G:OP1	1.80	0.79
34:2:8:U:O4	34:2:15:U:O4	2.01	0.79
34:2:264:A:C2	34:2:287:A:N6	2.50	0.78
6:F:125:VAL:HG11	26:Z:59:TYR:HB3	1.65	0.78
34:2:1258:U:C2'	34:2:1259:U:C5	2.66	0.78
34:2:564:C:H2'	34:2:576:G:N2	1.98	0.78
34:2:1258:U:C6	34:2:1259:U:O4	2.36	0.78
34:2:883:A:H2'	34:2:884:G:C5'	2.12	0.78
34:2:267:C:H42	34:2:286:G:H1	1.29	0.77
34:2:565:C:H2'	34:2:566:A:C8	2.19	0.77
34:2:1173:C:N3	34:2:1464:G:C2	2.53	0.77
34:2:883:A:C2'	34:2:884:G:C5'	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1258:U:H2'	34:2:1259:U:H5	1.49	0.77
34:2:1229:A:H2	34:2:1257:U:H6	1.33	0.77
10:J:14:THR:HG21	34:2:23:G:OP1	1.83	0.77
34:2:1082:G:C3'	34:2:1083:A:H5''	2.14	0.77
34:2:1229:A:C2	34:2:1257:U:H6	2.02	0.77
34:2:70:C:H2'	34:2:71:A:O4'	1.85	0.77
10:J:170:GLY:N	34:2:511:A:OP1	2.19	0.76
34:2:935:G:OP2	34:2:1073:G:N2	2.18	0.76
34:2:888:U:H2'	34:2:889:C:C6	2.21	0.76
16:P:18:LYS:O	19:S:95:GLY:N	2.18	0.76
26:Z:58:ARG:HH12	26:Z:103:ARG:HH22	1.29	0.76
34:2:1070:U:H5''	34:2:1071:C:OP1	1.86	0.76
8:H:70:TYR:O	8:H:74:GLN:N	2.19	0.76
34:2:1229:A:N3	34:2:1257:U:C6	2.54	0.76
34:2:1590:A:H2'	34:2:1591:A:C8	2.21	0.76
26:Z:53:GLU:HB3	26:Z:55:PRO:CD	2.15	0.76
34:2:208:U:C4	34:2:209:A:N7	2.54	0.75
34:2:65:A:H2'	34:2:83:G:N1	2.01	0.75
26:Z:52:LYS:HD2	26:Z:53:GLU:HG3	1.67	0.75
34:2:884:G:C2'	34:2:885:U:H4'	2.16	0.75
26:Z:58:ARG:CZ	26:Z:103:ARG:HH22	1.99	0.75
26:Z:104:ALA:HB1	26:Z:105:THR:CA	2.16	0.75
34:2:556:G:C6	34:2:558:C:N4	2.55	0.74
7:G:154:ARG:C	34:2:78:A:O5'	2.24	0.74
26:Z:60:VAL:HG12	26:Z:80:LEU:CD2	2.16	0.74
34:2:70:C:N4	34:2:71:A:N1	2.36	0.74
34:2:1255:A:N3	34:2:1257:U:O4	2.20	0.74
34:2:267:C:N3	34:2:286:G:N2	2.35	0.73
34:2:8:U:O2'	34:2:9:U:H5'	1.89	0.73
34:2:264:A:H2	34:2:288:U:H3	1.37	0.73
10:J:170:GLY:O	34:2:511:A:OP2	2.07	0.73
34:2:558:C:H2'	34:2:559:U:C6	2.24	0.72
34:2:560:G:H2'	34:2:561:G:H8	1.54	0.72
24:X:63:GLN:NE2	34:2:1753:A:H5'	2.05	0.72
34:2:560:G:H2'	34:2:561:G:C8	2.23	0.72
34:2:1221:C:O2	34:2:1261:U:C2	2.43	0.72
10:J:170:GLY:O	34:2:511:A:O5'	2.07	0.72
34:2:884:G:H2'	34:2:885:U:H4'	1.71	0.72
34:2:884:G:C5'	34:2:884:G:H8	2.03	0.71
9:I:160:GLN:HB3	9:I:166:LEU:HA	1.73	0.71
34:2:150:G:O6	34:2:162:G:O6	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:884:G:C3'	34:2:885:U:H4'	2.20	0.71
34:2:1082:G:O6	34:2:1083:A:C6	2.44	0.71
10:J:170:GLY:CA	34:2:511:A:P	2.78	0.71
26:Z:54:ALA:HB3	26:Z:88:ILE:HG21	1.72	0.71
34:2:1043:U:N3	34:2:1044:C:N4	2.38	0.71
34:2:214:A:N7	34:2:241:U:H2'	2.06	0.70
7:G:155:ASP:N	34:2:77:U:O3'	2.24	0.70
7:G:154:ARG:CA	34:2:78:A:H3'	2.21	0.70
34:2:1083:A:N1	34:2:1089:C:C4	2.59	0.70
26:Z:60:VAL:CG1	26:Z:80:LEU:HD21	2.21	0.70
26:Z:49:ARG:HG2	26:Z:49:ARG:NH1	1.96	0.70
34:2:564:C:H2'	34:2:576:G:C2	2.25	0.70
34:2:1363:G:N2	34:2:1364:C:C2	2.60	0.69
34:2:1082:G:C6	34:2:1083:A:C5	2.80	0.69
34:2:537:A:C8	34:2:542:C:C4	2.80	0.69
34:2:515:G:C6	34:2:536:G:N2	2.61	0.69
16:P:19:GLY:N	19:S:93:ASN:N	2.41	0.69
34:2:1229:A:C2	34:2:1257:U:C5	2.82	0.68
34:2:542:C:O2'	34:2:543:A:P	2.50	0.68
26:Z:61:SER:O	26:Z:64:VAL:N	2.25	0.68
34:2:148:C:H2'	34:2:149:U:C6	2.28	0.68
34:2:1499:C:C2	34:2:1505:G:N2	2.62	0.68
34:2:261:U:C4	34:2:262:C:N4	2.61	0.68
34:2:559:U:H2'	34:2:560:G:H8	1.58	0.68
34:2:884:G:H2'	34:2:885:U:C4'	2.23	0.68
34:2:1258:U:H2'	34:2:1259:U:C5	2.28	0.68
34:2:628:U:N3	34:2:969:A:N6	2.41	0.68
9:I:82:VAL:HG12	9:I:197:LEU:HD21	1.76	0.68
34:2:1042:A:N1	34:2:1075:A:N1	2.42	0.68
34:2:511:A:C3'	34:2:512:U:H5'	2.23	0.68
26:Z:53:GLU:CB	26:Z:55:PRO:HD2	2.20	0.68
34:2:537:A:N7	34:2:542:C:N4	2.42	0.67
34:2:261:U:C4	34:2:262:C:C4	2.82	0.67
34:2:299:A:H2'	34:2:300:A:C8	2.30	0.67
26:Z:61:SER:HB3	26:Z:64:VAL:HG23	1.75	0.67
34:2:406:A:O2'	34:2:1669:A:N3	2.26	0.67
34:2:269:C:H2'	34:2:270:A:C8	2.25	0.67
34:2:144:A:C2	34:2:170:A:C2	2.83	0.66
34:2:1082:G:O6	34:2:1083:A:C5	2.48	0.66
34:2:883:A:C3'	34:2:884:G:C5'	2.73	0.66
34:2:1218:A:N6	34:2:1263:G:C2'	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1215:C:O2'	34:2:1442:A:N6	2.28	0.66
34:2:1223:A:N6	34:2:1224:U:C4	2.64	0.66
34:2:139:C:H42	34:2:280:G:P	2.19	0.66
34:2:1084:G:N2	34:2:1088:U:N3	2.44	0.66
34:2:1074:C:O2	34:2:1074:C:C2'	2.42	0.65
34:2:1215:C:HO2'	34:2:1442:A:N6	1.93	0.65
10:J:170:GLY:HA3	34:2:511:A:O5'	1.96	0.65
16:P:17:TYR:N	19:S:92:VAL:O	2.29	0.65
34:2:1183:A:C2	34:2:1453:G:O4'	2.48	0.65
34:2:537:A:N7	34:2:542:C:C4	2.65	0.65
34:2:264:A:N1	34:2:288:U:C4	2.63	0.65
34:2:1417:G:C6	34:2:1418:C:N3	2.64	0.65
34:2:560:G:N3	34:2:561:G:C8	2.64	0.65
26:Z:60:VAL:CG1	26:Z:80:LEU:CD2	2.75	0.65
34:2:1223:A:C6	34:2:1224:U:C4	2.85	0.65
34:2:556:G:C2	34:2:558:C:C4	2.84	0.65
34:2:1044:C:C4	34:2:1072:G:N1	2.56	0.65
34:2:935:G:P	34:2:1074:C:N4	2.70	0.65
34:2:1040:G:N1	34:2:1076:C:N4	2.42	0.65
34:2:480:A:C2	34:2:506:U:C4	2.82	0.65
34:2:883:A:C6	34:2:884:G:C6	2.84	0.65
34:2:513:G:N7	34:2:536:G:N1	2.45	0.65
34:2:8:U:C2'	34:2:9:U:H5'	2.27	0.65
34:2:360:C:C2	34:2:383:G:N2	2.65	0.65
34:2:535:C:H2'	34:2:536:G:O4'	1.96	0.65
34:2:1601:U:H2'	34:2:1602:U:C6	2.32	0.64
34:2:1040:G:N2	34:2:1076:C:N3	2.44	0.64
26:Z:54:ALA:CB	26:Z:88:ILE:CG2	2.75	0.64
26:Z:55:PRO:O	26:Z:56:THR:OG1	2.12	0.64
34:2:1217:G:C8	34:2:1442:A:C5	2.85	0.64
34:2:1082:G:H3'	34:2:1083:A:C5'	2.27	0.64
26:Z:67:ASP:C	26:Z:69:PHE:H	1.82	0.64
34:2:560:G:O2'	34:2:561:G:H8	1.80	0.64
34:2:1464:G:N2	34:2:1465:C:C2	2.66	0.63
34:2:67:A:OP2	34:2:83:G:N2	2.31	0.63
34:2:152:G:C6	34:2:161:A:C6	2.87	0.63
34:2:363:G:N2	34:2:380:C:C2	2.67	0.63
34:2:151:U:N3	34:2:162:G:N7	2.47	0.63
34:2:537:A:C8	34:2:542:C:N4	2.67	0.63
34:2:883:A:C2'	34:2:884:G:H5''	2.28	0.63
26:Z:58:ARG:CZ	26:Z:103:ARG:NH2	2.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:559:U:H2'	34:2:560:G:C8	2.34	0.63
7:G:174:LYS:HA	34:2:79:C:O2'	1.99	0.63
34:2:264:A:H2	34:2:288:U:N3	1.96	0.62
34:2:264:A:C2	34:2:288:U:N3	2.67	0.62
34:2:70:C:C5	34:2:71:A:C5	2.87	0.62
34:2:363:G:C2	34:2:380:C:C2	2.88	0.62
34:2:1220:A:N1	34:2:1261:U:N3	2.48	0.62
34:2:168:A:C4	34:2:170:A:C8	2.87	0.62
34:2:823:G:N2	34:2:848:C:C2	2.67	0.62
7:G:154:ARG:HB3	34:2:77:U:H4'	1.80	0.62
24:X:102:VAL:HG22	24:X:124:VAL:HG13	1.81	0.62
7:G:155:ASP:H	34:2:78:A:H5''	1.60	0.62
7:G:188:ARG:NH1	34:2:283:G:O6	2.32	0.62
34:2:207:U:H2'	34:2:208:U:C6	2.35	0.61
34:2:1220:A:C6	34:2:1262:G:C6	2.88	0.61
34:2:1222:A:C4	34:2:1260:G:C2	2.88	0.61
34:2:1222:A:C5	34:2:1260:G:N1	2.68	0.61
34:2:171:C:O2'	34:2:172:A:O4'	2.15	0.61
34:2:1223:A:C6	34:2:1259:U:N3	2.68	0.61
6:F:53:VAL:HG13	6:F:133:GLN:HA	1.81	0.61
34:2:1229:A:H2	34:2:1257:U:C6	2.08	0.61
16:P:19:GLY:H	19:S:93:ASN:N	1.99	0.61
34:2:1378:U:O2'	34:2:1514:A:N1	2.32	0.61
34:2:480:A:C6	34:2:506:U:C4	2.86	0.61
16:P:17:TYR:C	19:S:92:VAL:O	2.39	0.61
34:2:1082:G:C3'	34:2:1083:A:C5'	2.78	0.60
6:F:188:ASN:HA	34:2:1533:U:C6	2.36	0.60
34:2:209:A:C2'	34:2:210:U:H5'	2.31	0.60
34:2:65:A:N1	34:2:83:G:H2'	2.16	0.60
24:X:96:VAL:HA	24:X:127:VAL:HG11	1.82	0.60
26:Z:54:ALA:N	26:Z:55:PRO:HD2	2.16	0.60
7:G:154:ARG:H	34:2:78:A:C4'	2.14	0.60
34:2:267:C:O2'	34:2:268:G:H5'	2.02	0.60
34:2:65:A:C2'	34:2:83:G:H1	2.10	0.60
7:G:154:ARG:N	34:2:78:A:C5'	2.64	0.60
20:T:68:ARG:NH1	34:2:1519:G:O6	2.33	0.60
26:Z:61:SER:O	26:Z:62:VAL:C	2.40	0.60
34:2:1130:A:H2'	34:2:1131:A:O4'	2.01	0.60
34:2:560:G:C4	34:2:561:G:N7	2.69	0.60
34:2:69:G:C6	34:2:70:C:C4	2.88	0.60
34:2:1044:C:C4	34:2:1072:G:N2	2.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:811:A:O4'	34:2:857:G:N2	2.34	0.60
34:2:1219:C:N3	34:2:1262:G:O6	2.35	0.60
34:2:987:A:H2'	34:2:988:U:C6	2.36	0.60
7:G:154:ARG:CB	34:2:77:U:H4'	2.32	0.60
34:2:1220:A:C5	34:2:1262:G:C6	2.90	0.59
34:2:1230:U:H5'	34:2:1258:U:H4'	1.83	0.59
34:2:561:G:H2'	34:2:562:U:H6	1.67	0.59
34:2:969:A:N6	34:2:970:A:C4	2.70	0.59
34:2:12:U:H2'	34:2:13:C:C6	2.37	0.59
34:2:1024:A:O2'	34:2:1771:C:O2'	2.20	0.59
34:2:70:C:H42	34:2:81:G:H1	1.50	0.59
34:2:65:A:C2'	34:2:83:G:N1	2.66	0.59
9:I:107:THR:N	9:I:108:PRO:HD2	2.17	0.59
26:Z:59:TYR:CZ	26:Z:64:VAL:CG2	2.85	0.59
34:2:70:C:N4	34:2:71:A:C6	2.70	0.59
34:2:1464:G:N1	34:2:1465:C:C4	2.71	0.59
26:Z:59:TYR:CZ	26:Z:64:VAL:HG21	2.37	0.59
34:2:1231:U:OP1	34:2:1257:U:O3'	2.21	0.59
34:2:157:U:C4	34:2:419:A:H4'	2.38	0.59
7:G:154:ARG:H	34:2:78:A:C5'	2.16	0.59
10:J:173:ALA:HA	34:2:510:A:OP2	2.03	0.59
34:2:1671:G:C6	34:2:1672:C:N4	2.70	0.59
34:2:886:A:H2'	34:2:887:U:O4'	2.02	0.59
34:2:1217:G:O6	34:2:1442:A:H5"	2.03	0.59
34:2:1462:G:N2	34:2:1463:C:C2	2.71	0.59
34:2:266:U:O2	34:2:287:A:C2	2.56	0.59
24:X:41:SER:O	24:X:43:PHE:N	2.36	0.59
26:Z:54:ALA:HB1	26:Z:89:ILE:HD11	1.83	0.59
34:2:1218:A:H62	34:2:1263:G:H2'	1.68	0.58
34:2:749:U:H2'	34:2:750:U:C6	2.37	0.58
17:Q:36:ILE:HD11	17:Q:48:VAL:HG12	1.85	0.58
34:2:1082:G:C6	34:2:1083:A:N7	2.71	0.58
3:C:50:VAL:HG21	3:C:73:ILE:HG23	1.85	0.58
34:2:958:U:H2'	34:2:958:U:O2	2.03	0.58
9:I:83:TYR:CZ	9:I:196:ARG:HG2	2.37	0.58
34:2:1215:C:H2'	34:2:1442:A:N1	2.19	0.58
34:2:1103:U:H2'	34:2:1104:C:O4'	2.04	0.58
34:2:1120:C:C2	34:2:1126:G:C2	2.92	0.58
34:2:1349:G:C2	34:2:1374:C:O2	2.57	0.58
34:2:1462:G:N1	34:2:1463:C:C4	2.72	0.58
24:X:63:GLN:HG3	24:X:64:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:105:THR:O	26:Z:105:THR:HG22	2.01	0.58
34:2:291:U:H2'	34:2:292:U:C6	2.39	0.58
7:G:171:LYS:CE	34:2:71:A:H61	2.12	0.58
34:2:1086:A:H2'	34:2:1087:A:C8	2.38	0.58
34:2:561:G:C2	34:2:583:C:C2	2.93	0.57
34:2:561:G:C2	34:2:583:C:O2	2.57	0.57
34:2:1223:A:N6	34:2:1224:U:O4	2.37	0.57
34:2:1222:A:N1	34:2:1260:G:C5	2.73	0.57
34:2:1256:U:C6	34:2:1257:U:H1'	2.40	0.57
15:O:81:ILE:HB	15:O:115:ILE:HG22	1.87	0.57
34:2:70:C:C4	34:2:71:A:C6	2.93	0.57
1:A:120:LEU:HD11	1:A:144:ILE:HD12	1.87	0.57
34:2:556:G:N2	34:2:558:C:C2	2.73	0.57
34:2:1757:C:H2'	34:2:1758:G:O4'	2.05	0.57
9:I:76:THR:HG21	9:I:104:ILE:HG23	1.86	0.57
26:Z:54:ALA:CB	26:Z:88:ILE:HG21	2.32	0.57
34:2:1215:C:O2'	34:2:1442:A:C6	2.58	0.57
34:2:1793:U:O3'	34:2:1795:A:N1	2.38	0.57
34:2:513:G:N7	34:2:536:G:C2	2.73	0.57
1:A:129:ASP:O	1:A:132:ALA:N	2.35	0.56
34:2:1349:G:C6	34:2:1374:C:N3	2.73	0.56
1:A:18:LEU:HD22	18:R:106:THR:HG23	1.86	0.56
25:Y:40:LEU:HD13	25:Y:60:PHE:CZ	2.39	0.56
34:2:137:U:N3	34:2:138:A:N6	2.53	0.56
9:I:99:ALA:N	9:I:170:ILE:O	2.36	0.56
12:L:99:ARG:HB2	24:X:12:ALA:HB2	1.87	0.56
34:2:1671:G:C2	34:2:1672:C:C2	2.94	0.56
16:P:121:ILE:HD11	19:S:125:ILE:HD13	1.88	0.56
34:2:1182:A:N3	34:2:1209:C:O2'	2.26	0.56
34:2:1218:A:N6	34:2:1263:G:H2'	2.19	0.56
24:X:69:ARG:NH1	24:X:116:ASP:OD2	2.38	0.56
34:2:1012:A:H2'	34:2:1013:G:C1'	2.36	0.56
34:2:908:U:H2'	34:2:909:C:C5	2.40	0.56
34:2:1218:A:N7	34:2:1264:G:H1'	2.20	0.56
34:2:884:G:H2'	34:2:885:U:O2'	2.06	0.56
3:C:170:VAL:HG11	3:C:215:THR:HA	1.87	0.56
23:W:40:VAL:HG11	23:W:103:ILE:HD12	1.86	0.56
34:2:556:G:C2	34:2:558:C:N3	2.74	0.56
34:2:564:C:O2'	34:2:565:C:OP2	2.22	0.56
34:2:823:G:C2	34:2:848:C:N3	2.74	0.56
7:G:153:VAL:HG21	7:G:178:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:82:LYS:O	23:W:84:ALA:N	2.37	0.56
34:2:1154:G:C2	34:2:1622:C:C2	2.94	0.56
34:2:1277:G:C2	34:2:1278:C:C2	2.95	0.55
34:2:511:A:C2'	34:2:512:U:C5'	2.76	0.55
34:2:1042:A:C6	34:2:1043:U:C4	2.93	0.55
7:G:136:LYS:HZ2	34:2:65:A:P	2.20	0.55
34:2:1239:U:O2'	34:2:1241:A:C8	2.59	0.55
34:2:1230:U:C5'	34:2:1258:U:H4'	2.35	0.55
34:2:1173:C:N4	34:2:1464:G:C6	2.75	0.55
34:2:1586:G:N1	34:2:1587:C:C2	2.73	0.55
34:2:209:A:C6	34:2:210:U:C4	2.94	0.55
1:A:14:ALA:O	1:A:18:LEU:HG	2.06	0.55
16:P:19:GLY:HA3	19:S:94:ASP:C	2.26	0.55
34:2:150:G:C2	34:2:163:A:C5	2.95	0.55
34:2:50:C:O2	34:2:429:G:C2	2.60	0.55
23:W:55:ASP:O	23:W:57:ARG:N	2.39	0.55
34:2:1042:A:C2	34:2:1043:U:C2	2.95	0.55
34:2:1173:C:C2	34:2:1464:G:C2	2.94	0.55
34:2:1223:A:C4	34:2:1259:U:O2	2.59	0.55
6:F:185:ALA:HB2	6:F:192:ILE:HG23	1.89	0.55
34:2:1081:C:O2'	34:2:1082:G:H5''	2.06	0.55
34:2:1292:U:O4	34:2:1293:G:C4	2.60	0.55
34:2:976:A:H2'	34:2:977:A:O4'	2.07	0.55
11:K:46:LEU:HD13	11:K:66:TYR:CE2	2.42	0.55
34:2:884:G:C3'	34:2:885:U:C4'	2.85	0.55
34:2:990:G:O2'	34:2:1012:A:N6	2.39	0.55
34:2:1042:A:C6	34:2:1043:U:N3	2.75	0.55
34:2:1257:U:H2'	34:2:1258:U:O4'	2.06	0.55
34:2:884:G:H3'	34:2:885:U:C4'	2.37	0.55
26:Z:58:ARG:NH1	26:Z:103:ARG:CZ	2.68	0.55
34:2:69:G:C2	34:2:70:C:C2	2.95	0.54
34:2:1183:A:C2	34:2:1452:G:N3	2.74	0.54
34:2:1343:A:H2'	34:2:1344:A:C8	2.42	0.54
25:Y:121:THR:OG1	34:2:148:C:OP1	2.20	0.54
34:2:1778:G:HO2'	34:2:1779:A:H8	1.53	0.54
34:2:262:C:O2'	34:2:263:G:O4'	2.25	0.54
34:2:161:A:C6	34:2:162:G:C6	2.95	0.54
34:2:65:A:HO2'	34:2:83:G:N2	2.06	0.54
1:A:49:ASN:O	1:A:53:THR:HG23	2.08	0.54
34:2:562:U:H2'	34:2:563:G:C8	2.43	0.54
7:G:131:LYS:HB3	34:2:165:C:O2'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:594:G:C6	34:2:595:C:N4	2.76	0.54
10:J:170:GLY:CA	34:2:511:A:O5'	2.56	0.54
34:2:1072:G:N2	34:2:1073:G:C6	2.75	0.54
34:2:1220:A:H2'	34:2:1221:C:C6	2.43	0.54
34:2:147:U:H2'	34:2:148:C:O4'	2.08	0.54
24:X:63:GLN:NE2	34:2:1753:A:P	2.54	0.54
34:2:1043:U:H3	34:2:1044:C:N4	2.05	0.54
34:2:1726:U:H2'	34:2:1727:C:C6	2.43	0.54
34:2:268:G:C6	34:2:269:C:C4	2.96	0.54
34:2:168:A:C5	34:2:170:A:C8	2.95	0.54
34:2:65:A:H2'	34:2:83:G:C6	2.43	0.54
3:C:173:ARG:NH1	34:2:1096:U:O3'	2.41	0.54
34:2:1219:C:O2	34:2:1262:G:N1	2.41	0.54
34:2:1333:U:H2'	34:2:1334:U:O4'	2.08	0.54
34:2:1499:C:C2	34:2:1505:G:C2	2.95	0.54
34:2:922:A:N1	34:2:923:A:C6	2.76	0.54
34:2:1222:A:C2	34:2:1260:G:C4	2.96	0.53
34:2:1378:U:H2'	34:2:1379:U:C6	2.44	0.53
7:G:155:ASP:HB2	34:2:78:A:OP2	2.08	0.53
26:Z:52:LYS:HD2	26:Z:53:GLU:CG	2.37	0.53
34:2:121:U:H2'	34:2:122:U:C6	2.43	0.53
34:2:1772:G:H2'	34:2:1773:U:O4'	2.08	0.53
7:G:171:LYS:HE3	34:2:71:A:N6	2.18	0.53
34:2:150:G:C6	34:2:163:A:C6	2.96	0.53
23:W:75:ILE:HD11	23:W:125:ILE:HB	1.90	0.53
6:F:53:VAL:HG12	6:F:53:VAL:O	2.08	0.53
23:W:16:ASN:O	23:W:20:THR:HG23	2.08	0.53
34:2:1363:G:N1	34:2:1364:C:C4	2.77	0.53
34:2:1794:C:O2	34:2:1794:C:O4'	2.25	0.53
34:2:394:U:H2'	34:2:395:G:O4'	2.08	0.53
34:2:70:C:N4	34:2:71:A:C2	2.77	0.53
9:I:82:VAL:HG12	9:I:197:LEU:CD2	2.37	0.53
34:2:1671:G:C5	34:2:1672:C:C4	2.97	0.53
34:2:1671:G:C6	34:2:1672:C:C4	2.97	0.53
34:2:143:G:C6	34:2:170:A:N6	2.68	0.53
26:Z:104:ALA:CB	26:Z:105:THR:HA	2.21	0.53
6:F:97:ASN:HB3	34:2:1609:A:O2'	2.09	0.53
34:2:170:A:H2'	34:2:171:C:C6	2.44	0.53
34:2:1653:A:N6	34:2:1743:G:O2'	2.42	0.53
34:2:22:A:C2	34:2:23:G:C8	2.97	0.53
34:2:1494:U:O2	34:2:1509:G:O6	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1231:U:C4	34:2:1253:U:C6	2.97	0.52
34:2:406:A:H2'	34:2:407:C:C6	2.44	0.52
34:2:478:C:H2'	34:2:479:G:O4'	2.09	0.52
7:G:155:ASP:O	7:G:157:VAL:HB	2.08	0.52
10:J:121:SER:O	10:J:123:HIS:N	2.41	0.52
34:2:1277:G:C6	34:2:1278:C:C4	2.97	0.52
34:2:150:G:N1	34:2:162:G:N7	2.57	0.52
7:G:190:GLN:NE2	34:2:266:U:O4	2.42	0.52
34:2:582:C:O2	34:2:582:C:H2'	2.08	0.52
34:2:1146:A:H2'	34:2:1147:C:O4'	2.09	0.52
34:2:467:A:N1	34:2:593:A:O2'	2.38	0.52
34:2:565:C:H2'	34:2:566:A:H8	1.74	0.52
34:2:700:C:C2	34:2:739:G:N1	2.77	0.52
34:2:886:A:C5	34:2:887:U:C4	2.98	0.52
6:F:115:ILE:O	6:F:119:THR:HG23	2.08	0.52
34:2:1338:C:O2'	34:2:1340:A:N7	2.29	0.52
34:2:150:G:C6	34:2:163:A:N6	2.77	0.52
34:2:25:C:O4'	34:2:25:C:O2	2.26	0.52
34:2:268:G:C2	34:2:269:C:C2	2.97	0.52
34:2:628:U:C2	34:2:969:A:N6	2.77	0.52
34:2:86:A:H2'	34:2:87:C:C6	2.45	0.52
5:E:149:TYR:HB3	7:G:208:TYR:CD1	2.44	0.52
26:Z:56:THR:O	26:Z:57:TYR:HB2	2.10	0.52
34:2:266:U:O2	34:2:267:C:C5	2.63	0.52
34:2:1771:C:C2	34:2:1787:G:C2	2.97	0.52
34:2:519:A:N1	34:2:532:U:C2	2.77	0.52
34:2:700:C:N3	34:2:739:G:C6	2.78	0.52
34:2:884:G:C4	34:2:885:U:H1'	2.44	0.52
9:I:142:ARG:NH2	34:2:196:A:N1	2.57	0.52
34:2:1137:A:H2'	34:2:1138:A:C8	2.44	0.52
34:2:1671:G:H2'	34:2:1672:C:C6	2.45	0.52
34:2:360:C:C2	34:2:383:G:C2	2.97	0.52
26:Z:54:ALA:N	26:Z:55:PRO:CD	2.73	0.52
34:2:1041:G:H2'	34:2:1042:A:O4'	2.10	0.52
34:2:255:A:H2'	34:2:256:A:C8	2.45	0.52
34:2:560:G:O6	34:2:584:A:C6	2.63	0.52
34:2:508:G:H2'	34:2:509:G:O4'	2.09	0.52
34:2:1014:U:C6	34:2:1015:C:N3	2.78	0.52
34:2:1586:G:C6	34:2:1587:C:C4	2.97	0.52
34:2:214:A:C5	34:2:241:U:C6	2.97	0.52
34:2:431:G:C6	34:2:432:C:N3	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:509:G:C6	34:2:510:A:N7	2.78	0.52
34:2:309:C:C2	34:2:356:G:C2	2.98	0.51
34:2:624:C:H2'	34:2:625:U:C6	2.45	0.51
15:O:123:SER:O	34:2:884:G:N2	2.41	0.51
26:Z:103:ARG:O	26:Z:104:ALA:O	2.28	0.51
34:2:1137:A:C4	34:2:1138:A:N7	2.78	0.51
34:2:1651:C:C2	34:2:1746:G:C2	2.98	0.51
34:2:820:U:H2'	34:2:821:U:C6	2.45	0.51
8:H:93:LEU:HD21	8:H:125:ILE:HG23	1.92	0.51
12:L:101:GLU:OE2	24:X:13:ARG:N	2.43	0.51
14:N:94:LYS:O	14:N:98:VAL:HG23	2.09	0.51
34:2:1012:A:C2'	34:2:1013:G:O4'	2.53	0.51
7:G:174:LYS:HD3	34:2:65:A:H5'	1.93	0.51
7:G:83:CYS:N	34:2:161:A:OP1	2.43	0.51
9:I:68:ALA:HB1	12:L:20:PHE:CZ	2.46	0.51
34:2:1266:G:O2'	34:2:1446:G:O2'	2.27	0.51
34:2:520:A:C2	34:2:531:U:N3	2.78	0.51
2:B:99:ASN:O	2:B:101:HIS:N	2.43	0.51
34:2:1349:G:N1	34:2:1374:C:C2	2.78	0.51
34:2:28:A:H2'	34:2:29:U:O4'	2.10	0.51
34:2:849:A:C2	34:2:850:U:C2	2.98	0.51
34:2:1070:U:H5''	34:2:1071:C:P	2.50	0.51
34:2:214:A:C5	34:2:215:U:C5	2.98	0.51
34:2:776:G:N2	34:2:777:C:C2	2.79	0.51
34:2:928:A:P	34:2:930:C:N4	2.84	0.51
34:2:150:G:N2	34:2:163:A:C4	2.79	0.51
34:2:480:A:N1	34:2:506:U:C5	2.76	0.51
15:O:123:SER:HB3	34:2:884:G:H1'	1.92	0.51
34:2:1020:C:C4	34:2:1021:C:C4	2.99	0.51
34:2:1120:C:O2	34:2:1126:G:C2	2.63	0.51
34:2:1353:G:C6	34:2:1354:C:C4	2.99	0.51
34:2:273:G:C6	34:2:274:C:N4	2.79	0.51
34:2:425:G:N2	34:2:426:C:C2	2.79	0.51
34:2:885:U:H2'	34:2:886:A:O4'	2.10	0.51
34:2:1558:U:O2	34:2:1558:U:O4'	2.28	0.51
34:2:541:A:H2'	34:2:542:C:H3'	1.93	0.51
34:2:642:G:C2	34:2:692:C:O2	2.63	0.51
8:H:107:ARG:HD3	34:2:698:U:H1'	1.93	0.51
3:C:86:MET:HA	3:C:86:MET:HE3	1.92	0.51
34:2:85:A:O2'	34:2:147:U:O3'	2.22	0.51
34:2:1611:U:C5	34:2:1612:A:C2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:70:C:C4	34:2:71:A:C5	2.98	0.51
16:P:34:VAL:HG21	16:P:45:PHE:CG	2.45	0.51
24:X:63:GLN:HB3	24:X:64:PRO:HD2	1.93	0.51
34:2:1137:A:H2'	34:2:1138:A:H8	1.76	0.50
34:2:1363:G:C2	34:2:1364:C:C4	2.99	0.50
1:A:148:ASP:OD1	1:A:151:SER:N	2.44	0.50
26:Z:54:ALA:CB	26:Z:88:ILE:HG22	2.41	0.50
34:2:980:U:O2'	34:2:1122:C:N3	2.45	0.50
34:2:72:A:H2'	34:2:72:A:N3	2.26	0.50
24:X:65:ASN:HB3	34:2:574:C:H41	1.76	0.50
34:2:887:U:O4	34:2:888:U:O4	2.28	0.50
34:2:89:G:C6	34:2:90:C:C4	3.00	0.50
34:2:1173:C:C2	34:2:1464:G:N2	2.79	0.50
24:X:63:GLN:HG3	24:X:64:PRO:CD	2.41	0.50
26:Z:104:ALA:HB1	26:Z:105:THR:OG1	2.12	0.50
34:2:1353:G:C2	34:2:1354:C:C2	2.99	0.50
34:2:281:C:H2'	34:2:282:U:O4'	2.12	0.50
34:2:65:A:C5	34:2:83:G:C5	3.00	0.50
6:F:192:ILE:HD11	34:2:1471:U:H5'	1.94	0.50
15:O:129:LYS:HA	34:2:989:C:H4'	1.94	0.50
23:W:87:GLU:O	23:W:90:THR:HG22	2.12	0.50
34:2:137:U:C2	34:2:138:A:C6	2.99	0.50
34:2:150:G:N1	34:2:163:A:C6	2.80	0.50
34:2:1666:G:H2'	34:2:1667:U:O4'	2.11	0.50
1:A:18:LEU:HD22	18:R:106:THR:CG2	2.41	0.50
21:U:34:LEU:HD11	21:U:89:ARG:HG3	1.94	0.50
34:2:1471:U:O2	34:2:1471:U:C2'	2.59	0.50
34:2:261:U:N3	34:2:262:C:C4	2.80	0.50
34:2:508:G:H2'	34:2:509:G:C8	2.47	0.50
34:2:542:C:HO2'	34:2:543:A:P	2.33	0.50
34:2:883:A:C3'	34:2:884:G:H5'	2.40	0.50
7:G:155:ASP:N	34:2:78:A:H5''	2.23	0.50
34:2:515:G:O6	34:2:536:G:N2	2.45	0.50
34:2:700:C:O2	34:2:739:G:C2	2.65	0.50
7:G:154:ARG:C	34:2:78:A:H3'	2.32	0.50
17:Q:50:GLU:N	17:Q:51:PRO:CD	2.74	0.50
6:F:194:GLU:OE2	26:Z:59:TYR:HE2	1.95	0.50
34:2:1238:U:H1'	34:2:1247:C:N4	2.27	0.49
7:G:173:PRO:HA	34:2:66:U:O4'	2.11	0.49
34:2:1005:C:C6	34:2:1006:C:C5	3.00	0.49
34:2:1417:G:C2	34:2:1418:C:O2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1661:G:C6	34:2:1662:C:C4	3.00	0.49
34:2:564:C:C4	34:2:575:G:C8	3.00	0.49
34:2:150:G:C2	34:2:163:A:C4	3.00	0.49
34:2:1611:U:O2	34:2:1611:U:O4'	2.27	0.49
34:2:266:U:H3	34:2:267:C:H41	1.60	0.49
34:2:38:C:O2	34:2:469:A:N1	2.44	0.49
1:A:73:VAL:HG13	1:A:120:LEU:HD12	1.94	0.49
13:M:56:VAL:HG22	13:M:85:ALA:HB2	1.94	0.49
34:2:1015:C:O4'	34:2:1015:C:O2	2.29	0.49
34:2:39:A:O2'	34:2:468:C:N4	2.46	0.49
34:2:782:G:N2	34:2:783:C:C2	2.81	0.49
34:2:921:G:C6	34:2:922:A:C6	3.00	0.49
34:2:1292:U:C5	34:2:1321:A:C2	3.01	0.49
34:2:1396:U:H3'	34:2:1397:C:H5'	1.95	0.49
34:2:1527:C:H2'	34:2:1528:C:C6	2.46	0.49
6:F:189:ILE:HG23	34:2:1533:U:O2	2.12	0.49
34:2:561:G:H2'	34:2:562:U:C6	2.46	0.49
10:J:62:ARG:HB2	10:J:69:ARG:HG2	1.95	0.49
17:Q:52:LEU:HD22	17:Q:60:PHE:CZ	2.47	0.49
34:2:1183:A:H2	34:2:1453:G:O4'	1.95	0.49
34:2:70:C:C5	34:2:71:A:C6	3.00	0.49
15:O:123:SER:HA	34:2:928:A:C5	2.47	0.49
34:2:932:A:N7	34:2:934:U:H1'	2.26	0.49
34:2:1083:A:H2'	34:2:1084:G:O4'	2.13	0.49
34:2:1346:U:O2	34:2:1514:A:H5'	2.13	0.49
16:P:115:TYR:OH	34:2:1554:A:OP1	2.29	0.49
34:2:30:G:H2'	34:2:31:C:O4'	2.13	0.49
34:2:922:A:C2	34:2:923:A:C6	3.01	0.49
34:2:1222:A:N6	34:2:1260:G:O6	2.46	0.49
34:2:1571:A:O4'	34:2:1572:G:C2	2.65	0.49
34:2:1671:G:C5	34:2:1672:C:N4	2.80	0.49
34:2:560:G:N3	34:2:561:G:N7	2.60	0.49
7:G:171:LYS:CE	34:2:71:A:N6	2.75	0.49
34:2:886:A:C6	34:2:887:U:C4	3.01	0.49
13:M:24:VAL:HG22	13:M:124:ARG:HD3	1.94	0.49
34:2:925:A:H4'	34:2:1015:C:O2'	2.13	0.49
34:2:1255:A:H1'	34:2:1257:U:O4	2.12	0.49
34:2:767:U:O4'	34:2:767:U:O2	2.30	0.49
34:2:94:U:H2'	34:2:95:G:O4'	2.13	0.49
34:2:1131:A:C2	34:2:1132:A:C4	3.01	0.49
34:2:390:A:O2'	34:2:1728:A:O2'	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:334:U:H2'	34:2:335:G:O4'	2.12	0.49
34:2:261:U:O4	34:2:262:C:N4	2.46	0.48
20:T:31:PRO:HG3	20:T:54:PHE:CZ	2.48	0.48
34:2:1501:A:O2'	34:2:1502:G:OP1	2.26	0.48
34:2:1637:C:H2'	34:2:1638:C:O4'	2.13	0.48
34:2:975:G:H1	34:2:1022:A:HO2'	1.59	0.48
34:2:1046:G:N1	34:2:1071:C:C2	2.81	0.48
34:2:522:G:H8	34:2:522:G:O5'	1.97	0.48
34:2:89:G:C2	34:2:90:C:C2	3.01	0.48
25:Y:132:ARG:O	25:Y:135:ASP:N	2.46	0.48
34:2:1175:G:C2	34:2:1176:C:C2	3.02	0.48
34:2:150:G:N1	34:2:163:A:C5	2.81	0.48
34:2:1032:C:N4	34:2:1033:C:N4	2.61	0.48
34:2:1306:U:O2	34:2:1306:U:O4'	2.31	0.48
7:G:136:LYS:HB3	34:2:167:A:H4'	1.96	0.48
34:2:888:U:O4'	34:2:987:A:H4'	2.14	0.48
14:N:35:GLU:HA	14:N:38:ILE:HG12	1.95	0.48
19:S:143:ARG:NH1	34:2:1460:G:N7	2.62	0.48
34:2:1222:A:C6	34:2:1260:G:N1	2.82	0.48
34:2:1400:G:C6	34:2:1401:C:C4	3.02	0.48
34:2:14:C:C2	34:2:1140:G:C2	3.02	0.48
34:2:487:G:C2	34:2:499:C:C2	3.02	0.48
34:2:594:G:C2	34:2:595:C:N3	2.81	0.48
34:2:637:U:O4'	34:2:637:U:O2	2.31	0.48
34:2:763:G:O6	34:2:772:G:O6	2.30	0.48
6:F:203:ALA:HA	6:F:213:ILE:HD11	1.96	0.48
34:2:9:U:H2'	34:2:11:A:OP2	2.13	0.48
34:2:1220:A:C5	34:2:1221:C:C4	3.02	0.48
34:2:1786:G:H2'	34:2:1787:G:O4'	2.14	0.48
34:2:388:G:C2	34:2:408:C:C2	3.02	0.48
34:2:963:U:O4'	34:2:964:U:C5	2.66	0.48
10:J:80:LEU:O	10:J:83:ILE:HG22	2.13	0.48
34:2:1255:A:O4'	34:2:1257:U:C5	2.67	0.48
34:2:1499:C:N3	34:2:1505:G:C2	2.82	0.48
34:2:1661:G:C2	34:2:1662:C:C2	3.02	0.48
25:Y:43:LYS:O	25:Y:46:GLU:HG3	2.14	0.48
34:2:511:A:C6	34:2:512:U:C4	3.02	0.48
19:S:42:TYR:CE1	19:S:101:LEU:HD11	2.49	0.48
34:2:151:U:O2	34:2:162:G:C8	2.67	0.47
34:2:152:G:H2'	34:2:153:G:C8	2.49	0.47
34:2:1620:G:C2	34:2:1621:C:C2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:65:ASN:CB	34:2:574:C:H41	2.27	0.47
24:X:19:ARG:HA	24:X:19:ARG:HD2	1.57	0.47
34:2:1138:A:H2'	34:2:1139:G:O4'	2.14	0.47
34:2:1586:G:C2	34:2:1587:C:C2	3.02	0.47
34:2:1670:G:C2	34:2:1671:G:C5	3.03	0.47
34:2:30:G:C6	34:2:31:C:C4	3.02	0.47
34:2:84:A:H2'	34:2:85:A:O4'	2.14	0.47
34:2:921:G:H2'	34:2:922:A:C8	2.49	0.47
18:R:25:THR:O	18:R:27:ASP:N	2.47	0.47
34:2:1262:G:C2	34:2:1263:G:H1'	2.49	0.47
13:M:55:LEU:HD22	13:M:79:LEU:HD22	1.96	0.47
34:2:1044:C:C4	34:2:1072:G:C2	3.02	0.47
34:2:204:U:C2	34:2:205:A:C8	3.03	0.47
34:2:1083:A:N6	34:2:1089:C:N4	2.62	0.47
34:2:1497:G:C6	34:2:1498:C:C4	3.02	0.47
34:2:1533:U:O2	34:2:1533:U:O4'	2.31	0.47
34:2:212:A:C6	34:2:252:A:C6	3.03	0.47
34:2:560:G:C2'	34:2:561:G:C8	2.82	0.47
34:2:96:G:C6	34:2:97:C:C4	3.03	0.47
34:2:1042:A:C5	34:2:1043:U:C4	3.02	0.47
34:2:1240:G:H2'	34:2:1241:A:O5'	2.15	0.47
34:2:1220:A:N6	34:2:1261:U:O4	2.47	0.47
34:2:207:U:O2	34:2:208:U:C2	2.67	0.47
34:2:360:C:N3	34:2:383:G:C2	2.82	0.47
34:2:565:C:O2'	34:2:566:A:O4'	2.25	0.47
9:I:10:LYS:O	9:I:11:ARG:C	2.52	0.47
26:Z:52:LYS:CD	26:Z:53:GLU:HG3	2.41	0.47
34:2:935:G:OP1	34:2:1044:C:O4'	2.33	0.47
34:2:1218:A:C5	34:2:1264:G:H1'	2.49	0.47
7:G:179:VAL:HG11	34:2:139:C:H1'	1.97	0.47
34:2:1231:U:C2	34:2:1253:U:H1'	2.50	0.47
34:2:1437:C:H2'	34:2:1438:C:C6	2.49	0.47
34:2:567:G:C6	34:2:575:G:C2	3.03	0.47
34:2:988:U:C4	34:2:989:C:N4	2.83	0.47
26:Z:104:ALA:CB	26:Z:105:THR:CA	2.85	0.47
26:Z:52:LYS:HG3	26:Z:52:LYS:O	2.14	0.47
34:2:1038:A:N6	34:2:1077:C:H42	2.12	0.47
6:F:91:ILE:HG12	34:2:1443:G:C5	90.86	0.47
34:2:1444:A:N7	34:2:1446:G:C5	2.82	0.47
34:2:1454:C:O2	34:2:1454:C:O4'	2.33	0.47
34:2:564:C:H2'	34:2:576:G:H21	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:71:A:C2	34:2:72:A:C6	3.02	0.47
34:2:925:A:H3'	34:2:926:C:C6	2.50	0.47
7:G:136:LYS:NZ	34:2:65:A:P	2.84	0.47
7:G:173:PRO:HB2	7:G:175:ILE:HD12	1.95	0.47
34:2:1040:G:H2'	34:2:1041:G:C8	2.50	0.47
34:2:1222:A:N6	34:2:1260:G:C6	2.82	0.47
34:2:1400:G:C2	34:2:1401:C:C2	3.03	0.47
34:2:1588:G:C2	34:2:1589:C:C2	3.03	0.47
9:I:100:ALA:O	9:I:170:ILE:HD12	2.14	0.47
10:J:148:VAL:HG11	10:J:156:ILE:HD11	1.96	0.47
34:2:1183:A:C2	34:2:1452:G:N2	2.82	0.47
34:2:1496:G:O6	34:2:1507:C:N4	2.48	0.47
1:A:164:ASN:HA	1:A:170:ILE:HD11	1.96	0.47
26:Z:104:ALA:HB1	26:Z:105:THR:CB	2.45	0.47
34:2:1081:C:O2'	34:2:1082:G:C5'	2.62	0.46
34:2:1239:U:O4'	34:2:1245:C:N4	2.48	0.46
34:2:1560:G:C6	34:2:1561:C:C4	3.03	0.46
34:2:214:A:C5	34:2:241:U:C5	3.03	0.46
34:2:967:U:H5''	34:2:1032:C:O2'	2.16	0.46
34:2:1598:A:H1'	34:2:1599:G:H5'	1.98	0.46
10:J:172:VAL:N	34:2:511:A:OP2	2.48	0.46
10:J:66:ASP:HB3	10:J:67:PRO:CD	2.45	0.46
20:T:18:TYR:CD2	20:T:135:ILE:HD13	2.50	0.46
34:2:1175:G:C6	34:2:1176:C:C4	3.04	0.46
34:2:142:G:H2'	34:2:143:G:C8	2.50	0.46
34:2:1578:C:H2'	34:2:1579:C:O4'	2.15	0.46
34:2:274:C:N4	34:2:275:C:N4	2.64	0.46
34:2:585:G:C6	34:2:586:C:C4	3.03	0.46
34:2:980:U:H2'	34:2:981:U:C6	2.50	0.46
3:C:169:SER:OG	3:C:169:SER:O	2.34	0.46
34:2:1222:A:N3	34:2:1260:G:C2	2.84	0.46
34:2:1363:G:C6	34:2:1364:C:N4	2.83	0.46
34:2:1620:G:C6	34:2:1621:C:C4	3.04	0.46
34:2:1670:G:H2'	34:2:1671:G:C8	2.50	0.46
34:2:254:U:C4	34:2:255:A:N7	2.84	0.46
34:2:585:G:C2	34:2:586:C:C2	3.03	0.46
7:G:160:ARG:NE	34:2:68:A:C8	2.83	0.46
34:2:884:G:C8	34:2:884:G:C5'	2.85	0.46
34:2:935:G:C6	34:2:936:C:C4	3.03	0.46
7:G:175:ILE:HG22	34:2:78:A:N3	2.31	0.46
9:I:68:ALA:HB2	9:I:183:TYR:OH	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:33:ALA:CB	34:2:532:U:H4'	2.46	0.46
34:2:1203:A:H2'	34:2:1203:A:N3	2.31	0.46
34:2:1290:G:H2'	34:2:1291:G:H8	1.81	0.46
34:2:149:U:O2'	34:2:150:G:O4'	2.23	0.46
34:2:284:G:N2	34:2:285:C:C2	2.84	0.46
34:2:266:U:O2	34:2:287:A:N1	2.48	0.46
34:2:887:U:C4	34:2:888:U:C4	3.04	0.46
16:P:79:HIS:O	16:P:81:ARG:N	2.49	0.46
25:Y:90:ARG:HA	25:Y:93:ARG:HD3	1.98	0.46
24:X:7:ARG:NH2	34:2:1099:G:O4'	2.48	0.46
34:2:210:U:H2'	34:2:211:U:C6	2.51	0.46
34:2:268:G:O6	34:2:285:C:N3	2.49	0.46
34:2:30:G:C2	34:2:31:C:C2	3.04	0.46
34:2:458:G:H3'	34:2:459:A:C5'	2.45	0.46
34:2:642:G:N1	34:2:692:C:C2	2.84	0.46
7:G:155:ASP:HB2	34:2:78:A:P	2.55	0.46
21:U:95:ALA:HB1	21:U:99:ILE:HG21	1.96	0.46
16:P:122:THR:HG21	34:2:1452:G:H4'	1.98	0.46
34:2:1643:G:N2	34:2:1644:C:C2	2.84	0.46
34:2:266:U:C2	34:2:287:A:N1	2.83	0.46
34:2:89:G:N1	34:2:90:C:C2	2.84	0.46
9:I:139:ASN:HB2	34:2:186:G:H2'	1.98	0.46
24:X:63:GLN:CB	24:X:64:PRO:HD2	2.46	0.46
26:Z:54:ALA:HB1	26:Z:89:ILE:CD1	2.46	0.46
34:2:1289:U:H2'	34:2:1290:G:C8	2.51	0.46
7:G:74:LYS:HA	7:G:96:SER:HA	1.97	0.46
14:N:98:VAL:CG1	14:N:115:LEU:HB2	2.46	0.46
25:Y:59:GLY:O	25:Y:60:PHE:HB2	2.16	0.46
34:2:1589:C:C2	34:2:1590:A:C8	3.04	0.46
34:2:209:A:O2'	34:2:210:U:H5'	2.15	0.46
34:2:214:A:C4	34:2:241:U:C5	3.04	0.46
34:2:988:U:H2'	34:2:989:C:C2	2.51	0.46
7:G:4:ASN:HB3	7:G:110:ALA:HA	1.98	0.46
34:2:1082:G:O6	34:2:1083:A:N6	2.49	0.46
34:2:1083:A:H2'	34:2:1084:G:C8	2.51	0.46
34:2:1603:G:C6	34:2:1604:C:C4	3.03	0.46
34:2:1778:G:O2'	34:2:1779:A:H8	1.98	0.46
7:G:153:VAL:HA	34:2:78:A:H5'	1.98	0.46
34:2:987:A:C2	34:2:988:U:C2	3.04	0.46
34:2:935:G:OP1	34:2:1074:C:N4	2.49	0.45
19:S:41:ARG:HD2	34:2:1563:C:H5"	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1074:C:O2	34:2:1074:C:H2'	2.10	0.45
34:2:1647:G:H2'	34:2:1648:U:C6	2.51	0.45
34:2:1733:U:H2'	34:2:1734:G:O4'	2.16	0.45
34:2:991:A:H4'	34:2:1783:U:O2'	2.16	0.45
6:F:119:THR:HG22	6:F:193:ALA:O	2.16	0.45
21:U:103:ILE:O	21:U:106:ILE:O	2.34	0.45
34:2:1042:A:N1	34:2:1043:U:C2	2.84	0.45
34:2:1223:A:C6	34:2:1259:U:C2	3.04	0.45
34:2:1439:C:H2'	34:2:1440:U:O4'	2.16	0.45
34:2:85:A:N3	34:2:147:U:H1'	2.31	0.45
34:2:623:G:C2	34:2:624:C:C2	3.04	0.45
8:H:116:ARG:NH2	34:2:855:A:O2'	2.49	0.45
34:2:89:G:C6	34:2:90:C:N3	2.84	0.45
15:O:41:ARG:NH2	34:2:915:U:O2	2.49	0.45
34:2:123:G:C5	34:2:124:A:C8	3.04	0.45
34:2:1730:A:H2'	34:2:1731:C:C6	2.51	0.45
34:2:403:G:C2	34:2:404:C:C2	3.05	0.45
10:J:62:ARG:HB2	10:J:69:ARG:CG	2.46	0.45
34:2:1220:A:C2	34:2:1262:G:C4	3.05	0.45
34:2:1598:A:H1'	34:2:1599:G:C5'	2.47	0.45
34:2:1783:U:H2'	34:2:1784:G:C8	2.52	0.45
34:2:626:C:H2'	34:2:627:G:O4'	2.16	0.45
6:F:63:TYR:CE1	6:F:167:LEU:HD11	2.52	0.45
12:L:94:VAL:CG2	24:X:12:ALA:HB1	2.47	0.45
19:S:116:LEU:HA	19:S:119:ILE:HG12	1.97	0.45
25:Y:130:ALA:O	25:Y:133:ASN:HB2	2.16	0.45
34:2:1185:U:C4	34:2:1207:A:N6	2.84	0.45
34:2:1217:G:C4	34:2:1442:A:C8	3.04	0.45
34:2:266:U:C2	34:2:267:C:C5	3.04	0.45
34:2:96:G:C2	34:2:97:C:C2	3.05	0.45
3:C:183:ILE:HG21	3:C:190:LYS:HA	1.98	0.45
25:Y:29:HIS:CD2	25:Y:35:VAL:HG13	2.51	0.45
34:2:1007:G:H2'	34:2:1008:U:C6	2.51	0.45
34:2:1220:A:N1	34:2:1261:U:C4	2.85	0.45
34:2:1269:G:C2	34:2:1439:C:O2	2.70	0.45
34:2:137:U:O2	34:2:137:U:C2'	2.64	0.45
7:G:183:ARG:NH1	34:2:266:U:OP1	2.50	0.45
34:2:269:C:C2'	34:2:270:A:H8	2.17	0.45
34:2:45:U:O2'	34:2:46:A:H2'	2.17	0.45
34:2:1170:A:H2'	34:2:1171:G:C8	2.52	0.45
34:2:1560:G:C2	34:2:1561:C:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:N	2:B:194:ASN:OD1	2.48	0.45
16:P:79:HIS:CE1	16:P:97:TYR:CD2	3.04	0.45
26:Z:54:ALA:HB1	26:Z:89:ILE:CG1	2.47	0.45
34:2:1447:U:H2'	34:2:1448:U:O4'	2.17	0.45
34:2:1497:G:C2	34:2:1498:C:C2	3.05	0.45
34:2:48:G:C2	34:2:49:C:C2	3.05	0.45
34:2:48:G:C6	34:2:49:C:C4	3.05	0.45
34:2:782:G:C2	34:2:783:C:C2	3.05	0.45
5:E:134:LYS:N	34:2:252:A:OP1	2.50	0.45
9:I:76:THR:HG23	9:I:108:PRO:HG2	1.99	0.45
10:J:108:ARG:NH2	10:J:145:SER:OG	2.50	0.45
23:W:99:PHE:HB3	23:W:130:TYR:CE1	2.52	0.45
34:2:1223:A:N6	34:2:1259:U:H3	2.14	0.44
34:2:1442:A:N3	34:2:1442:A:H2'	2.32	0.44
34:2:1781:C:H2'	34:2:1782:C:C6	2.51	0.44
34:2:208:U:N3	34:2:209:A:N7	2.65	0.44
34:2:520:A:C2'	34:2:521:U:O5'	2.65	0.44
34:2:70:C:N4	34:2:81:G:H1	2.14	0.44
34:2:932:A:C6	34:2:934:U:C2	3.05	0.44
34:2:991:A:C5'	34:2:991:A:N3	2.80	0.44
4:D:98:ALA:HA	4:D:188:ILE:HD13	1.98	0.44
34:2:1126:G:C6	34:2:1127:C:C4	3.05	0.44
34:2:1269:G:C2	34:2:1439:C:C2	3.06	0.44
26:Z:97:LYS:NZ	34:2:1471:U:OP2	2.49	0.44
9:I:140:THR:CG2	34:2:185:C:H3'	2.47	0.44
7:G:155:ASP:OD2	34:2:77:U:O2'	2.34	0.44
1:A:124:THR:OG1	1:A:125:ASP:N	2.51	0.44
34:2:1307:G:C2	34:2:1308:C:C2	3.05	0.44
34:2:1584:A:C2	34:2:1609:A:N7	2.86	0.44
34:2:798:A:C2	34:2:799:U:C2	3.05	0.44
34:2:878:G:C2	34:2:879:C:C2	3.05	0.44
26:Z:51:MET:O	26:Z:53:GLU:CB	2.64	0.44
34:2:1603:G:C2	34:2:1604:C:C2	3.05	0.44
34:2:515:G:O6	34:2:536:G:C2	2.70	0.44
34:2:560:G:C6	34:2:584:A:C6	3.06	0.44
34:2:883:A:N6	34:2:884:G:C6	2.84	0.44
34:2:935:G:C2	34:2:936:C:C2	3.05	0.44
6:F:109:LYS:HB2	34:2:1608:G:C5'	2.48	0.44
26:Z:103:ARG:C	26:Z:104:ALA:O	2.54	0.44
26:Z:59:TYR:HA	26:Z:101:TYR:O	2.17	0.44
34:2:1031:G:C6	34:2:1032:C:C4	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1042:A:C6	34:2:1075:A:N1	2.85	0.44
16:P:43:ARG:NH2	34:2:1550:U:OP2	2.50	0.44
34:2:269:C:H42	34:2:284:G:H1	1.64	0.44
34:2:954:A:H2'	34:2:955:C:O4'	2.17	0.44
6:F:78:ARG:NH2	34:2:1410:G:OP1	2.51	0.44
7:G:175:ILE:HD13	34:2:78:A:O2'	2.16	0.44
21:U:39:ALA:HA	21:U:42:ILE:HG12	1.99	0.44
10:J:140:ILE:HD12	25:Y:65:GLY:HA3	1.99	0.44
26:Z:49:ARG:CG	26:Z:49:ARG:HH11	2.12	0.44
34:2:1218:A:N6	34:2:1264:G:H4'	2.32	0.44
34:2:1219:C:C4	34:2:1263:G:N2	2.86	0.44
34:2:1498:C:N3	34:2:1499:C:C5	2.86	0.44
34:2:251:U:O2'	34:2:252:A:O4'	2.31	0.44
34:2:267:C:N4	34:2:286:G:N1	2.47	0.44
34:2:288:U:C2	34:2:289:G:C8	3.06	0.44
34:2:560:G:C6	34:2:584:A:N1	2.86	0.44
34:2:734:A:H2'	34:2:735:C:C6	2.53	0.44
34:2:952:G:H2'	34:2:953:G:C8	2.52	0.44
23:W:75:ILE:HA	34:2:1099:G:O2'	2.17	0.44
34:2:1014:U:C5	34:2:1015:C:N3	2.86	0.44
34:2:1080:A:C6	34:2:1090:A:C6	3.06	0.44
34:2:1209:C:H2'	34:2:1210:A:C8	2.52	0.44
34:2:268:G:N2	34:2:269:C:C2	2.86	0.44
34:2:268:G:O6	34:2:286:G:C4	2.71	0.44
34:2:508:G:H2'	34:2:509:G:C1'	2.47	0.44
34:2:564:C:C5	34:2:575:G:C8	3.06	0.44
8:H:41:LEU:HD22	8:H:70:TYR:CD2	2.52	0.44
6:F:125:VAL:CG1	26:Z:59:TYR:HB3	2.44	0.44
26:Z:61:SER:O	26:Z:63:SER:N	2.51	0.44
34:2:1218:A:C8	34:2:1263:G:N2	2.85	0.44
34:2:157:U:H4'	34:2:158:U:OP1	2.18	0.44
34:2:514:A:C6	34:2:542:C:C6	3.06	0.44
34:2:515:G:C6	34:2:536:G:C2	3.06	0.44
34:2:922:A:C6	34:2:923:A:N6	2.86	0.44
7:G:5:ILE:HD12	7:G:16:ILE:HD13	2.00	0.44
34:2:1232:G:N2	34:2:1252:U:H1'	2.32	0.44
34:2:1287:G:N7	34:2:1313:U:H2'	2.33	0.44
34:2:1671:G:C4	34:2:1672:C:C5	3.06	0.44
34:2:53:G:C6	34:2:54:C:C4	3.05	0.44
34:2:955:C:H2'	34:2:956:G:C8	2.52	0.44
34:2:8:U:H3'	34:2:9:U:H5'	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:103:ASN:O	19:S:106:GLU:HG2	2.18	0.44
16:P:18:LYS:HA	19:S:91:ASP:C	2.37	0.44
34:2:1042:A:C6	34:2:1075:A:C2	3.06	0.43
34:2:168:A:C8	34:2:170:A:N7	2.86	0.43
34:2:911:U:O2	34:2:911:U:C2'	2.66	0.43
34:2:979:G:H2'	34:2:980:U:O4'	2.18	0.43
34:2:1217:G:C5'	34:2:1442:A:H62	2.31	0.43
34:2:1316:C:H2'	34:2:1317:G:O4'	2.18	0.43
34:2:151:U:O2	34:2:162:G:H8	2.00	0.43
34:2:429:G:C2	34:2:430:C:C2	3.06	0.43
34:2:519:A:C2	34:2:532:U:O2	2.71	0.43
34:2:53:G:C2	34:2:54:C:C2	3.06	0.43
34:2:623:G:C6	34:2:624:C:C4	3.06	0.43
34:2:776:G:N1	34:2:777:C:C4	2.86	0.43
34:2:782:G:C6	34:2:783:C:C4	3.05	0.43
10:J:11:THR:HB	10:J:12:TYR:CE1	2.53	0.43
6:F:113:VAL:HG12	17:Q:43:ILE:HD11	2.00	0.43
16:P:19:GLY:C	19:S:93:ASN:H	2.21	0.43
26:Z:96:SER:O	26:Z:97:LYS:HG3	2.18	0.43
34:2:1015:C:H2'	34:2:1016:U:O4'	2.18	0.43
34:2:1123:A:C6	34:2:1124:A:C6	3.06	0.43
1:A:162:CYS:SG	1:A:163:ASN:N	2.91	0.43
25:Y:121:THR:N	34:2:148:C:OP1	2.50	0.43
34:2:1046:G:C2	34:2:1071:C:O2	2.72	0.43
34:2:1437:C:C2	34:2:1438:C:C5	3.06	0.43
7:G:136:LYS:O	7:G:175:ILE:HG23	2.18	0.43
20:T:99:SER:HA	20:T:102:ARG:NH2	2.33	0.43
34:2:1031:G:C2	34:2:1032:C:C2	3.06	0.43
34:2:1270:G:C2	34:2:1438:C:C2	3.06	0.43
34:2:1417:G:H2'	34:2:1418:C:O4'	2.18	0.43
34:2:551:G:C2	34:2:572:C:C2	3.06	0.43
34:2:886:A:C2	34:2:925:A:C2	3.06	0.43
14:N:127:ARG:NH2	34:2:628:U:OP1	2.51	0.43
34:2:1217:G:C5	34:2:1442:A:C8	3.06	0.43
34:2:1222:A:C2	34:2:1260:G:C2	3.07	0.43
34:2:1482:G:N2	34:2:1483:C:C2	2.86	0.43
34:2:1540:G:O2'	34:2:1541:A:O4'	2.35	0.43
34:2:1546:G:C2	34:2:1547:C:C2	3.07	0.43
34:2:213:G:C5'	34:2:241:U:O2	2.66	0.43
34:2:266:U:H3	34:2:267:C:N4	2.17	0.43
34:2:452:U:O2	34:2:452:U:H2'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG13	1:A:150:ASP:HB3	2.00	0.43
10:J:109:LEU:HD11	10:J:134:ILE:HG21	1.98	0.43
34:2:1222:A:N1	34:2:1259:U:C2	2.86	0.43
34:2:207:U:N3	34:2:208:U:C4	2.87	0.43
34:2:560:G:O6	34:2:584:A:N6	2.51	0.43
1:A:53:THR:HA	1:A:161:PRO:HD2	2.00	0.43
6:F:194:GLU:OE2	26:Z:59:TYR:CE2	2.72	0.43
34:2:1182:A:C2	34:2:1209:C:O2	2.72	0.43
34:2:1210:A:H2'	34:2:1211:G:O4'	2.18	0.43
34:2:366:A:H2'	34:2:367:U:O4'	2.19	0.43
34:2:828:A:O2'	34:2:829:U:OP2	2.37	0.43
2:B:137:ILE:HG21	2:B:176:VAL:HG21	1.99	0.43
7:G:174:LYS:CD	34:2:65:A:H5'	2.48	0.43
17:Q:47:LYS:O	17:Q:50:GLU:HB2	2.18	0.43
26:Z:61:SER:H	26:Z:64:VAL:HB	1.84	0.43
34:2:1220:A:C4	34:2:1262:G:C2	3.07	0.43
16:P:79:HIS:HB2	34:2:1240:G:C8	2.54	0.43
34:2:1292:U:O4	34:2:1293:G:C5	2.72	0.43
34:2:1598:A:H4'	34:2:1599:G:OP1	2.18	0.43
34:2:1785:C:H2'	34:2:1786:G:C8	2.54	0.43
34:2:252:A:O2'	34:2:253:A:O4'	2.35	0.43
34:2:429:G:C6	34:2:430:C:C4	3.07	0.43
34:2:452:U:O2	34:2:452:U:C2'	2.66	0.43
34:2:1171:G:C2	34:2:1172:C:C2	3.06	0.43
34:2:1178:G:C2	34:2:1179:C:C2	3.07	0.43
34:2:1258:U:C6	34:2:1259:U:C4	3.06	0.43
34:2:1222:A:N1	34:2:1260:G:C6	2.87	0.43
34:2:1783:U:H2'	34:2:1784:G:H8	1.83	0.43
7:G:173:PRO:HG3	34:2:66:U:C2	2.54	0.43
34:2:978:A:N3	34:2:1773:U:O2'	2.42	0.43
10:J:126:ARG:HD3	10:J:144:PRO:HB3	2.01	0.43
10:J:149:ARG:O	10:J:151:GLU:N	2.49	0.43
11:K:42:VAL:HG12	11:K:46:LEU:HD12	2.01	0.43
34:2:1073:G:O2'	34:2:1074:C:H5''	2.19	0.42
34:2:1240:G:C2'	34:2:1241:A:O5'	2.65	0.42
34:2:1551:G:N1	34:2:1554:A:OP2	2.52	0.42
34:2:851:C:H2'	34:2:852:G:O4'	2.19	0.42
1:A:25:GLY:O	1:A:26:ALA:HB3	2.19	0.42
9:I:9:HIS:O	9:I:10:LYS:HB2	2.19	0.42
23:W:2:THR:N	34:2:1033:C:HO2'	2.16	0.42
34:2:1079:U:H3	34:2:1090:A:H61	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1482:G:C6	34:2:1483:C:N4	2.88	0.42
34:2:1590:A:C2	34:2:1602:U:N3	2.87	0.42
34:2:144:A:C6	34:2:170:A:C6	3.07	0.42
34:2:1784:G:C6	34:2:1785:C:N3	2.87	0.42
34:2:535:C:C2'	34:2:536:G:O4'	2.65	0.42
34:2:556:G:N1	34:2:558:C:C4	2.87	0.42
34:2:571:C:C4	34:2:572:C:C5	3.07	0.42
1:A:15:GLN:HG3	18:R:117:LEU:HD23	2.00	0.42
6:F:125:VAL:HG11	26:Z:59:TYR:CB	2.43	0.42
10:J:7:THR:HG21	34:2:758:U:H5''	2.00	0.42
14:N:4:MET:SD	14:N:124:ARG:NH1	2.92	0.42
34:2:1083:A:C2	34:2:1089:C:N3	2.87	0.42
34:2:1218:A:H62	34:2:1263:G:C2'	2.26	0.42
34:2:1460:G:C2	34:2:1461:C:C2	3.07	0.42
34:2:1491:A:O2'	34:2:1492:C:OP2	2.28	0.42
34:2:515:G:C5	34:2:536:G:N2	2.85	0.42
34:2:513:G:N1	34:2:542:C:C4	2.57	0.42
34:2:566:A:C2	34:2:582:C:H1'	2.55	0.42
34:2:549:A:C2	34:2:588:C:C6	3.07	0.42
16:P:18:LYS:N	19:S:93:ASN:O	2.41	0.42
12:L:99:ARG:CB	24:X:12:ALA:HB2	2.49	0.42
25:Y:29:HIS:N	25:Y:30:PRO:CD	2.82	0.42
34:2:1460:G:C6	34:2:1461:C:C4	3.07	0.42
34:2:1672:C:H2'	34:2:1673:C:C6	2.54	0.42
9:I:96:LEU:HD11	9:I:180:CYS:SG	2.59	0.42
34:2:1073:G:O2'	34:2:1074:C:O5'	2.37	0.42
34:2:1074:C:O2'	34:2:1074:C:O2	2.37	0.42
34:2:1083:A:C2	34:2:1089:C:C2	3.07	0.42
34:2:1126:G:C2	34:2:1127:C:C2	3.08	0.42
34:2:1230:U:O3'	34:2:1258:U:H5'	2.19	0.42
34:2:1307:G:C6	34:2:1308:C:N4	2.87	0.42
34:2:1444:A:C8	34:2:1446:G:C5	3.08	0.42
34:2:1154:G:N2	34:2:1622:C:C2	2.87	0.42
34:2:127:G:O2'	34:2:178:A:N7	2.46	0.42
34:2:506:U:O4'	34:2:506:U:O2	2.37	0.42
34:2:630:G:C5	34:2:631:U:C4	3.07	0.42
34:2:1171:G:C6	34:2:1172:C:C4	3.07	0.42
34:2:1185:U:O4	34:2:1199:G:N2	2.51	0.42
34:2:1315:G:C2	34:2:1316:C:C2	3.07	0.42
34:2:647:G:N3	34:2:647:G:H2'	2.34	0.42
16:P:19:GLY:H	19:S:92:VAL:C	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:20:VAL:N	19:S:94:ASP:H	2.18	0.42
18:R:45:ARG:NH2	34:2:1413:U:OP1	2.52	0.42
16:P:17:TYR:CA	19:S:92:VAL:O	2.68	0.42
34:2:1588:G:N2	34:2:1589:C:C2	2.87	0.42
34:2:407:C:HO2'	34:2:1730:A:HO2'	1.66	0.42
34:2:1629:A:N6	34:2:1761:A:O2'	2.53	0.42
34:2:16:G:C2	34:2:17:C:N3	2.87	0.42
34:2:564:C:C4	34:2:576:G:C5	3.07	0.42
6:F:138:ALA:HA	6:F:203:ALA:HB1	2.01	0.42
7:G:160:ARG:HB3	7:G:171:LYS:HB2	2.01	0.42
17:Q:49:TYR:O	17:Q:52:LEU:HG	2.20	0.42
34:2:1217:G:H2'	34:2:1442:A:N6	2.34	0.42
34:2:1378:U:H2'	34:2:1379:U:O4'	2.19	0.42
34:2:549:A:C6	34:2:556:G:O6	2.73	0.42
34:2:566:A:C2'	34:2:567:G:O4'	2.60	0.42
34:2:885:U:N3	34:2:886:A:C5	2.87	0.42
13:M:21:LEU:HD21	13:M:80:ILE:HD13	2.01	0.42
19:S:38:VAL:HG22	19:S:101:LEU:HB3	2.02	0.42
34:2:1431:G:H2'	34:2:1432:U:O4'	2.19	0.42
34:2:1531:C:H4'	34:2:1537:G:C6	2.55	0.42
34:2:1602:U:C4	34:2:1603:G:N7	2.88	0.42
34:2:922:A:H2'	34:2:923:A:O4'	2.19	0.42
34:2:941:G:C2	34:2:942:C:C2	3.08	0.42
34:2:1070:U:O3'	34:2:1071:C:O4'	2.38	0.42
34:2:63:G:O2'	34:2:64:U:O5'	2.38	0.42
34:2:1083:A:C6	34:2:1089:C:N4	2.88	0.41
34:2:1255:A:C1'	34:2:1257:U:C5	3.02	0.41
34:2:1220:A:C2	34:2:1262:G:C5	3.08	0.41
34:2:15:U:H2'	34:2:16:G:O4'	2.21	0.41
34:2:363:G:C2	34:2:380:C:N3	2.88	0.41
34:2:60:U:H4'	34:2:454:C:N4	2.35	0.41
34:2:629:A:C8	34:2:630:G:C8	3.08	0.41
34:2:922:A:N1	34:2:923:A:N6	2.67	0.41
10:J:127:VAL:HG21	34:2:477:A:H5'	2.02	0.41
18:R:110:VAL:HG13	18:R:117:LEU:HD22	2.02	0.41
24:X:63:GLN:CG	24:X:64:PRO:HD2	2.49	0.41
34:2:1040:G:C5	34:2:1076:C:N4	2.86	0.41
34:2:1183:A:O2'	34:2:1184:U:H4'	2.21	0.41
34:2:1260:G:C5	34:2:1261:U:C4	3.08	0.41
34:2:391:G:C2	34:2:392:C:C2	3.08	0.41
34:2:50:C:N3	34:2:429:G:C6	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:584:A:N6	34:2:585:G:O6	2.53	0.41
9:I:5:ARG:NH1	9:I:29:LEU:O	2.44	0.41
10:J:171:ARG:N	10:J:171:ARG:HD2	2.35	0.41
23:W:76:SER:CB	23:W:77:PRO:CD	2.98	0.41
34:2:1073:G:O2'	34:2:1074:C:C5'	2.68	0.41
34:2:1222:A:C2	34:2:1260:G:N3	2.88	0.41
34:2:1441:U:H4'	34:2:1444:A:N3	2.35	0.41
34:2:268:G:C5	34:2:269:C:C5	3.09	0.41
34:2:300:A:H2'	34:2:301:U:O4'	2.20	0.41
34:2:31:C:N4	34:2:32:U:C4	2.88	0.41
34:2:407:C:H2'	34:2:408:C:C6	2.54	0.41
1:A:185:ARG:HG3	22:V:45:ALA:HB3	2.01	0.41
34:2:1206:C:C2	34:2:1207:A:C6	3.09	0.41
34:2:1315:G:C6	34:2:1316:C:C4	3.08	0.41
34:2:1560:G:N2	34:2:1561:C:C2	2.89	0.41
34:2:511:A:C3'	34:2:512:U:C5'	2.96	0.41
34:2:642:G:C6	34:2:692:C:N3	2.88	0.41
34:2:878:G:C6	34:2:879:C:C4	3.08	0.41
34:2:978:A:C2	34:2:1773:U:H4'	2.55	0.41
1:A:124:THR:HG22	1:A:174:TRP:HE1	1.85	0.41
3:C:144:ILE:CD1	3:C:196:ALA:HB1	2.51	0.41
13:M:45:LEU:HD13	13:M:71:LEU:HB3	2.02	0.41
26:Z:66:VAL:HA	26:Z:67:ASP:HA	1.56	0.41
34:2:1471:U:O2	34:2:1471:U:H2'	2.19	0.41
34:2:146:A:C5	34:2:147:U:C5	3.08	0.41
34:2:146:A:C6	34:2:147:U:C5	3.08	0.41
5:E:47:PHE:CE2	5:E:52:LEU:HD11	2.56	0.41
10:J:133:HIS:HB2	10:J:134:ILE:HD12	2.02	0.41
24:X:53:VAL:HG13	24:X:72:VAL:HG13	2.02	0.41
34:2:1290:G:C2	34:2:1324:A:C2	3.08	0.41
34:2:1463:C:C5	34:2:1464:G:C8	3.09	0.41
34:2:59:C:O2'	34:2:60:U:C6	2.72	0.41
34:2:690:A:H2'	34:2:691:U:O4'	2.20	0.41
34:2:8:U:C3'	34:2:9:U:C5'	2.90	0.41
34:2:8:U:HO2'	34:2:9:U:H5'	1.85	0.41
16:P:98:ASN:O	34:2:1182:A:N6	2.54	0.41
34:2:1250:U:C2	34:2:1251:C:C5	3.08	0.41
34:2:1307:G:C6	34:2:1308:C:C4	3.09	0.41
34:2:1546:G:N2	34:2:1547:C:C2	2.89	0.41
34:2:209:A:H2'	34:2:210:U:H5'	2.00	0.41
34:2:211:U:C2	34:2:253:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:46:A:N1	34:2:431:G:O2'	2.45	0.41
34:2:566:A:C8	34:2:575:G:N2	2.86	0.41
34:2:776:G:C2	34:2:777:C:C2	3.08	0.41
23:W:8:ALA:HA	23:W:74:VAL:HG21	2.01	0.41
34:2:1255:A:O4'	34:2:1257:U:H5	2.04	0.41
21:U:70:THR:HG22	34:2:1279:C:O2'	2.20	0.41
19:S:41:ARG:NH1	34:2:1563:C:OP1	2.46	0.41
34:2:556:G:N2	34:2:558:C:N3	2.68	0.41
34:2:564:C:C2'	34:2:576:G:N2	2.78	0.41
34:2:885:U:O4	34:2:886:A:N6	2.54	0.41
1:A:102:PHE:CE2	1:A:132:ALA:HA	2.55	0.41
4:D:20:GLU:HG2	11:K:61:TRP:CZ3	2.55	0.41
15:O:124:ASP:OD1	34:2:926:C:O2'	2.33	0.41
34:2:391:G:C6	34:2:392:C:C4	3.08	0.41
34:2:564:C:C5	34:2:576:G:C5	3.09	0.41
7:G:36:VAL:HB	7:G:50:PHE:HB2	2.03	0.41
7:G:56:ASN:ND2	7:G:61:PHE:O	2.54	0.41
11:K:3:ILE:HG21	11:K:8:ARG:HB2	2.02	0.41
15:O:50:ALA:O	15:O:52:ARG:N	2.53	0.41
25:Y:35:VAL:HG21	25:Y:40:LEU:HD11	2.02	0.41
34:2:1002:A:O2'	34:2:1004:A:N7	2.44	0.41
34:2:935:G:P	34:2:1074:C:N3	2.91	0.41
34:2:1041:G:H1	34:2:1075:A:H2	1.69	0.41
34:2:1245:C:C4	34:2:1246:U:O2	2.74	0.41
34:2:1464:G:C6	34:2:1465:C:C4	3.08	0.41
34:2:151:U:C2	34:2:162:G:C8	3.08	0.41
34:2:1592:G:OP2	34:2:1594:C:N4	2.54	0.41
34:2:185:C:O2	34:2:185:C:H2'	2.21	0.41
34:2:216:A:N1	34:2:844:G:H1'	2.36	0.41
10:J:173:ALA:HB3	34:2:511:A:OP1	2.20	0.41
13:M:70:GLY:O	13:M:73:THR:OG1	2.39	0.41
34:2:1038:A:H61	34:2:1077:C:N4	2.19	0.41
34:2:1187:G:C6	34:2:1197:G:C6	3.09	0.41
34:2:268:G:O6	34:2:286:G:N3	2.54	0.41
34:2:403:G:C6	34:2:404:C:C4	3.09	0.41
34:2:425:G:C2	34:2:426:C:C2	3.09	0.41
34:2:425:G:C6	34:2:426:C:C4	3.09	0.41
34:2:821:U:C4	34:2:822:G:C2	3.09	0.41
13:M:55:LEU:HB3	13:M:68:VAL:HG11	2.03	0.41
23:W:4:THR:O	23:W:5:SER:C	2.58	0.41
34:2:1076:C:HO2'	34:2:1077:C:C5'	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1570:G:N3	34:2:1570:G:H5''	2.36	0.40
34:2:179:A:H2'	34:2:180:A:O4'	2.20	0.40
34:2:26:A:HO2'	34:2:27:U:C5'	2.34	0.40
34:2:99:C:C2	34:2:360:C:C5	3.09	0.40
34:2:883:A:O2'	34:2:884:G:H5''	2.21	0.40
34:2:947:G:C2	34:2:948:C:C2	3.09	0.40
8:H:20:VAL:HG21	8:H:46:ILE:HD13	2.02	0.40
25:Y:20:ARG:CZ	25:Y:74:LEU:HD13	2.51	0.40
34:2:16:G:C2	34:2:17:C:C2	3.09	0.40
34:2:16:G:C6	34:2:17:C:N4	2.89	0.40
3:C:156:PRO:HG3	22:V:9:VAL:HG11	2.04	0.40
6:F:122:ILE:HD12	26:Z:59:TYR:CE2	2.55	0.40
16:P:18:LYS:C	19:S:93:ASN:C	2.80	0.40
34:2:1140:G:H2'	34:2:1141:A:C8	2.57	0.40
34:2:1354:C:H2'	34:2:1355:U:O4'	2.21	0.40
34:2:1437:C:H2'	34:2:1438:C:H6	1.86	0.40
34:2:149:U:C4	34:2:150:G:N7	2.90	0.40
34:2:1588:G:C6	34:2:1589:C:C4	3.10	0.40
9:I:138:LYS:NZ	34:2:186:G:O2'	2.45	0.40
34:2:392:C:H2'	34:2:393:C:C6	2.56	0.40
34:2:531:U:H2'	34:2:532:U:O4'	2.21	0.40
34:2:566:A:N1	34:2:582:C:H1'	2.36	0.40
34:2:65:A:H2	34:2:84:A:N7	2.19	0.40
34:2:776:G:C6	34:2:777:C:C4	3.09	0.40
34:2:946:U:H2'	34:2:947:G:O4'	2.21	0.40
34:2:958:U:C2'	34:2:958:U:O2	2.69	0.40
5:E:126:VAL:HG13	5:E:139:VAL:CG2	2.52	0.40
6:F:98:SER:HB2	6:F:178:THR:HG21	2.03	0.40
6:F:66:ILE:HG22	6:F:66:ILE:O	2.21	0.40
34:2:1020:C:H2'	34:2:1021:C:O4'	2.22	0.40
34:2:1256:U:C5	34:2:1257:U:H1'	2.57	0.40
34:2:1231:U:P	34:2:1258:U:H5'	2.62	0.40
34:2:208:U:C2	34:2:209:A:C8	3.09	0.40
34:2:941:G:C6	34:2:942:C:C4	3.09	0.40
26:Z:67:ASP:CA	26:Z:69:PHE:H	2.35	0.40
34:2:1040:G:C6	34:2:1041:G:C6	3.09	0.40
34:2:1072:G:N3	34:2:1073:G:N7	2.64	0.40
34:2:1765:G:H4'	34:2:1766:G:O5'	2.21	0.40
34:2:214:A:C4	34:2:241:U:C4	3.09	0.40
34:2:604:A:C4	34:2:605:A:C2	3.09	0.40
34:2:65:A:O2'	34:2:83:G:N1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:ALA:HA	6:F:203:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	168 (82%)	25 (12%)	11 (5%)	2	30
2	B	212/214 (99%)	174 (82%)	32 (15%)	6 (3%)	6	47
3	C	215/217 (99%)	187 (87%)	21 (10%)	7 (3%)	5	43
4	D	221/223 (99%)	198 (90%)	17 (8%)	6 (3%)	6	48
5	E	258/260 (99%)	214 (83%)	36 (14%)	8 (3%)	5	45
6	F	204/206 (99%)	174 (85%)	21 (10%)	9 (4%)	3	35
7	G	224/226 (99%)	186 (83%)	29 (13%)	9 (4%)	4	38
8	H	182/184 (99%)	155 (85%)	16 (9%)	11 (6%)	2	27
9	I	184/200 (92%)	154 (84%)	22 (12%)	8 (4%)	3	35
10	J	180/182 (99%)	151 (84%)	17 (9%)	12 (7%)	1	25
11	K	94/96 (98%)	80 (85%)	7 (7%)	7 (7%)	1	21
12	L	153/155 (99%)	129 (84%)	17 (11%)	7 (5%)	3	34
13	M	120/122 (98%)	94 (78%)	21 (18%)	5 (4%)	3	36
14	N	148/150 (99%)	130 (88%)	14 (10%)	4 (3%)	6	48
15	O	125/127 (98%)	108 (86%)	11 (9%)	6 (5%)	3	32
16	P	121/123 (98%)	96 (79%)	16 (13%)	9 (7%)	1	21
17	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	4	41
18	R	127/129 (98%)	106 (84%)	14 (11%)	7 (6%)	2	29
19	S	143/145 (99%)	119 (83%)	17 (12%)	7 (5%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	141/143 (99%)	126 (89%)	10 (7%)	5 (4%)	4	42
21	U	104/106 (98%)	93 (89%)	7 (7%)	4 (4%)	4	39
22	V	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	23
23	W	127/129 (98%)	107 (84%)	14 (11%)	6 (5%)	3	33
24	X	143/145 (99%)	121 (85%)	15 (10%)	7 (5%)	3	32
25	Y	132/134 (98%)	113 (86%)	9 (7%)	10 (8%)	1	20
26	Z	68/70 (97%)	58 (85%)	5 (7%)	5 (7%)	1	21
27	a	98/100 (98%)	74 (76%)	13 (13%)	11 (11%)	0	10
28	b	80/82 (98%)	64 (80%)	12 (15%)	4 (5%)	3	31
29	c	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
30	d	51/53 (96%)	41 (80%)	10 (20%)	0	100	100
31	e	53/55 (96%)	47 (89%)	3 (6%)	3 (6%)	2	28
32	f	67/69 (97%)	50 (75%)	11 (16%)	6 (9%)	1	16
33	g	312/324 (96%)	261 (84%)	44 (14%)	7 (2%)	8	52
All	All	4776/4866 (98%)	4024 (84%)	534 (11%)	218 (5%)	5	34

All (218) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ALA
2	B	100	PHE
3	C	149	TRP
4	D	164	VAL
6	F	59	SER
6	F	206	GLY
7	G	154	ARG
8	H	32	PRO
8	H	64	VAL
8	H	74	GLN
9	I	10	LYS
10	J	121	SER
11	K	88	PRO
12	L	105	LYS
14	N	24	ALA
14	N	133	SER
15	O	91	SER
16	P	20	VAL

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Mol	Chain	Res	Type
16	P	29	PRO
17	Q	40	GLN
17	Q	138	PHE
18	R	26	MET
18	R	121	VAL
19	S	92	VAL
20	T	11	ALA
21	U	107	THR
21	U	118	ILE
22	V	30	SER
23	W	83	ILE
24	X	42	PRO
24	X	64	PRO
24	X	131	SER
25	Y	30	PRO
25	Y	60	PHE
26	Z	73	GLY
26	Z	104	ALA
27	a	18	VAL
27	a	75	ILE
27	a	81	ALA
27	a	86	VAL
28	b	21	LEU
32	f	143	HIS
1	A	26	ALA
1	A	72	ASP
1	A	94	GLY
3	C	141	VAL
3	C	153	LEU
4	D	217	VAL
5	E	38	LEU
5	E	195	ILE
5	E	201	HIS
7	G	122	GLU
8	H	10	SER
8	H	13	PRO
8	H	53	GLY
8	H	132	PRO
9	I	11	ARG
9	I	153	ILE
10	J	65	LYS
10	J	118	LEU

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Mol	Chain	Res	Type
11	K	81	ASN
11	K	83	PRO
12	L	5	LEU
12	L	7	VAL
12	L	55	ASP
13	M	48	GLY
13	M	82	VAL
13	M	85	ALA
16	P	12	PHE
16	P	101	VAL
17	Q	27	GLY
18	R	127	VAL
19	S	26	ILE
19	S	51	ASP
20	T	43	ASN
22	V	22	ARG
23	W	5	SER
23	W	57	ARG
23	W	120	HIS
24	X	130	VAL
25	Y	64	TYR
27	a	10	ARG
27	a	83	ILE
27	a	85	ARG
32	f	89	LYS
32	f	97	LYS
32	f	111	GLU
33	g	293	ASP
1	A	35	PRO
2	B	209	ASN
3	C	41	VAL
3	C	111	ASP
4	D	44	THR
4	D	93	ASP
5	E	80	THR
5	E	95	THR
5	E	120	SER
5	E	205	PHE
6	F	53	VAL
6	F	101	MET
7	G	89	ASN
8	H	29	ASN

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Mol	Chain	Res	Type
9	I	22	ARG
9	I	40	THR
9	I	52	ASN
10	J	97	LEU
10	J	171	ARG
12	L	133	LYS
13	M	78	PRO
15	O	18	ARG
15	O	124	ASP
17	Q	116	LEU
20	T	50	SER
22	V	4	ASP
22	V	44	ARG
23	W	107	SER
25	Y	61	ARG
25	Y	63	GLN
27	a	8	ASN
31	e	11	ALA
31	e	61	SER
32	f	88	PRO
33	g	4	SER
33	g	244	LYS
1	A	9	LEU
1	A	39	LYS
1	A	103	THR
1	A	167	LYS
1	A	193	GLN
2	B	148	ASN
2	B	210	VAL
5	E	77	ARG
6	F	83	ARG
7	G	165	GLY
7	G	173	PRO
7	G	177	ARG
8	H	110	GLN
9	I	116	HIS
10	J	35	GLY
10	J	120	LYS
10	J	147	MET
15	O	51	ASP
16	P	28	MET
16	P	80	LEU

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Mol	Chain	Res	Type
16	P	121	ILE
17	Q	115	THR
18	R	100	LEU
20	T	39	THR
21	U	21	LYS
25	Y	34	ASN
26	Z	56	THR
26	Z	57	TYR
27	a	16	GLY
28	b	3	LEU
32	f	106	TYR
33	g	168	ASP
1	A	68	PRO
2	B	190	PRO
3	C	44	THR
3	C	65	SER
6	F	40	GLN
6	F	52	ASP
6	F	102	ASN
7	G	8	PRO
7	G	70	PRO
7	G	224	ALA
10	J	18	PRO
10	J	67	PRO
10	J	122	VAL
10	J	134	ILE
11	K	54	PHE
11	K	87	PHE
11	K	94	GLY
12	L	30	LYS
14	N	70	LYS
15	O	114	ARG
18	R	72	LYS
19	S	14	ILE
19	S	144	ARG
21	U	71	PRO
24	X	4	GLY
25	Y	51	GLU
25	Y	133	ASN
28	b	62	VAL
31	e	47	VAL
2	B	221	PRO

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Mol	Chain	Res	Type
4	D	4	ILE
11	K	2	LEU
12	L	113	PRO
14	N	3	ARG
15	O	25	ASP
16	P	69	GLU
19	S	12	GLN
20	T	45	LEU
22	V	46	ILE
22	V	82	VAL
24	X	144	ARG
25	Y	31	ASN
26	Z	62	VAL
27	a	84	VAL
33	g	139	GLY
27	a	36	ILE
33	g	278	ILE
6	F	77	GLY
8	H	8	ILE
13	M	97	ILE
18	R	38	ILE
18	R	124	VAL
23	W	76	SER
4	D	163	PRO
8	H	98	ILE
9	I	39	GLY
24	X	63	GLN
28	b	39	GLY
33	g	31	PRO
16	P	53	PRO
19	S	76	PRO
25	Y	29	HIS

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	A	174/174 (100%)	160 (92%)	14 (8%)	15	54
2	B	196/196 (100%)	182 (93%)	14 (7%)	18	59
3	C	176/176 (100%)	154 (88%)	22 (12%)	6	33
4	D	185/185 (100%)	165 (89%)	20 (11%)	8	41
5	E	223/223 (100%)	204 (92%)	19 (8%)	13	52
6	F	174/174 (100%)	158 (91%)	16 (9%)	11	48
7	G	192/192 (100%)	175 (91%)	17 (9%)	12	50
8	H	164/164 (100%)	149 (91%)	15 (9%)	12	48
9	I	148/158 (94%)	126 (85%)	22 (15%)	4	26
10	J	153/153 (100%)	135 (88%)	18 (12%)	6	35
11	K	88/88 (100%)	82 (93%)	6 (7%)	20	61
12	L	136/136 (100%)	126 (93%)	10 (7%)	17	57
13	M	97/97 (100%)	91 (94%)	6 (6%)	23	64
14	N	127/127 (100%)	116 (91%)	11 (9%)	13	50
15	O	96/96 (100%)	90 (94%)	6 (6%)	22	63
16	P	105/106 (99%)	96 (91%)	9 (9%)	13	51
17	Q	117/117 (100%)	109 (93%)	8 (7%)	20	61
18	R	117/117 (100%)	104 (89%)	13 (11%)	8	39
19	S	128/128 (100%)	111 (87%)	17 (13%)	5	31
20	T	117/117 (100%)	106 (91%)	11 (9%)	11	47
21	U	96/96 (100%)	92 (96%)	4 (4%)	36	74
22	V	73/73 (100%)	69 (94%)	4 (6%)	27	68
23	W	110/110 (100%)	97 (88%)	13 (12%)	6	35
24	X	120/120 (100%)	105 (88%)	15 (12%)	6	33
25	Y	108/108 (100%)	94 (87%)	14 (13%)	5	32
26	Z	60/60 (100%)	55 (92%)	5 (8%)	14	52
27	a	85/85 (100%)	73 (86%)	12 (14%)	4	29
28	b	72/72 (100%)	68 (94%)	4 (6%)	26	67
29	c	55/55 (100%)	52 (94%)	3 (6%)	27	68
30	d	46/46 (100%)	42 (91%)	4 (9%)	13	50
31	e	49/49 (100%)	45 (92%)	4 (8%)	14	53
32	f	58/60 (97%)	48 (83%)	10 (17%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	265/270 (98%)	251 (95%)	14 (5%)	28	69
All	All	4110/4128 (100%)	3730 (91%)	380 (9%)	16	48

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	21	ARG
1	A	32	HIS
1	A	56	LYS
1	A	59	LEU
1	A	79	ARG
1	A	108	THR
1	A	109	ASN
1	A	135	GLU
1	A	146	LEU
1	A	151	SER
1	A	177	LEU
1	A	198	MET
1	A	205	ARG
2	B	47	LEU
2	B	48	VAL
2	B	70	LEU
2	B	84	VAL
2	B	96	LEU
2	B	100	PHE
2	B	120	LEU
2	B	127	VAL
2	B	167	VAL
2	B	179	SER
2	B	181	LEU
2	B	191	GLU
2	B	194	ASN
2	B	228	LEU
3	C	43	VAL
3	C	49	LEU
3	C	51	LYS
3	C	58	ILE
3	C	59	GLU
3	C	71	PHE
3	C	86	MET
3	C	92	GLN

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Mol	Chain	Res	Type
3	C	93	LYS
3	C	94	GLN
3	C	99	GLN
3	C	100	ARG
3	C	111	ASP
3	C	122	THR
3	C	142	ILE
3	C	145	ARG
3	C	149	TRP
3	C	166	LYS
3	C	167	CYS
3	C	190	LYS
3	C	223	ILE
3	C	235	TRP
4	D	5	ILE
4	D	7	LYS
4	D	11	LEU
4	D	17	PHE
4	D	51	ARG
4	D	65	ARG
4	D	101	GLN
4	D	113	LEU
4	D	122	VAL
4	D	134	CYS
4	D	135	GLU
4	D	141	LYS
4	D	143	ARG
4	D	146	ARG
4	D	157	LEU
4	D	162	GLN
4	D	173	ARG
4	D	178	ARG
4	D	179	GLN
4	D	222	VAL
5	E	6	LYS
5	E	9	LEU
5	E	11	ARG
5	E	18	TRP
5	E	37	LYS
5	E	38	LEU
5	E	42	LEU
5	E	51	ARG

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Mol	Chain	Res	Type
5	E	68	ARG
5	E	77	ARG
5	E	79	ASP
5	E	123	LEU
5	E	133	LYS
5	E	143	ASP
5	E	187	ARG
5	E	208	VAL
5	E	225	VAL
5	E	245	LYS
5	E	247	THR
6	F	81	ASN
6	F	94	ARG
6	F	101	MET
6	F	114	ARG
6	F	121	GLU
6	F	158	ARG
6	F	165	SER
6	F	173	SER
6	F	186	PHE
6	F	187	ARG
6	F	188	ASN
6	F	192	ILE
6	F	196	LEU
6	F	210	SER
6	F	211	TYR
6	F	220	GLU
7	G	52	ILE
7	G	75	LEU
7	G	92	ARG
7	G	96	SER
7	G	97	VAL
7	G	136	LYS
7	G	141	ILE
7	G	152	ASP
7	G	153	VAL
7	G	155	ASP
7	G	159	ARG
7	G	164	LYS
7	G	178	LEU
7	G	180	THR
7	G	182	GLN

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Mol	Chain	Res	Type
7	G	183	ARG
7	G	215	ARG
8	H	11	GLN
8	H	16	LEU
8	H	24	PHE
8	H	27	LEU
8	H	33	GLU
8	H	47	ARG
8	H	80	GLU
8	H	81	LEU
8	H	93	LEU
8	H	114	ARG
8	H	122	HIS
8	H	126	LEU
8	H	129	LEU
8	H	139	ARG
8	H	174	ASN
9	I	8	ARG
9	I	10	LYS
9	I	24	LYS
9	I	25	ARG
9	I	29	LEU
9	I	35	ASN
9	I	62	THR
9	I	66	SER
9	I	72	VAL
9	I	75	LYS
9	I	77	ARG
9	I	86	SER
9	I	96	LEU
9	I	107	THR
9	I	138	LYS
9	I	140	THR
9	I	144	TRP
9	I	159	SER
9	I	160	GLN
9	I	161	PHE
9	I	170	ILE
9	I	190	LEU
10	J	8	TYR
10	J	11	THR
10	J	28	LEU

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Mol	Chain	Res	Type
10	J	30	LEU
10	J	37	LYS
10	J	49	LEU
10	J	61	THR
10	J	64	GLU
10	J	69	ARG
10	J	89	ASP
10	J	97	LEU
10	J	126	ARG
10	J	132	ARG
10	J	145	SER
10	J	149	ARG
10	J	153	GLU
10	J	175	LYS
10	J	176	ARG
11	K	15	LEU
11	K	40	LEU
11	K	59	PHE
11	K	76	LEU
11	K	80	LEU
11	K	86	ILE
12	L	8	GLN
12	L	10	GLU
12	L	80	MET
12	L	83	THR
12	L	84	ILE
12	L	87	ARG
12	L	94	VAL
12	L	101	GLU
12	L	105	LYS
12	L	136	ARG
13	M	55	LEU
13	M	67	LEU
13	M	69	GLN
13	M	91	TRP
13	M	104	ARG
13	M	105	LYS
14	N	3	ARG
14	N	12	SER
14	N	25	TRP
14	N	36	GLN
14	N	64	LYS

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Mol	Chain	Res	Type
14	N	88	LEU
14	N	89	TYR
14	N	115	LEU
14	N	121	ARG
14	N	139	TRP
14	N	142	GLU
15	O	53	ASP
15	O	67	VAL
15	O	71	CYS
15	O	114	ARG
15	O	124	ASP
15	O	127	ARG
16	P	17	TYR
16	P	40	ARG
16	P	52	LYS
16	P	57	MET
16	P	77	ARG
16	P	79	HIS
16	P	84	ILE
16	P	111	MET
16	P	127	ARG
17	Q	8	GLN
17	Q	19	VAL
17	Q	46	PHE
17	Q	53	LEU
17	Q	55	VAL
17	Q	121	SER
17	Q	128	LYS
17	Q	142	TYR
18	R	6	THR
18	R	16	LEU
18	R	17	ILE
18	R	27	ASP
18	R	36	ASP
18	R	45	ARG
18	R	47	ARG
18	R	66	VAL
18	R	67	ARG
18	R	88	VAL
18	R	127	VAL
18	R	128	ARG
18	R	130	ARG

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Mol	Chain	Res	Type
19	S	16	ARG
19	S	25	ASN
19	S	36	ARG
19	S	38	VAL
19	S	41	ARG
19	S	49	LYS
19	S	73	MET
19	S	74	GLN
19	S	85	PHE
19	S	93	ASN
19	S	96	LYS
19	S	100	SER
19	S	105	LEU
19	S	126	ARG
19	S	128	PHE
19	S	131	LEU
19	S	144	ARG
20	T	45	LEU
20	T	53	TRP
20	T	57	ARG
20	T	63	ARG
20	T	68	ARG
20	T	85	ASN
20	T	86	ARG
20	T	100	ILE
20	T	102	ARG
20	T	124	ILE
20	T	139	THR
21	U	52	LYS
21	U	84	MET
21	U	94	GLU
21	U	103	ILE
22	V	12	TYR
22	V	33	GLN
22	V	38	GLN
22	V	50	TYR
23	W	6	VAL
23	W	7	LEU
23	W	11	LEU
23	W	15	ASN
23	W	19	LYS
23	W	23	ARG

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Mol	Chain	Res	Type
23	W	24	GLN
23	W	25	VAL
23	W	28	ARG
23	W	61	ILE
23	W	66	ASN
23	W	70	ASN
23	W	107	SER
24	X	9	LEU
24	X	17	VAL
24	X	19	ARG
24	X	63	GLN
24	X	64	PRO
24	X	70	LYS
24	X	73	ARG
24	X	93	LEU
24	X	98	GLU
24	X	99	ASN
24	X	102	VAL
24	X	107	PHE
24	X	109	ARG
24	X	114	LYS
24	X	130	VAL
25	Y	3	ASP
25	Y	6	THR
25	Y	15	ASN
25	Y	29	HIS
25	Y	31	ASN
25	Y	35	VAL
25	Y	46	GLU
25	Y	57	VAL
25	Y	74	LEU
25	Y	98	GLU
25	Y	110	GLN
25	Y	113	ASN
25	Y	116	LYS
25	Y	125	ILE
26	Z	49	ARG
26	Z	59	TYR
26	Z	63	SER
26	Z	68	ARG
26	Z	97	LYS
27	a	1	MET

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Mol	Chain	Res	Type
27	a	5	ARG
27	a	7	SER
27	a	8	ASN
27	a	18	VAL
27	a	30	VAL
27	a	32	LYS
27	a	33	ASP
27	a	34	LYS
27	a	39	MET
27	a	64	LEU
27	a	75	ILE
28	b	7	LEU
28	b	9	HIS
28	b	26	GLN
28	b	67	THR
29	c	16	LEU
29	c	32	PHE
29	c	56	LEU
30	d	21	CYS
30	d	40	ARG
30	d	45	GLU
30	d	49	ASP
31	e	17	GLN
31	e	22	GLU
31	e	33	ARG
31	e	53	LYS
32	f	82	LYS
32	f	89	LYS
32	f	99	LYS
32	f	103	LEU
32	f	106	TYR
32	f	113	LYS
32	f	117	LEU
32	f	120	GLU
32	f	136	ARG
32	f	139	CYS
33	g	27	SER
33	g	43	LEU
33	g	55	PHE
33	g	60	ARG
33	g	67	HIS
33	g	99	ASN

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Mol	Chain	Res	Type
33	g	175	VAL
33	g	188	LEU
33	g	244	LYS
33	g	273	GLU
33	g	275	GLU
33	g	292	GLN
33	g	299	LEU
33	g	321	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	109	ASN
2	B	160	HIS
5	E	224	ASN
6	F	141	ASN
6	F	202	ASN
7	G	4	ASN
7	G	190	GLN
14	N	78	ASN
15	O	29	HIS
16	P	79	HIS
16	P	98	ASN
17	Q	83	GLN
19	S	89	GLN
20	T	25	GLN
23	W	92	ASN
24	X	18	HIS
24	X	22	ASN
24	X	63	GLN
24	X	79	ASN
25	Y	29	HIS
25	Y	34	ASN
28	b	49	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	2	1778/1780 (99%)	767 (43%)	111 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	i	184/192 (95%)	107 (58%)	0
All	All	1962/1972 (99%)	874 (44%)	111 (5%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	2	2	A
34	2	3	U
34	2	4	C
34	2	5	U
34	2	9	U
34	2	10	G
34	2	14	C
34	2	17	C
34	2	25	C
34	2	26	A
34	2	32	U
34	2	34	G
34	2	39	A
34	2	40	A
34	2	42	G
34	2	45	U
34	2	47	A
34	2	51	A
34	2	57	G
34	2	59	C
34	2	60	U
34	2	61	A
34	2	63	G
34	2	64	U
34	2	65	A
34	2	66	U
34	2	67	A
34	2	68	A
34	2	69	G
34	2	71	A
34	2	72	A
34	2	73	U
34	2	74	U
34	2	75	U
34	2	76	A
34	2	77	U

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Mol	Chain	Res	Type
34	2	78	A
34	2	80	A
34	2	81	G
34	2	82	U
34	2	86	A
34	2	93	A
34	2	101	U
34	2	104	A
34	2	111	U
34	2	113	U
34	2	114	C
34	2	115	G
34	2	123	G
34	2	124	A
34	2	125	U
34	2	127	G
34	2	129	U
34	2	130	C
34	2	131	C
34	2	132	U
34	2	133	U
34	2	134	U
34	2	136	C
34	2	137	U
34	2	138	A
34	2	139	C
34	2	140	A
34	2	141	U
34	2	146	A
34	2	148	C
34	2	149	U
34	2	150	G
34	2	152	G
34	2	153	G
34	2	154	U
34	2	155	A
34	2	157	U
34	2	158	U
34	2	159	C
34	2	160	U
34	2	161	A
34	2	167	A

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Mol	Chain	Res	Type
34	2	169	U
34	2	170	A
34	2	173	U
34	2	175	C
34	2	176	U
34	2	177	U
34	2	178	A
34	2	180	A
34	2	183	C
34	2	184	U
34	2	186	G
34	2	187	A
34	2	190	C
34	2	191	U
34	2	192	U
34	2	194	G
34	2	195	G
34	2	198	G
34	2	199	A
34	2	203	G
34	2	205	A
34	2	210	U
34	2	217	A
34	2	218	A
34	2	220	A
34	2	224	A
34	2	225	A
34	2	226	U
34	2	228	U
34	2	230	U
34	2	231	U
34	2	232	C
34	2	233	G
34	2	234	G
34	2	235	A
34	2	239	C
34	2	240	U
34	2	241	U
34	2	249	C
34	2	253	A
34	2	256	A
34	2	259	U

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Mol	Chain	Res	Type
34	2	264	A
34	2	265	A
34	2	266	U
34	2	267	C
34	2	268	G
34	2	269	C
34	2	270	A
34	2	274	C
34	2	275	C
34	2	276	U
34	2	277	U
34	2	278	G
34	2	279	U
34	2	280	G
34	2	284	G
34	2	286	G
34	2	288	U
34	2	294	A
34	2	298	A
34	2	301	U
34	2	305	U
34	2	308	C
34	2	309	C
34	2	311	A
34	2	312	U
34	2	313	C
34	2	314	A
34	2	315	A
34	2	319	U
34	2	320	C
34	2	321	G
34	2	322	A
34	2	328	G
34	2	332	A
34	2	336	G
34	2	337	C
34	2	342	C
34	2	351	A
34	2	359	A
34	2	360	C
34	2	374	U
34	2	377	A

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Mol	Chain	Res	Type
34	2	382	G
34	2	389	G
34	2	392	C
34	2	397	G
34	2	399	A
34	2	400	A
34	2	401	C
34	2	403	G
34	2	406	A
34	2	410	C
34	2	411	A
34	2	412	U
34	2	414	C
34	2	415	A
34	2	416	A
34	2	417	G
34	2	419	A
34	2	421	G
34	2	422	G
34	2	423	C
34	2	424	A
34	2	425	G
34	2	433	G
34	2	436	A
34	2	438	U
34	2	442	C
34	2	443	C
34	2	444	A
34	2	447	C
34	2	452	U
34	2	458	G
34	2	459	A
34	2	460	G
34	2	463	A
34	2	467	A
34	2	474	A
34	2	476	A
34	2	479	G
34	2	480	A
34	2	483	C
34	2	490	C
34	2	491	A

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Mol	Chain	Res	Type
34	2	492	U
34	2	493	U
34	2	494	C
34	2	497	G
34	2	499	C
34	2	500	U
34	2	503	U
34	2	504	A
34	2	505	A
34	2	506	U
34	2	507	U
34	2	509	G
34	2	510	A
34	2	512	U
34	2	513	G
34	2	514	A
34	2	516	U
34	2	518	C
34	2	521	U
34	2	524	A
34	2	526	A
34	2	527	U
34	2	532	U
34	2	533	A
34	2	534	A
34	2	535	C
34	2	536	G
34	2	537	A
34	2	538	G
34	2	539	G
34	2	540	A
34	2	541	A
34	2	542	C
34	2	543	A
34	2	544	A
34	2	545	C
34	2	547	G
34	2	548	G
34	2	550	G
34	2	551	G
34	2	553	C
34	2	554	A

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Mol	Chain	Res	Type
34	2	556	G
34	2	557	U
34	2	558	C
34	2	561	G
34	2	564	C
34	2	565	C
34	2	570	G
34	2	573	G
34	2	574	C
34	2	575	G
34	2	576	G
34	2	577	U
34	2	578	A
34	2	579	A
34	2	581	U
34	2	593	A
34	2	594	G
34	2	596	G
34	2	600	A
34	2	605	A
34	2	606	G
34	2	607	U
34	2	610	U
34	2	613	C
34	2	618	A
34	2	619	A
34	2	622	A
34	2	623	G
34	2	629	A
34	2	632	U
34	2	634	A
34	2	637	U
34	2	638	U
34	2	639	U
34	2	640	G
34	2	642	G
34	2	647	G
34	2	648	U
34	2	649	U
34	2	652	C
34	2	653	C
34	2	654	G

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Mol	Chain	Res	Type
34	2	655	G
34	2	677	G
34	2	678	U
34	2	679	U
34	2	683	C
34	2	684	A
34	2	691	U
34	2	694	U
34	2	695	U
34	2	696	C
34	2	697	C
34	2	698	U
34	2	701	U
34	2	704	C
34	2	705	U
34	2	708	C
34	2	709	C
34	2	710	U
34	2	712	U
34	2	713	A
34	2	714	C
34	2	716	C
34	2	717	C
34	2	718	U
34	2	719	U
34	2	722	G
34	2	724	G
34	2	725	U
34	2	727	C
34	2	731	C
34	2	732	G
34	2	733	A
34	2	734	A
34	2	735	C
34	2	736	C
34	2	737	A
34	2	738	G
34	2	740	A
34	2	741	C
34	2	742	U
34	2	743	U
34	2	754	A

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Mol	Chain	Res	Type
34	2	756	A
34	2	765	G
34	2	766	U
34	2	767	U
34	2	769	A
34	2	771	A
34	2	774	A
34	2	778	G
34	2	779	A
34	2	780	A
34	2	781	A
34	2	782	G
34	2	785	C
34	2	786	G
34	2	787	A
34	2	788	A
34	2	789	U
34	2	792	A
34	2	793	U
34	2	794	U
34	2	795	A
34	2	802	A
34	2	806	A
34	2	809	G
34	2	811	A
34	2	812	U
34	2	813	A
34	2	815	G
34	2	817	C
34	2	819	U
34	2	820	U
34	2	821	U
34	2	822	G
34	2	823	G
34	2	825	U
34	2	826	C
34	2	828	A
34	2	829	U
34	2	830	U
34	2	831	U
34	2	832	U
34	2	834	U

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Mol	Chain	Res	Type
34	2	837	G
34	2	840	U
34	2	842	U
34	2	844	G
34	2	845	G
34	2	848	C
34	2	849	A
34	2	852	G
34	2	855	A
34	2	859	U
34	2	860	U
34	2	861	A
34	2	862	A
34	2	863	U
34	2	872	U
34	2	875	G
34	2	876	G
34	2	884	G
34	2	885	U
34	2	887	U
34	2	894	G
34	2	895	U
34	2	897	A
34	2	903	G
34	2	904	A
34	2	905	A
34	2	906	A
34	2	908	U
34	2	909	C
34	2	910	U
34	2	912	G
34	2	913	G
34	2	914	A
34	2	915	U
34	2	919	U
34	2	920	U
34	2	927	U
34	2	928	A
34	2	929	A
34	2	931	U
34	2	932	A
34	2	934	U

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Mol	Chain	Res	Type
34	2	935	G
34	2	936	C
34	2	939	A
34	2	941	G
34	2	943	A
34	2	944	U
34	2	950	A
34	2	958	U
34	2	959	U
34	2	964	U
34	2	965	A
34	2	969	A
34	2	972	A
34	2	980	U
34	2	981	U
34	2	983	G
34	2	985	G
34	2	987	A
34	2	990	G
34	2	991	A
34	2	992	A
34	2	993	G
34	2	994	A
34	2	999	C
34	2	1003	U
34	2	1004	A
34	2	1005	C
34	2	1009	C
34	2	1010	G
34	2	1011	U
34	2	1012	A
34	2	1013	G
34	2	1015	C
34	2	1020	C
34	2	1024	A
34	2	1026	A
34	2	1027	C
34	2	1028	U
34	2	1030	U
34	2	1031	G
34	2	1037	U
34	2	1038	A

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Mol	Chain	Res	Type
34	2	1039	G
34	2	1041	G
34	2	1042	A
34	2	1044	C
34	2	1045	G
34	2	1046	G
34	2	1050	G
34	2	1051	U
34	2	1052	G
34	2	1056	U
34	2	1057	U
34	2	1058	C
34	2	1059	U
34	2	1060	U
34	2	1063	G
34	2	1070	U
34	2	1071	C
34	2	1073	G
34	2	1074	C
34	2	1075	A
34	2	1076	C
34	2	1080	A
34	2	1081	C
34	2	1082	G
34	2	1083	A
34	2	1084	G
34	2	1087	A
34	2	1090	A
34	2	1091	A
34	2	1092	A
34	2	1094	U
34	2	1096	U
34	2	1097	U
34	2	1098	U
34	2	1099	G
34	2	1100	G
34	2	1107	G
34	2	1108	G
34	2	1110	G
34	2	1113	G
34	2	1118	G
34	2	1121	G

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Mol	Chain	Res	Type
34	2	1123	A
34	2	1130	A
34	2	1137	A
34	2	1142	A
34	2	1145	G
34	2	1149	G
34	2	1150	A
34	2	1157	C
34	2	1158	C
34	2	1159	A
34	2	1162	A
34	2	1163	G
34	2	1166	G
34	2	1174	U
34	2	1175	G
34	2	1183	A
34	2	1184	U
34	2	1185	U
34	2	1189	C
34	2	1190	U
34	2	1192	A
34	2	1193	A
34	2	1195	A
34	2	1196	C
34	2	1198	G
34	2	1199	G
34	2	1200	G
34	2	1201	A
34	2	1202	A
34	2	1203	A
34	2	1204	C
34	2	1211	G
34	2	1212	G
34	2	1213	U
34	2	1215	C
34	2	1216	A
34	2	1217	G
34	2	1218	A
34	2	1219	C
34	2	1222	A
34	2	1224	U
34	2	1226	A

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Mol	Chain	Res	Type
34	2	1227	G
34	2	1228	G
34	2	1229	A
34	2	1230	U
34	2	1231	U
34	2	1234	C
34	2	1236	G
34	2	1238	U
34	2	1240	G
34	2	1241	A
34	2	1242	G
34	2	1243	A
34	2	1244	G
34	2	1245	C
34	2	1247	C
34	2	1250	U
34	2	1253	U
34	2	1254	G
34	2	1257	U
34	2	1258	U
34	2	1259	U
34	2	1265	U
34	2	1266	G
34	2	1268	U
34	2	1269	G
34	2	1274	A
34	2	1282	U
34	2	1284	U
34	2	1296	G
34	2	1306	U
34	2	1310	U
34	2	1313	U
34	2	1314	U
34	2	1317	G
34	2	1319	U
34	2	1320	A
34	2	1321	A
34	2	1322	C
34	2	1324	A
34	2	1336	A
34	2	1339	U
34	2	1340	A

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Mol	Chain	Res	Type
34	2	1343	A
34	2	1344	A
34	2	1345	A
34	2	1347	A
34	2	1349	G
34	2	1353	G
34	2	1356	G
34	2	1358	C
34	2	1359	A
34	2	1360	C
34	2	1361	U
34	2	1362	U
34	2	1363	G
34	2	1364	C
34	2	1366	G
34	2	1369	U
34	2	1370	G
34	2	1371	A
34	2	1374	C
34	2	1380	A
34	2	1388	U
34	2	1393	G
34	2	1396	U
34	2	1397	C
34	2	1398	A
34	2	1400	G
34	2	1404	A
34	2	1410	G
34	2	1411	U
34	2	1412	U
34	2	1413	U
34	2	1416	G
34	2	1417	G
34	2	1425	A
34	2	1426	G
34	2	1428	U
34	2	1430	U
34	2	1432	U
34	2	1433	G
34	2	1434	A
34	2	1435	U
34	2	1442	A

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Mol	Chain	Res	Type
34	2	1443	G
34	2	1444	A
34	2	1445	C
34	2	1446	G
34	2	1449	C
34	2	1452	G
34	2	1454	C
34	2	1455	C
34	2	1456	G
34	2	1457	C
34	2	1458	A
34	2	1461	C
34	2	1464	G
34	2	1467	A
34	2	1468	C
34	2	1469	A
34	2	1471	U
34	2	1475	G
34	2	1476	G
34	2	1481	A
34	2	1484	G
34	2	1485	A
34	2	1487	U
34	2	1488	A
34	2	1489	C
34	2	1490	A
34	2	1491	A
34	2	1492	C
34	2	1494	U
34	2	1495	U
34	2	1498	C
34	2	1502	G
34	2	1506	U
34	2	1507	C
34	2	1508	U
34	2	1509	G
34	2	1512	U
34	2	1513	A
34	2	1514	A
34	2	1519	G
34	2	1521	G
34	2	1522	A

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Mol	Chain	Res	Type
34	2	1523	A
34	2	1527	C
34	2	1531	C
34	2	1532	G
34	2	1533	U
34	2	1534	G
34	2	1535	C
34	2	1537	G
34	2	1538	G
34	2	1540	G
34	2	1543	A
34	2	1552	U
34	2	1555	U
34	2	1557	A
34	2	1565	U
34	2	1566	C
34	2	1569	C
34	2	1570	G
34	2	1571	A
34	2	1580	U
34	2	1583	U
34	2	1588	G
34	2	1589	C
34	2	1594	C
34	2	1595	A
34	2	1597	C
34	2	1598	A
34	2	1599	G
34	2	1602	U
34	2	1603	G
34	2	1605	G
34	2	1612	A
34	2	1614	G
34	2	1616	C
34	2	1623	C
34	2	1626	U
34	2	1629	A
34	2	1633	A
34	2	1635	C
34	2	1640	G
34	2	1643	G
34	2	1655	U

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Mol	Chain	Res	Type
34	2	1656	G
34	2	1667	U
34	2	1676	A
34	2	1679	A
34	2	1682	U
34	2	1685	U
34	2	1686	U
34	2	1687	A
34	2	1688	G
34	2	1692	A
34	2	1693	G
34	2	1694	G
34	2	1696	G
34	2	1697	G
34	2	1698	C
34	2	1699	A
34	2	1700	A
34	2	1701	C
34	2	1702	U
34	2	1703	C
34	2	1706	U
34	2	1707	C
34	2	1708	U
34	2	1709	C
34	2	1710	A
34	2	1711	G
34	2	1712	A
34	2	1725	G
34	2	1730	A
34	2	1740	U
34	2	1743	G
34	2	1748	A
34	2	1753	A
34	2	1754	A
34	2	1755	G
34	2	1756	U
34	2	1758	G
34	2	1759	U
34	2	1763	A
34	2	1764	A
34	2	1766	G
34	2	1767	U

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Mol	Chain	Res	Type
34	2	1770	C
34	2	1774	A
34	2	1776	G
34	2	1777	U
34	2	1778	G
34	2	1779	A
34	2	1780	A
34	2	1781	C
34	2	1784	G
34	2	1789	A
34	2	1790	G
34	2	1791	G
34	2	1792	A
34	2	1793	U
34	2	1794	C
34	2	1796	U
34	2	1798	A
35	i	6033	A
35	i	6034	A
35	i	6037	U
35	i	6039	A
35	i	6044	G
35	i	6046	U
35	i	6049	U
35	i	6052	A
35	i	6053	U
35	i	6056	A
35	i	6058	U
35	i	6061	U
35	i	6062	G
35	i	6063	A
35	i	6067	G
35	i	6068	U
35	i	6075	A
35	i	6076	U
35	i	6077	U
35	i	6079	C
35	i	6080	A
35	i	6081	A
35	i	6084	A
35	i	6086	U
35	i	6087	G

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Mol	Chain	Res	Type
35	i	6088	C
35	i	6090	A
35	i	6094	U
35	i	6098	A
35	i	6099	U
35	i	6101	U
35	i	6102	A
35	i	6104	G
35	i	6105	U
35	i	6106	U
35	i	6107	A
35	i	6108	G
35	i	6109	C
35	i	6110	U
35	i	6112	U
35	i	6114	U
35	i	6118	U
35	i	6119	U
35	i	6121	A
35	i	6122	C
35	i	6123	G
35	i	6124	U
35	i	6128	A
35	i	6129	G
35	i	6130	G
35	i	6132	U
35	i	6133	G
35	i	6135	C
35	i	6136	U
35	i	6137	A
35	i	6138	G
35	i	6139	U
35	i	6140	G
35	i	6142	C
35	i	6143	A
35	i	6144	G
35	i	6145	C
35	i	6146	C
35	i	6147	C
35	i	6148	C
35	i	6149	A
35	i	6153	U

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Mol	Chain	Res	Type
35	i	6154	A
35	i	6155	U
35	i	6157	C
35	i	6158	A
35	i	6159	G
35	i	6160	G
35	i	6162	A
35	i	6163	G
35	i	6165	C
35	i	6166	C
35	i	6168	C
35	i	6169	U
35	i	6170	C
35	i	6171	U
35	i	6172	G
35	i	6173	C
35	i	6174	G
35	i	6176	C
35	i	6178	U
35	i	6179	U
35	i	6180	U
35	i	6181	C
35	i	6183	G
35	i	6184	A
35	i	6186	U
35	i	6187	A
35	i	6192	G
35	i	6197	A
35	i	6198	A
35	i	6199	A
35	i	6200	A
35	i	6202	C
35	i	6210	U
35	i	6211	U
35	i	6212	U
35	i	6213	A
35	i	6218	C
35	i	6219	U
35	i	6220	A
35	i	6221	C

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	2	3	U
34	2	44	U
34	2	59	C
34	2	63	G
34	2	65	A
34	2	66	U
34	2	70	C
34	2	71	A
34	2	72	A
34	2	73	U
34	2	129	U
34	2	130	C
34	2	137	U
34	2	139	C
34	2	148	C
34	2	149	U
34	2	157	U
34	2	169	U
34	2	177	U
34	2	186	G
34	2	216	A
34	2	217	A
34	2	239	C
34	2	248	U
34	2	258	U
34	2	262	C
34	2	263	G
34	2	264	A
34	2	265	A
34	2	269	C
34	2	271	U
34	2	277	U
34	2	279	U
34	2	321	G
34	2	399	A
34	2	454	C
34	2	497	G
34	2	509	G
34	2	513	G
34	2	532	U
34	2	537	A
34	2	542	C
34	2	556	G

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Mol	Chain	Res	Type
34	2	557	U
34	2	563	G
34	2	564	C
34	2	576	G
34	2	577	U
34	2	578	A
34	2	579	A
34	2	605	A
34	2	621	A
34	2	638	U
34	2	695	U
34	2	700	C
34	2	704	C
34	2	708	C
34	2	710	U
34	2	721	U
34	2	740	A
34	2	766	U
34	2	779	A
34	2	792	A
34	2	794	U
34	2	809	G
34	2	811	A
34	2	826	C
34	2	828	A
34	2	854	A
34	2	862	A
34	2	884	G
34	2	909	C
34	2	911	U
34	2	912	G
34	2	913	G
34	2	927	U
34	2	963	U
34	2	1003	U
34	2	1010	G
34	2	1027	C
34	2	1044	C
34	2	1060	U
34	2	1073	G
34	2	1080	A
34	2	1083	A

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Mol	Chain	Res	Type
34	2	1107	G
34	2	1184	U
34	2	1189	C
34	2	1195	A
34	2	1217	G
34	2	1230	U
34	2	1243	A
34	2	1264	G
34	2	1343	A
34	2	1429	C
34	2	1455	C
34	2	1470	C
34	2	1491	A
34	2	1501	A
34	2	1532	G
34	2	1534	G
34	2	1556	U
34	2	1598	A
34	2	1613	C
34	2	1628	U
34	2	1634	C
34	2	1655	U
34	2	1678	G
34	2	1763	A
34	2	1765	G
34	2	1791	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 83 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	657:C	O3'	676:G	P	17.80