



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J0Q
EMDB ID: : EMD-5329
Title : Core of mammalian 80S pre-ribosome in complex with tRNAs fitted to a 10.6A cryo-em map: rotated PRE state 2
Authors : Budkevich, T.; Giesebrecht, J.; Altman, R.; Munro, J.; Mielke, T.; Nierhaus, K.; Blanchard, S.; Spahn, C.M.
Deposited on : 2011-10-11
Resolution : 10.60 Å(reported)
Based on PDB ID : 2XZM, 3O58

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) : trunk27241

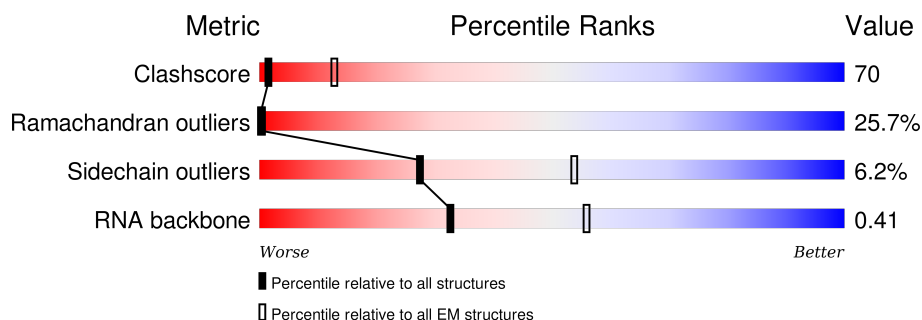
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.60 Å.

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



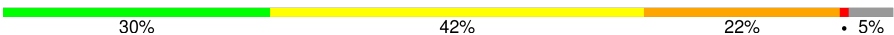
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	48	65% 25% 6% .
2	c	17	71% 29%
3	d	7	71% 14% 14%
4	g	31	71% 23% 6%
5	G	13	38% 46% 15%
6	f	21	76% 24%
7	h	111	88% 11% .
8	S	125	32% 62% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	L	141	
10	X	68	
11	2	112	
12	3	12	
13	9	19	
14	7	50	
15	B	213	
16	J	219	
17	k	165	
18	W	77	
18	Y	77	
19	y	3	
20	w	2	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 18327 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	48	Total	C	N	O	P	0	0
			1029	459	190	332	48		

- Molecule 2 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	17	Total	C	N	O	P	0	0
			362	162	66	117	17		

- Molecule 3 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	7	Total	C	N	O	P	0	0
			155	69	33	46	7		

- Molecule 4 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	31	Total	C	N	O	P	0	0
			660	295	118	216	31		

- Molecule 5 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	13	Total	C	N	O	P	0	0
			276	123	49	91	13		

- Molecule 6 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	21	Total	C	N	O	P	0	0
			452	200	79	152	21		

- Molecule 7 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	111	Total	C	N	O	P	0	0
			2368	1060	431	766	111		

- Molecule 8 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	125	Total	C	N	O	S	0	0
			985	632	173	176	4		

- Molecule 9 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	141	Total	C	N	O	S	0	0
			1097	691	221	180	5		

- Molecule 10 is a protein called Ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	68	Total	C	N	O	S	0	0
			554	350	113	90	1		

- Molecule 11 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	112	Total	C	N	O	P	0	0
			2392	1070	435	775	112		

- Molecule 12 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	12	Total	C	N	O	P	0	0
			259	116	50	81	12		

- Molecule 13 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	9	19	Total	C	N	O	P	0	0
			408	183	78	128	19		

- Molecule 14 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	50	Total	C	N	O	P	0	0
			1054	471	173	360	50		

- Molecule 15 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	213	Total	C	N	O		0	0
			1055	629	213	213			

- Molecule 16 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	208	Total	C	N	O		0	0
			1027	611	208	208			

- Molecule 17 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	165	Total	C	N	O		0	0
			810	480	165	165			

- Molecule 18 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
18	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 19 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	y	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

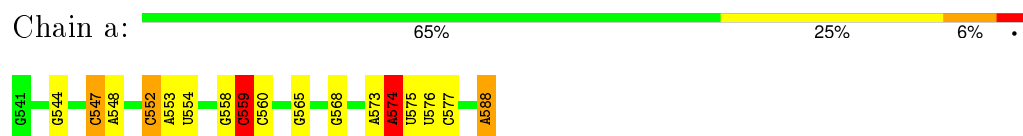
- Molecule 20 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	2	Total	C	N	O	P	0	0
			44	20	10	12	2		

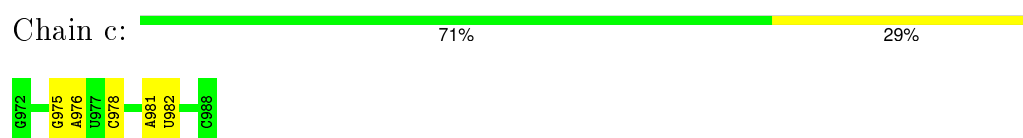
3 Residue-property plots [i](#)

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.

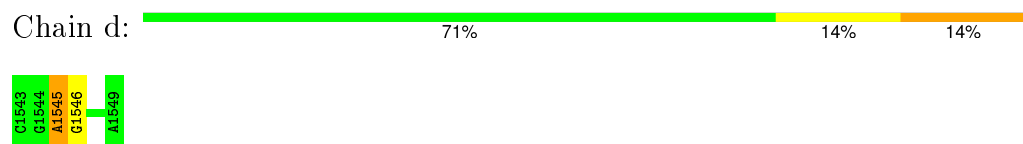
- Molecule 1: 40S ribosomal RNA fragment



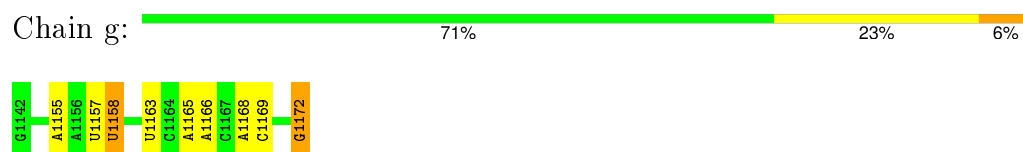
- Molecule 2: 40S ribosomal RNA fragment



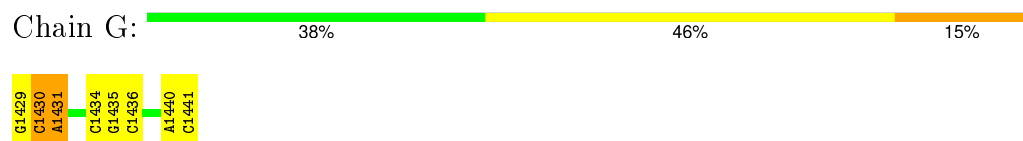
- Molecule 3: 40S ribosomal RNA fragment



- Molecule 4: 40S ribosomal RNA fragment

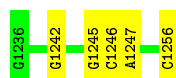


- Molecule 5: 40S ribosomal RNA fragment



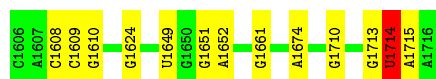
- Molecule 6: 40S ribosomal RNA fragment





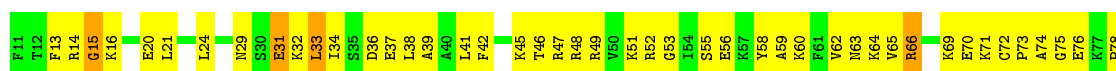
- Molecule 7: 40S ribosomal RNA fragment

Chain h: 88% 11%



- Molecule 8: Ribosomal protein S15

Chain S: 32% 62% 5%



- Molecule 9: Ribosomal protein S23

Chain L: 33% 51% 16%



- Molecule 10: Ribosomal protein S30

Chain X: 41% 51% 7%

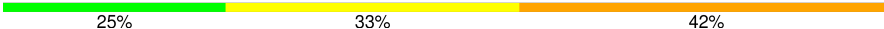


- Molecule 11: 60S ribosomal RNA fragment

Chain 2: 36% 49% 13%



- Molecule 12: 60S ribosomal RNA fragment

Chain 3: 

G2477
C2478
C2479
G2480
G2481
U2482
G2483
A2484
A2485
U2486
U2487
A2488

- Molecule 13: 60S ribosomal RNA fragment

Chain 9: 

U2668
G2669
G2670
A2671
G2672
G2673
A2674
C2675
A2676
G2677
A2678
A2679
A2680
U2681
G2682
U2683
C2684
C2685
A2686

- Molecule 14: 60S ribosomal RNA fragment

Chain 7: 

G2834
C2835
U2836
U2837
G2838
G2839
G2840
G2841
U2842
U2843
C2844
C2845
U2846
A2847
G2848
C2849
G2850
A2851
C2852
A2853
U2854
U2855
G2856
C2857
U2858
P2859
U2860
U2861
U2862
G2863
A2864
U2865
U2866
G2867
U2868
U2869
C2870
G2871
A2872
U2873

- Molecule 15: Ribosomal protein L10a

Chain B: 

I4
T5
H12
E22
T23
K24
K25
R26
N27
V32
V36
K39
N40
Y41
D42
P43
Q44
R45
D46
A2847
G2848
C2849
G2850
A2851
C2852
A2853
U2854
U2855
G2856
C2857
U2858
P2859
U2860
U2861
U2862
G2863
A2864
U2865
U2866
G2867
U2868
U2869
C2870
G2871
A2872
U2873

S104
K105
Y107
M108
A109
A112
V115
L116
I117
V120
P121
R122
L123
L124
G125
P126
Q127
L128
S129
K130
A131
G132
P135
T136
P137
D143
L144
Y145
V146
V148
V151
R152
S153
T154
I155
K156
L158
A159
V167
A168
V169
M174
D177
V178
M181
Q182
S186
V187

M188
F189
V190
V191
S192
L193
L194
K195
M197
V201
G202
S203
L204
V205
V206
K207
S208
S209
M210
G211
P212
A213
L216

- Molecule 16: Ribosomal protein L10

Chain J: 

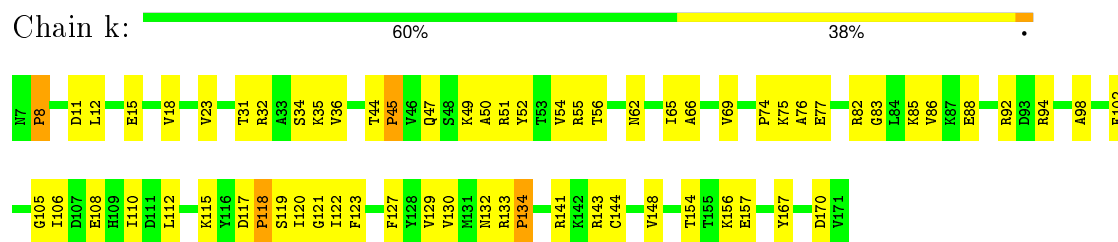
R3
R4
P5
A6
R7
C8
Y9
R10
Y11
Q12
K13
N14
K15
P16
Y17
P18
R19
S20
R21
Y22
M23
R24
A25
V26
P27
D28
S29

C71
A72
M73
K74
Y75
M76
T77
Y78
V79
D83
A84
R85
R86
L87
R88
V89
R90
V91
R92
P93
F94
R95
A96
G161
Q162
R98
R99
M100
K101
M102
LEU
SER
CYS
ALA
GLY
ASP
ARG
LEU
GLN
Q113
G114
M115
R116
G117
G120
K121
P122
H123
A126
L60
R128
A195
V129
D130
I131
T135
R69
F136

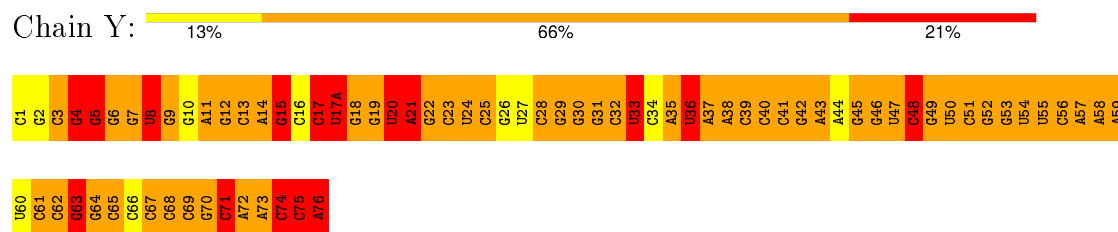
S137
V138
R139
T140
K141
D142
S143
N144
K145
V146
D147
V148
A149
E150
L152
R153
R154
A155
K158
F159
P160
G161
Q162
R164
I165
K169
K170
W171
G172
F173
T174
N175
L176
D177
R178
P179
Y181
K184
R185
E186
E189
V190
K191
D192
D193
G194
F196
S201
K202
K203
G204

S205
L206
E207
M208
E212
F213
F214
E215
F216
F217
A218
A219
Q220
A221

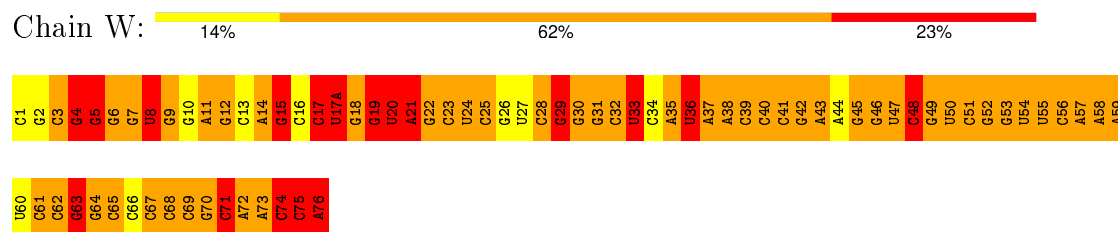
- Molecule 17: Ribosomal protein L11



- Molecule 18: tRNA



- Molecule 18: tRNA



- Molecule 19: mRNA fragment



There are no outlier residues recorded for this chain.

- Molecule 20: mRNA fragment



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	23347	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF CORRECTION OF EACH DEFOCUS GROUP VOLUME PRIOR TO BACK PROJECTION	Depositor
Microscope	FEI POLARA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.69	2/1151 (0.2%)	0.99	8/1793 (0.4%)
10	X	0.35	0/566	0.71	0/753
11	2	1.10	4/2677 (0.1%)	1.68	69/4170 (1.7%)
12	3	0.19	0/290	0.43	0/450
13	9	1.04	0/457	2.15	29/710 (4.1%)
14	7	1.07	2/1174 (0.2%)	2.34	33/1825 (1.8%)
15	B	0.34	0/1054	0.63	9/1468 (0.6%)
16	J	0.66	0/1025	0.89	8/1424 (0.6%)
17	k	0.56	0/809	0.86	5/1122 (0.4%)
18	W	2.74	133/1832 (7.3%)	2.54	183/2855 (6.4%)
18	Y	2.74	134/1832 (7.3%)	2.54	181/2855 (6.3%)
19	y	0.41	0/65	0.70	0/98
2	c	0.63	0/404	0.91	1/627 (0.2%)
20	w	0.40	0/49	0.79	0/74
3	d	0.49	0/174	0.84	0/270
4	g	0.60	0/737	0.87	2/1146 (0.2%)
5	G	0.52	0/307	0.82	0/476
6	f	0.58	0/504	0.87	0/785
7	h	0.45	0/2650	0.74	1/4127 (0.0%)
8	S	0.39	0/1003	0.66	1/1342 (0.1%)
9	L	0.43	0/1114	0.74	0/1485
All	All	1.34	275/19874 (1.4%)	1.56	530/29855 (1.8%)

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	3
17	k	0	1
18	W	0	5
18	Y	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
4	g	0	2
7	h	0	2
All	All	0	19

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	59	A	N9-C4	-13.26	1.29	1.37
18	W	59	A	N9-C4	-13.23	1.29	1.37
18	Y	2	G	C8-N7	-13.20	1.23	1.30
18	W	2	G	C8-N7	-13.15	1.23	1.30
18	W	40	C	N1-C6	-12.03	1.29	1.37
18	Y	40	C	N1-C6	-11.94	1.29	1.37
14	7	2845	A	C6-N1	-10.99	1.27	1.35
18	W	22	G	N7-C5	-10.55	1.32	1.39
18	Y	22	G	N7-C5	-10.43	1.32	1.39
18	W	72	A	N9-C4	-10.03	1.31	1.37
18	Y	72	A	N9-C4	-9.96	1.31	1.37
18	W	49	G	N9-C8	-9.53	1.31	1.37
18	Y	49	G	N9-C8	-9.52	1.31	1.37
18	Y	24	U	C4-O4	-9.35	1.16	1.23
18	W	24	U	C4-O4	-9.30	1.16	1.23
18	Y	16	C	N1-C6	-9.26	1.31	1.37
18	Y	49	G	N7-C5	-9.15	1.33	1.39
18	W	49	G	N7-C5	-9.14	1.33	1.39
18	W	16	C	N1-C6	-9.08	1.31	1.37
18	W	57	A	N7-C5	-8.94	1.33	1.39
18	Y	57	A	N7-C5	-8.93	1.33	1.39
18	Y	10	G	C5-C6	-8.72	1.33	1.42
18	W	10	G	C5-C6	-8.71	1.33	1.42
18	Y	30	G	C2'-C1'	-8.68	1.43	1.53
18	W	30	G	C2'-C1'	-8.63	1.43	1.53
18	W	48	C	C2-N3	-8.58	1.28	1.35
18	Y	48	C	C2-N3	-8.53	1.28	1.35
18	W	9	G	N7-C5	-8.53	1.34	1.39
18	Y	9	G	N7-C5	-8.41	1.34	1.39
18	W	51	C	C2-N3	-8.34	1.29	1.35
18	Y	51	C	C2-N3	-8.23	1.29	1.35
18	Y	21	A	N9-C4	-8.19	1.32	1.37
18	W	21	A	N9-C4	-8.17	1.32	1.37
18	W	27	U	C2-N3	-8.16	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	27	U	C2-N3	-8.08	1.32	1.37
18	W	61	C	C5-C6	-8.01	1.27	1.34
18	Y	61	C	C5-C6	-7.99	1.27	1.34
18	Y	3	C	N3-C4	-7.88	1.28	1.33
18	W	3	C	N3-C4	-7.85	1.28	1.33
18	Y	31	G	C8-N7	-7.78	1.26	1.30
18	W	15	G	C6-N1	-7.71	1.34	1.39
18	W	31	G	C8-N7	-7.71	1.26	1.30
18	Y	15	G	C6-N1	-7.67	1.34	1.39
18	W	33	U	C2-N3	-7.59	1.32	1.37
18	Y	33	U	C2-N3	-7.58	1.32	1.37
18	Y	39	C	C4-N4	-7.57	1.27	1.33
18	W	39	C	C4-N4	-7.57	1.27	1.33
18	Y	65	C	C4-C5	-7.57	1.36	1.43
18	W	62	C	C4-C5	-7.57	1.36	1.43
18	Y	69	C	C2-N3	-7.54	1.29	1.35
18	W	65	C	C4-C5	-7.52	1.36	1.43
18	W	35	A	N7-C5	-7.51	1.34	1.39
18	W	58	A	N3-C4	-7.51	1.30	1.34
18	Y	62	C	C4-C5	-7.50	1.36	1.43
18	W	57	A	N9-C4	-7.46	1.33	1.37
18	W	69	C	C2-N3	-7.46	1.29	1.35
18	Y	57	A	N9-C4	-7.41	1.33	1.37
18	W	36	U	C3'-C2'	-7.40	1.44	1.52
18	Y	58	A	N3-C4	-7.38	1.30	1.34
18	Y	36	U	C3'-C2'	-7.36	1.44	1.52
18	Y	35	A	N7-C5	-7.32	1.34	1.39
18	W	73	A	C5-C4	-7.31	1.33	1.38
18	Y	67	C	P-O5'	-7.29	1.52	1.59
18	Y	71	C	N1-C2	-7.29	1.32	1.40
18	Y	73	A	C5-C4	-7.28	1.33	1.38
18	W	71	C	N1-C2	-7.23	1.32	1.40
18	Y	69	C	N3-C4	7.19	1.39	1.33
18	W	67	C	P-O5'	-7.17	1.52	1.59
18	W	69	C	N3-C4	7.17	1.39	1.33
18	Y	53	G	N7-C5	-7.17	1.34	1.39
18	W	38	A	C8-N7	-7.10	1.26	1.31
18	W	53	G	N7-C5	-7.08	1.34	1.39
18	Y	38	A	C8-N7	-7.08	1.26	1.31
18	W	43	A	N3-C4	-7.08	1.30	1.34
18	W	39	C	N1-C6	-7.07	1.32	1.37
18	Y	30	G	C6-O6	-7.03	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	22	G	C4'-C3'	-7.02	1.45	1.53
18	Y	22	G	C4'-C3'	-7.00	1.45	1.53
18	Y	39	C	N1-C6	-6.98	1.32	1.37
18	Y	43	A	N3-C4	-6.97	1.30	1.34
18	W	19	G	C2-N3	-6.97	1.27	1.32
18	Y	10	G	P-O5'	-6.93	1.52	1.59
18	W	30	G	C6-O6	-6.92	1.18	1.24
18	Y	19	G	C2-N3	-6.92	1.27	1.32
18	W	45	G	N9-C4	-6.90	1.32	1.38
18	W	10	G	P-O5'	-6.89	1.52	1.59
18	Y	45	G	N9-C4	-6.85	1.32	1.38
18	W	18	G	N9-C4	-6.85	1.32	1.38
18	Y	63	G	C5-C6	-6.78	1.35	1.42
18	W	63	G	C5-C6	-6.78	1.35	1.42
18	Y	18	G	N9-C4	-6.78	1.32	1.38
18	Y	30	G	N3-C4	-6.74	1.30	1.35
18	Y	34	C	N1-C6	-6.74	1.33	1.37
18	W	30	G	N3-C4	-6.73	1.30	1.35
18	Y	7	G	P-O5'	-6.71	1.53	1.59
18	W	7	G	P-O5'	-6.67	1.53	1.59
18	W	32	C	N3-C4	-6.66	1.29	1.33
18	Y	32	C	N3-C4	-6.65	1.29	1.33
18	W	58	A	P-O5'	-6.62	1.53	1.59
18	W	17(A)	U	C2-N3	-6.61	1.33	1.37
18	W	17	C	C2'-C1'	-6.60	1.46	1.53
18	Y	17	C	C2'-C1'	-6.60	1.46	1.53
18	Y	59	A	C8-N7	-6.59	1.26	1.31
18	W	25	C	C2-O2	-6.58	1.18	1.24
18	Y	58	A	P-O5'	-6.57	1.53	1.59
18	Y	17(A)	U	C2-N3	-6.57	1.33	1.37
18	W	34	C	N1-C6	-6.53	1.33	1.37
18	Y	72	A	N9-C8	-6.53	1.32	1.37
18	W	12	G	N7-C5	-6.51	1.35	1.39
18	Y	25	C	C2-O2	-6.51	1.18	1.24
18	W	12	G	C8-N7	-6.50	1.27	1.30
18	W	16	C	C4-C5	6.48	1.48	1.43
18	Y	41	C	C2-O2	-6.48	1.18	1.24
18	Y	12	G	C8-N7	-6.48	1.27	1.30
18	W	59	A	C8-N7	-6.46	1.27	1.31
18	W	72	A	N9-C8	-6.45	1.32	1.37
18	W	41	C	C2-O2	-6.44	1.18	1.24
18	Y	16	C	C4-C5	6.43	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	18	G	C3'-C2'	-6.41	1.45	1.52
18	Y	12	G	N7-C5	-6.40	1.35	1.39
18	W	8	U	C4-C5	-6.39	1.37	1.43
18	Y	8	U	C4-C5	-6.39	1.37	1.43
18	W	64	G	C6-N1	-6.37	1.35	1.39
18	W	56	C	C4'-C3'	-6.35	1.46	1.53
18	Y	64	G	C6-N1	-6.35	1.35	1.39
18	Y	18	G	C3'-C2'	-6.34	1.45	1.52
18	Y	8	U	C2-O2	-6.34	1.16	1.22
18	W	5	G	C8-N7	-6.33	1.27	1.30
18	W	12	G	N3-C4	-6.33	1.31	1.35
18	Y	56	C	C4'-C3'	-6.33	1.46	1.53
18	W	8	U	C2-O2	-6.33	1.16	1.22
18	Y	18	G	C5-C4	-6.27	1.33	1.38
18	Y	32	C	C3'-C2'	-6.26	1.45	1.52
18	Y	41	C	C4-N4	-6.26	1.28	1.33
18	W	41	C	C4-N4	-6.25	1.28	1.33
18	W	44	A	C5-C4	-6.24	1.34	1.38
18	W	32	C	C3'-C2'	-6.24	1.45	1.52
18	Y	12	G	N3-C4	-6.24	1.31	1.35
18	W	18	G	C5-C4	-6.22	1.33	1.38
18	Y	5	G	C8-N7	-6.20	1.27	1.30
18	Y	33	U	C4'-C3'	-6.20	1.46	1.53
18	Y	44	A	C5-C4	-6.19	1.34	1.38
18	W	3	C	C4-C5	-6.18	1.38	1.43
11	2	2283	G	N9-C8	6.17	1.42	1.37
18	W	33	U	C4'-C3'	-6.15	1.46	1.53
18	Y	3	C	C4-C5	-6.13	1.38	1.43
18	Y	34	C	C4-C5	-6.10	1.38	1.43
18	W	72	A	N7-C5	-6.10	1.35	1.39
18	W	34	C	C4-C5	-6.04	1.38	1.43
18	Y	63	G	P-O5'	-5.99	1.53	1.59
18	Y	72	A	N7-C5	-5.98	1.35	1.39
18	W	44	A	C8-N7	-5.98	1.27	1.31
18	Y	3	C	C3'-C2'	-5.97	1.46	1.52
18	Y	42	G	C8-N7	-5.97	1.27	1.30
18	Y	73	A	C8-N7	-5.96	1.27	1.31
18	Y	36	U	C2-O2	-5.93	1.17	1.22
18	W	73	A	C8-N7	-5.93	1.27	1.31
18	Y	14	A	C6-N1	-5.93	1.31	1.35
18	Y	44	A	C8-N7	-5.92	1.27	1.31
18	Y	11	A	N1-C2	-5.91	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	63	G	P-O5'	-5.89	1.53	1.59
18	W	14	A	C6-N1	-5.89	1.31	1.35
18	Y	76	A	C8-N7	-5.88	1.27	1.31
18	W	14	A	P-O5'	-5.88	1.53	1.59
18	Y	63	G	C8-N7	-5.88	1.27	1.30
18	W	42	G	C8-N7	-5.88	1.27	1.30
18	W	3	C	C3'-C2'	-5.87	1.46	1.52
18	W	36	U	C2-O2	-5.86	1.17	1.22
18	W	76	A	C8-N7	-5.86	1.27	1.31
18	W	58	A	N9-C8	-5.84	1.33	1.37
18	W	11	A	N1-C2	-5.84	1.29	1.34
18	Y	14	A	P-O5'	-5.84	1.53	1.59
18	W	43	A	N7-C5	-5.83	1.35	1.39
18	W	63	G	C8-N7	-5.83	1.27	1.30
18	W	11	A	P-O5'	-5.82	1.53	1.59
18	Y	36	U	P-O5'	-5.81	1.53	1.59
18	Y	58	A	N9-C8	-5.80	1.33	1.37
18	Y	71	C	C4-C5	-5.80	1.38	1.43
18	W	9	G	C8-N7	-5.80	1.27	1.30
18	Y	46	G	N1-C2	-5.79	1.33	1.37
18	W	36	U	P-O5'	-5.78	1.53	1.59
18	Y	11	A	P-O5'	-5.77	1.53	1.59
18	Y	11	A	O4'-C1'	-5.77	1.34	1.41
18	Y	9	G	C8-N7	-5.76	1.27	1.30
18	W	21	A	C2-N3	-5.75	1.28	1.33
18	W	46	G	N1-C2	-5.75	1.33	1.37
18	Y	25	C	C4'-C3'	-5.74	1.46	1.52
18	W	58	A	N1-C2	-5.72	1.29	1.34
18	W	71	C	C4-C5	-5.72	1.38	1.43
18	W	11	A	O4'-C1'	-5.72	1.34	1.41
18	Y	43	A	N7-C5	-5.71	1.35	1.39
18	Y	58	A	N1-C2	-5.71	1.29	1.34
18	Y	21	A	C2-N3	-5.70	1.28	1.33
18	Y	21	A	C5-C6	-5.67	1.35	1.41
18	W	25	C	C4'-C3'	-5.66	1.46	1.52
18	Y	30	G	C4'-C3'	-5.63	1.47	1.52
18	W	21	A	C5-C6	-5.62	1.35	1.41
18	W	30	G	C4'-C3'	-5.60	1.47	1.52
18	Y	9	G	N9-C8	-5.59	1.33	1.37
18	W	45	G	C6-N1	-5.58	1.35	1.39
18	Y	45	G	C6-N1	-5.54	1.35	1.39
18	Y	45	G	C1'-N9	-5.53	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	9	G	N9-C8	-5.52	1.33	1.37
18	Y	55	U	C5-C6	-5.51	1.29	1.34
18	Y	28	C	C4'-C3'	-5.50	1.47	1.52
18	W	70	G	C8-N7	-5.50	1.27	1.30
18	W	45	G	C1'-N9	-5.49	1.39	1.46
18	Y	70	G	C8-N7	-5.47	1.27	1.30
18	W	17(A)	U	C2-O2	-5.46	1.17	1.22
18	W	28	C	C4'-C3'	-5.44	1.47	1.52
18	W	55	U	C5-C6	-5.41	1.29	1.34
18	W	56	C	N3-C4	-5.40	1.30	1.33
1	a	565	G	N9-C4	5.39	1.42	1.38
18	Y	11	A	C8-N7	-5.39	1.27	1.31
18	W	27	U	C4'-C3'	5.39	1.59	1.53
18	Y	27	U	C4'-C3'	5.38	1.59	1.53
18	Y	56	C	C5-C6	-5.37	1.30	1.34
18	W	61	C	C4'-C3'	-5.35	1.47	1.52
18	W	64	G	C8-N7	-5.35	1.27	1.30
18	Y	64	G	C8-N7	-5.35	1.27	1.30
18	Y	17(A)	U	C2-O2	-5.34	1.17	1.22
18	Y	62	C	C4'-C3'	-5.34	1.47	1.52
18	Y	46	G	C3'-C2'	-5.34	1.46	1.52
18	Y	61	C	C4'-C3'	-5.33	1.47	1.52
18	W	62	C	C4'-C3'	-5.32	1.47	1.52
18	Y	43	A	C5-C6	-5.30	1.36	1.41
18	Y	57	A	N9-C8	-5.29	1.33	1.37
18	W	57	A	N9-C8	-5.28	1.33	1.37
18	W	56	C	C5-C6	-5.28	1.30	1.34
18	Y	14	A	C1'-N9	-5.27	1.39	1.46
18	W	43	A	C5-C6	-5.27	1.36	1.41
18	W	32	C	N1-C2	-5.27	1.34	1.40
18	Y	56	C	N3-C4	-5.26	1.30	1.33
18	W	46	G	C3'-C2'	-5.26	1.47	1.52
18	Y	53	G	C2-N3	-5.25	1.28	1.32
18	W	45	G	N3-C4	-5.24	1.31	1.35
18	W	14	A	C1'-N9	-5.24	1.39	1.46
18	W	11	A	C8-N7	-5.23	1.27	1.31
18	Y	45	G	N3-C4	-5.22	1.31	1.35
18	Y	74	C	C4'-O4'	-5.22	1.38	1.45
18	W	74	C	C4'-O4'	-5.21	1.38	1.45
18	W	50	U	N3-C4	-5.20	1.33	1.38
18	Y	73	A	N1-C2	-5.19	1.29	1.34
18	Y	59	A	C6-N6	-5.19	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	22	G	C3'-C2'	-5.19	1.47	1.52
18	W	23	C	C4'-C3'	-5.18	1.47	1.52
18	Y	50	U	N3-C4	-5.18	1.33	1.38
11	2	2302	G	C6-N1	-5.17	1.35	1.39
18	Y	22	G	C3'-C2'	-5.17	1.47	1.52
18	Y	23	C	C4'-C3'	-5.17	1.47	1.52
18	W	22	G	N9-C8	-5.17	1.34	1.37
18	Y	32	C	N1-C2	-5.15	1.35	1.40
18	W	53	G	C2-N3	-5.15	1.28	1.32
18	W	11	A	C5-C4	-5.14	1.35	1.38
18	Y	46	G	N9-C4	-5.14	1.33	1.38
18	W	18	G	N9-C8	5.14	1.41	1.37
18	W	59	A	C6-N6	-5.13	1.29	1.33
11	2	2279	A	N7-C5	-5.12	1.36	1.39
18	Y	49	G	N3-C4	-5.11	1.31	1.35
18	W	73	A	N1-C2	-5.10	1.29	1.34
18	Y	19	G	C6-O6	-5.10	1.19	1.24
18	Y	37	A	C2-N3	-5.10	1.28	1.33
18	Y	22	G	N9-C8	-5.09	1.34	1.37
18	W	46	G	N9-C4	-5.09	1.33	1.38
1	a	565	G	C2-N3	5.07	1.36	1.32
18	Y	26	G	C8-N7	-5.06	1.27	1.30
18	W	19	G	C6-O6	-5.06	1.19	1.24
18	W	40	C	P-O5'	-5.05	1.54	1.59
18	Y	40	C	P-O5'	-5.04	1.54	1.59
18	W	29	G	N7-C5	-5.04	1.36	1.39
18	W	37	A	C2-N3	-5.04	1.29	1.33
18	Y	18	G	N9-C8	5.03	1.41	1.37
14	7	2830	G	N3-C4	-5.02	1.31	1.35
18	Y	15	G	N1-C2	5.01	1.41	1.37
11	2	2283	G	C8-N7	5.00	1.33	1.30

All (530) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	2845	A	N1-C6-N6	39.32	142.19	118.60
14	7	2845	A	C6-N1-C2	38.58	141.75	118.60
14	7	2845	A	C5-C6-N1	-33.94	100.73	117.70
14	7	2845	A	N1-C2-N3	-22.70	117.95	129.30
13	9	2681	U	C2-N1-C1'	14.58	135.19	117.70
18	Y	54	U	C5-C6-N1	13.56	129.48	122.70
18	W	54	U	C5-C6-N1	13.48	129.44	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	2681	U	C6-N1-C1'	-13.14	102.80	121.20
18	Y	43	A	C8-N9-C4	-12.70	100.72	105.80
18	W	43	A	C8-N9-C4	-12.68	100.73	105.80
14	7	2845	A	C5-C6-N6	-12.67	113.56	123.70
18	Y	43	A	N1-C2-N3	-11.53	123.53	129.30
18	W	43	A	N1-C2-N3	-11.53	123.54	129.30
18	Y	43	A	C2-N3-C4	10.92	116.06	110.60
18	W	43	A	C2-N3-C4	10.91	116.05	110.60
18	Y	37	A	C5-N7-C8	10.87	109.33	103.90
18	W	37	A	C5-N7-C8	10.81	109.31	103.90
18	W	74	C	N3-C4-C5	-10.59	117.66	121.90
18	Y	74	C	N3-C4-C5	-10.46	117.72	121.90
11	2	2195	C	N3-C4-C5	10.38	126.05	121.90
18	W	37	A	N7-C8-N9	-10.12	108.74	113.80
18	Y	37	A	N7-C8-N9	-10.08	108.76	113.80
11	2	2289	U	C2-N3-C4	-10.07	120.96	127.00
13	9	2681	U	C5-C4-O4	-10.04	119.88	125.90
18	W	31	G	C5-C6-O6	-9.96	122.62	128.60
18	Y	31	G	C5-C6-O6	-9.90	122.66	128.60
11	2	2245	C	C6-N1-C2	-9.86	116.36	120.30
11	2	2283	G	C8-N9-C4	-9.85	102.46	106.40
18	W	18	G	C5-C6-N1	9.52	116.26	111.50
18	Y	18	G	C5-C6-N1	9.50	116.25	111.50
11	2	2278	C	N1-C2-O2	9.47	124.58	118.90
18	W	72	A	C5-C6-N1	9.46	122.43	117.70
18	Y	12	G	C2-N3-C4	9.46	116.63	111.90
18	W	12	G	C2-N3-C4	9.44	116.62	111.90
13	9	2671	A	C5-C6-N6	-9.37	116.21	123.70
18	Y	72	A	C5-C6-N1	9.30	122.35	117.70
18	Y	61	C	N3-C4-C5	-9.29	118.18	121.90
18	W	61	C	N3-C4-C5	-9.26	118.20	121.90
18	W	1	C	C6-N1-C2	-9.22	116.61	120.30
18	Y	1	C	C6-N1-C2	-9.13	116.65	120.30
18	W	18	G	C5-C6-O6	-9.02	123.19	128.60
18	W	31	G	C2-N3-C4	8.97	116.39	111.90
18	Y	18	G	C5-C6-O6	-8.96	123.22	128.60
18	Y	31	G	C2-N3-C4	8.96	116.38	111.90
18	W	66	C	C6-N1-C2	8.95	123.88	120.30
11	2	2277	C	C5-C6-N1	-8.95	116.53	121.00
18	Y	66	C	C6-N1-C2	8.88	123.85	120.30
14	7	2835	U	C2-N1-C1'	8.88	128.35	117.70
18	W	76	A	N1-C6-N6	8.80	123.88	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	1714	U	N1-C1'-C2'	8.79	125.42	114.00
18	Y	76	A	N1-C6-N6	8.74	123.84	118.60
11	2	2247	G	C5-C6-O6	-8.71	123.37	128.60
18	Y	43	A	N9-C4-C5	8.70	109.28	105.80
18	W	6	G	C4-C5-N7	8.66	114.26	110.80
11	2	2302	G	N1-C6-O6	-8.64	114.72	119.90
18	W	43	A	N9-C4-C5	8.61	109.24	105.80
18	Y	6	G	C4-C5-N7	8.58	114.23	110.80
13	9	2683	U	C5-C4-O4	-8.49	120.81	125.90
14	7	2828	G	N1-C6-O6	8.47	124.98	119.90
18	Y	49	G	N7-C8-N9	8.47	117.33	113.10
14	7	2867	C	N1-C2-O2	-8.46	113.82	118.90
18	Y	68	C	C6-N1-C2	-8.44	116.92	120.30
14	7	2828	G	C5-C6-O6	-8.40	123.56	128.60
11	2	2283	G	N3-C2-N2	-8.38	114.03	119.90
18	W	68	C	C6-N1-C2	-8.38	116.95	120.30
18	Y	16	C	C6-N1-C2	8.38	123.65	120.30
18	W	49	G	N7-C8-N9	8.36	117.28	113.10
18	W	51	C	C2-N3-C4	8.36	124.08	119.90
18	Y	51	C	C2-N3-C4	8.29	124.05	119.90
11	2	2247	G	C4-C5-N7	8.28	114.11	110.80
14	7	2837	A	N1-C6-N6	-8.28	113.63	118.60
18	W	16	C	C6-N1-C2	8.28	123.61	120.30
18	W	18	G	C5-N7-C8	-8.27	100.17	104.30
18	Y	18	G	C5-N7-C8	-8.26	100.17	104.30
11	2	2303	A	C8-N9-C4	8.23	109.09	105.80
18	W	2	G	N9-C4-C5	-8.11	102.16	105.40
18	Y	2	G	N9-C4-C5	-8.09	102.17	105.40
18	W	9	G	C5-N7-C8	7.96	108.28	104.30
18	W	9	G	C4-C5-N7	-7.94	107.62	110.80
18	Y	9	G	C4-C5-N7	-7.93	107.63	110.80
18	Y	70	G	C4-C5-N7	-7.92	107.63	110.80
18	Y	63	G	N3-C4-N9	7.91	130.75	126.00
18	W	63	G	N3-C4-N9	7.90	130.74	126.00
18	Y	15	G	N1-C6-O6	-7.88	115.17	119.90
18	Y	59	A	C8-N9-C4	7.86	108.94	105.80
18	W	15	G	N1-C6-O6	-7.86	115.19	119.90
18	Y	9	G	C5-N7-C8	7.85	108.22	104.30
18	Y	76	A	C5-C6-N1	-7.84	113.78	117.70
18	W	59	A	C8-N9-C4	7.84	108.94	105.80
13	9	2671	A	N1-C6-N6	7.82	123.29	118.60
18	W	70	G	C4-C5-N7	-7.81	107.68	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	21	A	C2-N3-C4	7.80	114.50	110.60
18	Y	6	G	C5-C6-O6	-7.79	123.93	128.60
11	2	2283	G	N1-C6-O6	7.76	124.56	119.90
11	2	2290	C	N1-C2-O2	-7.75	114.25	118.90
18	W	21	A	C2-N3-C4	7.74	114.47	110.60
18	W	76	A	C5-C6-N1	-7.72	113.84	117.70
14	7	2851	A	N1-C6-N6	-7.70	113.98	118.60
18	Y	73	A	N7-C8-N9	-7.70	109.95	113.80
18	W	52	G	C5-C6-N1	7.69	115.34	111.50
18	W	6	G	C5-C6-O6	-7.69	123.99	128.60
18	Y	54	U	C4-C5-C6	-7.68	115.09	119.70
14	7	2835	U	C5-C4-O4	-7.67	121.30	125.90
18	Y	52	G	C5-C6-N1	7.66	115.33	111.50
18	W	18	G	C4-C5-N7	7.66	113.86	110.80
18	W	54	U	C4-C5-C6	-7.62	115.12	119.70
18	Y	18	G	C4-C5-N7	7.60	113.84	110.80
18	Y	17	C	C5-C6-N1	7.60	124.80	121.00
11	2	2247	G	C6-C5-N7	-7.59	125.84	130.40
18	Y	38	A	N9-C4-C5	-7.58	102.77	105.80
11	2	2277	C	C2-N3-C4	-7.58	116.11	119.90
18	Y	62	C	C6-N1-C2	7.58	123.33	120.30
18	W	73	A	N7-C8-N9	-7.56	110.02	113.80
18	W	62	C	C6-N1-C2	7.55	123.32	120.30
14	7	2835	U	N3-C4-O4	7.55	124.68	119.40
18	Y	62	C	C4-C5-C6	7.54	121.17	117.40
18	W	17	C	C5-C6-N1	7.53	124.77	121.00
18	W	62	C	C4-C5-C6	7.53	121.17	117.40
18	Y	72	A	N1-C6-N6	-7.52	114.09	118.60
11	2	2283	G	N3-C4-N9	-7.50	121.50	126.00
18	W	72	A	N1-C6-N6	-7.50	114.10	118.60
18	W	38	A	N9-C4-C5	-7.49	102.80	105.80
18	W	4	G	O4'-C1'-N9	7.48	114.18	108.20
11	2	2201	G	N1-C6-O6	7.47	124.38	119.90
13	9	2683	U	C2-N1-C1'	7.47	126.66	117.70
18	Y	4	G	O4'-C1'-N9	7.42	114.13	108.20
18	W	5	G	N9-C4-C5	-7.38	102.45	105.40
17	k	8	PRO	N-CA-CB	7.38	112.15	103.30
18	Y	24	U	C5-C4-O4	7.38	130.32	125.90
11	2	2241	U	C5-C4-O4	7.37	130.32	125.90
13	9	2679	A	N1-C6-N6	7.37	123.02	118.60
18	Y	62	C	C5-C6-N1	-7.34	117.33	121.00
18	W	5	G	C8-N9-C4	7.33	109.33	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	5	G	N9-C4-C5	-7.33	102.47	105.40
18	Y	49	G	C8-N9-C4	-7.32	103.47	106.40
18	W	8	U	C6-N1-C2	-7.31	116.61	121.00
18	W	24	U	C5-C4-O4	7.31	130.29	125.90
18	W	62	C	C5-C6-N1	-7.30	117.35	121.00
13	9	2683	U	C6-N1-C1'	-7.28	111.01	121.20
18	W	17	C	C3'-C2'-C1'	7.27	107.32	101.50
18	Y	17	C	C3'-C2'-C1'	7.26	107.31	101.50
11	2	2302	G	C6-C5-N7	7.24	134.75	130.40
13	9	2681	U	N1-C2-N3	-7.24	110.56	114.90
18	Y	5	G	C8-N9-C4	7.24	109.29	106.40
18	Y	55	U	C5-C6-N1	7.22	126.31	122.70
18	W	53	G	C6-N1-C2	7.21	129.43	125.10
18	Y	8	U	C6-N1-C2	-7.19	116.69	121.00
18	W	49	G	C8-N9-C4	-7.16	103.53	106.40
18	Y	53	G	C6-N1-C2	7.16	129.40	125.10
18	W	55	U	C5-C6-N1	7.12	126.26	122.70
11	2	2267	C	N1-C2-O2	-7.12	114.63	118.90
13	9	2673	A	C5-C6-N6	-7.10	118.02	123.70
13	9	2669	G	C6-C5-N7	-7.08	126.15	130.40
11	2	2247	G	N1-C6-O6	7.03	124.12	119.90
18	Y	6	G	N9-C4-C5	-7.02	102.59	105.40
18	W	6	G	N9-C4-C5	-6.99	102.60	105.40
18	W	31	G	N1-C2-N3	-6.96	119.72	123.90
4	g	1172	G	N9-C1'-C2'	6.91	122.98	114.00
18	Y	12	G	C5-C6-N1	6.91	114.95	111.50
18	Y	31	G	N1-C2-N3	-6.91	119.76	123.90
11	2	2248	C	N1-C2-O2	-6.87	114.78	118.90
18	Y	31	G	N3-C4-N9	6.87	130.12	126.00
18	W	31	G	N3-C4-N9	6.86	130.12	126.00
11	2	2283	G	N7-C8-N9	6.83	116.52	113.10
18	W	12	G	C5-C6-N1	6.82	114.91	111.50
2	c	981	A	N9-C1'-C2'	6.82	122.86	114.00
13	9	2681	U	N3-C4-O4	6.82	124.17	119.40
11	2	2277	C	N1-C2-O2	-6.81	114.82	118.90
18	W	61	C	C4-C5-C6	6.77	120.79	117.40
1	a	588	A	N9-C1'-C2'	6.76	122.79	114.00
14	7	2824	G	C6-N1-C2	6.76	129.16	125.10
14	7	2830	G	C5-C6-N1	-6.74	108.13	111.50
13	9	2669	G	C4-C5-N7	6.73	113.49	110.80
11	2	2304	C	C6-N1-C2	-6.70	117.62	120.30
18	Y	61	C	C4-C5-C6	6.69	120.74	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	23	C	O4'-C1'-N1	6.67	113.54	108.20
18	Y	23	C	O4'-C1'-N1	6.66	113.53	108.20
1	a	559	C	N1-C1'-C2'	6.63	122.62	114.00
18	W	75	C	C4-C5-C6	6.58	120.69	117.40
18	Y	61	C	N3-C4-N4	6.56	122.59	118.00
18	Y	75	C	C4-C5-C6	6.55	120.68	117.40
18	W	28	C	O4'-C1'-N1	6.54	113.43	108.20
11	2	2289	U	N3-C4-C5	6.54	118.52	114.60
18	W	61	C	N3-C4-N4	6.54	122.58	118.00
11	2	2278	C	N1-C2-N3	-6.53	114.63	119.20
18	Y	28	C	O4'-C1'-N1	6.51	113.41	108.20
11	2	2277	C	C6-N1-C2	6.50	122.90	120.30
18	W	1	C	C5-C6-N1	6.49	124.25	121.00
18	W	22	G	O4'-C1'-N9	6.49	113.39	108.20
18	Y	22	G	O4'-C1'-N9	6.48	113.38	108.20
18	W	15	G	N3-C4-C5	-6.46	125.37	128.60
18	Y	55	U	N1-C2-N3	-6.46	111.03	114.90
14	7	2845	A	C2-N3-C4	-6.45	107.38	110.60
18	W	66	C	C2-N3-C4	6.44	123.12	119.90
18	Y	1	C	C5-C6-N1	6.42	124.21	121.00
18	Y	68	C	C5-C6-N1	6.41	124.20	121.00
17	k	45	PRO	N-CA-CB	6.41	110.99	103.30
15	B	56	PRO	N-CA-CB	6.40	110.98	103.30
14	7	2847	A	C8-N9-C4	-6.40	103.24	105.80
1	a	565	G	N3-C2-N2	6.37	124.36	119.90
18	W	55	U	N1-C2-N3	-6.36	111.08	114.90
18	Y	1	C	C5-C4-N4	6.35	124.64	120.20
18	Y	66	C	C2-N3-C4	6.35	123.07	119.90
18	Y	15	G	N3-C4-C5	-6.34	125.43	128.60
18	W	37	A	C5-C6-N1	-6.34	114.53	117.70
18	W	68	C	C5-C6-N1	6.34	124.17	121.00
18	Y	75	C	O5'-P-OP1	-6.33	100.00	105.70
18	W	52	G	C4-C5-C6	-6.33	115.00	118.80
14	7	2865	U	N1-C2-O2	-6.32	118.38	122.80
18	Y	37	A	C5-C6-N1	-6.32	114.54	117.70
18	W	15	G	C5-C6-O6	6.32	132.39	128.60
11	2	2218	G	C5-C6-N1	6.31	114.66	111.50
18	Y	52	G	C4-C5-C6	-6.31	115.01	118.80
18	W	1	C	C5-C4-N4	6.31	124.62	120.20
18	Y	15	G	C5-C6-O6	6.29	132.38	128.60
18	W	75	C	O5'-P-OP1	-6.29	100.04	105.70
18	W	26	G	C2-N3-C4	-6.28	108.76	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	64	G	N3-C2-N2	-6.27	115.51	119.90
18	W	64	G	N3-C2-N2	-6.27	115.51	119.90
11	2	2248	C	C6-N1-C2	6.27	122.81	120.30
18	Y	4	G	N9-C4-C5	6.26	107.90	105.40
14	7	2857	C	N3-C4-C5	6.25	124.40	121.90
4	g	1172	G	C2'-C3'-O3'	6.25	123.70	113.70
18	W	4	G	N9-C4-C5	6.25	107.90	105.40
18	W	65	C	N1-C2-O2	-6.24	115.15	118.90
16	J	179	PRO	N-CA-CB	6.22	110.76	103.30
13	9	2681	U	N1-C2-O2	6.20	127.14	122.80
11	2	2278	C	C6-N1-C1'	-6.20	113.37	120.80
18	Y	76	A	C4-C5-C6	6.19	120.09	117.00
11	2	2278	C	C2-N1-C1'	6.18	125.60	118.80
18	Y	26	G	C2-N3-C4	-6.18	108.81	111.90
1	a	574	A	N9-C1'-C2'	6.17	122.03	114.00
18	W	76	A	C4-C5-C6	6.16	120.08	117.00
18	W	76	A	C4-C5-N7	-6.14	107.63	110.70
16	J	47	PRO	N-CA-CB	6.14	110.67	103.30
14	7	2837	A	C8-N9-C4	6.12	108.25	105.80
18	W	72	A	C4-C5-C6	-6.12	113.94	117.00
11	2	2280	A	C8-N9-C4	-6.12	103.35	105.80
18	Y	65	C	N1-C2-O2	-6.12	115.23	118.90
13	9	2669	G	N9-C4-C5	-6.12	102.95	105.40
14	7	2837	A	N7-C8-N9	-6.11	110.75	113.80
18	Y	20	U	N1-C2-O2	6.11	127.07	122.80
18	W	71	C	N1-C2-N3	-6.10	114.93	119.20
18	Y	71	C	N1-C2-N3	-6.09	114.94	119.20
18	W	19	G	C8-N9-C4	6.08	108.83	106.40
18	W	37	A	C8-N9-C4	6.08	108.23	105.80
18	W	13	C	C5-C4-N4	-6.08	115.94	120.20
18	Y	69	C	N1-C1'-C2'	-6.07	105.32	112.00
18	W	71	C	C2-N3-C4	6.06	122.93	119.90
18	Y	76	A	C4-C5-N7	-6.05	107.67	110.70
15	B	61	PRO	N-CA-CB	6.05	110.56	103.30
18	W	69	C	N1-C1'-C2'	-6.04	105.35	112.00
11	2	2289	U	C5-C6-N1	-6.04	119.68	122.70
18	Y	13	C	C5-C4-N4	-6.04	115.97	120.20
15	B	135	PRO	N-CA-CB	6.04	110.54	103.30
18	Y	19	G	C8-N9-C4	6.04	108.81	106.40
11	2	2278	C	C2-N3-C4	6.03	122.91	119.90
14	7	2869	U	N3-C2-O2	-6.02	117.98	122.20
18	Y	57	A	C5-C6-N1	6.02	120.71	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	20	U	N1-C2-O2	6.02	127.01	122.80
18	Y	72	A	C4-C5-C6	-6.02	113.99	117.00
11	2	2196	C	C6-N1-C2	-6.01	117.89	120.30
18	Y	12	G	C5-C6-O6	-6.01	124.99	128.60
15	B	121	PRO	N-CA-CB	6.01	110.51	103.30
11	2	2194	G	C8-N9-C4	6.01	108.80	106.40
11	2	2283	G	C5-N7-C8	-6.01	101.30	104.30
18	Y	37	A	C8-N9-C4	6.00	108.20	105.80
14	7	2835	U	C6-N1-C1'	-6.00	112.81	121.20
13	9	2669	G	C4-N9-C1'	6.00	134.29	126.50
13	9	2669	G	N3-C4-N9	5.99	129.60	126.00
18	W	21	A	N3-C4-N9	5.99	132.19	127.40
18	W	56	C	C5-C4-N4	-5.99	116.01	120.20
18	W	74	C	C3'-C2'-C1'	5.99	106.29	101.50
18	Y	10	G	C8-N9-C4	5.98	108.79	106.40
18	Y	74	C	C3'-C2'-C1'	5.98	106.29	101.50
18	Y	56	C	C5-C4-N4	-5.97	116.02	120.20
18	Y	63	G	C6-C5-N7	-5.97	126.82	130.40
18	Y	61	C	C2-N3-C4	5.96	122.88	119.90
18	Y	71	C	C2-N3-C4	5.96	122.88	119.90
18	Y	44	A	N9-C4-C5	-5.96	103.42	105.80
18	W	8	U	C2-N3-C4	5.95	130.57	127.00
18	W	10	G	C8-N9-C4	5.95	108.78	106.40
15	B	126	PRO	N-CA-CB	5.94	110.43	103.30
18	W	63	G	C6-C5-N7	-5.94	126.84	130.40
18	W	22	G	N3-C4-C5	5.93	131.56	128.60
14	7	2868	U	N3-C2-O2	5.92	126.35	122.20
18	W	12	G	C5-C6-O6	-5.92	125.05	128.60
18	W	18	G	O4'-C1'-N9	-5.92	103.46	108.20
18	Y	18	G	O4'-C1'-N9	-5.91	103.47	108.20
18	Y	8	U	C2-N3-C4	5.90	130.54	127.00
18	W	57	A	C5-C6-N1	5.90	120.65	117.70
18	Y	21	A	N3-C4-N9	5.90	132.12	127.40
18	W	61	C	C2-N3-C4	5.89	122.84	119.90
18	W	12	G	N9-C4-C5	-5.88	103.05	105.40
18	W	59	A	N1-C2-N3	-5.88	126.36	129.30
11	2	2303	A	N9-C4-C5	-5.88	103.45	105.80
15	B	43	PRO	N-CA-CB	5.88	110.36	103.30
18	Y	22	G	N3-C4-C5	5.86	131.53	128.60
15	B	137	PRO	N-CA-CB	5.86	110.33	103.30
13	9	2671	A	C6-N1-C2	-5.85	115.09	118.60
14	7	2867	C	N3-C2-O2	5.85	125.99	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2201	G	C5-C6-O6	-5.84	125.09	128.60
18	W	44	A	O4'-C1'-N9	-5.84	103.52	108.20
15	B	212	PRO	N-CA-CB	5.84	110.31	103.30
18	Y	59	A	N1-C2-N3	-5.83	126.38	129.30
17	k	74	PRO	N-CA-CB	5.83	110.30	103.30
18	W	66	C	N1-C2-N3	-5.83	115.12	119.20
15	B	59	PRO	N-CA-CB	5.82	110.28	103.30
11	2	2241	U	C6-N1-C1'	5.80	129.32	121.20
18	Y	44	A	O4'-C1'-N9	-5.80	103.56	108.20
18	Y	70	G	C5-N7-C8	5.80	107.20	104.30
11	2	2302	G	C5-C6-N1	5.80	114.40	111.50
13	9	2669	G	C8-N9-C1'	-5.80	119.47	127.00
18	W	44	A	N9-C4-C5	-5.79	103.48	105.80
18	W	18	G	C2-N3-C4	5.78	114.79	111.90
16	J	122	PRO	N-CA-CB	5.78	110.24	103.30
18	Y	48	C	N1-C2-O2	-5.78	115.43	118.90
1	a	558	G	N9-C1'-C2'	5.78	121.51	114.00
18	Y	51	C	C4'-C3'-C2'	5.78	108.38	102.60
18	W	51	C	C4'-C3'-C2'	5.78	108.38	102.60
18	W	48	C	N1-C2-O2	-5.78	115.44	118.90
16	J	18	PRO	N-CA-CB	5.77	110.23	103.30
18	Y	50	U	N3-C4-O4	-5.76	115.37	119.40
11	2	2283	G	N1-C2-N2	5.75	121.37	116.20
18	Y	66	C	N1-C2-N3	-5.75	115.18	119.20
11	2	2290	C	C2-N3-C4	-5.75	117.03	119.90
18	W	55	U	O4'-C1'-N1	5.74	112.79	108.20
18	W	58	A	N9-C4-C5	-5.73	103.51	105.80
11	2	2302	G	N3-C4-N9	-5.73	122.56	126.00
18	W	10	G	N9-C4-C5	-5.73	103.11	105.40
18	W	70	G	C5-N7-C8	5.72	107.16	104.30
18	W	64	G	N1-C2-N3	5.72	127.33	123.90
18	Y	12	G	N9-C4-C5	-5.72	103.11	105.40
18	Y	64	G	N1-C2-N3	5.72	127.33	123.90
18	Y	55	U	O4'-C1'-N1	5.71	112.77	108.20
18	Y	71	C	C6-N1-C2	5.71	122.58	120.30
11	2	2283	G	C2-N3-C4	-5.71	109.05	111.90
18	Y	18	G	C2-N3-C4	5.71	114.75	111.90
14	7	2837	A	C4-C5-N7	-5.70	107.85	110.70
18	W	50	U	N3-C4-O4	-5.69	115.42	119.40
18	W	6	G	C5-N7-C8	-5.68	101.46	104.30
18	Y	58	A	N9-C4-C5	-5.68	103.53	105.80
11	2	2290	C	N3-C4-C5	5.68	124.17	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2248	C	N3-C2-O2	5.67	125.87	121.90
1	a	565	G	N1-C2-N2	-5.67	111.10	116.20
18	W	50	U	C4-C5-C6	-5.67	116.30	119.70
18	Y	44	A	C4-C5-N7	5.67	113.53	110.70
18	Y	10	G	N9-C4-C5	-5.66	103.14	105.40
18	Y	13	C	O4'-C1'-N1	-5.66	103.67	108.20
18	W	71	C	C6-N1-C2	5.66	122.56	120.30
18	Y	18	G	C4-C5-C6	-5.65	115.41	118.80
18	W	18	G	C4-C5-C6	-5.65	115.41	118.80
1	a	552	C	N1-C1'-C2'	5.64	121.34	114.00
16	J	16	PRO	N-CA-CB	5.64	110.07	103.30
18	Y	8	U	N3-C4-C5	-5.64	111.21	114.60
18	W	8	U	N3-C4-C5	-5.64	111.22	114.60
11	2	2301	U	C6-N1-C2	5.64	124.38	121.00
18	Y	6	G	C5-N7-C8	-5.63	101.48	104.30
18	Y	50	U	C4-C5-C6	-5.63	116.32	119.70
16	J	214	PRO	N-CA-CB	5.62	110.05	103.30
18	Y	73	A	C8-N9-C4	5.62	108.05	105.80
18	W	10	G	C4-C5-N7	5.62	113.05	110.80
13	9	2679	A	N9-C4-C5	-5.60	103.56	105.80
18	W	13	C	O4'-C1'-N1	-5.60	103.72	108.20
11	2	2196	C	N3-C4-C5	5.59	124.14	121.90
18	W	44	A	C4-C5-N7	5.59	113.50	110.70
11	2	2197	C	N3-C2-O2	5.58	125.81	121.90
13	9	2668	U	C2-N1-C1'	5.58	124.40	117.70
18	Y	10	G	C4-C5-N7	5.58	113.03	110.80
18	Y	75	C	N1-C2-O2	-5.57	115.56	118.90
11	2	2300	G	C8-N9-C1'	-5.56	119.77	127.00
18	W	73	A	C8-N9-C4	5.56	108.03	105.80
18	Y	63	G	N3-C4-C5	-5.56	125.82	128.60
11	2	2246	G	C5-C6-N1	5.56	114.28	111.50
14	7	2853	A	N1-C6-N6	5.56	121.93	118.60
18	W	63	G	N7-C8-N9	5.55	115.88	113.10
18	Y	63	G	N7-C8-N9	5.55	115.88	113.10
18	Y	42	G	N1-C6-O6	-5.54	116.58	119.90
18	Y	64	G	C6-N1-C2	-5.53	121.78	125.10
11	2	2241	U	N1-C2-N3	5.52	118.21	114.90
11	2	2301	U	N3-C2-O2	5.52	126.06	122.20
18	W	65	C	N3-C2-O2	5.52	125.76	121.90
18	W	31	G	C5-N7-C8	5.52	107.06	104.30
18	W	13	C	N3-C4-N4	5.51	121.86	118.00
18	Y	13	C	N3-C4-N4	5.51	121.86	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	53	G	C5-C6-N1	-5.50	108.75	111.50
18	W	21	A	C1'-O4'-C4'	-5.50	105.50	109.90
18	W	75	C	N1-C2-O2	-5.50	115.60	118.90
18	Y	64	G	C8-N9-C4	-5.49	104.20	106.40
18	W	44	A	C2-N3-C4	-5.49	107.86	110.60
18	W	64	G	C6-N1-C2	-5.49	121.81	125.10
17	k	134	PRO	N-CA-CB	5.49	109.88	103.30
18	Y	21	A	C1'-O4'-C4'	-5.49	105.51	109.90
18	Y	4	G	N9-C1'-C2'	-5.48	105.97	112.00
18	Y	6	G	C4-C5-C6	-5.48	115.51	118.80
18	Y	44	A	C2-N3-C4	-5.48	107.86	110.60
18	W	4	G	N9-C1'-C2'	-5.48	105.97	112.00
18	W	74	C	C4-C5-C6	5.47	120.14	117.40
18	W	6	G	C4-C5-C6	-5.47	115.52	118.80
14	7	2830	G	C2-N3-C4	-5.47	109.17	111.90
18	W	17(A)	U	C2-N3-C4	5.47	130.28	127.00
18	Y	20	U	N3-C4-O4	-5.46	115.58	119.40
11	2	2274	U	N3-C2-O2	-5.45	118.38	122.20
18	W	23	C	N3-C4-C5	-5.45	119.72	121.90
18	W	53	G	C5-C6-N1	-5.45	108.77	111.50
11	2	2195	C	C5-C4-N4	-5.45	116.39	120.20
18	W	72	A	C6-C5-N7	5.45	136.11	132.30
18	W	63	G	N3-C4-C5	-5.44	125.88	128.60
18	W	64	G	C8-N9-C4	-5.44	104.22	106.40
18	Y	18	G	C3'-C2'-C1'	5.43	105.85	101.50
18	Y	12	G	N3-C4-N9	5.43	129.26	126.00
18	Y	17(A)	U	C2-N3-C4	5.42	130.25	127.00
18	W	12	G	N3-C4-N9	5.42	129.25	126.00
18	Y	65	C	N3-C2-O2	5.42	125.69	121.90
11	2	2289	U	C5-C4-O4	-5.42	122.65	125.90
18	W	18	G	C3'-C2'-C1'	5.42	105.83	101.50
13	9	2671	A	C5-C6-N1	5.41	120.41	117.70
18	W	42	G	N1-C6-O6	-5.41	116.65	119.90
11	2	2301	U	N1-C2-O2	-5.41	119.01	122.80
11	2	2283	G	N3-C4-C5	5.41	131.30	128.60
18	Y	50	U	N3-C4-C5	5.41	117.84	114.60
18	Y	31	G	C5-C6-N1	5.40	114.20	111.50
18	Y	23	C	N3-C4-C5	-5.40	119.74	121.90
18	Y	74	C	N3-C4-N4	5.39	121.78	118.00
18	W	50	U	N3-C4-C5	5.39	117.83	114.60
11	2	2194	G	N7-C8-N9	-5.39	110.41	113.10
18	Y	68	C	N1-C2-N3	5.39	122.97	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	72	A	C6-C5-N7	5.39	136.07	132.30
18	Y	31	G	C5-N7-C8	5.38	106.99	104.30
18	W	71	C	C4-C5-C6	-5.38	114.71	117.40
14	7	2869	U	C2-N1-C1'	5.37	124.15	117.70
18	W	5	G	N7-C8-N9	-5.37	110.42	113.10
18	W	17	C	C4-C5-C6	-5.37	114.72	117.40
18	W	20	U	N3-C4-O4	-5.37	115.64	119.40
18	Y	65	C	C4-C5-C6	5.36	120.08	117.40
18	Y	74	C	C4-C5-C6	5.35	120.08	117.40
18	W	74	C	N3-C4-N4	5.35	121.75	118.00
18	Y	43	A	N7-C8-N9	5.35	116.47	113.80
18	W	68	C	N1-C2-N3	5.35	122.94	119.20
18	Y	67	C	C6-N1-C2	-5.34	118.16	120.30
18	Y	5	G	N7-C8-N9	-5.34	110.43	113.10
18	Y	17	C	C4-C5-C6	-5.34	114.73	117.40
17	k	118	PRO	N-CA-CB	5.33	109.70	103.30
18	Y	3	C	C5-C6-N1	-5.33	118.33	121.00
18	Y	70	G	C6-C5-N7	5.33	133.60	130.40
18	W	59	A	N1-C6-N6	-5.33	115.41	118.60
18	W	43	A	N7-C8-N9	5.32	116.46	113.80
18	Y	15	G	C6-N1-C2	-5.31	121.91	125.10
11	2	2275	A	C5-C6-N1	-5.31	115.05	117.70
11	2	2303	A	C5-C6-N1	5.31	120.36	117.70
11	2	2247	G	C5-N7-C8	-5.30	101.65	104.30
14	7	2859	U	N3-C2-O2	5.29	125.91	122.20
18	W	31	G	C5-C6-N1	5.29	114.15	111.50
18	Y	59	A	N1-C6-N6	-5.29	115.43	118.60
18	W	65	C	C4-C5-C6	5.29	120.05	117.40
13	9	2671	A	N9-C4-C5	-5.28	103.69	105.80
18	Y	71	C	C4-C5-C6	-5.28	114.76	117.40
18	W	71	C	C5'-C4'-C3'	-5.28	107.55	116.00
18	Y	71	C	C5'-C4'-C3'	-5.28	107.55	116.00
18	Y	37	A	C4-C5-C6	5.28	119.64	117.00
18	W	15	G	C6-N1-C2	-5.26	121.94	125.10
18	W	21	A	N3-C4-C5	-5.26	123.12	126.80
18	Y	44	A	C5-N7-C8	-5.25	101.27	103.90
18	W	74	C	C2-N3-C4	5.25	122.53	119.90
18	W	70	G	C6-C5-N7	5.25	133.55	130.40
18	W	38	A	N7-C8-N9	5.25	116.42	113.80
11	2	2246	G	N3-C4-N9	5.25	129.15	126.00
18	Y	21	A	N3-C4-C5	-5.25	123.13	126.80
13	9	2683	U	C2-N3-C4	-5.24	123.86	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	31	G	N1-C6-O6	5.24	123.05	119.90
18	W	4	G	C3'-C2'-C1'	5.24	105.69	101.50
18	W	37	A	C4-C5-C6	5.24	119.62	117.00
18	W	3	C	C5-C6-N1	-5.23	118.38	121.00
18	Y	24	U	P-O5'-C5'	-5.23	112.53	120.90
18	Y	21	A	N1-C6-N6	-5.23	115.46	118.60
18	W	44	A	C5-N7-C8	-5.23	101.28	103.90
18	W	4	G	C5'-C4'-C3'	-5.22	107.64	116.00
18	W	21	A	N1-C6-N6	-5.22	115.47	118.60
18	W	24	U	P-O5'-C5'	-5.22	112.55	120.90
18	Y	38	A	N7-C8-N9	5.21	116.41	113.80
18	W	24	U	N3-C2-O2	-5.21	118.56	122.20
18	W	67	C	C6-N1-C2	-5.20	118.22	120.30
18	Y	20	U	O4'-C1'-N1	5.20	112.36	108.20
18	Y	32	C	N1-C2-O2	-5.20	115.78	118.90
18	W	20	U	O4'-C1'-N1	5.19	112.35	108.20
18	Y	24	U	N3-C2-O2	-5.19	118.57	122.20
18	Y	4	G	C5'-C4'-C3'	-5.18	107.71	116.00
18	Y	74	C	C2-N3-C4	5.18	122.49	119.90
18	Y	4	G	C3'-C2'-C1'	5.16	105.63	101.50
18	Y	53	G	C4-C5-N7	5.15	112.86	110.80
13	9	2671	A	N3-C4-N9	5.14	131.52	127.40
18	W	14	A	C6-N1-C2	5.14	121.69	118.60
18	W	71	C	C4'-C3'-C2'	-5.14	97.46	102.60
18	Y	14	A	C6-N1-C2	5.14	121.69	118.60
18	Y	31	G	N3-C4-C5	-5.14	126.03	128.60
11	2	2215	A	C2-N3-C4	-5.14	108.03	110.60
18	W	69	C	C2-N3-C4	5.13	122.47	119.90
18	Y	71	C	C4'-C3'-C2'	-5.13	97.47	102.60
18	W	31	G	N3-C4-C5	-5.12	126.04	128.60
18	Y	17(A)	U	N1-C2-O2	5.12	126.38	122.80
18	Y	56	C	N3-C4-C5	5.12	123.95	121.90
18	W	17(A)	U	N1-C2-O2	5.12	126.38	122.80
16	J	27	PRO	N-CA-CB	5.12	109.44	103.30
18	W	32	C	N1-C2-O2	-5.11	115.83	118.90
13	9	2672	G	C4-C5-N7	5.11	112.84	110.80
18	Y	31	G	N1-C6-O6	5.09	122.96	119.90
18	W	56	C	N3-C4-C5	5.08	123.93	121.90
13	9	2685	C	C2-N1-C1'	5.08	124.38	118.80
18	W	26	G	N3-C4-N9	-5.08	122.95	126.00
11	2	2281	A	C4-C5-C6	5.07	119.53	117.00
18	W	10	G	C5-C6-O6	-5.07	125.56	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	11	A	N1-C6-N6	5.06	121.64	118.60
16	J	178	ARG	N-CA-C	5.05	124.65	111.00
18	Y	69	C	C2-N3-C4	5.05	122.43	119.90
14	7	2828	G	C8-N9-C1'	-5.05	120.44	127.00
18	W	63	G	N9-C4-C5	-5.05	103.38	105.40
8	S	131	THR	N-CA-C	5.04	124.61	111.00
14	7	2869	U	C6-N1-C2	-5.04	117.97	121.00
18	W	2	G	N3-C4-N9	5.03	129.02	126.00
18	W	11	A	N1-C6-N6	5.03	121.62	118.60
18	Y	73	A	C5-N7-C8	5.03	106.42	103.90
18	W	53	G	C4-C5-N7	5.03	112.81	110.80
1	a	559	C	O4'-C1'-N1	5.03	112.22	108.20
18	Y	4	G	C4-C5-N7	-5.02	108.79	110.80
11	2	2261	G	N1-C6-O6	5.02	122.91	119.90
18	Y	59	A	N9-C4-C5	-5.01	103.80	105.80
13	9	2672	G	N9-C4-C5	-5.01	103.40	105.40
14	7	2824	G	C5-C6-N1	-5.01	109.00	111.50
18	W	1	C	N1-C1'-C2'	5.00	120.50	114.00
11	2	2290	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	W	15	G	Sidechain
18	W	29	G	Sidechain
18	W	33	U	Sidechain
18	W	4	G	Sidechain
18	W	8	U	Sidechain
18	Y	15	G	Sidechain
18	Y	29	G	Sidechain
18	Y	33	U	Sidechain
18	Y	4	G	Sidechain
18	Y	8	U	Sidechain
1	a	547	C	Sidechain
1	a	559	C	Sidechain
1	a	574	A	Sidechain
3	d	1545	A	Sidechain
4	g	1157	U	Sidechain
4	g	1158	U	Sidechain
7	h	1610	G	Sidechain
7	h	1714	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
17	k	51	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1029	0	521	0	0
2	c	362	0	185	0	0
3	d	155	0	77	0	0
4	g	660	0	335	0	0
5	G	276	0	142	10	0
6	f	452	0	226	0	0
7	h	2368	0	1196	0	0
8	S	985	0	1026	98	0
9	L	1097	0	1169	102	0
10	X	554	0	604	42	0
11	2	2392	0	1208	402	0
12	3	259	0	125	92	0
13	9	408	0	199	109	0
14	7	1054	0	529	186	0
15	B	1055	0	449	125	0
16	J	1027	0	468	105	0
17	k	810	0	353	0	0
18	W	1640	0	825	117	0
18	Y	1640	0	825	146	0
19	y	60	0	31	0	0
20	w	44	0	23	0	0
All	All	18327	0	10516	1371	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 70.

All (1371) 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)
12:3:2481:G:O5'	15:B:102:LYS:CB	1.65	1.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:2484:A:H5'	15:B:122:ARG:C	1.34	1.43
11:2:2253:G:OP1	18:Y:13:C:C4'	1.64	1.43
14:7:2828:G:N1	18:Y:76:A:H1'	1.33	1.39
12:3:2481:G:H8	15:B:102:LYS:CB	1.34	1.39
12:3:2481:G:C8	15:B:102:LYS:CA	2.04	1.38
16:J:177:ASP:HA	16:J:179:PRO:N	1.35	1.37
12:3:2483:G:N3	15:B:97:LYS:HA	1.38	1.36
13:9:2673:A:N6	13:9:2681:U:O4	1.61	1.32
14:7:2863:G:H5'	18:Y:75:C:C3'	1.49	1.28
11:2:2253:G:H5'	18:Y:13:C:O2'	1.27	1.27
18:Y:20:U:O2	18:Y:37:A:C4	41.18	1.25
14:7:2863:G:H5'	18:Y:75:C:O3'	1.35	1.22
12:3:2482:U:O4	15:B:101:LYS:CB	1.88	1.21
14:7:2863:G:H5'	18:Y:75:C:C4'	1.71	1.20
12:3:2484:A:H5'	15:B:122:ARG:CA	1.67	1.19
12:3:2481:G:H8	15:B:102:LYS:CA	1.43	1.19
14:7:2830:G:H5'	18:Y:76:A:N6	1.57	1.19
14:7:2863:G:C5'	18:Y:75:C:H4'	1.73	1.18
13:9:2684:C:H5'	13:9:2684:C:C6	1.77	1.17
12:3:2481:G:C8	15:B:102:LYS:HA	1.74	1.16
12:3:2481:G:C8	15:B:102:LYS:CB	2.27	1.16
18:Y:17:C:H5''	18:Y:17(A):U:H6	1.12	1.14
13:9:2684:C:C5'	13:9:2684:C:H6	1.59	1.14
12:3:2481:G:C8	15:B:102:LYS:N	2.16	1.13
14:7:2863:G:C5'	18:Y:75:C:O3'	1.97	1.12
18:W:17:C:H5''	18:W:17(A):U:H6	1.12	1.12
18:W:17:C:H5''	18:W:17(A):U:C6	1.85	1.12
12:3:2483:G:C8	15:B:96:ASN:N	2.19	1.11
18:Y:17:C:H5''	18:Y:17(A):U:C6	1.85	1.11
11:2:2262:A:H3'	11:2:2263:C:H5''	1.31	1.11
18:Y:20:U:C2	18:Y:37:A:N3	40.47	1.10
12:3:2484:A:H3'	15:B:127:GLN:CB	1.80	1.10
11:2:2250:G:N2	11:2:2267:C:O2	1.82	1.10
13:9:2684:C:H2'	13:9:2685:C:H6	1.08	1.10
12:3:2481:G:N7	15:B:102:LYS:HA	1.66	1.10
11:2:2270:A:C8	11:2:2270:A:H5''	1.87	1.09
12:3:2484:A:C5'	15:B:122:ARG:C	2.21	1.09
11:2:2213:A:H2'	11:2:2214:A:H8	1.16	1.08
9:L:9:ILE:H	9:L:9:ILE:HD12	0.97	1.08
14:7:2828:G:C6	18:Y:76:A:H1'	1.82	1.08
11:2:2271:A:C2'	11:2:2272:G:H5''	1.84	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2271:A:H2'	11:2:2272:G:H5''	1.30	1.07
13:9:2684:C:H5'	13:9:2684:C:H6	1.04	1.06
14:7:2828:G:H1	18:Y:76:A:C1'	1.69	1.06
9:L:116:ILE:HG21	9:L:119:VAL:HB	1.33	1.05
11:2:2213:A:H2'	11:2:2214:A:C8	1.89	1.05
18:Y:20:U:O2	18:Y:37:A:N3	41.35	1.05
18:Y:46:G:H4'	18:Y:47:U:H5	1.20	1.04
14:7:2863:G:H5''	18:Y:74:C:O2'	1.57	1.04
18:W:21:A:H61	18:W:46:G:H2'	1.17	1.03
18:Y:21:A:H61	18:Y:46:G:H2'	1.17	1.02
18:W:46:G:H4'	18:W:47:U:H5	1.20	1.02
16:J:161:GLY:HA2	16:J:162:GLN:CB	1.89	1.02
13:9:2673:A:N6	13:9:2681:U:C4	2.28	1.01
9:L:19:ARG:HH11	9:L:19:ARG:HA	1.26	1.00
13:9:2684:C:H2'	13:9:2685:C:C6	1.95	1.00
9:L:9:ILE:CD1	9:L:9:ILE:H	1.71	1.00
11:2:2223:A:O2'	11:2:2224:A:H8	1.45	0.99
18:W:17:C:H6	18:W:17(A):U:H5	1.11	0.98
9:L:19:ARG:NH1	9:L:19:ARG:HA	1.78	0.98
18:W:14:A:C2	18:W:37:A:C6	33.43	0.98
14:7:2854:U:C5'	16:J:160:PRO:HA	1.93	0.98
14:7:2854:U:H5''	16:J:160:PRO:HA	1.45	0.98
11:2:2304:C:O2'	11:2:2305:G:H5'	1.64	0.98
14:7:2863:G:N7	18:Y:76:A:O3'	1.97	0.97
11:2:2253:G:P	18:Y:13:C:H4'	2.04	0.97
9:L:9:ILE:N	9:L:9:ILE:HD12	1.79	0.97
12:3:2483:G:N3	15:B:97:LYS:CA	2.27	0.97
14:7:2829:U:O2'	18:Y:75:C:C4	2.18	0.97
14:7:2828:G:N1	18:Y:76:A:C1'	2.24	0.96
11:2:2285:C:H5	11:2:2286:U:C2	1.83	0.96
14:7:2863:G:H5''	18:Y:75:C:H4'	1.44	0.96
12:3:2482:U:C5	15:B:101:LYS:N	2.22	0.95
18:Y:17:C:H6	18:Y:17(A):U:H5	1.11	0.95
12:3:2483:G:C5	15:B:127:GLN:CB	2.49	0.95
11:2:2276:G:C5	11:2:2277:C:C5	2.55	0.95
13:9:2678:A:N7	18:Y:56:C:OP1	1.97	0.95
12:3:2484:A:H4'	15:B:127:GLN:H	1.31	0.95
11:2:2270:A:H8	11:2:2270:A:H5''	1.25	0.95
11:2:2252:A:H2'	11:2:2253:G:H8	1.33	0.94
18:W:14:A:N3	18:W:37:A:C6	33.05	0.94
16:J:89:VAL:O	16:J:136:PHE:HA	1.68	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:93:PRO:HA	16:J:127:ALA:HB2	1.50	0.94
11:2:2268:U:H2'	11:2:2269:U:H5	1.33	0.94
18:Y:20:U:O2	18:Y:37:A:N9	41.53	0.94
14:7:2863:G:H5'	18:Y:75:C:H4'	1.36	0.93
12:3:2484:A:C3'	15:B:127:GLN:CB	2.46	0.93
10:X:7:THR:HG21	10:X:10:LYS:HB2	1.51	0.92
14:7:2850:G:OP1	14:7:2850:G:H4'	1.68	0.92
11:2:2251:G:H1'	11:2:2252:A:OP1	1.68	0.92
18:Y:20:U:O2	18:Y:37:A:H1'	42.91	0.91
15:B:67:ILE:HA	15:B:112:ALA:HB2	1.52	0.91
12:3:2482:U:C4	15:B:101:LYS:N	2.38	0.91
14:7:2869:U:H5''	14:7:2870:C:OP2	1.71	0.91
12:3:2481:G:P	15:B:102:LYS:CB	2.60	0.90
12:3:2483:G:C8	15:B:127:GLN:CB	2.53	0.90
11:2:2253:G:C5'	18:Y:13:C:O2'	2.19	0.90
12:3:2483:G:C4	15:B:127:GLN:CB	2.54	0.90
11:2:2253:G:O6	11:2:2263:C:N4	2.04	0.90
13:9:2680:A:OP2	13:9:2681:U:C5	2.25	0.90
18:Y:20:U:C2	18:Y:37:A:C4	40.32	0.90
11:2:2251:G:O2'	11:2:2252:A:H5''	1.72	0.90
18:Y:20:U:O2	18:Y:37:A:C1'	42.13	0.90
14:7:2862:U:O3'	18:Y:75:C:O5'	1.90	0.90
5:G:1434:C:OP1	18:W:30:G:H5''	1.73	0.89
11:2:2299:A:C5	11:2:2300:G:C8	2.60	0.89
9:L:71:VAL:HG21	9:L:95:LEU:HD13	1.53	0.89
11:2:2254:U:O2	11:2:2261:G:N2	2.05	0.89
14:7:2833:A:H2'	14:7:2834:G:H5'	1.55	0.89
14:7:2847:A:H5'	14:7:2848:G:OP2	1.73	0.88
11:2:2270:A:H2'	11:2:2271:A:C8	2.07	0.88
14:7:2830:G:C5'	18:Y:76:A:N6	2.37	0.88
13:9:2680:A:P	13:9:2681:U:C5	2.66	0.88
11:2:2252:A:H2'	11:2:2253:G:C8	2.08	0.88
16:J:177:ASP:CA	16:J:179:PRO:N	2.32	0.87
14:7:2826:U:O2'	14:7:2827:U:H5'	1.72	0.87
9:L:58:ILE:HG21	9:L:117:PRO:HG3	1.54	0.87
11:2:2253:G:OP1	18:Y:13:C:H4'	0.69	0.87
11:2:2215:A:H2'	11:2:2215:A:N3	1.87	0.86
11:2:2262:A:H3'	11:2:2263:C:C5'	2.03	0.86
12:3:2482:U:O4	15:B:101:LYS:N	2.07	0.86
18:Y:17:C:H6	18:Y:17(A):U:C5	1.93	0.86
12:3:2486:A:N7	15:B:101:LYS:CB	2.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:2483:G:O5'	15:B:96:ASN:CA	2.20	0.86
11:2:2293:C:H5	11:2:2294:U:H5	1.20	0.86
9:L:69:LYS:HZ2	9:L:69:LYS:HB3	1.40	0.86
18:W:17:C:H6	18:W:17(A):U:C5	1.93	0.86
12:3:2484:A:H4'	15:B:127:GLN:N	1.90	0.86
14:7:2834:G:O2'	14:7:2835:U:H6	1.56	0.86
15:B:178:VAL:O	15:B:182:GLN:CB	2.23	0.86
18:Y:71:C:H2'	18:Y:71:C:O2	1.75	0.85
11:2:2287:C:O2	11:2:2298:U:O4'	1.94	0.85
18:W:71:C:O2	18:W:71:C:H2'	1.75	0.85
11:2:2253:G:OP1	18:Y:13:C:C5'	2.24	0.85
11:2:2259:A:H3'	11:2:2260:U:C6	2.11	0.85
18:W:75:C:C6	18:W:76:A:C8	2.65	0.84
18:Y:75:C:C6	18:Y:76:A:C8	2.65	0.84
13:9:2684:C:C6	13:9:2684:C:C5'	2.47	0.84
11:2:2205:U:H2'	11:2:2206:G:H5'	1.58	0.84
18:W:46:G:H4'	18:W:47:U:C5	2.12	0.84
13:9:2678:A:C8	13:9:2679:A:C2	2.65	0.84
15:B:154:THR:HA	15:B:155:ILE:O	1.76	0.84
12:3:2483:G:O5'	15:B:96:ASN:HA	1.70	0.84
14:7:2828:G:H1	18:Y:76:A:H1'	0.83	0.84
13:9:2675:C:H41	13:9:2676:A:N6	1.75	0.84
15:B:45:ARG:CB	18:W:54:U:H5''	2.07	0.84
11:2:2272:G:N3	11:2:2272:G:H5'	1.91	0.83
12:3:2482:U:H5''	15:B:93:LEU:C	1.98	0.83
8:S:105:LYS:HG3	8:S:106:GLU:HG2	1.60	0.83
14:7:2851:A:H2'	14:7:2852:C:O4'	1.77	0.83
11:2:2232:A:H2'	11:2:2233:A:O4'	1.79	0.83
12:3:2484:A:H5'	15:B:123:LEU:N	1.93	0.83
11:2:2278:C:N4	11:2:2305:G:N7	2.27	0.83
11:2:2253:G:N7	11:2:2254:U:C4	2.47	0.82
11:2:2293:C:C5	11:2:2294:U:H5	1.97	0.82
11:2:2223:A:O2'	11:2:2224:A:C8	2.29	0.82
8:S:101:VAL:HG21	8:S:121:LEU:HD11	1.60	0.82
12:3:2483:G:C5'	15:B:96:ASN:CB	2.45	0.82
11:2:2224:A:H2'	11:2:2225:U:O4'	1.79	0.82
16:J:65:LEU:O	16:J:68:ALA:HB3	1.79	0.82
11:2:2253:G:H5'	18:Y:13:C:HO2'	1.45	0.82
11:2:2268:U:H2'	11:2:2269:U:C5	2.14	0.81
18:Y:46:G:H4'	18:Y:47:U:C5	2.12	0.81
12:3:2482:U:O4	15:B:101:LYS:CA	2.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:120:VAL:O	18:W:56:C:O3'	1.91	0.81
9:L:3:VAL:HG12	9:L:4:GLY:H	1.45	0.81
11:2:2285:C:C5	11:2:2286:U:C2	2.68	0.81
13:9:2678:A:H8	13:9:2679:A:N3	1.79	0.81
13:9:2680:A:H3'	13:9:2681:U:H5'	1.62	0.81
9:L:62:GLN:HB3	9:L:63:PRO:HD3	1.63	0.81
9:L:75:LEU:HD21	9:L:82:ILE:HD12	1.63	0.81
9:L:24:TRP:CH2	9:L:33:LEU:HD13	2.16	0.81
11:2:2271:A:H2'	11:2:2272:G:C5'	2.11	0.80
11:2:2253:G:H3'	11:2:2254:U:C5	2.16	0.80
13:9:2676:A:H4'	13:9:2677:G:C8	2.15	0.80
11:2:2272:G:H4'	11:2:2273:G:OP1	1.81	0.79
9:L:40:ASN:HB2	9:L:41:PRO:HD2	1.62	0.79
14:7:2842:U:O2	14:7:2842:U:H2'	1.82	0.79
13:9:2680:A:OP1	13:9:2681:U:H5	1.65	0.79
18:Y:46:G:O3'	18:Y:47:U:H6	1.66	0.79
13:9:2680:A:OP1	13:9:2681:U:C5	2.36	0.79
11:2:2245:C:H2'	11:2:2246:G:O4'	1.83	0.78
8:S:55:SER:HB2	8:S:58:TYR:CD2	2.18	0.78
14:7:2837:A:H2'	14:7:2845:A:N1	1.98	0.78
9:L:62:GLN:HB3	9:L:63:PRO:CD	2.14	0.78
15:B:177:ASP:O	15:B:181:ASN:CB	2.31	0.78
15:B:45:ARG:CB	18:W:54:U:H4'	2.14	0.78
16:J:181:TYR:O	16:J:184:LYS:N	2.16	0.78
11:2:2293:C:C5	11:2:2294:U:C5	2.72	0.78
14:7:2825:C:H5'	14:7:2826:U:OP2	1.83	0.78
13:9:2682:C:N3	13:9:2683:U:C5	2.52	0.78
18:W:46:G:O3'	18:W:47:U:H6	1.66	0.78
12:3:2482:U:C4	15:B:101:LYS:CB	2.67	0.78
12:3:2484:A:C5'	15:B:123:LEU:N	2.45	0.78
13:9:2680:A:H3'	13:9:2681:U:C5'	2.13	0.78
11:2:2269:U:O2	11:2:2269:U:H2'	1.84	0.78
11:2:2286:U:C4	11:2:2288:G:H1'	2.18	0.78
11:2:2251:G:C1'	11:2:2252:A:OP1	2.32	0.77
9:L:92:LEU:O	9:L:92:LEU:HD12	1.84	0.77
14:7:2838:A:C2	14:7:2851:A:C4	2.72	0.77
10:X:50:LEU:HD23	10:X:57:ARG:HH12	1.47	0.77
9:L:96:ALA:HB3	9:L:99:ASP:OD2	1.85	0.77
14:7:2863:G:C5'	18:Y:75:C:C4'	2.44	0.77
12:3:2485:A:H5'	15:B:129:SER:N	1.89	0.77
18:W:53:G:O2'	18:W:54:U:H5'	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:9:2676:A:O2'	13:9:2677:G:H5''	1.85	0.77
11:2:2215:A:C2	11:2:2216:G:C8	2.73	0.77
13:9:2675:C:H5	13:9:2676:A:C6	2.03	0.76
14:7:2858:U:H2'	14:7:2859:U:C5	2.20	0.76
18:Y:53:G:O2'	18:Y:54:U:H5'	1.84	0.76
11:2:2253:G:H3'	11:2:2254:U:C6	2.20	0.76
13:9:2676:A:H2	13:9:2680:A:C6	2.03	0.76
11:2:2253:G:C6	11:2:2254:U:C2	2.73	0.76
12:3:2483:G:O6	15:B:128:LEU:CB	2.34	0.76
11:2:2280:A:C5	11:2:2282:U:H5	2.02	0.76
10:X:34:ARG:NH1	10:X:34:ARG:HB3	2.00	0.76
12:3:2481:G:N7	15:B:102:LYS:CA	2.36	0.76
14:7:2834:G:C4	14:7:2835:U:C5	2.74	0.75
18:W:14:A:C2	18:W:37:A:C5	33.65	0.75
13:9:2676:A:H2	13:9:2680:A:N1	1.85	0.75
15:B:44:GLN:CB	18:W:55:U:OP1	2.34	0.75
8:S:46:THR:HG23	8:S:89:ILE:HD13	1.67	0.75
8:S:97:GLY:O	8:S:112:VAL:HG23	1.86	0.75
12:3:2483:G:H5'	15:B:96:ASN:CB	2.16	0.75
14:7:2829:U:H2'	14:7:2830:G:H5'	1.67	0.75
11:2:2260:U:H2'	11:2:2261:G:N7	2.02	0.75
11:2:2278:C:N4	11:2:2305:G:C8	2.55	0.75
9:L:52:VAL:HG13	9:L:71:VAL:CG1	2.17	0.75
11:2:2287:C:C2	11:2:2298:U:O2	2.40	0.75
8:S:38:LEU:HB3	8:S:42:PHE:HE1	1.52	0.75
11:2:2279:A:H4'	11:2:2280:A:H5'	1.69	0.74
13:9:2673:A:H61	13:9:2681:U:H3	1.34	0.74
11:2:2249:G:H2'	11:2:2250:G:C1'	2.17	0.74
9:L:116:ILE:CG2	9:L:119:VAL:HB	2.13	0.74
11:2:2280:A:C5	11:2:2282:U:C5	2.76	0.74
11:2:2257:C:H3'	11:2:2258:U:H6	1.52	0.74
8:S:55:SER:HB2	8:S:58:TYR:HD2	1.50	0.74
11:2:2270:A:C2	11:2:2271:A:C4	2.76	0.74
12:3:2484:A:N7	18:W:57:A:C4	2.40	0.74
12:3:2484:A:N7	18:W:19:G:N1	2.35	0.74
16:J:69:ARG:O	16:J:72:ALA:HB3	1.88	0.73
18:Y:17:C:C6	18:Y:17(A):U:H5	2.02	0.73
18:W:21:A:N6	18:W:46:G:H2'	1.99	0.73
11:2:2296:A:O2'	11:2:2297:U:H5'	1.87	0.73
10:X:50:LEU:HD23	10:X:57:ARG:NH1	2.03	0.73
16:J:177:ASP:HA	16:J:178:ARG:C	2.09	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:63:HIS:O	10:X:65:GLY:N	2.21	0.73
14:7:2854:U:H5'	16:J:160:PRO:HA	1.68	0.73
14:7:2872:A:C4'	14:7:2873:U:OP1	2.35	0.73
18:W:6:G:H1	18:W:67:C:H42	1.36	0.73
13:9:2680:A:OP2	13:9:2681:U:C4	2.42	0.73
14:7:2854:U:O2'	14:7:2855:U:H5'	1.89	0.73
18:W:14:A:N3	18:W:37:A:N1	32.98	0.73
14:7:2863:G:O5'	18:Y:75:C:O3'	2.06	0.73
11:2:2279:A:O5'	11:2:2280:A:H5''	1.88	0.73
18:W:5:G:N2	18:W:69:C:C2	2.57	0.73
12:3:2483:G:C2	15:B:97:LYS:HA	2.22	0.73
16:J:155:ALA:O	16:J:158:LYS:N	2.21	0.73
11:2:2293:C:H5	11:2:2294:U:C5	2.05	0.72
5:G:1430:C:O2'	5:G:1431:A:H5'	1.87	0.72
11:2:2266:U:N3	11:2:2267:C:N4	2.36	0.72
11:2:2294:U:H5'	11:2:2295:A:OP2	1.90	0.72
18:W:68:C:H2'	18:W:69:C:C6	2.25	0.72
9:L:101:VAL:CG1	9:L:123:VAL:HG13	2.18	0.72
11:2:2281:A:O2'	11:2:2282:U:H5''	1.90	0.72
11:2:2289:U:O2'	11:2:2290:C:H5'	1.88	0.72
18:Y:21:A:N6	18:Y:46:G:H2'	1.99	0.72
13:9:2678:A:O4'	13:9:2679:A:H2	1.72	0.72
12:3:2483:G:O6	15:B:100:ILE:CB	2.37	0.72
10:X:63:HIS:C	10:X:65:GLY:H	1.93	0.72
11:2:2222:A:HO2'	11:2:2223:A:H8	1.31	0.72
11:2:2278:C:H2'	11:2:2279:A:H5''	1.70	0.72
11:2:2288:G:C4	11:2:2289:U:C5	2.78	0.72
9:L:69:LYS:NZ	9:L:69:LYS:HB3	2.04	0.72
18:Y:6:G:H1	18:Y:67:C:H42	1.36	0.72
13:9:2676:A:C2	13:9:2680:A:C6	2.78	0.71
18:Y:20:U:H3'	18:Y:21:A:H5'	1.72	0.71
12:3:2482:U:H5''	15:B:94:ASN:N	2.06	0.71
8:S:46:THR:HG23	8:S:89:ILE:CD1	2.19	0.71
13:9:2673:A:H2	13:9:2674:A:C5	2.08	0.71
11:2:2271:A:C3'	11:2:2272:G:H5''	2.20	0.71
18:W:17:C:C6	18:W:17(A):U:H5	2.02	0.71
14:7:2852:C:C5	14:7:2853:A:C4	2.78	0.71
9:L:19:ARG:HH12	9:L:22:GLN:HB2	1.54	0.71
18:Y:68:C:H2'	18:Y:69:C:C6	2.25	0.71
13:9:2682:C:H5'	13:9:2683:U:OP2	1.87	0.71
12:3:2483:G:N7	15:B:127:GLN:CB	2.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:5:G:N2	18:Y:69:C:C2	2.57	0.71
14:7:2853:A:C6	14:7:2854:U:N3	2.58	0.71
11:2:2267:C:H2'	11:2:2268:U:O4'	1.90	0.71
11:2:2269:U:C6	11:2:2272:G:O6	2.44	0.71
11:2:2294:U:O2	11:2:2296:A:H2'	1.90	0.71
8:S:16:LYS:O	8:S:16:LYS:HG3	1.90	0.71
14:7:2863:G:C5	18:Y:76:A:O3'	2.43	0.71
18:Y:3:C:H2'	18:Y:4:G:H5'	1.73	0.70
8:S:98:ILE:O	8:S:98:ILE:HG13	1.90	0.70
18:W:20:U:H3'	18:W:21:A:H5'	1.72	0.70
11:2:2301:U:H2'	11:2:2302:G:H8	1.55	0.70
15:B:121:PRO:O	18:W:57:A:O4'	2.10	0.70
14:7:2834:G:N3	14:7:2835:U:C6	2.59	0.70
12:3:2482:U:O5'	15:B:95:LYS:N	2.23	0.70
14:7:2834:G:O2'	14:7:2835:U:O5'	2.08	0.70
13:9:2676:A:H2	13:9:2680:A:C2	2.09	0.70
12:3:2484:A:C5'	15:B:122:ARG:CA	2.57	0.70
14:7:2847:A:H3'	14:7:2848:G:H8	1.55	0.70
14:7:2854:U:OP1	16:J:160:PRO:CB	2.40	0.70
11:2:2295:A:N6	11:2:2296:A:N6	2.40	0.70
18:W:3:C:H2'	18:W:4:G:H5'	1.73	0.70
12:3:2483:G:C6	15:B:100:ILE:CB	2.75	0.70
11:2:2284:C:H2'	11:2:2285:C:O2	1.90	0.70
11:2:2218:G:O2'	11:2:2219:A:H5'	1.92	0.70
13:9:2673:A:H2	13:9:2674:A:C6	2.09	0.69
11:2:2256:A:O2'	11:2:2257:C:P	2.49	0.69
9:L:58:ILE:HG21	9:L:117:PRO:CG	2.22	0.69
14:7:2846:U:O2	14:7:2850:G:O6	2.09	0.69
13:9:2678:A:H8	13:9:2679:A:C2	2.04	0.69
16:J:161:GLY:CA	16:J:162:GLN:CB	2.69	0.69
8:S:100:GLY:HA2	8:S:108:VAL:O	1.92	0.69
12:3:2481:G:H3'	15:B:99:LEU:O	1.92	0.69
11:2:2252:A:C2	11:2:2253:G:C5	2.81	0.69
11:2:2253:G:C8	11:2:2254:U:C5	2.81	0.69
14:7:2872:A:H4'	14:7:2873:U:OP1	1.91	0.69
14:7:2837:A:C8	14:7:2845:A:C2	2.81	0.69
11:2:2287:C:N3	11:2:2298:U:O2	2.25	0.69
13:9:2684:C:C2	13:9:2685:C:C6	2.80	0.69
12:3:2485:A:H5'	15:B:129:SER:H	1.57	0.69
8:S:33:LEU:HD11	8:S:59:ALA:HA	1.74	0.69
13:9:2677:G:N1	13:9:2679:A:C5	2.60	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:2481:G:N7	15:B:102:LYS:N	2.39	0.69
14:7:2861:U:H2'	14:7:2862:U:H6	1.58	0.69
11:2:2222:A:O2'	11:2:2223:A:C8	2.46	0.69
11:2:2221:G:N2	11:2:2225:U:N3	2.41	0.69
11:2:2285:C:H5	11:2:2286:U:N3	1.90	0.69
11:2:2207:A:H8	11:2:2237:C:O2	1.75	0.68
9:L:19:ARG:O	9:L:23:ARG:HB2	1.92	0.68
18:Y:20:U:C3'	18:Y:21:A:H5'	2.23	0.68
12:3:2483:G:N9	15:B:127:GLN:CB	2.56	0.68
11:2:2259:A:H3'	11:2:2260:U:H6	1.57	0.68
9:L:112:ALA:HB2	9:L:119:VAL:O	1.92	0.68
11:2:2196:C:N4	11:2:2242:A:N7	2.40	0.68
18:Y:20:U:C2	18:Y:37:A:C2	40.09	0.68
11:2:2249:G:O4'	11:2:2272:G:H8	1.76	0.68
12:3:2482:U:O2	15:B:97:LYS:CB	2.29	0.68
11:2:2239:G:O2'	11:2:2240:G:H5'	1.93	0.68
18:W:20:U:C3'	18:W:21:A:H5'	2.23	0.68
14:7:2826:U:C2'	14:7:2827:U:H5'	2.22	0.68
14:7:2841:G:C6	14:7:2844:C:C4	2.82	0.68
13:9:2673:A:C2	13:9:2674:A:C5	2.81	0.68
16:J:37:GLY:HA3	16:J:86:HIS:H	1.58	0.68
18:Y:68:C:H2'	18:Y:69:C:H6	1.58	0.67
16:J:75:TYR:O	16:J:76:MET:C	2.32	0.67
13:9:2682:C:C4	13:9:2683:U:C5	2.82	0.67
13:9:2682:C:C4	13:9:2683:U:H5	2.12	0.67
11:2:2294:U:O2	11:2:2294:U:H2'	1.92	0.67
5:G:1429:G:OP2	5:G:1430:C:H5	1.78	0.67
13:9:2684:C:C2	13:9:2685:C:C5	2.82	0.67
11:2:2251:G:N3	11:2:2252:A:C8	2.63	0.67
11:2:2249:G:O4'	11:2:2272:G:C8	2.48	0.67
11:2:2226:U:HO2'	11:2:2227:C:H6	1.41	0.67
13:9:2684:C:O2'	13:9:2685:C:O4'	2.11	0.67
18:W:68:C:H2'	18:W:69:C:H6	1.58	0.67
9:L:58:ILE:CG2	9:L:117:PRO:HG3	2.24	0.67
14:7:2858:U:H2'	14:7:2859:U:C6	2.30	0.67
11:2:2295:A:C5	11:2:2296:A:N6	2.63	0.67
18:W:75:C:C6	18:W:76:A:N7	2.63	0.67
14:7:2853:A:H4'	16:J:159:PHE:H	1.59	0.67
11:2:2269:U:C4	11:2:2272:G:N1	2.61	0.67
11:2:2222:A:O2'	11:2:2223:A:H8	1.78	0.67
18:W:14:A:C2	18:W:36:U:N3	37.52	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:17:C:C5'	18:W:17(A):U:H6	2.01	0.66
11:2:2279:A:C8	11:2:2288:G:C6	2.83	0.66
11:2:2295:A:C6	11:2:2296:A:N6	2.62	0.66
11:2:2255:A:N7	18:Y:25:C:O2'	2.29	0.66
18:Y:75:C:C6	18:Y:76:A:N7	2.63	0.66
13:9:2673:A:N1	13:9:2676:A:C8	2.63	0.66
11:2:2282:U:H5'	11:2:2282:U:C6	2.30	0.66
11:2:2299:A:C4	11:2:2300:G:C8	2.84	0.66
14:7:2836:C:H5	14:7:2853:A:N1	1.93	0.66
11:2:2280:A:C6	11:2:2282:U:C5	2.83	0.66
9:L:34:LEU:O	9:L:36:SER:N	2.29	0.66
11:2:2221:G:H3'	11:2:2221:G:C8	2.31	0.66
18:W:46:G:O3'	18:W:47:U:C6	2.47	0.66
18:Y:75:C:C5	18:Y:76:A:N7	2.64	0.66
18:Y:17:C:C5'	18:Y:17(A):U:H6	2.01	0.66
11:2:2276:G:C6	11:2:2277:C:C4	2.84	0.66
9:L:52:VAL:HG13	9:L:71:VAL:HG13	1.77	0.66
11:2:2254:U:H2'	11:2:2261:G:H1	1.60	0.66
14:7:2868:U:H2'	14:7:2869:U:H6	1.61	0.66
18:W:75:C:C5	18:W:76:A:N7	2.64	0.66
8:S:132:THR:HG22	8:S:133:HIS:H	1.61	0.66
13:9:2673:A:C2	13:9:2674:A:C6	2.84	0.65
11:2:2262:A:H5''	11:2:2263:C:H5'	1.76	0.65
11:2:2223:A:C2	11:2:2224:A:C4	2.84	0.65
11:2:2225:U:O2'	11:2:2226:U:H5'	1.95	0.65
18:W:75:C:C6	18:W:76:A:H8	2.14	0.65
11:2:2288:G:C6	11:2:2289:U:O4	2.50	0.65
16:J:146:ASP:O	16:J:147:VAL:O	2.14	0.65
18:Y:46:G:O3'	18:Y:47:U:C6	2.47	0.65
11:2:2194:G:C2'	11:2:2195:C:H5'	2.27	0.65
9:L:53:THR:O	9:L:54:GLU:HB3	1.96	0.65
18:W:61:C:O2'	18:W:62:C:H5'	1.97	0.65
13:9:2676:A:C2	13:9:2680:A:N1	2.64	0.65
11:2:2254:U:O2	11:2:2261:G:C2	2.50	0.65
9:L:69:LYS:NZ	9:L:92:LEU:HD23	2.12	0.65
14:7:2830:G:C8	18:Y:76:A:N1	2.65	0.64
8:S:42:PHE:CE2	8:S:118:GLY:HA2	2.32	0.64
15:B:53:LEU:CB	15:B:54:LYS:HA	2.26	0.64
16:J:184:LYS:C	16:J:186:GLU:H	2.00	0.64
8:S:14:ARG:HB3	8:S:114:PHE:CD2	2.31	0.64
9:L:54:GLU:OE2	9:L:56:ILE:HD11	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:133:ALA:O	9:L:139:LYS:HB2	1.98	0.64
13:9:2676:A:C4'	13:9:2677:G:C8	2.80	0.64
5:G:1429:G:N3	5:G:1429:G:H2'	2.11	0.64
8:S:91:ILE:HG23	8:S:92:PRO:HD2	1.80	0.64
15:B:120:VAL:O	18:W:56:C:H4'	1.98	0.64
11:2:2251:G:N2	11:2:2252:A:C4	2.66	0.64
9:L:19:ARG:HH11	9:L:19:ARG:CA	2.08	0.64
18:Y:61:C:O2'	18:Y:62:C:H5'	1.96	0.64
11:2:2253:G:C5	11:2:2254:U:C4	2.86	0.64
11:2:2276:G:C6	11:2:2277:C:C5	2.86	0.64
11:2:2285:C:C5	11:2:2286:U:N3	2.66	0.64
14:7:2864:A:C5	14:7:2865:U:C5	2.86	0.64
18:W:3:C:H42	18:W:70:G:H1	1.45	0.64
11:2:2197:C:N4	11:2:2241:U:H2'	2.13	0.64
10:X:66:LYS:HD2	10:X:69:LYS:HD2	1.79	0.64
18:Y:47:U:H3'	18:Y:48:C:H5'	1.80	0.64
11:2:2255:A:C2	11:2:2260:U:O4	2.51	0.64
11:2:2278:C:C2'	11:2:2279:A:H5''	2.27	0.64
11:2:2259:A:H5''	11:2:2260:U:H5	1.63	0.63
18:W:47:U:H3'	18:W:48:C:H5'	1.80	0.63
11:2:2289:U:C2	11:2:2290:C:C5	2.86	0.63
11:2:2262:A:N3	11:2:2263:C:H5''	2.13	0.63
16:J:175:ASN:CB	16:J:176:LEU:HA	2.27	0.63
11:2:2246:G:C2	11:2:2247:G:C8	2.86	0.63
15:B:101:LYS:O	15:B:105:LYS:N	2.31	0.63
11:2:2211:U:H2'	11:2:2212:C:O4'	1.99	0.63
13:9:2677:G:N2	13:9:2679:A:C4	2.67	0.63
9:L:86:VAL:HG12	9:L:91:CYS:HB3	1.80	0.63
14:7:2830:G:C4	14:7:2831:G:C8	2.86	0.63
14:7:2830:G:H5'	18:Y:76:A:C6	2.33	0.63
14:7:2830:G:O2'	14:7:2831:G:H5'	1.98	0.63
5:G:1430:C:O2'	5:G:1431:A:C5'	2.47	0.63
16:J:144:ASN:O	16:J:147:VAL:CB	2.47	0.63
16:J:87:LEU:HA	16:J:138:VAL:CB	2.29	0.63
14:7:2828:G:C6	18:Y:76:A:C1'	2.56	0.63
11:2:2294:U:C5'	11:2:2295:A:OP2	2.47	0.63
16:J:191:LYS:HA	16:J:192:ASP:CB	2.27	0.63
12:3:2484:A:C4	18:W:57:A:N7	2.51	0.63
9:L:117:PRO:HG2	9:L:118:GLY:H	1.61	0.63
11:2:2277:C:O2'	11:2:2278:C:O5'	2.13	0.63
11:2:2279:A:N1	11:2:2283:G:N2	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:58:TYR:O	8:S:62:VAL:HG23	1.99	0.63
16:J:20:SER:O	16:J:22:TYR:N	2.32	0.63
12:3:2482:U:C1'	15:B:97:LYS:H	2.11	0.62
11:2:2279:A:H2	11:2:2285:C:H41	1.46	0.62
9:L:60:SER:OG	9:L:64:ASN:HB2	1.99	0.62
9:L:78:ASN:HD21	9:L:80:LYS:HG3	1.64	0.62
11:2:2251:G:C6	11:2:2266:U:O2	2.52	0.62
18:Y:71:C:O2	18:Y:71:C:C2'	2.41	0.62
8:S:83:THR:HG23	8:S:85:TYR:H	1.64	0.62
11:2:2289:U:C2'	11:2:2290:C:H5'	2.29	0.62
11:2:2301:U:H2'	11:2:2302:G:C8	2.32	0.62
15:B:95:LYS:HA	15:B:100:ILE:N	2.15	0.62
18:Y:75:C:C6	18:Y:76:A:H8	2.14	0.62
14:7:2839:G:C5	14:7:2850:G:N2	2.68	0.62
8:S:31:GLU:HG3	8:S:32:LYS:H	1.63	0.62
11:2:2209:U:C6	11:2:2209:U:OP2	2.52	0.62
13:9:2681:U:O2'	13:9:2682:C:H5''	1.99	0.62
11:2:2249:G:C4	11:2:2272:G:N7	2.67	0.62
9:L:101:VAL:HG13	9:L:123:VAL:HG13	1.81	0.62
9:L:97:GLU:O	9:L:98:ASN:HB2	1.99	0.62
9:L:6:PRO:HG2	9:L:15:LEU:HD21	1.81	0.62
12:3:2486:A:N7	15:B:97:LYS:O	2.33	0.62
12:3:2486:A:N7	15:B:98:LYS:HA	1.97	0.62
14:7:2857:C:H2'	14:7:2858:U:H6	1.65	0.62
11:2:2279:A:H2	11:2:2285:C:N4	1.98	0.62
8:S:78:PRO:HB2	8:S:98:ILE:HG12	1.82	0.62
16:J:97:LEU:O	16:J:123:HIS:N	2.32	0.62
13:9:2682:C:C2	13:9:2683:U:C5	2.88	0.62
8:S:86:ARG:NH1	8:S:122:ALA:HB1	2.15	0.62
8:S:24:LEU:HG	8:S:37:GLU:HB3	1.81	0.62
13:9:2678:A:H3'	13:9:2679:A:N3	2.14	0.62
16:J:77:THR:O	16:J:79:VAL:N	2.32	0.62
12:3:2486:A:OP1	15:B:131:ALA:C	2.36	0.61
14:7:2830:G:H1	14:7:2858:U:H3	1.48	0.61
11:2:2214:A:H2'	11:2:2215:A:H8	1.64	0.61
8:S:124:PHE:N	8:S:124:PHE:CD1	2.68	0.61
18:Y:3:C:H42	18:Y:70:G:H1	1.45	0.61
10:X:44:ARG:HG3	10:X:45:TYR:N	2.14	0.61
11:2:2235:C:C4	11:2:2236:G:C6	2.89	0.61
13:9:2678:A:H5''	13:9:2679:A:C2	2.35	0.61
12:3:2481:G:H3'	15:B:102:LYS:CB	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2215:A:N3	11:2:2216:G:C8	2.68	0.61
14:7:2863:G:C8	18:Y:76:A:H4'	2.36	0.61
15:B:45:ARG:CB	18:W:54:U:C5'	2.77	0.61
9:L:62:GLN:CB	9:L:63:PRO:CD	2.78	0.61
15:B:95:LYS:CB	15:B:124:LEU:HA	2.31	0.61
11:2:2197:C:H4'	11:2:2198:A:C8	2.35	0.61
11:2:2270:A:C2	11:2:2271:A:N3	2.69	0.61
10:X:50:LEU:CD2	10:X:57:ARG:HH12	2.13	0.61
14:7:2847:A:C4	14:7:2848:G:C8	2.88	0.61
13:9:2675:C:C5	13:9:2676:A:C6	2.88	0.60
13:9:2678:A:C8	13:9:2679:A:N3	2.66	0.60
11:2:2255:A:C8	18:Y:25:C:O2'	2.51	0.60
12:3:2483:G:C5	15:B:100:ILE:CB	2.85	0.60
11:2:2258:U:O2	11:2:2258:U:H2'	2.01	0.60
14:7:2831:G:C6	14:7:2832:C:C4	2.90	0.60
16:J:61:SER:HA	16:J:126:ALA:CB	2.31	0.60
16:J:12:GLN:O	16:J:14:ASN:N	2.34	0.60
14:7:2851:A:H3'	14:7:2852:C:H5''	1.82	0.60
13:9:2674:A:H2'	13:9:2674:A:N3	2.16	0.60
11:2:2258:U:H3'	11:2:2259:A:H8	1.66	0.60
16:J:159:PHE:O	16:J:161:GLY:N	2.34	0.60
18:W:52:G:C2	18:W:53:G:C8	2.90	0.60
11:2:2219:A:C2'	11:2:2220:A:H5'	2.31	0.60
11:2:2219:A:H2'	11:2:2220:A:H5'	1.83	0.60
15:B:54:LYS:HA	15:B:55:LEU:CB	2.31	0.60
14:7:2859:U:H4'	14:7:2860:U:OP1	2.01	0.60
18:W:14:A:H1'	18:W:22:G:N2	2.17	0.60
12:3:2483:G:N7	15:B:100:ILE:CB	2.65	0.60
14:7:2830:G:N7	18:Y:76:A:N1	2.49	0.60
18:Y:52:G:C2	18:Y:53:G:C8	2.90	0.60
8:S:69:LYS:HZ1	8:S:94:LEU:C	2.05	0.60
18:Y:14:A:H1'	18:Y:22:G:N2	2.17	0.60
14:7:2869:U:H2'	14:7:2869:U:O2	2.00	0.60
15:B:55:LEU:N	15:B:186:SER:HA	2.17	0.60
9:L:116:ILE:HG23	9:L:117:PRO:HD2	1.84	0.59
11:2:2280:A:H4'	11:2:2281:A:OP1	2.02	0.59
11:2:2290:C:C2	11:2:2303:A:C2	2.90	0.59
14:7:2834:G:O2'	14:7:2835:U:C6	2.41	0.59
9:L:47:HIS:ND1	9:L:104:ALA:HB2	2.17	0.59
8:S:73:PRO:C	8:S:75:GLY:H	2.05	0.59
11:2:2204:C:H6	11:2:2204:C:O5'	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:38:LYS:O	16:J:39:LYS:O	2.20	0.59
11:2:2253:G:H5'	18:Y:13:C:C2'	2.30	0.59
14:7:2861:U:H2'	14:7:2862:U:O4'	2.02	0.59
10:X:63:HIS:C	10:X:65:GLY:N	2.56	0.59
18:W:17:C:C6	18:W:17(A):U:C5	2.83	0.59
8:S:83:THR:HG23	8:S:85:TYR:N	2.18	0.59
15:B:188:ASN:C	15:B:190:PHE:H	2.05	0.59
11:2:2269:U:O2	11:2:2269:U:C2'	2.50	0.59
14:7:2836:C:O2	14:7:2836:C:C2'	2.51	0.59
8:S:69:LYS:HE2	8:S:97:GLY:N	2.17	0.59
11:2:2253:G:C8	11:2:2254:U:C4	2.91	0.59
18:W:14:A:C4	18:W:37:A:N6	33.25	0.59
14:7:2829:U:O2'	18:Y:75:C:C5	2.44	0.59
13:9:2677:G:N2	13:9:2678:A:H5'	2.18	0.59
13:9:2681:U:O2'	13:9:2682:C:P	2.61	0.59
18:Y:75:C:H2'	18:Y:76:A:H8	1.66	0.59
11:2:2202:C:O2	11:2:2202:C:H2'	2.02	0.59
14:7:2853:A:OP1	16:J:67:ALA:HB2	2.03	0.59
9:L:78:ASN:ND2	9:L:80:LYS:CG	2.66	0.59
8:S:66:ARG:NH1	8:S:93:GLU:HB3	2.17	0.59
14:7:2842:U:O2	14:7:2842:U:C2'	2.49	0.59
11:2:2260:U:C2'	11:2:2261:G:N7	2.65	0.58
11:2:2226:U:O2'	11:2:2227:C:H6	1.86	0.58
18:W:75:C:H2'	18:W:76:A:H8	1.66	0.58
10:X:31:PRO:HG3	10:X:39:ILE:HD11	1.83	0.58
14:7:2853:A:N6	14:7:2854:U:H3	2.00	0.58
13:9:2677:G:N3	13:9:2677:G:H3'	2.19	0.58
12:3:2482:U:N1	15:B:97:LYS:N	2.34	0.58
11:2:2299:A:C5	11:2:2300:G:N7	2.71	0.58
13:9:2684:C:C2'	13:9:2685:C:H6	2.00	0.58
12:3:2483:G:C4	15:B:97:LYS:HA	2.30	0.58
11:2:2244:A:O2'	11:2:2245:C:H5'	2.04	0.58
18:Y:74:C:O2'	18:Y:75:C:H4'	2.03	0.58
18:Y:30:G:N2	18:Y:31:G:H1'	2.19	0.58
8:S:36:ASP:O	8:S:39:ALA:HB3	2.03	0.58
16:J:53:VAL:H	16:J:164:LYS:CB	2.17	0.58
18:Y:75:C:H2'	18:Y:76:A:C8	2.38	0.58
8:S:132:THR:HG22	8:S:133:HIS:N	2.18	0.58
16:J:68:ALA:O	16:J:72:ALA:HB2	2.04	0.58
11:2:2285:C:C5	11:2:2286:U:C4	2.91	0.58
9:L:54:GLU:HG3	9:L:56:ILE:HG13	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2288:G:N3	11:2:2289:U:C5	2.72	0.58
18:W:3:C:C2'	18:W:4:G:H5'	2.34	0.58
18:W:74:C:O2'	18:W:75:C:H4'	2.03	0.58
16:J:91:VAL:O	16:J:92:HIS:CB	2.51	0.58
11:2:2196:C:O2'	11:2:2271:A:O4'	2.22	0.58
14:7:2836:C:O2	14:7:2837:A:C8	2.57	0.58
10:X:34:ARG:HH11	10:X:34:ARG:HB3	1.66	0.58
14:7:2849:C:H2'	14:7:2849:C:O2	2.03	0.58
11:2:2199:G:C6	11:2:2200:U:C4	2.92	0.58
11:2:2248:C:C4'	11:2:2271:A:H2	2.17	0.58
18:Y:4:G:O2'	18:Y:5:G:C8	2.56	0.58
8:S:95:VAL:HG21	8:S:117:ILE:HD11	1.85	0.58
16:J:174:THR:O	16:J:175:ASN:C	2.42	0.58
11:2:2260:U:H3'	11:2:2261:G:C8	2.39	0.57
18:W:30:G:N2	18:W:31:G:H1'	2.18	0.57
11:2:2294:U:C6	11:2:2297:U:H5	2.20	0.57
14:7:2827:U:O2	14:7:2827:U:H2'	2.02	0.57
13:9:2675:C:H5	13:9:2676:A:N6	2.02	0.57
11:2:2253:G:H3'	11:2:2254:U:H5	1.69	0.57
11:2:2269:U:N3	11:2:2272:G:N1	2.45	0.57
11:2:2285:C:H5	11:2:2286:U:N1	2.02	0.57
9:L:71:VAL:HG23	9:L:86:VAL:CG2	2.34	0.57
9:L:37:ARG:HG2	9:L:44:GLY:HA2	1.86	0.57
12:3:2482:U:C5'	15:B:95:LYS:N	2.68	0.57
11:2:2194:G:H1'	11:2:2274:U:O2	2.04	0.57
11:2:2290:C:H2'	11:2:2291:A:H8	1.70	0.57
11:2:2202:C:H5''	11:2:2203:U:OP2	2.04	0.57
11:2:2261:G:N2	11:2:2263:C:C4	2.72	0.57
9:L:101:VAL:HA	9:L:125:CYS:O	2.04	0.57
9:L:51:LEU:HD21	9:L:76:ARG:HE	1.70	0.57
13:9:2677:G:H2'	13:9:2678:A:O5'	2.05	0.57
12:3:2484:A:H5''	15:B:123:LEU:N	2.18	0.57
11:2:2287:C:O2	11:2:2298:U:O2	2.22	0.57
18:W:4:G:O2'	18:W:5:G:C8	2.56	0.57
10:X:42:ASN:HA	10:X:46:ALA:HB2	1.87	0.57
18:W:75:C:H2'	18:W:76:A:C8	2.38	0.57
16:J:135:ILE:O	16:J:137:SER:N	2.38	0.57
11:2:2253:G:C5	11:2:2254:U:N3	2.72	0.57
11:2:2270:A:C8	11:2:2270:A:C5'	2.76	0.57
18:Y:3:C:C2'	18:Y:4:G:H5'	2.34	0.57
15:B:45:ARG:CB	18:W:54:U:C4'	2.81	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:29:G:O2'	18:Y:30:G:H5'	2.05	0.57
16:J:7:ARG:C	16:J:9:TYR:H	2.07	0.57
13:9:2675:C:C5	13:9:2676:A:N6	2.72	0.57
11:2:2210:G:C6	11:2:2211:U:C4	2.92	0.57
11:2:2288:G:C2	11:2:2289:U:C4	2.93	0.57
13:9:2686:A:H8	13:9:2686:A:O5'	1.88	0.57
9:L:81:LYS:O	9:L:81:LYS:HD2	2.05	0.57
11:2:2299:A:C6	11:2:2300:G:C8	2.93	0.56
10:X:38:ARG:HG2	10:X:42:ASN:HD21	1.69	0.56
13:9:2676:A:C2	13:9:2680:A:C2	2.93	0.56
11:2:2265:C:N4	11:2:2266:U:N3	2.53	0.56
18:Y:17:C:C6	18:Y:17(A):U:C5	2.83	0.56
11:2:2204:C:H2'	11:2:2205:U:H5''	1.86	0.56
11:2:2210:G:C6	11:2:2236:G:N2	2.73	0.56
8:S:74:ALA:C	8:S:76:GLU:H	2.07	0.56
13:9:2678:A:OP2	13:9:2678:A:H4'	2.05	0.56
11:2:2246:G:N3	11:2:2247:G:C8	2.73	0.56
14:7:2856:G:H2'	14:7:2857:C:C6	2.39	0.56
10:X:58:LYS:HD3	10:X:62:TRP:CH2	2.40	0.56
14:7:2833:A:C6	14:7:2834:G:N7	2.74	0.56
11:2:2288:G:H2'	11:2:2289:U:C6	2.40	0.56
18:W:71:C:C2'	18:W:71:C:O2	2.41	0.56
9:L:34:LEU:O	9:L:35:GLY:C	2.44	0.56
11:2:2304:C:C4	11:2:2305:G:N2	2.72	0.56
13:9:2681:U:O2'	13:9:2682:C:C5'	2.54	0.56
16:J:121:LYS:O	16:J:122:PRO:C	2.42	0.56
12:3:2481:G:C5'	15:B:102:LYS:CB	2.78	0.56
14:7:2842:U:C6	14:7:2842:U:O5'	2.58	0.56
11:2:2286:U:C4	11:2:2288:G:C1'	2.88	0.56
10:X:34:ARG:HG2	10:X:34:ARG:O	2.04	0.56
11:2:2254:U:OP2	11:2:2254:U:C6	2.58	0.56
11:2:2283:G:H1'	11:2:2284:C:H5	1.70	0.56
14:7:2868:U:C5	14:7:2869:U:H5	2.24	0.56
14:7:2833:A:N1	14:7:2834:G:C8	2.74	0.56
18:W:14:A:C2	18:W:37:A:N6	33.36	0.56
16:J:146:ASP:O	16:J:147:VAL:C	2.43	0.56
9:L:56:ILE:HG22	9:L:57:GLY:N	2.20	0.56
11:2:2260:U:C3'	11:2:2261:G:C8	2.88	0.56
11:2:2266:U:C4	11:2:2267:C:N4	2.73	0.56
9:L:112:ALA:CB	9:L:119:VAL:O	2.53	0.56
11:2:2221:G:C3'	11:2:2221:G:C8	2.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:2484:A:C3'	15:B:127:GLN:CA	2.56	0.55
11:2:2260:U:H4'	11:2:2261:G:OP2	2.06	0.55
18:W:29:G:O2'	18:W:30:G:H5'	2.05	0.55
11:2:2223:A:O2'	11:2:2224:A:O5'	2.25	0.55
8:S:92:PRO:O	8:S:95:VAL:HG23	2.07	0.55
8:S:86:ARG:HB3	8:S:122:ALA:HB2	1.88	0.55
8:S:70:GLU:HG3	8:S:71:LYS:H	1.71	0.55
16:J:34:TYR:O	16:J:35:ASP:CB	2.54	0.55
11:2:2275:A:H3'	11:2:2276:G:O4'	2.06	0.55
8:S:31:GLU:HG3	8:S:32:LYS:HG2	1.88	0.55
11:2:2194:G:C1'	11:2:2274:U:O2	2.54	0.55
11:2:2215:A:C4	11:2:2216:G:C8	2.94	0.55
16:J:61:SER:HA	16:J:126:ALA:HB1	1.87	0.55
11:2:2247:G:C6	11:2:2248:C:C4	2.95	0.55
11:2:2260:U:C2'	11:2:2261:G:C8	2.89	0.55
8:S:49:ARG:HH22	8:S:87:SER:HB2	1.70	0.55
11:2:2295:A:H62	11:2:2296:A:N6	2.05	0.55
8:S:91:ILE:O	8:S:94:LEU:HB2	2.06	0.55
13:9:2677:G:N2	13:9:2679:A:N3	2.54	0.55
13:9:2677:G:H21	13:9:2678:A:H5'	1.72	0.55
11:2:2270:A:N1	11:2:2271:A:C2	2.75	0.55
11:2:2240:G:H2'	11:2:2241:U:O5'	2.07	0.55
11:2:2221:G:N2	11:2:2225:U:C2	2.75	0.55
11:2:2282:U:O2'	11:2:2283:G:C5'	2.54	0.55
8:S:66:ARG:HH12	8:S:93:GLU:CB	2.19	0.55
11:2:2265:C:N4	11:2:2266:U:C4	2.75	0.55
14:7:2862:U:O2	18:Y:75:C:H2'	2.06	0.55
11:2:2214:A:H2'	11:2:2215:A:C8	2.41	0.55
11:2:2280:A:C4	11:2:2282:U:H5	2.25	0.55
11:2:2290:C:O2'	11:2:2291:A:O4'	2.20	0.55
11:2:2217:U:O2'	11:2:2218:G:H5'	2.07	0.55
18:W:49:G:H1	18:W:65:C:H42	1.55	0.55
11:2:2290:C:C2	11:2:2291:A:C8	2.96	0.54
15:B:155:ILE:HA	15:B:156:LYS:CB	2.37	0.54
11:2:2196:C:C4	11:2:2242:A:N7	2.75	0.54
18:Y:23:C:O2'	18:Y:24:U:H5'	2.07	0.54
14:7:2847:A:C2	14:7:2848:G:H1'	2.42	0.54
18:W:62:C:H2'	18:W:63:G:O4'	2.07	0.54
14:7:2837:A:C8	14:7:2845:A:N1	2.75	0.54
11:2:2269:U:H2'	11:2:2270:A:H5'	1.89	0.54
14:7:2833:A:C6	14:7:2834:G:C8	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:7:THR:CG2	10:X:10:LYS:HB2	2.34	0.54
9:L:75:LEU:HD11	9:L:82:ILE:CD1	2.38	0.54
8:S:33:LEU:HD22	8:S:62:VAL:HG21	1.89	0.54
13:9:2682:C:N4	13:9:2683:U:O4	2.40	0.54
11:2:2269:U:C5	11:2:2272:G:O6	2.60	0.54
18:Y:49:G:H1	18:Y:65:C:H42	1.55	0.54
18:W:23:C:O2'	18:W:24:U:H5'	2.07	0.54
14:7:2836:C:O2	14:7:2836:C:H3'	2.08	0.54
14:7:2838:A:C2	14:7:2851:A:N9	2.76	0.54
11:2:2290:C:N3	11:2:2303:A:N1	2.56	0.54
18:Y:62:C:H2'	18:Y:63:G:O4'	2.07	0.54
16:J:7:ARG:C	16:J:9:TYR:N	2.61	0.54
16:J:207:GLU:O	16:J:208:ASN:C	2.46	0.54
13:9:2671:A:N6	13:9:2672:G:O6	2.40	0.54
14:7:2853:A:N6	14:7:2854:U:N3	2.56	0.54
11:2:2223:A:C2'	11:2:2224:A:C8	2.89	0.54
8:S:101:VAL:CG2	8:S:121:LEU:HD11	2.34	0.54
8:S:90:VAL:HB	8:S:117:ILE:HA	1.90	0.54
10:X:40:LEU:HA	10:X:43:ARG:HG2	1.90	0.54
8:S:82:LYS:HB3	8:S:107:PHE:CE2	2.43	0.54
15:B:192:SER:HA	15:B:197:ASN:O	2.06	0.54
9:L:132:LEU:HD21	9:L:136:LYS:HE3	1.89	0.54
11:2:2254:U:C5	11:2:2254:U:OP2	2.61	0.54
14:7:2834:G:HO2'	14:7:2835:U:H6	0.73	0.54
12:3:2482:U:H3'	15:B:95:LYS:CA	2.00	0.54
11:2:2261:G:N2	11:2:2263:C:N3	2.56	0.54
16:J:99:ILE:O	16:J:120:GLY:HA2	2.08	0.54
16:J:42:THR:C	16:J:44:ASP:H	2.12	0.54
18:W:47:U:H3'	18:W:48:C:C5'	2.37	0.54
14:7:2838:A:N1	14:7:2851:A:C8	2.75	0.54
13:9:2678:A:O4'	13:9:2679:A:C2	2.59	0.53
11:2:2259:A:H3'	11:2:2260:U:C5	2.42	0.53
14:7:2833:A:H2'	14:7:2833:A:N3	2.23	0.53
18:Y:47:U:H3'	18:Y:48:C:C5'	2.37	0.53
14:7:2861:U:C2	14:7:2862:U:C6	2.96	0.53
14:7:2834:G:N3	14:7:2835:U:C5	2.76	0.53
9:L:6:PRO:HG2	9:L:15:LEU:CD2	2.38	0.53
18:Y:7:G:H8	18:Y:7:G:H5''	1.74	0.53
13:9:2673:A:C2	13:9:2674:A:N6	2.76	0.53
11:2:2270:A:H2'	11:2:2271:A:H8	1.71	0.53
11:2:2270:A:O2'	11:2:2271:A:H5'	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2257:C:H3'	11:2:2258:U:C6	2.40	0.53
11:2:2257:C:H5'	11:2:2258:U:H5	1.72	0.53
16:J:66:GLU:O	16:J:69:ARG:N	2.42	0.53
11:2:2252:A:C2	11:2:2253:G:C4	2.97	0.53
14:7:2850:G:C8	14:7:2850:G:H5''	2.44	0.53
8:S:88:MET:SD	8:S:89:ILE:N	2.81	0.53
18:Y:39:C:H2'	18:Y:40:C:H6	1.74	0.53
14:7:2868:U:H5''	14:7:2869:U:OP2	2.08	0.53
14:7:2841:G:H3'	14:7:2842:U:H5'	1.91	0.53
16:J:121:LYS:O	16:J:122:PRO:O	2.26	0.53
10:X:53:ASP:OD2	10:X:56:LYS:HD2	2.09	0.53
14:7:2833:A:C2'	14:7:2834:G:H5'	2.35	0.53
14:7:2872:A:H1'	14:7:2873:U:H5'	1.90	0.53
8:S:86:ARG:O	8:S:122:ALA:HB2	2.08	0.53
14:7:2866:U:H1'	14:7:2867:C:H5	1.74	0.53
18:W:7:G:H5''	18:W:7:G:H8	1.74	0.53
11:2:2233:A:C8	11:2:2234:G:C8	2.97	0.53
18:W:35:A:O2'	18:W:36:U:H5'	2.09	0.53
9:L:47:HIS:CE1	9:L:104:ALA:HB2	2.43	0.53
9:L:107:GLY:O	9:L:108:ARG:O	2.26	0.53
16:J:17:TYR:O	16:J:19:LYS:N	2.42	0.53
9:L:29:PHE:CZ	9:L:33:LEU:HD12	2.44	0.53
15:B:120:VAL:O	18:W:56:C:C4'	2.57	0.53
11:2:2299:A:C6	11:2:2300:G:N7	2.76	0.53
8:S:49:ARG:NH1	8:S:87:SER:O	2.42	0.53
16:J:73:ASN:O	16:J:74:LYS:C	2.47	0.53
9:L:42:PHE:HB3	9:L:45:ALA:HB3	1.92	0.52
12:3:2487:U:H4'	12:3:2488:A:OP2	2.08	0.52
11:2:2250:G:N2	11:2:2267:C:C2	2.60	0.52
14:7:2847:A:N3	14:7:2847:A:H2'	2.25	0.52
11:2:2300:G:C6	11:2:2301:U:C4	2.97	0.52
14:7:2841:G:C4	14:7:2844:C:N4	2.77	0.52
10:X:36:TYR:CE2	10:X:40:LEU:HD11	2.44	0.52
16:J:47:PRO:O	16:J:140:THR:O	2.28	0.52
13:9:2676:A:H2'	13:9:2677:G:OP2	2.09	0.52
12:3:2483:G:C4	15:B:97:LYS:CA	2.90	0.52
11:2:2259:A:C5	11:2:2260:U:C2	2.98	0.52
14:7:2852:C:H5	14:7:2853:A:C5	2.27	0.52
9:L:55:LYS:H	9:L:55:LYS:HD3	1.74	0.52
16:J:184:LYS:C	16:J:186:GLU:N	2.62	0.52
8:S:56:GLU:N	8:S:56:GLU:CD	2.63	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2252:A:C4	11:2:2253:G:C8	2.98	0.52
11:2:2302:G:C6	11:2:2303:A:C5	2.98	0.52
9:L:26:ASP:HB3	9:L:29:PHE:HB3	1.92	0.52
16:J:155:ALA:O	16:J:158:LYS:O	2.27	0.52
18:Y:35:A:O2'	18:Y:36:U:H5'	2.09	0.52
18:Y:20:U:N3	18:Y:37:A:C2	40.28	0.52
11:2:2271:A:C3'	11:2:2272:G:C5'	2.86	0.52
8:S:47:ARG:O	8:S:51:LYS:HB2	2.09	0.52
16:J:24:ARG:O	16:J:25:ALA:HB2	2.10	0.52
14:7:2836:C:O2	14:7:2836:C:H2'	2.10	0.52
18:Y:70:G:H2'	18:Y:71:C:H6	1.75	0.52
18:W:73:A:H8	18:W:73:A:O5'	1.93	0.52
11:2:2291:A:C2	11:2:2292:U:C2	2.97	0.52
12:3:2482:U:H5''	15:B:95:LYS:H	1.75	0.52
14:7:2833:A:C2	14:7:2834:G:C8	2.97	0.52
11:2:2290:C:C2'	11:2:2291:A:O5'	2.58	0.52
11:2:2304:C:O2'	11:2:2305:G:C5'	2.48	0.52
16:J:94:PHE:O	16:J:126:ALA:O	2.27	0.52
11:2:2207:A:H8	11:2:2237:C:C2	2.28	0.52
9:L:101:VAL:HG11	9:L:123:VAL:HG13	1.90	0.52
8:S:86:ARG:CZ	8:S:122:ALA:HB1	2.40	0.52
16:J:98:ARG:CB	16:J:120:GLY:HA3	2.40	0.52
10:X:47:PRO:O	10:X:51:ALA:HB2	2.10	0.52
18:W:39:C:H2'	18:W:40:C:H6	1.74	0.52
16:J:56:GLU:O	16:J:57:LEU:C	2.47	0.52
14:7:2863:G:H5''	18:Y:74:C:HO2'	1.68	0.51
11:2:2215:A:N3	11:2:2215:A:C2'	2.65	0.51
16:J:37:GLY:HA3	16:J:86:HIS:N	2.25	0.51
16:J:17:TYR:C	16:J:19:LYS:H	2.12	0.51
8:S:42:PHE:HE2	8:S:118:GLY:HA2	1.75	0.51
8:S:15:GLY:N	8:S:114:PHE:HE2	2.09	0.51
15:B:4:ILE:O	15:B:5:THR:C	2.48	0.51
13:9:2678:A:C4	18:Y:56:C:H5'	2.45	0.51
11:2:2200:U:C2	11:2:2201:G:C8	2.98	0.51
11:2:2255:A:C4'	11:2:2256:A:OP1	2.56	0.51
11:2:2262:A:C5'	11:2:2263:C:OP2	2.58	0.51
11:2:2279:A:H4'	11:2:2280:A:C5'	2.40	0.51
16:J:17:TYR:C	16:J:19:LYS:N	2.63	0.51
9:L:106:LEU:HD21	9:L:121:PHE:C	2.31	0.51
18:Y:73:A:O5'	18:Y:73:A:H8	1.93	0.51
15:B:121:PRO:O	18:W:57:A:C5'	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2253:G:C5	11:2:2254:U:C2	2.97	0.51
11:2:2253:G:C6	11:2:2254:U:N3	2.78	0.51
14:7:2861:U:H2'	14:7:2862:U:C6	2.41	0.51
11:2:2299:A:H2'	11:2:2300:G:O5'	2.11	0.51
11:2:2304:C:HO2'	11:2:2305:G:H5'	1.72	0.51
9:L:55:LYS:HB2	9:L:92:LEU:HD21	1.91	0.51
8:S:33:LEU:CD2	8:S:62:VAL:HG21	2.41	0.51
8:S:38:LEU:O	8:S:42:PHE:CD1	2.64	0.51
11:2:2297:U:C2	11:2:2299:A:C6	2.99	0.51
18:W:70:G:H2'	18:W:71:C:H6	1.75	0.51
13:9:2673:A:C2	13:9:2674:A:N7	2.78	0.51
13:9:2675:C:N4	13:9:2676:A:N6	2.51	0.51
11:2:2251:G:C2	11:2:2252:A:C8	2.98	0.51
10:X:59:SER:O	10:X:61:ASN:N	2.44	0.51
11:2:2279:A:N7	11:2:2288:G:C6	2.79	0.51
9:L:75:LEU:HD11	9:L:82:ILE:HD11	1.91	0.51
12:3:2482:U:O5'	15:B:94:ASN:C	2.48	0.51
14:7:2863:G:OP1	18:Y:74:C:O2'	2.28	0.51
16:J:170:LYS:H	16:J:177:ASP:C	2.12	0.51
16:J:66:GLU:O	16:J:67:ALA:C	2.49	0.51
11:2:2279:A:C2	11:2:2283:G:C2	2.99	0.51
9:L:52:VAL:HG22	9:L:71:VAL:HG11	1.91	0.51
14:7:2841:G:C5	14:7:2844:C:C4	2.99	0.51
8:S:38:LEU:O	8:S:42:PHE:HD1	1.93	0.51
11:2:2206:G:H2'	11:2:2207:A:H5'	1.93	0.51
14:7:2836:C:C5	14:7:2853:A:C2	2.99	0.51
11:2:2280:A:O2'	11:2:2281:A:P	2.68	0.51
11:2:2289:U:H2'	11:2:2290:C:H5'	1.92	0.51
8:S:60:LYS:HD3	8:S:64:LYS:HE3	1.93	0.51
14:7:2837:A:H2'	14:7:2845:A:C2	2.46	0.51
14:7:2864:A:C6	14:7:2865:U:C4	2.99	0.51
16:J:170:LYS:CB	16:J:171:TRP:C	2.80	0.51
8:S:48:ARG:O	8:S:52:ARG:HB2	2.10	0.51
13:9:2673:A:C2	13:9:2676:A:C8	3.00	0.50
14:7:2857:C:H2'	14:7:2858:U:C6	2.45	0.50
16:J:170:LYS:CB	16:J:172:GLY:N	2.74	0.50
14:7:2847:A:N3	14:7:2848:G:C8	2.79	0.50
14:7:2868:U:C4	14:7:2869:U:H5	2.27	0.50
18:W:76:A:OP1	18:W:76:A:H4'	2.11	0.50
9:L:75:LEU:CD2	9:L:82:ILE:HD12	2.39	0.50
15:B:59:PRO:O	15:B:60:ARG:CB	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:127:THR:HG22	8:S:127:THR:O	2.11	0.50
14:7:2862:U:O3'	18:Y:75:C:P	2.68	0.50
8:S:58:TYR:HB3	8:S:88:MET:CE	2.41	0.50
11:2:2209:U:H6	11:2:2209:U:H3'	1.76	0.50
12:3:2484:A:C4'	15:B:127:GLN:H	2.14	0.50
11:2:2198:A:C4	11:2:2199:G:C8	2.99	0.50
11:2:2249:G:N9	11:2:2272:G:C8	2.79	0.50
10:X:59:SER:C	10:X:61:ASN:H	2.15	0.50
11:2:2204:C:C2'	11:2:2205:U:H5''	2.41	0.50
9:L:40:ASN:CB	9:L:41:PRO:HD2	2.38	0.50
13:9:2677:G:C2'	13:9:2678:A:O5'	2.60	0.50
13:9:2684:C:H4'	13:9:2684:C:OP1	2.12	0.50
18:W:7:G:H5''	18:W:7:G:C8	2.46	0.50
11:2:2249:G:H2'	11:2:2250:G:H1'	1.92	0.50
11:2:2297:U:N3	11:2:2299:A:C6	2.79	0.50
14:7:2827:U:O2	14:7:2827:U:C2'	2.60	0.50
16:J:35:ASP:O	16:J:36:LEU:C	2.50	0.50
18:Y:39:C:H6	18:Y:39:C:O5'	1.94	0.50
8:S:60:LYS:HZ3	8:S:64:LYS:CE	2.25	0.50
12:3:2484:A:C5'	15:B:122:ARG:HA	2.11	0.50
10:X:7:THR:HG22	10:X:8:LEU:H	1.75	0.50
8:S:60:LYS:NZ	8:S:64:LYS:HE3	2.27	0.50
11:2:2253:G:H3'	11:2:2254:U:H6	1.74	0.50
14:7:2852:C:H5	14:7:2853:A:C4	2.29	0.50
15:B:54:LYS:CA	15:B:55:LEU:CB	2.89	0.50
12:3:2486:A:C8	15:B:101:LYS:CB	2.95	0.49
11:2:2222:A:O5'	11:2:2222:A:H8	1.95	0.49
18:Y:30:G:H21	18:Y:31:G:H1'	1.77	0.49
16:J:205:SER:N	16:J:206:LEU:HA	2.26	0.49
8:S:56:GLU:CD	8:S:56:GLU:H	2.14	0.49
12:3:2484:A:H4'	15:B:126:PRO:CB	2.17	0.49
11:2:2264:U:O2'	11:2:2265:C:H5'	2.13	0.49
9:L:61:LYS:HD2	9:L:117:PRO:HA	1.93	0.49
14:7:2841:G:N1	14:7:2844:C:N3	2.60	0.49
12:3:2484:A:N7	18:W:19:G:C2	2.80	0.49
11:2:2294:U:H3'	11:2:2295:A:H5''	1.94	0.49
14:7:2856:G:C2	14:7:2857:C:C4	3.00	0.49
11:2:2207:A:C8	11:2:2237:C:C2	3.00	0.49
11:2:2223:A:C2'	11:2:2224:A:H8	2.20	0.49
18:W:39:C:O5'	18:W:39:C:H6	1.94	0.49
14:7:2851:A:H5''	14:7:2851:A:C8	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:205:SER:CB	16:J:206:LEU:HA	2.43	0.49
13:9:2672:G:C8	13:9:2672:G:H3'	2.47	0.49
11:2:2252:A:N3	11:2:2253:G:C8	2.80	0.49
18:Y:76:A:OP1	18:Y:76:A:H4'	2.11	0.49
9:L:69:LYS:NZ	9:L:92:LEU:HB3	2.28	0.49
12:3:2484:A:OP2	15:B:122:ARG:CB	2.60	0.49
11:2:2221:G:H8	11:2:2221:G:H5''	1.76	0.49
11:2:2285:C:H5	11:2:2286:U:C4	2.27	0.49
18:Y:32:C:C4	18:Y:33:U:C5	3.01	0.49
11:2:2247:G:N3	11:2:2247:G:H2'	2.27	0.49
11:2:2276:G:N7	11:2:2277:C:C5	2.80	0.49
11:2:2280:A:O2'	11:2:2281:A:O5'	2.26	0.49
18:Y:7:G:H5''	18:Y:7:G:C8	2.46	0.49
14:7:2858:U:C2'	14:7:2859:U:C5	2.94	0.49
11:2:2198:A:O2'	11:2:2199:G:H5'	2.13	0.49
11:2:2264:U:H6	11:2:2264:U:O5'	1.96	0.49
9:L:71:VAL:CG2	9:L:95:LEU:HD13	2.36	0.49
13:9:2679:A:O4'	13:9:2679:A:OP1	2.30	0.48
10:X:66:LYS:O	10:X:70:MET:HB2	2.13	0.48
15:B:155:ILE:HA	15:B:156:LYS:C	2.32	0.48
13:9:2684:C:N3	13:9:2685:C:C5	2.81	0.48
11:2:2206:G:N2	11:2:2207:A:C8	2.81	0.48
11:2:2206:G:N3	11:2:2206:G:H2'	2.28	0.48
8:S:101:VAL:HG21	8:S:121:LEU:CD1	2.38	0.48
18:W:61:C:H2'	18:W:62:C:H6	1.78	0.48
9:L:42:PHE:CZ	9:L:103:VAL:HG23	2.47	0.48
5:G:1440:A:H2'	5:G:1441:C:C6	2.48	0.48
12:3:2482:U:H2'	15:B:97:LYS:N	2.17	0.48
9:L:3:VAL:HG12	9:L:4:GLY:N	2.21	0.48
9:L:87:PRO:O	9:L:88:MET:O	2.30	0.48
14:7:2841:G:C5	14:7:2844:C:N4	2.81	0.48
18:Y:57:A:H2'	18:Y:58:A:H5'	1.96	0.48
11:2:2253:G:C4	11:2:2254:U:C6	3.01	0.48
18:W:32:C:C4	18:W:33:U:C5	3.01	0.48
14:7:2847:A:C2	14:7:2848:G:C1'	2.97	0.48
14:7:2847:A:C5'	14:7:2848:G:OP2	2.55	0.48
8:S:46:THR:CG2	8:S:89:ILE:HD13	2.41	0.48
9:L:73:VAL:HG12	9:L:74:LEU:N	2.28	0.48
16:J:170:LYS:O	16:J:178:ARG:N	2.47	0.48
18:W:30:G:H21	18:W:31:G:H1'	1.77	0.48
18:W:14:A:N3	18:W:37:A:N6	33.01	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:85:TYR:HD1	8:S:85:TYR:H	1.61	0.48
11:2:2255:A:N1	11:2:2258:U:H5'	2.28	0.48
8:S:45:LYS:O	8:S:48:ARG:HB3	2.13	0.48
13:9:2677:G:N1	13:9:2679:A:C4	2.81	0.48
11:2:2270:A:C2'	11:2:2271:A:C8	2.89	0.48
14:7:2834:G:C6	14:7:2855:U:C4	3.01	0.48
11:2:2276:G:O6	11:2:2277:C:C4	2.67	0.48
11:2:2279:A:C8	11:2:2288:G:C5	3.01	0.48
11:2:2299:A:C4	11:2:2300:G:H8	2.31	0.48
14:7:2869:U:C2'	14:7:2869:U:O2	2.62	0.48
8:S:73:PRO:C	8:S:75:GLY:N	2.67	0.48
18:Y:38:A:O2'	18:Y:39:C:H5'	2.13	0.48
14:7:2860:U:O2	14:7:2860:U:H2'	2.13	0.48
11:2:2213:A:C2'	11:2:2214:A:C8	2.81	0.48
11:2:2290:C:C4	11:2:2303:A:N1	2.82	0.48
8:S:42:PHE:CD2	8:S:118:GLY:HA2	2.49	0.48
16:J:184:LYS:O	16:J:186:GLU:N	2.47	0.48
13:9:2683:U:H2'	13:9:2683:U:O2	2.14	0.48
11:2:2254:U:O2'	11:2:2255:A:P	2.71	0.48
11:2:2254:U:C2'	11:2:2255:A:OP1	2.62	0.48
11:2:2261:G:N2	11:2:2263:C:C2	2.82	0.48
8:S:32:LYS:O	8:S:34:ILE:N	2.47	0.48
18:W:57:A:H2'	18:W:58:A:H5'	1.96	0.47
14:7:2826:U:N3	14:7:2827:U:C5	2.81	0.47
13:9:2681:U:H2'	13:9:2681:U:H6	1.08	0.47
12:3:2482:U:H3'	15:B:96:ASN:N	1.79	0.47
12:3:2482:U:C5'	15:B:93:LEU:C	2.77	0.47
18:W:38:A:O2'	18:W:39:C:H5'	2.13	0.47
14:7:2854:U:HO2'	14:7:2855:U:H5'	1.79	0.47
16:J:219:ALA:C	16:J:221:ALA:H	2.17	0.47
11:2:2205:U:C2'	11:2:2206:G:H5'	2.37	0.47
14:7:2852:C:C5	14:7:2853:A:C5	3.03	0.47
8:S:13:PHE:O	8:S:14:ARG:HD3	2.14	0.47
11:2:2194:G:H2'	11:2:2195:C:H5'	1.97	0.47
11:2:2199:G:C4	11:2:2200:U:C5	3.03	0.47
11:2:2215:A:C2	11:2:2216:G:N9	2.83	0.47
9:L:42:PHE:HZ	9:L:103:VAL:HG23	1.79	0.47
16:J:57:LEU:HA	16:J:129:VAL:O	2.15	0.47
5:G:1434:C:H2'	5:G:1434:C:O2	2.15	0.47
18:W:71:C:N4	18:W:72:A:C6	2.83	0.47
18:W:54:U:C2'	18:W:55:U:H5'	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:54:U:C2'	18:Y:55:U:H5'	2.45	0.47
9:L:85:PHE:HE1	9:L:87:PRO:HA	1.78	0.47
12:3:2482:U:C3'	15:B:96:ASN:N	2.37	0.47
15:B:101:LYS:O	15:B:102:LYS:C	2.53	0.47
11:2:2197:C:H4'	11:2:2198:A:H8	1.79	0.47
11:2:2248:C:C4'	11:2:2271:A:C2	2.96	0.47
11:2:2266:U:H5''	11:2:2267:C:OP2	2.14	0.47
18:Y:17:C:H5	18:Y:17(A):U:O4	1.98	0.47
11:2:2295:A:C6	11:2:2296:A:C6	3.02	0.47
15:B:53:LEU:CB	15:B:54:LYS:CA	2.91	0.47
18:Y:61:C:H2'	18:Y:62:C:H6	1.78	0.47
16:J:45:GLU:O	16:J:47:PRO:N	2.48	0.47
16:J:153:ARG:O	16:J:154:ARG:C	2.52	0.47
13:9:2678:A:C5'	13:9:2679:A:C2	2.97	0.47
13:9:2684:C:O2'	13:9:2685:C:O5'	2.32	0.47
13:9:2678:A:C2	18:Y:56:C:C5'	2.97	0.47
12:3:2483:G:C2	15:B:97:LYS:O	2.68	0.47
11:2:2249:G:C1'	11:2:2272:G:C8	2.97	0.47
9:L:29:PHE:O	9:L:33:LEU:HB2	2.14	0.47
8:S:59:ALA:O	8:S:62:VAL:HB	2.15	0.47
11:2:2248:C:H4'	11:2:2271:A:C2	2.49	0.47
18:W:20:U:C3'	18:W:21:A:C5'	2.93	0.47
14:7:2853:A:O2'	16:J:159:PHE:N	2.48	0.47
18:W:14:A:H2	18:W:36:U:H3	37.42	0.47
11:2:2288:G:C2	11:2:2289:U:C5	3.03	0.47
18:Y:71:C:N4	18:Y:72:A:C6	2.83	0.47
8:S:69:LYS:NZ	8:S:93:GLU:O	2.45	0.47
15:B:55:LEU:HA	15:B:167:VAL:HA	1.96	0.47
16:J:206:LEU:O	16:J:207:GLU:C	2.53	0.47
11:2:2249:G:C2	11:2:2272:G:O6	2.68	0.47
10:X:7:THR:CG2	10:X:8:LEU:H	2.25	0.47
16:J:61:SER:HA	16:J:126:ALA:HB2	1.96	0.47
13:9:2673:A:C2	13:9:2676:A:H8	2.32	0.46
12:3:2482:U:C5'	15:B:95:LYS:H	2.26	0.46
11:2:2215:A:C2	11:2:2216:G:C1'	2.98	0.46
14:7:2836:C:H5	14:7:2853:A:C2	2.33	0.46
18:W:14:A:H2	18:W:36:U:N3	37.51	0.46
10:X:13:LYS:O	10:X:17:GLN:HG3	2.15	0.46
18:W:50:U:O2'	18:W:51:C:H5'	2.16	0.46
18:Y:20:U:C3'	18:Y:21:A:C5'	2.93	0.46
14:7:2830:G:C8	18:Y:76:A:C6	3.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:2834:G:O2'	14:7:2835:U:O4'	2.34	0.46
8:S:55:SER:HB2	8:S:58:TYR:CE2	2.50	0.46
11:2:2250:G:H2'	11:2:2250:G:N3	2.31	0.46
11:2:2223:A:N3	11:2:2224:A:C4	2.83	0.46
8:S:38:LEU:HA	8:S:41:LEU:HD12	1.97	0.46
8:S:65:VAL:HG21	8:S:94:LEU:HD21	1.96	0.46
11:2:2252:A:C4	11:2:2253:G:N7	2.84	0.46
11:2:2255:A:H8	18:Y:25:C:H4'	1.80	0.46
18:W:17:C:H5	18:W:17(A):U:O4	1.98	0.46
11:2:2225:U:C2	11:2:2226:U:C5	3.03	0.46
11:2:2294:U:C2	11:2:2296:A:OP2	2.69	0.46
18:Y:4:G:O2'	18:Y:5:G:P	2.73	0.46
18:W:4:G:O2'	18:W:5:G:P	2.74	0.46
9:L:106:LEU:CD2	9:L:122:LYS:HB2	2.45	0.46
11:2:2196:C:N4	11:2:2242:A:C8	2.83	0.46
10:X:62:TRP:CH2	10:X:63:HIS:NE2	2.83	0.46
11:2:2289:U:C2'	11:2:2290:C:C5'	2.94	0.46
8:S:95:VAL:CG2	8:S:117:ILE:HD11	2.45	0.46
12:3:2482:U:C4	15:B:98:LYS:C	2.87	0.46
11:2:2257:C:C2	11:2:2258:U:C6	3.04	0.46
16:J:69:ARG:O	16:J:70:ILE:O	2.33	0.46
11:2:2300:G:C2	11:2:2301:U:C2	3.04	0.46
9:L:29:PHE:CZ	9:L:33:LEU:CD1	2.98	0.46
16:J:33:ILE:O	16:J:34:TYR:CB	2.61	0.46
11:2:2234:G:C5	11:2:2235:C:C5	3.04	0.46
10:X:7:THR:O	10:X:8:LEU:HB2	2.16	0.46
9:L:27:ASN:O	9:L:31:LYS:HB2	2.15	0.46
15:B:128:LEU:O	15:B:131:ALA:HB3	2.15	0.46
11:2:2240:G:C2'	11:2:2241:U:O5'	2.64	0.46
11:2:2259:A:H5''	11:2:2260:U:C5	2.47	0.46
11:2:2285:C:H5	11:2:2286:U:C6	2.33	0.46
11:2:2289:U:N3	11:2:2290:C:C5	2.84	0.46
11:2:2290:C:N3	11:2:2303:A:C2	2.84	0.46
18:Y:28:C:O2	18:Y:43:A:C2	2.69	0.46
11:2:2291:A:N1	11:2:2292:U:C2	2.84	0.46
8:S:42:PHE:CD2	8:S:46:THR:HG21	2.51	0.46
8:S:98:ILE:HG22	8:S:111:GLU:HG2	1.97	0.46
10:X:35:SER:O	10:X:38:ARG:HB3	2.16	0.46
14:7:2830:G:N7	18:Y:76:A:C2	2.84	0.46
10:X:44:ARG:HA	10:X:49:ILE:HD12	1.98	0.46
11:2:2232:A:H3'	11:2:2232:A:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:66:ARG:HH12	8:S:93:GLU:HB3	1.78	0.46
9:L:56:ILE:CG2	9:L:57:GLY:N	2.78	0.46
14:7:2825:C:H42	14:7:2864:A:N6	2.12	0.45
10:X:35:SER:O	10:X:39:ILE:HG13	2.16	0.45
18:Y:50:U:O2'	18:Y:51:C:H5'	2.16	0.45
13:9:2681:U:HO2'	13:9:2682:C:H5''	1.81	0.45
11:2:2301:U:O2'	11:2:2302:G:H5'	2.16	0.45
11:2:2235:C:H2'	11:2:2236:G:C8	2.52	0.45
11:2:2222:A:O2'	11:2:2223:A:H5''	2.16	0.45
14:7:2840:C:N4	14:7:2841:G:C5	2.85	0.45
10:X:34:ARG:CZ	10:X:34:ARG:HB3	2.46	0.45
11:2:2255:A:H4'	11:2:2256:A:OP1	2.11	0.45
11:2:2250:G:N1	11:2:2267:C:N3	2.55	0.45
18:W:28:C:O2	18:W:43:A:C2	2.69	0.45
15:B:120:VAL:O	18:W:56:C:C3'	2.64	0.45
16:J:159:PHE:O	16:J:160:PRO:C	2.54	0.45
11:2:2295:A:H2'	11:2:2296:A:C8	2.52	0.45
8:S:33:LEU:HD11	8:S:59:ALA:CA	2.46	0.45
14:7:2872:A:O4'	14:7:2873:U:OP1	2.35	0.45
18:W:59:A:H2'	18:W:60:U:H5'	1.98	0.45
18:Y:17:C:C5	18:Y:17(A):U:O4	2.70	0.45
14:7:2852:C:N4	14:7:2853:A:N3	2.64	0.45
11:2:2297:U:O2	11:2:2299:A:C5	2.70	0.45
11:2:2302:G:H2'	11:2:2303:A:O4'	2.16	0.45
10:X:31:PRO:O	10:X:36:TYR:HB2	2.16	0.45
18:Y:41:C:O2'	18:Y:42:G:H5'	2.17	0.45
13:9:2672:G:C8	13:9:2672:G:C3'	3.00	0.45
13:9:2676:A:C2'	13:9:2677:G:OP2	2.64	0.45
11:2:2247:G:H5''	11:2:2248:C:OP2	2.17	0.45
18:W:17:C:C5	18:W:17(A):U:O4	2.70	0.45
9:L:29:PHE:CE1	9:L:33:LEU:HD12	2.52	0.45
8:S:60:LYS:NZ	8:S:64:LYS:CE	2.80	0.45
12:3:2483:G:O5'	15:B:96:ASN:CB	2.58	0.45
11:2:2240:G:H2'	11:2:2241:U:C5'	2.47	0.45
14:7:2837:A:H2'	14:7:2845:A:C6	2.52	0.45
18:Y:4:G:O2'	18:Y:5:G:H8	2.00	0.45
11:2:2287:C:O2	11:2:2298:U:H5''	2.17	0.45
16:J:142:ASP:C	16:J:144:ASN:H	2.20	0.45
16:J:152:LEU:O	16:J:153:ARG:C	2.53	0.45
18:Y:11:A:O2'	18:Y:12:G:H5'	2.17	0.45
18:W:11:A:O2'	18:W:12:G:H5'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:9:2679:A:OP1	13:9:2679:A:C4'	2.65	0.44
11:2:2249:G:H2'	11:2:2250:G:O4'	2.16	0.44
11:2:2279:A:C3'	11:2:2280:A:C5'	2.94	0.44
15:B:68:PHE:HA	15:B:73:ASP:CB	2.46	0.44
16:J:56:GLU:N	16:J:131:ILE:HA	2.32	0.44
18:Y:59:A:H2'	18:Y:60:U:H5'	1.98	0.44
13:9:2678:A:C2	18:Y:56:C:H5''	2.52	0.44
11:2:2211:U:O2'	11:2:2212:C:H5'	2.17	0.44
14:7:2850:G:H8	14:7:2850:G:H5''	1.79	0.44
8:S:91:ILE:CG2	8:S:92:PRO:HD2	2.45	0.44
8:S:60:LYS:HZ3	8:S:64:LYS:HE3	1.81	0.44
13:9:2673:A:N3	13:9:2674:A:N7	2.65	0.44
11:2:2253:G:C3'	11:2:2254:U:C6	2.97	0.44
18:W:15:G:H8	18:W:15:G:O5'	2.00	0.44
16:J:24:ARG:O	16:J:25:ALA:CB	2.65	0.44
18:Y:15:G:H8	18:Y:15:G:O5'	2.00	0.44
9:L:135:PHE:CE1	10:X:15:ARG:NH1	2.85	0.44
11:2:2209:U:N1	11:2:2209:U:OP2	2.50	0.44
13:9:2674:A:H2	13:9:2675:C:C6	2.36	0.44
18:Y:38:A:H2'	18:Y:39:C:O4'	2.18	0.44
11:2:2270:A:C6	11:2:2271:A:C6	3.05	0.44
16:J:66:GLU:O	16:J:68:ALA:N	2.51	0.44
11:2:2279:A:C2	11:2:2283:G:N2	2.86	0.44
11:2:2280:A:HO2'	11:2:2281:A:H3'	1.82	0.44
11:2:2278:C:C4	11:2:2305:G:C5	3.06	0.44
18:Y:5:G:N2	18:Y:69:C:N3	2.65	0.44
18:W:5:G:N2	18:W:69:C:N3	2.65	0.44
11:2:2252:A:N1	11:2:2253:G:C6	2.86	0.44
11:2:2285:C:H41	11:2:2286:U:H3	1.65	0.44
10:X:7:THR:HG22	10:X:8:LEU:N	2.33	0.44
11:2:2298:U:O4'	11:2:2298:U:O2	2.35	0.44
8:S:85:TYR:N	8:S:85:TYR:CD1	2.85	0.44
16:J:202:LYS:O	16:J:203:LYS:CB	2.65	0.44
13:9:2671:A:C6	13:9:2672:G:N7	2.86	0.44
18:W:41:C:O2'	18:W:42:G:H5'	2.17	0.44
14:7:2836:C:C3'	14:7:2836:C:O2	2.65	0.44
14:7:2839:G:C6	14:7:2850:G:C2	3.04	0.44
14:7:2851:A:H3'	14:7:2852:C:C5'	2.48	0.44
11:2:2278:C:O2'	11:2:2279:A:H5''	2.17	0.44
11:2:2300:G:N3	11:2:2300:G:H2'	2.32	0.44
9:L:95:LEU:HD23	9:L:126:VAL:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:78:ASN:O	9:L:79:SER:HB2	2.16	0.44
8:S:86:ARG:HD2	8:S:102:TYR:O	2.17	0.44
18:W:38:A:H2'	18:W:39:C:O4'	2.18	0.44
11:2:2197:C:N3	11:2:2242:A:C2	2.86	0.44
11:2:2255:A:C2	11:2:2258:U:OP2	2.71	0.44
11:2:2223:A:C2	11:2:2224:A:C5	3.06	0.44
8:S:121:LEU:HD12	8:S:121:LEU:O	2.17	0.44
9:L:124:VAL:O	9:L:124:VAL:HG12	2.18	0.44
14:7:2830:G:H2'	14:7:2831:G:H8	1.83	0.44
11:2:2289:U:O2'	11:2:2290:C:C5'	2.62	0.44
5:G:1430:C:O2'	5:G:1431:A:O5'	2.36	0.44
11:2:2218:G:C4	11:2:2228:A:C2	3.06	0.44
18:W:7:G:H3'	18:W:8:U:C5'	2.47	0.44
18:W:35:A:C4	18:W:36:U:C5	3.06	0.43
16:J:164:LYS:O	16:J:165:ILE:C	2.57	0.43
16:J:83:ASP:O	16:J:84:ALA:HB2	2.17	0.43
14:7:2835:U:O2	14:7:2835:U:H2'	2.17	0.43
16:J:114:GLY:O	16:J:115:MET:CB	2.65	0.43
13:9:2677:G:C2	13:9:2678:A:H5'	2.53	0.43
11:2:2257:C:O4'	11:2:2257:C:O2	2.36	0.43
14:7:2856:G:N2	14:7:2857:C:C2	2.87	0.43
16:J:69:ARG:O	16:J:70:ILE:C	2.56	0.43
5:G:1430:C:O2'	5:G:1431:A:P	2.77	0.43
11:2:2217:U:H2'	11:2:2218:G:H8	1.83	0.43
16:J:215:GLU:C	16:J:217:PHE:N	2.72	0.43
13:9:2672:G:O6	13:9:2683:U:O4	2.36	0.43
18:Y:35:A:C4	18:Y:36:U:C5	3.06	0.43
18:Y:39:C:H2'	18:Y:40:C:C6	2.54	0.43
12:3:2482:U:C2'	15:B:97:LYS:H	2.31	0.43
14:7:2863:G:C8	18:Y:76:A:C4'	3.01	0.43
14:7:2850:G:OP1	14:7:2850:G:C4'	2.53	0.43
11:2:2281:A:H1'	11:2:2282:U:OP1	2.18	0.43
11:2:2201:G:C4	11:2:2202:C:C6	3.07	0.43
11:2:2246:G:C4	11:2:2247:G:C8	3.06	0.43
14:7:2846:U:H2'	14:7:2847:A:OP2	2.19	0.43
9:L:69:LYS:HZ2	9:L:92:LEU:HD23	1.84	0.43
8:S:101:VAL:O	8:S:108:VAL:N	2.44	0.43
11:2:2218:G:C5	11:2:2228:A:C2	3.06	0.43
9:L:44:GLY:O	9:L:45:ALA:O	2.36	0.43
9:L:131:LEU:O	9:L:132:LEU:C	2.57	0.43
18:Y:59:A:C2'	18:Y:60:U:H5'	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2284:C:C5'	11:2:2285:C:OP2	2.66	0.43
9:L:75:LEU:HD12	9:L:78:ASN:HD22	1.83	0.43
13:9:2677:G:C2	13:9:2679:A:C4	3.06	0.43
11:2:2197:C:C2	11:2:2242:A:C2	3.06	0.43
18:Y:24:U:H2'	18:Y:25:C:H6	1.84	0.43
14:7:2828:G:H2'	14:7:2829:U:O5'	2.18	0.43
14:7:2831:G:C2	14:7:2832:C:C2	3.06	0.43
11:2:2276:G:C4	11:2:2277:C:C5	3.05	0.43
11:2:2209:U:C3'	11:2:2209:U:C6	3.01	0.43
11:2:2249:G:N9	11:2:2272:G:N7	2.66	0.43
14:7:2857:C:C2	14:7:2858:U:C6	3.06	0.43
9:L:95:LEU:CD2	9:L:126:VAL:HG22	2.48	0.43
8:S:29:ASN:O	8:S:31:GLU:HG2	2.19	0.43
16:J:56:GLU:O	16:J:58:GLU:N	2.52	0.43
8:S:60:LYS:CD	8:S:64:LYS:HE3	2.49	0.43
14:7:2843:U:P	14:7:2843:U:H3'	2.59	0.43
11:2:2249:G:C4	11:2:2272:G:C5	3.07	0.43
11:2:2255:A:N1	11:2:2260:U:O4	2.52	0.43
11:2:2256:A:O2'	11:2:2257:C:OP2	2.36	0.43
14:7:2830:G:H2'	14:7:2831:G:O5'	2.19	0.43
10:X:31:PRO:CG	10:X:39:ILE:HD11	2.47	0.43
16:J:56:GLU:H	16:J:131:ILE:HA	1.84	0.43
5:G:1435:G:C2	5:G:1436:C:C5	3.07	0.43
11:2:2247:G:C6	11:2:2248:C:N4	2.87	0.43
14:7:2868:U:C4	14:7:2869:U:C5	3.06	0.43
18:Y:9:G:N3	18:Y:45:G:H2'	2.34	0.43
16:J:203:LYS:HA	16:J:204:GLY:HA2	1.81	0.43
10:X:28:ARG:HD3	10:X:28:ARG:HA	1.58	0.43
11:2:2199:G:C2	11:2:2200:U:C6	3.06	0.42
11:2:2260:U:O2'	11:2:2261:G:C8	2.71	0.42
11:2:2214:A:C2'	11:2:2215:A:H8	2.32	0.42
11:2:2300:G:N2	11:2:2301:U:H1'	2.34	0.42
15:B:68:PHE:H	15:B:112:ALA:HB2	1.83	0.42
15:B:188:ASN:C	15:B:190:PHE:N	2.72	0.42
9:L:5:LYS:NZ	9:L:18:HIS:NE2	2.66	0.42
15:B:101:LYS:O	15:B:104:SER:N	2.52	0.42
11:2:2212:C:O2'	11:2:2233:A:N6	2.51	0.42
14:7:2834:G:C4	14:7:2835:U:H5	2.35	0.42
14:7:2853:A:C6	14:7:2854:U:C2	3.07	0.42
11:2:2218:G:C6	11:2:2228:A:C6	3.07	0.42
16:J:147:VAL:O	16:J:148:VAL:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:174:THR:C	16:J:176:LEU:CB	2.87	0.42
18:W:24:U:H2'	18:W:25:C:H6	1.84	0.42
12:3:2488:A:N3	12:3:2488:A:H2'	2.33	0.42
15:B:32:VAL:HA	15:B:208:SER:HA	2.00	0.42
11:2:2273:G:H1'	11:2:2274:U:H5	1.85	0.42
11:2:2224:A:H3'	11:2:2225:U:H6	1.83	0.42
11:2:2279:A:C4'	11:2:2280:A:C5'	2.97	0.42
18:Y:3:C:N4	18:Y:70:G:H1	2.16	0.42
13:9:2671:A:C6	13:9:2684:C:N4	2.87	0.42
11:2:2196:C:C2	11:2:2242:A:N6	2.88	0.42
11:2:2262:A:C2	11:2:2263:C:O4'	2.72	0.42
9:L:139:LYS:O	9:L:140:GLU:HG3	2.19	0.42
18:W:59:A:C2'	18:W:60:U:H5'	2.49	0.42
8:S:81:VAL:O	8:S:99:VAL:HG13	2.19	0.42
15:B:145:TYR:HA	15:B:148:VAL:CB	2.50	0.42
11:2:2229:A:H2'	11:2:2230:C:N1	2.35	0.42
11:2:2252:A:C2	11:2:2265:C:O2	2.72	0.42
11:2:2254:U:H2'	11:2:2255:A:OP1	2.18	0.42
11:2:2213:A:N6	11:2:2232:A:C4	2.88	0.42
14:7:2834:G:C2	14:7:2835:U:C5	3.08	0.42
11:2:2222:A:C2	11:2:2223:A:C6	3.08	0.42
11:2:2279:A:C4'	11:2:2280:A:H5'	2.43	0.42
16:J:89:VAL:O	16:J:136:PHE:CA	2.54	0.42
18:W:49:G:H1	18:W:65:C:N4	2.18	0.42
16:J:151:GLY:O	16:J:152:LEU:C	2.58	0.42
9:L:17:ARG:NH2	9:L:20:LYS:HB3	2.34	0.42
14:7:2864:A:C5	14:7:2865:U:C4	3.07	0.42
18:Y:70:G:C5	18:Y:71:C:C5	3.08	0.42
18:W:9:G:N3	18:W:45:G:H2'	2.34	0.42
14:7:2830:G:H8	18:Y:76:A:C6	2.38	0.42
14:7:2834:G:C4	14:7:2835:U:C6	3.07	0.42
14:7:2872:A:H1'	14:7:2873:U:C5'	2.50	0.42
8:S:15:GLY:CA	8:S:114:PHE:HE2	2.33	0.42
13:9:2674:A:H2'	13:9:2675:C:H5''	2.02	0.42
11:2:2259:A:C6	11:2:2260:U:C2	3.08	0.42
14:7:2828:G:C2'	14:7:2829:U:O5'	2.68	0.42
14:7:2828:G:N1	18:Y:76:A:N9	2.66	0.42
11:2:2211:U:H2'	11:2:2212:C:C6	2.54	0.42
18:W:35:A:C6	18:W:36:U:C4	3.08	0.42
11:2:2276:G:H2'	11:2:2277:C:H5'	2.02	0.42
11:2:2285:C:C5	11:2:2286:U:C6	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:2286:U:O4	11:2:2288:G:H1'	2.18	0.42
11:2:2262:A:H5''	11:2:2263:C:OP2	2.20	0.42
15:B:167:VAL:O	15:B:168:ALA:HB2	2.19	0.42
18:Y:35:A:C6	18:Y:36:U:C4	3.08	0.42
11:2:2273:G:O2'	11:2:2274:U:P	2.78	0.42
11:2:2288:G:C6	11:2:2289:U:C4	3.08	0.42
14:7:2868:U:C6	14:7:2869:U:H5	2.38	0.42
9:L:90:GLY:O	9:L:91:CYS:C	2.59	0.42
18:Y:20:U:N3	18:Y:37:A:C4	40.57	0.41
14:7:2834:G:C2	14:7:2835:U:C6	3.07	0.41
14:7:2837:A:C8	14:7:2845:A:H2	2.36	0.41
11:2:2290:C:O2'	11:2:2291:A:O5'	2.38	0.41
14:7:2840:C:C4	14:7:2841:G:C5	3.08	0.41
8:S:21:LEU:HA	8:S:24:LEU:CB	2.50	0.41
18:Y:64:G:C6	18:Y:65:C:C4	3.08	0.41
10:X:25:ASP:O	10:X:26:LYS:C	2.58	0.41
16:J:28:ASP:O	16:J:29:SER:O	2.38	0.41
13:9:2674:A:N1	13:9:2676:A:N7	2.69	0.41
13:9:2684:C:H5''	13:9:2684:C:H6	1.66	0.41
14:7:2829:U:OP1	16:J:4:ARG:O	2.38	0.41
8:S:46:THR:HG23	8:S:89:ILE:HD12	1.98	0.41
9:L:87:PRO:HB2	9:L:88:MET:H	1.66	0.41
18:Y:46:G:H3'	18:Y:46:G:C8	2.55	0.41
11:2:2196:C:C5'	11:2:2197:C:OP2	2.69	0.41
14:7:2831:G:C5	14:7:2832:C:C5	3.08	0.41
9:L:78:ASN:ND2	9:L:80:LYS:HG2	2.34	0.41
16:J:144:ASN:O	16:J:145:LYS:C	2.57	0.41
13:9:2680:A:C8	13:9:2680:A:H3'	2.55	0.41
13:9:2680:A:H8	13:9:2680:A:H3'	1.85	0.41
12:3:2485:A:H4'	15:B:131:ALA:H	1.86	0.41
14:7:2856:G:N1	14:7:2857:C:C4	2.88	0.41
18:W:70:G:C5	18:W:71:C:C5	3.08	0.41
8:S:51:LYS:HD3	8:S:51:LYS:HA	1.87	0.41
18:W:64:G:C6	18:W:65:C:C4	3.08	0.41
15:B:12:HIS:CB	15:B:213:ALA:HB1	2.50	0.41
8:S:72:CYS:SG	8:S:79:VAL:HG23	2.60	0.41
13:9:2685:C:H2'	13:9:2685:C:O2	2.20	0.41
11:2:2194:G:N9	11:2:2274:U:O2	2.53	0.41
11:2:2249:G:C8	11:2:2272:G:C8	3.09	0.41
14:7:2856:G:C6	14:7:2857:C:N4	2.89	0.41
11:2:2210:G:C5	11:2:2211:U:C5	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:29:G:H8	18:Y:29:G:O5'	2.04	0.41
18:Y:7:G:H3'	18:Y:8:U:C5'	2.47	0.41
11:2:2273:G:O2'	11:2:2274:U:OP2	2.37	0.41
11:2:2213:A:C6	11:2:2214:A:C6	3.09	0.41
14:7:2824:G:H5''	14:7:2825:C:P	2.59	0.41
9:L:6:PRO:HG3	9:L:14:LYS:HG2	2.03	0.41
11:2:2270:A:H2'	11:2:2271:A:O4'	2.20	0.41
11:2:2213:A:C6	11:2:2214:A:N6	2.89	0.41
10:X:39:ILE:HA	10:X:42:ASN:HD22	1.85	0.41
9:L:81:LYS:C	9:L:81:LYS:HD2	2.41	0.41
12:3:2482:U:C2'	15:B:97:LYS:N	2.84	0.41
11:2:2258:U:H3'	11:2:2259:A:C8	2.50	0.41
16:J:169:LYS:CB	16:J:177:ASP:O	2.69	0.41
18:W:29:G:H8	18:W:29:G:O5'	2.04	0.41
11:2:2236:G:H2'	11:2:2237:C:O5'	2.21	0.41
14:7:2854:U:H5'	16:J:160:PRO:CA	2.46	0.41
11:2:2280:A:H8	11:2:2280:A:H3'	1.85	0.41
11:2:2276:G:N7	11:2:2277:C:H5	2.19	0.41
11:2:2285:C:C5	11:2:2286:U:N1	2.87	0.41
10:X:8:LEU:C	10:X:10:LYS:N	2.73	0.41
18:W:4:G:O2'	18:W:5:G:H8	2.00	0.41
8:S:63:ASN:HA	8:S:66:ARG:HB2	2.02	0.41
8:S:92:PRO:HA	8:S:117:ILE:HD13	2.03	0.41
16:J:217:PHE:O	16:J:220:GLN:N	2.54	0.41
13:9:2680:A:OP2	13:9:2681:U:C6	2.72	0.41
11:2:2253:G:N1	11:2:2263:C:N3	2.57	0.41
18:W:41:C:H2'	18:W:42:G:O4'	2.21	0.41
18:W:14:A:C4	18:W:37:A:C6	33.23	0.41
14:7:2826:U:C4	14:7:2827:U:C4	3.08	0.41
18:W:70:G:H2'	18:W:71:C:O4'	2.21	0.41
9:L:131:LEU:O	9:L:134:LEU:N	2.53	0.41
13:9:2675:C:OP2	13:9:2676:A:H5''	2.21	0.40
13:9:2673:A:N6	13:9:2681:U:H3	2.07	0.40
18:Y:36:U:C2'	18:Y:37:A:O5'	2.70	0.40
11:2:2201:G:C5	11:2:2202:C:C5	3.09	0.40
11:2:2260:U:C4'	11:2:2260:U:OP1	2.68	0.40
11:2:2299:A:C2'	11:2:2300:G:O5'	2.68	0.40
18:W:71:C:H5'	18:W:72:A:OP2	2.21	0.40
18:Y:49:G:H1	18:Y:65:C:N4	2.18	0.40
18:W:39:C:H2'	18:W:40:C:C6	2.54	0.40
12:3:2483:G:O6	15:B:128:LEU:CA	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:2857:C:H2'	14:7:2858:U:O4'	2.21	0.40
18:W:3:C:N4	18:W:70:G:H1	2.16	0.40
8:S:16:LYS:HG3	8:S:20:GLU:OE1	2.21	0.40
8:S:21:LEU:HA	8:S:24:LEU:HB3	2.03	0.40
16:J:215:GLU:O	16:J:217:PHE:N	2.55	0.40
13:9:2675:C:H5	13:9:2676:A:C5	2.36	0.40
10:X:65:GLY:HA2	10:X:70:MET:HE1	2.03	0.40
18:W:46:G:C8	18:W:46:G:H3'	2.55	0.40
11:2:2291:A:C6	11:2:2292:U:N3	2.90	0.40
14:7:2843:U:OP2	14:7:2843:U:H3'	2.21	0.40
14:7:2830:G:H8	14:7:2830:G:H5'	1.87	0.40
18:W:36:U:C2'	18:W:37:A:O5'	2.69	0.40
18:W:38:A:C6	18:W:39:C:C2	3.09	0.40
13:9:2684:C:C2'	13:9:2685:C:O5'	2.70	0.40
12:3:2484:A:C5'	18:W:56:C:C2	3.03	0.40
16:J:148:VAL:O	16:J:149:VAL:C	2.59	0.40
14:7:2849:C:C2'	14:7:2849:C:O2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	123/125 (98%)	90 (73%)	25 (20%)	8 (6%)	1	25
9	L	139/141 (99%)	106 (76%)	18 (13%)	15 (11%)	0	11
10	X	66/68 (97%)	48 (73%)	12 (18%)	6 (9%)	1	17
15	B	211/213 (99%)	76 (36%)	67 (32%)	68 (32%)	0	0
16	J	204/219 (93%)	80 (39%)	52 (26%)	72 (35%)	0	0
17	k	163/165 (99%)	57 (35%)	42 (26%)	64 (39%)	0	0
All	All	906/931 (97%)	457 (50%)	216 (24%)	233 (26%)	0	1

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	15	GLY
9	L	45	ALA
9	L	62	GLN
9	L	87	PRO
9	L	88	MET
9	L	89	ASP
9	L	107	GLY
9	L	108	ARG
9	L	117	PRO
10	X	8	LEU
10	X	64	ALA
15	B	24	LYS
15	B	36	VAL
15	B	39	LYS
15	B	42	ASP
15	B	43	PRO
15	B	55	LEU
15	B	56	PRO
15	B	58	CYS
15	B	59	PRO
15	B	60	ARG
15	B	61	PRO
15	B	109	ALA
15	B	115	VAL
15	B	120	VAL
15	B	122	ARG
15	B	124	LEU
15	B	126	PRO
15	B	127	GLN
15	B	128	LEU
15	B	129	SER
15	B	135	PRO
15	B	143	ASP
15	B	151	VAL
15	B	174	MET
15	B	201	VAL
15	B	207	LYS
15	B	208	SER
15	B	209	SER
15	B	210	MET
15	B	212	PRO
16	J	5	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	J	11	TYR
16	J	13	LYS
16	J	14	ASN
16	J	16	PRO
16	J	17	TYR
16	J	25	ALA
16	J	29	SER
16	J	34	TYR
16	J	39	LYS
16	J	43	VAL
16	J	46	PHE
16	J	48	LEU
16	J	57	LEU
16	J	61	SER
16	J	70	ILE
16	J	92	HIS
16	J	115	MET
16	J	136	PHE
16	J	145	LYS
16	J	147	VAL
16	J	160	PRO
16	J	162	GLN
16	J	169	LYS
16	J	178	ARG
16	J	190	VAL
16	J	201	SER
16	J	208	ASN
17	k	8	PRO
17	k	15	GLU
17	k	18	VAL
17	k	23	VAL
17	k	32	ARG
17	k	34	SER
17	k	45	PRO
17	k	47	GLN
17	k	49	LYS
17	k	50	ALA
17	k	52	TYR
17	k	54	VAL
17	k	55	ARG
17	k	56	THR
17	k	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	k	65	ILE
17	k	66	ALA
17	k	69	VAL
17	k	76	ALA
17	k	85	LYS
17	k	86	VAL
17	k	88	GLU
17	k	102	PHE
17	k	108	GLU
17	k	110	ILE
17	k	115	LYS
17	k	118	PRO
17	k	120	ILE
17	k	122	ILE
17	k	129	VAL
17	k	132	ASN
17	k	133	ARG
17	k	134	PRO
17	k	143	ARG
17	k	148	VAL
17	k	154	THR
8	S	31	GLU
8	S	33	LEU
9	L	35	GLY
9	L	54	GLU
9	L	76	ARG
9	L	138	LYS
10	X	24	LYS
15	B	25	LYS
15	B	26	ARG
15	B	41	TYR
15	B	44	GLN
15	B	47	LYS
15	B	67	ILE
15	B	77	ALA
15	B	96	ASN
15	B	117	ILE
15	B	123	LEU
15	B	169	VAL
15	B	193	LEU
15	B	194	LEU
15	B	196	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	B	197	ASN
15	B	204	LEU
15	B	206	VAL
16	J	12	GLN
16	J	21	ARG
16	J	28	ASP
16	J	35	ASP
16	J	36	LEU
16	J	78	THR
16	J	84	ALA
16	J	86	HIS
16	J	93	PRO
16	J	95	HIS
16	J	143	SER
16	J	175	ASN
16	J	177	ASP
16	J	185	ARG
16	J	189	GLU
16	J	196	PHE
16	J	207	GLU
17	k	11	ASP
17	k	31	THR
17	k	77	GLU
17	k	82	ARG
17	k	83	GLY
17	k	92	ARG
17	k	94	ARG
17	k	112	LEU
17	k	121	GLY
17	k	123	PHE
17	k	127	PHE
17	k	141	ARG
17	k	170	ASP
8	S	130	PRO
9	L	91	CYS
9	L	109	GLN
10	X	60	PRO
15	B	22	GLU
15	B	49	PHE
15	B	57	ASN
15	B	101	LYS
15	B	102	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	B	152	ARG
15	B	202	GLY
16	J	15	LYS
16	J	47	PRO
16	J	56	GLU
16	J	85	PHE
16	J	94	PHE
16	J	181	TYR
16	J	205	SER
16	J	214	PRO
17	k	35	LYS
17	k	119	SER
17	k	156	LYS
17	k	167	TYR
10	X	25	ASP
15	B	27	ASN
15	B	107	TYR
15	B	132	GLY
15	B	155	ILE
15	B	165	LEU
15	B	189	PHE
15	B	213	ALA
16	J	20	SER
16	J	60	LEU
16	J	66	GLU
16	J	91	VAL
16	J	154	ARG
16	J	163	GLN
17	k	98	ALA
17	k	106	ILE
17	k	144	CYS
8	S	123	GLU
10	X	26	LYS
15	B	5	THR
15	B	45	ARG
15	B	92	LYS
15	B	108	ASN
15	B	154	THR
16	J	8	CYS
16	J	41	ALA
16	J	67	ALA
16	J	171	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	J	212	GLU
17	k	12	LEU
17	k	44	THR
17	k	130	VAL
8	S	85	TYR
17	k	36	VAL
17	k	75	LYS
17	k	157	GLU
8	S	104	GLY
16	J	4	ARG
16	J	172	GLY
16	J	194	GLY
15	B	69	GLY
9	L	110	GLY
15	B	65	ILE
16	J	18	PRO
16	J	117	GLY
16	J	131	ILE
17	k	105	GLY
17	k	117	ASP
8	S	53	GLY
16	J	27	PRO
16	J	89	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	L	113/113 (100%)	102 (90%)	11 (10%)	10	40
10	X	57/57 (100%)	55 (96%)	2 (4%)	43	74
All	All	275/275 (100%)	258 (94%)	17 (6%)	27	60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	66	ARG
8	S	83	THR
8	S	85	TYR
8	S	124	PHE
9	L	9	ILE
9	L	19	ARG
9	L	33	LEU
9	L	55	LYS
9	L	69	LYS
9	L	81	LYS
9	L	82	ILE
9	L	89	ASP
9	L	92	LEU
9	L	106	LEU
9	L	132	LEU
10	X	34	ARG
10	X	62	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
8	S	29	ASN
8	S	84	HIS
8	S	133	HIS
9	L	62	GLN
9	L	78	ASN
9	L	98	ASN
10	X	42	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	47/48 (97%)	15 (31%)	0
11	2	111/112 (99%)	54 (48%)	9 (8%)
12	3	11/12 (91%)	6 (54%)	1 (9%)
13	9	18/19 (94%)	13 (72%)	1 (5%)
14	7	49/50 (98%)	29 (59%)	5 (10%)
18	W	76/77 (98%)	17 (22%)	0
18	Y	76/77 (98%)	17 (22%)	0
19	y	2/3 (66%)	0	0
2	c	16/17 (94%)	4 (25%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	w	1/2 (50%)	0	0
3	d	6/7 (85%)	2 (33%)	0
4	g	30/31 (96%)	8 (26%)	0
5	G	12/13 (92%)	2 (16%)	1 (8%)
6	f	20/21 (95%)	5 (25%)	0
7	h	110/111 (99%)	12 (10%)	0
All	All	585/600 (97%)	184 (31%)	17 (2%)

All (184) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	544	G
1	a	547	C
1	a	548	A
1	a	552	C
1	a	553	A
1	a	554	U
1	a	559	C
1	a	560	C
1	a	568	G
1	a	573	A
1	a	574	A
1	a	575	U
1	a	576	U
1	a	577	C
1	a	588	A
2	c	975	G
2	c	976	A
2	c	978	C
2	c	982	U
3	d	1545	A
3	d	1546	G
4	g	1155	A
4	g	1158	U
4	g	1163	U
4	g	1165	A
4	g	1166	A
4	g	1168	A
4	g	1169	C
4	g	1172	G
5	G	1430	C
5	G	1431	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	1242	G
6	f	1245	G
6	f	1246	C
6	f	1247	A
6	f	1256	C
7	h	1608	C
7	h	1609	C
7	h	1624	G
7	h	1649	U
7	h	1651	G
7	h	1652	A
7	h	1661	G
7	h	1674	A
7	h	1710	G
7	h	1713	G
7	h	1714	U
7	h	1715	A
11	2	2195	C
11	2	2201	G
11	2	2205	U
11	2	2206	G
11	2	2207	A
11	2	2208	A
11	2	2209	U
11	2	2210	G
11	2	2211	U
11	2	2215	A
11	2	2222	A
11	2	2223	A
11	2	2224	A
11	2	2227	C
11	2	2237	C
11	2	2244	A
11	2	2247	G
11	2	2248	C
11	2	2249	G
11	2	2250	G
11	2	2252	A
11	2	2254	U
11	2	2255	A
11	2	2256	A
11	2	2257	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2	2259	A
11	2	2260	U
11	2	2261	G
11	2	2262	A
11	2	2263	C
11	2	2264	U
11	2	2266	U
11	2	2270	A
11	2	2272	G
11	2	2273	G
11	2	2275	A
11	2	2276	G
11	2	2277	C
11	2	2280	A
11	2	2281	A
11	2	2282	U
11	2	2283	G
11	2	2286	U
11	2	2288	G
11	2	2290	C
11	2	2291	A
11	2	2292	U
11	2	2295	A
11	2	2296	A
11	2	2297	U
11	2	2298	U
11	2	2299	A
11	2	2300	G
11	2	2303	A
12	3	2479	C
12	3	2484	A
12	3	2485	A
12	3	2486	A
12	3	2487	U
12	3	2488	A
13	9	2671	A
13	9	2672	G
13	9	2675	C
13	9	2676	A
13	9	2677	G
13	9	2678	A
13	9	2679	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	9	2681	U
13	9	2682	C
13	9	2683	U
13	9	2684	C
13	9	2685	C
13	9	2686	A
14	7	2825	C
14	7	2826	U
14	7	2828	G
14	7	2829	U
14	7	2830	G
14	7	2833	A
14	7	2834	G
14	7	2835	U
14	7	2836	C
14	7	2838	A
14	7	2839	G
14	7	2840	C
14	7	2842	U
14	7	2843	U
14	7	2844	C
14	7	2845	A
14	7	2846	U
14	7	2847	A
14	7	2849	C
14	7	2850	G
14	7	2851	A
14	7	2852	C
14	7	2859	U
14	7	2860	U
14	7	2867	C
14	7	2870	C
14	7	2871	G
14	7	2872	A
14	7	2873	U
18	Y	4	G
18	Y	5	G
18	Y	8	U
18	Y	17	C
18	Y	17(A)	U
18	Y	18	G
18	Y	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Y	20	U
18	Y	21	A
18	Y	36	U
18	Y	47	U
18	Y	48	C
18	Y	63	G
18	Y	71	C
18	Y	74	C
18	Y	75	C
18	Y	76	A
18	W	4	G
18	W	5	G
18	W	8	U
18	W	17	C
18	W	17(A)	U
18	W	18	G
18	W	19	G
18	W	20	U
18	W	21	A
18	W	36	U
18	W	47	U
18	W	48	C
18	W	63	G
18	W	71	C
18	W	74	C
18	W	75	C
18	W	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	G	1430	C
11	2	2211	U
11	2	2251	G
11	2	2254	U
11	2	2255	A
11	2	2270	A
11	2	2280	A
11	2	2281	A
11	2	2290	C
11	2	2297	U
12	3	2487	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	9	2684	C
14	7	2834	G
14	7	2850	G
14	7	2851	A
14	7	2859	U
14	7	2872	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.