



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:41 AM GMT

PDB ID : 3I22  
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting  
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.  
Deposited on : 2009-06-28  
Resolution : 3.71 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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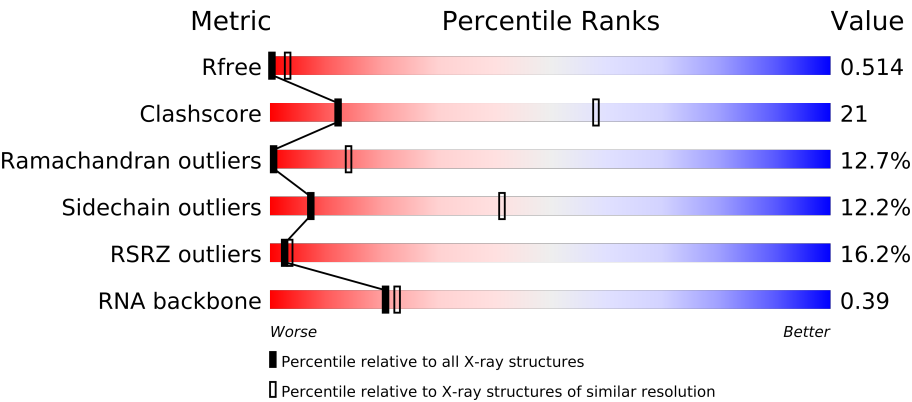
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.71 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
Ramachandran outliers	78287	1082 (4.00-3.44)
Sidechain outliers	78261	1075 (4.00-3.44)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	117	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	I	142	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	0	57	
28	1	55	
29	2	46	
30	3	65	
31	4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2905	-	X
32	MG	A	2909	-	X
32	MG	A	2914	-	X
32	MG	A	2917	-	X
32	MG	A	2923	-	X
32	MG	A	2929	-	X
32	MG	A	2933	-	X
32	MG	A	2935	-	X
32	MG	A	2958	-	X
32	MG	A	2960	-	X
32	MG	A	2961	-	X
32	MG	A	2966	-	X
32	MG	A	2967	-	X
32	MG	A	2983	-	X
32	MG	A	2984	-	X
32	MG	A	2989	-	X
32	MG	A	2997	-	X
32	MG	A	2999	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	3000	-	X
32	MG	A	3001	-	X
32	MG	A	3011	-	X
32	MG	A	3019	-	X
32	MG	A	3022	-	X
32	MG	A	3026	-	X
32	MG	A	3030	-	X
32	MG	A	3032	-	X
32	MG	A	3036	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90428 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	94	Total	C	N	O	S			
			753	479	137	134	3	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	79	Total	C	N	O	S			
			596	367	120	108	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	77	Total	C	N	O	S			
			625	388	129	106	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S			
			444	269	94	80	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	1	Total	Mg	0	0
			1	1		
32	A	133	Total	Mg	0	0
			133	133		
32	C	2	Total	Mg	0	0
			2	2		
32	J	1	Total	Mg	0	0
			1	1		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

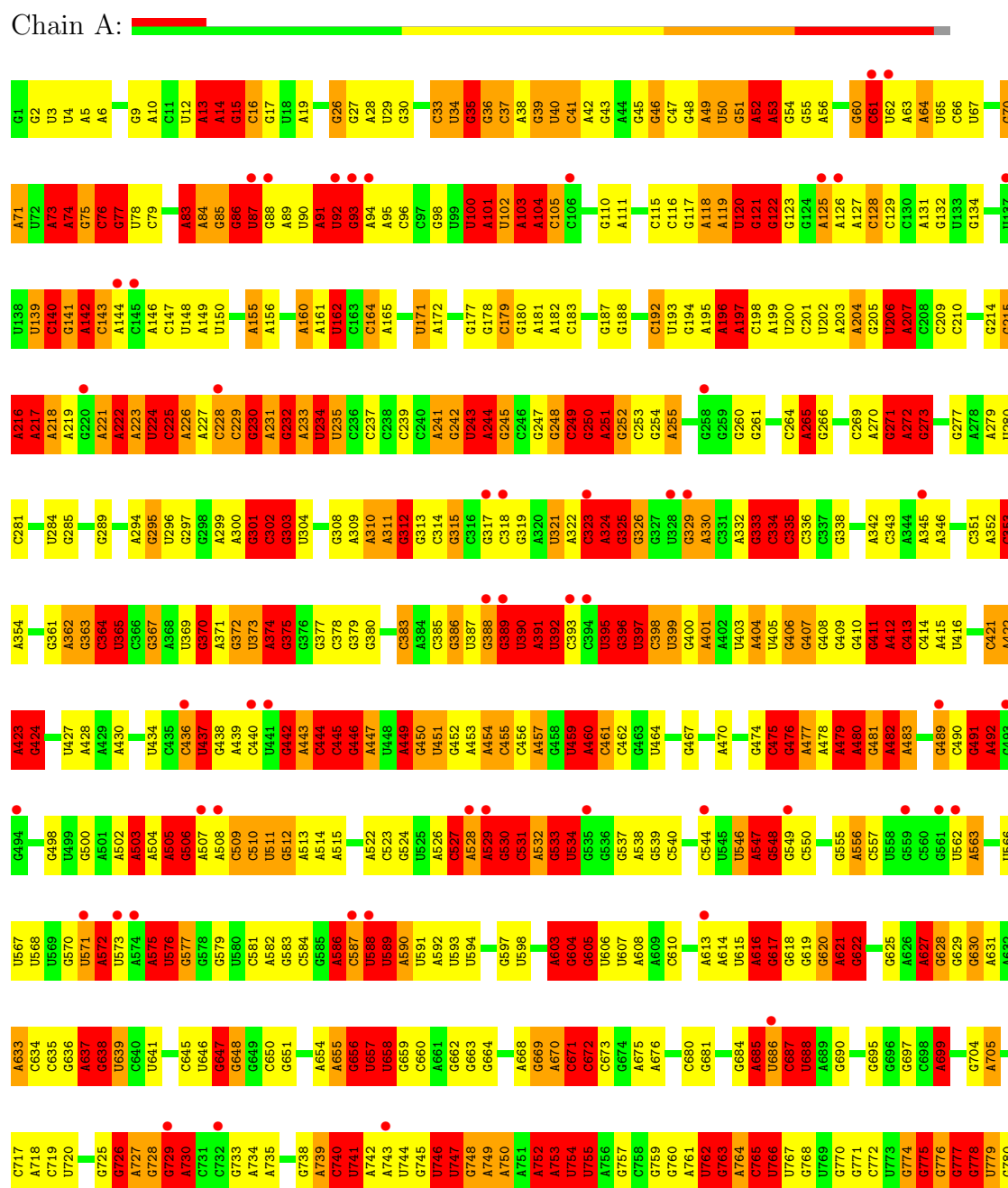
- Molecule 34 is water.

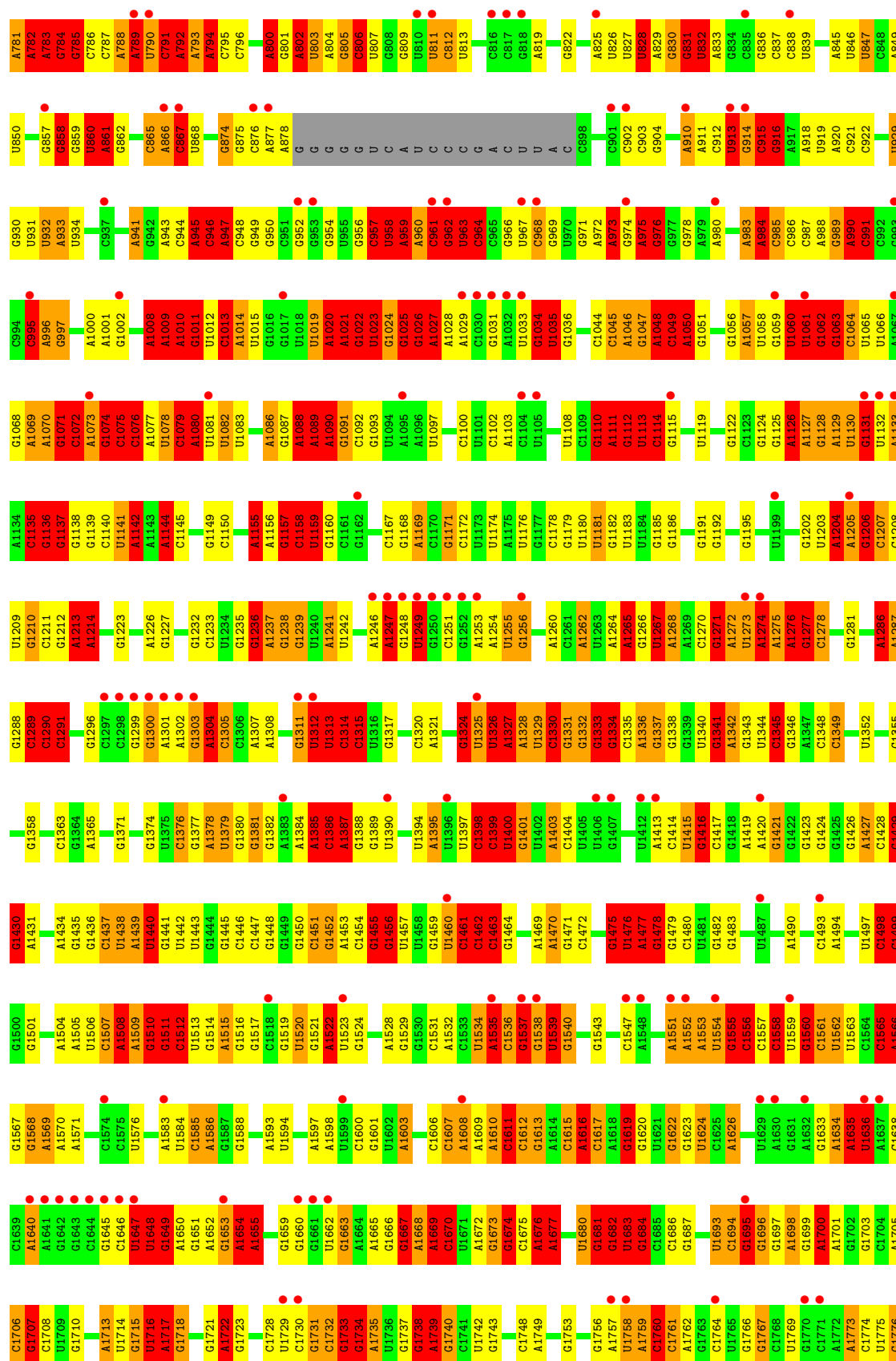
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	603	Total O 603 603	0	0
34	B	5	Total O 5 5	0	0
34	C	10	Total O 10 10	0	0
34	D	2	Total O 2 2	0	0
34	E	3	Total O 3 3	0	0
34	J	6	Total O 6 6	0	0
34	L	4	Total O 4 4	0	0
34	N	2	Total O 2 2	0	0
34	T	2	Total O 2 2	0	0
34	U	1	Total O 1 1	0	0
34	2	1	Total O 1 1	0	0
34	3	1	Total O 1 1	0	0
34	4	3	Total O 3 3	0	0

### 3 Residue-property plots

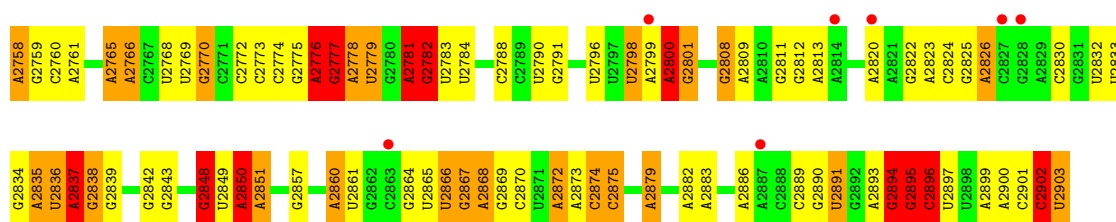
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: 23S rRNA



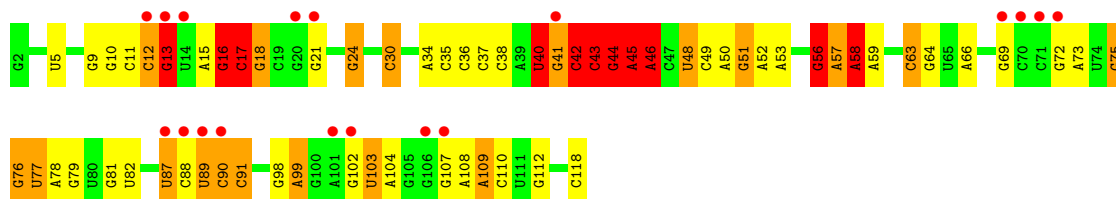






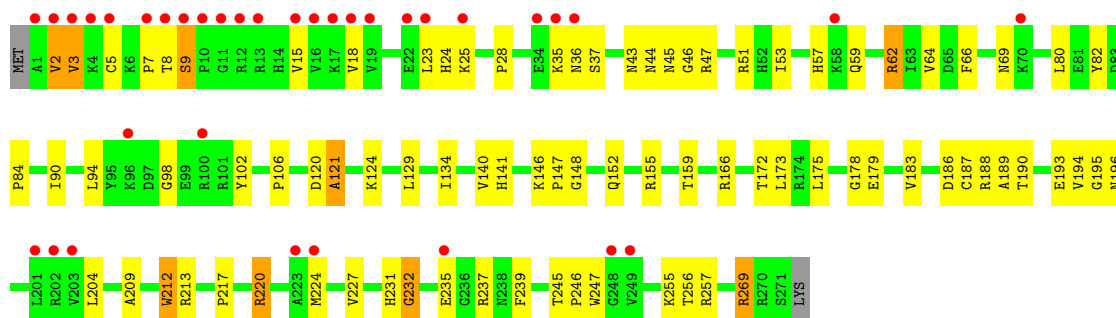
• Molecule 2: 5S rRNA

Chain B:



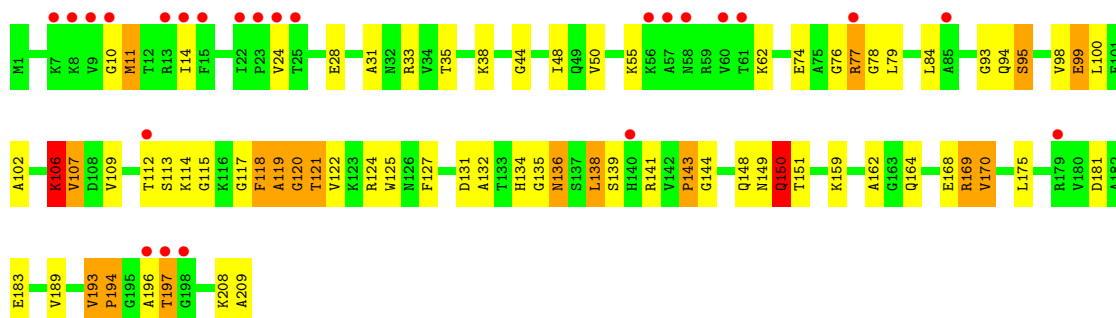
• Molecule 3: 50S ribosomal protein L2

Chain C:



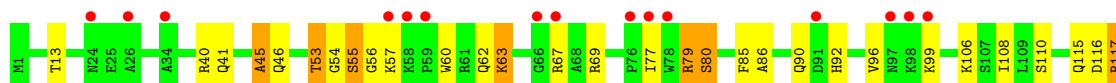
• Molecule 4: 50S ribosomal protein L3

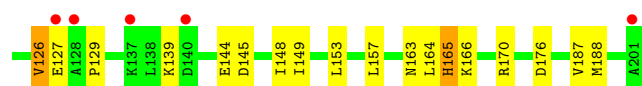
Chain D:



• Molecule 5: 50S ribosomal protein L4

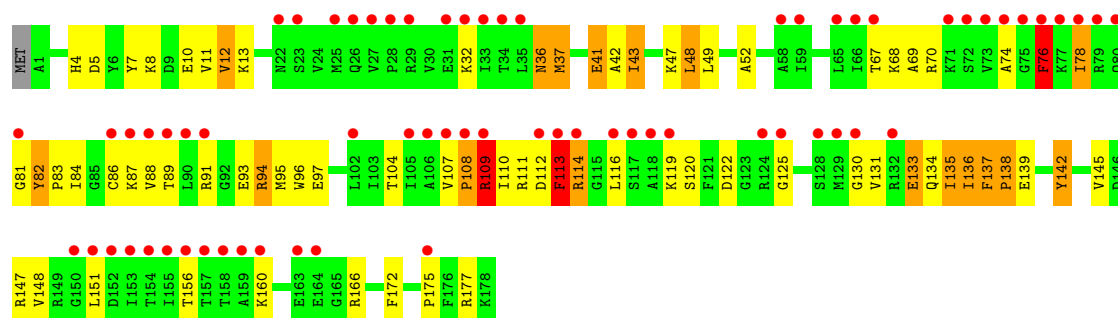
Chain E:





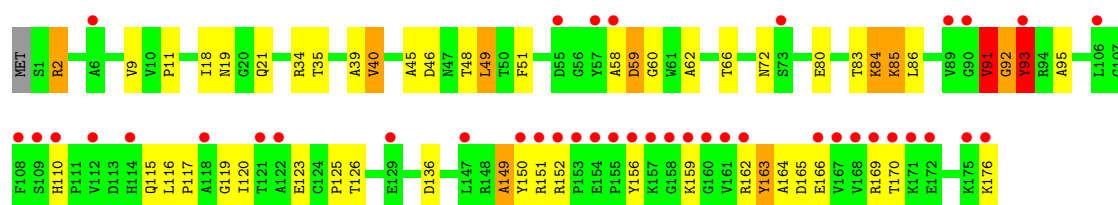
• Molecule 6: 50S ribosomal protein L5

Chain F:



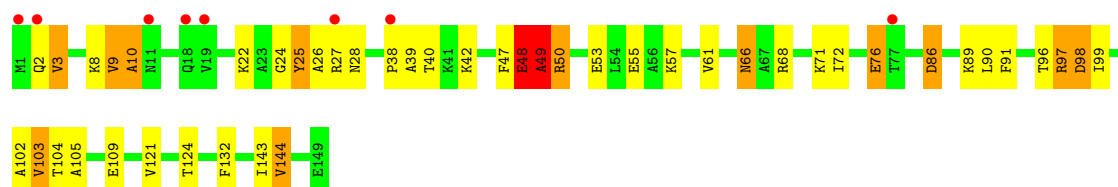
• Molecule 7: 50S ribosomal protein L6

Chain G:



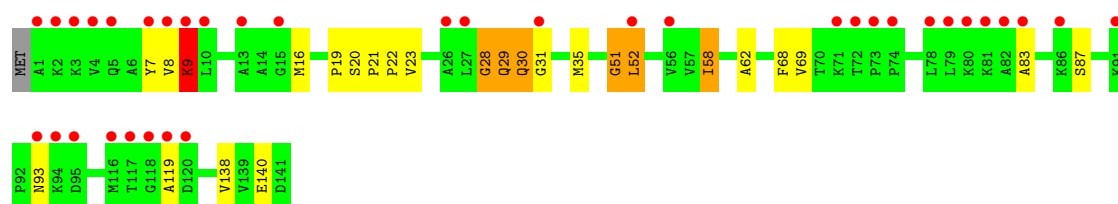
• Molecule 8: 50S ribosomal protein L9

Chain H:



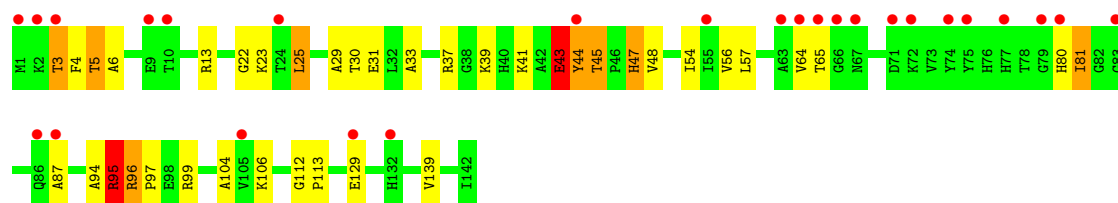
• Molecule 9: 50S ribosomal protein L11

Chain I:



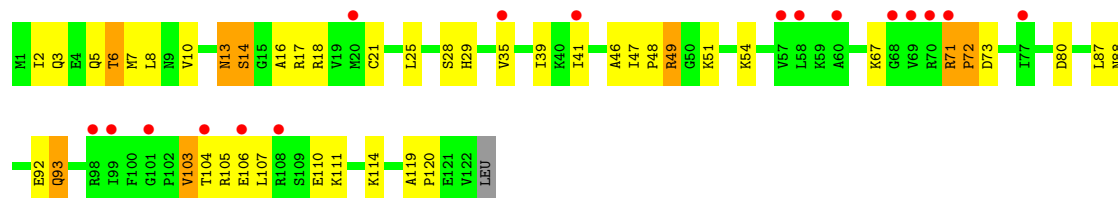
• Molecule 10: 50S ribosomal protein L13

Chain J:



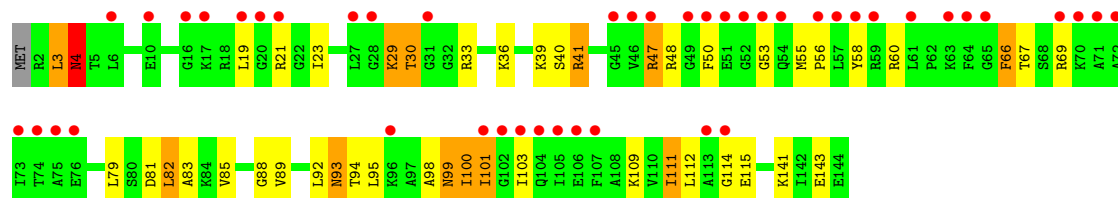
• Molecule 11: 50S ribosomal protein L14

Chain K:



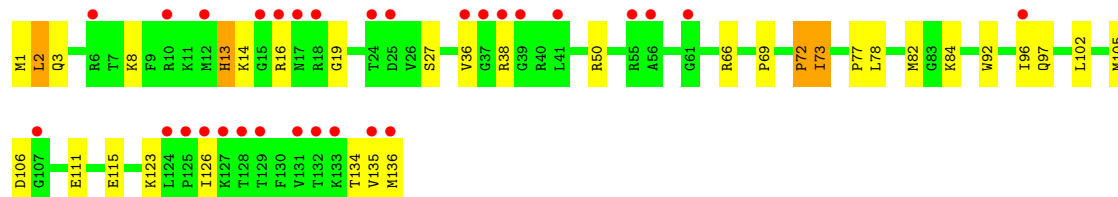
• Molecule 12: 50S ribosomal protein L15

Chain L:



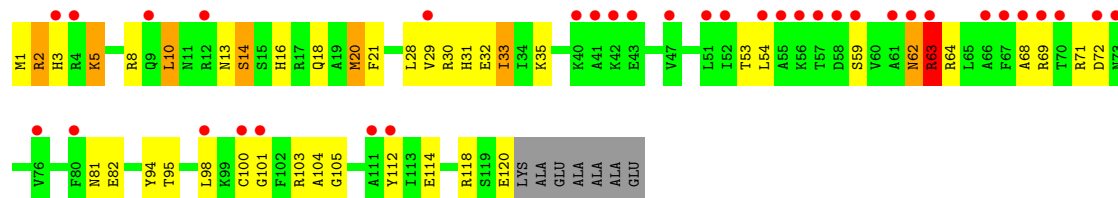
• Molecule 13: 50S ribosomal protein L16

Chain M:



• Molecule 14: 50S ribosomal protein L17

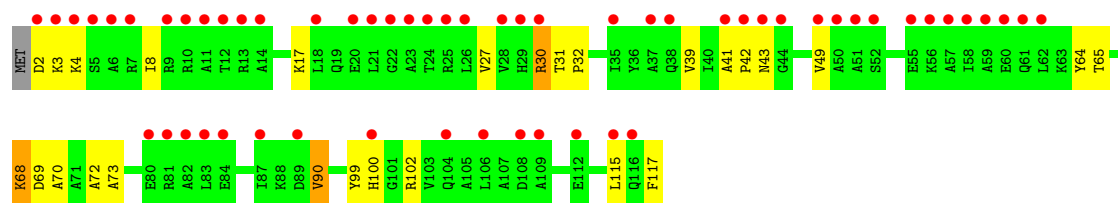
Chain N:



• Molecule 15: 50S ribosomal protein L18

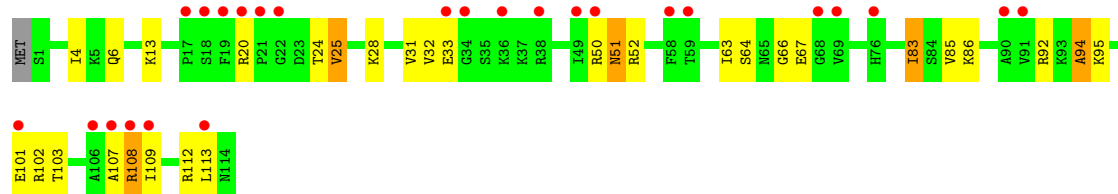
Chain O:





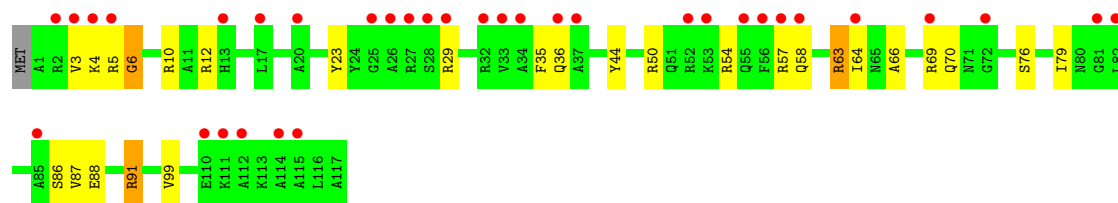
• Molecule 16: 50S ribosomal protein L19

Chain P:



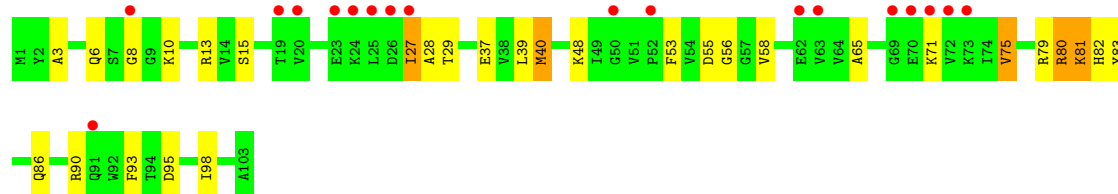
• Molecule 17: 50S ribosomal protein L20

Chain Q:



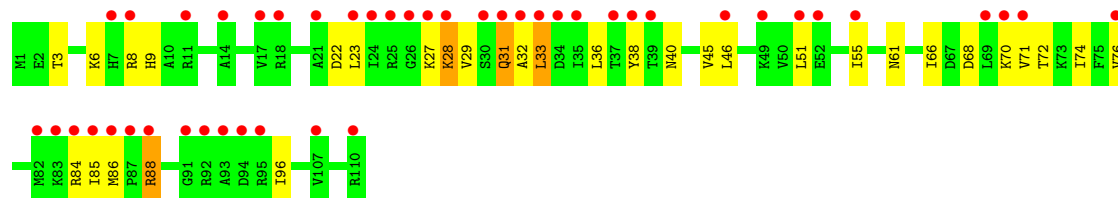
• Molecule 18: 50S ribosomal protein L21

Chain R:



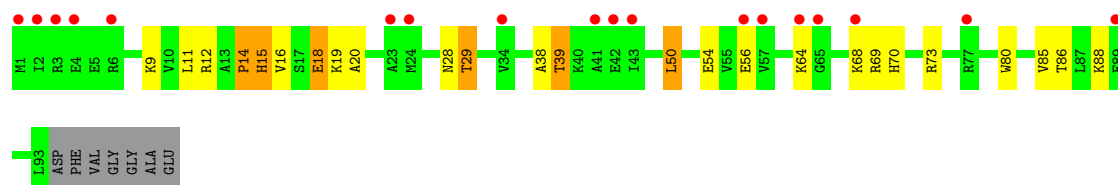
• Molecule 19: 50S ribosomal protein L22

Chain S:



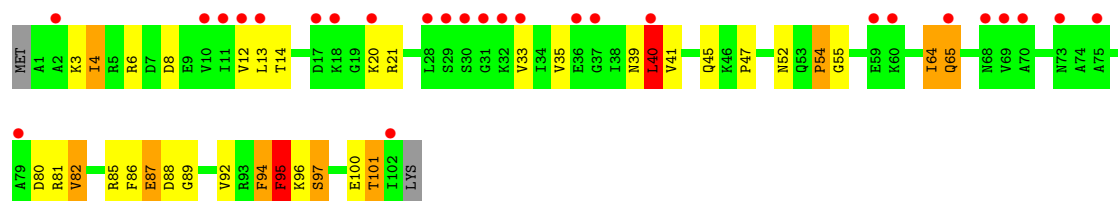
• Molecule 20: 50S ribosomal protein L23

Chain T:



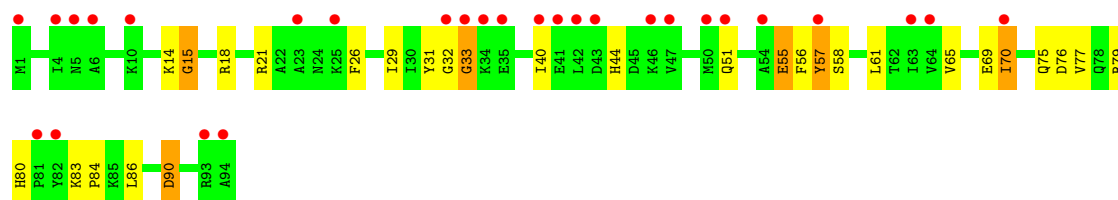
- Molecule 21: 50S ribosomal protein L24

Chain U:



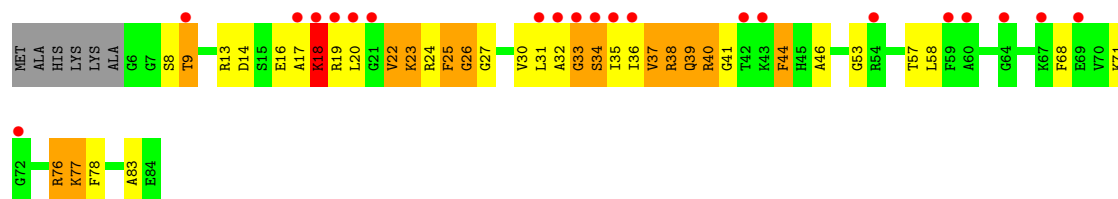
- Molecule 22: 50S ribosomal protein L25

Chain V:



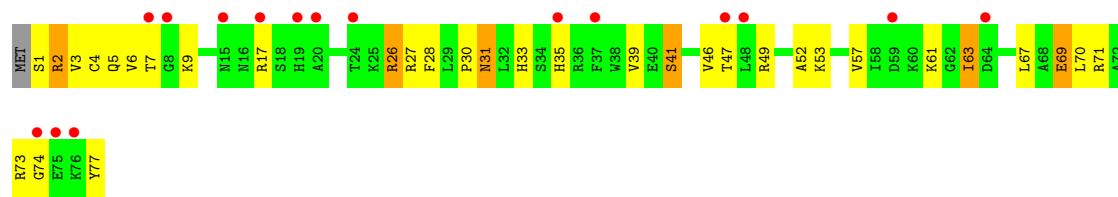
- Molecule 23: 50S ribosomal protein L27

Chain W:



- Molecule 24: 50S ribosomal protein L28

Chain X:



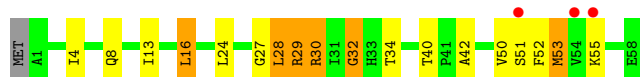
- Molecule 25: 50S ribosomal protein L29

Chain Y:



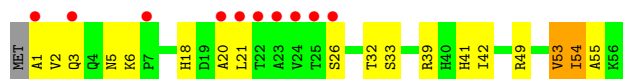
- Molecule 26: 50S ribosomal protein L30

Chain Z: 



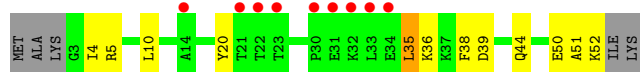
- Molecule 27: 50S ribosomal protein L32

Chain 0: 



- Molecule 28: 50S ribosomal protein L33

Chain 1: 



- Molecule 29: 50S ribosomal protein L34

Chain 2: 



- Molecule 30: 50S ribosomal protein L35

Chain 3: 



- Molecule 31: 50S ribosomal protein L36

Chain 4: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.227 , 0.268 0.508 , 0.514	Depositor DCC
$R_{free}$ test set	9145 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 80.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 452802 reflections	Xtriage
$F_o, F_c$ correlation	0.58	EDS
Total number of atoms	90428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.53	1/68314 (0.0%)	1.46	1365/106569 (1.3%)
2	B	0.52	0/2803	1.35	52/4371 (1.2%)
3	C	0.33	0/2121	0.54	0/2852
4	D	0.31	0/1586	0.55	0/2134
5	E	0.25	0/1571	0.47	0/2113
6	F	0.35	0/1444	0.73	5/1937 (0.3%)
7	G	0.23	0/1343	0.46	0/1816
8	H	0.53	3/1122 (0.3%)	0.67	3/1515 (0.2%)
9	I	0.23	0/1046	0.44	0/1410
10	J	0.28	0/1152	0.55	0/1551
11	K	0.31	0/947	0.54	0/1268
12	L	0.27	0/1054	0.51	0/1403
13	M	0.31	0/1093	0.48	0/1460
14	N	0.27	0/973	0.49	0/1301
15	O	0.24	0/902	0.44	0/1209
16	P	0.28	0/929	0.49	0/1242
17	Q	0.28	0/960	0.46	0/1278
18	R	0.28	0/829	0.50	0/1107
19	S	0.29	0/864	0.54	0/1156
20	T	0.25	0/744	0.49	0/994
21	U	0.25	0/787	0.47	0/1051
22	V	0.38	0/766	0.54	0/1025
23	W	0.26	0/603	0.47	0/797
24	X	0.30	0/635	0.55	0/848
25	Y	0.23	0/510	0.44	0/677
26	Z	0.28	0/453	0.51	0/605
27	0	0.28	0/450	0.51	0/599
28	1	0.28	0/416	0.46	0/554
29	2	0.28	0/380	0.55	0/498
30	3	0.26	0/513	0.51	0/676
31	4	0.30	0/303	0.49	0/397
All	All	0.48	4/97613 (0.0%)	1.29	1425/146413 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	49	ALA	CA-CB	-7.88	1.35	1.52
1	A	1060	U	C2-N3	6.91	1.42	1.37
8	H	48	GLU	CB-CG	6.81	1.65	1.52
8	H	50	ARG	CB-CG	-5.09	1.38	1.52

All (1425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	109	ARG	NE-CZ-NH1	-14.18	113.21	120.30
1	A	2283	C	N1-C1'-C2'	-14.13	95.63	114.00
1	A	861	A	P-O3'-C3'	-13.83	103.11	119.70
1	A	2586	U	N1-C1'-C2'	-13.74	96.14	114.00
1	A	1956	U	N1-C1'-C2'	-13.43	96.54	114.00
1	A	1499	C	N1-C1'-C2'	-13.40	96.58	114.00
6	F	109	ARG	NE-CZ-NH2	13.28	126.94	120.30
1	A	832	U	N1-C1'-C2'	-13.26	96.76	114.00
1	A	1536	C	P-O3'-C3'	13.22	135.57	119.70
1	A	2441	U	N1-C1'-C2'	-13.20	96.84	114.00
1	A	1267	U	N1-C1'-C2'	-13.20	96.85	114.00
1	A	741	U	N1-C1'-C2'	-13.18	96.86	114.00
1	A	2403	C	N1-C1'-C2'	-13.16	96.89	114.00
1	A	964	C	N1-C1'-C2'	-13.16	96.89	114.00
1	A	1060	U	C5-C4-O4	-13.15	118.01	125.90
1	A	1612	C	N1-C1'-C2'	-13.10	96.97	114.00
1	A	1556	C	N1-C1'-C2'	-12.85	97.29	114.00
1	A	1023	U	N1-C1'-C2'	-12.83	97.32	114.00
1	A	2061	G	P-O3'-C3'	12.80	135.06	119.70
1	A	2504	U	N1-C1'-C2'	-12.75	97.42	114.00
1	A	1611	C	N1-C1'-C2'	-12.74	97.43	114.00
1	A	2063	C	N1-C1'-C2'	-12.71	97.48	114.00
1	A	1963	U	N1-C1'-C2'	-12.55	97.68	114.00
2	B	90	C	N1-C1'-C2'	-12.52	97.72	114.00
1	A	2493	U	N1-C1'-C2'	-12.48	97.78	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2568	U	N1-C1'-C2'	-12.46	97.80	114.00
1	A	813	U	N1-C1'-C2'	-12.45	97.82	114.00
1	A	784	G	P-O3'-C3'	12.40	134.58	119.70
1	A	76	C	N1-C1'-C2'	-12.37	97.92	114.00
1	A	807	U	N1-C1'-C2'	-12.37	97.92	114.00
1	A	87	U	N1-C1'-C2'	-12.27	98.05	114.00
1	A	2520	C	N1-C1'-C2'	-12.17	98.17	114.00
1	A	658	U	N1-C1'-C2'	-12.14	98.22	114.00
1	A	375	G	P-O3'-C3'	-12.14	105.14	119.70
1	A	460	A	P-O3'-C3'	-12.05	105.24	119.70
1	A	534	U	N1-C1'-C2'	-11.94	98.48	114.00
1	A	2261	C	N1-C1'-C2'	-11.94	98.48	114.00
1	A	392	U	N1-C1'-C2'	-11.91	98.51	114.00
1	A	1539	U	N1-C1'-C2'	-11.91	98.52	114.00
1	A	313	G	P-O3'-C3'	-11.85	105.48	119.70
1	A	1916	A	P-O3'-C3'	-11.83	105.51	119.70
1	A	2429	G	P-O3'-C3'	-11.80	105.54	119.70
1	A	576	U	N1-C1'-C2'	-11.78	98.69	114.00
1	A	364	C	N1-C1'-C2'	-11.77	98.70	114.00
1	A	413	C	N1-C1'-C2'	-11.77	98.71	114.00
1	A	1655	A	P-O3'-C3'	-11.75	105.60	119.70
1	A	1462	C	N1-C1'-C2'	-11.68	98.81	114.00
1	A	437	U	N1-C1'-C2'	-11.67	98.83	114.00
1	A	1683	U	N1-C1'-C2'	-11.65	98.85	114.00
1	A	128	C	N1-C1'-C2'	-11.59	98.93	114.00
1	A	2402	U	N1-C1'-C2'	-11.52	99.03	114.00
1	A	225	C	N1-C1'-C2'	-11.47	99.08	114.00
1	A	2348	U	N1-C1'-C2'	-11.45	99.11	114.00
1	A	617	G	P-O3'-C3'	-11.44	105.97	119.70
1	A	325	G	P-O3'-C3'	-11.44	105.97	119.70
1	A	672	C	N1-C1'-C2'	-11.44	99.13	114.00
1	A	1799	G	P-O3'-C3'	11.35	133.32	119.70
1	A	2339	C	N1-C1'-C2'	-11.34	99.25	114.00
1	A	2896	C	N1-C1'-C2'	-11.31	99.30	114.00
1	A	1788	C	N1-C1'-C2'	-11.28	99.34	114.00
1	A	2616	C	N1-C1'-C2'	-11.12	99.55	114.00
1	A	1997	C	N1-C1'-C2'	-11.07	99.61	114.00
1	A	1556	C	P-O3'-C3'	-11.05	106.44	119.70
1	A	1046	A	P-O3'-C3'	11.04	132.95	119.70
1	A	946	C	N1-C1'-C2'	-11.03	99.67	114.00
1	A	234	U	N1-C1'-C2'	-11.02	99.68	114.00
1	A	789	A	P-O3'-C3'	11.01	132.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1478	G	P-O3'-C3'	-11.01	106.49	119.70
1	A	991	C	N1-C1'-C2'	-11.00	99.70	114.00
1	A	1300	G	P-O3'-C3'	10.98	132.88	119.70
1	A	2499	C	N1-C1'-C2'	-10.96	99.75	114.00
1	A	765	C	N1-C1'-C2'	-10.93	99.79	114.00
1	A	311	A	P-O3'-C3'	10.92	132.80	119.70
1	A	444	C	N1-C1'-C2'	-10.88	99.85	114.00
2	B	46	A	P-O3'-C3'	-10.86	106.67	119.70
1	A	775	G	P-O3'-C3'	10.85	132.72	119.70
1	A	2612	C	N1-C1'-C2'	-10.84	99.91	114.00
1	A	1400	U	N1-C1'-C2'	-10.79	99.98	114.00
1	A	1552	A	O4'-C1'-N9	10.78	116.82	108.20
1	A	1439	A	C5-C6-N1	-10.77	112.31	117.70
1	A	1956	U	O4'-C1'-N1	10.77	116.81	108.20
1	A	2240	U	O4'-C1'-N1	10.77	116.81	108.20
1	A	1566	A	P-O3'-C3'	10.76	132.62	119.70
1	A	1684	G	P-O3'-C3'	-10.73	106.83	119.70
1	A	2728	U	O4'-C1'-N1	10.70	116.76	108.20
1	A	1967	C	N1-C1'-C2'	-10.69	100.10	114.00
1	A	1013	C	N1-C1'-C2'	-10.69	100.11	114.00
1	A	1304	A	P-O3'-C3'	-10.68	106.88	119.70
1	A	2586	U	P-O3'-C3'	-10.68	106.89	119.70
1	A	1816	C	N1-C1'-C2'	-10.67	100.13	114.00
1	A	397	U	N1-C1'-C2'	-10.66	100.14	114.00
1	A	1708	C	N1-C1'-C2'	-10.65	100.16	114.00
1	A	2778	A	P-O3'-C3'	10.64	132.47	119.70
1	A	2314	A	P-O3'-C3'	-10.63	106.94	119.70
1	A	622	G	P-O3'-C3'	-10.61	106.97	119.70
1	A	1126	A	P-O3'-C3'	10.57	132.39	119.70
1	A	1648	U	N1-C1'-C2'	-10.52	100.33	114.00
1	A	421	C	P-O3'-C3'	10.49	132.29	119.70
1	A	2267	A	N1-C6-N6	10.43	124.86	118.60
1	A	964	C	O4'-C1'-N1	10.41	116.53	108.20
1	A	1499	C	O4'-C1'-N1	10.41	116.53	108.20
1	A	321	U	O4'-C1'-N1	10.41	116.53	108.20
1	A	225	C	O4'-C1'-N1	10.40	116.52	108.20
1	A	2692	G	P-O3'-C3'	-10.38	107.24	119.70
1	A	206	U	N1-C1'-C2'	-10.38	100.51	114.00
1	A	2068	U	N1-C1'-C2'	-10.36	100.53	114.00
1	A	436	C	O4'-C1'-N1	10.36	116.48	108.20
1	A	2261	C	P-O3'-C3'	-10.34	107.29	119.70
1	A	2226	C	N1-C1'-C2'	-10.33	100.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2611	C	N1-C1'-C2'	-10.33	100.57	114.00
1	A	2447	G	P-O3'-C3'	10.32	132.09	119.70
1	A	1315	C	N1-C1'-C2'	-10.31	100.60	114.00
1	A	1561	C	N1-C1'-C2'	-10.29	100.62	114.00
1	A	1667	G	P-O3'-C3'	10.27	132.03	119.70
1	A	2064	C	N1-C1'-C2'	-10.25	100.67	114.00
1	A	2064	C	P-O3'-C3'	-10.23	107.42	119.70
1	A	687	C	N1-C1'-C2'	-10.22	100.71	114.00
1	A	2214	C	N1-C1'-C2'	-10.22	100.71	114.00
1	A	234	U	O4'-C1'-N1	10.21	116.37	108.20
1	A	53	A	P-O3'-C3'	-10.18	107.49	119.70
1	A	792	A	P-O3'-C3'	10.18	131.91	119.70
1	A	1049	C	N1-C1'-C2'	-10.16	100.79	114.00
1	A	1957	C	P-O3'-C3'	-10.11	107.57	119.70
1	A	2064	C	O4'-C1'-N1	10.11	116.28	108.20
1	A	548	G	P-O3'-C3'	-10.09	107.59	119.70
1	A	1114	C	N1-C1'-C2'	-10.08	100.90	114.00
1	A	2581	G	P-O3'-C3'	10.06	131.77	119.70
1	A	459	U	N1-C1'-C2'	-10.05	100.93	114.00
1	A	2440	C	N1-C1'-C2'	-10.05	100.94	114.00
1	A	997	G	P-O3'-C3'	-10.03	107.67	119.70
1	A	445	C	N1-C1'-C2'	-10.01	100.99	114.00
1	A	2023	C	N1-C1'-C2'	-9.99	101.01	112.00
1	A	273	G	P-O3'-C3'	-9.96	107.75	119.70
1	A	179	C	N1-C1'-C2'	-9.93	101.07	112.00
1	A	915	C	N1-C1'-C2'	-9.91	101.10	112.00
1	A	1265	A	P-O3'-C3'	9.90	131.58	119.70
1	A	831	G	P-O3'-C3'	-9.89	107.83	119.70
1	A	229	C	N1-C1'-C2'	-9.87	101.14	112.00
1	A	2758	A	P-O3'-C3'	-9.86	107.86	119.70
1	A	2339	C	O4'-C1'-N1	9.86	116.09	108.20
1	A	1819	A	P-O3'-C3'	9.84	131.50	119.70
1	A	860	U	N1-C1'-C2'	-9.82	101.20	112.00
1	A	392	U	P-O3'-C3'	-9.81	107.92	119.70
1	A	2215	C	P-O3'-C3'	-9.81	107.92	119.70
1	A	916	G	P-O3'-C3'	-9.81	107.93	119.70
1	A	2347	C	N1-C1'-C2'	-9.81	101.21	112.00
1	A	1035	U	P-O3'-C3'	-9.78	107.97	119.70
1	A	2615	U	N1-C1'-C2'	-9.78	101.25	112.00
1	A	2568	U	P-O3'-C3'	-9.77	107.97	119.70
1	A	1387	A	P-O3'-C3'	-9.76	107.99	119.70
1	A	2408	U	N1-C1'-C2'	-9.75	101.27	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1476	U	O4'-C1'-N1	9.74	115.99	108.20
1	A	2798	U	P-O3'-C3'	9.73	131.38	119.70
1	A	1475	G	P-O3'-C3'	9.72	131.37	119.70
1	A	1119	U	O4'-C1'-N1	9.70	115.96	108.20
1	A	790	U	O4'-C1'-N1	9.69	115.95	108.20
1	A	1137	G	P-O3'-C3'	-9.69	108.07	119.70
1	A	1345	C	N1-C1'-C2'	-9.69	101.34	112.00
1	A	2267	A	C5-C6-N6	-9.67	115.97	123.70
1	A	364	C	P-O3'-C3'	-9.66	108.10	119.70
1	A	179	C	O4'-C1'-N1	9.66	115.92	108.20
1	A	1399	C	N1-C1'-C2'	-9.66	101.38	112.00
1	A	2572	A	P-O3'-C3'	9.66	131.29	119.70
1	A	1982	U	N1-C1'-C2'	-9.65	101.38	112.00
1	A	2868	A	P-O3'-C3'	-9.64	108.13	119.70
1	A	1020	A	P-O3'-C3'	9.64	131.27	119.70
1	A	2094	A	P-O3'-C3'	-9.63	108.14	119.70
1	A	766	U	N1-C1'-C2'	-9.63	101.41	112.00
1	A	217	A	P-O3'-C3'	-9.62	108.16	119.70
2	B	104	A	P-O3'-C3'	-9.59	108.19	119.70
1	A	688	U	N1-C1'-C2'	-9.57	101.47	112.00
1	A	2136	G	P-O3'-C3'	-9.57	108.22	119.70
1	A	589	U	N1-C1'-C2'	-9.57	101.47	112.00
1	A	2348	U	O4'-C1'-N1	9.57	115.85	108.20
1	A	1456	G	P-O3'-C3'	-9.56	108.23	119.70
1	A	413	C	P-O3'-C3'	-9.55	108.24	119.70
1	A	2338	C	O4'-C1'-N1	9.54	115.83	108.20
1	A	1214	A	P-O3'-C3'	-9.54	108.25	119.70
1	A	335	C	N1-C1'-C2'	-9.53	101.52	112.00
1	A	688	U	P-O3'-C3'	-9.52	108.28	119.70
1	A	142	A	P-O3'-C3'	-9.51	108.29	119.70
1	A	2498	C	N1-C1'-C2'	-9.50	101.55	112.00
1	A	527	C	O4'-C1'-N1	9.48	115.79	108.20
1	A	1249	U	N1-C1'-C2'	-9.48	101.57	112.00
1	A	1708	C	P-O3'-C3'	-9.48	108.33	119.70
1	A	2875	C	N1-C1'-C2'	-9.48	101.57	112.00
1	A	1498	C	N1-C1'-C2'	-9.47	101.58	112.00
1	A	1810	A	P-O3'-C3'	-9.47	108.34	119.70
1	A	2657	A	P-O3'-C3'	-9.45	108.36	119.70
1	A	243	U	N1-C1'-C2'	-9.42	101.64	112.00
1	A	2497	A	P-O3'-C3'	9.41	130.99	119.70
1	A	1980	G	P-O3'-C3'	9.40	130.99	119.70
1	A	1290	C	N1-C1'-C2'	-9.40	101.66	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2493	U	P-O3'-C3'	-9.39	108.43	119.70
1	A	1636	U	P-O3'-C3'	-9.39	108.44	119.70
1	A	741	U	O4'-C1'-N1	9.38	115.71	108.20
1	A	1072	C	N1-C1'-C2'	-9.38	101.68	112.00
1	A	1607	C	P-O3'-C3'	9.38	130.95	119.70
1	A	1131	G	P-O3'-C3'	9.36	130.93	119.70
1	A	1400	U	P-O3'-C3'	-9.36	108.47	119.70
1	A	104	A	P-O3'-C3'	-9.35	108.48	119.70
1	A	1867	G	P-O3'-C3'	-9.34	108.49	119.70
1	A	658	U	O4'-C1'-N1	9.34	115.67	108.20
1	A	1050	A	P-O3'-C3'	-9.33	108.50	119.70
1	A	164	C	N1-C1'-C2'	-9.31	101.76	112.00
1	A	730	A	P-O3'-C3'	-9.27	108.58	119.70
1	A	2313	C	N1-C1'-C2'	-9.27	101.80	112.00
1	A	2334	U	P-O3'-C3'	9.25	130.80	119.70
1	A	945	A	P-O3'-C3'	9.24	130.79	119.70
1	A	1080	A	P-O3'-C3'	-9.23	108.62	119.70
1	A	2339	C	P-O3'-C3'	-9.23	108.62	119.70
2	B	17	C	O4'-C1'-N1	9.22	115.58	108.20
1	A	1019	U	O4'-C1'-N1	9.19	115.56	108.20
1	A	1815	A	P-O3'-C3'	9.19	130.73	119.70
1	A	2409	G	P-O3'-C3'	-9.17	108.70	119.70
1	A	1289	C	N1-C1'-C2'	-9.16	101.92	112.00
1	A	1971	U	N1-C1'-C2'	-9.16	101.93	112.00
1	A	1708	C	O4'-C1'-N1	9.14	115.52	108.20
1	A	424	G	P-O3'-C3'	-9.13	108.74	119.70
1	A	437	U	O4'-C1'-N1	9.12	115.49	108.20
1	A	2298	A	P-O3'-C3'	-9.11	108.76	119.70
1	A	2198	A	P-O3'-C3'	9.11	130.63	119.70
1	A	483	A	P-O3'-C3'	-9.10	108.78	119.70
1	A	1822	C	N1-C1'-C2'	-9.07	102.02	112.00
1	A	77	G	P-O3'-C3'	-9.06	108.83	119.70
1	A	2215	C	N1-C1'-C2'	-9.06	102.03	112.00
1	A	1158	C	N1-C1'-C2'	-9.03	102.07	112.00
1	A	73	A	P-O3'-C3'	-9.02	108.87	119.70
1	A	739	A	P-O3'-C3'	9.02	130.53	119.70
1	A	867	C	N1-C1'-C2'	-9.02	102.08	112.00
1	A	1957	C	N1-C1'-C2'	-9.01	102.09	112.00
1	A	1060	U	N3-C4-O4	8.99	125.69	119.40
1	A	207	A	P-O3'-C3'	-8.98	108.92	119.70
1	A	976	G	P-O3'-C3'	-8.97	108.93	119.70
1	A	397	U	P-O3'-C3'	-8.97	108.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1023	U	P-O5'-C5'	-8.96	106.57	120.90
1	A	2713	U	N1-C1'-C2'	8.95	125.64	114.00
1	A	1079	C	N1-C1'-C2'	-8.95	102.16	112.00
1	A	128	C	P-O3'-C3'	-8.94	108.97	119.70
1	A	2631	G	P-O3'-C3'	-8.93	108.98	119.70
1	A	1314	C	N1-C1'-C2'	-8.93	102.18	112.00
1	A	2713	U	P-O3'-C3'	8.93	130.42	119.70
1	A	1914	C	N1-C1'-C2'	-8.92	102.18	112.00
1	A	1315	C	P-O3'-C3'	-8.92	108.99	119.70
1	A	1013	C	P-O3'-C3'	-8.90	109.02	119.70
1	A	754	U	N1-C1'-C2'	-8.89	102.22	112.00
1	A	2021	C	N1-C1'-C2'	8.87	125.53	114.00
1	A	140	C	N1-C1'-C2'	8.85	125.51	114.00
1	A	1271	G	P-O3'-C3'	8.82	130.29	119.70
1	A	2753	A	P-O3'-C3'	-8.82	109.11	119.70
1	A	1076	C	P-O3'-C3'	-8.80	109.14	119.70
1	A	312	G	P-O3'-C3'	-8.79	109.14	119.70
1	A	1943	U	P-O3'-C3'	8.78	130.24	119.70
1	A	2851	A	P-O3'-C3'	-8.76	109.19	119.70
1	A	510	C	N1-C1'-C2'	-8.76	102.36	112.00
1	A	1239	G	P-O3'-C3'	-8.75	109.20	119.70
1	A	2387	U	P-O3'-C3'	-8.75	109.20	119.70
1	A	755	U	P-O3'-C3'	-8.74	109.21	119.70
1	A	2322	A	P-O3'-C3'	-8.74	109.22	119.70
1	A	2691	C	N1-C1'-C2'	-8.72	102.41	112.00
1	A	2728	U	N1-C1'-C2'	-8.71	102.42	112.00
1	A	1114	C	P-O3'-C3'	-8.71	109.25	119.70
1	A	2656	U	N1-C1'-C2'	-8.70	102.43	112.00
1	A	2837	A	P-O3'-C3'	-8.69	109.28	119.70
1	A	60	G	P-O3'-C3'	8.67	130.10	119.70
1	A	1993	U	N1-C1'-C2'	-8.64	102.49	112.00
1	A	1606	C	O4'-C1'-N1	8.64	115.11	108.20
1	A	1113	U	O4'-C1'-N1	8.64	115.11	108.20
1	A	1274	A	P-O3'-C3'	-8.62	109.36	119.70
1	A	451	U	O4'-C1'-N1	8.61	115.09	108.20
1	A	766	U	P-O3'-C3'	-8.59	109.40	119.70
1	A	2612	C	P-O3'-C3'	-8.57	109.41	119.70
1	A	1681	G	P-O3'-C3'	8.57	129.98	119.70
1	A	1386	C	N1-C1'-C2'	-8.56	102.58	112.00
1	A	784	G	O4'-C1'-N9	8.54	115.03	108.20
1	A	791	C	P-O3'-C3'	-8.52	109.47	119.70
1	A	749	A	P-O3'-C3'	-8.52	109.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	A	C8-N9-C4	-8.51	102.40	105.80
1	A	865	C	P-O3'-C3'	8.50	129.90	119.70
1	A	2348	U	P-O3'-C3'	-8.50	109.50	119.70
1	A	1206	G	P-O3'-C3'	-8.49	109.51	119.70
1	A	100	U	P-O3'-C3'	8.48	129.88	119.70
1	A	1636	U	O4'-C1'-N1	8.47	114.98	108.20
2	B	24	G	P-O3'-C3'	8.46	129.85	119.70
1	A	774	G	P-O3'-C3'	8.46	129.85	119.70
1	A	1141	U	P-O3'-C3'	8.46	129.85	119.70
1	A	2031	A	P-O3'-C3'	8.45	129.83	119.70
1	A	1636	U	N1-C1'-C2'	-8.42	102.74	112.00
1	A	778	G	P-O3'-C3'	-8.41	109.60	119.70
1	A	2226	C	O4'-C1'-N1	8.38	114.90	108.20
1	A	273	G	N9-C1'-C2'	-8.36	102.80	112.00
1	A	2261	C	O4'-C1'-N1	8.36	114.89	108.20
1	A	629	G	P-O3'-C3'	-8.34	109.70	119.70
1	A	1946	U	N1-C1'-C2'	-8.34	102.83	112.00
1	A	2458	G	P-O3'-C3'	8.34	129.71	119.70
1	A	1954	G	P-O3'-C3'	8.33	129.70	119.70
1	A	503	A	P-O3'-C3'	8.33	129.69	119.70
1	A	957	C	P-O3'-C3'	8.30	129.66	119.70
1	A	2034	U	N1-C1'-C2'	-8.30	102.87	112.00
1	A	2612	C	O4'-C1'-N1	8.29	114.83	108.20
1	A	2492	U	N1-C1'-C2'	-8.28	102.89	112.00
1	A	445	C	O4'-C1'-N1	8.28	114.82	108.20
1	A	766	U	O4'-C1'-N1	8.27	114.81	108.20
1	A	2441	U	P-O3'-C3'	-8.27	109.78	119.70
1	A	389	G	P-O3'-C3'	-8.24	109.81	119.70
1	A	444	C	O4'-C1'-N1	8.24	114.79	108.20
1	A	1113	U	N1-C1'-C2'	-8.23	102.94	112.00
1	A	1110	G	P-O3'-C3'	8.22	129.56	119.70
1	A	2616	C	O4'-C1'-N1	8.21	114.77	108.20
1	A	1760	C	N1-C1'-C2'	-8.21	102.97	112.00
1	A	1334	G	P-O3'-C3'	-8.20	109.86	119.70
1	A	588	U	N1-C1'-C2'	-8.19	102.99	112.00
1	A	1063	G	P-O3'-C3'	-8.19	109.87	119.70
2	B	104	A	O4'-C1'-N9	8.19	114.75	108.20
1	A	2387	U	N1-C1'-C2'	-8.17	103.01	112.00
1	A	805	G	P-O3'-C3'	8.17	129.50	119.70
1	A	1035	U	N1-C1'-C2'	-8.15	103.03	112.00
1	A	1616	A	P-O3'-C3'	8.15	129.48	119.70
1	A	492	A	P-O3'-C3'	-8.14	109.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2603	G	P-O3'-C3'	-8.13	109.94	119.70
1	A	1073	A	P-O3'-C3'	-8.12	109.95	119.70
1	A	1782	U	N1-C1'-C2'	-8.12	103.06	112.00
1	A	1415	U	P-O3'-C3'	8.11	129.44	119.70
1	A	1839	G	P-O3'-C3'	-8.12	109.96	119.70
1	A	2902	C	O4'-C1'-N1	8.11	114.69	108.20
1	A	1499	C	P-O3'-C3'	-8.11	109.97	119.70
1	A	755	U	N1-C1'-C2'	-8.11	103.08	112.00
1	A	1838	C	O4'-C1'-N1	8.10	114.68	108.20
1	A	2277	G	P-O3'-C3'	-8.10	109.99	119.70
1	A	2382	G	P-O3'-C3'	8.07	129.39	119.70
1	A	392	U	O4'-C1'-N1	8.07	114.66	108.20
1	A	1076	C	O4'-C1'-N1	8.05	114.64	108.20
1	A	2782	G	P-O3'-C3'	-8.05	110.04	119.70
1	A	2692	G	N9-C1'-C2'	-8.04	103.15	112.00
1	A	122	G	P-O3'-C3'	-8.00	110.10	119.70
1	A	411	G	P-O3'-C3'	8.00	129.30	119.70
1	A	658	U	P-O3'-C3'	-8.00	110.10	119.70
2	B	40	U	P-O3'-C3'	7.99	129.29	119.70
1	A	1290	C	O4'-C1'-N1	7.99	114.59	108.20
1	A	2499	C	P-O3'-C3'	-7.99	110.11	119.70
1	A	50	U	P-O3'-C3'	7.97	129.27	119.70
1	A	2712	C	P-O3'-C3'	7.97	129.27	119.70
1	A	335	C	P-O3'-C3'	-7.97	110.14	119.70
1	A	1325	U	P-O3'-C3'	7.97	129.26	119.70
1	A	527	C	P-O3'-C3'	7.96	129.26	119.70
1	A	2249	U	P-O3'-C3'	7.96	129.26	119.70
1	A	2503	A	P-O3'-C3'	7.96	129.26	119.70
1	A	1330	C	N1-C1'-C2'	-7.96	103.24	112.00
1	A	605	G	N9-C1'-C2'	-7.95	103.26	112.00
1	A	2024	G	P-O3'-C3'	-7.94	110.18	119.70
1	A	633	A	N1-C6-N6	7.93	123.36	118.60
1	A	1440	U	O4'-C1'-N1	7.93	114.55	108.20
1	A	2728	U	P-O3'-C3'	-7.92	110.19	119.70
1	A	1539	U	P-O3'-C3'	-7.92	110.20	119.70
1	A	534	U	P-O3'-C3'	-7.91	110.21	119.70
1	A	2559	C	P-O3'-C3'	-7.90	110.22	119.70
1	A	2505	G	P-O3'-C3'	-7.90	110.22	119.70
1	A	1942	C	P-O3'-C3'	-7.89	110.23	119.70
1	A	2267	A	C6-C5-N7	-7.89	126.78	132.30
1	A	2023	C	O4'-C1'-N1	7.88	114.51	108.20
1	A	2238	G	P-O3'-C3'	7.88	129.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1430	G	P-O3'-C3'	-7.88	110.25	119.70
1	A	2629	U	P-O3'-C3'	7.88	129.15	119.70
1	A	61	C	N1-C1'-C2'	-7.86	103.35	112.00
1	A	811	U	P-O3'-C3'	7.85	129.12	119.70
1	A	2585	U	P-O3'-C3'	7.83	129.09	119.70
1	A	224	U	N1-C1'-C2'	-7.82	103.39	112.00
1	A	828	U	O4'-C1'-N1	7.81	114.45	108.20
1	A	423	A	P-O3'-C3'	-7.80	110.34	119.70
1	A	646	U	P-O3'-C3'	7.80	129.06	119.70
1	A	2860	A	N1-C6-N6	7.79	123.28	118.60
1	A	1462	C	O4'-C1'-N1	7.79	114.43	108.20
1	A	1913	A	P-O3'-C3'	7.79	129.05	119.70
2	B	17	C	N1-C1'-C2'	-7.78	103.44	112.00
1	A	2758	A	N9-C1'-C2'	-7.77	103.46	112.00
1	A	990	A	P-O3'-C3'	-7.76	110.39	119.70
1	A	1463	C	O4'-C1'-N1	7.76	114.41	108.20
1	A	1674	G	P-O3'-C3'	7.76	129.01	119.70
1	A	271	G	P-O3'-C3'	7.75	129.01	119.70
1	A	1088	A	C5-C6-N1	-7.75	113.82	117.70
1	A	1816	C	P-O3'-C3'	-7.75	110.40	119.70
1	A	1946	U	P-O3'-C3'	-7.75	110.40	119.70
1	A	1972	G	P-O3'-C3'	-7.75	110.40	119.70
1	A	91	A	P-O3'-C3'	7.75	129.00	119.70
1	A	1075	C	N1-C1'-C2'	-7.73	103.50	112.00
1	A	395	U	N1-C1'-C2'	7.71	124.03	114.00
1	A	1010	A	P-O3'-C3'	-7.71	110.44	119.70
1	A	1089	A	P-O3'-C3'	7.70	128.94	119.70
1	A	688	U	O4'-C1'-N1	7.69	114.35	108.20
1	A	2460	U	O4'-C1'-N1	7.69	114.35	108.20
1	A	1941	C	N1-C1'-C2'	-7.68	103.55	112.00
1	A	1937	A	P-O3'-C3'	7.67	128.90	119.70
1	A	1971	U	P-O3'-C3'	-7.66	110.51	119.70
1	A	1684	G	N9-C1'-C2'	-7.65	103.58	112.00
1	A	2143	C	P-O3'-C3'	7.65	128.88	119.70
1	A	2347	C	P-O3'-C3'	-7.65	110.52	119.70
1	A	1236	G	P-O3'-C3'	7.64	128.87	119.70
1	A	2093	G	N9-C1'-C2'	-7.64	103.59	112.00
1	A	1963	U	O4'-C1'-N1	7.64	114.31	108.20
1	A	2726	A	P-O3'-C3'	7.64	128.86	119.70
1	A	813	U	P-O3'-C3'	-7.63	110.54	119.70
1	A	2896	C	O4'-C1'-N1	7.63	114.31	108.20
1	A	1272	A	P-O3'-C3'	7.63	128.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	U	P-O3'-C3'	7.62	128.84	119.70
1	A	777	G	N9-C1'-C2'	-7.62	103.62	112.00
1	A	1565	C	P-O3'-C3'	7.62	128.84	119.70
1	A	741	U	P-O3'-C3'	-7.62	110.56	119.70
1	A	958	U	N1-C1'-C2'	-7.61	103.63	112.00
1	A	2210	U	P-O3'-C3'	7.61	128.83	119.70
1	A	1439	A	C4-C5-C6	7.57	120.79	117.00
1	A	2035	G	P-O3'-C3'	-7.57	110.61	119.70
1	A	2850	A	P-O3'-C3'	-7.54	110.65	119.70
2	B	43	C	P-O3'-C3'	-7.54	110.65	119.70
1	A	1320	C	P-O3'-C3'	7.54	128.75	119.70
1	A	2447	G	C6-N1-C2	-7.53	120.58	125.10
1	A	2566	A	P-O3'-C3'	7.53	128.73	119.70
1	A	480	A	P-O3'-C3'	-7.53	110.67	119.70
1	A	1276	A	P-O3'-C3'	-7.52	110.67	119.70
1	A	93	G	P-O3'-C3'	-7.52	110.67	119.70
1	A	482	A	P-O3'-C3'	-7.50	110.70	119.70
1	A	1326	U	N1-C1'-C2'	-7.48	103.77	112.00
1	A	1535	A	P-O3'-C3'	7.48	128.68	119.70
1	A	1674	G	C4-N9-C1'	7.48	136.22	126.50
1	A	2310	C	N1-C1'-C2'	-7.48	103.77	112.00
1	A	1782	U	O4'-C1'-N1	7.48	114.18	108.20
2	B	56	G	P-O3'-C3'	7.47	128.66	119.70
1	A	1649	G	P-O3'-C3'	-7.46	110.75	119.70
1	A	1387	A	N9-C1'-C2'	-7.46	103.80	112.00
1	A	2713	U	O4'-C1'-N1	-7.46	102.23	108.20
1	A	92	U	N1-C1'-C2'	-7.45	103.80	112.00
1	A	963	U	O4'-C1'-N1	7.45	114.16	108.20
1	A	995	C	P-O3'-C3'	7.45	128.64	119.70
1	A	2716	C	O4'-C1'-N1	7.45	114.16	108.20
1	A	1696	G	P-O3'-C3'	-7.45	110.77	119.70
1	A	2282	G	P-O3'-C3'	7.44	128.63	119.70
1	A	2307	G	P-O3'-C3'	7.44	128.62	119.70
1	A	1345	C	O4'-C1'-N1	7.42	114.14	108.20
1	A	2874	C	P-O3'-C3'	-7.41	110.81	119.70
1	A	404	A	P-O3'-C3'	7.41	128.59	119.70
1	A	989	G	P-O3'-C3'	7.41	128.59	119.70
1	A	1477	A	P-O3'-C3'	-7.39	110.83	119.70
1	A	777	G	P-O3'-C3'	-7.39	110.84	119.70
1	A	1312	U	P-O3'-C3'	7.38	128.56	119.70
1	A	534	U	O4'-C1'-N1	7.38	114.10	108.20
1	A	1076	C	N1-C1'-C2'	-7.38	103.89	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	G	P-O3'-C3'	7.37	128.54	119.70
1	A	2428	G	P-O3'-C3'	-7.34	110.89	119.70
1	A	1286	A	P-O3'-C3'	7.33	128.50	119.70
1	A	86	G	P-O3'-C3'	-7.33	110.90	119.70
1	A	321	U	P-O3'-C3'	7.33	128.50	119.70
1	A	325	G	N9-C1'-C2'	-7.32	103.94	112.00
1	A	958	U	P-O3'-C3'	-7.31	110.92	119.70
1	A	2037	A	P-O3'-C3'	-7.30	110.93	119.70
1	A	2069	G	N9-C1'-C2'	-7.29	103.98	112.00
1	A	2460	U	N1-C1'-C2'	-7.29	103.98	112.00
1	A	2283	C	P-O3'-C3'	-7.29	110.95	119.70
1	A	991	C	P-O3'-C3'	-7.28	110.96	119.70
1	A	2521	C	N1-C1'-C2'	-7.27	104.00	112.00
1	A	2439	A	P-O3'-C3'	7.26	128.41	119.70
1	A	973	A	P-O3'-C3'	7.26	128.41	119.70
1	A	1936	A	P-O3'-C3'	7.25	128.40	119.70
1	A	589	U	O4'-C1'-N1	7.25	114.00	108.20
1	A	603	A	P-O3'-C3'	7.25	128.40	119.70
1	A	2181	U	O4'-C1'-N1	7.25	114.00	108.20
1	A	2391	G	P-O3'-C3'	7.23	128.38	119.70
1	A	445	C	P-O3'-C3'	-7.23	111.03	119.70
1	A	945	A	O4'-C1'-N9	7.22	113.98	108.20
1	A	1758	U	P-O3'-C3'	7.22	128.37	119.70
1	A	1965	C	N1-C1'-C2'	-7.22	104.06	112.00
1	A	1780	A	P-O3'-C3'	7.21	128.35	119.70
1	A	396	G	N9-C1'-C2'	-7.20	104.08	112.00
1	A	1158	C	O4'-C1'-N1	7.19	113.95	108.20
1	A	436	C	N1-C1'-C2'	-7.19	104.09	112.00
1	A	975	A	P-O3'-C3'	-7.18	111.08	119.70
1	A	627	A	P-O3'-C3'	7.18	128.31	119.70
1	A	790	U	P-O3'-C3'	-7.18	111.09	119.70
1	A	1946	U	O4'-C1'-N1	7.16	113.93	108.20
1	A	1576	U	O4'-C1'-N1	7.16	113.92	108.20
1	A	1249	U	O4'-C1'-N1	7.15	113.92	108.20
1	A	1931	U	N1-C1'-C2'	-7.14	104.14	112.00
1	A	832	U	P-O5'-C5'	-7.14	109.47	120.90
1	A	647	G	P-O3'-C3'	-7.13	111.15	119.70
1	A	1569	A	P-O3'-C3'	-7.13	111.14	119.70
1	A	2350	C	O4'-C1'-N1	7.13	113.90	108.20
2	B	58	A	P-O3'-C3'	-7.12	111.15	119.70
1	A	1304	A	N9-C1'-C2'	-7.11	104.17	112.00
1	A	1615	C	P-O3'-C3'	7.11	128.24	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1822	C	O4'-C1'-N1	7.11	113.88	108.20
1	A	2069	G	P-O3'-C3'	-7.09	111.19	119.70
1	A	2267	A	N9-C4-C5	-7.09	102.96	105.80
1	A	2275	C	O4'-C1'-N1	7.09	113.88	108.20
1	A	228	C	O4'-C1'-N1	7.09	113.87	108.20
1	A	2408	U	O4'-C1'-N1	7.09	113.87	108.20
1	A	1287	A	P-O3'-C3'	7.07	128.18	119.70
1	A	15	G	P-O3'-C3'	-7.05	111.24	119.70
1	A	1674	G	C8-N9-C1'	-7.05	117.84	127.00
1	A	933	A	P-O3'-C3'	-7.04	111.25	119.70
1	A	2447	G	C5-C6-N1	7.03	115.02	111.50
1	A	2542	A	P-O3'-C3'	7.03	128.14	119.70
1	A	984	A	P-O3'-C3'	7.03	128.13	119.70
1	A	1758	U	N1-C1'-C2'	7.02	123.13	114.00
1	A	265	A	O4'-C1'-N9	7.02	113.81	108.20
1	A	755	U	O4'-C1'-N1	7.01	113.81	108.20
1	A	2611	C	P-O3'-C3'	-7.01	111.29	119.70
1	A	437	U	P-O3'-C3'	-7.00	111.30	119.70
1	A	1108	U	O4'-C1'-N1	7.00	113.80	108.20
1	A	775	G	O4'-C1'-N9	6.99	113.80	108.20
1	A	1716	U	N1-C1'-C2'	-6.99	104.31	112.00
1	A	2613	U	P-O3'-C3'	6.99	128.09	119.70
1	A	1539	U	O4'-C1'-N1	6.99	113.79	108.20
1	A	740	C	P-O3'-C3'	6.99	128.08	119.70
1	A	617	G	N9-C1'-C2'	-6.97	104.33	112.00
1	A	1669	A	P-O3'-C3'	-6.97	111.33	119.70
1	A	2616	C	P-O3'-C3'	-6.97	111.33	119.70
1	A	335	C	O4'-C1'-N1	6.97	113.78	108.20
1	A	302	C	N1-C1'-C2'	-6.96	104.34	112.00
1	A	2225	A	P-O3'-C3'	6.96	128.05	119.70
1	A	1256	G	P-O3'-C3'	-6.95	111.36	119.70
1	A	2334	U	O4'-C1'-N1	6.95	113.76	108.20
1	A	232	G	P-O3'-C3'	6.95	128.04	119.70
1	A	807	U	P-O3'-C3'	-6.94	111.37	119.70
1	A	2267	A	N3-C4-N9	6.93	132.94	127.40
1	A	1962	C	P-O3'-C3'	6.92	128.00	119.70
1	A	1722	A	P-O3'-C3'	-6.92	111.40	119.70
1	A	1734	G	P-O3'-C3'	-6.92	111.40	119.70
1	A	2060	A	P-O3'-C3'	6.92	128.00	119.70
1	A	605	G	P-O3'-C3'	-6.91	111.40	119.70
1	A	2875	C	P-O3'-C3'	-6.91	111.41	119.70
2	B	76	G	N3-C4-N9	-6.91	121.86	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2896	C	P-O3'-C3'	-6.91	111.41	119.70
1	A	913	U	P-O3'-C3'	6.90	127.98	119.70
1	A	1460	U	P-O3'-C3'	6.90	127.98	119.70
1	A	2283	C	O4'-C1'-N1	6.90	113.72	108.20
1	A	1942	C	N1-C1'-C2'	-6.90	104.41	112.00
1	A	424	G	N9-C1'-C2'	-6.89	104.42	112.00
1	A	2333	A	P-O3'-C3'	6.89	127.97	119.70
1	A	1511	G	P-O3'-C3'	-6.89	111.44	119.70
1	A	1683	U	O4'-C1'-N1	6.88	113.71	108.20
1	A	1839	G	N9-C1'-C2'	-6.88	104.43	112.00
1	A	1970	A	P-O3'-C3'	6.85	127.92	119.70
1	A	1556	C	O4'-C1'-N1	6.84	113.67	108.20
1	A	2280	G	P-O3'-C3'	-6.83	111.50	119.70
1	A	2314	A	N9-C1'-C2'	-6.83	104.48	112.00
1	A	746	U	N1-C1'-C2'	6.83	122.88	114.00
1	A	1929	G	P-O3'-C3'	6.82	127.89	119.70
1	A	2143	C	O4'-C1'-N1	6.82	113.65	108.20
2	B	44	G	P-O3'-C3'	6.82	127.88	119.70
1	A	1136	G	N9-C1'-C2'	-6.82	104.50	112.00
1	A	2753	A	N9-C1'-C2'	-6.80	104.52	112.00
1	A	460	A	N9-C1'-C2'	-6.80	104.52	112.00
1	A	2682	A	C3'-C2'-C1'	6.80	106.94	101.50
8	H	49	ALA	CB-CA-C	-6.80	99.91	110.10
1	A	531	C	N1-C1'-C2'	6.79	122.83	114.00
1	A	2041	U	C2-N3-C4	-6.79	122.92	127.00
1	A	807	U	O4'-C1'-N1	6.79	113.63	108.20
1	A	729	G	P-O3'-C3'	-6.79	111.55	119.70
1	A	2021	C	O4'-C1'-N1	6.79	113.63	108.20
1	A	2272	U	O4'-C1'-N1	-6.78	102.78	108.20
1	A	1515	A	O4'-C1'-N9	6.77	113.62	108.20
1	A	2289	G	P-O3'-C3'	-6.76	111.59	119.70
1	A	531	C	C2-N1-C1'	-6.76	111.37	118.80
2	B	16	G	P-O3'-C3'	-6.76	111.59	119.70
1	A	1554	U	O4'-C1'-N1	6.75	113.60	108.20
1	A	832	U	O4'-C1'-N1	6.75	113.60	108.20
1	A	1818	U	P-O3'-C3'	6.75	127.80	119.70
1	A	1451	C	P-O3'-C3'	6.75	127.80	119.70
1	A	1092	C	O4'-C1'-N1	6.74	113.59	108.20
1	A	1456	G	N9-C1'-C2'	-6.73	104.59	112.00
1	A	913	U	N1-C1'-C2'	6.73	122.75	114.00
1	A	1738	G	P-O3'-C3'	6.73	127.77	119.70
1	A	2403	C	P-O3'-C3'	-6.72	111.63	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	A	P-O3'-C3'	6.72	127.77	119.70
1	A	2053	G	N3-C4-N9	-6.71	121.97	126.00
1	A	1778	U	P-O3'-C3'	6.71	127.75	119.70
1	A	116	C	O4'-C1'-N1	6.71	113.57	108.20
1	A	2021	C	P-O3'-C3'	6.71	127.75	119.70
1	A	704	G	P-O3'-C3'	6.68	127.72	119.70
1	A	2498	C	O4'-C1'-N1	6.68	113.55	108.20
1	A	783	A	C3'-C2'-C1'	6.68	106.84	101.50
2	B	91	C	O4'-C1'-N1	6.68	113.54	108.20
1	A	2386	A	P-O3'-C3'	-6.68	111.69	119.70
1	A	1268	A	P-O3'-C3'	-6.68	111.69	119.70
1	A	1647	U	P-O3'-C3'	6.67	127.71	119.70
1	A	60	G	O4'-C1'-N9	6.67	113.54	108.20
1	A	547	A	P-O3'-C3'	6.67	127.70	119.70
1	A	1536	C	O4'-C1'-N1	-6.67	102.87	108.20
1	A	2312	U	N3-C2-O2	-6.66	117.53	122.20
1	A	1327	A	P-O3'-C3'	-6.66	111.71	119.70
1	A	1957	C	O4'-C1'-N1	6.66	113.53	108.20
1	A	509	C	C2-N1-C1'	6.66	126.12	118.80
2	B	104	A	C4-C5-C6	6.66	120.33	117.00
1	A	931	U	O4'-C1'-N1	6.65	113.52	108.20
2	B	51	G	O4'-C1'-N9	6.64	113.51	108.20
1	A	1653	G	P-O3'-C3'	6.63	127.66	119.70
1	A	301	G	N3-C4-N9	-6.63	122.02	126.00
1	A	1619	G	N9-C1'-C2'	-6.63	104.71	112.00
1	A	621	A	P-O3'-C3'	-6.62	111.75	119.70
1	A	2857	G	C2-N3-C4	-6.62	108.59	111.90
1	A	251	A	C3'-C2'-C1'	6.61	106.79	101.50
1	A	915	C	P-O3'-C3'	-6.60	111.78	119.70
1	A	334	C	O4'-C1'-N1	6.60	113.48	108.20
1	A	1561	C	P-O3'-C3'	-6.59	111.78	119.70
1	A	37	C	O4'-C1'-N1	6.59	113.47	108.20
1	A	427	U	O4'-C1'-N1	6.59	113.47	108.20
1	A	575	A	P-O3'-C3'	-6.59	111.79	119.70
1	A	1943	U	N1-C1'-C2'	-6.59	104.75	112.00
1	A	2258	C	P-O3'-C3'	6.59	127.60	119.70
1	A	2423	U	N1-C1'-C2'	6.58	122.55	114.00
2	B	43	C	O4'-C1'-N1	6.57	113.45	108.20
1	A	2266	A	P-O3'-C3'	6.57	127.58	119.70
1	A	461	C	C2-N1-C1'	6.56	126.02	118.80
1	A	1809	A	P-O3'-C3'	-6.56	111.82	119.70
1	A	1214	A	N9-C1'-C2'	-6.56	104.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	976	G	N9-C1'-C2'	-6.56	104.79	112.00
1	A	1522	A	N1-C6-N6	6.56	122.53	118.60
1	A	250	G	P-O3'-C3'	-6.55	111.84	119.70
1	A	1865	U	C2-N3-C4	-6.54	123.07	127.00
1	A	301	G	C8-N9-C1'	6.54	135.50	127.00
1	A	53	A	N9-C1'-C2'	-6.54	104.81	112.00
1	A	370	G	N3-C4-N9	-6.54	122.08	126.00
1	A	861	A	N9-C1'-C2'	-6.54	104.81	112.00
1	A	334	C	P-O3'-C3'	-6.53	111.86	119.70
1	A	1707	G	P-O3'-C3'	6.53	127.54	119.70
1	A	685	A	P-O3'-C3'	6.53	127.53	119.70
2	B	46	A	N9-C1'-C2'	-6.53	104.82	112.00
1	A	1275	A	P-O3'-C3'	6.52	127.53	119.70
1	A	2092	U	P-O3'-C3'	6.52	127.52	119.70
1	A	2493	U	O4'-C1'-N1	6.52	113.41	108.20
1	A	2681	C	P-O3'-C3'	6.52	127.52	119.70
1	A	74	A	P-O3'-C3'	6.51	127.52	119.70
1	A	531	C	C6-N1-C2	6.51	122.90	120.30
1	A	1025	G	P-O3'-C3'	6.50	127.50	119.70
1	A	2581	G	O4'-C1'-N9	6.50	113.40	108.20
1	A	1615	C	N1-C1'-C2'	6.49	122.44	114.00
1	A	13	A	P-O3'-C3'	6.49	127.49	119.70
1	A	389	G	N9-C1'-C2'	-6.49	104.86	112.00
1	A	2790	U	O4'-C1'-N1	6.49	113.39	108.20
1	A	1478	G	N9-C1'-C2'	-6.49	104.87	112.00
1	A	1674	G	C6-C5-N7	-6.48	126.51	130.40
1	A	225	C	P-O3'-C3'	-6.48	111.93	119.70
1	A	931	U	P-O3'-C3'	6.48	127.47	119.70
1	A	1277	G	C3'-C2'-C1'	6.47	106.68	101.50
1	A	1788	C	P-O3'-C3'	-6.47	111.94	119.70
8	H	48	GLU	CA-C-N	-6.47	102.97	117.20
1	A	1717	A	P-O3'-C3'	-6.46	111.94	119.70
1	A	1437	C	O4'-C1'-N1	6.46	113.36	108.20
1	A	2043	C	O4'-C1'-N1	-6.45	103.04	108.20
1	A	961	C	P-O3'-C3'	6.45	127.44	119.70
1	A	239	C	O4'-C1'-N1	6.44	113.35	108.20
1	A	1962	C	N1-C1'-C2'	6.44	122.38	114.00
1	A	230	G	P-O3'-C3'	-6.44	111.97	119.70
1	A	1049	C	O4'-C1'-N1	6.44	113.35	108.20
1	A	1082	U	O4'-C1'-N1	6.44	113.35	108.20
1	A	302	C	O4'-C1'-N1	6.42	113.34	108.20
2	B	104	A	N1-C6-N6	6.42	122.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2199	A	P-O3'-C3'	-6.42	112.00	119.70
1	A	140	C	P-O3'-C3'	6.42	127.40	119.70
1	A	2573	C	C6-N1-C2	-6.41	117.73	120.30
1	A	1925	C	O4'-C1'-N1	6.41	113.33	108.20
1	A	2311	A	P-O5'-C5'	6.41	131.15	120.90
1	A	301	G	C4-N9-C1'	-6.41	118.17	126.50
1	A	2030	A	P-O3'-C3'	6.40	127.38	119.70
1	A	2352	A	N1-C6-N6	6.39	122.44	118.60
1	A	2094	A	N9-C1'-C2'	-6.39	104.97	112.00
1	A	964	C	P-O3'-C3'	-6.38	112.04	119.70
1	A	1867	G	N9-C1'-C2'	-6.38	104.98	112.00
1	A	61	C	C3'-C2'-C1'	6.37	106.60	101.50
1	A	2387	U	O4'-C1'-N1	6.37	113.30	108.20
1	A	2092	U	O4'-C1'-N1	6.37	113.29	108.20
1	A	396	G	C3'-C2'-C1'	6.36	106.59	101.50
1	A	947	A	P-O3'-C3'	-6.36	112.06	119.70
1	A	1786	A	O4'-C1'-N9	6.36	113.29	108.20
1	A	1385	A	C6-N1-C2	6.36	122.42	118.60
1	A	2403	C	O4'-C1'-N1	6.36	113.29	108.20
1	A	249	C	P-O3'-C3'	6.36	127.33	119.70
1	A	1079	C	P-O3'-C3'	-6.36	112.07	119.70
1	A	2275	C	P-O3'-C3'	6.34	127.31	119.70
1	A	271	G	C4-N9-C1'	-6.34	118.26	126.50
1	A	2800	A	C3'-C2'-C1'	6.34	106.57	101.50
1	A	531	C	P-O3'-C3'	6.33	127.30	119.70
1	A	860	U	P-O3'-C3'	-6.33	112.10	119.70
1	A	1607	C	N1-C1'-C2'	6.33	122.23	114.00
1	A	1996	C	P-O3'-C3'	6.33	127.30	119.70
1	A	2401	U	P-O3'-C3'	6.33	127.30	119.70
1	A	121	G	P-O3'-C3'	-6.33	112.11	119.70
1	A	216	A	P-O3'-C3'	-6.33	112.11	119.70
1	A	1291	C	O4'-C1'-N1	6.32	113.26	108.20
1	A	2267	A	C6-N1-C2	-6.32	114.81	118.60
1	A	1802	A	C3'-C2'-C1'	6.31	106.55	101.50
1	A	1996	C	O4'-C1'-N1	6.31	113.25	108.20
1	A	749	A	N9-C1'-C2'	-6.31	105.06	112.00
1	A	234	U	P-O3'-C3'	-6.31	112.13	119.70
1	A	370	G	C4-N9-C1'	-6.31	118.30	126.50
1	A	1722	A	N9-C1'-C2'	-6.30	105.06	112.00
1	A	1246	A	C6-N1-C2	-6.30	114.82	118.60
1	A	2630	G	C3'-C2'-C1'	6.30	106.54	101.50
1	A	222	A	P-O3'-C3'	6.30	127.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	U	P-O3'-C3'	-6.29	112.15	119.70
1	A	1828	G	P-O3'-C3'	6.29	127.25	119.70
1	A	1324	G	P-O3'-C3'	6.29	127.25	119.70
1	A	1993	U	C3'-C2'-C1'	6.29	106.53	101.50
1	A	1945	G	C3'-C2'-C1'	6.28	106.52	101.50
1	A	1021	A	N9-C1'-C2'	-6.28	105.10	112.00
1	A	1915	U	N1-C1'-C2'	-6.28	105.10	112.00
1	A	2260	C	O4'-C1'-N1	6.28	113.22	108.20
1	A	2457	U	O4'-C1'-N1	6.28	113.22	108.20
1	A	1832	C	O4'-C1'-N1	6.27	113.22	108.20
1	A	1461	C	P-O3'-C3'	-6.27	112.17	119.70
1	A	959	A	P-O3'-C3'	-6.27	112.18	119.70
1	A	1398	C	P-O3'-C3'	-6.27	112.18	119.70
2	B	41	G	P-O3'-C3'	-6.27	112.18	119.70
1	A	1816	C	O4'-C1'-N1	6.26	113.21	108.20
1	A	2214	C	P-O3'-C3'	-6.26	112.19	119.70
1	A	303	G	C3'-C2'-C1'	6.26	106.50	101.50
1	A	2277	G	N9-C1'-C2'	-6.26	105.12	112.00
1	A	2144	G	P-O3'-C3'	6.25	127.20	119.70
1	A	2460	U	C3'-C2'-C1'	6.25	106.50	101.50
1	A	1993	U	O4'-C1'-N1	6.25	113.20	108.20
1	A	2053	G	N9-C4-C5	6.25	107.90	105.40
1	A	1090	A	C3'-C2'-C1'	6.25	106.50	101.50
1	A	647	G	C3'-C2'-C1'	6.24	106.49	101.50
1	A	1341	G	C3'-C2'-C1'	6.24	106.49	101.50
1	A	1733	G	P-O3'-C3'	-6.24	112.22	119.70
6	F	109	ARG	CG-CD-NE	-6.23	98.72	111.80
1	A	2895	G	C3'-C2'-C1'	6.22	106.48	101.50
1	A	301	G	P-O3'-C3'	6.22	127.17	119.70
1	A	375	G	N9-C1'-C2'	-6.22	105.16	112.00
1	A	1839	G	C3'-C2'-C1'	6.22	106.47	101.50
1	A	1416	G	O4'-C1'-N9	6.21	113.17	108.20
1	A	1341	G	P-O3'-C3'	6.21	127.15	119.70
1	A	2447	G	O4'-C1'-N9	6.21	113.17	108.20
1	A	2656	U	P-O3'-C3'	-6.21	112.25	119.70
1	A	2610	C	N1-C1'-C2'	6.21	122.07	114.00
1	A	1315	C	P-O5'-C5'	-6.20	110.97	120.90
1	A	2459	A	C3'-C2'-C1'	6.20	106.46	101.50
1	A	763	G	P-O3'-C3'	-6.19	112.27	119.70
1	A	794	A	C3'-C2'-C1'	6.19	106.45	101.50
1	A	35	G	P-O3'-C3'	-6.18	112.29	119.70
1	A	2492	U	C3'-C2'-C1'	6.17	106.43	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1255	U	O4'-C1'-N1	6.16	113.13	108.20
1	A	2544	G	C3'-C2'-C1'	6.16	106.43	101.50
1	A	87	U	O4'-C1'-N1	6.16	113.13	108.20
1	A	1206	G	N9-C1'-C2'	-6.16	105.22	112.00
8	H	48	GLU	CB-CA-C	-6.16	98.09	110.40
1	A	671	C	N1-C1'-C2'	-6.15	105.23	112.00
1	A	1135	C	N1-C1'-C2'	-6.14	105.24	112.00
1	A	1137	G	N9-C1'-C2'	-6.14	105.24	112.00
1	A	1739	A	P-O3'-C3'	-6.14	112.33	119.70
1	A	244	A	P-O3'-C3'	-6.14	112.33	119.70
1	A	1932	A	N1-C6-N6	6.14	122.28	118.60
1	A	52	A	P-O3'-C3'	-6.13	112.34	119.70
1	A	2689	U	P-O3'-C3'	6.13	127.05	119.70
1	A	1624	U	O4'-C1'-N1	6.12	113.10	108.20
1	A	1961	C	O4'-C1'-N1	6.12	113.10	108.20
1	A	2691	C	C3'-C2'-C1'	6.12	106.40	101.50
2	B	42	C	P-O3'-C3'	-6.12	112.36	119.70
1	A	1072	C	P-O3'-C3'	-6.12	112.36	119.70
1	A	2289	G	C3'-C2'-C1'	6.12	106.39	101.50
1	A	1802	A	P-O3'-C3'	-6.11	112.37	119.70
1	A	2289	G	N9-C1'-C2'	-6.11	105.28	112.00
1	A	1960	A	N1-C6-N6	-6.11	114.94	118.60
1	A	1142	A	C5-N7-C8	-6.11	100.85	103.90
1	A	1739	A	C3'-C2'-C1'	6.10	106.38	101.50
1	A	446	G	P-O3'-C3'	6.10	127.02	119.70
1	A	1619	G	P-O3'-C3'	-6.10	112.38	119.70
1	A	1303	G	P-O3'-C3'	-6.10	112.38	119.70
1	A	2631	G	N9-C1'-C2'	-6.10	105.29	112.00
1	A	2851	A	N9-C1'-C2'	-6.09	105.30	112.00
1	A	1769	U	O4'-C1'-N1	6.09	113.08	108.20
1	A	65	U	O4'-C1'-N1	6.09	113.07	108.20
1	A	2250	G	O4'-C1'-N9	-6.09	103.33	108.20
1	A	687	C	C3'-C2'-C1'	6.09	106.37	101.50
1	A	1395	A	P-O3'-C3'	6.08	127.00	119.70
1	A	1649	G	N9-C1'-C2'	-6.08	105.31	112.00
1	A	1060	U	C2-N3-C4	-6.08	123.35	127.00
1	A	1683	U	P-O3'-C3'	-6.08	112.41	119.70
1	A	1241	A	P-O5'-C5'	-6.07	111.18	120.90
1	A	2582	G	C3'-C2'-C1'	6.07	106.36	101.50
1	A	629	G	N9-C1'-C2'	-6.07	105.33	112.00
1	A	1786	A	P-O3'-C3'	6.07	126.98	119.70
1	A	1385	A	C5-C6-N6	6.06	128.55	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1314	C	C3'-C2'-C1'	6.06	106.34	101.50
1	A	1760	C	C3'-C2'-C1'	6.05	106.34	101.50
1	A	2440	C	C3'-C2'-C1'	6.05	106.34	101.50
1	A	1386	C	C3'-C2'-C1'	6.05	106.34	101.50
1	A	1477	A	C3'-C2'-C1'	6.05	106.34	101.50
1	A	2312	U	O5'-P-OP1	-6.05	100.26	105.70
1	A	197	A	C3'-C2'-C1'	6.04	106.33	101.50
1	A	443	A	P-O3'-C3'	-6.04	112.45	119.70
1	A	397	U	O4'-C1'-N1	6.04	113.03	108.20
1	A	622	G	N9-C1'-C2'	-6.02	105.38	112.00
1	A	2148	G	P-O3'-C3'	-6.02	112.48	119.70
1	A	482	A	N9-C1'-C2'	-6.01	105.38	112.00
2	B	45	A	P-O3'-C3'	-6.01	112.48	119.70
1	A	2615	U	C3'-C2'-C1'	6.01	106.31	101.50
1	A	2889	C	O4'-C1'-N1	6.00	113.00	108.20
1	A	1158	C	C3'-C2'-C1'	6.00	106.30	101.50
2	B	42	C	N1-C1'-C2'	-6.00	105.40	112.00
1	A	2251	G	C3'-C2'-C1'	5.99	106.30	101.50
1	A	2611	C	C3'-C2'-C1'	5.99	106.29	101.50
1	A	2226	C	C3'-C2'-C1'	5.99	106.29	101.50
1	A	303	G	P-O3'-C3'	-5.99	112.51	119.70
1	A	406	G	P-O3'-C3'	-5.99	112.52	119.70
1	A	1787	A	C3'-C2'-C1'	5.99	106.29	101.50
1	A	1654	A	C3'-C2'-C1'	5.98	106.28	101.50
1	A	1992	G	P-O3'-C3'	5.98	126.88	119.70
1	A	459	U	C3'-C2'-C1'	5.98	106.28	101.50
1	A	1019	U	C2-N3-C4	-5.98	123.41	127.00
1	A	2267	A	N9-C1'-C2'	-5.98	105.42	112.00
1	A	530	G	P-O3'-C3'	-5.98	112.53	119.70
1	A	2257	U	P-O3'-C3'	5.98	126.87	119.70
1	A	461	C	O4'-C1'-N1	-5.97	103.42	108.20
1	A	1788	C	O4'-C1'-N1	5.97	112.98	108.20
1	A	962	G	P-O3'-C3'	5.97	126.87	119.70
1	A	35	G	C3'-C2'-C1'	5.97	106.28	101.50
1	A	449	A	P-O3'-C3'	-5.97	112.53	119.70
1	A	14	A	P-O3'-C3'	-5.97	112.54	119.70
1	A	421	C	N1-C1'-C2'	5.97	121.76	114.00
1	A	1694	C	N1-C2-O2	5.97	122.48	118.90
1	A	244	A	C3'-C2'-C1'	5.96	106.27	101.50
1	A	1997	C	C3'-C2'-C1'	5.96	106.27	101.50
1	A	576	U	C3'-C2'-C1'	5.96	106.26	101.50
1	A	269	C	O4'-C1'-N1	5.96	112.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	947	A	C3'-C2'-C1'	5.95	106.26	101.50
1	A	2214	C	C3'-C2'-C1'	5.95	106.26	101.50
1	A	390	U	P-O3'-C3'	5.95	126.84	119.70
1	A	2781	A	C3'-C2'-C1'	5.95	106.26	101.50
1	A	1676	A	C3'-C2'-C1'	5.94	106.25	101.50
1	A	1695	G	P-O3'-C3'	-5.94	112.57	119.70
1	A	1759	A	C3'-C2'-C1'	5.94	106.25	101.50
1	A	2022	U	O4'-C1'-N1	-5.94	103.45	108.20
1	A	2245	U	O4'-C1'-N1	5.94	112.95	108.20
2	B	58	A	C3'-C2'-C1'	5.94	106.25	101.50
1	A	1330	C	P-O3'-C3'	-5.94	112.57	119.70
1	A	2093	G	C3'-C2'-C1'	5.94	106.25	101.50
2	B	87	U	O4'-C1'-N1	5.94	112.95	108.20
1	A	1654	A	O4'-C1'-N9	5.93	112.94	108.20
1	A	310	A	P-O3'-C3'	5.93	126.81	119.70
1	A	1821	A	P-O3'-C3'	-5.92	112.59	119.70
1	A	230	G	C3'-C2'-C1'	5.92	106.24	101.50
1	A	449	A	C3'-C2'-C1'	5.92	106.24	101.50
1	A	604	G	N9-C1'-C2'	-5.92	105.49	112.00
1	A	1788	C	C3'-C2'-C1'	5.92	106.23	101.50
1	A	2630	G	N9-C1'-C2'	-5.92	105.49	112.00
1	A	60	G	C8-N9-C1'	5.91	134.69	127.00
1	A	1010	A	C3'-C2'-C1'	5.91	106.23	101.50
1	A	1129	A	C3'-C2'-C1'	5.91	106.23	101.50
1	A	2543	G	C3'-C2'-C1'	5.91	106.23	101.50
1	A	1050	A	N9-C1'-C2'	-5.91	105.50	112.00
1	A	1706	C	O4'-C1'-N1	5.90	112.92	108.20
1	A	2267	A	C4-C5-N7	5.90	113.65	110.70
1	A	271	G	C8-N9-C1'	5.90	134.67	127.00
1	A	1555	G	C3'-C2'-C1'	5.90	106.22	101.50
1	A	390	U	N1-C1'-C2'	5.90	121.67	114.00
1	A	2521	C	O4'-C1'-N1	5.90	112.92	108.20
1	A	779	U	O4'-C1'-N1	5.89	112.92	108.20
1	A	1290	C	C3'-C2'-C1'	5.89	106.22	101.50
1	A	1626	A	P-O3'-C3'	5.89	126.77	119.70
1	A	1965	C	P-O3'-C3'	-5.89	112.63	119.70
1	A	1303	G	C3'-C2'-C1'	5.89	106.21	101.50
1	A	1507	C	O4'-C1'-N1	-5.89	103.49	108.20
1	A	1670	C	P-O3'-C3'	5.88	126.76	119.70
1	A	1206	G	C3'-C2'-C1'	5.88	106.21	101.50
1	A	1785	A	C3'-C2'-C1'	5.88	106.21	101.50
1	A	1034	G	C3'-C2'-C1'	5.88	106.21	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2402	U	P-O3'-C3'	-5.88	112.65	119.70
1	A	2447	G	C5-C6-O6	-5.88	125.08	128.60
1	A	374	A	C3'-C2'-C1'	5.87	106.20	101.50
1	A	2312	U	P-O3'-C3'	-5.87	112.65	119.70
1	A	2312	U	C6-N1-C2	-5.87	117.47	121.00
1	A	1114	C	O4'-C1'-N1	5.87	112.90	108.20
1	A	2337	G	P-O3'-C3'	-5.87	112.66	119.70
1	A	2903	U	O4'-C1'-N1	5.87	112.89	108.20
1	A	2504	U	C3'-C2'-C1'	5.87	106.19	101.50
1	A	2620	C	C6-N1-C2	5.87	122.65	120.30
1	A	413	C	O4'-C1'-N1	5.86	112.89	108.20
1	A	1363	C	O4'-C1'-N1	-5.86	103.51	108.20
1	A	1941	C	P-O3'-C3'	-5.86	112.67	119.70
1	A	802	A	C3'-C2'-C1'	5.86	106.19	101.50
1	A	2727	A	P-O3'-C3'	-5.86	112.67	119.70
1	A	1612	C	O4'-C1'-N1	5.85	112.88	108.20
1	A	370	G	C8-N9-C1'	5.85	134.61	127.00
1	A	587	C	P-O3'-C3'	5.85	126.72	119.70
1	A	1812	U	O4'-C1'-N1	5.85	112.88	108.20
1	A	197	A	P-O3'-C3'	-5.85	112.68	119.70
1	A	1607	C	O4'-C1'-N1	-5.84	103.53	108.20
1	A	1157	G	C3'-C2'-C1'	5.84	106.17	101.50
2	B	17	C	P-O3'-C3'	-5.84	112.70	119.70
1	A	2059	A	P-O3'-C3'	5.83	126.70	119.70
1	A	858	G	P-O3'-C3'	5.83	126.70	119.70
1	A	990	A	C3'-C2'-C1'	5.83	106.16	101.50
1	A	1822	C	C3'-C2'-C1'	5.83	106.16	101.50
1	A	2037	A	C3'-C2'-C1'	5.83	106.16	101.50
1	A	2267	A	P-O3'-C3'	-5.83	112.70	119.70
1	A	1716	U	P-O3'-C3'	-5.83	112.71	119.70
1	A	2434	A	P-O3'-C3'	5.83	126.69	119.70
1	A	2573	C	N1-C1'-C2'	-5.83	105.59	112.00
2	B	45	A	C3'-C2'-C1'	5.83	106.16	101.50
1	A	52	A	C3'-C2'-C1'	5.82	106.15	101.50
1	A	2756	U	P-O3'-C3'	5.81	126.68	119.70
1	A	221	A	P-O3'-C3'	5.81	126.67	119.70
1	A	1273	U	N1-C1'-C2'	-5.81	105.61	112.00
1	A	1399	C	C3'-C2'-C1'	5.81	106.15	101.50
1	A	1060	U	C2-N1-C1'	5.81	124.67	117.70
1	A	2848	G	P-O3'-C3'	5.80	126.66	119.70
1	A	785	G	N9-C1'-C2'	-5.80	105.62	112.00
1	A	1333	G	C3'-C2'-C1'	5.80	106.14	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	G	P-O3'-C3'	-5.80	112.74	119.70
1	A	832	U	P-O3'-C3'	-5.80	112.74	119.70
1	A	2136	G	N9-C1'-C2'	-5.80	105.62	112.00
1	A	2313	C	P-O3'-C3'	-5.80	112.74	119.70
1	A	479	A	O4'-C1'-N9	5.79	112.83	108.20
1	A	2039	U	O4'-C1'-N1	5.79	112.83	108.20
1	A	1553	A	O4'-C1'-N9	5.79	112.83	108.20
1	A	2638	G	P-O3'-C3'	5.79	126.64	119.70
1	A	672	C	C3'-C2'-C1'	5.78	106.12	101.50
1	A	2267	A	C8-N9-C1'	-5.78	117.30	127.70
1	A	509	C	N1-C1'-C2'	-5.78	105.64	112.00
2	B	5	U	O4'-C1'-N1	5.77	112.82	108.20
1	A	250	G	C3'-C2'-C1'	5.77	106.12	101.50
1	A	656	G	C3'-C2'-C1'	5.77	106.12	101.50
1	A	1021	A	C3'-C2'-C1'	5.77	106.12	101.50
1	A	1008	A	P-O3'-C3'	5.77	126.62	119.70
1	A	1060	U	C6-N1-C1'	-5.77	113.12	121.20
1	A	434	U	N1-C1'-C2'	5.76	121.49	114.00
1	A	1455	G	C3'-C2'-C1'	5.76	106.11	101.50
1	A	726	G	O4'-C1'-N9	5.76	112.81	108.20
1	A	1717	A	C3'-C2'-C1'	5.76	106.11	101.50
1	A	2033	A	C6-N1-C2	5.76	122.06	118.60
2	B	45	A	N9-C1'-C2'	-5.76	105.67	112.00
1	A	2777	G	C3'-C2'-C1'	5.76	106.10	101.50
2	B	87	U	P-O3'-C3'	5.76	126.61	119.70
1	A	142	A	N9-C1'-C2'	-5.75	105.67	112.00
1	A	2308	G	P-O3'-C3'	5.75	126.60	119.70
1	A	2657	A	N9-C1'-C2'	-5.75	105.67	112.00
1	A	271	G	N3-C4-N9	-5.75	122.55	126.00
1	A	1022	G	O4'-C1'-N9	5.75	112.80	108.20
1	A	1647	U	O4'-C1'-N1	5.75	112.80	108.20
1	A	572	A	C3'-C2'-C1'	5.74	106.09	101.50
1	A	2549	G	P-O3'-C3'	5.74	126.59	119.70
1	A	505	A	C3'-C2'-C1'	5.74	106.09	101.50
1	A	1213	A	C3'-C2'-C1'	5.74	106.09	101.50
1	A	491	G	P-O3'-C3'	-5.73	112.82	119.70
1	A	2499	C	C3'-C2'-C1'	5.73	106.09	101.50
1	A	1080	A	N9-C1'-C2'	-5.73	105.70	112.00
1	A	1325	U	N1-C1'-C2'	5.73	121.45	114.00
1	A	1011	G	C4-N9-C1'	-5.72	119.06	126.50
1	A	1683	U	C3'-C2'-C1'	5.72	106.08	101.50
1	A	1611	C	P-O3'-C3'	-5.71	112.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1455	G	P-O3'-C3'	-5.71	112.84	119.70
1	A	2691	C	O4'-C1'-N1	5.71	112.77	108.20
1	A	1537	G	C3'-C2'-C1'	5.71	106.07	101.50
1	A	1071	G	C3'-C2'-C1'	5.71	106.07	101.50
1	A	60	G	C4-N9-C1'	-5.71	119.08	126.50
1	A	1334	G	N9-C1'-C2'	-5.71	105.72	112.00
1	A	1635	A	C3'-C2'-C1'	5.71	106.06	101.50
1	A	1315	C	O4'-C1'-N1	5.70	112.76	108.20
1	A	2324	U	P-O3'-C3'	5.70	126.55	119.70
1	A	754	U	O4'-C1'-N1	5.70	112.76	108.20
1	A	2752	C	O4'-C1'-N1	5.70	112.76	108.20
1	A	529	A	C5-N7-C8	-5.70	101.05	103.90
1	A	2757	A	C3'-C2'-C1'	5.70	106.06	101.50
1	A	122	G	C3'-C2'-C1'	5.70	106.06	101.50
1	A	491	G	C3'-C2'-C1'	5.70	106.06	101.50
1	A	1276	A	C3'-C2'-C1'	5.69	106.06	101.50
1	A	93	G	C3'-C2'-C1'	5.69	106.06	101.50
1	A	370	G	C6-C5-N7	5.69	133.81	130.40
1	A	1439	A	C6-N1-C2	5.69	122.02	118.60
1	A	646	U	O4'-C1'-N1	-5.69	103.65	108.20
1	A	224	U	P-O3'-C3'	-5.69	112.87	119.70
1	A	1700	A	C3'-C2'-C1'	5.69	106.05	101.50
1	A	2215	C	O4'-C1'-N1	5.69	112.75	108.20
1	A	2752	C	N1-C1'-C2'	-5.69	105.74	112.00
1	A	1713	A	P-O3'-C3'	5.69	126.52	119.70
1	A	656	G	P-O3'-C3'	-5.68	112.88	119.70
1	A	2272	U	N3-C2-O2	5.68	126.18	122.20
1	A	777	G	C3'-C2'-C1'	5.68	106.05	101.50
1	A	1778	U	C2-N3-C4	-5.68	123.59	127.00
1	A	1674	G	C4-C5-N7	5.68	113.07	110.80
1	A	788	A	P-O3'-C3'	5.67	126.51	119.70
1	A	1568	G	C3'-C2'-C1'	5.67	106.04	101.50
1	A	2267	A	C4-N9-C1'	5.67	136.51	126.30
1	A	1313	U	C3'-C2'-C1'	5.67	106.03	101.50
1	A	2458	G	O4'-C1'-N9	5.67	112.73	108.20
1	A	2875	C	O4'-C1'-N1	5.67	112.73	108.20
1	A	1649	G	C3'-C2'-C1'	5.67	106.03	101.50
1	A	1027	A	C3'-C2'-C1'	5.67	106.03	101.50
1	A	1511	G	C3'-C2'-C1'	5.67	106.03	101.50
1	A	672	C	P-O3'-C3'	-5.66	112.90	119.70
1	A	575	A	C3'-C2'-C1'	5.66	106.03	101.50
1	A	2714	G	P-O3'-C3'	-5.66	112.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	C	C3'-C2'-C1'	5.66	106.02	101.50
1	A	699	A	O4'-C1'-N9	-5.66	103.67	108.20
1	A	1327	A	C3'-C2'-C1'	5.66	106.03	101.50
1	A	1462	C	C3'-C2'-C1'	5.65	106.02	101.50
1	A	2603	G	C3'-C2'-C1'	5.65	106.02	101.50
1	A	1634	A	P-O3'-C3'	5.65	126.48	119.70
1	A	628	G	P-O3'-C3'	5.65	126.48	119.70
1	A	1512	C	O4'-C1'-N1	5.65	112.72	108.20
1	A	637	A	P-O3'-C3'	5.64	126.47	119.70
1	A	2251	G	P-O3'-C3'	-5.64	112.93	119.70
1	A	2313	C	C3'-C2'-C1'	5.64	106.01	101.50
1	A	192	C	P-O3'-C3'	5.64	126.47	119.70
1	A	1159	U	O4'-C1'-N1	5.64	112.71	108.20
1	A	442	G	P-O3'-C3'	5.64	126.47	119.70
1	A	2189	U	O4'-C1'-N1	5.64	112.71	108.20
1	A	103	A	C3'-C2'-C1'	5.63	106.01	101.50
1	A	313	G	N9-C1'-C2'	-5.63	105.80	112.00
1	A	646	U	N1-C1'-C2'	5.63	121.33	114.00
1	A	461	C	C6-N1-C1'	-5.63	114.04	120.80
1	A	546	U	P-O3'-C3'	5.63	126.46	119.70
1	A	671	C	O5'-P-OP2	-5.63	100.63	105.70
1	A	2312	U	N3-C4-C5	-5.63	111.22	114.60
2	B	43	C	C3'-C2'-C1'	5.63	106.00	101.50
1	A	77	G	N9-C1'-C2'	-5.62	105.81	112.00
1	A	964	C	P-O5'-C5'	-5.62	111.90	120.90
1	A	2283	C	C3'-C2'-C1'	5.62	106.00	101.50
1	A	621	A	C3'-C2'-C1'	5.62	106.00	101.50
1	A	2380	C	O4'-C1'-N1	5.62	112.69	108.20
1	A	2409	G	N9-C1'-C2'	-5.62	105.82	112.00
1	A	164	C	C3'-C2'-C1'	5.62	105.99	101.50
1	A	763	G	C6-C5-N7	-5.62	127.03	130.40
1	A	2638	G	N1-C2-N2	5.62	121.25	116.20
1	A	1277	G	P-O3'-C3'	-5.61	112.97	119.70
1	A	1074	G	P-O3'-C3'	5.61	126.42	119.70
1	A	2063	C	C3'-C2'-C1'	5.60	105.98	101.50
1	A	1676	A	P-O3'-C3'	-5.59	112.99	119.70
1	A	301	G	C6-C5-N7	5.59	133.75	130.40
1	A	1136	G	C3'-C2'-C1'	5.59	105.97	101.50
1	A	2215	C	C3'-C2'-C1'	5.59	105.97	101.50
1	A	1027	A	P-O3'-C3'	-5.58	113.00	119.70
1	A	1136	G	P-O3'-C3'	-5.58	113.00	119.70
1	A	2520	C	C3'-C2'-C1'	5.58	105.96	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1698	A	P-O3'-C3'	5.58	126.39	119.70
1	A	510	C	C3'-C2'-C1'	5.58	105.96	101.50
1	A	2518	A	P-O3'-C3'	5.58	126.39	119.70
1	A	139	U	P-O3'-C3'	5.57	126.39	119.70
2	B	75	G	P-O3'-C3'	-5.57	113.02	119.70
1	A	915	C	C3'-C2'-C1'	5.57	105.95	101.50
1	A	705	A	N1-C6-N6	5.56	121.94	118.60
1	A	548	G	N9-C1'-C2'	-5.56	105.88	112.00
1	A	806	C	C6-N1-C2	5.56	122.53	120.30
1	A	2450	A	C3'-C2'-C1'	5.56	105.95	101.50
1	A	2891	U	O4'-C1'-N1	5.56	112.65	108.20
1	A	1213	A	P-O3'-C3'	-5.55	113.03	119.70
1	A	2056	G	N1-C6-O6	-5.55	116.57	119.90
1	A	2613	U	O4'-C1'-N1	5.55	112.64	108.20
1	A	1673	G	P-O3'-C3'	5.55	126.36	119.70
1	A	2240	U	P-O3'-C3'	-5.55	113.04	119.70
1	A	548	G	C4-N9-C1'	5.55	133.72	126.50
1	A	2302	U	O4'-C1'-N1	5.55	112.64	108.20
1	A	92	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	630	G	C2-N3-C4	-5.54	109.13	111.90
1	A	1305	C	O4'-C1'-N1	5.54	112.63	108.20
1	A	1611	C	C3'-C2'-C1'	5.54	105.93	101.50
1	A	1916	A	N9-C1'-C2'	-5.53	105.91	112.00
1	A	1267	U	P-O3'-C3'	-5.53	113.06	119.70
1	A	1330	C	C3'-C2'-C1'	5.53	105.92	101.50
1	A	2874	C	C3'-C2'-C1'	5.53	105.92	101.50
1	A	2896	C	C3'-C2'-C1'	5.53	105.92	101.50
1	A	2902	C	P-O3'-C3'	5.53	126.33	119.70
1	A	2568	U	O4'-C1'-N1	5.52	112.62	108.20
1	A	445	C	C3'-C2'-C1'	5.52	105.92	101.50
1	A	2572	A	O4'-C1'-N9	5.52	112.62	108.20
1	A	1931	U	C3'-C2'-C1'	5.52	105.92	101.50
2	B	43	C	N1-C1'-C2'	-5.52	105.93	112.00
1	A	2498	C	P-O3'-C3'	-5.52	113.08	119.70
1	A	963	U	P-O3'-C3'	-5.52	113.08	119.70
1	A	1023	U	P-O3'-C3'	-5.52	113.08	119.70
1	A	460	A	P-O5'-C5'	-5.51	112.08	120.90
1	A	388	G	P-O3'-C3'	-5.51	113.08	119.70
1	A	1510	G	C3'-C2'-C1'	5.51	105.91	101.50
1	A	1551	A	C6-N1-C2	5.51	121.91	118.60
1	A	406	G	C3'-C2'-C1'	5.50	105.90	101.50
1	A	2338	C	N1-C1'-C2'	-5.50	105.95	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1648	U	C3'-C2'-C1'	5.50	105.90	101.50
6	F	78	ILE	CB-CA-C	-5.50	100.60	111.60
1	A	1558	C	P-O3'-C3'	5.50	126.30	119.70
1	A	1113	U	P-O3'-C3'	-5.50	113.10	119.70
1	A	207	A	C3'-C2'-C1'	5.50	105.90	101.50
1	A	1669	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	1733	G	C3'-C2'-C1'	5.49	105.89	101.50
1	A	2837	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	2148	G	C3'-C2'-C1'	5.49	105.89	101.50
1	A	373	U	N1-C1'-C2'	-5.49	105.96	112.00
1	A	1558	C	N1-C1'-C2'	5.49	121.14	114.00
1	A	2383	G	P-O3'-C3'	-5.49	113.11	119.70
1	A	2135	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	2311	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	2573	C	C3'-C2'-C1'	5.48	105.88	101.50
1	A	510	C	P-O3'-C3'	-5.47	113.13	119.70
1	A	2505	G	N9-C1'-C2'	-5.47	105.98	112.00
1	A	754	U	C3'-C2'-C1'	5.47	105.88	101.50
1	A	1695	G	C3'-C2'-C1'	5.47	105.88	101.50
1	A	1838	C	P-O3'-C3'	5.47	126.27	119.70
1	A	374	A	P-O3'-C3'	-5.46	113.14	119.70
1	A	741	U	C3'-C2'-C1'	5.46	105.87	101.50
1	A	1662	U	O4'-C1'-N1	5.46	112.57	108.20
1	A	2875	C	C3'-C2'-C1'	5.46	105.87	101.50
1	A	2034	U	C3'-C2'-C1'	5.46	105.87	101.50
1	A	1560	G	P-O3'-C3'	-5.45	113.16	119.70
2	B	72	G	C2-N3-C4	-5.45	109.17	111.90
1	A	2197	U	P-O3'-C3'	5.45	126.24	119.70
1	A	1144	A	C3'-C2'-C1'	5.45	105.86	101.50
1	A	1239	G	N9-C1'-C2'	-5.45	106.01	112.00
1	A	791	C	P-O5'-C5'	-5.45	112.19	120.90
1	A	1026	G	P-O3'-C3'	-5.45	113.17	119.70
1	A	1816	C	C3'-C2'-C1'	5.45	105.86	101.50
2	B	90	C	C3'-C2'-C1'	5.44	105.86	101.50
1	A	514	A	N1-C6-N6	5.44	121.86	118.60
1	A	1779	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	1888	G	O4'-C1'-N9	5.44	112.55	108.20
1	A	1183	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	2385	C	P-O3'-C3'	-5.43	113.18	119.70
1	A	629	G	C3'-C2'-C1'	5.43	105.85	101.50
1	A	1829	A	P-O3'-C3'	5.43	126.22	119.70
1	A	334	C	N1-C1'-C2'	-5.43	106.03	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2798	U	O4'-C1'-N1	-5.43	103.86	108.20
1	A	2096	C	O4'-C1'-N1	5.43	112.54	108.20
1	A	1963	U	P-O3'-C3'	-5.42	113.19	119.70
1	A	139	U	N1-C1'-C2'	5.42	121.05	114.00
1	A	616	A	P-O3'-C3'	-5.42	113.19	119.70
2	B	118	C	O4'-C1'-N1	5.42	112.54	108.20
1	A	1181	U	P-O3'-C3'	-5.42	113.20	119.70
1	A	1063	G	N9-C1'-C2'	-5.42	106.04	112.00
1	A	1498	C	C3'-C2'-C1'	5.42	105.83	101.50
1	A	2067	G	P-O3'-C3'	5.42	126.20	119.70
1	A	967	U	O4'-C1'-N1	5.42	112.53	108.20
1	A	2800	A	N9-C1'-C2'	-5.42	106.04	112.00
1	A	476	G	C3'-C2'-C1'	5.42	105.83	101.50
1	A	916	G	N9-C1'-C2'	-5.41	106.05	112.00
1	A	991	C	O4'-C1'-N1	5.41	112.53	108.20
1	A	1734	G	C3'-C2'-C1'	5.41	105.83	101.50
1	A	752	A	P-O3'-C3'	5.40	126.18	119.70
1	A	763	G	C3'-C2'-C1'	5.40	105.82	101.50
1	A	2521	C	C3'-C2'-C1'	5.40	105.82	101.50
1	A	783	A	O4'-C1'-N9	5.40	112.52	108.20
1	A	2322	A	N9-C1'-C2'	-5.40	106.06	112.00
1	A	475	C	P-O3'-C3'	-5.39	113.23	119.70
1	A	2567	G	P-O3'-C3'	5.39	126.17	119.70
1	A	2576	G	P-O3'-C3'	5.39	126.17	119.70
1	A	509	C	N1-C2-O2	5.39	122.14	118.90
1	A	616	A	C3'-C2'-C1'	5.39	105.81	101.50
1	A	800	A	P-O3'-C3'	5.39	126.17	119.70
2	B	16	G	C3'-C2'-C1'	5.39	105.81	101.50
1	A	1551	A	C5-C6-N6	5.38	128.01	123.70
1	A	1395	A	O4'-C1'-N9	5.38	112.51	108.20
1	A	1508	A	P-O3'-C3'	5.38	126.16	119.70
1	A	1612	C	C3'-C2'-C1'	5.38	105.80	101.50
1	A	1865	U	O4'-C1'-N1	5.38	112.50	108.20
1	A	217	A	N9-C1'-C2'	-5.38	106.08	112.00
1	A	272	A	P-O3'-C3'	-5.38	113.25	119.70
1	A	1023	U	C3'-C2'-C1'	5.38	105.80	101.50
1	A	1914	C	C3'-C2'-C1'	5.38	105.80	101.50
1	A	1029	A	N1-C6-N6	5.38	121.83	118.60
1	A	1009	A	P-O3'-C3'	-5.37	113.25	119.70
1	A	638	G	C3'-C2'-C1'	5.37	105.80	101.50
1	A	1345	C	C3'-C2'-C1'	5.37	105.80	101.50
2	B	76	G	N3-C4-C5	5.37	131.28	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	G	C3'-C2'-C1'	5.37	105.79	101.50
1	A	73	A	C3'-C2'-C1'	5.36	105.79	101.50
1	A	1480	C	O4'-C1'-N1	5.36	112.49	108.20
1	A	2699	C	O4'-C1'-N1	5.36	112.49	108.20
1	A	140	C	O4'-C1'-N1	-5.36	103.91	108.20
1	A	1256	G	C3'-C2'-C1'	5.36	105.79	101.50
1	A	1561	C	C3'-C2'-C1'	5.36	105.79	101.50
1	A	929	U	O4'-C1'-N1	5.35	112.48	108.20
1	A	2868	A	N9-C1'-C2'	-5.35	106.11	112.00
1	A	365	U	C5-C4-O4	-5.35	122.69	125.90
1	A	2147	A	P-O3'-C3'	-5.35	113.28	119.70
1	A	2499	C	C2-N1-C1'	5.35	124.68	118.80
1	A	2610	C	P-O3'-C3'	5.35	126.12	119.70
1	A	86	G	C3'-C2'-C1'	5.35	105.78	101.50
1	A	1882	U	O4'-C1'-N1	5.35	112.48	108.20
1	A	763	G	C4-C5-N7	5.34	112.94	110.80
1	A	509	C	C3'-C2'-C1'	5.34	105.77	101.50
1	A	2507	C	O4'-C1'-N1	5.34	112.47	108.20
1	A	391	A	P-O3'-C3'	-5.34	113.30	119.70
1	A	1636	U	C3'-C2'-C1'	5.34	105.77	101.50
1	A	103	A	P-O3'-C3'	-5.33	113.30	119.70
1	A	1135	C	P-O3'-C3'	-5.33	113.30	119.70
1	A	1558	C	O4'-C1'-N1	5.33	112.47	108.20
1	A	2493	U	C3'-C2'-C1'	5.33	105.77	101.50
1	A	2850	A	C3'-C2'-C1'	5.33	105.76	101.50
1	A	1429	G	C3'-C2'-C1'	5.33	105.76	101.50
1	A	1669	A	N1-C2-N3	-5.33	126.64	129.30
1	A	2689	U	N1-C1'-C2'	5.33	120.93	114.00
1	A	401	A	O4'-C1'-N9	5.33	112.46	108.20
1	A	1783	A	C3'-C2'-C1'	5.33	105.76	101.50
1	A	1167	C	O4'-C1'-N1	5.31	112.45	108.20
1	A	1787	A	P-O3'-C3'	-5.31	113.32	119.70
1	A	2036	C	N1-C1'-C2'	-5.31	106.16	112.00
1	A	26	G	C2-N3-C4	-5.31	109.24	111.90
1	A	2830	C	O4'-C1'-N1	5.31	112.45	108.20
1	A	586	A	P-O3'-C3'	5.31	126.07	119.70
1	A	480	A	N9-C1'-C2'	-5.31	106.16	112.00
1	A	1655	A	C3'-C2'-C1'	5.30	105.74	101.50
1	A	2782	G	N9-C1'-C2'	-5.30	106.17	112.00
1	A	533	G	C3'-C2'-C1'	5.30	105.74	101.50
1	A	2580	U	P-O3'-C3'	5.30	126.06	119.70
1	A	530	G	C3'-C2'-C1'	5.29	105.73	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	109	ARG	CB-CA-C	5.29	120.98	110.40
1	A	2631	G	C3'-C2'-C1'	5.29	105.73	101.50
1	A	437	U	C3'-C2'-C1'	5.29	105.73	101.50
1	A	76	C	C3'-C2'-C1'	5.28	105.72	101.50
1	A	1062	G	P-O3'-C3'	-5.28	113.36	119.70
1	A	1080	A	C3'-C2'-C1'	5.28	105.72	101.50
1	A	1011	G	C8-N9-C1'	5.28	133.86	127.00
1	A	2555	U	O4'-C1'-N1	5.28	112.42	108.20
1	A	63	A	P-O3'-C3'	-5.27	113.37	119.70
1	A	492	A	N9-C1'-C2'	-5.27	106.20	112.00
1	A	481	G	N3-C4-C5	-5.27	125.96	128.60
1	A	782	A	P-O3'-C3'	5.27	126.03	119.70
1	A	224	U	C3'-C2'-C1'	5.27	105.72	101.50
1	A	1049	C	P-O3'-C3'	-5.27	113.38	119.70
1	A	101	A	C3'-C2'-C1'	5.27	105.72	101.50
1	A	243	U	C3'-C2'-C1'	5.27	105.71	101.50
1	A	589	U	C3'-C2'-C1'	5.27	105.72	101.50
1	A	657	U	N1-C1'-C2'	-5.27	106.21	112.00
1	A	1430	G	C3'-C2'-C1'	5.27	105.71	101.50
1	A	2726	A	O4'-C1'-N9	5.27	112.42	108.20
1	A	1799	G	N9-C4-C5	5.27	107.51	105.40
1	A	2297	A	C3'-C2'-C1'	5.27	105.71	101.50
1	A	2262	U	O4'-C1'-N1	5.26	112.41	108.20
1	A	2199	A	C3'-C2'-C1'	5.26	105.71	101.50
1	A	406	G	N9-C1'-C2'	-5.26	106.22	112.00
1	A	15	G	C3'-C2'-C1'	5.26	105.70	101.50
1	A	1267	U	C3'-C2'-C1'	5.25	105.70	101.50
1	A	2727	A	C3'-C2'-C1'	5.25	105.70	101.50
1	A	324	A	C3'-C2'-C1'	5.25	105.70	101.50
1	A	1551	A	C5-C6-N1	-5.25	115.08	117.70
1	A	787	C	C5-C4-N4	5.25	123.87	120.20
1	A	120	U	P-O5'-C5'	-5.25	112.51	120.90
1	A	529	A	C4-C5-C6	-5.24	114.38	117.00
1	A	104	A	N9-C1'-C2'	-5.24	106.23	112.00
1	A	272	A	C3'-C2'-C1'	5.24	105.69	101.50
1	A	503	A	N1-C6-N6	-5.24	115.46	118.60
1	A	778	G	C3'-C2'-C1'	5.24	105.69	101.50
1	A	2386	A	C3'-C2'-C1'	5.24	105.69	101.50
1	A	750	A	P-O3'-C3'	-5.23	113.42	119.70
1	A	150	U	O4'-C1'-N1	5.23	112.39	108.20
1	A	753	A	C3'-C2'-C1'	5.23	105.69	101.50
1	A	1818	U	N1-C1'-C2'	5.23	120.80	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	A	C3'-C2'-C1'	5.23	105.68	101.50
1	A	963	U	N1-C1'-C2'	-5.23	106.25	112.00
1	A	2613	U	N1-C1'-C2'	5.23	120.80	114.00
1	A	2675	A	P-O3'-C3'	-5.23	113.43	119.70
1	A	229	C	C3'-C2'-C1'	5.23	105.68	101.50
1	A	2024	G	C3'-C2'-C1'	5.23	105.68	101.50
1	A	492	A	P-O5'-C5'	-5.22	112.55	120.90
1	A	2611	C	O4'-C1'-N1	5.22	112.38	108.20
1	A	77	G	C3'-C2'-C1'	5.22	105.67	101.50
1	A	1865	U	C5-C4-O4	-5.22	122.77	125.90
2	B	104	A	N3-C4-C5	-5.22	123.15	126.80
1	A	747	U	O4'-C1'-N1	-5.21	104.03	108.20
1	A	1048	A	C3'-C2'-C1'	5.21	105.67	101.50
1	A	2428	G	C3'-C2'-C1'	5.21	105.67	101.50
1	A	2714	G	C3'-C2'-C1'	5.21	105.67	101.50
1	A	403	U	P-O3'-C3'	5.21	125.95	119.70
1	A	959	A	C3'-C2'-C1'	5.21	105.67	101.50
1	A	1112	G	C3'-C2'-C1'	5.21	105.67	101.50
1	A	1239	G	C3'-C2'-C1'	5.21	105.67	101.50
1	A	216	A	C3'-C2'-C1'	5.21	105.67	101.50
1	A	1782	U	P-O3'-C3'	-5.21	113.45	119.70
2	B	44	G	N3-C4-N9	-5.21	122.88	126.00
1	A	479	A	P-O3'-C3'	5.20	125.94	119.70
2	B	41	G	C3'-C2'-C1'	5.20	105.66	101.50
1	A	1144	A	N9-C1'-C2'	-5.20	106.28	112.00
1	A	1247	A	O4'-C1'-N9	5.20	112.36	108.20
1	A	1682	G	C3'-C2'-C1'	5.20	105.66	101.50
1	A	1722	A	C3'-C2'-C1'	5.20	105.66	101.50
1	A	2052	A	N9-C1'-C2'	-5.20	106.28	112.00
1	A	2776	A	P-O3'-C3'	5.20	125.94	119.70
1	A	2781	A	N9-C1'-C2'	-5.20	106.28	112.00
2	B	40	U	O4'-C1'-N1	5.20	112.36	108.20
1	A	1476	U	P-O3'-C3'	5.19	125.93	119.70
1	A	234	U	C3'-C2'-C1'	5.19	105.65	101.50
1	A	370	G	P-O3'-C3'	5.19	125.93	119.70
1	A	604	G	C3'-C2'-C1'	5.19	105.65	101.50
1	A	1635	A	P-O5'-C5'	-5.19	112.59	120.90
1	A	1956	U	C3'-C2'-C1'	5.19	105.65	101.50
1	A	964	C	C3'-C2'-C1'	5.19	105.65	101.50
1	A	506	G	P-O3'-C3'	-5.19	113.47	119.70
1	A	2450	A	P-O3'-C3'	-5.18	113.48	119.70
1	A	2319	G	P-O3'-C3'	5.18	125.92	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2610	C	O4'-C1'-N1	-5.18	104.06	108.20
1	A	968	C	O4'-C1'-N1	5.18	112.34	108.20
1	A	333	G	C3'-C2'-C1'	5.17	105.64	101.50
1	A	1915	U	C3'-C2'-C1'	5.17	105.64	101.50
1	A	2894	G	C3'-C2'-C1'	5.17	105.64	101.50
2	B	17	C	C3'-C2'-C1'	5.17	105.64	101.50
1	A	577	G	N7-C8-N9	5.17	115.68	113.10
1	A	1415	U	O4'-C1'-N1	5.17	112.33	108.20
1	A	1554	U	P-O3'-C3'	5.17	125.90	119.70
1	A	2402	U	C3'-C2'-C1'	5.17	105.63	101.50
1	A	206	U	C3'-C2'-C1'	5.16	105.63	101.50
1	A	2286	G	P-O3'-C3'	5.16	125.90	119.70
1	A	2589	A	N1-C6-N6	-5.16	115.50	118.60
1	A	105	C	O4'-C1'-N1	5.16	112.33	108.20
1	A	832	U	C3'-C2'-C1'	5.16	105.63	101.50
1	A	589	U	P-O3'-C3'	-5.16	113.51	119.70
1	A	1386	C	P-O3'-C3'	-5.16	113.51	119.70
1	A	1560	G	C3'-C2'-C1'	5.16	105.63	101.50
1	A	2427	C	C3'-C2'-C1'	5.16	105.62	101.50
1	A	230	G	N9-C1'-C2'	-5.15	106.33	112.00
1	A	533	G	N9-C1'-C2'	-5.15	106.33	112.00
1	A	483	A	N9-C1'-C2'	-5.15	106.34	112.00
1	A	1606	C	P-O3'-C3'	5.15	125.88	119.70
1	A	87	U	C3'-C2'-C1'	5.15	105.62	101.50
1	A	975	A	C3'-C2'-C1'	5.15	105.62	101.50
1	A	997	G	N9-C1'-C2'	-5.15	106.34	112.00
1	A	2477	U	O4'-C1'-N1	5.15	112.32	108.20
1	A	2267	A	C4-C5-C6	5.15	119.57	117.00
1	A	1155	A	O4'-C1'-N9	5.14	112.31	108.20
1	A	2272	U	C5-C4-O4	-5.14	122.81	125.90
1	A	92	U	C3'-C2'-C1'	5.14	105.61	101.50
1	A	2053	G	N1-C6-O6	-5.14	116.82	119.90
1	A	2408	U	P-O3'-C3'	-5.14	113.53	119.70
1	A	1963	U	C3'-C2'-C1'	5.14	105.61	101.50
1	A	1334	G	C3'-C2'-C1'	5.13	105.61	101.50
1	A	162	U	N1-C1'-C2'	5.13	120.67	114.00
1	A	480	A	C3'-C2'-C1'	5.13	105.60	101.50
1	A	1569	A	N9-C1'-C2'	-5.13	106.36	112.00
1	A	1957	C	N3-C2-O2	-5.13	118.31	121.90
1	A	2603	G	N9-C1'-C2'	-5.13	106.36	112.00
1	A	179	C	C3'-C2'-C1'	5.12	105.60	101.50
1	A	656	G	N9-C1'-C2'	-5.12	106.36	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	A	C3'-C2'-C1'	5.12	105.60	101.50
1	A	831	G	C3'-C2'-C1'	5.12	105.60	101.50
1	A	1696	G	C3'-C2'-C1'	5.12	105.60	101.50
1	A	2459	A	N9-C1'-C2'	-5.12	106.37	112.00
1	A	444	C	C3'-C2'-C1'	5.12	105.60	101.50
1	A	577	G	N3-C4-N9	5.12	129.07	126.00
1	A	867	C	C3'-C2'-C1'	5.12	105.59	101.50
1	A	1111	A	P-O3'-C3'	-5.11	113.56	119.70
1	A	64	A	N1-C6-N6	-5.11	115.53	118.60
1	A	1390	U	O4'-C1'-N1	5.11	112.29	108.20
1	A	60	G	N9-C4-C5	5.11	107.44	105.40
1	A	503	A	O4'-C1'-N9	5.11	112.29	108.20
2	B	42	C	C3'-C2'-C1'	5.11	105.59	101.50
1	A	1634	A	O3'-P-O5'	-5.10	94.30	104.00
1	A	1075	C	P-O3'-C3'	-5.10	113.58	119.70
1	A	1677	A	P-O3'-C3'	-5.10	113.58	119.70
1	A	783	A	P-O3'-C3'	-5.10	113.58	119.70
1	A	318	C	O4'-C1'-N1	5.10	112.28	108.20
1	A	482	A	C3'-C2'-C1'	5.10	105.58	101.50
2	B	77	U	O4'-C1'-N1	5.10	112.28	108.20
1	A	2440	C	O4'-C1'-N1	5.09	112.27	108.20
1	A	142	A	C3'-C2'-C1'	5.09	105.57	101.50
1	A	1063	G	C3'-C2'-C1'	5.08	105.57	101.50
1	A	1268	A	N9-C1'-C2'	-5.08	106.41	112.00
1	A	2492	U	O4'-C1'-N1	5.08	112.27	108.20
1	A	1942	C	C3'-C2'-C1'	5.08	105.56	101.50
1	A	164	C	P-O3'-C3'	-5.08	113.61	119.70
1	A	74	A	C3'-C2'-C1'	5.08	105.56	101.50
1	A	1941	C	C3'-C2'-C1'	5.08	105.56	101.50
1	A	1965	C	C3'-C2'-C1'	5.08	105.56	101.50
2	B	103	U	N1-C1'-C2'	5.08	120.60	114.00
1	A	312	G	C3'-C2'-C1'	5.07	105.56	101.50
1	A	1019	U	N1-C2-N3	5.07	117.94	114.90
1	A	388	G	C3'-C2'-C1'	5.07	105.56	101.50
1	A	687	C	P-O3'-C3'	-5.07	113.61	119.70
1	A	1048	A	P-O3'-C3'	-5.07	113.61	119.70
1	A	1957	C	C3'-C2'-C1'	5.07	105.56	101.50
1	A	2337	G	C3'-C2'-C1'	5.07	105.56	101.50
1	A	1767	G	N1-C6-O6	-5.07	116.86	119.90
1	A	2778	A	C3'-C2'-C1'	5.07	105.55	101.50
1	A	2425	A	O4'-C1'-N9	5.07	112.25	108.20
1	A	2832	U	O4'-C1'-N1	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	C	O4'-C1'-N1	5.06	112.25	108.20
1	A	1972	G	C3'-C2'-C1'	5.06	105.55	101.50
1	A	2616	C	C3'-C2'-C1'	5.06	105.55	101.50
1	A	1082	U	C2-N3-C4	-5.06	123.96	127.00
1	A	2770	G	C6-C5-N7	-5.06	127.36	130.40
2	B	13	G	C3'-C2'-C1'	5.06	105.55	101.50
1	A	1378	A	P-O3'-C3'	5.05	125.77	119.70
1	A	1439	A	C6-C5-N7	-5.05	128.76	132.30
2	B	44	G	C6-C5-N7	5.05	133.43	130.40
1	A	26	G	P-O3'-C3'	5.05	125.76	119.70
1	A	1865	U	N1-C1'-C2'	5.05	120.57	114.00
1	A	2210	U	O3'-P-O5'	5.05	113.60	104.00
2	B	43	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1507	C	C2-N3-C4	5.05	122.42	119.90
1	A	2036	C	P-O3'-C3'	-5.05	113.64	119.70
1	A	2260	C	C6-N1-C2	-5.04	118.28	120.30
1	A	657	U	C3'-C2'-C1'	5.04	105.53	101.50
1	A	783	A	N9-C1'-C2'	-5.04	106.45	112.00
1	A	2239	G	C3'-C2'-C1'	5.04	105.53	101.50
1	A	1900	A	P-O3'-C3'	5.04	125.75	119.70
1	A	1439	A	N1-C6-N6	5.04	121.62	118.60
1	A	813	U	O4'-C1'-N1	5.04	112.23	108.20
1	A	1062	G	C8-N9-C4	-5.04	104.39	106.40
1	A	2586	U	C3'-C2'-C1'	5.04	105.53	101.50
1	A	2616	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1204	A	P-O3'-C3'	5.03	125.74	119.70
1	A	6	A	C6-N1-C2	5.03	121.62	118.60
1	A	373	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	2312	U	N1-C2-O2	5.03	126.32	122.80
1	A	2241	A	O4'-C1'-N9	5.03	112.22	108.20
2	B	104	A	C2-N3-C4	5.03	113.11	110.60
1	A	2496	C	O4'-C1'-N1	5.02	112.22	108.20
1	A	41	C	O4'-C1'-N1	5.02	112.22	108.20
1	A	1838	C	N1-C1'-C2'	5.02	120.53	114.00
1	A	353	C	N1-C1'-C2'	5.02	120.52	114.00
1	A	1799	G	C4-C5-N7	-5.02	108.79	110.80
1	A	2322	A	C3'-C2'-C1'	5.02	105.51	101.50
1	A	1507	C	N1-C2-O2	5.02	121.91	118.90
1	A	1738	G	O4'-C1'-N9	5.01	112.21	108.20
1	A	1061	U	P-O3'-C3'	-5.01	113.69	119.70
1	A	83	A	P-O3'-C3'	5.01	125.71	119.70
1	A	2277	G	C3'-C2'-C1'	5.01	105.51	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	C	C3'-C2'-C1'	5.01	105.51	101.50
1	A	483	A	C3'-C2'-C1'	5.01	105.51	101.50
1	A	812	C	C6-N1-C2	5.01	122.30	120.30
1	A	1061	U	C5-C6-N1	5.01	125.20	122.70
1	A	2033	A	P-O3'-C3'	5.01	125.71	119.70
1	A	2064	C	C3'-C2'-C1'	5.01	105.51	101.50
1	A	2312	U	C3'-C2'-C1'	5.01	105.50	101.50
1	A	1238	G	P-O3'-C3'	5.00	125.71	119.70
1	A	2339	C	P-O5'-C5'	-5.00	112.89	120.90
1	A	1311	G	P-O3'-C3'	5.00	125.70	119.70
1	A	1400	U	C3'-C2'-C1'	5.00	105.50	101.50
1	A	2441	U	C3'-C2'-C1'	5.00	105.50	101.50
1	A	2645	G	N3-C4-C5	5.00	131.10	128.60
1	A	1078	U	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	47	PHE	Peptide
8	H	48	GLU	Peptide
8	H	49	ALA	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60995	0	0	1569	0
2	B	2507	0	0	52	0
3	C	2082	0	0	34	0
4	D	1565	0	0	33	0
5	E	1552	0	0	15	0
6	F	1420	0	0	23	0
7	G	1323	0	0	15	0
8	H	1111	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1032	0	0	4	0
10	J	1129	0	0	20	0
11	K	938	0	0	11	0
12	L	1045	0	0	25	0
13	M	1074	0	0	12	0
14	N	960	0	0	15	0
15	O	892	0	0	12	0
16	P	917	0	0	8	0
17	Q	947	0	0	10	0
18	R	816	0	0	8	0
19	S	857	0	0	9	0
20	T	738	0	0	8	0
21	U	779	0	0	10	0
22	V	753	0	0	18	0
23	W	596	0	0	17	0
24	X	625	0	0	19	0
25	Y	509	0	0	7	0
26	Z	449	0	0	6	0
27	0	444	0	0	11	0
28	1	409	0	0	4	0
29	2	377	0	0	10	0
30	3	504	0	0	11	0
31	4	302	0	0	5	0
32	A	133	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	J	1	0	0	0	0
33	4	1	0	0	0	0
34	2	1	0	0	0	0
34	3	1	0	0	0	0
34	4	3	0	0	0	0
34	A	603	0	0	11	0
34	B	5	0	0	0	0
34	C	10	0	0	0	0
34	D	2	0	0	0	0
34	E	3	0	0	0	0
34	J	6	0	0	0	0
34	L	4	0	0	0	0
34	N	2	0	0	1	0
34	T	2	0	0	0	0
34	U	1	0	0	0	0
All	All	90428	0	0	1905	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (1905) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1439:A:N1	1:A:1552:A:C5	2.13	1.15
6:F:109:ARG:CB	6:F:109:ARG:CZ	2.34	1.04
1:A:1439:A:C2	1:A:1552:A:C6	2.48	1.01
1:A:1439:A:C2	1:A:1552:A:C5	2.50	0.99
1:A:1476:U:O2'	1:A:1477:A:O5'	1.84	0.95
1:A:1439:A:C6	1:A:1552:A:N7	2.35	0.95
1:A:445:C:O2'	1:A:446:G:O4'	1.88	0.92
1:A:2036:C:O2'	1:A:2037:A:C8	2.25	0.90
1:A:216:A:O2'	1:A:217:A:C8	2.25	0.89
1:A:2308:G:O6	1:A:2311:A:N6	2.06	0.89
1:A:272:A:O2'	1:A:273:G:C8	2.27	0.86
1:A:1312:U:O2'	1:A:1314:C:N4	2.08	0.86
1:A:1062:G:O2'	1:A:1063:G:C8	2.29	0.85
1:A:1062:G:O4'	1:A:1088:A:N7	2.10	0.84
1:A:1439:A:N1	1:A:1552:A:N7	2.24	0.83
1:A:1324:G:O2'	1:A:1616:A:C6	2.31	0.83
1:A:302:C:O2'	1:A:303:G:C8	2.34	0.81
1:A:670:A:O2'	1:A:671:C:OP2	2.00	0.79
1:A:1131:G:O2'	1:A:1133:A:N7	2.15	0.79
1:A:2386:A:O2'	1:A:2387:U:C6	2.36	0.79
1:A:1809:A:O2'	1:A:1810:A:C8	2.36	0.79
1:A:1429:G:O2'	1:A:1430:G:C8	2.35	0.78
1:A:479:A:O2'	1:A:480:A:C5'	2.31	0.78
1:A:2385:C:O2'	1:A:2386:A:C8	2.37	0.78
1:A:1669:A:C2'	1:A:1669:A:N3	2.48	0.77
1:A:1716:U:O2'	1:A:1717:A:C8	2.38	0.77
1:A:2197:U:O2'	1:A:2198:A:C8	2.38	0.77
1:A:1062:G:C8	1:A:1088:A:C8	2.73	0.76
1:A:2516:A:C2	1:A:2569:G:C2	2.73	0.76
1:A:2408:U:O2'	1:A:2409:G:C8	2.39	0.76
1:A:1847:A:O2'	1:A:1848:A:C8	2.38	0.76
1:A:983:A:N6	1:A:984:A:N1	2.34	0.75
1:A:2056:G:N2	27:0:1:ALA:N	2.34	0.75
1:A:589:U:O2'	1:A:590:A:C8	2.40	0.74
1:A:2543:G:C6	1:A:2765:A:C5	2.76	0.74
2:B:50:A:OP1	15:O:68:LYS:N	2.20	0.74
1:A:391:A:O2'	1:A:392:U:C5'	2.36	0.74
1:A:2311:A:C2'	1:A:2311:A:N3	2.50	0.74
1:A:668:A:C5	1:A:670:A:N7	2.56	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:604:G:O2'	1:A:605:G:C5'	2.37	0.73
1:A:1313:U:C6	1:A:1610:A:C8	2.77	0.73
1:A:223:A:N6	1:A:422:A:C6	2.57	0.72
1:A:482:A:N6	1:A:506:G:C4	2.58	0.72
18:R:82:HIS:O	18:R:82:HIS:CG	2.40	0.72
1:A:1271:G:OP2	34:A:3238:HOH:O	2.06	0.72
1:A:1737:G:C6	1:A:1738:G:N1	2.58	0.72
1:A:1223:G:N2	1:A:1226:A:OP2	2.22	0.72
1:A:379:G:C6	1:A:396:G:O6	2.43	0.72
1:A:77:G:O2'	1:A:78:U:O4'	2.06	0.72
1:A:1802:A:N6	1:A:1817:G:N2	2.38	0.72
6:F:136:ILE:O	6:F:137:PHE:O	2.07	0.71
1:A:828:U:C4	1:A:829:A:N6	2.58	0.71
1:A:1552:A:C2	1:A:1553:A:C8	2.80	0.70
1:A:2259:U:O2'	1:A:2260:C:C6	2.44	0.70
1:A:1439:A:C6	1:A:1552:A:C5	2.80	0.70
1:A:655:A:O2'	1:A:656:G:C8	2.44	0.70
1:A:202:U:C4	1:A:203:A:C6	2.79	0.70
1:A:379:G:C6	1:A:396:G:C6	2.80	0.69
1:A:1788:C:O2'	1:A:1789:A:O4'	2.10	0.69
1:A:983:A:N6	1:A:984:A:C2	2.61	0.69
1:A:741:U:O2'	1:A:742:A:O4'	2.09	0.69
1:A:1439:A:N7	1:A:1440:U:C6	2.60	0.69
1:A:118:A:C8	1:A:119:A:C8	2.80	0.69
1:A:529:A:C8	1:A:2023:C:N4	2.60	0.69
22:V:29:ILE:CD1	22:V:31:TYR:CE2	2.75	0.69
1:A:2788:C:O2'	1:A:2809:A:N3	2.26	0.69
1:A:1327:A:O2'	1:A:1328:A:O4'	2.11	0.69
1:A:1021:A:C2	1:A:1023:U:C2	2.81	0.69
1:A:1071:G:N7	1:A:1089:A:C6	2.61	0.68
1:A:2657:A:O3'	7:G:159:LYS:NZ	2.26	0.68
1:A:782:A:OP1	1:A:782:A:C8	2.46	0.68
1:A:442:G:C6	1:A:444:C:N4	2.62	0.68
1:A:745:G:O2'	1:A:748:G:O2'	2.11	0.68
1:A:395:U:O2'	1:A:396:G:C8	2.46	0.68
1:A:478:A:C6	1:A:480:A:C5	2.82	0.67
1:A:789:A:N1	34:A:3160:HOH:O	2.26	0.67
1:A:2285:C:C5	28:1:5:ARG:NH2	2.62	0.67
1:A:85:G:O2'	1:A:86:G:C8	2.47	0.67
1:A:1439:A:N6	1:A:1551:A:C2	2.63	0.67
1:A:271:G:O2'	1:A:272:A:C5'	2.43	0.67
1:A:627:A:O2'	1:A:628:G:O4'	2.13	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:364:C:O2'	1:A:365:U:O4'	2.13	0.67
1:A:476:G:O2'	1:A:477:A:O5'	2.12	0.67
1:A:2056:G:C2	1:A:2057:G:C8	2.83	0.66
1:A:373:U:O2'	1:A:374:A:C8	2.48	0.66
1:A:303:G:O2'	1:A:304:U:O4'	2.12	0.66
1:A:397:U:O2'	1:A:398:C:O4'	2.12	0.66
1:A:1281:G:C6	1:A:1290:C:N4	2.63	0.66
1:A:1956:U:O2'	1:A:1957:C:C5'	2.44	0.66
1:A:2313:C:O2'	1:A:2314:A:C5'	2.43	0.66
1:A:1296:G:N2	1:A:1645:G:C4	2.64	0.66
23:W:40:ARG:NH1	23:W:40:ARG:CG	2.58	0.66
1:A:2460:U:O2'	1:A:2461:A:O4'	2.12	0.66
13:M:27:SER:N	13:M:66:ARG:NH2	2.43	0.66
1:A:1552:A:N3	1:A:1552:A:C2'	2.59	0.66
1:A:1784:A:C4'	1:A:1785:A:O5'	2.44	0.66
1:A:2037:A:O2'	1:A:2038:G:O4'	2.13	0.65
1:A:1277:G:O2'	1:A:1278:C:O4'	2.14	0.65
1:A:752:A:O2'	1:A:753:A:P	2.54	0.65
1:A:2264:C:C2	1:A:2277:G:N2	2.63	0.65
1:A:1270:C:N4	1:A:1648:U:O4	2.29	0.65
1:A:2064:C:O2'	1:A:2065:C:O4'	2.15	0.65
1:A:2308:G:O6	1:A:2311:A:C6	2.49	0.65
1:A:13:A:O2'	1:A:15:G:N7	2.29	0.65
1:A:1832:C:N4	1:A:1833:C:C4	2.64	0.65
1:A:1079:C:N4	1:A:1088:A:N3	2.45	0.65
1:A:2520:C:O2'	1:A:2521:C:C6	2.49	0.65
1:A:121:G:C2	1:A:131:A:C5	2.85	0.65
1:A:734:A:C4	1:A:735:A:C8	2.84	0.65
1:A:390:U:O2'	1:A:391:A:C8	2.50	0.65
1:A:2260:C:O2'	1:A:2261:C:C6	2.50	0.65
13:M:136:MET:OXT	13:M:136:MET:CG	2.45	0.65
2:B:79:G:N7	22:V:14:LYS:NZ	2.45	0.65
1:A:1555:G:N2	1:A:1556:C:C2	2.65	0.65
1:A:1608:A:C8	1:A:1611:C:N4	2.65	0.65
1:A:2572:A:O2'	1:A:2573:C:OP2	2.15	0.65
1:A:1386:C:O2'	1:A:1387:A:C8	2.50	0.65
1:A:1787:A:C2	1:A:1788:C:C4	2.85	0.65
1:A:1113:U:O2'	1:A:1114:C:C6	2.50	0.65
1:A:752:A:O2'	1:A:753:A:OP2	2.15	0.64
1:A:604:G:O2'	1:A:605:G:C8	2.50	0.64
1:A:2519:U:C6	1:A:2542:A:N6	2.64	0.64
1:A:2728:U:O2'	1:A:2729:G:C8	2.50	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2895:G:O2'	1:A:2896:C:C6	2.50	0.64
1:A:1654:A:O2'	1:A:1655:A:C8	2.49	0.64
1:A:764:A:N1	1:A:1789:A:O2'	2.31	0.64
1:A:2543:G:O6	1:A:2765:A:C5	2.50	0.64
1:A:1835:G:N2	1:A:1836:C:C2	2.65	0.64
1:A:572:A:OP1	34:A:3442:HOH:O	2.15	0.64
6:F:107:VAL:C	6:F:109:ARG:N	2.51	0.64
1:A:2259:U:C4	1:A:2427:C:N4	2.65	0.64
1:A:2093:G:N2	1:A:2094:A:C4	2.66	0.64
1:A:2148:G:O2'	1:A:2149:U:C6	2.51	0.64
1:A:1080:A:O2'	1:A:1081:U:O4'	2.16	0.64
1:A:1439:A:N1	1:A:1552:A:C4	2.65	0.64
1:A:2287:A:O2'	1:A:2288:A:C3'	2.46	0.64
1:A:225:C:O2'	1:A:226:A:O4'	2.16	0.64
22:V:55:GLU:O	22:V:57:TYR:N	2.31	0.64
1:A:2712:C:C2	1:A:2715:C:OP1	2.50	0.63
1:A:2421:G:N7	30:3:30:HIS:CD2	2.66	0.63
1:A:2902:C:O2'	1:A:2903:U:C5'	2.46	0.63
1:A:437:U:O2'	1:A:438:G:O4'	2.15	0.63
2:B:40:U:O2'	2:B:45:A:N6	2.31	0.63
1:A:556:A:C8	1:A:556:A:OP2	2.52	0.63
1:A:2592:G:C5	1:A:2593:U:C5	2.86	0.63
1:A:983:A:C6	1:A:984:A:C2	2.87	0.63
1:A:2010:G:C6	1:A:2011:U:C4	2.87	0.63
1:A:776:G:C8	1:A:793:A:C4	2.86	0.63
4:D:124:ARG:NH1	4:D:125:TRP:CZ2	2.67	0.63
1:A:374:A:O2'	1:A:375:G:O4'	2.17	0.63
1:A:2726:A:O2'	11:K:67:LYS:NZ	2.31	0.63
3:C:175:LEU:O	3:C:178:GLY:N	2.31	0.63
4:D:124:ARG:CD	4:D:125:TRP:CD1	2.82	0.63
1:A:2053:G:N2	1:A:2054:A:C4	2.66	0.63
1:A:1079:C:C4	1:A:1088:A:C2	2.87	0.63
1:A:1439:A:N7	1:A:1440:U:N1	2.47	0.63
1:A:1809:A:C2	1:A:1810:A:C4	2.87	0.63
2:B:11:C:C5	2:B:12:C:C5	2.86	0.63
1:A:2748:A:C4	1:A:2757:A:N6	2.67	0.62
20:T:15:HIS:CE1	20:T:80:TRP:CH2	2.87	0.62
1:A:1352:U:C5	1:A:1377:G:C6	2.87	0.62
1:A:1980:G:C5	1:A:1982:U:O4	2.53	0.62
1:A:1895:C:C2	1:A:1896:G:C8	2.87	0.62
1:A:832:U:OP1	12:L:39:LYS:N	2.33	0.62
1:A:1082:U:N3	1:A:1086:A:C5	2.67	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:397:U:OP1	24:X:30:PRO:CA	2.48	0.62
1:A:2287:A:C5	1:A:2289:G:C8	2.87	0.62
1:A:345:A:O2'	1:A:346:A:C2	2.53	0.62
7:G:93:TYR:N	7:G:93:TYR:CD2	2.67	0.62
1:A:2867:G:N3	1:A:2867:G:C2'	2.61	0.62
1:A:1440:U:C2	1:A:1441:G:C8	2.88	0.62
1:A:1906:G:C2	1:A:1925:C:O2	2.53	0.62
1:A:753:A:C2	1:A:754:U:N3	2.68	0.62
1:A:84:A:C5	1:A:103:A:N6	2.68	0.62
1:A:2638:G:O2'	1:A:2639:A:C8	2.53	0.62
1:A:2686:G:C2	1:A:2687:U:C2	2.87	0.62
1:A:987:C:O2'	1:A:1000:A:N3	2.32	0.62
1:A:740:C:O2'	1:A:741:U:C5'	2.47	0.61
1:A:500:G:N2	1:A:503:A:C8	2.68	0.61
1:A:2468:A:O2'	1:A:2469:A:C8	2.53	0.61
1:A:866:A:O2'	1:A:867:C:C6	2.53	0.61
1:A:2093:G:C6	1:A:2225:A:C8	2.88	0.61
1:A:460:A:OP2	29:2:41:ARG:NH1	2.33	0.61
1:A:1461:C:O2'	1:A:1462:C:C6	2.53	0.61
1:A:2297:A:N6	1:A:2319:G:O2'	2.33	0.61
1:A:1570:A:C6	1:A:1571:A:C6	2.89	0.61
1:A:2240:U:O2'	1:A:2241:A:O4'	2.18	0.61
1:A:946:C:O2'	1:A:947:A:C8	2.53	0.61
1:A:1683:U:O2'	1:A:1684:G:C8	2.53	0.61
1:A:33:C:O2	1:A:447:A:N6	2.34	0.61
1:A:972:A:N1	1:A:973:A:N6	2.48	0.61
1:A:2517:C:O2'	1:A:2518:A:C3'	2.48	0.61
1:A:537:G:N2	1:A:557:C:N4	2.48	0.61
1:A:1676:A:O2'	1:A:1677:A:O4'	2.19	0.61
1:A:1287:A:O2'	1:A:1288:G:C5'	2.48	0.61
8:H:49:ALA:O	8:H:53:GLU:N	2.34	0.61
23:W:33:GLY:O	23:W:34:SER:CB	2.48	0.61
1:A:1441:G:C6	1:A:1442:U:C4	2.89	0.61
1:A:1809:A:C2'	1:A:1810:A:C8	2.84	0.61
1:A:76:C:O2'	1:A:77:G:C5'	2.49	0.61
1:A:2267:A:N6	1:A:2271:G:O6	2.34	0.61
8:H:97:ARG:O	8:H:98:ASP:CB	2.49	0.61
1:A:2333:A:C2	1:A:2335:A:N6	2.69	0.61
1:A:2643:G:C5	1:A:2644:G:N7	2.68	0.61
1:A:1014:A:C5	1:A:1015:U:C5	2.89	0.61
1:A:2611:C:O2'	1:A:2612:C:O4'	2.18	0.61
1:A:2093:G:C5	1:A:2225:A:C5	2.89	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:671:C:O2'	1:A:672:C:C6	2.54	0.60
1:A:2336:A:N7	23:W:40:ARG:NH2	2.49	0.60
1:A:2531:A:C4	1:A:2532:G:C8	2.89	0.60
1:A:2571:U:C4	1:A:2574:G:C8	2.89	0.60
1:A:2259:U:C2	1:A:2260:C:C5	2.89	0.60
2:B:38:C:C4'	15:O:100:HIS:NE2	2.63	0.60
1:A:396:G:OP2	24:X:9:LYS:NZ	2.35	0.60
1:A:2287:A:O2'	1:A:2288:A:O5'	2.20	0.60
1:A:571:U:C2	1:A:2030:A:C5	2.89	0.60
1:A:1071:G:N7	1:A:1089:A:C5	2.70	0.60
1:A:1738:G:O2'	1:A:1739:A:C8	2.55	0.60
1:A:396:G:O2'	1:A:397:U:C6	2.55	0.60
1:A:832:U:O2'	1:A:833:A:O4'	2.19	0.60
1:A:1057:A:N6	1:A:1087:G:OP1	2.35	0.60
24:X:1:SER:O	24:X:3:VAL:N	2.35	0.60
1:A:647:G:O2'	1:A:648:G:O4'	2.17	0.60
1:A:860:U:C4	1:A:2268:A:C4	2.90	0.60
22:V:31:TYR:O	22:V:31:TYR:CD1	2.54	0.60
1:A:1439:A:C2	1:A:1552:A:C4	2.89	0.59
1:A:49:A:N6	1:A:177:G:C5	2.70	0.59
1:A:279:A:N6	1:A:361:G:O2'	2.35	0.59
1:A:1844:C:C2	1:A:1845:G:C8	2.90	0.59
2:B:73:A:N6	22:V:31:TYR:CE2	2.71	0.59
1:A:1343:G:C5	1:A:1597:A:N6	2.70	0.59
1:A:617:G:O2'	1:A:618:G:O4'	2.21	0.59
17:Q:4:LYS:NZ	17:Q:6:GLY:CA	2.65	0.59
1:A:1206:G:C2	1:A:1207:C:C2	2.91	0.59
1:A:1074:G:OP2	1:A:1074:G:C8	2.56	0.59
1:A:1439:A:N1	1:A:1552:A:C8	2.71	0.59
1:A:2093:G:N7	1:A:2225:A:C4	2.70	0.59
1:A:780:G:O2'	1:A:783:A:N6	2.36	0.59
1:A:1521:G:C6	1:A:1522:A:N6	2.71	0.59
1:A:1341:G:O2'	1:A:1398:C:C5'	2.50	0.59
1:A:1682:G:O2'	1:A:1683:U:C6	2.55	0.59
3:C:8:THR:O	3:C:9:SER:CB	2.50	0.59
10:J:45:THR:C	10:J:47:HIS:N	2.56	0.59
1:A:2836:U:C2	1:A:2837:A:N7	2.71	0.59
1:A:1034:G:O2'	1:A:1035:U:O4'	2.20	0.59
1:A:1001:A:C8	1:A:1002:G:C8	2.90	0.59
1:A:2415:G:C2	1:A:2416:C:C2	2.91	0.59
1:A:46:G:N2	1:A:47:C:C2	2.71	0.59
1:A:2508:G:C2	1:A:2582:G:C6	2.91	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2623:G:N2	27:0:18:HIS:CE1	2.71	0.58
1:A:478:A:N6	1:A:480:A:C6	2.71	0.58
8:H:24:GLY:O	8:H:26:ALA:O	2.22	0.58
1:A:729:G:C2'	1:A:729:G:N3	2.66	0.58
1:A:380:G:C2	1:A:395:U:O2	2.55	0.58
4:D:149:ASN:O	4:D:151:THR:N	2.36	0.58
1:A:2686:G:C5	1:A:2687:U:C4	2.92	0.58
1:A:2643:G:C4	1:A:2644:G:C8	2.91	0.58
1:A:2774:C:N4	1:A:2775:G:C6	2.71	0.58
1:A:657:U:O2'	1:A:658:U:C6	2.57	0.58
1:A:1008:A:N6	1:A:1136:G:C6	2.71	0.58
1:A:1075:C:O2'	1:A:1076:C:C5'	2.51	0.58
1:A:1079:C:O2'	1:A:1080:A:C8	2.57	0.58
1:A:2687:U:C4	1:A:2688:G:C6	2.90	0.58
1:A:2446:G:C2	1:A:2501:C:C5	2.92	0.58
1:A:1565:C:O2'	1:A:1566:A:C8	2.57	0.58
1:A:2315:G:C2	1:A:2316:G:C4	2.91	0.58
1:A:1087:G:C5	1:A:1089:A:C2	2.92	0.58
1:A:75:G:O2'	1:A:76:C:C6	2.56	0.58
1:A:2348:U:O2'	1:A:2349:G:O4'	2.22	0.58
1:A:1826:G:C6	1:A:1827:U:C4	2.90	0.58
1:A:583:G:C6	1:A:584:C:C4	2.92	0.58
6:F:109:ARG:NH1	6:F:135:ILE:CG2	2.66	0.58
6:F:135:ILE:O	6:F:137:PHE:N	2.37	0.58
1:A:1476:U:O2'	1:A:1477:A:P	2.61	0.58
1:A:2077:A:C8	1:A:2435:A:C4	2.91	0.58
1:A:2253:G:C6	1:A:2254:C:C4	2.92	0.58
1:A:2653:U:C4	1:A:2654:A:C6	2.92	0.58
1:A:54:G:C6	1:A:55:G:N7	2.72	0.58
7:G:163:TYR:N	7:G:163:TYR:CD2	2.72	0.58
1:A:1331:G:C4	1:A:1333:G:N7	2.72	0.58
4:D:208:LYS:O	4:D:209:ALA:CB	2.52	0.58
1:A:1950:G:N1	1:A:1954:G:C8	2.72	0.57
1:A:975:A:C4	1:A:990:A:N7	2.72	0.57
1:A:1889:A:N3	1:A:2086:U:O2'	2.37	0.57
1:A:2812:G:C2	1:A:2813:A:C4	2.92	0.57
1:A:1623:G:C2	1:A:1624:U:C6	2.91	0.57
4:D:118:PHE:CD1	4:D:119:ALA:N	2.72	0.57
1:A:2212:A:C8	1:A:2214:C:N4	2.72	0.57
1:A:2214:C:O2'	1:A:2215:C:C5'	2.52	0.57
1:A:121:G:N2	1:A:131:A:C4	2.72	0.57
1:A:233:A:O2'	1:A:234:U:C6	2.57	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2595:G:N1	1:A:2599:G:C6	2.72	0.57
1:A:2601:C:C2	1:A:2603:G:N7	2.72	0.57
1:A:2461:A:N1	1:A:2490:G:N2	2.52	0.57
1:A:324:A:O2'	1:A:325:G:O4'	2.23	0.57
24:X:26:ARG:NH1	24:X:28:PHE:CD2	2.72	0.57
1:A:379:G:C6	1:A:380:G:C5	2.92	0.57
1:A:2336:A:N7	23:W:40:ARG:CZ	2.67	0.57
1:A:100:U:O2'	1:A:101:A:O5'	2.21	0.57
8:H:2:GLN:O	8:H:3:VAL:O	2.23	0.57
2:B:17:C:O2'	2:B:18:G:O4'	2.22	0.57
1:A:442:G:O6	1:A:444:C:N4	2.37	0.57
1:A:2543:G:N1	1:A:2765:A:C8	2.72	0.57
1:A:972:A:C6	1:A:973:A:C6	2.93	0.57
1:A:1974:C:C2	1:A:1975:G:C8	2.92	0.57
1:A:2886:A:N7	27:O:39:ARG:NE	2.53	0.57
1:A:1508:A:C4'	1:A:1509:A:OP1	2.53	0.57
1:A:1731:G:N3	1:A:1733:G:C8	2.73	0.57
1:A:93:G:O2'	1:A:94:A:O4'	2.23	0.57
1:A:745:G:C2	1:A:753:A:N6	2.73	0.57
1:A:2544:G:O2'	1:A:2545:G:O4'	2.22	0.57
1:A:1651:G:C6	1:A:1652:A:C6	2.93	0.57
1:A:782:A:C2	3:C:224:MET:SD	2.98	0.56
1:A:1845:G:C6	1:A:1896:G:C6	2.93	0.56
1:A:1682:G:C8	1:A:1757:A:C2	2.92	0.56
1:A:2447:G:O6	1:A:2504:U:O4	2.22	0.56
1:A:1734:G:O2'	1:A:1735:A:C8	2.58	0.56
1:A:2287:A:C6	1:A:2289:G:C5	2.93	0.56
1:A:2287:A:C4	1:A:2289:G:N7	2.74	0.56
1:A:226:A:C2	1:A:230:G:O6	2.58	0.56
1:A:1331:G:O2'	1:A:1332:G:C5'	2.53	0.56
3:C:66:PHE:CZ	3:C:155:ARG:NH1	2.74	0.56
1:A:110:G:C4	1:A:111:A:C8	2.93	0.56
1:A:117:G:C6	1:A:119:A:C6	2.93	0.56
1:A:233:A:O2'	1:A:234:U:O5'	2.23	0.56
1:A:265:A:C5	1:A:428:A:C8	2.93	0.56
1:A:1203:U:N3	1:A:1204:A:N6	2.53	0.56
1:A:250:G:C2'	1:A:251:A:C8	2.87	0.56
1:A:2823:A:C5	1:A:2824:C:C5	2.93	0.56
21:U:95:PHE:O	21:U:97:SER:N	2.38	0.56
1:A:2540:C:C2	1:A:2541:A:C8	2.94	0.56
1:A:2023:C:O2'	1:A:2024:G:C8	2.59	0.56
1:A:1019:U:O2'	1:A:1021:A:C2	2.59	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2547:A:C1'	1:A:2566:A:C6	2.88	0.56
2:B:58:A:C2'	2:B:59:A:C8	2.89	0.56
1:A:2543:G:C6	1:A:2765:A:C4	2.94	0.56
1:A:117:G:N1	1:A:119:A:N6	2.53	0.56
1:A:2287:A:C5	1:A:2289:G:N7	2.74	0.56
1:A:1168:G:C6	1:A:1182:G:C6	2.93	0.56
1:A:1203:U:N3	1:A:1204:A:C6	2.73	0.56
1:A:2592:G:C4	1:A:2593:U:C5	2.94	0.56
1:A:2849:U:OP1	16:P:92:ARG:NH1	2.39	0.56
1:A:2080:A:C2	1:A:2081:U:C2	2.94	0.56
1:A:1236:G:O2'	1:A:1237:A:C8	2.58	0.56
8:H:9:VAL:CG1	8:H:10:ALA:N	2.68	0.56
1:A:33:C:O2'	1:A:34:U:C5'	2.53	0.56
1:A:658:U:O2'	1:A:659:G:O4'	2.24	0.56
1:A:374:A:C6	1:A:401:A:C8	2.94	0.56
1:A:2572:A:C8	4:D:149:ASN:ND2	2.74	0.56
1:A:1128:G:O6	1:A:2491:U:C5	2.59	0.56
1:A:690:G:O2'	1:A:780:G:OP1	2.23	0.56
1:A:333:G:O2'	1:A:334:C:C5'	2.54	0.56
1:A:1867:G:O2'	1:A:1868:C:O4'	2.24	0.56
11:K:73:ASP:N	11:K:73:ASP:OD1	2.39	0.56
1:A:1439:A:N6	1:A:1440:U:C2	2.74	0.55
1:A:604:G:C6	1:A:625:G:C6	2.94	0.55
1:A:177:G:N2	1:A:177:G:OP2	2.39	0.55
1:A:2051:A:C4'	1:A:2052:A:OP1	2.54	0.55
1:A:508:A:N6	19:S:9:HIS:CE1	2.74	0.55
1:A:2230:G:C6	1:A:2231:U:C4	2.95	0.55
1:A:695:G:C4	1:A:768:G:C2	2.95	0.55
4:D:124:ARG:CD	4:D:125:TRP:NE1	2.69	0.55
1:A:2499:C:O2'	1:A:2500:U:O4'	2.24	0.55
15:O:69:ASP:O	15:O:73:ALA:N	2.39	0.55
1:A:74:A:O2'	1:A:88:G:C8	2.60	0.55
1:A:1011:G:C6	1:A:1013:C:C4	2.94	0.55
31:4:19:ARG:O	31:4:20:ASP:CB	2.54	0.55
4:D:10:GLY:O	4:D:11:MET:CB	2.54	0.55
1:A:1439:A:N6	1:A:1551:A:N1	2.54	0.55
1:A:482:A:C6	1:A:506:G:C4	2.95	0.55
1:A:76:C:N3	1:A:111:A:C2	2.74	0.55
1:A:54:G:C4	1:A:55:G:C8	2.95	0.55
1:A:2065:C:N4	1:A:2066:C:N4	2.55	0.55
21:U:95:PHE:N	21:U:95:PHE:CD1	2.74	0.55
1:A:1663:G:C6	1:A:1992:G:N7	2.75	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1213:A:O2'	1:A:1214:A:C5'	2.55	0.55
24:X:31:ASN:ND2	24:X:31:ASN:N	2.54	0.55
1:A:2447:G:C8	1:A:2500:U:C6	2.94	0.55
1:A:247:G:C4'	1:A:386:G:C5	2.89	0.55
1:A:1049:C:O2'	1:A:1050:A:C5'	2.54	0.55
1:A:2616:C:O2'	1:A:2617:U:O4'	2.24	0.55
1:A:672:C:C2	1:A:809:G:N2	2.75	0.55
1:A:1238:G:N3	1:A:1239:G:C8	2.74	0.55
3:C:146:LYS:O	3:C:148:GLY:N	2.39	0.55
1:A:825:A:C2	1:A:826:U:C2	2.94	0.55
10:J:4:PHE:O	10:J:44:TYR:CZ	2.60	0.55
3:C:43:ASN:ND2	3:C:44:ASN:N	2.55	0.55
1:A:216:A:O2'	1:A:217:A:O5'	2.24	0.55
1:A:301:G:C6	1:A:302:C:N4	2.75	0.55
1:A:1286:A:C5	1:A:1289:C:N4	2.75	0.55
1:A:2837:A:O2'	1:A:2838:G:O4'	2.24	0.55
1:A:1079:C:N4	1:A:1088:A:C2	2.75	0.55
1:A:1324:G:O2'	1:A:1616:A:C5	2.59	0.55
1:A:2539:C:C4	1:A:2540:C:C5	2.94	0.55
1:A:2240:U:O2'	1:A:2241:A:O5'	2.25	0.55
1:A:1838:C:C6	1:A:1899:A:C6	2.95	0.55
1:A:2770:G:C8	1:A:2770:G:O5'	2.60	0.55
1:A:2611:C:O2'	1:A:2612:C:C5'	2.55	0.55
1:A:1251:C:C6	17:Q:5:ARG:NH1	2.75	0.55
1:A:1954:G:O2'	1:A:1956:U:O4	2.25	0.54
1:A:1276:A:C2	1:A:1277:G:C5	2.95	0.54
1:A:874:G:C2	1:A:904:G:C2	2.95	0.54
1:A:271:G:C6	1:A:272:A:N6	2.75	0.54
1:A:973:A:OP1	1:A:973:A:O4'	2.24	0.54
1:A:1079:C:N3	1:A:1088:A:C2	2.76	0.54
1:A:54:G:C5	1:A:55:G:C8	2.96	0.54
1:A:2902:C:O2'	1:A:2903:U:O5'	2.26	0.54
1:A:508:A:N6	19:S:9:HIS:NE2	2.56	0.54
1:A:2524:G:O2'	1:A:2741:A:N1	2.40	0.54
1:A:2615:U:C4	27:O:2:VAL:C	2.80	0.54
1:A:1022:G:O2'	1:A:1023:U:OP2	2.25	0.54
1:A:161:A:C5	1:A:162:U:C4	2.96	0.54
1:A:1022:G:N2	1:A:1142:A:C2	2.76	0.54
1:A:1984:G:C6	1:A:1985:C:C4	2.96	0.54
1:A:70:G:O2'	1:A:71:A:C5'	2.56	0.54
1:A:2809:A:OP2	1:A:2890:G:N1	2.41	0.54
1:A:2237:G:O2'	1:A:2239:G:N7	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:A:C2	29:2:35:ARG:NH1	2.76	0.54
1:A:1935:G:C1'	1:A:1964:G:N2	2.70	0.54
6:F:76:PHE:N	6:F:76:PHE:CD2	2.75	0.54
1:A:90:U:C4	1:A:91:A:C5	2.96	0.54
1:A:1290:C:O2'	1:A:1291:C:O4'	2.26	0.54
1:A:1399:C:O2'	1:A:1400:U:C5'	2.56	0.54
1:A:2835:A:N7	1:A:2879:A:C2	2.76	0.54
1:A:529:A:C5	1:A:2023:C:C4	2.95	0.54
1:A:1623:G:C6	1:A:1624:U:C5	2.96	0.54
1:A:1782:U:O2'	1:A:1783:A:C5'	2.55	0.54
6:F:107:VAL:N	6:F:108:PRO:CD	2.71	0.54
1:A:762:U:N3	1:A:1431:A:OP1	2.41	0.54
1:A:84:A:C4	1:A:103:A:N6	2.76	0.54
1:A:84:A:O2'	1:A:85:G:O4'	2.26	0.54
1:A:2015:A:C2	27:0:2:VAL:CG1	2.91	0.54
1:A:1059:G:C5	1:A:1060:U:C2	2.96	0.54
2:B:73:A:N6	22:V:31:TYR:CD2	2.76	0.54
1:A:1355:G:C6	1:A:1377:G:N2	2.76	0.54
4:D:117:GLY:O	4:D:119:ALA:N	2.41	0.54
1:A:1535:A:N1	1:A:1537:G:N7	2.56	0.54
1:A:1450:G:N2	1:A:1462:C:C2	2.76	0.53
1:A:804:A:C2'	1:A:806:C:C4	2.91	0.53
1:A:197:A:N7	1:A:2430:A:C5	2.76	0.53
1:A:422:A:C6	1:A:423:A:N6	2.77	0.53
1:A:2520:C:C2	1:A:2521:C:C5	2.97	0.53
1:A:2052:A:C2	1:A:2053:G:C8	2.97	0.53
1:A:1352:U:C6	1:A:1377:G:C6	2.96	0.53
1:A:1439:A:N7	1:A:1440:U:C2	2.76	0.53
2:B:17:C:O2'	2:B:18:G:C5'	2.57	0.53
14:N:62:ASN:O	14:N:63:ARG:CB	2.56	0.53
1:A:1420:A:C2	1:A:2211:A:N7	2.76	0.53
1:A:1649:G:O6	1:A:2009:A:N6	2.41	0.53
1:A:571:U:C5	1:A:575:A:C6	2.97	0.53
1:A:2077:A:C5	1:A:2435:A:C5	2.96	0.53
1:A:695:G:N3	1:A:768:G:C2	2.77	0.53
1:A:1416:G:C6	1:A:1417:C:C4	2.96	0.53
1:A:2750:A:O2'	1:A:2752:C:N4	2.42	0.53
1:A:2752:C:O2'	1:A:2753:A:O4'	2.26	0.53
1:A:1638:C:O2	1:A:2698:U:O2'	2.27	0.53
1:A:1808:A:N7	24:X:27:ARG:NH1	2.57	0.53
1:A:957:C:C2	1:A:2459:A:O4'	2.62	0.53
1:A:241:A:O2'	1:A:242:G:O5'	2.26	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:G:C6	1:A:378:C:C4	2.96	0.53
1:A:2307:G:O2'	1:A:2308:G:C8	2.62	0.53
1:A:364:C:C2'	1:A:365:U:C6	2.91	0.53
1:A:1608:A:C5	1:A:1611:C:C4	2.96	0.53
1:A:1352:U:C5	1:A:1377:G:C5	2.95	0.53
1:A:616:A:C2'	1:A:617:G:C8	2.92	0.53
7:G:149:ALA:O	7:G:151:ARG:N	2.42	0.53
23:W:17:ALA:O	23:W:18:LYS:CB	2.56	0.53
1:A:2370:G:C6	1:A:2371:G:C6	2.97	0.53
1:A:579:G:C2	1:A:1262:A:C4	2.97	0.53
1:A:1919:A:O5'	1:A:1919:A:C8	2.60	0.53
1:A:2418:A:C2	1:A:2419:U:C2	2.97	0.53
1:A:1439:A:C8	1:A:1440:U:C6	2.97	0.53
1:A:739:A:O2'	1:A:740:C:C5	2.61	0.53
1:A:2239:G:O2'	1:A:2240:U:C6	2.62	0.53
1:A:1946:U:O2'	1:A:1947:C:O4'	2.27	0.53
1:A:444:C:O2'	1:A:445:C:C5'	2.56	0.53
1:A:201:C:C5	1:A:202:U:C5	2.97	0.53
1:A:1135:C:N4	1:A:1139:G:C6	2.76	0.53
1:A:616:A:O2'	1:A:617:G:C5'	2.56	0.53
1:A:2536:G:C6	1:A:2537:U:C4	2.97	0.53
1:A:1511:G:O2'	1:A:1512:C:O4'	2.27	0.53
13:M:19:GLY:N	13:M:38:ARG:NH2	2.56	0.53
4:D:124:ARG:NH1	4:D:125:TRP:CE2	2.77	0.53
1:A:1670:C:O2	4:D:134:HIS:NE2	2.41	0.53
1:A:948:C:O2	1:A:984:A:O2'	2.27	0.53
1:A:656:G:O2'	1:A:657:U:C5'	2.57	0.53
1:A:1667:G:N2	1:A:1992:G:OP2	2.42	0.53
1:A:1992:G:N2	1:A:1995:U:C5	2.77	0.53
1:A:1274:A:C6	1:A:1302:A:C2	2.97	0.53
1:A:1439:A:N6	1:A:1440:U:O2	2.42	0.52
1:A:1178:C:C2	1:A:1179:G:C8	2.98	0.52
1:A:1439:A:N3	1:A:1552:A:C6	2.77	0.52
1:A:1071:G:O4'	1:A:1088:A:O2'	2.28	0.52
1:A:1358:G:O6	1:A:1371:G:C8	2.63	0.52
1:A:1267:U:OP2	1:A:2012:G:N1	2.42	0.52
1:A:1539:U:O2'	1:A:1540:G:O4'	2.27	0.52
1:A:2026:U:O2	1:A:2038:G:N2	2.43	0.52
1:A:1654:A:O2'	1:A:1655:A:O5'	2.28	0.52
14:N:28:LEU:O	14:N:32:GLU:N	2.42	0.52
1:A:2577:A:C2	27:O:1:ALA:N	2.77	0.52
1:A:1286:A:C5	1:A:1289:C:C4	2.97	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:45:A:C2'	2:B:46:A:C8	2.92	0.52
1:A:1651:G:C6	1:A:1652:A:C5	2.98	0.52
1:A:1127:A:N7	1:A:2488:G:O2'	2.41	0.52
1:A:160:A:C6	1:A:161:A:C6	2.97	0.52
1:A:2370:G:O6	1:A:2371:G:C6	2.62	0.52
1:A:910:A:C6	1:A:911:A:C6	2.98	0.52
1:A:2048:G:C6	1:A:2049:G:C5	2.98	0.52
12:L:81:ASP:O	12:L:83:ALA:N	2.42	0.52
1:A:200:U:O4	1:A:248:G:C2	2.63	0.52
1:A:1776:G:N2	1:A:1789:A:C4	2.78	0.52
1:A:866:A:C5	1:A:914:G:N7	2.77	0.52
1:A:975:A:O2'	1:A:976:G:C5'	2.58	0.52
1:A:197:A:N6	1:A:2430:A:C2'	2.73	0.52
1:A:637:A:C4'	1:A:638:G:O5'	2.57	0.52
1:A:2585:U:O2'	1:A:2586:U:C5'	2.57	0.52
1:A:1478:G:C6	1:A:1514:G:C2	2.97	0.52
1:A:604:G:C2	1:A:605:G:C5	2.98	0.52
1:A:197:A:C5	1:A:2430:A:C4	2.98	0.52
5:E:170:ARG:CZ	5:E:176:ASP:OD2	2.57	0.52
31:4:3:VAL:O	31:4:4:ARG:CB	2.57	0.52
13:M:1:MET:O	13:M:2:LEU:O	2.27	0.52
1:A:753:A:C2	1:A:754:U:C2	2.98	0.52
1:A:2566:A:O2'	1:A:2567:G:OP2	2.28	0.52
1:A:2811:G:C2	1:A:2812:G:C4	2.98	0.52
1:A:1923:U:C2	1:A:1924:C:C5	2.97	0.52
3:C:189:ALA:O	3:C:190:THR:CB	2.56	0.52
1:A:2264:C:C2	1:A:2277:G:C2	2.97	0.52
1:A:83:A:N6	1:A:101:A:C5'	2.73	0.52
1:A:48:G:C6	1:A:178:G:O6	2.62	0.52
1:A:2711:A:N6	1:A:2714:G:C5	2.77	0.52
1:A:1158:C:O2'	1:A:1159:U:O4'	2.28	0.52
5:E:79:ARG:O	5:E:80:SER:C	2.48	0.52
1:A:1475:G:O2'	1:A:1476:U:C6	2.63	0.52
1:A:216:A:C2'	1:A:217:A:C8	2.93	0.52
1:A:476:G:C4	1:A:478:A:OP2	2.63	0.52
1:A:1570:A:C6	1:A:1571:A:N1	2.78	0.52
1:A:2392:A:C2	12:L:55:MET:SD	3.03	0.52
1:A:2720:U:C2	1:A:2872:A:C5	2.98	0.52
1:A:680:C:O2	1:A:681:G:C8	2.63	0.52
1:A:697:G:C2	1:A:766:U:O2	2.63	0.52
1:A:766:U:O2'	1:A:767:U:O4'	2.28	0.52
1:A:1296:G:N2	1:A:1645:G:C5	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1386:C:O2'	1:A:1387:A:O5'	2.28	0.52
1:A:2592:G:C6	1:A:2593:U:C4	2.98	0.52
1:A:2349:G:N1	1:A:2350:C:C2	2.77	0.52
1:A:616:A:O2'	1:A:617:G:O4'	2.28	0.52
1:A:1827:U:O4'	1:A:1970:A:O2'	2.28	0.52
1:A:686:U:C6	1:A:788:A:N1	2.77	0.52
1:A:985:C:N4	1:A:986:C:N4	2.58	0.52
1:A:2860:A:O5'	1:A:2860:A:C8	2.62	0.52
1:A:684:G:C2	1:A:794:A:C2	2.98	0.52
6:F:136:ILE:CG2	6:F:142:TYR:CG	2.93	0.51
1:A:2337:G:OP1	1:A:2385:C:OP2	2.28	0.51
1:A:1809:A:C6	1:A:1810:A:C6	2.98	0.51
1:A:475:C:C2'	1:A:476:G:C8	2.92	0.51
1:A:1973:G:C5	1:A:1974:C:C5	2.98	0.51
1:A:161:A:C6	1:A:162:U:O4	2.62	0.51
10:J:30:THR:CG2	10:J:31:GLU:N	2.73	0.51
1:A:590:A:OP1	5:E:90:GLN:NE2	2.43	0.51
1:A:1900:A:C2	1:A:1970:A:C5	2.97	0.51
2:B:75:G:N1	2:B:102:G:N2	2.58	0.51
1:A:1953:A:C6	1:A:2550:G:O4'	2.63	0.51
1:A:2283:C:C4	1:A:2389:G:C5	2.99	0.51
1:A:120:U:C2	1:A:149:A:C6	2.98	0.51
1:A:2140:G:C6	1:A:2152:G:C6	2.98	0.51
6:F:107:VAL:O	6:F:109:ARG:N	2.44	0.51
1:A:1775:U:C2'	1:A:1776:G:O5'	2.58	0.51
1:A:2568:U:O2'	1:A:2569:G:O4'	2.27	0.51
1:A:160:A:C2	1:A:161:A:C4	2.99	0.51
12:L:94:THR:O	12:L:98:ALA:N	2.44	0.51
1:A:392:U:O2'	1:A:393:C:O4'	2.28	0.51
1:A:529:A:C8	1:A:2042:A:N1	2.79	0.51
1:A:2074:U:N3	1:A:2075:U:C4	2.78	0.51
19:S:8:ARG:O	19:S:9:HIS:CB	2.57	0.51
4:D:113:SER:OG	4:D:114:LYS:N	2.44	0.51
1:A:1180:U:N3	1:A:1181:U:C2	2.79	0.51
10:J:95:ARG:O	10:J:96:ARG:C	2.48	0.51
6:F:113:PHE:O	6:F:114:ARG:CB	2.59	0.51
1:A:845:A:N6	1:A:932:U:N3	2.59	0.51
1:A:2700:A:C2	1:A:2708:G:C2	2.98	0.51
1:A:2337:G:N3	1:A:2337:G:C2'	2.73	0.51
1:A:647:G:C2'	1:A:648:G:C8	2.94	0.51
8:H:24:GLY:O	8:H:25:TYR:C	2.48	0.51
1:A:2079:U:C2	1:A:2080:A:C8	2.98	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1821:A:O2'	1:A:1822:C:O5'	2.27	0.51
10:J:94:ALA:O	10:J:95:ARG:CB	2.58	0.51
1:A:2667:C:O2'	7:G:110:HIS:CE1	2.63	0.51
1:A:1680:U:O4	1:A:1681:G:C2	2.64	0.51
1:A:1024:G:C6	1:A:1025:G:C6	2.99	0.51
1:A:1438:U:C4	1:A:1552:A:N1	2.78	0.51
1:A:225:C:O2'	1:A:226:A:C5'	2.58	0.51
1:A:2052:A:N6	1:A:2618:G:C2	2.78	0.51
1:A:533:G:C2	1:A:534:U:C2	2.99	0.51
1:A:1562:U:C4	1:A:1563:U:C4	2.98	0.51
13:M:72:PRO:O	13:M:73:ILE:CB	2.59	0.51
1:A:35:G:C2'	1:A:36:G:O5'	2.58	0.51
1:A:1816:C:O3'	1:A:1817:G:C8	2.64	0.51
1:A:571:U:C6	1:A:575:A:N6	2.79	0.51
1:A:680:C:C2	1:A:681:G:C8	2.99	0.51
1:A:1558:C:C2	1:A:1560:G:C6	2.99	0.51
1:A:2782:G:N2	1:A:2783:U:C2	2.79	0.51
1:A:1686:C:N3	1:A:1703:G:C2	2.78	0.51
1:A:628:G:C6	1:A:636:G:C2	2.99	0.51
1:A:973:A:C8	1:A:973:A:OP1	2.63	0.51
10:J:43:GLU:O	10:J:45:THR:N	2.43	0.51
21:U:94:PHE:O	21:U:95:PHE:C	2.48	0.51
3:C:212:TRP:CD1	3:C:212:TRP:C	2.84	0.51
1:A:1707:G:C8	1:A:1756:G:C5	2.99	0.51
1:A:1716:U:O2'	1:A:1717:A:C5'	2.59	0.51
1:A:223:A:N6	1:A:422:A:C5	2.78	0.51
1:A:910:A:N6	1:A:911:A:N1	2.59	0.51
1:A:28:A:C6	1:A:29:U:C2	2.99	0.51
2:B:52:A:O2'	2:B:53:A:C8	2.64	0.51
1:A:1498:C:O2'	1:A:1499:C:C5'	2.59	0.51
1:A:2331:G:N1	1:A:2385:C:N4	2.58	0.51
1:A:410:G:N1	1:A:2407:A:N6	2.59	0.51
1:A:2748:A:C2	1:A:2757:A:C5	2.99	0.51
1:A:449:A:O2'	1:A:450:G:C5'	2.59	0.51
2:B:49:C:OP1	15:O:102:ARG:N	2.44	0.51
15:O:99:TYR:O	15:O:99:TYR:CD1	2.64	0.51
22:V:31:TYR:OH	22:V:90:ASP:CB	2.60	0.50
1:A:1435:G:N2	1:A:1558:C:N4	2.59	0.50
1:A:1853:A:N6	1:A:1888:G:O2'	2.45	0.50
1:A:1191:G:N2	1:A:1192:G:C4	2.79	0.50
1:A:2864:G:C5	1:A:2865:U:C4	2.99	0.50
1:A:301:G:C6	1:A:317:G:C6	2.99	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:781:A:N1	1:A:1776:G:O2'	2.44	0.50
1:A:232:G:C4'	1:A:233:A:OP1	2.59	0.50
12:L:93:ASN:O	12:L:95:LEU:N	2.44	0.50
1:A:1998:A:C5	1:A:1999:C:C5	2.99	0.50
1:A:289:G:C2	1:A:352:A:C2	2.99	0.50
1:A:260:G:C6	1:A:261:G:N7	2.79	0.50
4:D:135:GLY:O	4:D:136:ASN:O	2.29	0.50
2:B:66:A:OP2	2:B:108:A:N6	2.44	0.50
1:A:301:G:O2'	1:A:302:C:P	2.70	0.50
1:A:2653:U:N3	1:A:2654:A:C6	2.79	0.50
1:A:2550:G:C6	1:A:2551:C:C4	2.99	0.50
1:A:2674:G:C5	1:A:2675:A:N7	2.79	0.50
1:A:43:G:C2	1:A:437:U:C2	2.99	0.50
8:H:96:THR:O	8:H:97:ARG:CG	2.60	0.50
1:A:1206:G:N2	1:A:1207:C:C2	2.80	0.50
1:A:1203:U:C4	1:A:1204:A:C6	3.00	0.50
1:A:961:C:C5	1:A:2031:A:C2	2.99	0.50
1:A:1047:G:C2	1:A:1110:G:C5	3.00	0.50
1:A:146:A:C2	1:A:147:C:C2	3.00	0.50
11:K:71:ARG:CB	11:K:72:PRO:CD	2.90	0.50
1:A:1027:A:O2'	1:A:1028:A:C8	2.64	0.50
1:A:489:G:C6	1:A:491:G:C6	2.99	0.50
1:A:656:G:C5	1:A:657:U:C4	2.99	0.50
1:A:2009:A:N1	1:A:2010:G:C5	2.79	0.50
2:B:98:G:N1	22:V:14:LYS:CB	2.75	0.50
1:A:1835:G:C2	1:A:1836:C:C2	3.00	0.50
1:A:2267:A:N6	1:A:2271:G:C6	2.79	0.50
1:A:1935:G:C2	1:A:1962:C:C2	3.00	0.50
1:A:2515:C:O2	1:A:2570:G:C2	2.65	0.50
1:A:38:A:C5	1:A:39:G:C8	2.99	0.50
1:A:36:G:N2	1:A:445:C:C2	2.79	0.50
1:A:475:C:N3	1:A:479:A:N7	2.59	0.50
1:A:422:A:C6	1:A:423:A:C6	2.99	0.50
1:A:1814:G:C6	1:A:1815:A:C6	3.00	0.50
1:A:1683:U:O2'	1:A:1684:G:O5'	2.29	0.50
1:A:1622:G:C2	1:A:1623:G:C8	2.99	0.50
1:A:100:U:O2'	1:A:101:A:P	2.69	0.50
1:A:1168:G:C2	1:A:1182:G:C2	3.00	0.50
1:A:1026:G:O2'	1:A:1027:A:C5'	2.60	0.50
1:A:1312:U:C2	1:A:1603:A:C6	3.00	0.50
25:Y:30:MET:O	25:Y:30:MET:SD	2.70	0.50
1:A:754:U:O2'	1:A:755:U:C6	2.64	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2285:C:O4'	1:A:2288:A:C2	2.65	0.50
1:A:2686:G:C6	1:A:2687:U:C4	2.99	0.50
10:J:43:GLU:CG	10:J:43:GLU:O	2.59	0.50
1:A:1731:G:O2'	1:A:1732:C:C5'	2.59	0.50
1:A:352:A:C6	1:A:353:C:C2	3.00	0.50
30:3:18:LYS:CG	30:3:19:GLY:N	2.75	0.50
1:A:2422:C:N4	1:A:2424:C:N3	2.60	0.50
1:A:2630:G:C5	1:A:2894:G:C6	3.00	0.50
1:A:1613:G:C2	1:A:1617:C:C2	2.99	0.50
1:A:1613:G:N1	1:A:1617:C:C2	2.80	0.50
12:L:3:LEU:O	12:L:4:ASN:C	2.49	0.50
25:Y:47:ARG:O	25:Y:50:VAL:N	2.45	0.50
1:A:1470:A:C8	1:A:1470:A:OP2	2.65	0.50
1:A:1789:A:OP2	3:C:220:ARG:NH1	2.45	0.50
1:A:754:U:O2'	1:A:755:U:C5'	2.60	0.50
4:D:118:PHE:CG	4:D:119:ALA:N	2.80	0.50
9:I:8:VAL:C	9:I:9:LYS:CG	2.80	0.50
1:A:1996:C:C4'	1:A:1997:C:OP1	2.60	0.50
1:A:2339:C:O2'	1:A:2340:A:O4'	2.30	0.50
6:F:36:ASN:O	6:F:37:MET:CB	2.59	0.50
2:B:77:U:OP1	22:V:18:ARG:CG	2.60	0.50
1:A:2900:A:C6	1:A:2901:C:C4	2.99	0.49
1:A:1819:A:C1'	1:A:1821:A:C6	2.95	0.49
1:A:1667:G:OP2	1:A:1667:G:C8	2.65	0.49
1:A:1885:A:C6	1:A:1886:U:C2	3.00	0.49
1:A:1342:A:C4	1:A:1345:C:N4	2.80	0.49
12:L:40:SER:O	12:L:41:ARG:O	2.30	0.49
24:X:69:GLU:O	24:X:71:ARG:N	2.45	0.49
1:A:2135:A:C2'	1:A:2136:G:O4'	2.60	0.49
1:A:860:U:O2'	1:A:861:A:C5'	2.60	0.49
10:J:44:TYR:O	10:J:45:THR:CB	2.60	0.49
1:A:1333:G:O2'	1:A:1334:G:C8	2.65	0.49
28:1:51:ALA:O	28:1:52:LYS:CB	2.60	0.49
1:A:1329:U:O2'	1:A:1330:C:OP1	2.29	0.49
1:A:2184:A:C2	1:A:2185:U:C2	3.00	0.49
5:E:55:SER:OG	5:E:56:GLY:N	2.45	0.49
3:C:231:HIS:O	3:C:232:GLY:C	2.50	0.49
1:A:1072:C:O2'	1:A:1093:G:O6	2.31	0.49
1:A:2516:A:C4	1:A:2569:G:N2	2.80	0.49
1:A:2745:C:C4	1:A:2746:U:O4	2.66	0.49
1:A:1112:G:O2'	1:A:1113:U:C6	2.66	0.49
1:A:910:A:C2	13:M:13:HIS:CE1	2.99	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2455:G:N1	1:A:2498:C:N4	2.60	0.49
1:A:2511:U:O2'	4:D:143:PRO:O	2.29	0.49
11:K:14:SER:OG	11:K:51:LYS:N	2.45	0.49
1:A:1930:G:O2'	1:A:1968:G:N1	2.46	0.49
1:A:319:G:C6	1:A:333:G:C6	3.00	0.49
1:A:197:A:C8	1:A:2430:A:C5	3.00	0.49
1:A:1416:G:C6	1:A:1417:C:N4	2.81	0.49
1:A:1264:A:N7	1:A:1265:A:C5	2.81	0.49
1:A:1469:A:C2'	1:A:1470:A:C8	2.96	0.49
1:A:1335:C:N4	34:A:3248:HOH:O	2.46	0.49
1:A:725:G:N1	1:A:726:G:N2	2.61	0.49
14:N:5:LYS:O	34:N:780:HOH:O	2.20	0.49
1:A:581:C:C2	1:A:582:A:C8	3.00	0.49
1:A:671:C:C5	12:L:33:ARG:NH2	2.80	0.49
1:A:2902:C:O2'	1:A:2903:U:O4'	2.29	0.49
1:A:2436:G:C2	1:A:2437:G:C8	3.01	0.49
1:A:2630:G:O2'	1:A:2631:G:O5'	2.30	0.49
1:A:142:A:C2'	1:A:143:C:C6	2.95	0.49
1:A:309:A:C2	1:A:329:G:O2'	2.66	0.49
1:A:204:A:C8	1:A:206:U:C4	3.00	0.49
22:V:70:ILE:N	22:V:70:ILE:CD1	2.75	0.49
1:A:35:G:O2'	1:A:36:G:O5'	2.30	0.49
1:A:1071:G:O6	1:A:1091:G:N7	2.45	0.49
1:A:104:A:O2'	1:A:105:C:O4'	2.31	0.49
1:A:1521:G:C6	1:A:1522:A:C6	3.01	0.49
1:A:1264:A:C6	1:A:1265:A:N6	2.80	0.49
1:A:2373:G:C6	1:A:2374:C:C4	3.01	0.49
23:W:25:PHE:O	23:W:27:GLY:N	2.46	0.49
1:A:2056:G:N2	1:A:2057:G:N9	2.61	0.49
1:A:655:A:O2'	1:A:656:G:N7	2.46	0.49
1:A:2896:C:O2'	1:A:2897:U:C5'	2.61	0.49
1:A:2639:A:N6	1:A:2640:G:C2	2.81	0.49
1:A:233:A:C2'	1:A:234:U:C6	2.96	0.49
1:A:1707:G:C5	1:A:1756:G:C6	3.01	0.49
7:G:115:GLN:CG	7:G:116:LEU:N	2.76	0.49
1:A:669:G:N2	1:A:670:A:C2	2.80	0.49
1:A:1130:U:O2'	1:A:1131:G:C8	2.66	0.49
1:A:1014:A:C4	1:A:1015:U:C5	3.00	0.49
1:A:1331:G:N3	1:A:1333:G:C8	2.81	0.49
1:A:2550:G:O6	1:A:2551:C:N4	2.45	0.49
1:A:491:G:C2'	1:A:492:A:C8	2.95	0.49
1:A:607:U:C5	1:A:619:G:C4	3.01	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:A:N3	1:A:457:A:O2'	2.45	0.49
1:A:2496:C:N4	34:A:3400:HOH:O	2.46	0.49
1:A:1125:G:C6	1:A:1126:A:N6	2.80	0.49
29:2:11:LYS:O	29:2:14:ARG:N	2.46	0.49
1:A:214:G:O2'	1:A:216:A:O3'	2.31	0.49
1:A:2331:G:C6	1:A:2385:C:N4	2.81	0.49
1:A:2065:C:C4	1:A:2066:C:N4	2.81	0.49
1:A:1906:G:N2	1:A:1925:C:O2	2.46	0.49
1:A:2779:U:O4'	1:A:2781:A:N7	2.46	0.49
1:A:2691:C:O2'	1:A:2692:G:C5'	2.60	0.49
1:A:2692:G:O2'	1:A:2693:G:O4'	2.29	0.49
1:A:271:G:C4	1:A:367:G:C2	3.01	0.49
1:A:303:G:C2	1:A:304:U:C2	3.00	0.49
1:A:64:A:N1	1:A:91:A:N6	2.60	0.49
1:A:2093:G:C6	1:A:2225:A:N7	2.81	0.49
1:A:1332:G:C6	1:A:1609:A:N7	2.81	0.49
2:B:52:A:OP2	15:O:64:TYR:CD1	2.66	0.49
1:A:206:U:O2'	1:A:207:A:C5'	2.61	0.49
1:A:1780:A:C4'	1:A:1781:U:OP2	2.61	0.49
1:A:1659:G:C5	1:A:1660:G:C8	3.01	0.49
11:K:13:ASN:ND2	11:K:13:ASN:N	2.60	0.49
1:A:2093:G:O2'	1:A:2094:A:C5'	2.61	0.48
30:3:41:ARG:CG	30:3:41:ARG:NH2	2.75	0.48
10:J:44:TYR:C	10:J:44:TYR:CD2	2.86	0.48
1:A:811:U:O4	12:L:21:ARG:NH1	2.46	0.48
1:A:370:G:C6	1:A:424:G:C5	3.01	0.48
1:A:155:A:C6	1:A:172:A:N6	2.81	0.48
7:G:48:THR:O	7:G:49:LEU:CB	2.61	0.48
1:A:591:U:C2	1:A:592:A:C8	3.01	0.48
1:A:1570:A:C5	1:A:1571:A:C6	3.00	0.48
1:A:1953:A:C2	1:A:2550:G:O4'	2.66	0.48
1:A:2283:C:N4	1:A:2389:G:C6	2.81	0.48
29:2:11:LYS:O	29:2:12:ARG:C	2.51	0.48
16:P:107:ALA:O	16:P:108:ARG:C	2.51	0.48
1:A:40:U:C4	1:A:41:C:C4	3.00	0.48
13:M:3:GLN:NE2	13:M:92:TRP:CD1	2.81	0.48
1:A:771:G:C4	1:A:772:C:C5	3.00	0.48
1:A:753:A:O2'	1:A:754:U:C6	2.66	0.48
1:A:503:A:C2	1:A:505:A:C4	3.02	0.48
1:A:2435:A:C2	1:A:2436:G:C4	3.02	0.48
1:A:324:A:N6	1:A:338:G:C2'	2.75	0.48
1:A:1149:G:C2	1:A:1150:C:C2	3.01	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:A:N1	1:A:369:U:O2'	2.47	0.48
1:A:1799:G:C8	3:C:179:GLU:OE1	2.66	0.48
3:C:134:ILE:O	3:C:166:ARG:NH1	2.46	0.48
8:H:40:THR:O	8:H:42:LYS:N	2.45	0.48
1:A:1059:G:C2	1:A:1080:A:C2	3.02	0.48
1:A:1057:A:N3	1:A:1082:U:C2	2.81	0.48
1:A:1142:A:C8	1:A:1144:A:N7	2.82	0.48
2:B:43:C:O2'	2:B:45:A:N7	2.46	0.48
1:A:777:G:N7	1:A:793:A:C2	2.81	0.48
1:A:2867:G:O2'	1:A:2868:A:OP2	2.31	0.48
1:A:2315:G:N1	1:A:2316:G:C5	2.82	0.48
1:A:2653:U:C4	1:A:2654:A:C5	3.01	0.48
1:A:92:U:O2'	1:A:93:G:C5'	2.62	0.48
1:A:638:G:O2'	1:A:639:U:O4'	2.30	0.48
1:A:785:G:C6	1:A:786:C:C4	3.01	0.48
1:A:194:G:C6	1:A:195:A:C6	3.01	0.48
1:A:959:A:O2'	1:A:960:A:O4'	2.32	0.48
3:C:62:ARG:CG	3:C:62:ARG:NH2	2.77	0.48
1:A:2838:G:OP1	34:A:3636:HOH:O	2.20	0.48
1:A:17:G:C6	1:A:524:G:C6	3.01	0.48
3:C:245:THR:O	3:C:247:TRP:N	2.47	0.48
1:A:1910:G:C6	1:A:1921:G:C6	3.01	0.48
12:L:66:PHE:CG	12:L:67:THR:N	2.81	0.48
1:A:1062:G:O2'	1:A:1063:G:O5'	2.31	0.48
1:A:2901:C:N4	1:A:2902:C:N4	2.62	0.48
1:A:251:A:C2'	1:A:252:G:O4'	2.60	0.48
1:A:52:A:N1	1:A:178:G:O2'	2.47	0.48
1:A:533:G:N2	17:Q:44:TYR:CD1	2.82	0.48
1:A:2359:C:O2	12:L:60:ARG:NH2	2.47	0.48
24:X:52:ALA:O	24:X:53:LYS:CB	2.60	0.48
1:A:2303:G:C4	1:A:2304:G:C8	3.01	0.48
1:A:444:C:O2'	1:A:445:C:C6	2.67	0.48
1:A:1057:A:C4	1:A:1082:U:N3	2.81	0.48
1:A:1809:A:O2'	1:A:1810:A:O5'	2.31	0.48
1:A:2725:A:O2'	1:A:2726:A:C8	2.67	0.48
1:A:1343:G:O2'	1:A:1344:U:C6	2.67	0.48
1:A:1537:G:C2'	1:A:1538:G:C4'	2.92	0.48
1:A:1504:A:C2	1:A:1505:A:C8	3.01	0.48
1:A:89:A:C2	1:A:90:U:C2	3.02	0.48
1:A:2850:A:OP2	1:A:2866:U:N3	2.46	0.48
1:A:866:A:N6	1:A:913:U:O2'	2.46	0.48
1:A:2838:G:C4	1:A:2839:G:C8	3.01	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:845:A:N6	1:A:932:U:C2	2.81	0.48
1:A:309:A:N3	1:A:329:G:O2'	2.46	0.48
1:A:1695:G:C8	3:C:7:PRO:O	2.67	0.48
6:F:109:ARG:NH2	6:F:109:ARG:CB	2.74	0.48
1:A:2408:U:O2'	1:A:2409:G:O5'	2.32	0.48
1:A:88:G:C2	1:A:89:A:C8	3.02	0.48
1:A:49:A:N6	1:A:177:G:C4	2.82	0.48
1:A:866:A:C8	1:A:914:G:O6	2.67	0.48
1:A:1009:A:C2	1:A:1010:A:C2	3.02	0.48
1:A:1011:G:OP1	17:Q:76:SER:CB	2.62	0.48
1:A:2753:A:O2'	1:A:2754:U:C5'	2.62	0.48
1:A:132:G:N2	1:A:148:U:C2	2.82	0.48
1:A:439:A:C5	1:A:440:C:C4	3.02	0.48
11:K:6:THR:O	11:K:8:LEU:CD1	2.62	0.48
26:Z:32:GLY:C	26:Z:34:THR:N	2.66	0.48
1:A:1448:G:C2	1:A:1464:G:C2	3.02	0.48
1:A:2067:G:C4	1:A:2444:G:N2	2.82	0.48
1:A:2069:G:C2	1:A:2443:C:C2	3.01	0.48
1:A:1807:G:OP1	3:C:47:ARG:NH1	2.46	0.48
1:A:1716:U:O2	1:A:1717:A:C8	2.67	0.48
1:A:2748:A:N6	1:A:2749:A:C6	2.82	0.48
1:A:234:U:O2'	1:A:235:U:O5'	2.32	0.48
1:A:1127:A:O2'	1:A:1128:G:C5'	2.62	0.48
1:A:2630:G:O2'	1:A:2631:G:C8	2.66	0.48
1:A:726:G:O2'	1:A:727:A:P	2.72	0.48
1:A:308:G:N1	1:A:309:A:C2	2.82	0.48
1:A:2067:G:C4'	1:A:2068:U:OP2	2.62	0.48
1:A:27:G:C6	1:A:512:G:C6	3.02	0.48
1:A:2226:C:O2'	1:A:2227:A:C5'	2.62	0.48
1:A:753:A:O2'	1:A:754:U:O5'	2.32	0.47
1:A:15:G:C2	1:A:16:C:C2	3.02	0.47
1:A:2868:A:O2'	1:A:2869:G:O4'	2.31	0.47
1:A:978:G:O4'	1:A:1001:A:C2	2.67	0.47
1:A:332:A:O2'	1:A:334:C:OP2	2.32	0.47
1:A:2417:C:C2	1:A:2418:A:C8	3.02	0.47
1:A:2283:C:C4	1:A:2389:G:C6	3.02	0.47
1:A:140:C:O2'	1:A:141:G:P	2.72	0.47
1:A:2478:A:N7	1:A:2529:G:C6	2.82	0.47
1:A:2808:G:N2	1:A:2891:U:C6	2.82	0.47
1:A:630:G:N2	1:A:634:C:C4	2.82	0.47
1:A:1633:G:C5	1:A:1635:A:C5	3.02	0.47
1:A:1994:C:OP1	4:D:132:ALA:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:761:A:N6	34:A:3143:HOH:O	2.46	0.47
15:O:30:ARG:CG	15:O:30:ARG:NH1	2.76	0.47
1:A:2386:A:O2'	1:A:2387:U:O5'	2.31	0.47
1:A:379:G:C2	1:A:396:G:C5	3.02	0.47
1:A:659:G:C6	1:A:660:C:N4	2.82	0.47
1:A:2756:U:O2'	1:A:2757:A:C5'	2.62	0.47
1:A:49:A:C6	1:A:177:G:C5	3.02	0.47
1:A:1327:A:O2'	1:A:1328:A:O5'	2.32	0.47
1:A:1649:G:C6	1:A:2009:A:C6	3.02	0.47
1:A:2212:A:N7	1:A:2214:C:N4	2.62	0.47
1:A:1822:C:O2'	1:A:1823:G:O4'	2.31	0.47
1:A:2550:G:C6	1:A:2551:C:N4	2.82	0.47
1:A:1681:G:O2'	1:A:1762:A:C2'	2.62	0.47
1:A:1423:G:C4	1:A:1424:G:C8	3.02	0.47
1:A:2100:G:C6	1:A:2190:G:C5	3.02	0.47
1:A:566:U:O2'	1:A:809:G:OP2	2.31	0.47
1:A:478:A:C6	1:A:480:A:C6	3.03	0.47
1:A:49:A:C6	1:A:177:G:C6	3.02	0.47
2:B:42:C:C2'	2:B:43:C:C6	2.96	0.47
1:A:2686:G:C6	1:A:2687:U:N3	2.83	0.47
1:A:1180:U:C4	1:A:1181:U:N3	2.83	0.47
2:B:37:C:N3	2:B:49:C:O4'	2.47	0.47
1:A:2345:G:C4	1:A:2381:A:C2	3.02	0.47
1:A:2189:U:C2	1:A:2190:G:C8	3.02	0.47
1:A:1915:U:C2'	1:A:1916:A:C8	2.97	0.47
3:C:159:THR:N	3:C:194:VAL:CG1	2.78	0.47
1:A:836:G:C6	1:A:837:C:C4	3.01	0.47
1:A:2234:G:C6	1:A:2235:G:C5	3.03	0.47
20:T:69:ARG:NE	20:T:70:HIS:CD2	2.82	0.47
1:A:2026:U:C2	1:A:2038:G:N2	2.82	0.47
1:A:379:G:C5	1:A:396:G:C6	3.02	0.47
1:A:396:G:O2'	1:A:397:U:C5'	2.62	0.47
1:A:2748:A:C6	1:A:2749:A:C5	3.02	0.47
1:A:2287:A:N7	1:A:2289:G:C8	2.82	0.47
1:A:2064:C:C2	1:A:2450:A:N6	2.82	0.47
1:A:2603:G:C2	1:A:2604:U:C2	3.02	0.47
2:B:13:G:N2	2:B:16:G:C4	2.83	0.47
1:A:40:U:C4	1:A:41:C:N4	2.83	0.47
4:D:169:ARG:O	4:D:170:VAL:O	2.32	0.47
5:E:115:GLN:O	5:E:117:ARG:N	2.47	0.47
5:E:144:GLU:O	5:E:145:ASP:C	2.53	0.47
1:A:1760:C:O2'	1:A:1761:C:C5'	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1672:A:N6	1:A:1673:G:C6	2.83	0.47
1:A:2516:A:C2	1:A:2569:G:N3	2.82	0.47
1:A:2239:G:C4	1:A:2240:U:C5	3.02	0.47
1:A:647:G:N2	1:A:2350:C:O2'	2.47	0.47
1:A:1343:G:C4	1:A:1597:A:C6	3.03	0.47
1:A:1137:G:O2'	1:A:1138:G:O4'	2.33	0.47
1:A:2483:C:N3	13:M:123:LYS:NZ	2.63	0.47
1:A:1069:A:O2'	1:A:1070:A:C5'	2.62	0.47
1:A:971:G:O6	1:A:972:A:C2	2.67	0.47
2:B:102:G:C6	2:B:103:U:C4	3.03	0.47
1:A:222:A:C6	1:A:224:U:C2	3.02	0.47
12:L:29:LYS:O	12:L:30:THR:OG1	2.33	0.47
12:L:100:ILE:O	12:L:101:ILE:CB	2.62	0.47
1:A:296:U:C2	1:A:297:G:C8	3.03	0.47
7:G:84:LYS:O	7:G:85:LYS:CB	2.62	0.47
1:A:828:U:C5	1:A:829:A:N6	2.83	0.47
1:A:54:G:C6	1:A:117:G:N2	2.83	0.47
1:A:1019:U:C5	1:A:1020:A:N7	2.83	0.47
1:A:2547:A:C8	1:A:2566:A:N7	2.82	0.47
1:A:2571:U:O4	1:A:2574:G:C8	2.67	0.47
1:A:571:U:C2	1:A:575:A:N7	2.83	0.47
1:A:100:U:O2'	1:A:101:A:C5'	2.63	0.47
1:A:2370:G:C6	1:A:2371:G:C5	3.03	0.47
1:A:910:A:N6	1:A:911:A:C6	2.82	0.47
1:A:771:G:C5	1:A:772:C:C5	3.03	0.47
1:A:1635:A:O2'	1:A:1636:U:C5'	2.63	0.47
16:P:64:SER:O	16:P:66:GLY:N	2.47	0.47
1:A:586:A:C8	1:A:586:A:O5'	2.68	0.47
1:A:1693:U:O4	1:A:1977:A:C5	2.67	0.47
1:A:1378:A:N7	1:A:1380:G:C6	2.83	0.47
1:A:675:A:N6	1:A:676:A:N6	2.63	0.47
1:A:1802:A:C2'	1:A:1803:A:C8	2.97	0.47
1:A:1832:C:C4	1:A:1833:C:C5	3.02	0.47
1:A:2848:G:N3	1:A:2849:U:C5	2.83	0.47
1:A:2849:U:O4	1:A:2867:G:C8	2.68	0.47
1:A:1009:A:O2'	1:A:1010:A:C8	2.68	0.47
1:A:1345:C:O2'	1:A:1346:G:C5'	2.62	0.47
1:A:1247:A:C5	1:A:1249:U:C4	3.02	0.47
1:A:2825:G:C4	1:A:2826:A:C8	3.03	0.47
1:A:56:A:C2	1:A:115:C:C2	3.03	0.47
19:S:68:ASP:N	19:S:68:ASP:OD1	2.48	0.47
1:A:2331:G:C2	1:A:2332:C:C2	3.03	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:A:C6	1:A:422:A:N7	2.83	0.47
1:A:740:C:C4	1:A:1981:A:C2	3.03	0.47
1:A:2520:C:N4	1:A:2567:G:C5	2.83	0.47
1:A:2053:G:C2	1:A:2054:A:C4	3.02	0.47
1:A:775:G:C2	1:A:794:A:C8	3.03	0.47
1:A:2660:A:C2	1:A:2661:G:C5	3.03	0.47
1:A:2776:A:C4'	1:A:2777:G:O5'	2.63	0.47
5:E:40:ARG:NH2	5:E:92:HIS:NE2	2.63	0.47
2:B:109:A:C5	2:B:110:C:C4	3.03	0.47
1:A:1476:U:C5	1:A:1514:G:C2	3.03	0.47
1:A:85:G:C5	1:A:98:G:C2	3.03	0.47
1:A:1113:U:O2'	1:A:1114:C:O5'	2.33	0.47
1:A:1570:A:C2	1:A:1571:A:C2	3.03	0.47
1:A:2544:G:C5'	1:A:2645:G:N7	2.78	0.47
1:A:571:U:C4	1:A:2030:A:C6	3.02	0.47
1:A:1435:G:C2	1:A:1558:C:N4	2.83	0.47
2:B:48:U:C4	2:B:49:C:N4	2.83	0.47
1:A:963:U:O2'	1:A:964:C:O5'	2.32	0.47
1:A:2067:G:C6	1:A:2069:G:N7	2.83	0.47
1:A:1760:C:O2'	1:A:1761:C:O4'	2.31	0.47
25:Y:1:MET:CE	25:Y:1:MET:N	2.78	0.47
1:A:1553:A:C8	1:A:1555:G:C5	3.03	0.46
1:A:2261:C:C2	1:A:2280:G:N2	2.83	0.46
1:A:202:U:C4	1:A:203:A:N1	2.83	0.46
1:A:54:G:C6	1:A:55:G:C5	3.03	0.46
1:A:2836:U:O2'	1:A:2837:A:C5'	2.63	0.46
1:A:1651:G:N2	1:A:2007:U:C2	2.83	0.46
1:A:836:G:C5	1:A:837:C:C4	3.03	0.46
1:A:335:C:O2'	1:A:336:C:C5'	2.63	0.46
10:J:29:ALA:O	10:J:33:ALA:N	2.48	0.46
1:A:747:U:C2	1:A:2613:U:O4	2.68	0.46
1:A:1286:A:O2'	1:A:1288:G:N2	2.47	0.46
1:A:776:G:C8	1:A:793:A:C5	3.03	0.46
1:A:2725:A:C4	1:A:2727:A:C8	3.03	0.46
1:A:197:A:C8	1:A:2430:A:N7	2.83	0.46
1:A:1416:G:O2'	1:A:1417:C:O5'	2.34	0.46
1:A:964:C:O3'	1:A:2273:A:O2'	2.33	0.46
1:A:2630:G:C6	1:A:2894:G:O6	2.68	0.46
1:A:1633:G:C6	1:A:1635:A:C5	3.03	0.46
1:A:1633:G:C6	1:A:1635:A:C6	3.03	0.46
1:A:792:A:N3	1:A:2072:C:O2'	2.48	0.46
24:X:39:VAL:O	24:X:41:SER:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:532:A:N3	1:A:532:A:C2'	2.78	0.46
1:A:1665:A:N6	34:A:3278:HOH:O	2.47	0.46
1:A:33:C:N4	1:A:446:G:O2'	2.48	0.46
1:A:1090:A:C6	1:A:1102:C:O2	2.68	0.46
1:A:110:G:C2	1:A:111:A:C8	3.04	0.46
1:A:1326:U:O2'	1:A:1327:A:C8	2.68	0.46
1:A:2093:G:C8	1:A:2225:A:C4	3.03	0.46
1:A:2592:G:C4	1:A:2593:U:C6	3.03	0.46
1:A:1450:G:C2	1:A:1462:C:N3	2.83	0.46
1:A:1011:G:C6	1:A:1013:C:N3	2.83	0.46
1:A:2414:G:N2	12:L:66:PHE:CZ	2.84	0.46
1:A:1873:G:N2	1:A:1874:C:C2	2.84	0.46
4:D:193:VAL:O	4:D:194:PRO:O	2.33	0.46
1:A:2275:C:O2'	13:M:84:LYS:CA	2.63	0.46
18:R:39:LEU:O	18:R:40:MET:CB	2.63	0.46
14:N:1:MET:O	14:N:2:ARG:CB	2.62	0.46
1:A:1722:A:C6	1:A:1739:A:C8	3.03	0.46
1:A:972:A:C6	1:A:973:A:N6	2.84	0.46
29:2:15:SER:O	29:2:16:HIS:ND1	2.48	0.46
1:A:1413:A:C6	1:A:1414:C:N4	2.83	0.46
3:C:24:HIS:ND1	3:C:25:LYS:N	2.62	0.46
1:A:2738:A:C2	1:A:2766:A:N6	2.83	0.46
1:A:687:C:O2'	1:A:688:U:C5'	2.64	0.46
1:A:1430:G:O2'	1:A:1431:A:O4'	2.32	0.46
1:A:588:U:O2'	1:A:589:U:C6	2.68	0.46
1:A:1290:C:O2'	1:A:1291:C:C6	2.68	0.46
1:A:2593:U:N3	1:A:2594:C:C5	2.83	0.46
1:A:1512:C:C4	1:A:1513:U:C4	3.02	0.46
1:A:2455:G:C6	1:A:2498:C:N4	2.84	0.46
1:A:630:G:OP1	30:3:22:LYS:NZ	2.49	0.46
1:A:2660:A:C2	1:A:2661:G:C8	3.03	0.46
3:C:24:HIS:N	3:C:80:LEU:O	2.48	0.46
24:X:4:CYS:SG	24:X:4:CYS:O	2.73	0.46
1:A:96:C:C4'	25:Y:41:HIS:CD2	2.98	0.46
12:L:47:ARG:CG	12:L:47:ARG:NH2	2.77	0.46
2:B:21:G:C2	2:B:63:C:C2	3.03	0.46
1:A:1059:G:C5	1:A:1060:U:N3	2.84	0.46
1:A:482:A:N6	1:A:506:G:N9	2.63	0.46
1:A:51:G:N3	1:A:119:A:C2	2.84	0.46
1:A:734:A:C5	1:A:735:A:C8	3.04	0.46
1:A:2900:A:C2	1:A:2901:C:C2	3.04	0.46
1:A:777:G:N2	1:A:778:G:C4	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:858:G:C4	1:A:2268:A:C2	3.03	0.46
1:A:1331:G:C4	1:A:1333:G:C8	3.03	0.46
1:A:83:A:C6	1:A:101:A:OP1	2.68	0.46
1:A:73:A:C8	1:A:73:A:O5'	2.68	0.46
1:A:563:A:N3	17:Q:36:GLN:NE2	2.64	0.46
1:A:1797:G:O3'	3:C:255:LYS:O	2.33	0.46
18:R:27:ILE:CG2	18:R:28:ALA:N	2.79	0.46
1:A:802:A:C2'	1:A:803:U:C6	2.98	0.46
1:A:122:G:O2'	1:A:123:G:C5'	2.64	0.46
1:A:838:C:C2	1:A:941:A:C2	3.04	0.46
1:A:1080:A:C5	1:A:1081:U:C4	3.03	0.46
1:A:1787:A:C2	1:A:1788:C:C5	3.03	0.46
1:A:589:U:O2'	1:A:590:A:C5'	2.64	0.46
1:A:1739:A:C2'	1:A:1740:G:C8	2.98	0.46
1:A:2748:A:C6	1:A:2749:A:C6	3.03	0.46
1:A:1281:G:N1	1:A:1290:C:C4	2.83	0.46
2:B:10:G:C6	2:B:11:C:N3	2.84	0.46
1:A:1450:G:C2	1:A:1462:C:C2	3.04	0.46
1:A:570:G:O6	1:A:2499:C:OP1	2.34	0.46
1:A:2811:G:C4	1:A:2812:G:C8	3.03	0.46
1:A:450:G:O6	34:A:3075:HOH:O	2.20	0.46
1:A:1930:G:C4	1:A:1968:G:C6	3.03	0.46
1:A:607:U:C5	1:A:619:G:C5	3.03	0.46
1:A:950:G:C6	1:A:968:C:N3	2.84	0.46
21:U:86:PHE:CG	21:U:87:GLU:N	2.83	0.46
1:A:2383:G:O2'	1:A:2384:U:C6	2.69	0.46
1:A:454:A:O2'	1:A:455:C:OP1	2.33	0.46
1:A:604:G:C6	1:A:625:G:N1	2.84	0.46
2:B:42:C:C5	6:F:87:LYS:NZ	2.84	0.46
1:A:237:C:C2	1:A:261:G:C2	3.03	0.46
1:A:949:G:C2	1:A:969:G:C2	3.04	0.46
3:C:82:TYR:O	3:C:84:PRO:CD	2.64	0.46
1:A:515:A:C2	1:A:1260:A:N3	2.84	0.46
1:A:1445:G:C2	1:A:1547:C:N3	2.83	0.46
1:A:547:A:C3'	1:A:548:G:C5'	2.94	0.46
1:A:1388:G:C2	1:A:1389:G:C8	3.04	0.46
1:A:399:U:C4	1:A:400:G:C6	3.03	0.46
1:A:2547:A:C8	1:A:2566:A:C5	3.04	0.46
1:A:2093:G:C2	1:A:2094:A:C5	3.03	0.46
2:B:43:C:O2'	2:B:45:A:C8	2.68	0.46
1:A:2315:G:C2	1:A:2316:G:N9	2.84	0.46
1:A:1358:G:C8	1:A:1371:G:O6	2.68	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:U:C2	1:A:788:A:N6	2.84	0.46
1:A:811:U:C4	12:L:21:ARG:NH2	2.84	0.46
8:H:38:PRO:O	8:H:40:THR:N	2.49	0.46
1:A:297:G:C6	1:A:342:A:N1	2.84	0.46
1:A:1665:A:C2	1:A:1666:G:C4	3.04	0.46
23:W:13:ARG:CG	23:W:14:ASP:N	2.79	0.46
1:A:750:A:OP1	1:A:1615:C:N4	2.49	0.46
1:A:1071:G:C8	1:A:1089:A:C5	3.04	0.46
1:A:1800:C:C2	1:A:1802:A:C8	3.04	0.46
1:A:628:G:C6	1:A:636:G:N1	2.84	0.46
1:A:325:G:O2'	1:A:326:G:C5'	2.63	0.46
1:A:1731:G:C4'	1:A:1732:C:OP1	2.63	0.46
1:A:1149:G:C6	1:A:1150:C:N4	2.84	0.46
1:A:2104:C:O2	1:A:2105:U:C5	2.68	0.46
1:A:30:G:C6	1:A:511:U:O2	2.69	0.46
1:A:915:C:C2'	1:A:916:G:C8	2.99	0.46
11:K:92:GLU:O	11:K:93:GLN:O	2.34	0.46
1:A:2516:A:N3	1:A:2569:G:N2	2.64	0.45
23:W:37:VAL:CG2	23:W:38:ARG:NH1	2.79	0.45
1:A:2519:U:C6	1:A:2542:A:C6	3.04	0.45
1:A:1895:C:N3	1:A:1896:G:N7	2.65	0.45
1:A:2435:A:N1	1:A:2436:G:C5	2.84	0.45
1:A:324:A:N6	1:A:338:G:O2'	2.49	0.45
1:A:903:C:C2	1:A:904:G:C8	3.04	0.45
1:A:1857:G:C4	1:A:1884:G:N1	2.85	0.45
4:D:121:THR:CG2	4:D:127:PHE:CD1	2.99	0.45
1:A:2842:G:C6	1:A:2843:G:C5	3.04	0.45
24:X:67:LEU:O	24:X:77:TYR:OH	2.33	0.45
31:4:7:VAL:CG1	31:4:8:LYS:N	2.79	0.45
1:A:55:G:N2	1:A:127:A:C2	2.85	0.45
2:B:43:C:C2'	2:B:45:A:N7	2.80	0.45
1:A:2869:G:C6	1:A:2870:C:C4	3.04	0.45
1:A:1076:C:O2'	1:A:1077:A:C4	2.70	0.45
1:A:1205:A:C5	5:E:165:HIS:CE1	3.05	0.45
1:A:197:A:C5	1:A:2430:A:C5	3.05	0.45
1:A:353:C:N4	1:A:354:A:N6	2.64	0.45
1:A:725:G:C6	1:A:726:G:N1	2.84	0.45
1:A:581:C:N3	1:A:582:A:C5	2.84	0.45
1:A:204:A:C8	1:A:206:U:N3	2.84	0.45
1:A:621:A:O2'	1:A:622:G:O4'	2.34	0.45
1:A:192:C:OP1	1:A:2243:U:OP1	2.34	0.45
1:A:719:C:C2	1:A:720:U:C6	3.04	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1299:G:N1	1:A:1640:A:OP2	2.48	0.45
1:A:2772:C:N3	1:A:2773:C:C5	2.84	0.45
1:A:2056:G:N2	1:A:2057:G:C8	2.84	0.45
1:A:2259:U:C2	1:A:2427:C:N3	2.85	0.45
1:A:2520:C:O2'	1:A:2521:C:C5'	2.64	0.45
1:A:230:G:C2	1:A:231:A:C8	3.04	0.45
1:A:1826:G:C5	1:A:1827:U:C4	3.04	0.45
1:A:323:C:OP1	1:A:324:A:C8	2.69	0.45
1:A:2031:A:O2'	1:A:2032:G:P	2.74	0.45
1:A:2627:G:O2'	1:A:2781:A:N1	2.49	0.45
1:A:171:U:O2	1:A:172:A:C8	2.70	0.45
11:K:92:GLU:O	11:K:93:GLN:C	2.54	0.45
1:A:2441:U:O2'	1:A:2442:C:C5'	2.65	0.45
1:A:467:G:O2'	1:A:796:C:O2'	2.34	0.45
1:A:770:G:O4'	1:A:1379:U:C5	2.70	0.45
1:A:2108:A:OP2	1:A:2108:A:C8	2.69	0.45
1:A:866:A:N7	1:A:914:G:N7	2.64	0.45
1:A:1684:G:C2	1:A:1705:A:C2	3.04	0.45
1:A:571:U:C5	1:A:575:A:C5	3.05	0.45
1:A:641:U:O2'	1:A:2350:C:OP1	2.35	0.45
1:A:1520:U:O4	1:A:1521:G:C6	2.69	0.45
1:A:1010:A:O2'	1:A:1011:G:C5'	2.64	0.45
1:A:2603:G:C6	1:A:2604:U:C4	3.05	0.45
1:A:1731:G:N3	1:A:1731:G:O4'	2.46	0.45
1:A:838:C:C2	1:A:941:A:N1	2.84	0.45
5:E:45:ALA:O	5:E:46:GLN:CB	2.64	0.45
1:A:539:G:C6	1:A:540:C:C4	3.04	0.45
2:B:9:G:C2	2:B:112:G:C2	3.04	0.45
1:A:1439:A:N6	1:A:1552:A:C8	2.84	0.45
1:A:374:A:C2'	1:A:375:G:C8	2.99	0.45
1:A:500:G:C2	1:A:503:A:C8	3.05	0.45
1:A:1341:G:OP2	1:A:1394:U:O2'	2.34	0.45
1:A:975:A:C5	1:A:990:A:N7	2.85	0.45
1:A:1050:A:O2'	1:A:1051:G:C5'	2.64	0.45
1:A:160:A:N1	1:A:161:A:C2	2.85	0.45
1:A:2418:A:C6	1:A:2419:U:C4	3.04	0.45
22:V:32:GLY:O	22:V:33:GLY:C	2.55	0.45
24:X:70:LEU:O	24:X:74:GLY:N	2.49	0.45
7:G:58:ALA:O	7:G:59:ASP:C	2.55	0.45
1:A:271:G:O4'	1:A:367:G:N2	2.49	0.45
1:A:1087:G:N2	1:A:1103:A:C1'	2.80	0.45
1:A:1739:A:O2'	1:A:1740:G:O4'	2.35	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:753:A:C2	1:A:754:U:C4	3.04	0.45
4:D:149:ASN:OD1	4:D:150:GLN:N	2.49	0.45
1:A:2836:U:O2'	1:A:2837:A:C8	2.70	0.45
1:A:1136:G:O2'	1:A:1137:G:C8	2.70	0.45
1:A:1783:A:C2	1:A:2588:G:O4'	2.69	0.45
1:A:244:A:C2	1:A:255:A:C4	3.04	0.45
1:A:684:G:OP1	29:2:16:HIS:CD2	2.70	0.45
6:F:93:GLU:O	6:F:95:MET:N	2.49	0.45
2:B:81:G:C5	2:B:82:U:C5	3.04	0.45
9:I:28:GLY:O	9:I:29:GLN:C	2.54	0.45
1:A:1475:G:O2'	1:A:1476:U:OP2	2.35	0.45
1:A:1289:C:O2'	1:A:1290:C:C6	2.70	0.45
1:A:575:A:O2'	1:A:576:U:C5'	2.64	0.45
10:J:4:PHE:CG	10:J:5:THR:N	2.85	0.45
1:A:1799:G:OP1	3:C:257:ARG:NH1	2.50	0.45
1:A:749:A:C4	1:A:750:A:C8	3.05	0.45
1:A:413:C:O2'	1:A:414:C:O4'	2.34	0.45
5:E:53:THR:OG1	5:E:54:GLY:N	2.50	0.45
25:Y:58:ASN:C	25:Y:60:LYS:N	2.70	0.45
1:A:1060:U:C4'	1:A:1061:U:C5'	2.95	0.45
1:A:301:G:C5	1:A:302:C:N4	2.85	0.45
1:A:1130:U:O2'	1:A:1131:G:N7	2.50	0.45
1:A:478:A:C2	1:A:480:A:C8	3.04	0.45
2:B:50:A:C5	2:B:51:G:C8	3.05	0.45
1:A:604:G:O6	1:A:625:G:C6	2.70	0.45
1:A:1816:C:O2'	1:A:1817:G:P	2.74	0.45
1:A:2459:A:O2'	1:A:2460:U:C5'	2.65	0.45
1:A:2685:G:C2	1:A:2725:A:C2	3.05	0.45
1:A:1875:G:OP2	1:A:1875:G:C8	2.70	0.45
1:A:244:A:C2'	1:A:245:G:O5'	2.65	0.45
1:A:1510:G:O2'	1:A:1511:G:O4'	2.35	0.45
1:A:527:C:O2'	1:A:528:A:C5	2.70	0.45
1:A:567:U:C4	1:A:568:U:C4	3.05	0.45
1:A:1438:U:O4	1:A:1552:A:N1	2.50	0.45
1:A:1062:G:OP1	1:A:1070:A:OP2	2.35	0.45
1:A:2748:A:C4	1:A:2757:A:C6	3.05	0.45
1:A:1021:A:C2	1:A:1023:U:O2	2.69	0.45
1:A:746:U:C5'	1:A:748:G:O4'	2.65	0.45
1:A:372:G:N2	1:A:401:A:OP2	2.50	0.45
13:M:136:MET:CE	22:V:75:GLN:C	2.86	0.45
1:A:2886:A:N7	27:0:39:ARG:CZ	2.80	0.45
1:A:377:G:C5	1:A:378:C:C4	3.05	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1264:A:C5	1:A:1265:A:C6	3.04	0.45
5:E:170:ARG:NH2	5:E:176:ASP:OD2	2.50	0.45
1:A:788:A:OP1	1:A:791:C:N4	2.50	0.45
4:D:76:GLY:O	4:D:77:ARG:C	2.53	0.45
1:A:5:A:C2	1:A:2899:A:C2	3.05	0.45
1:A:1941:C:C6	1:A:1965:C:C4	3.05	0.45
1:A:2147:A:OP1	1:A:2147:A:C4'	2.64	0.45
1:A:456:C:O2'	20:T:73:ARG:CG	2.64	0.45
1:A:303:G:C6	1:A:315:G:C6	3.05	0.45
1:A:2408:U:O2'	1:A:2409:G:C5'	2.65	0.45
1:A:1950:G:C2	1:A:1954:G:C8	3.04	0.45
1:A:1400:U:C2'	1:A:1401:G:O4'	2.65	0.45
1:A:1819:A:OP1	3:C:155:ARG:N	2.50	0.45
1:A:464:U:C2	1:A:788:A:C6	3.05	0.45
1:A:1423:G:C2	1:A:1424:G:C4	3.05	0.45
1:A:125:A:OP2	29:2:19:ARG:NH2	2.50	0.45
1:A:2581:G:C6	1:A:2610:C:O2	2.70	0.45
1:A:218:A:N6	1:A:219:A:N6	2.65	0.44
1:A:2543:G:O6	1:A:2765:A:C6	2.71	0.44
1:A:223:A:C6	1:A:422:A:C5	3.05	0.44
1:A:54:G:C5	1:A:55:G:N7	2.85	0.44
1:A:2489:U:C4	1:A:2490:G:N1	2.85	0.44
1:A:2625:G:C5	1:A:2626:C:C4	3.05	0.44
1:A:196:A:O2'	1:A:197:A:OP1	2.34	0.44
1:A:1953:A:N1	1:A:2550:G:O4'	2.50	0.44
1:A:792:A:C8	1:A:2440:C:C2	3.05	0.44
1:A:310:A:C2'	1:A:312:G:N7	2.80	0.44
1:A:1071:G:O2'	1:A:1072:C:C5'	2.66	0.44
1:A:121:G:C2	1:A:131:A:C4	3.05	0.44
1:A:2148:G:O3'	1:A:2149:U:O4'	2.35	0.44
1:A:1517:G:N2	1:A:1732:C:C5	2.85	0.44
1:A:243:U:O2'	1:A:244:A:C5'	2.64	0.44
1:A:638:G:C6	1:A:651:G:C6	3.05	0.44
3:C:245:THR:C	3:C:247:TRP:N	2.70	0.44
1:A:1914:C:O2'	1:A:1915:U:O4'	2.35	0.44
1:A:802:A:O2'	1:A:803:U:O4'	2.35	0.44
15:O:39:VAL:N	15:O:49:VAL:O	2.51	0.44
1:A:699:A:N6	1:A:733:G:O2'	2.51	0.44
1:A:2800:A:O2'	1:A:2801:G:C4'	2.65	0.44
28:1:38:PHE:CD2	28:1:39:ASP:N	2.85	0.44
10:J:80:HIS:O	10:J:81:ILE:O	2.34	0.44
14:N:16:HIS:O	14:N:20:MET:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1839:G:O2'	1:A:1840:G:C5'	2.65	0.44
1:A:188:G:C2	1:A:209:C:N3	2.86	0.44
1:A:2459:A:C4	1:A:2460:U:C5	3.06	0.44
1:A:1333:G:O2'	1:A:1334:G:C5'	2.65	0.44
1:A:241:A:N9	1:A:243:U:C4	2.85	0.44
1:A:725:G:C6	1:A:726:G:C2	3.05	0.44
1:A:2345:G:C2	1:A:2381:A:C5	3.05	0.44
1:A:608:A:C5	1:A:621:A:C5	3.05	0.44
3:C:5:CYS:SG	3:C:15:VAL:O	2.75	0.44
1:A:1440:U:O2	1:A:1441:G:C8	2.71	0.44
1:A:2024:G:C2'	1:A:2025:C:C6	3.01	0.44
1:A:1270:C:N3	1:A:1648:U:C4	2.86	0.44
2:B:16:G:O6	2:B:69:G:C6	2.70	0.44
3:C:43:ASN:CG	3:C:44:ASN:N	2.71	0.44
1:A:141:G:C3'	1:A:142:A:O4'	2.66	0.44
1:A:1210:G:N3	1:A:1212:G:N2	2.66	0.44
1:A:1529:G:O6	1:A:1543:G:N2	2.51	0.44
1:A:1796:U:O2	1:A:1824:G:C2	2.70	0.44
1:A:530:G:N2	1:A:2034:U:O3'	2.50	0.44
1:A:593:U:C4	1:A:594:U:O4	2.70	0.44
1:A:2407:A:C2	1:A:2408:U:N3	2.85	0.44
1:A:372:G:P	24:X:61:LYS:NZ	2.90	0.44
1:A:9:G:C6	1:A:2895:G:O6	2.70	0.44
1:A:2148:G:O2'	1:A:2149:U:N1	2.50	0.44
1:A:860:U:C2	1:A:2268:A:C8	3.05	0.44
1:A:1519:G:N1	1:A:1520:U:C2	2.86	0.44
1:A:2782:G:N2	1:A:2783:U:O2	2.50	0.44
1:A:2511:U:C6	1:A:2511:U:C3'	3.01	0.44
1:A:26:G:C6	1:A:27:G:C2	3.06	0.44
1:A:1317:G:C2	1:A:1336:A:C2	3.05	0.44
1:A:996:A:C5'	17:Q:91:ARG:NH1	2.80	0.44
1:A:49:A:C2	1:A:118:A:N1	2.85	0.44
1:A:529:A:C4	1:A:2023:C:C5	3.05	0.44
1:A:1623:G:C5	1:A:1624:U:C5	3.06	0.44
1:A:2750:A:O2'	1:A:2752:C:C5	2.70	0.44
1:A:1191:G:C2	1:A:1192:G:C4	3.05	0.44
1:A:261:G:O2'	1:A:610:C:O2'	2.35	0.44
1:A:581:C:N4	1:A:582:A:N6	2.65	0.44
1:A:996:A:N6	1:A:1160:G:C6	2.86	0.44
1:A:2666:C:O2	1:A:2666:C:O4'	2.36	0.44
1:A:182:A:C2	1:A:183:C:C2	3.05	0.44
4:D:131:ASP:N	4:D:131:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:A:O2'	1:A:273:G:O5'	2.35	0.44
1:A:1080:A:C6	1:A:1081:U:C4	3.06	0.44
1:A:604:G:C2	1:A:605:G:N7	2.85	0.44
1:A:422:A:C2'	1:A:423:A:C8	3.01	0.44
1:A:422:A:O2'	1:A:423:A:C8	2.71	0.44
1:A:740:C:C2	1:A:1981:A:C2	3.06	0.44
1:A:628:G:C5	1:A:636:G:N2	2.86	0.44
1:A:2053:G:N2	1:A:2054:A:N3	2.66	0.44
1:A:1008:A:C4'	1:A:1009:A:OP1	2.66	0.44
1:A:101:A:O2'	1:A:102:U:P	2.76	0.44
1:A:1912:A:N6	1:A:1918:A:C1'	2.81	0.44
3:C:212:TRP:CD1	3:C:212:TRP:O	2.70	0.44
1:A:962:G:O2'	1:A:963:U:C5'	2.65	0.44
1:A:705:A:O5'	1:A:705:A:C8	2.71	0.44
1:A:538:A:N6	1:A:555:G:O2'	2.51	0.44
1:A:919:U:C2'	1:A:920:A:C8	3.01	0.44
1:A:1748:C:C2	1:A:1749:A:C8	3.06	0.44
1:A:1439:A:C2	1:A:1552:A:N1	2.83	0.44
1:A:1439:A:C8	1:A:1439:A:C3'	3.01	0.44
1:A:1195:G:O2'	1:A:1226:A:N1	2.50	0.44
1:A:85:G:C6	1:A:98:G:C2	3.06	0.44
1:A:2625:G:C4	1:A:2626:C:C5	3.06	0.44
1:A:562:U:C2	1:A:572:A:C8	3.06	0.44
1:A:975:A:C8	1:A:990:A:N6	2.85	0.44
1:A:1180:U:C4	1:A:1181:U:C4	3.05	0.44
1:A:370:G:N1	1:A:424:G:C5	2.85	0.44
1:A:959:A:C2'	1:A:960:A:C8	3.01	0.44
24:X:77:TYR:CD1	24:X:77:TYR:C	2.91	0.44
1:A:593:U:N3	1:A:594:U:C4	2.86	0.44
1:A:663:G:C6	1:A:664:G:C5	3.05	0.44
1:A:1337:G:OP2	1:A:1337:G:C8	2.71	0.44
4:D:181:ASP:C	4:D:183:GLU:N	2.70	0.44
1:A:273:G:N2	1:A:365:U:C2	2.85	0.44
12:L:23:ILE:CG1	18:R:82:HIS:CE1	3.01	0.44
1:A:659:G:C6	1:A:660:C:C4	3.06	0.44
1:A:1022:G:C6	1:A:1140:C:C5	3.06	0.44
1:A:1385:A:C6	1:A:1403:A:C5	3.05	0.44
1:A:776:G:N7	1:A:793:A:C4	2.86	0.44
20:T:14:PRO:O	20:T:15:HIS:CB	2.66	0.44
1:A:1651:G:C2	1:A:2007:U:N3	2.86	0.44
1:A:1202:G:C5	1:A:1203:U:C5	3.05	0.44
2:B:58:A:O2'	2:B:59:A:C5'	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:2:28:ARG:O	29:2:31:LEU:N	2.50	0.44
14:N:21:PHE:N	14:N:21:PHE:CD1	2.86	0.44
1:A:2509:G:C6	1:A:2510:C:C5	3.05	0.44
1:A:1062:G:OP1	1:A:1070:A:C4'	2.66	0.43
1:A:739:A:O2'	1:A:740:C:C6	2.71	0.43
1:A:2460:U:O2'	1:A:2461:A:C5'	2.66	0.43
1:A:675:A:C6	1:A:676:A:C6	3.06	0.43
1:A:2635:A:C2	1:A:2784:U:C2	3.06	0.43
1:A:2548:U:C4	1:A:2549:G:N7	2.86	0.43
1:A:1456:G:C6	1:A:1457:U:C4	3.06	0.43
1:A:531:C:C5	1:A:2035:G:C2	3.06	0.43
1:A:2:G:C6	1:A:3:U:C4	3.05	0.43
19:S:88:ARG:CG	19:S:88:ARG:NH2	2.77	0.43
1:A:1808:A:O2'	1:A:1809:A:OP1	2.36	0.43
18:R:81:LYS:O	18:R:82:HIS:C	2.57	0.43
1:A:1286:A:C4	1:A:1289:C:N4	2.87	0.43
1:A:103:A:O2'	1:A:104:A:O4'	2.36	0.43
1:A:2093:G:C5	1:A:2225:A:N7	2.86	0.43
1:A:783:A:O2'	1:A:784:G:C4'	2.65	0.43
1:A:1973:G:C6	1:A:1974:C:C4	3.07	0.43
1:A:2835:A:C6	1:A:2879:A:C4	3.06	0.43
1:A:1668:A:N3	1:A:1670:C:C4	2.86	0.43
1:A:2675:A:C2	1:A:2676:C:C2	3.06	0.43
1:A:2031:A:N3	1:A:2455:G:O2'	2.51	0.43
1:A:2716:C:C2	1:A:2717:C:C5	3.07	0.43
6:F:5:ASP:C	6:F:7:TYR:N	2.70	0.43
21:U:3:LYS:O	21:U:4:ILE:C	2.56	0.43
1:A:303:G:N1	1:A:315:G:C6	2.86	0.43
1:A:15:G:OP1	27:0:20:ALA:CB	2.66	0.43
23:W:31:LEU:C	23:W:33:GLY:N	2.71	0.43
1:A:2232:C:P	24:X:26:ARG:NH1	2.91	0.43
1:A:1045:C:O4'	1:A:1111:A:N6	2.51	0.43
1:A:1048:A:O2'	1:A:1049:C:C6	2.71	0.43
1:A:1825:U:O3'	3:C:231:HIS:CE1	2.71	0.43
1:A:2373:G:C6	1:A:2381:A:N1	2.86	0.43
1:A:1315:C:C2	1:A:1338:G:C2	3.06	0.43
20:T:29:THR:OG1	20:T:86:THR:N	2.51	0.43
1:A:121:G:N2	1:A:131:A:N9	2.66	0.43
2:B:98:G:O6	22:V:14:LYS:N	2.51	0.43
24:X:1:SER:C	24:X:3:VAL:N	2.72	0.43
1:A:94:A:C2	1:A:95:A:C4	3.07	0.43
1:A:197:A:N7	1:A:2430:A:C4	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:A:O2'	1:A:245:G:O4'	2.36	0.43
1:A:579:G:C2	1:A:1262:A:C5	3.06	0.43
1:A:761:A:OP2	34:A:3142:HOH:O	2.21	0.43
1:A:2483:C:C5	1:A:2484:G:C8	3.06	0.43
30:3:24:LYS:O	30:3:25:HIS:CD2	2.71	0.43
6:F:41:GLU:O	6:F:43:ILE:N	2.51	0.43
6:F:4:HIS:CE1	6:F:96:TRP:CZ2	3.06	0.43
1:A:2208:C:C2	1:A:2217:G:N2	2.86	0.43
1:A:66:C:N4	1:A:67:U:N3	2.67	0.43
1:A:2077:A:N1	1:A:2078:C:C4	2.87	0.43
1:A:1265:A:C8	1:A:1267:U:C2	3.06	0.43
1:A:2711:A:N6	1:A:2714:G:N7	2.66	0.43
1:A:2092:U:C5	1:A:2226:C:OP2	2.72	0.43
1:A:838:C:C4	1:A:839:U:C4	3.07	0.43
1:A:3:U:C5	1:A:4:U:C5	3.06	0.43
3:C:2:VAL:O	3:C:3:VAL:CB	2.66	0.43
29:2:43:THR:O	29:2:44:VAL:C	2.57	0.43
5:E:106:LYS:O	5:E:110:SER:N	2.51	0.43
1:A:2060:A:C8	5:E:63:LYS:NZ	2.87	0.43
1:A:2209:G:C2	1:A:2210:U:O4	2.71	0.43
18:R:79:ARG:O	18:R:80:ARG:CB	2.67	0.43
9:I:20:SER:N	9:I:21:PRO:CD	2.81	0.43
1:A:1931:U:O2'	1:A:1932:A:O4'	2.37	0.43
1:A:223:A:C2	1:A:407:G:N3	2.87	0.43
1:A:1800:C:C2	1:A:1818:U:O2	2.71	0.43
1:A:1202:G:C6	1:A:1203:U:C4	3.06	0.43
1:A:1907:G:C2	1:A:1924:C:C2	3.07	0.43
1:A:2282:G:O2'	1:A:2283:C:OP2	2.37	0.43
1:A:2422:C:N4	1:A:2424:C:C4	2.86	0.43
1:A:1914:C:C4	1:A:1915:U:C4	3.07	0.43
1:A:1829:A:C8	1:A:1830:C:C5	3.07	0.43
1:A:996:A:N3	1:A:997:G:C8	2.86	0.43
1:A:300:A:N6	34:A:3435:HOH:O	2.51	0.43
22:V:44:HIS:NE2	22:V:86:LEU:O	2.52	0.43
8:H:71:LYS:N	8:H:71:LYS:CD	2.82	0.43
1:A:2757:A:N1	7:G:66:THR:CG2	2.82	0.43
1:A:2869:G:C6	1:A:2870:C:N3	2.87	0.43
1:A:460:A:N3	1:A:470:A:C6	2.87	0.43
12:L:93:ASN:CG	12:L:94:THR:N	2.72	0.43
12:L:40:SER:O	12:L:41:ARG:C	2.56	0.43
24:X:4:CYS:SG	24:X:7:THR:OG1	2.77	0.43
23:W:8:SER:O	23:W:9:THR:CB	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:55:ASP:CG	18:R:56:GLY:N	2.72	0.43
1:A:1687:G:N1	1:A:1700:A:OP1	2.51	0.43
1:A:117:G:C2	1:A:119:A:N6	2.87	0.43
1:A:13:A:C5'	1:A:14:A:OP1	2.67	0.43
1:A:2547:A:C8	1:A:2566:A:C8	3.07	0.43
1:A:2078:C:C4	1:A:2079:U:C4	3.06	0.43
2:B:16:G:C6	2:B:69:G:C4	3.07	0.43
2:B:16:G:O2'	2:B:17:C:C5'	2.66	0.43
1:A:1867:G:O6	1:A:1875:G:N2	2.52	0.43
1:A:1951:U:C2'	1:A:1953:A:OP2	2.66	0.43
1:A:527:C:O2'	1:A:528:A:N7	2.51	0.43
4:D:76:GLY:O	4:D:78:GLY:N	2.52	0.43
4:D:115:GLY:O	14:N:3:HIS:CE1	2.72	0.43
1:A:294:A:C2'	1:A:295:G:O5'	2.67	0.43
26:Z:8:GLN:OE1	26:Z:30:ARG:O	2.37	0.43
1:A:763:G:C5	1:A:765:C:C4	3.07	0.43
1:A:478:A:N1	1:A:480:A:C4	2.87	0.43
1:A:2458:G:C4	1:A:2490:G:C6	3.07	0.43
1:A:1648:U:O2'	1:A:1649:G:O4'	2.37	0.43
1:A:2542:A:C2	1:A:2567:G:O6	2.72	0.43
1:A:2869:G:C5	1:A:2870:C:C4	3.06	0.43
1:A:1462:C:O2'	1:A:1463:C:C5'	2.66	0.43
1:A:2654:A:N3	1:A:2656:U:C4	2.87	0.43
4:D:119:ALA:O	4:D:120:GLY:O	2.37	0.43
1:A:251:A:O2'	1:A:252:G:O5'	2.36	0.43
1:A:1945:G:N2	1:A:1946:U:C2	2.87	0.43
1:A:308:G:C2	1:A:309:A:C2	3.06	0.43
1:A:1695:G:N3	1:A:1695:G:C2'	2.82	0.43
1:A:1413:A:C5	1:A:1414:C:N4	2.87	0.43
1:A:1766:G:C4	1:A:1987:A:C2	3.06	0.43
4:D:98:VAL:O	4:D:99:GLU:C	2.58	0.43
1:A:1348:C:C5	1:A:1349:C:C2	3.06	0.43
25:Y:31:GLN:C	25:Y:33:ALA:N	2.72	0.43
1:A:1936:A:C4	1:A:1940:U:C5	3.07	0.43
1:A:822:G:O6	1:A:943:A:C2	2.72	0.43
31:4:1:MET:N	31:4:1:MET:SD	2.92	0.43
1:A:422:A:N1	1:A:423:A:C6	2.87	0.43
1:A:1142:A:C8	1:A:1144:A:C5	3.07	0.43
1:A:2350:C:C5	30:3:41:ARG:NH1	2.87	0.43
1:A:94:A:C6	1:A:95:A:C6	3.06	0.43
1:A:695:G:C2	1:A:768:G:C2	3.07	0.43
5:E:170:ARG:NH2	5:E:176:ASP:CB	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:50:PHE:CE2	12:L:53:GLY:N	2.86	0.43
26:Z:40:THR:C	26:Z:42:ALA:N	2.71	0.43
1:A:2746:U:N3	1:A:2759:G:N1	2.67	0.42
1:A:627:A:O2'	1:A:628:G:C8	2.72	0.42
1:A:2458:G:O2'	1:A:2460:U:O4	2.36	0.42
2:B:42:C:O2	6:F:89:THR:N	2.52	0.42
1:A:831:G:O2'	1:A:832:U:C5'	2.67	0.42
1:A:617:G:C4	1:A:618:G:C8	3.07	0.42
10:J:45:THR:OG1	10:J:48:VAL:N	2.52	0.42
1:A:2654:A:C4	1:A:2656:U:C4	3.07	0.42
1:A:249:C:C5'	1:A:2394:C:O2'	2.66	0.42
1:A:242:G:P	30:3:2:LYS:NZ	2.92	0.42
1:A:2693:G:C2	1:A:2694:G:N7	2.87	0.42
1:A:531:C:C6	1:A:2035:G:C2	3.07	0.42
4:D:196:ALA:O	4:D:197:THR:C	2.57	0.42
1:A:1593:A:C6	1:A:1594:U:C4	3.07	0.42
1:A:1223:G:O6	18:R:71:LYS:NZ	2.51	0.42
1:A:656:G:C2'	1:A:657:U:C6	3.02	0.42
1:A:2023:C:O2'	1:A:2024:G:O5'	2.35	0.42
1:A:2459:A:C5	1:A:2460:U:C5	3.07	0.42
1:A:2582:G:O2'	1:A:2583:G:C5'	2.67	0.42
1:A:2315:G:C6	1:A:2316:G:C5	3.08	0.42
1:A:1782:U:O2'	1:A:1783:A:O5'	2.37	0.42
1:A:389:G:C6	1:A:2413:G:O2'	2.71	0.42
1:A:1455:G:C2	1:A:1456:G:C4	3.07	0.42
9:I:51:GLY:O	9:I:52:LEU:CB	2.66	0.42
16:P:102:ARG:O	16:P:103:THR:CB	2.67	0.42
1:A:1031:G:N2	1:A:1124:G:C4	2.87	0.42
26:Z:28:LEU:N	26:Z:28:LEU:CD2	2.82	0.42
1:A:2307:G:C8	1:A:2312:U:C5	3.07	0.42
1:A:765:C:O2'	1:A:766:U:O4'	2.37	0.42
1:A:2625:G:C6	1:A:2626:C:C4	3.07	0.42
1:A:1654:A:N3	1:A:1655:A:C8	2.87	0.42
1:A:793:A:OP2	1:A:2071:A:O2'	2.37	0.42
1:A:2848:G:OP2	16:P:94:ALA:CB	2.68	0.42
1:A:61:C:C4	1:A:94:A:N1	2.87	0.42
1:A:247:G:C6	1:A:249:C:O2'	2.72	0.42
1:A:1171:G:C4	1:A:1179:G:N2	2.87	0.42
1:A:310:A:C2	1:A:330:A:C4	3.06	0.42
1:A:918:A:C5	1:A:919:U:C1'	3.01	0.42
1:A:1471:G:C6	1:A:1472:C:C4	3.07	0.42
1:A:1208:C:N3	1:A:1209:U:C5	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:39:ASN:O	21:U:40:LEU:C	2.57	0.42
1:A:1438:U:C2'	1:A:1439:A:O4'	2.67	0.42
1:A:668:A:N7	1:A:670:A:N7	2.67	0.42
1:A:475:C:C6	1:A:475:C:O5'	2.72	0.42
1:A:2520:C:C4	1:A:2567:G:C5	3.07	0.42
1:A:230:G:C2	1:A:231:A:N7	2.87	0.42
1:A:503:A:C2	1:A:505:A:C2	3.07	0.42
1:A:2030:A:C2	1:A:2499:C:OP1	2.72	0.42
1:A:2074:U:C2	1:A:2436:G:C2	3.07	0.42
1:A:976:G:O6	1:A:988:A:C2	2.73	0.42
1:A:2360:G:O4'	12:L:60:ARG:NH2	2.53	0.42
1:A:956:G:C2	1:A:962:G:O6	2.72	0.42
1:A:38:A:N6	1:A:39:G:C5	2.88	0.42
1:A:1910:G:N1	1:A:1921:G:C5	2.87	0.42
1:A:2104:C:O2'	1:A:2105:U:C6	2.73	0.42
31:4:7:VAL:O	31:4:8:LYS:O	2.37	0.42
1:A:1773:A:C8	1:A:1829:A:C8	3.08	0.42
1:A:411:G:C4'	1:A:412:A:OP1	2.67	0.42
6:F:11:VAL:CG1	6:F:12:VAL:N	2.83	0.42
1:A:2733:A:C2	1:A:2734:A:C4	3.08	0.42
23:W:77:LYS:O	23:W:78:PHE:CB	2.67	0.42
6:F:74:ALA:CB	6:F:78:ILE:CD1	2.98	0.42
1:A:1939:U:O4'	1:A:2591:C:O2'	2.37	0.42
1:A:216:A:N3	1:A:217:A:C8	2.88	0.42
1:A:75:G:O2'	1:A:76:C:O5'	2.38	0.42
1:A:89:A:C6	1:A:90:U:C4	3.08	0.42
1:A:2040:G:C6	1:A:2041:U:C4	3.08	0.42
1:A:2297:A:O2'	1:A:2298:A:C5'	2.67	0.42
1:A:1427:A:N6	1:A:1571:A:OP2	2.51	0.42
1:A:2323:G:N2	1:A:2335:A:C2	2.88	0.42
1:A:2454:G:C2	1:A:2499:C:N3	2.87	0.42
1:A:2229:U:C2	1:A:2230:G:C8	3.08	0.42
1:A:962:G:N2	13:M:82:MET:CE	2.82	0.42
1:A:1505:A:C2	1:A:1506:U:C2	3.08	0.42
1:A:1247:A:N7	1:A:1249:U:O4	2.53	0.42
1:A:2530:A:C8	7:G:156:TYR:OH	2.73	0.42
19:S:36:LEU:C	19:S:38:TYR:N	2.72	0.42
1:A:1307:A:C6	1:A:1308:A:C5	3.08	0.42
15:O:41:ALA:O	15:O:43:ASN:N	2.52	0.42
14:N:35:LYS:NZ	14:N:112:TYR:CE1	2.88	0.42
26:Z:51:SER:C	26:Z:53:MET:N	2.72	0.42
1:A:668:A:N3	1:A:670:A:N6	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1815:A:C4	1:A:1817:G:C6	3.07	0.42
1:A:2489:U:C5	1:A:2490:G:C6	3.08	0.42
1:A:2093:G:C5	1:A:2225:A:C8	3.08	0.42
1:A:579:G:N2	1:A:1262:A:C4	2.88	0.42
1:A:705:A:C2	1:A:727:A:O4'	2.72	0.42
1:A:1710:G:C2	1:A:1749:A:C2	3.07	0.42
1:A:522:A:C4	1:A:523:C:C5	3.08	0.42
1:A:1304:A:C6	1:A:1305:C:C4	3.07	0.42
1:A:759:G:C2	1:A:760:G:C4	3.08	0.42
27:0:53:VAL:O	27:0:54:ILE:O	2.37	0.42
2:B:30:C:O2'	2:B:57:A:N1	2.53	0.42
1:A:1534:U:C2'	1:A:1534:U:O2	2.67	0.42
1:A:597:G:C6	1:A:598:U:C2	3.07	0.42
1:A:1717:A:C2'	1:A:1718:G:O4'	2.68	0.42
1:A:223:A:N6	1:A:422:A:N6	2.67	0.42
1:A:2788:C:O2	1:A:2809:A:C2	2.72	0.42
1:A:1296:G:OP1	1:A:2709:G:O2'	2.36	0.42
1:A:2336:A:N7	23:W:40:ARG:NE	2.67	0.42
1:A:2467:C:N4	1:A:2468:A:N1	2.67	0.42
1:A:631:A:N3	1:A:2415:G:O2'	2.53	0.42
1:A:1918:A:O2'	1:A:1919:A:N7	2.53	0.42
2:B:75:G:N2	2:B:102:G:N2	2.68	0.42
1:A:743:A:C6	1:A:744:U:C4	3.07	0.42
16:P:51:ASN:O	16:P:52:ARG:NH1	2.53	0.42
1:A:954:G:O2'	1:A:2274:A:N1	2.53	0.42
1:A:763:G:O2'	1:A:764:A:O5'	2.38	0.42
1:A:2406:A:C2	12:L:69:ARG:NH2	2.87	0.42
1:A:1008:A:N6	1:A:1136:G:N1	2.67	0.42
1:A:2077:A:C5	1:A:2435:A:C6	3.08	0.42
1:A:2077:A:C2	1:A:2078:C:C2	3.08	0.42
1:A:1731:G:C2	1:A:1733:G:N7	2.88	0.42
1:A:1920:C:C2	1:A:1921:G:C8	3.07	0.42
1:A:650:C:O4'	30:3:22:LYS:NZ	2.53	0.42
4:D:98:VAL:O	4:D:100:LEU:N	2.52	0.42
11:K:28:SER:O	11:K:29:HIS:CB	2.68	0.42
1:A:1232:G:C6	1:A:1233:C:C4	3.08	0.42
5:E:85:PHE:O	5:E:86:ALA:C	2.58	0.42
1:A:1585:C:C2'	1:A:1586:A:O5'	2.68	0.42
1:A:77:G:C4	1:A:110:G:C2	3.08	0.42
15:O:69:ASP:O	15:O:70:ALA:C	2.57	0.42
1:A:241:A:C4	1:A:243:U:O4	2.72	0.42
1:A:1941:C:C5	1:A:1942:C:N4	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1155:A:C4	1:A:1157:G:C8	3.07	0.42
17:Q:63:ARG:O	17:Q:66:ALA:N	2.53	0.42
1:A:2061:G:C2	1:A:2063:C:C4	3.07	0.42
1:A:280:U:O2	1:A:280:U:O4'	2.37	0.42
1:A:1438:U:C4	1:A:1555:G:N1	2.88	0.42
1:A:303:G:C6	1:A:315:G:O6	2.73	0.42
1:A:670:A:O2'	1:A:671:C:P	2.78	0.42
1:A:1787:A:N3	1:A:1788:C:C5	2.88	0.42
1:A:422:A:C2	1:A:423:A:C5	3.07	0.42
22:V:31:TYR:CD1	22:V:31:TYR:C	2.93	0.42
23:W:32:ALA:O	23:W:34:SER:N	2.52	0.42
10:J:41:LYS:C	10:J:43:GLU:N	2.73	0.42
1:A:2886:A:N6	27:0:39:ARG:CD	2.83	0.42
1:A:1262:A:N3	27:0:6:LYS:NZ	2.68	0.42
1:A:2800:A:C2	1:A:2801:G:N3	2.87	0.42
1:A:857:G:O2'	23:W:19:ARG:CZ	2.68	0.42
1:A:1446:C:N4	1:A:1447:C:N4	2.67	0.42
1:A:2016:U:C4	1:A:2017:U:O4	2.73	0.42
23:W:44:PHE:CE2	23:W:76:ARG:NE	2.88	0.42
1:A:991:C:C4	1:A:1185:G:C6	3.08	0.42
14:N:31:HIS:O	14:N:33:ILE:N	2.53	0.42
1:A:217:A:O2'	1:A:218:A:O4'	2.37	0.41
1:A:762:U:C4'	1:A:763:G:O5'	2.68	0.41
1:A:605:G:O2'	1:A:606:U:O4'	2.38	0.41
1:A:2624:G:C5	1:A:2625:G:C8	3.08	0.41
1:A:526:A:N6	1:A:2626:C:C4'	2.83	0.41
1:A:866:A:O2'	1:A:867:C:C5'	2.68	0.41
8:H:53:GLU:C	8:H:55:GLU:N	2.74	0.41
1:A:2644:G:C6	1:A:2645:G:C2	3.08	0.41
1:A:1889:A:C6	1:A:1890:A:C6	3.07	0.41
1:A:1517:G:N2	1:A:1732:C:C6	2.88	0.41
1:A:963:U:O2'	1:A:964:C:C6	2.72	0.41
1:A:1613:G:C6	1:A:1619:G:C6	3.08	0.41
24:X:4:CYS:O	24:X:6:VAL:N	2.53	0.41
1:A:770:G:O2'	1:A:1379:U:O4	2.38	0.41
1:A:1601:G:OP1	20:T:64:LYS:NZ	2.53	0.41
1:A:2423:U:C1'	1:A:2425:A:N7	2.83	0.41
1:A:2397:G:C6	1:A:2420:C:N3	2.87	0.41
1:A:1653:G:O6	14:N:10:LEU:O	2.38	0.41
1:A:2062:A:C6	1:A:2503:A:N7	2.88	0.41
1:A:1421:G:OP2	1:A:1421:G:C8	2.73	0.41
1:A:36:G:N1	1:A:445:C:C4	2.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:G:C4	1:A:302:C:C4	3.08	0.41
1:A:2541:A:O2'	1:A:2765:A:N1	2.54	0.41
1:A:603:A:C4'	1:A:604:G:O5'	2.68	0.41
1:A:379:G:N1	1:A:396:G:C6	2.88	0.41
1:A:1270:C:C4	1:A:1648:U:C4	3.08	0.41
1:A:2574:G:C5	1:A:2575:C:C5	3.08	0.41
1:A:2837:A:N6	1:A:2882:A:C6	2.88	0.41
1:A:1238:G:C2	1:A:1239:G:C5	3.08	0.41
1:A:1680:U:C4	1:A:1681:G:C2	3.08	0.41
1:A:142:A:C4	1:A:143:C:C5	3.07	0.41
1:A:1149:G:C6	1:A:1150:C:C4	3.08	0.41
1:A:2665:A:C2	1:A:2666:C:C2	3.08	0.41
1:A:1452:G:O2'	1:A:1457:U:O4	2.38	0.41
20:T:85:VAL:O	20:T:86:THR:OG1	2.39	0.41
1:A:1766:G:C2	1:A:1987:A:N3	2.88	0.41
1:A:2027:G:C6	1:A:2028:U:C4	3.08	0.41
1:A:1767:G:N2	1:A:1986:C:C2	2.88	0.41
1:A:1437:C:C2	1:A:1438:U:C5	3.08	0.41
1:A:1477:A:C2'	1:A:1478:G:O4'	2.68	0.41
1:A:1057:A:C6	1:A:1058:U:C4	3.08	0.41
1:A:1848:A:C2	1:A:1849:G:C4	3.09	0.41
1:A:395:U:O2'	1:A:396:G:O5'	2.38	0.41
1:A:657:U:O2'	1:A:658:U:C5'	2.68	0.41
1:A:1288:G:C8	1:A:1327:A:N6	2.88	0.41
1:A:2348:U:O2'	1:A:2349:G:C5'	2.69	0.41
1:A:2006:C:C2	1:A:2007:U:C5	3.08	0.41
1:A:120:U:C2	1:A:149:A:C5	3.08	0.41
1:A:2822:G:O2'	1:A:2825:G:N1	2.53	0.41
11:K:88:ASN:N	11:K:92:GLU:O	2.53	0.41
1:A:2800:A:N1	1:A:2801:G:N3	2.68	0.41
1:A:635:C:C5	12:L:109:LYS:NZ	2.89	0.41
1:A:36:G:C2	1:A:445:C:C4	3.09	0.41
1:A:1103:A:C8	1:A:1103:A:O5'	2.73	0.41
1:A:2197:U:O2'	1:A:2198:A:O5'	2.38	0.41
1:A:1313:U:C2'	1:A:1313:U:O2	2.66	0.41
1:A:2489:U:O4	1:A:2490:G:N1	2.52	0.41
22:V:14:LYS:O	22:V:15:GLY:C	2.58	0.41
7:G:92:GLY:O	7:G:93:TYR:C	2.59	0.41
1:A:249:C:P	1:A:2394:C:O2'	2.79	0.41
3:C:44:ASN:O	3:C:46:GLY:N	2.53	0.41
1:A:964:C:O2'	1:A:2273:A:N3	2.53	0.41
1:A:1941:C:O2'	1:A:1942:C:C5'	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:G:O2'	1:A:1254:A:OP1	2.39	0.41
1:A:633:A:C8	1:A:633:A:O5'	2.74	0.41
1:A:1809:A:O2'	1:A:1810:A:P	2.78	0.41
1:A:604:G:N3	1:A:605:G:C8	2.89	0.41
1:A:84:A:N1	1:A:98:G:O2'	2.53	0.41
1:A:2454:G:N2	1:A:2499:C:C2	2.88	0.41
1:A:197:A:N7	1:A:2430:A:C8	2.89	0.41
1:A:241:A:C1'	1:A:243:U:C4	3.03	0.41
1:A:1659:G:C2	1:A:2002:G:N3	2.88	0.41
1:A:771:G:N3	1:A:772:C:C6	2.88	0.41
1:A:800:A:N1	1:A:802:A:C8	2.88	0.41
1:A:945:A:C8	1:A:2448:A:C2	3.08	0.41
1:A:415:A:C6	1:A:416:U:C4	3.07	0.41
1:A:995:C:N3	10:J:3:THR:OG1	2.53	0.41
30:3:63:TYR:O	30:3:64:ALA:O	2.38	0.41
1:A:1742:U:C4	1:A:1743:G:C6	3.08	0.41
21:U:54:PRO:CG	21:U:55:GLY:N	2.83	0.41
1:A:215:G:O2'	1:A:216:A:O5'	2.39	0.41
1:A:302:C:O2'	1:A:303:G:O5'	2.38	0.41
1:A:2406:A:C4'	1:A:2407:A:O5'	2.68	0.41
1:A:738:G:N1	1:A:739:A:C2	2.89	0.41
1:A:1287:A:OP1	14:N:103:ARG:CG	2.69	0.41
1:A:2285:C:OP2	28:1:5:ARG:NH1	2.54	0.41
1:A:1355:G:C6	1:A:1377:G:C2	3.09	0.41
1:A:1844:C:N3	1:A:1845:G:N7	2.69	0.41
1:A:2850:A:N7	1:A:2868:A:O2'	2.53	0.41
1:A:61:C:N4	1:A:94:A:C6	2.89	0.41
1:A:2823:A:C4	1:A:2824:C:C6	3.08	0.41
1:A:1753:G:C2	1:A:1756:G:C2	3.09	0.41
1:A:1707:G:C8	1:A:1756:G:N7	2.89	0.41
2:B:66:A:C6	2:B:107:G:C4	3.09	0.41
1:A:1047:G:C2	1:A:1110:G:C4	3.08	0.41
1:A:620:G:O2'	1:A:622:G:N7	2.53	0.41
19:S:27:LYS:O	19:S:28:LYS:C	2.59	0.41
10:J:97:PRO:C	10:J:99:ARG:N	2.74	0.41
1:A:2029:G:N1	1:A:2033:A:OP2	2.53	0.41
21:U:100:GLU:O	21:U:101:THR:C	2.59	0.41
1:A:1475:G:N3	1:A:1514:G:O6	2.54	0.41
1:A:379:G:O6	1:A:380:G:C6	2.73	0.41
1:A:866:A:C8	1:A:914:G:C6	3.09	0.41
1:A:1398:C:O2'	1:A:1399:C:O5'	2.39	0.41
1:A:250:G:O6	1:A:386:G:N2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1127:A:N1	1:A:2463:C:O2'	2.54	0.41
1:A:71:A:C8	1:A:73:A:N6	2.89	0.41
1:A:2413:G:C4	1:A:2414:G:C8	3.09	0.41
2:B:76:G:O2'	22:V:21:ARG:NH2	2.53	0.41
1:A:958:U:O2'	2:B:89:U:C2	2.73	0.41
10:J:64:VAL:CG1	10:J:65:THR:N	2.83	0.41
1:A:2751:G:N3	7:G:2:ARG:NH2	2.69	0.41
1:A:728:G:C4	1:A:730:A:C8	3.09	0.41
6:F:48:LEU:O	6:F:52:ALA:CB	2.69	0.41
1:A:952:G:C4	1:A:966:G:N2	2.89	0.41
19:S:51:LEU:O	19:S:55:ILE:N	2.54	0.41
16:P:24:THR:O	16:P:25:VAL:C	2.58	0.41
1:A:1442:U:C4	1:A:1443:U:O4	2.74	0.41
1:A:1139:G:C6	1:A:1140:C:C4	3.08	0.41
1:A:42:A:C2	1:A:438:G:C2	3.09	0.41
1:A:961:C:O2'	1:A:962:G:OP1	2.39	0.41
1:A:2693:G:N3	1:A:2694:G:C8	2.89	0.41
1:A:1380:G:C2	1:A:1381:G:C8	3.09	0.41
1:A:527:C:C2'	1:A:527:C:O2	2.69	0.41
29:2:28:ARG:C	29:2:30:VAL:N	2.74	0.41
1:A:1715:G:O2'	1:A:1743:G:O6	2.39	0.41
1:A:1064:C:C4	1:A:1065:U:C4	3.09	0.41
1:A:2744:G:C6	1:A:2761:A:C6	3.09	0.41
14:N:100:CYS:SG	14:N:101:GLY:N	2.94	0.41
21:U:80:ASP:OD1	21:U:80:ASP:N	2.53	0.41
15:O:2:ASP:O	15:O:4:LYS:N	2.53	0.41
6:F:137:PHE:O	6:F:138:PRO:C	2.59	0.41
1:A:1477:A:C8	1:A:1515:A:N6	2.89	0.41
1:A:671:C:OP1	12:L:33:ARG:NH1	2.54	0.41
1:A:605:G:C5	1:A:606:U:C5	3.09	0.41
1:A:1721:G:O2'	1:A:1739:A:N6	2.53	0.41
1:A:2261:C:O2'	1:A:2262:U:C5'	2.69	0.41
1:A:2262:U:OP1	23:W:38:ARG:NH2	2.54	0.41
1:A:202:U:N3	1:A:203:A:C2	2.89	0.41
1:A:2023:C:O2'	1:A:2024:G:P	2.78	0.41
1:A:1276:A:N1	1:A:1277:G:C6	2.88	0.41
1:A:2902:C:O2'	1:A:2903:U:C6	2.73	0.41
1:A:2902:C:O2'	1:A:2903:U:P	2.79	0.41
1:A:1376:C:C4	1:A:1377:G:C6	3.09	0.41
1:A:1844:C:N3	1:A:1845:G:C8	2.89	0.41
1:A:2868:A:O2'	1:A:2869:G:C5'	2.69	0.41
1:A:459:U:O2'	1:A:460:A:C5'	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2349:G:C6	1:A:2350:C:C2	3.08	0.41
1:A:1136:G:O2'	1:A:1137:G:O5'	2.39	0.41
1:A:1138:G:O2'	10:J:104:ALA:O	2.38	0.41
1:A:2435:A:C4	1:A:2436:G:C8	3.08	0.41
1:A:2654:A:C4	1:A:2656:U:N3	2.88	0.41
1:A:2595:G:C6	1:A:2599:G:C6	3.09	0.41
1:A:2603:G:O2'	1:A:2604:U:O4'	2.39	0.41
2:B:16:G:O6	2:B:69:G:C5	2.73	0.41
1:A:2697:G:C5	1:A:2698:U:C5	3.08	0.41
1:A:1670:C:N4	1:A:1674:G:O5'	2.54	0.41
1:A:1171:G:C6	1:A:1179:G:C2	3.08	0.41
1:A:845:A:C2	1:A:847:U:N1	2.89	0.41
1:A:1435:G:C2	1:A:1436:G:C8	3.09	0.41
3:C:209:ALA:O	3:C:212:TRP:CD1	2.74	0.41
1:A:591:U:N3	1:A:592:A:C5	2.89	0.41
3:C:166:ARG:CG	3:C:166:ARG:O	2.69	0.41
1:A:2070:A:C2	1:A:2442:C:C2	3.08	0.41
1:A:2505:G:N2	1:A:2610:C:C2	2.89	0.41
20:T:28:ASN:O	20:T:29:THR:CG2	2.69	0.41
2:B:56:G:C4'	2:B:57:A:O5'	2.69	0.41
17:Q:66:ALA:O	17:Q:70:GLN:N	2.54	0.41
1:A:980:A:N6	1:A:2027:G:O2'	2.54	0.41
1:A:2363:G:C6	1:A:2364:C:C4	3.09	0.41
3:C:120:ASP:CG	3:C:121:ALA:N	2.75	0.41
30:3:50:SER:O	30:3:52:GLY:N	2.54	0.41
1:A:362:A:N7	1:A:363:G:N7	2.68	0.41
14:N:118:ARG:O	14:N:120:GLU:N	2.53	0.41
1:A:254:G:N7	30:3:4:LYS:CE	2.84	0.41
1:A:876:C:O4'	1:A:876:C:O2	2.38	0.41
1:A:1437:C:O2'	1:A:1516:G:O2'	2.38	0.41
1:A:2409:G:C6	1:A:2410:G:C5	3.08	0.41
1:A:2746:U:C2	1:A:2759:G:C2	3.09	0.41
1:A:117:G:C6	1:A:119:A:N6	2.89	0.41
1:A:529:A:C4	1:A:2023:C:C4	3.09	0.41
1:A:2459:A:N6	1:A:2494:G:C2	2.89	0.41
1:A:1000:A:N6	1:A:1001:A:C6	2.89	0.41
24:X:1:SER:O	24:X:2:ARG:C	2.59	0.41
1:A:1204:A:C4'	1:A:1205:A:O5'	2.69	0.41
1:A:2265:U:O2'	13:M:13:HIS:CE1	2.74	0.41
1:A:1169:A:C2	1:A:1181:U:O2	2.74	0.41
25:Y:45:GLN:C	25:Y:47:ARG:N	2.74	0.41
1:A:743:A:O2'	1:A:1659:G:OP1	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:G:N2	1:A:513:A:N7	2.69	0.41
1:A:412:A:N6	1:A:2411:A:C2'	2.84	0.41
17:Q:63:ARG:O	17:Q:64:ILE:C	2.59	0.41
1:A:991:C:OP2	1:A:1186:G:OP2	2.39	0.41
1:A:2084:C:C5	1:A:2085:U:C5	3.09	0.41
19:S:31:GLN:O	19:S:33:LEU:N	2.54	0.41
4:D:138:LEU:O	4:D:139:SER:OG	2.39	0.41
1:A:383:C:C2	1:A:385:C:C5	3.09	0.41
1:A:668:A:C5	1:A:670:A:C8	3.09	0.40
1:A:671:C:O2'	1:A:672:C:C5	2.74	0.40
1:A:1955:U:O2'	1:A:1956:U:P	2.78	0.40
1:A:2010:G:C5	1:A:2011:U:C5	3.10	0.40
4:D:150:GLN:O	4:D:151:THR:C	2.59	0.40
1:A:2644:G:N1	1:A:2645:G:N2	2.68	0.40
1:A:1344:U:O2	1:A:1384:A:O2'	2.39	0.40
1:A:1034:G:O6	1:A:1122:G:C6	2.75	0.40
2:B:13:G:N2	2:B:69:G:N2	2.68	0.40
3:C:44:ASN:C	3:C:46:GLY:N	2.74	0.40
1:A:1557:C:C4	1:A:1558:C:C2	3.09	0.40
1:A:2674:G:C4	1:A:2675:A:C8	3.09	0.40
1:A:2635:A:C2	1:A:2784:U:N3	2.89	0.40
2:B:44:G:OP1	6:F:91:ARG:NH1	2.54	0.40
10:J:22:GLY:O	10:J:23:LYS:C	2.59	0.40
4:D:94:GLN:O	4:D:95:SER:C	2.58	0.40
7:G:60:GLY:O	7:G:62:ALA:N	2.54	0.40
1:A:685:A:C5	1:A:774:G:N2	2.88	0.40
1:A:685:A:C8	1:A:774:G:N1	2.89	0.40
1:A:1616:A:C2	1:A:1647:U:C5	3.09	0.40
1:A:671:C:O2'	1:A:672:C:P	2.79	0.40
1:A:2198:A:O2'	1:A:2199:A:C8	2.74	0.40
1:A:410:G:C6	1:A:2407:A:N6	2.89	0.40
1:A:605:G:O2'	1:A:606:U:C5'	2.69	0.40
1:A:1956:U:O2'	1:A:1957:C:O5'	2.40	0.40
1:A:1296:G:C2	1:A:1645:G:C5	3.09	0.40
1:A:2460:U:C2'	1:A:2461:A:C8	3.04	0.40
1:A:1113:U:O2'	1:A:1114:C:P	2.80	0.40
7:G:91:VAL:N	7:G:93:TYR:CD2	2.90	0.40
1:A:861:A:O2'	1:A:862:G:C5'	2.69	0.40
1:A:2077:A:OP1	1:A:2238:G:N1	2.54	0.40
1:A:241:A:C8	1:A:243:U:N3	2.89	0.40
1:A:2345:G:C6	1:A:2347:C:N4	2.89	0.40
1:A:194:G:C6	1:A:195:A:C5	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1910:G:C2	1:A:1921:G:C4	3.09	0.40
1:A:1773:A:N7	1:A:1829:A:C1'	2.84	0.40
1:A:1456:G:N2	1:A:2704:C:C2	2.90	0.40
17:Q:63:ARG:NH1	17:Q:99:VAL:CG2	2.84	0.40
1:A:408:G:N3	1:A:409:G:C8	2.90	0.40
1:A:1878:G:C6	1:A:1879:C:C4	3.09	0.40
1:A:1415:U:C2	1:A:1588:G:N1	2.89	0.40
14:N:64:ARG:O	14:N:68:ALA:N	2.54	0.40
12:L:56:PRO:CB	12:L:58:TYR:CE2	3.03	0.40
11:K:80:ASP:CB	16:P:67:GLU:OE1	2.69	0.40
1:A:849:A:C4	1:A:850:U:C5	3.10	0.40
26:Z:16:LEU:CD2	26:Z:16:LEU:N	2.85	0.40
1:A:1442:U:C4	1:A:1443:U:C4	3.09	0.40
1:A:271:G:C4	1:A:272:A:N7	2.89	0.40
1:A:64:A:C6	1:A:91:A:N6	2.89	0.40
1:A:14:A:C6	1:A:526:A:C2	3.09	0.40
1:A:1385:A:C4'	1:A:1386:C:OP1	2.69	0.40
1:A:571:U:N3	1:A:2030:A:C6	2.89	0.40
1:A:1398:C:O2'	1:A:1399:C:C6	2.74	0.40
1:A:45:G:C5'	1:A:46:G:OP1	2.69	0.40
1:A:1203:U:C4	1:A:1204:A:C5	3.09	0.40
1:A:1345:C:C2	1:A:1346:G:C8	3.09	0.40
23:W:25:PHE:CG	23:W:26:GLY:N	2.88	0.40
1:A:532:A:N1	1:A:2020:A:C1'	2.84	0.40
1:A:996:A:C4	1:A:997:G:C8	3.10	0.40
21:U:64:ILE:O	21:U:65:GLN:O	2.40	0.40
2:B:78:A:C2	2:B:99:A:C4	3.09	0.40
1:A:2560:A:C6	1:A:2561:U:C4	3.10	0.40
22:V:80:HIS:CD2	22:V:83:LYS:N	2.89	0.40
1:A:929:U:N3	1:A:930:G:C5	2.89	0.40
2:B:51:G:O6	15:O:32:PRO:CB	2.70	0.40
1:A:74:A:C4'	1:A:75:G:O5'	2.69	0.40
1:A:249:C:OP2	1:A:2394:C:O2'	2.40	0.40
1:A:252:G:N2	1:A:253:C:C2	2.89	0.40
1:A:825:A:C6	1:A:826:U:N3	2.89	0.40
1:A:52:A:O2'	1:A:53:A:O4'	2.40	0.40
1:A:1047:G:N2	1:A:1110:G:C4	2.89	0.40
1:A:38:A:C6	1:A:39:G:C5	3.10	0.40
1:A:567:U:N3	1:A:568:U:C4	2.89	0.40
1:A:19:A:N1	1:A:522:A:C6	2.90	0.40
1:A:1959:G:C6	1:A:1960:A:C5	3.10	0.40
1:A:2102:G:C2	1:A:2188:U:C2	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:106:LYS:O	4:D:107:VAL:CB	2.69	0.40
1:A:187:G:C2	1:A:210:C:C2	3.10	0.40
1:A:2024:G:C5	1:A:2040:G:C2	3.10	0.40
1:A:86:G:C2	1:A:87:U:C5	3.10	0.40
1:A:2298:A:N1	1:A:2321:U:C5	2.90	0.40
1:A:2074:U:C4	1:A:2075:U:O4	2.73	0.40
1:A:1048:A:N6	1:A:1111:A:C5	2.89	0.40
1:A:197:A:C6	1:A:2430:A:N3	2.89	0.40
2:B:102:G:C5	2:B:103:U:C5	3.10	0.40
1:A:1951:U:C2	1:A:1953:A:OP2	2.74	0.40
1:A:961:C:C4	1:A:2031:A:C4	3.10	0.40
1:A:370:G:O6	1:A:424:G:C6	2.75	0.40
1:A:539:G:C2	1:A:540:C:C2	3.10	0.40
14:N:14:SER:C	14:N:16:HIS:N	2.75	0.40
2:B:34:A:C5	2:B:44:G:N7	2.89	0.40
1:A:2558:C:C4	1:A:2559:C:C4	3.09	0.40
1:A:2768:U:C4	1:A:2769:U:C4	3.10	0.40
10:J:37:ARG:NH2	10:J:39:LYS:NZ	2.69	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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	C	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	1	21
4	D	207/209 (99%)	129 (62%)	48 (23%)	30 (14%)	0	10
5	E	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	1	18
6	F	176/179 (98%)	94 (53%)	43 (24%)	39 (22%)	0	2
7	G	174/177 (98%)	109 (63%)	36 (21%)	29 (17%)	0	7
8	H	147/149 (99%)	78 (53%)	48 (33%)	21 (14%)	0	11
9	I	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	12
10	J	140/142 (99%)	95 (68%)	31 (22%)	14 (10%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	120/123 (98%)	79 (66%)	22 (18%)	19 (16%)	0	8
12	L	141/144 (98%)	80 (57%)	42 (30%)	19 (14%)	0	12
13	M	134/136 (98%)	89 (66%)	32 (24%)	13 (10%)	1	22
14	N	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	1	17
15	O	114/117 (97%)	80 (70%)	28 (25%)	6 (5%)	3	43
16	P	112/115 (97%)	67 (60%)	30 (27%)	15 (13%)	0	12
17	Q	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	2	34
18	R	101/103 (98%)	71 (70%)	20 (20%)	10 (10%)	1	21
19	S	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	1	25
20	T	91/100 (91%)	47 (52%)	30 (33%)	14 (15%)	0	9
21	U	100/104 (96%)	49 (49%)	29 (29%)	22 (22%)	0	2
22	V	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	1	26
23	W	77/85 (91%)	34 (44%)	25 (32%)	18 (23%)	0	2
24	X	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	1	25
25	Y	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	1	28
26	Z	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	1	14
27	0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	13
28	1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	28
29	2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	1	17
30	3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	29
31	4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	7
All	All	3310/3409 (97%)	2076 (63%)	813 (25%)	421 (13%)	0	14

All (421) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	9	SER
3	C	28	PRO
3	C	186	ASP
3	C	269	ARG
4	D	11	MET
4	D	14	ILE
4	D	31	ALA
4	D	74	GLU
4	D	77	ARG

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Mol	Chain	Res	Type
4	D	136	ASN
4	D	150	GLN
4	D	164	GLN
4	D	170	VAL
4	D	175	LEU
4	D	194	PRO
5	E	41	GLN
5	E	55	SER
5	E	99	LYS
5	E	116	ASP
6	F	10	GLU
6	F	12	VAL
6	F	32	LYS
6	F	36	ASN
6	F	42	ALA
6	F	112	ASP
6	F	114	ARG
6	F	120	SER
6	F	122	ASP
6	F	137	PHE
6	F	138	PRO
7	G	49	LEU
7	G	95	ALA
7	G	149	ALA
7	G	164	ALA
7	G	165	ASP
8	H	3	VAL
8	H	9	VAL
8	H	10	ALA
8	H	49	ALA
8	H	72	ILE
8	H	76	GLU
8	H	98	ASP
8	H	102	ALA
9	I	22	PRO
9	I	23	VAL
9	I	29	GLN
9	I	52	LEU
9	I	58	ILE
9	I	69	VAL
10	J	45	THR
10	J	81	ILE

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Mol	Chain	Res	Type
10	J	87	ALA
10	J	95	ARG
11	K	18	ARG
11	K	35	VAL
11	K	49	ARG
11	K	71	ARG
11	K	72	PRO
11	K	93	GLN
11	K	110	GLU
11	K	120	PRO
12	L	4	ASN
12	L	41	ARG
12	L	82	LEU
12	L	85	VAL
12	L	89	VAL
12	L	101	ILE
12	L	111	ILE
13	M	2	LEU
13	M	72	PRO
13	M	77	PRO
13	M	135	VAL
14	N	30	ARG
14	N	63	ARG
14	N	104	ALA
15	O	90	VAL
16	P	25	VAL
16	P	50	ARG
16	P	83	ILE
16	P	109	ILE
16	P	112	ARG
19	S	28	LYS
19	S	33	LEU
19	S	72	THR
20	T	14	PRO
20	T	15	HIS
20	T	20	ALA
20	T	29	THR
20	T	56	GLU
20	T	88	LYS
21	U	65	GLN
21	U	82	VAL
21	U	92	VAL

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Mol	Chain	Res	Type
21	U	95	PHE
21	U	96	LYS
21	U	97	SER
22	V	56	PHE
22	V	58	SER
23	W	9	THR
23	W	34	SER
23	W	35	ILE
24	X	2	ARG
26	Z	13	ILE
26	Z	30	ARG
27	0	54	ILE
30	3	29	ARG
31	4	8	LYS
31	4	20	ASP
3	C	3	VAL
3	C	37	SER
3	C	45	ASN
3	C	94	LEU
3	C	121	ALA
3	C	140	VAL
3	C	195	GLY
3	C	232	GLY
3	C	239	PHE
4	D	93	GLY
4	D	102	ALA
4	D	107	VAL
4	D	112	THR
4	D	118	PHE
4	D	119	ALA
4	D	120	GLY
5	E	62	GLN
5	E	79	ARG
5	E	80	SER
5	E	127	GLU
5	E	153	LEU
6	F	8	LYS
6	F	37	MET
6	F	43	ILE
6	F	67	THR
6	F	76	PHE
6	F	113	PHE

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Mol	Chain	Res	Type
6	F	133	GLU
6	F	145	VAL
6	F	148	VAL
7	G	59	ASP
7	G	80	GLU
7	G	83	THR
7	G	85	LYS
7	G	86	LEU
7	G	93	TYR
7	G	150	TYR
8	H	61	VAL
8	H	66	ASN
8	H	86	ASP
8	H	97	ARG
9	I	9	LYS
9	I	30	GLN
9	I	51	GLY
9	I	62	ALA
9	I	140	GLU
10	J	112	GLY
11	K	16	ALA
11	K	46	ALA
11	K	104	THR
12	L	29	LYS
13	M	14	LYS
13	M	73	ILE
14	N	8	ARG
14	N	105	GLY
15	O	3	LYS
15	O	8	ILE
15	O	72	ALA
16	P	32	VAL
16	P	33	GLU
16	P	85	VAL
16	P	108	ARG
17	Q	23	TYR
17	Q	86	SER
17	Q	88	GLU
17	Q	91	ARG
18	R	3	ALA
18	R	40	MET
19	S	3	THR

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Mol	Chain	Res	Type
19	S	40	ASN
20	T	39	THR
20	T	68	LYS
21	U	4	ILE
21	U	54	PRO
21	U	87	GLU
21	U	88	ASP
21	U	89	GLY
22	V	33	GLY
22	V	55	GLU
23	W	18	LYS
23	W	24	ARG
23	W	33	GLY
23	W	39	GLN
23	W	53	GLY
23	W	57	THR
23	W	71	LYS
23	W	83	ALA
24	X	41	SER
24	X	49	ARG
24	X	63	ILE
25	Y	9	LYS
25	Y	22	LEU
25	Y	37	LEU
26	Z	4	ILE
27	0	21	LEU
27	0	55	ALA
28	1	4	ILE
28	1	36	LYS
29	2	24	THR
29	2	40	ALA
30	3	3	ILE
30	3	6	VAL
30	3	51	LYS
31	4	4	ARG
3	C	36	ASN
3	C	59	GLN
3	C	69	ASN
3	C	98	GLY
3	C	141	HIS
3	C	147	PRO
3	C	237	ARG

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Mol	Chain	Res	Type
4	D	95	SER
4	D	99	GLU
4	D	162	ALA
5	E	13	THR
5	E	63	LYS
5	E	165	HIS
5	E	187	VAL
5	E	188	MET
6	F	41	GLU
6	F	70	ARG
6	F	116	LEU
7	G	9	VAL
7	G	11	PRO
7	G	46	ASP
7	G	91	VAL
7	G	117	PRO
7	G	125	PRO
7	G	169	ARG
8	H	99	ILE
8	H	144	VAL
9	I	35	MET
10	J	13	ARG
10	J	44	TYR
11	K	14	SER
11	K	17	ARG
11	K	103	VAL
12	L	19	LEU
12	L	99	ASN
12	L	100	ILE
12	L	115	GLU
13	M	16	ARG
13	M	111	GLU
14	N	2	ARG
14	N	5	LYS
14	N	10	LEU
14	N	13	ASN
16	P	94	ALA
16	P	113	LEU
17	Q	6	GLY
17	Q	29	ARG
17	Q	87	VAL
18	R	98	ILE

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Mol	Chain	Res	Type
19	S	61	ASN
20	T	19	LYS
20	T	38	ALA
21	U	8	ASP
21	U	40	LEU
22	V	79	ARG
23	W	36	ILE
23	W	46	ALA
24	X	35	HIS
24	X	69	GLU
27	0	32	THR
28	1	35	LEU
29	2	29	GLN
29	2	39	ARG
30	3	22	LYS
31	4	3	VAL
31	4	37	GLN
3	C	106	PRO
3	C	196	ASN
3	C	204	LEU
4	D	48	ILE
4	D	197	THR
5	E	69	ARG
5	E	96	VAL
5	E	126	VAL
5	E	148	ILE
6	F	94	ARG
6	F	104	THR
6	F	130	GLY
7	G	40	VAL
7	G	45	ALA
7	G	123	GLU
8	H	39	ALA
8	H	105	ALA
9	I	19	PRO
9	I	87	SER
9	I	119	ALA
10	J	5	THR
10	J	6	ALA
10	J	25	LEU
10	J	113	PRO
11	K	5	GLN

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Mol	Chain	Res	Type
11	K	6	THR
12	L	30	THR
13	M	13	HIS
13	M	106	ASP
14	N	82	GLU
16	P	20	ARG
16	P	51	ASN
17	Q	58	GLN
18	R	15	SER
18	R	29	THR
18	R	65	ALA
19	S	71	VAL
20	T	11	LEU
23	W	23	LYS
23	W	41	GLY
25	Y	2	LYS
25	Y	46	VAL
26	Z	52	PHE
27	0	26	SER
27	0	53	VAL
31	4	16	ILE
3	C	64	VAL
3	C	246	PRO
4	D	106	LYS
4	D	109	VAL
4	D	169	ARG
5	E	60	TRP
6	F	82	TYR
6	F	125	GLY
6	F	156	THR
7	G	39	ALA
7	G	119	GLY
7	G	126	THR
7	G	136	ASP
7	G	152	ARG
8	H	89	LYS
8	H	121	VAL
8	H	124	THR
8	H	143	ILE
10	J	43	GLU
11	K	119	ALA
12	L	48	ARG

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Mol	Chain	Res	Type
12	L	88	GLY
12	L	93	ASN
13	M	69	PRO
13	M	134	THR
14	N	59	SER
14	N	71	ARG
14	N	72	ASP
16	P	63	ILE
18	R	53	PHE
19	S	32	ALA
20	T	18	GLU
20	T	50	LEU
21	U	6	ARG
21	U	41	VAL
21	U	52	ASN
21	U	101	THR
24	X	17	ARG
26	Z	27	GLY
27	0	33	SER
28	1	50	GLU
5	E	45	ALA
6	F	68	LYS
6	F	69	ALA
6	F	83	PRO
6	F	86	CYS
7	G	92	GLY
7	G	170	THR
9	I	31	GLY
9	I	83	ALA
12	L	36	LYS
12	L	66	PHE
15	O	42	PRO
21	U	12	VAL
21	U	35	VAL
21	U	47	PRO
22	V	57	TYR
22	V	84	PRO
23	W	16	GLU
26	Z	29	ARG
26	Z	32	GLY
29	2	43	THR
4	D	44	GLY

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Mol	Chain	Res	Type
4	D	143	PRO
5	E	129	PRO
6	F	175	PRO
9	I	138	VAL
10	J	96	ARG
15	O	27	VAL
16	P	4	ILE
18	R	8	GLY
23	W	26	GLY
3	C	2	VAL
4	D	122	VAL
4	D	144	GLY
6	F	88	VAL
9	I	28	GLY
11	K	2	ILE
18	R	27	ILE
19	S	96	ILE
20	T	16	VAL
23	W	22	VAL
6	F	81	GLY
6	F	136	ILE
8	H	103	VAL
13	M	36	VAL
18	R	75	VAL
21	U	64	ILE
22	V	15	GLY
6	F	108	PRO
10	J	56	VAL
11	K	48	PRO
12	L	114	GLY
21	U	33	VAL
3	C	217	PRO
6	F	84	ILE
19	S	29	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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	C	216/218 (99%)	191 (88%)	25 (12%)	8	44
4	D	164/164 (100%)	144 (88%)	20 (12%)	7	41
5	E	165/165 (100%)	152 (92%)	13 (8%)	18	65
6	F	149/150 (99%)	124 (83%)	25 (17%)	3	24
7	G	137/138 (99%)	120 (88%)	17 (12%)	7	41
8	H	114/114 (100%)	95 (83%)	19 (17%)	3	24
9	I	109/110 (99%)	102 (94%)	7 (6%)	25	74
10	J	116/116 (100%)	106 (91%)	10 (9%)	15	62
11	K	103/104 (99%)	85 (82%)	18 (18%)	3	21
12	L	102/103 (99%)	90 (88%)	12 (12%)	8	43
13	M	109/109 (100%)	100 (92%)	9 (8%)	16	63
14	N	100/103 (97%)	85 (85%)	15 (15%)	4	30
15	O	86/87 (99%)	78 (91%)	8 (9%)	13	57
16	P	99/100 (99%)	91 (92%)	8 (8%)	17	64
17	Q	89/90 (99%)	79 (89%)	10 (11%)	9	46
18	R	84/84 (100%)	70 (83%)	14 (17%)	3	24
19	S	93/93 (100%)	79 (85%)	14 (15%)	4	30
20	T	80/84 (95%)	74 (92%)	6 (8%)	19	68
21	U	83/85 (98%)	72 (87%)	11 (13%)	6	37
22	V	78/78 (100%)	68 (87%)	10 (13%)	6	39
23	W	59/63 (94%)	44 (75%)	15 (25%)	1	8
24	X	67/68 (98%)	58 (87%)	9 (13%)	6	36
25	Y	55/55 (100%)	52 (94%)	3 (6%)	30	79
26	Z	48/49 (98%)	41 (85%)	7 (15%)	5	31
27	0	47/48 (98%)	42 (89%)	5 (11%)	10	49
28	1	45/49 (92%)	41 (91%)	4 (9%)	14	60
29	2	38/38 (100%)	34 (90%)	4 (10%)	10	49
30	3	51/52 (98%)	42 (82%)	9 (18%)	3	21
31	4	34/34 (100%)	29 (85%)	5 (15%)	4	31
All	All	2720/2751 (99%)	2388 (88%)	332 (12%)	7	41

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	18	VAL
3	C	23	LEU
3	C	35	LYS
3	C	51	ARG
3	C	53	ILE
3	C	57	HIS
3	C	62	ARG
3	C	90	ILE
3	C	102	TYR
3	C	124	LYS
3	C	129	LEU
3	C	152	GLN
3	C	172	THR
3	C	173	LEU
3	C	183	VAL
3	C	187	CYS
3	C	188	ARG
3	C	193	GLU
3	C	212	TRP
3	C	213	ARG
3	C	220	ARG
3	C	227	VAL
3	C	235	GLU
3	C	256	THR
3	C	269	ARG
4	D	24	VAL
4	D	28	GLU
4	D	33	ARG
4	D	35	THR
4	D	38	LYS
4	D	50	VAL
4	D	55	LYS
4	D	62	LYS
4	D	79	LEU
4	D	84	LEU
4	D	106	LYS
4	D	121	THR
4	D	138	LEU
4	D	141	ARG
4	D	148	GLN
4	D	150	GLN
4	D	159	LYS
4	D	168	GLU

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Mol	Chain	Res	Type
4	D	189	VAL
4	D	193	VAL
5	E	53	THR
5	E	57	LYS
5	E	67	ARG
5	E	77	ILE
5	E	108	ILE
5	E	117	ARG
5	E	126	VAL
5	E	139	LYS
5	E	149	ILE
5	E	157	LEU
5	E	163	ASN
5	E	164	LEU
5	E	166	LYS
6	F	13	LYS
6	F	47	LYS
6	F	48	LEU
6	F	49	LEU
6	F	76	PHE
6	F	82	TYR
6	F	94	ARG
6	F	97	GLU
6	F	109	ARG
6	F	110	ILE
6	F	111	ARG
6	F	113	PHE
6	F	119	LYS
6	F	131	VAL
6	F	133	GLU
6	F	134	GLN
6	F	135	ILE
6	F	139	GLU
6	F	142	TYR
6	F	147	ARG
6	F	151	LEU
6	F	160	LYS
6	F	166	ARG
6	F	172	PHE
6	F	177	ARG
7	G	2	ARG
7	G	18	ILE

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Mol	Chain	Res	Type
7	G	19	ASN
7	G	21	GLN
7	G	34	ARG
7	G	35	THR
7	G	40	VAL
7	G	51	PHE
7	G	72	ASN
7	G	84	LYS
7	G	91	VAL
7	G	93	TYR
7	G	120	ILE
7	G	162	ARG
7	G	163	TYR
7	G	166	GLU
7	G	176	LYS
8	H	8	LYS
8	H	22	LYS
8	H	25	TYR
8	H	27	ARG
8	H	28	ASN
8	H	48	GLU
8	H	50	ARG
8	H	57	LYS
8	H	66	ASN
8	H	68	ARG
8	H	76	GLU
8	H	86	ASP
8	H	90	LEU
8	H	91	PHE
8	H	103	VAL
8	H	104	THR
8	H	109	GLU
8	H	132	PHE
8	H	144	VAL
9	I	7	TYR
9	I	9	LYS
9	I	16	MET
9	I	30	GLN
9	I	58	ILE
9	I	68	PHE
9	I	93	ASN
10	J	3	THR

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Mol	Chain	Res	Type
10	J	25	LEU
10	J	43	GLU
10	J	47	HIS
10	J	54	ILE
10	J	57	LEU
10	J	95	ARG
10	J	106	LYS
10	J	129	GLU
10	J	139	VAL
11	K	3	GLN
11	K	7	MET
11	K	10	VAL
11	K	13	ASN
11	K	21	CYS
11	K	25	LEU
11	K	39	ILE
11	K	41	ILE
11	K	47	ILE
11	K	49	ARG
11	K	54	LYS
11	K	87	LEU
11	K	103	VAL
11	K	105	ARG
11	K	106	GLU
11	K	107	LEU
11	K	111	LYS
11	K	114	LYS
12	L	3	LEU
12	L	4	ASN
12	L	47	ARG
12	L	79	LEU
12	L	82	LEU
12	L	92	LEU
12	L	99	ASN
12	L	103	ILE
12	L	111	ILE
12	L	112	LEU
12	L	141	LYS
12	L	143	GLU
13	M	8	LYS
13	M	50	ARG
13	M	78	LEU

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Mol	Chain	Res	Type
13	M	96	ILE
13	M	97	GLN
13	M	102	LEU
13	M	105	MET
13	M	115	GLU
13	M	126	ILE
14	N	14	SER
14	N	18	GLN
14	N	20	MET
14	N	29	VAL
14	N	33	ILE
14	N	53	THR
14	N	54	LEU
14	N	62	ASN
14	N	63	ARG
14	N	69	ARG
14	N	81	ASN
14	N	94	TYR
14	N	95	THR
14	N	98	LEU
14	N	114	GLU
15	O	17	LYS
15	O	30	ARG
15	O	31	THR
15	O	65	THR
15	O	68	LYS
15	O	90	VAL
15	O	115	LEU
15	O	117	PHE
16	P	6	GLN
16	P	13	LYS
16	P	28	LYS
16	P	31	VAL
16	P	83	ILE
16	P	86	LYS
16	P	95	LYS
16	P	101	GLU
17	Q	3	VAL
17	Q	10	ARG
17	Q	12	ARG
17	Q	35	PHE
17	Q	50	ARG

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Mol	Chain	Res	Type
17	Q	54	ARG
17	Q	57	ARG
17	Q	63	ARG
17	Q	69	ARG
17	Q	79	ILE
18	R	6	GLN
18	R	10	LYS
18	R	13	ARG
18	R	37	GLU
18	R	48	LYS
18	R	58	VAL
18	R	75	VAL
18	R	80	ARG
18	R	81	LYS
18	R	83	TYR
18	R	86	GLN
18	R	90	ARG
18	R	93	PHE
18	R	95	ASP
19	S	6	LYS
19	S	22	ASP
19	S	23	LEU
19	S	31	GLN
19	S	45	VAL
19	S	46	LEU
19	S	66	ILE
19	S	70	LYS
19	S	74	ILE
19	S	76	VAL
19	S	84	ARG
19	S	85	ILE
19	S	86	MET
19	S	88	ARG
20	T	9	LYS
20	T	12	ARG
20	T	18	GLU
20	T	39	THR
20	T	50	LEU
20	T	54	GLU
21	U	13	LEU
21	U	14	THR
21	U	20	LYS

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Mol	Chain	Res	Type
21	U	21	ARG
21	U	40	LEU
21	U	45	GLN
21	U	81	ARG
21	U	82	VAL
21	U	85	ARG
21	U	94	PHE
21	U	95	PHE
22	V	26	PHE
22	V	40	ILE
22	V	51	GLN
22	V	61	LEU
22	V	65	VAL
22	V	69	GLU
22	V	70	ILE
22	V	76	ASP
22	V	77	VAL
22	V	90	ASP
23	W	18	LYS
23	W	20	LEU
23	W	22	VAL
23	W	23	LYS
23	W	25	PHE
23	W	30	VAL
23	W	37	VAL
23	W	38	ARG
23	W	39	GLN
23	W	40	ARG
23	W	44	PHE
23	W	58	LEU
23	W	68	PHE
23	W	76	ARG
23	W	77	LYS
24	X	5	GLN
24	X	26	ARG
24	X	31	ASN
24	X	33	HIS
24	X	46	VAL
24	X	47	THR
24	X	57	VAL
24	X	63	ILE
24	X	73	ARG

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Mol	Chain	Res	Type
25	Y	1	MET
25	Y	4	LYS
25	Y	28	LEU
26	Z	16	LEU
26	Z	24	LEU
26	Z	28	LEU
26	Z	29	ARG
26	Z	50	VAL
26	Z	53	MET
26	Z	55	LYS
27	0	3	GLN
27	0	5	ASN
27	0	41	HIS
27	0	42	ILE
27	0	49	ARG
28	1	10	LEU
28	1	20	TYR
28	1	35	LEU
28	1	44	GLN
29	2	8	SER
29	2	22	MET
29	2	26	ASN
29	2	33	ARG
30	3	12	ARG
30	3	14	LYS
30	3	27	ASN
30	3	29	ARG
30	3	41	ARG
30	3	46	LYS
30	3	48	MET
30	3	51	LYS
30	3	61	LEU
31	4	2	LYS
31	4	9	LYS
31	4	13	ASN
31	4	15	LYS
31	4	17	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2838/2903 (97%)	1020 (35%)	505 (17%)
2	B	116/117 (99%)	29 (25%)	13 (11%)
All	All	2954/3020 (97%)	1049 (35%)	518 (17%)

All (1049) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	15	G
1	A	16	C
1	A	34	U
1	A	35	G
1	A	36	G
1	A	37	C
1	A	39	G
1	A	40	U
1	A	46	G
1	A	49	A
1	A	50	U
1	A	51	G
1	A	52	A
1	A	53	A
1	A	60	G
1	A	61	C
1	A	62	U
1	A	70	G
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	76	C
1	A	77	G
1	A	79	C
1	A	83	A
1	A	84	A
1	A	85	G
1	A	86	G
1	A	87	U
1	A	91	A
1	A	92	U
1	A	93	G

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Mol	Chain	Res	Type
1	A	100	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	104	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	121	G
1	A	122	G
1	A	126	A
1	A	128	C
1	A	129	C
1	A	134	G
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	143	C
1	A	144	A
1	A	155	A
1	A	156	A
1	A	160	A
1	A	162	U
1	A	164	C
1	A	165	A
1	A	171	U
1	A	180	G
1	A	181	A
1	A	193	U
1	A	196	A
1	A	197	A
1	A	198	C
1	A	199	A
1	A	204	A
1	A	205	G
1	A	206	U
1	A	207	A
1	A	216	A
1	A	217	A
1	A	218	A
1	A	221	A

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Mol	Chain	Res	Type
1	A	222	A
1	A	223	A
1	A	224	U
1	A	225	C
1	A	226	A
1	A	227	A
1	A	228	C
1	A	229	C
1	A	230	G
1	A	231	A
1	A	233	A
1	A	234	U
1	A	235	U
1	A	241	A
1	A	242	G
1	A	243	U
1	A	244	A
1	A	245	G
1	A	248	G
1	A	249	C
1	A	250	G
1	A	251	A
1	A	252	G
1	A	255	A
1	A	264	C
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	273	G
1	A	277	G
1	A	281	C
1	A	284	U
1	A	285	G
1	A	295	G
1	A	299	A
1	A	301	G
1	A	302	C
1	A	303	G
1	A	311	A
1	A	312	G
1	A	314	C

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Mol	Chain	Res	Type
1	A	315	G
1	A	322	A
1	A	323	C
1	A	324	A
1	A	325	G
1	A	326	G
1	A	329	G
1	A	330	A
1	A	334	C
1	A	335	C
1	A	343	C
1	A	351	C
1	A	353	C
1	A	362	A
1	A	363	G
1	A	364	C
1	A	365	U
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	374	A
1	A	375	G
1	A	383	C
1	A	386	G
1	A	387	U
1	A	388	G
1	A	389	G
1	A	390	U
1	A	391	A
1	A	392	U
1	A	396	G
1	A	397	U
1	A	398	C
1	A	399	U
1	A	404	A
1	A	405	U
1	A	406	G
1	A	407	G
1	A	411	G
1	A	412	A
1	A	413	C

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Mol	Chain	Res	Type
1	A	421	C
1	A	422	A
1	A	423	A
1	A	424	G
1	A	430	A
1	A	437	U
1	A	442	G
1	A	443	A
1	A	444	C
1	A	445	C
1	A	446	G
1	A	447	A
1	A	449	A
1	A	450	G
1	A	451	U
1	A	452	G
1	A	455	C
1	A	457	A
1	A	459	U
1	A	460	A
1	A	461	C
1	A	462	C
1	A	475	C
1	A	476	G
1	A	477	A
1	A	479	A
1	A	480	A
1	A	481	G
1	A	482	A
1	A	489	G
1	A	490	C
1	A	491	G
1	A	492	A
1	A	498	G
1	A	502	A
1	A	503	A
1	A	504	A
1	A	505	A
1	A	506	G
1	A	507	A
1	A	509	C
1	A	510	C

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Mol	Chain	Res	Type
1	A	511	U
1	A	512	G
1	A	527	C
1	A	528	A
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	534	U
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	556	A
1	A	563	A
1	A	571	U
1	A	572	A
1	A	573	U
1	A	575	A
1	A	576	U
1	A	586	A
1	A	587	C
1	A	589	U
1	A	590	A
1	A	603	A
1	A	604	G
1	A	605	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	G
1	A	620	G
1	A	621	A
1	A	622	G
1	A	627	A
1	A	638	G
1	A	639	U
1	A	645	C

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Mol	Chain	Res	Type
1	A	647	G
1	A	648	G
1	A	654	A
1	A	655	A
1	A	656	G
1	A	657	U
1	A	658	U
1	A	662	G
1	A	669	G
1	A	670	A
1	A	671	C
1	A	672	C
1	A	673	C
1	A	686	U
1	A	687	C
1	A	688	U
1	A	699	A
1	A	717	C
1	A	718	A
1	A	727	A
1	A	728	G
1	A	729	G
1	A	730	A
1	A	740	C
1	A	741	U
1	A	746	U
1	A	747	U
1	A	748	G
1	A	752	A
1	A	753	A
1	A	754	U
1	A	755	U
1	A	757	G
1	A	763	G
1	A	764	A
1	A	765	C
1	A	766	U
1	A	775	G
1	A	776	G
1	A	777	G
1	A	778	G
1	A	779	U

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Mol	Chain	Res	Type
1	A	781	A
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	790	U
1	A	791	C
1	A	792	A
1	A	793	A
1	A	794	A
1	A	795	C
1	A	800	A
1	A	801	G
1	A	802	A
1	A	803	U
1	A	805	G
1	A	806	C
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	832	U
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	861	A
1	A	866	A
1	A	867	C
1	A	868	U
1	A	874	G
1	A	875	G
1	A	877	A
1	A	878	A
1	A	902	C
1	A	910	A
1	A	912	C
1	A	914	G
1	A	915	C

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Mol	Chain	Res	Type
1	A	916	G
1	A	921	C
1	A	922	C
1	A	932	U
1	A	933	A
1	A	934	U
1	A	941	A
1	A	944	C
1	A	946	C
1	A	947	A
1	A	958	U
1	A	959	A
1	A	960	A
1	A	961	C
1	A	962	G
1	A	964	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	976	G
1	A	983	A
1	A	985	C
1	A	990	A
1	A	991	C
1	A	995	C
1	A	996	A
1	A	1008	A
1	A	1009	A
1	A	1010	A
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1014	A
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1027	A
1	A	1033	U

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Mol	Chain	Res	Type
1	A	1034	G
1	A	1035	U
1	A	1036	G
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1049	C
1	A	1050	A
1	A	1056	G
1	A	1057	A
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1064	C
1	A	1066	U
1	A	1068	G
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1074	G
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1080	A
1	A	1083	U
1	A	1086	A
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1091	G
1	A	1097	U
1	A	1100	C
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1114	C
1	A	1115	G
1	A	1126	A
1	A	1127	A

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Mol	Chain	Res	Type
1	A	1128	G
1	A	1129	A
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1142	A
1	A	1144	A
1	A	1145	C
1	A	1155	A
1	A	1157	G
1	A	1158	C
1	A	1159	U
1	A	1169	A
1	A	1171	G
1	A	1172	C
1	A	1174	U
1	A	1176	U
1	A	1204	A
1	A	1205	A
1	A	1206	G
1	A	1207	C
1	A	1211	C
1	A	1213	A
1	A	1214	A
1	A	1227	G
1	A	1235	G
1	A	1236	G
1	A	1237	A
1	A	1241	A
1	A	1242	U
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1255	U
1	A	1256	G
1	A	1262	A
1	A	1265	A
1	A	1266	G

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Mol	Chain	Res	Type
1	A	1267	U
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1274	A
1	A	1275	A
1	A	1276	A
1	A	1277	G
1	A	1278	C
1	A	1286	A
1	A	1290	C
1	A	1291	C
1	A	1300	G
1	A	1301	A
1	A	1303	G
1	A	1304	A
1	A	1311	G
1	A	1313	U
1	A	1314	C
1	A	1315	C
1	A	1321	A
1	A	1324	G
1	A	1325	U
1	A	1326	U
1	A	1327	A
1	A	1328	A
1	A	1329	U
1	A	1330	C
1	A	1331	G
1	A	1332	G
1	A	1333	G
1	A	1334	G
1	A	1336	A
1	A	1337	G
1	A	1340	U
1	A	1341	G
1	A	1342	A
1	A	1345	C
1	A	1349	C
1	A	1365	A
1	A	1374	G

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Mol	Chain	Res	Type
1	A	1376	C
1	A	1379	U
1	A	1381	G
1	A	1382	G
1	A	1385	A
1	A	1386	C
1	A	1387	A
1	A	1397	U
1	A	1398	C
1	A	1399	C
1	A	1400	U
1	A	1401	G
1	A	1403	A
1	A	1404	C
1	A	1416	G
1	A	1419	A
1	A	1421	G
1	A	1426	G
1	A	1428	C
1	A	1430	G
1	A	1434	A
1	A	1438	U
1	A	1440	U
1	A	1452	G
1	A	1453	A
1	A	1454	C
1	A	1455	G
1	A	1456	G
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1462	C
1	A	1463	C
1	A	1470	A
1	A	1475	G
1	A	1476	U
1	A	1477	A
1	A	1478	G
1	A	1479	G
1	A	1482	G
1	A	1483	G
1	A	1490	A

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Mol	Chain	Res	Type
1	A	1493	C
1	A	1494	A
1	A	1497	U
1	A	1498	C
1	A	1499	C
1	A	1501	G
1	A	1507	C
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1511	G
1	A	1512	C
1	A	1520	U
1	A	1522	A
1	A	1523	U
1	A	1524	G
1	A	1528	A
1	A	1531	C
1	A	1532	A
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1540	G
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1561	C
1	A	1562	U
1	A	1565	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1598	A

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Mol	Chain	Res	Type
1	A	1600	C
1	A	1603	A
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1611	C
1	A	1612	C
1	A	1613	G
1	A	1616	A
1	A	1617	C
1	A	1620	G
1	A	1622	G
1	A	1626	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1640	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1650	A
1	A	1654	A
1	A	1655	A
1	A	1663	G
1	A	1667	G
1	A	1668	A
1	A	1669	A
1	A	1670	C
1	A	1674	G
1	A	1675	C
1	A	1676	A
1	A	1677	A
1	A	1680	U
1	A	1682	G
1	A	1683	U
1	A	1684	G
1	A	1694	C
1	A	1695	G
1	A	1696	G
1	A	1697	G
1	A	1698	A

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Mol	Chain	Res	Type
1	A	1699	G
1	A	1700	A
1	A	1701	A
1	A	1706	C
1	A	1707	G
1	A	1713	A
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1717	A
1	A	1718	G
1	A	1722	A
1	A	1723	G
1	A	1728	C
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1734	G
1	A	1735	A
1	A	1739	A
1	A	1740	G
1	A	1758	U
1	A	1759	A
1	A	1760	C
1	A	1761	C
1	A	1764	C
1	A	1773	A
1	A	1774	C
1	A	1776	G
1	A	1780	A
1	A	1781	U
1	A	1782	U
1	A	1783	A
1	A	1784	A
1	A	1785	A
1	A	1786	A
1	A	1788	C
1	A	1789	A
1	A	1800	C
1	A	1802	A

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Mol	Chain	Res	Type
1	A	1808	A
1	A	1809	A
1	A	1810	A
1	A	1811	G
1	A	1815	A
1	A	1816	C
1	A	1817	G
1	A	1819	A
1	A	1820	U
1	A	1821	A
1	A	1822	C
1	A	1829	A
1	A	1832	C
1	A	1833	C
1	A	1835	G
1	A	1839	G
1	A	1840	G
1	A	1847	A
1	A	1848	A
1	A	1857	G
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1873	G
1	A	1875	G
1	A	1877	A
1	A	1884	G
1	A	1886	U
1	A	1889	A
1	A	1906	G
1	A	1912	A
1	A	1914	C
1	A	1915	U
1	A	1916	A
1	A	1917	U
1	A	1919	A
1	A	1920	C
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1932	A

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Mol	Chain	Res	Type
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1941	C
1	A	1942	C
1	A	1943	U
1	A	1944	U
1	A	1945	G
1	A	1946	U
1	A	1954	G
1	A	1955	U
1	A	1956	U
1	A	1957	C
1	A	1963	U
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1968	G
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1980	G
1	A	1981	A
1	A	1982	U
1	A	1983	G
1	A	1991	U
1	A	1993	U
1	A	1994	C
1	A	1996	C
1	A	1997	C
1	A	1998	A
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2024	G
1	A	2030	A
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U

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Mol	Chain	Res	Type
1	A	2035	G
1	A	2036	C
1	A	2037	A
1	A	2038	G
1	A	2043	C
1	A	2050	C
1	A	2051	A
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2064	C
1	A	2068	U
1	A	2069	G
1	A	2070	A
1	A	2072	C
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2094	A
1	A	2100	G
1	A	2104	C
1	A	2105	U
1	A	2107	G
1	A	2108	A
1	A	2109	U
1	A	2110	G
1	A	2134	A
1	A	2135	A
1	A	2136	G
1	A	2138	G
1	A	2143	C
1	A	2144	G
1	A	2145	C
1	A	2147	A
1	A	2148	G
1	A	2149	U
1	A	2152	G
1	A	2153	C

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Mol	Chain	Res	Type
1	A	2154	A
1	A	2155	U
1	A	2156	G
1	A	2157	G
1	A	2180	U
1	A	2181	U
1	A	2183	A
1	A	2187	U
1	A	2190	G
1	A	2191	A
1	A	2192	U
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2204	G
1	A	2210	U
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2214	C
1	A	2215	C
1	A	2216	G
1	A	2226	C
1	A	2227	A
1	A	2238	G
1	A	2239	G
1	A	2240	U
1	A	2241	A
1	A	2249	U
1	A	2250	G
1	A	2251	G
1	A	2252	G
1	A	2259	U
1	A	2260	C
1	A	2261	C
1	A	2266	A
1	A	2267	A
1	A	2268	A
1	A	2275	C
1	A	2279	G
1	A	2283	C
1	A	2284	A

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Mol	Chain	Res	Type
1	A	2286	G
1	A	2288	A
1	A	2289	G
1	A	2290	G
1	A	2297	A
1	A	2298	A
1	A	2305	U
1	A	2308	G
1	A	2309	A
1	A	2310	C
1	A	2311	A
1	A	2312	U
1	A	2313	C
1	A	2314	A
1	A	2320	U
1	A	2321	U
1	A	2322	A
1	A	2323	G
1	A	2325	G
1	A	2334	U
1	A	2335	A
1	A	2337	G
1	A	2338	C
1	A	2339	C
1	A	2345	G
1	A	2347	C
1	A	2348	U
1	A	2357	G
1	A	2358	A
1	A	2361	G
1	A	2379	G
1	A	2382	G
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2386	A
1	A	2387	U
1	A	2392	A
1	A	2399	G
1	A	2401	U
1	A	2402	U
1	A	2403	C

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Mol	Chain	Res	Type
1	A	2405	G
1	A	2406	A
1	A	2407	A
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2424	C
1	A	2425	A
1	A	2426	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2450	A
1	A	2457	U
1	A	2459	A
1	A	2460	U
1	A	2461	A
1	A	2468	A
1	A	2475	C
1	A	2476	A
1	A	2490	G
1	A	2491	U
1	A	2492	U
1	A	2493	U
1	A	2494	G
1	A	2498	C
1	A	2499	C
1	A	2500	U
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2517	C

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Mol	Chain	Res	Type
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2521	C
1	A	2522	U
1	A	2529	G
1	A	2534	A
1	A	2543	G
1	A	2544	G
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2576	G
1	A	2578	G
1	A	2582	G
1	A	2583	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2604	U
1	A	2609	U
1	A	2610	C
1	A	2611	C
1	A	2612	C
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2616	C
1	A	2617	U
1	A	2629	U
1	A	2630	G
1	A	2631	G
1	A	2632	A
1	A	2645	G
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2656	U

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Mol	Chain	Res	Type
1	A	2657	A
1	A	2667	C
1	A	2682	A
1	A	2683	C
1	A	2689	U
1	A	2690	U
1	A	2691	C
1	A	2692	G
1	A	2713	U
1	A	2714	G
1	A	2715	C
1	A	2718	G
1	A	2726	A
1	A	2727	A
1	A	2728	U
1	A	2739	U
1	A	2748	A
1	A	2751	G
1	A	2752	C
1	A	2753	A
1	A	2756	U
1	A	2757	A
1	A	2758	A
1	A	2760	C
1	A	2765	A
1	A	2766	A
1	A	2777	G
1	A	2778	A
1	A	2779	U
1	A	2781	A
1	A	2782	G
1	A	2791	G
1	A	2796	U
1	A	2799	A
1	A	2800	A
1	A	2801	G
1	A	2808	G
1	A	2820	A
1	A	2826	A
1	A	2833	U
1	A	2834	G
1	A	2835	A

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Mol	Chain	Res	Type
1	A	2836	U
1	A	2837	A
1	A	2838	G
1	A	2848	G
1	A	2850	A
1	A	2851	A
1	A	2861	U
1	A	2866	U
1	A	2867	G
1	A	2872	A
1	A	2874	C
1	A	2875	C
1	A	2879	A
1	A	2883	A
1	A	2894	G
1	A	2895	G
1	A	2896	C
1	A	2902	C
2	B	12	C
2	B	13	G
2	B	15	A
2	B	16	G
2	B	17	C
2	B	18	G
2	B	24	G
2	B	30	C
2	B	35	C
2	B	36	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	46	A
2	B	48	U
2	B	57	A
2	B	58	A
2	B	63	C
2	B	64	G
2	B	87	U
2	B	88	C

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Mol	Chain	Res	Type
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	109	A

All (518) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	33	C
1	A	35	G
1	A	50	U
1	A	52	A
1	A	61	C
1	A	70	G
1	A	73	A
1	A	74	A
1	A	75	G
1	A	76	C
1	A	84	A
1	A	85	G
1	A	86	G
1	A	87	U
1	A	91	A
1	A	92	U
1	A	93	G
1	A	100	U
1	A	103	A
1	A	104	A
1	A	119	A
1	A	121	G
1	A	122	G
1	A	125	A
1	A	128	C
1	A	140	C
1	A	141	G
1	A	142	A
1	A	164	C
1	A	179	C

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Mol	Chain	Res	Type
1	A	196	A
1	A	197	A
1	A	204	A
1	A	206	U
1	A	207	A
1	A	215	G
1	A	216	A
1	A	222	A
1	A	223	A
1	A	224	U
1	A	225	C
1	A	227	A
1	A	229	C
1	A	230	G
1	A	232	G
1	A	234	U
1	A	241	A
1	A	243	U
1	A	244	A
1	A	249	C
1	A	250	G
1	A	251	A
1	A	271	G
1	A	272	A
1	A	301	G
1	A	302	C
1	A	303	G
1	A	311	A
1	A	312	G
1	A	321	U
1	A	324	A
1	A	325	G
1	A	329	G
1	A	333	G
1	A	334	C
1	A	364	C
1	A	370	G
1	A	374	A
1	A	386	G
1	A	388	G
1	A	389	G
1	A	390	U

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Mol	Chain	Res	Type
1	A	391	A
1	A	395	U
1	A	396	G
1	A	397	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	412	A
1	A	421	C
1	A	422	A
1	A	423	A
1	A	436	C
1	A	437	U
1	A	442	G
1	A	444	C
1	A	445	C
1	A	446	G
1	A	449	A
1	A	454	A
1	A	459	U
1	A	474	G
1	A	475	C
1	A	476	G
1	A	479	A
1	A	480	A
1	A	482	A
1	A	483	A
1	A	489	G
1	A	491	G
1	A	503	A
1	A	505	A
1	A	506	G
1	A	509	C
1	A	510	C
1	A	527	C
1	A	528	A
1	A	529	A
1	A	530	G
1	A	531	C
1	A	533	G
1	A	571	U
1	A	572	A

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Mol	Chain	Res	Type
1	A	575	A
1	A	588	U
1	A	589	U
1	A	603	A
1	A	604	G
1	A	605	G
1	A	616	A
1	A	620	G
1	A	621	A
1	A	637	A
1	A	638	G
1	A	647	G
1	A	655	A
1	A	656	G
1	A	657	U
1	A	670	A
1	A	672	C
1	A	685	A
1	A	687	C
1	A	726	G
1	A	730	A
1	A	752	A
1	A	753	A
1	A	754	U
1	A	762	U
1	A	763	G
1	A	765	C
1	A	766	U
1	A	775	G
1	A	777	G
1	A	778	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	791	C
1	A	792	A
1	A	794	A
1	A	800	A
1	A	802	A
1	A	830	G

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Mol	Chain	Res	Type
1	A	831	G
1	A	858	G
1	A	860	U
1	A	865	C
1	A	867	C
1	A	913	U
1	A	915	C
1	A	933	A
1	A	945	A
1	A	946	C
1	A	947	A
1	A	957	C
1	A	958	U
1	A	959	A
1	A	963	U
1	A	973	A
1	A	975	A
1	A	984	A
1	A	989	G
1	A	990	A
1	A	991	C
1	A	1008	A
1	A	1009	A
1	A	1010	A
1	A	1011	G
1	A	1013	C
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1035	U
1	A	1046	A
1	A	1048	A
1	A	1049	C
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1069	A

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Mol	Chain	Res	Type
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1089	A
1	A	1090	A
1	A	1110	G
1	A	1112	G
1	A	1113	U
1	A	1126	A
1	A	1129	A
1	A	1130	U
1	A	1131	G
1	A	1135	C
1	A	1136	G
1	A	1141	U
1	A	1144	A
1	A	1156	A
1	A	1157	G
1	A	1158	C
1	A	1204	A
1	A	1206	G
1	A	1210	G
1	A	1213	A
1	A	1236	G
1	A	1247	A
1	A	1249	U
1	A	1256	G
1	A	1265	A
1	A	1267	U
1	A	1272	A
1	A	1274	A
1	A	1275	A
1	A	1276	A
1	A	1277	G
1	A	1286	A
1	A	1289	C
1	A	1290	C
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1303	G
1	A	1312	U
1	A	1313	U
1	A	1314	C
1	A	1325	U
1	A	1326	U
1	A	1327	A
1	A	1330	C
1	A	1333	G
1	A	1340	U
1	A	1341	G
1	A	1345	C
1	A	1385	A
1	A	1386	C
1	A	1395	A
1	A	1399	C
1	A	1427	A
1	A	1429	G
1	A	1451	C
1	A	1455	G
1	A	1460	U
1	A	1462	C
1	A	1475	G
1	A	1476	U
1	A	1477	A
1	A	1478	G
1	A	1497	U
1	A	1498	C
1	A	1508	A
1	A	1510	G
1	A	1511	G
1	A	1536	C
1	A	1537	G
1	A	1539	U
1	A	1554	U
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1560	G
1	A	1561	C
1	A	1566	A
1	A	1568	G

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Mol	Chain	Res	Type
1	A	1569	A
1	A	1607	C
1	A	1611	C
1	A	1612	C
1	A	1616	A
1	A	1619	G
1	A	1634	A
1	A	1635	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1667	G
1	A	1669	A
1	A	1676	A
1	A	1681	G
1	A	1682	G
1	A	1683	U
1	A	1693	U
1	A	1695	G
1	A	1696	G
1	A	1698	A
1	A	1700	A
1	A	1713	A
1	A	1716	U
1	A	1717	A
1	A	1722	A
1	A	1731	G
1	A	1733	G
1	A	1734	G
1	A	1738	G
1	A	1739	A
1	A	1758	U
1	A	1759	A
1	A	1760	C
1	A	1780	A
1	A	1783	A
1	A	1784	A
1	A	1785	A
1	A	1786	A
1	A	1787	A
1	A	1788	C

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Mol	Chain	Res	Type
1	A	1799	G
1	A	1802	A
1	A	1808	A
1	A	1809	A
1	A	1810	A
1	A	1815	A
1	A	1816	C
1	A	1819	A
1	A	1838	C
1	A	1839	G
1	A	1857	G
1	A	1913	A
1	A	1914	C
1	A	1915	U
1	A	1916	A
1	A	1929	G
1	A	1931	U
1	A	1937	A
1	A	1941	C
1	A	1942	C
1	A	1943	U
1	A	1945	G
1	A	1954	G
1	A	1956	U
1	A	1962	C
1	A	1963	U
1	A	1964	G
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1980	G
1	A	1981	A
1	A	1982	U
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	C
1	A	2021	C
1	A	2023	C
1	A	2024	G

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Mol	Chain	Res	Type
1	A	2031	A
1	A	2034	U
1	A	2036	C
1	A	2037	A
1	A	2051	A
1	A	2061	G
1	A	2063	C
1	A	2064	C
1	A	2067	G
1	A	2068	U
1	A	2069	G
1	A	2092	U
1	A	2093	G
1	A	2135	A
1	A	2148	G
1	A	2179	C
1	A	2198	A
1	A	2199	A
1	A	2210	U
1	A	2214	C
1	A	2215	C
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2240	U
1	A	2249	U
1	A	2251	G
1	A	2258	C
1	A	2259	U
1	A	2260	C
1	A	2266	A
1	A	2267	A
1	A	2282	G
1	A	2283	C
1	A	2288	A
1	A	2289	G
1	A	2296	U
1	A	2297	A
1	A	2310	C
1	A	2311	A
1	A	2313	C

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Mol	Chain	Res	Type
1	A	2322	A
1	A	2334	U
1	A	2336	A
1	A	2337	G
1	A	2338	C
1	A	2344	U
1	A	2347	C
1	A	2382	G
1	A	2383	G
1	A	2386	A
1	A	2391	G
1	A	2401	U
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2408	U
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2439	A
1	A	2440	C
1	A	2447	G
1	A	2450	A
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2490	G
1	A	2492	U
1	A	2493	U
1	A	2497	A
1	A	2498	C
1	A	2499	C
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2518	A
1	A	2520	C
1	A	2521	C
1	A	2542	A
1	A	2543	G
1	A	2544	G
1	A	2566	A

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Mol	Chain	Res	Type
1	A	2572	A
1	A	2573	C
1	A	2581	G
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2601	C
1	A	2603	G
1	A	2610	C
1	A	2611	C
1	A	2613	U
1	A	2615	U
1	A	2616	C
1	A	2629	U
1	A	2630	G
1	A	2645	G
1	A	2654	A
1	A	2656	U
1	A	2657	A
1	A	2681	C
1	A	2682	A
1	A	2689	U
1	A	2691	C
1	A	2713	U
1	A	2714	G
1	A	2726	A
1	A	2727	A
1	A	2728	U
1	A	2750	A
1	A	2752	C
1	A	2756	U
1	A	2757	A
1	A	2776	A
1	A	2777	G
1	A	2778	A
1	A	2781	A
1	A	2782	G
1	A	2798	U
1	A	2800	A
1	A	2837	A
1	A	2848	G
1	A	2850	A

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Mol	Chain	Res	Type
1	A	2866	U
1	A	2867	G
1	A	2873	A
1	A	2874	C
1	A	2875	C
1	A	2893	A
1	A	2894	G
1	A	2895	G
1	A	2896	C
1	A	2902	C
2	B	12	C
2	B	13	G
2	B	16	G
2	B	17	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	43	C
2	B	45	A
2	B	56	G
2	B	58	A
2	B	87	U
2	B	90	C

## 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 ⓘ

Of 138 ligands modelled in this entry, 138 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2841/2903 (97%)	0.68	256 (9%) 10 9	132, 200, 303, 402	0
2	B	117/117 (100%)	0.94	18 (15%) 3 4	219, 294, 300, 302	0
3	C	271/273 (99%)	0.74	35 (12%) 4 5	133, 157, 179, 190	0
4	D	209/209 (100%)	0.67	24 (11%) 5 6	147, 200, 232, 242	0
5	E	201/201 (100%)	0.54	20 (9%) 8 8	154, 282, 335, 351	0
6	F	178/179 (99%)	1.63	67 (37%) 1 1	307, 314, 321, 323	0
7	G	176/177 (99%)	1.09	41 (23%) 1 2	186, 221, 245, 259	0
8	H	149/149 (100%)	0.26	8 (5%) 25 16	186, 240, 256, 260	0
9	I	141/142 (99%)	1.57	36 (25%) 1 2	367, 394, 412, 419	0
10	J	142/142 (100%)	0.83	26 (18%) 2 3	161, 201, 223, 233	0
11	K	122/123 (99%)	0.83	17 (13%) 4 4	151, 171, 189, 198	0
12	L	143/144 (99%)	1.34	45 (31%) 1 2	166, 240, 288, 297	0
13	M	136/136 (100%)	1.18	30 (22%) 1 2	144, 181, 210, 232	0
14	N	120/127 (94%)	1.59	35 (29%) 1 2	183, 222, 252, 266	0
15	O	116/117 (99%)	2.05	57 (49%) 1 1	286, 293, 297, 303	0
16	P	114/115 (99%)	1.19	25 (21%) 1 2	179, 203, 220, 230	0
17	Q	117/118 (99%)	1.43	34 (29%) 1 2	184, 211, 240, 247	0
18	R	103/103 (100%)	0.82	18 (17%) 2 3	173, 249, 271, 277	0
19	S	110/110 (100%)	1.89	45 (40%) 1 1	159, 223, 269, 278	0
20	T	93/100 (93%)	1.10	18 (19%) 2 2	206, 253, 285, 294	0
21	U	102/104 (98%)	1.31	27 (26%) 1 2	272, 312, 355, 358	0
22	V	94/94 (100%)	1.34	28 (29%) 1 2	228, 241, 252, 254	0
23	W	79/85 (92%)	1.42	21 (26%) 1 2	156, 216, 233, 252	0
24	X	77/78 (98%)	1.25	16 (20%) 1 2	157, 185, 209, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	63/63 (100%)	0.92	11 (17%) 2 3	264, 288, 316, 329	0
26	Z	58/59 (98%)	0.38	3 (5%) 26 17	188, 215, 238, 248	0
27	0	56/57 (98%)	0.88	10 (17%) 2 3	157, 230, 260, 265	0
28	1	50/55 (90%)	0.79	9 (18%) 2 3	174, 207, 228, 238	0
29	2	46/46 (100%)	1.54	16 (34%) 1 1	155, 182, 198, 202	0
30	3	64/65 (98%)	2.68	37 (57%) 0 1	180, 194, 211, 215	0
31	4	38/38 (100%)	1.63	11 (28%) 1 2	171, 187, 198, 203	0
All	All	6326/6429 (98%)	0.93	1044 (16%) 2 3	132, 211, 321, 419	0

All (1044) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	8	VAL	15.5
9	I	9	LYS	15.4
22	V	42	LEU	11.0
6	F	157	THR	10.6
1	A	1067	A	9.7
12	L	75	ALA	9.2
30	3	20	GLY	9.1
6	F	129	MET	8.8
1	A	914	G	8.6
30	3	22	LYS	8.4
7	G	171	LYS	8.1
1	A	1030	C	7.8
6	F	116	LEU	7.8
15	O	24	THR	7.6
21	U	31	GLY	7.6
9	I	3	LYS	7.4
1	A	1104	C	7.4
7	G	151	ARG	7.4
30	3	48	MET	7.4
22	V	43	ASP	7.2
22	V	33	GLY	7.1
21	U	69	VAL	7.0
10	J	2	LYS	7.0
31	4	11	CYS	7.0
30	3	47	ALA	6.9
21	U	32	LYS	6.9
15	O	56	LYS	6.8
23	W	18	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
7	G	170	THR	6.7
1	A	1547	C	6.7
6	F	125	GLY	6.7
30	3	15	LYS	6.7
4	D	197	THR	6.7
14	N	58	ASP	6.7
15	O	60	GLU	6.6
7	G	166	GLU	6.6
2	B	69	G	6.6
19	S	31	GLN	6.6
28	1	23	THR	6.6
6	F	155	ILE	6.5
8	H	1	MET	6.4
2	B	41	G	6.4
1	A	1002	G	6.4
27	0	24	VAL	6.3
30	3	35	LYS	6.3
15	O	23	ALA	6.2
7	G	150	TYR	6.2
14	N	63	ARG	6.2
4	D	14	ILE	6.2
9	I	119	ALA	6.2
13	M	17	ASN	6.1
31	4	9	LYS	6.1
16	P	19	PHE	6.1
12	L	104	GLN	6.0
2	B	88	C	6.0
14	N	62	ASN	5.9
22	V	34	LYS	5.9
19	S	38	TYR	5.9
23	W	59	PHE	5.9
9	I	1	ALA	5.9
6	F	158	THR	5.9
21	U	70	ALA	5.9
12	L	74	THR	5.9
18	R	24	LYS	5.8
9	I	80	LYS	5.8
31	4	10	LEU	5.8
1	A	2334	U	5.8
1	A	1643	G	5.7
25	Y	1	MET	5.7
9	I	94	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
6	F	164	GLU	5.7
12	L	51	GLU	5.7
15	O	21	LEU	5.7
4	D	196	ALA	5.7
1	A	1420	A	5.7
1	A	1298	C	5.7
19	S	110	ARG	5.7
13	M	16	ARG	5.6
5	E	59	PRO	5.6
1	A	1302	A	5.6
9	I	93	ASN	5.6
21	U	59	GLU	5.6
1	A	866	A	5.5
19	S	32	ALA	5.5
13	M	135	VAL	5.5
14	N	100	CYS	5.5
27	O	23	ALA	5.5
15	O	50	ALA	5.5
15	O	22	GLY	5.4
1	A	1061	U	5.4
1	A	2438	U	5.4
15	O	55	GLU	5.4
1	A	508	A	5.4
1	A	2001	C	5.4
24	X	47	THR	5.4
30	3	19	GLY	5.4
7	G	157	LYS	5.4
1	A	1460	U	5.4
18	R	70	GLU	5.4
14	N	59	SER	5.3
1	A	613	A	5.3
7	G	152	ARG	5.3
1	A	1249	U	5.3
7	G	110	HIS	5.3
13	M	136	MET	5.3
1	A	2002	G	5.3
9	I	95	ASP	5.3
18	R	71	LYS	5.3
6	F	118	ALA	5.2
14	N	54	LEU	5.2
7	G	159	LYS	5.2
1	A	441	U	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	2689	U	5.1
11	K	68	GLY	5.1
30	3	21	PHE	5.0
1	A	106	C	5.0
6	F	88	VAL	5.0
20	T	24	MET	5.0
4	D	8	LYS	4.9
7	G	169	ARG	4.9
7	G	122	ALA	4.9
9	I	2	LYS	4.9
22	V	47	VAL	4.9
17	Q	56	PHE	4.9
16	P	17	PRO	4.9
9	I	78	LEU	4.9
6	F	78	ILE	4.9
21	U	68	ASN	4.9
11	K	60	ALA	4.9
7	G	153	PRO	4.9
6	F	77	LYS	4.9
1	A	1729	U	4.8
27	0	25	THR	4.8
6	F	26	GLN	4.8
6	F	89	THR	4.8
30	3	23	HIS	4.8
21	U	13	LEU	4.8
13	M	126	ILE	4.8
17	Q	29	ARG	4.8
4	D	198	GLY	4.8
1	A	2000	C	4.8
1	A	1247	A	4.8
2	B	13	G	4.7
21	U	36	GLU	4.7
30	3	36	ALA	4.7
1	A	1629	U	4.7
1	A	2743	U	4.7
23	W	32	ALA	4.7
13	M	129	THR	4.7
1	A	1081	U	4.7
15	O	25	ARG	4.7
21	U	29	SER	4.7
22	V	57	TYR	4.6
15	O	29	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	2069	G	4.6
6	F	108	PRO	4.6
12	L	102	GLY	4.6
30	3	46	LYS	4.6
19	S	86	MET	4.6
14	N	76	VAL	4.6
1	A	961	C	4.6
1	A	1642	G	4.6
9	I	7	TYR	4.6
16	P	109	ILE	4.6
9	I	118	GLY	4.6
9	I	81	LYS	4.6
23	W	43	LYS	4.6
7	G	160	GLY	4.5
30	3	37	THR	4.5
15	O	3	LYS	4.5
15	O	57	ALA	4.5
2	B	70	C	4.5
9	I	31	GLY	4.5
22	V	46	LYS	4.5
1	A	1031	G	4.5
3	C	1	ALA	4.5
9	I	71	LYS	4.5
6	F	130	GLY	4.5
16	P	33	GLU	4.4
6	F	75	GLY	4.4
17	Q	82	LEU	4.4
18	R	91	GLN	4.4
17	Q	111	LYS	4.4
1	A	394	C	4.4
15	O	37	ALA	4.4
1	A	2585	U	4.4
2	B	14	U	4.4
23	W	35	ILE	4.4
13	M	15	GLY	4.3
1	A	507	A	4.3
8	H	18	GLN	4.3
16	P	18	SER	4.3
2	B	89	U	4.3
6	F	25	MET	4.3
17	Q	52	ARG	4.3
22	V	81	PRO	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	2676	C	4.3
17	Q	72	GLY	4.3
6	F	73	VAL	4.3
19	S	85	ILE	4.3
1	A	1535	A	4.3
1	A	1630	A	4.3
31	4	12	ARG	4.3
2	B	101	A	4.2
6	F	153	ILE	4.2
12	L	52	GLY	4.2
30	3	45	PRO	4.2
1	A	876	C	4.2
16	P	21	PRO	4.2
6	F	79	ARG	4.2
9	I	4	VAL	4.2
9	I	82	ALA	4.2
2	B	71	C	4.2
1	A	1131	G	4.2
1	A	1132	U	4.2
1	A	2363	G	4.2
13	M	38	ARG	4.2
13	M	125	PRO	4.2
7	G	154	GLU	4.2
1	A	1537	G	4.2
6	F	119	LYS	4.2
3	C	22	GLU	4.1
11	K	69	VAL	4.1
31	4	8	LYS	4.1
13	M	18	ARG	4.1
5	E	26	ALA	4.1
29	2	22	MET	4.1
2	B	72	G	4.1
3	C	4	LYS	4.1
18	R	8	GLY	4.1
9	I	72	THR	4.1
12	L	72	ALA	4.1
1	A	1301	A	4.1
23	W	42	THR	4.1
23	W	60	ALA	4.0
6	F	107	VAL	4.0
14	N	51	LEU	4.0
1	A	1095	A	4.0

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Mol	Chain	Res	Type	RSRZ
15	O	2	ASP	4.0
19	S	26	GLY	4.0
1	A	1583	A	4.0
6	F	106	ALA	4.0
6	F	74	ALA	4.0
1	A	1033	U	4.0
9	I	79	LEU	4.0
19	S	93	ALA	4.0
1	A	995	C	4.0
28	1	30	PRO	4.0
14	N	66	ALA	4.0
1	A	811	U	4.0
30	3	44	ARG	4.0
3	C	17	LYS	4.0
5	E	127	GLU	4.0
12	L	73	ILE	4.0
1	A	1248	G	4.0
1	A	1412	U	4.0
16	P	20	ARG	4.0
28	1	34	GLU	4.0
10	J	1	MET	3.9
4	D	23	PRO	3.9
1	A	61	C	3.9
17	Q	3	VAL	3.9
13	M	24	THR	3.9
1	A	2712	C	3.9
5	E	66	GLY	3.9
12	L	49	GLY	3.9
19	S	49	LYS	3.9
15	O	42	PRO	3.9
20	T	1	MET	3.9
15	O	82	ALA	3.9
19	S	84	ARG	3.9
30	3	40	LYS	3.9
19	S	14	ALA	3.9
2	B	20	G	3.9
1	A	1297	C	3.9
9	I	10	LEU	3.9
19	S	39	THR	3.9
16	P	101	GLU	3.8
29	2	42	LEU	3.8
1	A	1644	C	3.8

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Mol	Chain	Res	Type	RSRZ
15	O	11	ALA	3.8
1	A	2820	A	3.8
15	O	28	VAL	3.8
2	B	90	C	3.8
6	F	105	ILE	3.8
19	S	27	LYS	3.8
1	A	1647	U	3.8
1	A	2887	A	3.8
4	D	10	GLY	3.8
13	M	56	ALA	3.8
6	F	59	ILE	3.8
16	P	113	LEU	3.8
19	S	94	ASP	3.8
15	O	14	ALA	3.8
1	A	1661	G	3.8
3	C	18	VAL	3.8
30	3	13	PHE	3.8
1	A	1646	C	3.8
15	O	115	LEU	3.8
3	C	2	VAL	3.8
1	A	493	G	3.7
1	A	1059	G	3.7
3	C	7	PRO	3.7
1	A	2027	G	3.7
19	S	92	ARG	3.7
9	I	117	THR	3.7
15	O	61	GLN	3.7
3	C	36	ASN	3.7
1	A	1413	A	3.7
10	J	9	GLU	3.7
1	A	902	C	3.7
22	V	54	ALA	3.6
22	V	50	MET	3.6
30	3	51	LYS	3.6
9	I	13	ALA	3.6
21	U	17	ASP	3.6
23	W	34	SER	3.6
1	A	528	A	3.6
6	F	102	LEU	3.6
22	V	41	GLU	3.6
5	E	98	LYS	3.6
29	2	41	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
30	3	14	LYS	3.6
30	3	50	SER	3.6
22	V	6	ALA	3.6
14	N	57	THR	3.6
4	D	22	ILE	3.6
1	A	1730	C	3.6
18	R	26	ASP	3.6
1	A	317	G	3.6
7	G	57	TYR	3.6
15	O	83	LEU	3.6
16	P	58	PHE	3.6
1	A	2070	A	3.6
1	A	1299	G	3.5
12	L	28	GLY	3.5
30	3	57	VAL	3.5
19	S	35	ILE	3.5
7	G	162	ARG	3.5
23	W	19	ARG	3.5
14	N	72	ASP	3.5
5	E	140	ASP	3.5
6	F	35	LEU	3.5
25	Y	4	LYS	3.5
7	G	89	VAL	3.5
1	A	2713	U	3.5
18	R	72	VAL	3.5
6	F	124	ARG	3.5
12	L	20	GLY	3.5
1	A	2667	C	3.5
19	S	28	LYS	3.5
19	S	24	ILE	3.5
1	A	2569	G	3.5
6	F	128	SER	3.5
6	F	117	SER	3.5
4	D	9	VAL	3.5
1	A	817	C	3.5
12	L	16	GLY	3.5
2	B	102	G	3.4
1	A	2602	A	3.4
2	B	107	G	3.4
30	3	54	LEU	3.4
7	G	6	ALA	3.4
15	O	7	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
12	L	45	GLY	3.4
18	R	73	LYS	3.4
6	F	22	ASN	3.4
1	A	1396	U	3.4
14	N	4	ARG	3.4
19	S	52	GLU	3.4
5	E	67	ARG	3.4
19	S	95	ARG	3.4
30	3	56	LEU	3.4
1	A	1406	U	3.4
21	U	60	LYS	3.4
10	J	3	THR	3.4
12	L	103	ILE	3.4
16	P	76	HIS	3.4
19	S	34	ASP	3.4
1	A	2033	A	3.3
1	A	1554	U	3.3
22	V	4	ILE	3.3
21	U	65	GLN	3.3
13	M	127	LYS	3.3
1	A	2264	C	3.3
19	S	23	LEU	3.3
1	A	549	G	3.3
1	A	1574	C	3.3
1	A	2723	C	3.3
21	U	30	SER	3.3
24	X	8	GLY	3.3
14	N	12	ARG	3.3
28	1	14	ALA	3.3
11	K	70	ARG	3.3
30	3	39	ARG	3.3
5	E	77	ILE	3.3
12	L	57	LEU	3.3
14	N	52	ILE	3.3
12	L	64	PHE	3.3
1	A	686	U	3.3
1	A	1559	U	3.3
6	F	80	GLN	3.3
1	A	2274	A	3.3
9	I	27	LEU	3.3
26	Z	51	SER	3.3
30	3	55	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
22	V	51	GLN	3.3
1	A	2610	C	3.3
1	A	1548	A	3.3
1	A	93	G	3.3
4	D	13	ARG	3.2
6	F	28	PRO	3.2
8	H	19	VAL	3.2
1	A	2355	G	3.2
6	F	76	PHE	3.2
1	A	145	C	3.2
7	G	158	GLY	3.2
28	1	22	THR	3.2
31	4	26	ILE	3.2
1	A	2561	U	3.2
12	L	71	ALA	3.2
21	U	11	ILE	3.2
13	M	25	ASP	3.2
15	O	89	ASP	3.2
6	F	65	LEU	3.2
1	A	1390	U	3.2
2	B	87	U	3.2
5	E	34	ALA	3.2
19	S	37	THR	3.2
1	A	2452	C	3.2
9	I	86	LYS	3.2
21	U	79	ALA	3.2
20	T	2	ILE	3.2
17	Q	28	SER	3.2
17	Q	37	ALA	3.2
15	O	20	GLU	3.2
16	P	49	ILE	3.2
19	S	69	LEU	3.2
14	N	111	ALA	3.2
6	F	113	PHE	3.2
29	2	1	MET	3.2
1	A	535	G	3.2
1	A	1984	G	3.2
19	S	70	LYS	3.2
1	A	2042	A	3.2
20	T	65	GLY	3.2
6	F	58	ALA	3.2
1	A	974	G	3.2

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Mol	Chain	Res	Type	RSRZ
24	X	20	ALA	3.2
4	D	60	VAL	3.2
12	L	58	TYR	3.2
10	J	132	HIS	3.2
1	A	529	A	3.1
1	A	1253	A	3.1
1	A	1115	G	3.1
14	N	69	ARG	3.1
1	A	562	U	3.1
1	A	1523	U	3.1
3	C	35	LYS	3.1
16	P	69	VAL	3.1
1	A	1938	A	3.1
24	X	76	LYS	3.1
19	S	7	HIS	3.1
6	F	81	GLY	3.1
23	W	33	GLY	3.1
5	E	78	TRP	3.1
13	M	41	LEU	3.1
17	Q	26	ALA	3.1
2	B	12	C	3.1
6	F	86	CYS	3.1
20	T	34	VAL	3.1
21	U	75	ALA	3.1
1	A	2020	A	3.1
1	A	2827	C	3.1
17	Q	55	GLN	3.1
4	D	57	ALA	3.1
15	O	59	ALA	3.1
10	J	64	VAL	3.1
3	C	3	VAL	3.1
25	Y	41	HIS	3.1
15	O	49	VAL	3.1
9	I	5	GLN	3.1
15	O	44	GLY	3.1
19	S	8	ARG	3.1
21	U	37	GLY	3.0
20	T	57	VAL	3.0
22	V	70	ILE	3.0
27	O	20	ALA	3.0
1	A	1764	C	3.0
6	F	87	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	825	A	3.0
1	A	1757	A	3.0
9	I	15	GLY	3.0
13	M	37	GLY	3.0
1	A	2029	G	3.0
12	L	76	GLU	3.0
6	F	23	SER	3.0
1	A	2402	U	3.0
12	L	6	LEU	3.0
15	O	4	LYS	3.0
15	O	43	ASN	3.0
5	E	76	PRO	3.0
7	G	155	PRO	3.0
14	N	73	ASN	3.0
12	L	54	GLN	3.0
22	V	1	MET	3.0
30	3	49	VAL	3.0
1	A	587	C	3.0
16	P	50	ARG	3.0
19	S	88	ARG	3.0
1	A	1300	G	3.0
23	W	17	ALA	3.0
10	J	83	GLY	3.0
12	L	107	PHE	3.0
30	3	41	ARG	3.0
4	D	61	THR	3.0
17	Q	57	ARG	2.9
30	3	42	HIS	2.9
5	E	128	ALA	2.9
15	O	87	ILE	2.9
1	A	937	C	2.9
1	A	2031	A	2.9
1	A	2799	A	2.9
12	L	19	LEU	2.9
14	N	56	LYS	2.9
16	P	36	LYS	2.9
30	3	18	LYS	2.9
9	I	26	ALA	2.9
1	A	789	A	2.9
29	2	23	ALA	2.9
1	A	2690	U	2.9
30	3	34	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
18	R	69	GLY	2.9
1	A	2032	G	2.9
12	L	96	LYS	2.9
17	Q	64	ILE	2.9
19	S	55	ILE	2.9
7	G	147	LEU	2.9
1	A	1407	G	2.9
4	D	56	LYS	2.9
17	Q	5	ARG	2.9
1	A	1205	A	2.9
13	M	124	LEU	2.9
5	E	99	LYS	2.9
19	S	91	GLY	2.9
1	A	1032	A	2.9
1	A	2028	U	2.9
5	E	58	LYS	2.9
7	G	167	VAL	2.9
13	M	36	VAL	2.9
10	J	63	ALA	2.9
1	A	88	G	2.9
1	A	2510	C	2.9
19	S	107	VAL	2.9
1	A	816	C	2.9
1	A	1660	G	2.9
1	A	913	U	2.9
12	L	50	PHE	2.9
1	A	810	U	2.8
6	F	31	GLU	2.8
23	W	20	LEU	2.8
6	F	34	THR	2.8
16	P	68	GLY	2.8
6	F	33	ILE	2.8
12	L	106	GLU	2.8
13	M	12	MET	2.8
25	Y	5	GLU	2.8
12	L	69	ARG	2.8
17	Q	115	ALA	2.8
17	Q	25	GLY	2.8
6	F	159	ALA	2.8
7	G	118	ALA	2.8
17	Q	85	ALA	2.8
1	A	790	U	2.8

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Mol	Chain	Res	Type	RSRZ
12	L	47	ARG	2.8
1	A	389	G	2.8
1	A	2083	G	2.8
1	A	2642	G	2.8
15	O	6	ALA	2.8
5	E	24	ASN	2.8
19	S	83	LYS	2.8
1	A	1758	U	2.8
1	A	144	A	2.8
30	3	53	ASP	2.8
11	K	101	GLY	2.8
29	2	28	ARG	2.8
1	A	1632	A	2.8
17	Q	34	ALA	2.8
1	A	2339	C	2.8
7	G	129	GLU	2.8
23	W	31	LEU	2.8
9	I	56	VAL	2.8
7	G	175	LYS	2.8
1	A	1250	G	2.8
10	J	77	HIS	2.8
3	C	23	LEU	2.8
12	L	56	PRO	2.8
20	T	43	ILE	2.8
1	A	1312	U	2.8
12	L	46	VAL	2.8
27	0	1	ALA	2.8
17	Q	36	GLN	2.7
23	W	36	ILE	2.8
4	D	140	HIS	2.7
24	X	19	HIS	2.7
1	A	901	C	2.7
17	Q	69	ARG	2.7
24	X	75	GLU	2.7
13	M	128	THR	2.7
17	Q	32	ARG	2.7
29	2	19	ARG	2.7
1	A	867	C	2.7
6	F	90	LEU	2.7
7	G	121	THR	2.7
3	C	10	PRO	2.7
10	J	44	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
12	L	21	ARG	2.7
16	P	108	ARG	2.7
19	S	18	ARG	2.7
27	0	7	PRO	2.7
3	C	8	THR	2.7
23	W	69	GLU	2.7
17	Q	53	LYS	2.7
22	V	10	LYS	2.7
24	X	35	HIS	2.7
1	A	2084	C	2.7
24	X	59	ASP	2.7
1	A	1303	G	2.7
7	G	161	VAL	2.7
5	E	91	ASP	2.7
6	F	72	SER	2.7
1	A	489	G	2.7
1	A	1311	G	2.7
1	A	2437	G	2.7
15	O	81	ARG	2.7
22	V	93	ARG	2.7
13	M	132	THR	2.7
1	A	2030	A	2.7
1	A	393	C	2.7
14	N	67	PHE	2.7
3	C	12	ARG	2.7
27	0	26	SER	2.7
16	P	59	THR	2.7
21	U	20	LYS	2.7
1	A	571	U	2.7
1	A	2023	C	2.7
20	T	77	ARG	2.7
4	D	7	LYS	2.7
11	K	77	ILE	2.7
14	N	55	ALA	2.7
21	U	10	VAL	2.7
3	C	5	CYS	2.7
31	4	21	GLY	2.7
22	V	94	ALA	2.7
6	F	150	GLY	2.6
13	M	133	LYS	2.6
12	L	61	LEU	2.6
20	T	3	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
24	X	48	LEU	2.6
14	N	101	GLY	2.6
1	A	220	G	2.6
10	J	87	ALA	2.6
15	O	51	ALA	2.6
14	N	9	GLN	2.6
8	H	11	ASN	2.6
28	1	21	THR	2.6
9	I	120	ASP	2.6
15	O	9	ARG	2.6
1	A	818	G	2.6
6	F	109	ARG	2.6
30	3	12	ARG	2.6
11	K	106	GLU	2.6
1	A	388	G	2.6
1	A	1695	G	2.6
1	A	126	A	2.6
1	A	329	G	2.6
1	A	1645	G	2.6
1	A	1029	A	2.6
5	E	201	ALA	2.6
9	I	73	PRO	2.6
22	V	63	ILE	2.6
22	V	82	TYR	2.6
1	A	1807	G	2.6
2	B	21	G	2.6
3	C	58	LYS	2.6
6	F	67	THR	2.6
17	Q	2	ARG	2.6
1	A	440	C	2.6
12	L	114	GLY	2.6
1	A	2213	U	2.6
17	Q	17	LEU	2.6
19	S	76	VAL	2.5
25	Y	2	LYS	2.5
11	K	20	MET	2.5
15	O	109	ALA	2.5
24	X	37	PHE	2.5
15	O	116	GLN	2.5
27	0	22	THR	2.5
7	G	55	ASP	2.5
15	O	112	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
24	X	7	THR	2.5
4	D	24	VAL	2.5
6	F	27	VAL	2.5
1	A	1274	A	2.5
1	A	1637	A	2.5
17	Q	13	HIS	2.5
6	F	66	ILE	2.5
12	L	10	GLU	2.5
23	W	72	GLY	2.5
20	T	68	LYS	2.5
17	Q	33	VAL	2.5
18	R	52	PRO	2.5
18	R	27	ILE	2.5
29	2	25	LYS	2.5
1	A	1814	G	2.5
1	A	544	C	2.5
1	A	838	C	2.5
14	N	70	THR	2.5
1	A	137	U	2.5
1	A	1273	U	2.5
12	L	53	GLY	2.5
6	F	163	GLU	2.5
30	3	33	THR	2.5
24	X	74	GLY	2.5
27	0	3	GLN	2.5
1	A	2603	G	2.5
1	A	1636	U	2.5
1	A	1551	A	2.5
12	L	101	ILE	2.5
1	A	1518	C	2.5
1	A	1771	C	2.5
15	O	5	SER	2.5
18	R	23	GLU	2.5
1	A	1073	A	2.5
2	B	106	G	2.5
23	W	9	THR	2.5
18	R	62	GLU	2.5
29	2	33	ARG	2.5
3	C	16	VAL	2.5
1	A	2019	A	2.5
8	H	77	THR	2.5
9	I	52	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
6	F	32	LYS	2.5
1	A	2265	U	2.5
30	3	52	GLY	2.5
10	J	86	GLN	2.5
3	C	13	ARG	2.5
28	1	31	GLU	2.4
21	U	73	ASN	2.4
15	O	10	ARG	2.4
10	J	24	THR	2.4
20	T	42	GLU	2.4
1	A	993	G	2.4
1	A	2462	C	2.4
12	L	105	ILE	2.4
3	C	34	GLU	2.4
6	F	114	ARG	2.4
14	N	29	VAL	2.4
6	F	154	THR	2.4
15	O	35	ILE	2.4
19	S	11	ARG	2.4
7	G	176	LYS	2.4
14	N	61	ALA	2.4
1	A	1105	U	2.4
22	V	40	ILE	2.4
16	P	91	VAL	2.4
4	D	77	ARG	2.4
6	F	175	PRO	2.4
19	S	21	ALA	2.4
1	A	2601	C	2.4
10	J	75	TYR	2.4
3	C	19	VAL	2.4
10	J	80	HIS	2.4
12	L	63	LYS	2.4
14	N	40	LYS	2.4
14	N	43	GLU	2.4
10	J	72	LYS	2.4
1	A	1552	A	2.4
1	A	2273	A	2.4
3	C	96	LYS	2.4
5	E	137	LYS	2.4
20	T	89	GLU	2.4
1	A	2640	G	2.4
17	Q	110	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	94	A	2.4
6	F	71	LYS	2.4
3	C	248	GLY	2.4
7	G	114	HIS	2.4
1	A	573	U	2.4
11	K	41	ILE	2.4
15	O	38	GLN	2.4
10	J	105	VAL	2.4
7	G	108	PHE	2.4
1	A	2025	C	2.4
7	G	172	GLU	2.4
20	T	41	ALA	2.4
1	A	2428	G	2.4
22	V	64	VAL	2.4
3	C	70	LYS	2.4
15	O	106	LEU	2.4
3	C	202	ARG	2.4
29	2	29	GLN	2.4
3	C	203	VAL	2.3
21	U	28	LEU	2.3
28	1	33	LEU	2.3
11	K	108	ARG	2.3
1	A	1252	G	2.3
17	Q	4	LYS	2.3
30	3	11	LYS	2.3
1	A	328	U	2.3
1	A	345	A	2.3
6	F	156	THR	2.3
15	O	13	ARG	2.3
12	L	31	GLY	2.3
10	J	67	ASN	2.3
1	A	588	U	2.3
1	A	743	A	2.3
15	O	104	GLN	2.3
26	Z	54	VAL	2.3
6	F	152	ASP	2.3
1	A	877	A	2.3
1	A	1608	A	2.3
16	P	34	GLY	2.3
11	K	57	VAL	2.3
8	H	38	PRO	2.3
4	D	25	THR	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
15	O	52	SER	2.3
3	C	223	ALA	2.3
25	Y	19	LEU	2.3
7	G	109	SER	2.3
21	U	18	LYS	2.3
1	A	92	U	2.3
7	G	106	LEU	2.3
9	I	91	LYS	2.3
9	I	83	ALA	2.3
10	J	79	GLY	2.3
3	C	235	GLU	2.3
16	P	90	ALA	2.3
22	V	5	ASN	2.3
25	Y	3	ALA	2.3
8	H	2	GLN	2.3
10	J	66	GLY	2.3
15	O	30	ARG	2.3
16	P	107	ALA	2.3
21	U	33	VAL	2.3
24	X	15	ASN	2.3
22	V	35	GLU	2.3
31	4	30	GLU	2.3
1	A	494	G	2.3
1	A	1017	G	2.3
1	A	2024	G	2.3
24	X	24	THR	2.3
19	S	51	LEU	2.3
1	A	1251	C	2.3
6	F	29	ARG	2.3
7	G	58	ALA	2.3
12	L	113	ALA	2.3
29	2	40	ALA	2.3
1	A	2722	G	2.3
11	K	35	VAL	2.3
11	K	98	ARG	2.3
21	U	40	LEU	2.3
1	A	574	A	2.3
1	A	2062	A	2.3
1	A	1325	U	2.3
1	A	2244	U	2.3
11	K	99	ILE	2.2
15	O	80	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
12	L	65	GLY	2.2
30	3	16	THR	2.2
1	A	857	G	2.2
1	A	1133	A	2.2
1	A	1383	A	2.2
17	Q	27	ARG	2.2
1	A	2710	C	2.2
20	T	64	LYS	2.2
6	F	132	ARG	2.2
27	0	21	LEU	2.2
29	2	34	ARG	2.2
23	W	54	ARG	2.2
1	A	228	C	2.2
1	A	323	C	2.2
1	A	968	C	2.2
23	W	64	GLY	2.2
1	A	2688	G	2.2
11	K	58	LEU	2.2
10	J	65	THR	2.2
24	X	64	ASP	2.2
31	4	33	HIS	2.2
1	A	2863	C	2.2
3	C	15	VAL	2.2
25	Y	17	GLU	2.2
31	4	34	LYS	2.2
1	A	1538	G	2.2
1	A	62	U	2.2
15	O	18	LEU	2.2
4	D	15	PHE	2.2
17	Q	20	ALA	2.2
17	Q	81	GLY	2.2
19	S	82	MET	2.2
1	A	1641	A	2.2
29	2	24	THR	2.2
17	Q	58	GLN	2.2
7	G	73	SER	2.2
15	O	58	ILE	2.2
18	R	19	THR	2.2
20	T	6	ARG	2.2
1	A	953	G	2.2
1	A	2814	A	2.2
14	N	112	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
17	Q	112	ALA	2.2
1	A	318	C	2.2
17	Q	114	ALA	2.2
18	R	25	LEU	2.2
1	A	125	A	2.2
1	A	952	G	2.2
1	A	1770	G	2.2
22	V	23	ALA	2.2
5	E	57	LYS	2.2
14	N	98	LEU	2.2
13	M	10	ARG	2.2
19	S	25	ARG	2.2
28	1	32	LYS	2.2
21	U	12	VAL	2.2
1	A	835	C	2.2
20	T	56	GLU	2.2
7	G	112	VAL	2.2
1	A	2828	G	2.2
14	N	41	ALA	2.2
20	T	23	ALA	2.2
25	Y	37	LEU	2.2
18	R	63	VAL	2.1
6	F	112	ASP	2.1
6	F	160	LYS	2.1
22	V	32	GLY	2.1
1	A	87	U	2.1
5	E	97	ASN	2.1
29	2	26	ASN	2.1
4	D	112	THR	2.1
15	O	62	LEU	2.1
4	D	179	ARG	2.1
6	F	91	ARG	2.1
1	A	2063	C	2.1
19	S	87	PRO	2.1
7	G	168	VAL	2.1
1	A	967	U	2.1
18	R	20	VAL	2.1
19	S	30	SER	2.1
29	2	20	ALA	2.1
10	J	129	GLU	2.1
13	M	39	GLY	2.1
1	A	1199	U	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	249	VAL	2.1
19	S	17	VAL	2.1
12	L	17	LYS	2.1
4	D	85	ALA	2.1
1	A	732	C	2.1
12	L	70	LYS	2.1
15	O	26	LEU	2.1
21	U	102	ILE	2.1
20	T	4	GLU	2.1
1	A	2463	C	2.1
3	C	11	GLY	2.1
1	A	1979	U	2.1
6	F	151	LEU	2.1
10	J	55	ILE	2.1
1	A	258	G	2.1
13	M	131	VAL	2.1
3	C	25	LYS	2.1
26	Z	55	LYS	2.1
11	K	71	ARG	2.1
13	M	6	ARG	2.1
14	N	80	PHE	2.1
24	X	17	ARG	2.1
1	A	1256	G	2.1
3	C	224	MET	2.1
10	J	71	ASP	2.1
14	N	3	HIS	2.1
19	S	46	LEU	2.1
1	A	1640	A	2.1
7	G	90	GLY	2.1
22	V	25	LYS	2.1
1	A	559	G	2.1
1	A	561	G	2.1
1	A	2677	G	2.1
15	O	41	ALA	2.1
31	4	29	ALA	2.1
12	L	27	LEU	2.1
10	J	10	THR	2.1
11	K	104	THR	2.1
1	A	2600	A	2.1
1	A	2614	A	2.1
8	H	27	ARG	2.1
9	I	116	MET	2.1

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Mol	Chain	Res	Type	RSRZ
19	S	33	LEU	2.1
23	W	21	GLY	2.1
25	Y	21	LEU	2.1
1	A	1487	U	2.1
1	A	1599	U	2.1
1	A	2666	C	2.1
3	C	9	SER	2.1
18	R	50	GLY	2.1
15	O	108	ASP	2.1
13	M	55	ARG	2.0
13	M	107	GLY	2.0
19	S	71	VAL	2.0
4	D	58	ASN	2.0
1	A	436	C	2.0
14	N	42	LYS	2.0
13	M	96	ILE	2.0
7	G	93	TYR	2.0
9	I	74	PRO	2.0
1	A	980	A	2.0
1	A	1246	A	2.0
15	O	12	THR	2.0
16	P	38	ARG	2.0
1	A	1653	G	2.0
1	A	1662	U	2.0
14	N	47	VAL	2.0
1	A	2147	A	2.0
13	M	61	GLY	2.0
16	P	22	GLY	2.0
25	Y	36	GLN	2.0
1	A	2581	G	2.0
14	N	68	ALA	2.0
15	O	84	GLU	2.0
16	P	106	ALA	2.0
30	3	24	LYS	2.0
3	C	100	ARG	2.0
10	J	74	TYR	2.0
3	C	201	LEU	2.0
1	A	729	G	2.0
1	A	962	G	2.0
1	A	1162	G	2.0
1	A	2615	U	2.0
1	A	1493	C	2.0

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Mol	Chain	Res	Type	RSRZ
21	U	2	ALA	2.0
23	W	67	LYS	2.0
30	3	58	ILE	2.0
7	G	156	TYR	2.0
29	2	32	ALA	2.0
1	A	910	A	2.0
12	L	59	ARG	2.0
15	O	100	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	2933	1/1	1.43	1150.00	164,164,164,164	0
32	MG	A	2966	1/1	3.26	42.22	157,157,157,157	0
32	MG	A	2923	1/1	0.57	27.21	229,229,229,229	0
32	MG	A	3011	1/1	0.89	16.18	172,172,172,172	0
32	MG	A	3026	1/1	0.75	14.83	225,225,225,225	0
32	MG	A	3000	1/1	0.64	12.71	156,156,156,156	0
32	MG	A	3036	1/1	1.67	11.29	198,198,198,198	0
32	MG	A	3030	1/1	0.54	8.82	138,138,138,138	0
32	MG	A	2958	1/1	0.50	7.63	136,136,136,136	0
32	MG	A	2914	1/1	0.53	6.70	184,184,184,184	0
32	MG	A	2961	1/1	0.40	6.52	162,162,162,162	0
32	MG	A	2917	1/1	0.67	5.91	162,162,162,162	0
32	MG	A	2905	1/1	0.32	4.96	212,212,212,212	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2935	1/1	0.35	4.79	161,161,161,161	0
32	MG	A	2909	1/1	0.55	3.99	296,296,296,296	0
32	MG	A	3001	1/1	0.35	3.89	170,170,170,170	0
32	MG	A	2984	1/1	0.66	3.57	182,182,182,182	0
32	MG	A	2967	1/1	0.49	3.54	157,157,157,157	0
32	MG	A	2997	1/1	0.61	3.00	173,173,173,173	0
32	MG	A	3022	1/1	0.51	2.54	147,147,147,147	0
32	MG	A	2999	1/1	0.62	2.35	190,190,190,190	0
32	MG	A	2960	1/1	0.44	2.20	133,133,133,133	0
32	MG	A	3019	1/1	0.42	2.05	133,133,133,133	0
32	MG	A	3032	1/1	0.33	2.03	132,132,132,132	0
32	MG	A	2989	1/1	0.54	1.98	196,196,196,196	0
32	MG	A	2949	1/1	0.33	1.80	172,172,172,172	0
32	MG	A	2942	1/1	0.33	1.72	186,186,186,186	0
32	MG	A	2983	1/1	0.64	1.69	134,134,134,134	0
32	MG	A	3006	1/1	0.36	1.66	150,150,150,150	0
32	MG	A	2908	1/1	0.34	1.60	197,197,197,197	0
32	MG	A	3025	1/1	0.27	1.50	146,146,146,146	0
32	MG	A	2929	1/1	0.74	1.50	160,160,160,160	0
32	MG	A	2981	1/1	0.33	1.35	144,144,144,144	0
32	MG	A	2956	1/1	0.22	1.34	144,144,144,144	0
32	MG	A	2974	1/1	0.29	1.21	184,184,184,184	0
32	MG	A	2955	1/1	0.21	1.19	144,144,144,144	0
32	MG	A	3004	1/1	0.35	1.08	155,155,155,155	0
32	MG	A	3033	1/1	0.45	1.03	183,183,183,183	0
32	MG	A	2948	1/1	0.30	1.03	188,188,188,188	0
32	MG	A	3017	1/1	0.38	1.00	135,135,135,135	0
32	MG	A	2932	1/1	0.49	0.74	179,179,179,179	0
32	MG	A	3015	1/1	0.22	0.71	143,143,143,143	0
32	MG	A	2963	1/1	0.26	0.70	132,132,132,132	0
32	MG	A	2953	1/1	0.44	0.62	180,180,180,180	0
32	MG	A	3023	1/1	0.22	0.60	159,159,159,159	0
32	MG	A	3012	1/1	0.34	0.58	145,145,145,145	0
32	MG	A	2937	1/1	0.33	0.50	158,158,158,158	0
32	MG	A	2990	1/1	0.27	0.40	208,208,208,208	0
32	MG	A	2912	1/1	0.36	0.36	199,199,199,199	0
32	MG	A	2931	1/1	0.35	0.34	165,165,165,165	0
32	MG	A	2940	1/1	0.29	0.25	204,204,204,204	0
32	MG	A	3024	1/1	0.24	0.22	206,206,206,206	0
32	MG	A	3008	1/1	0.26	0.10	159,159,159,159	0
32	MG	A	3003	1/1	0.24	0.05	150,150,150,150	0
32	MG	A	2911	1/1	0.24	-0.06	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3005	1/1	0.24	-0.15	141,141,141,141	0
32	MG	A	2921	1/1	0.26	-0.29	248,248,248,248	0
32	MG	A	3031	1/1	0.32	-0.38	132,132,132,132	0
32	MG	A	2998	1/1	0.33	-0.41	152,152,152,152	0
32	MG	A	3009	1/1	0.21	-0.49	228,228,228,228	0
32	MG	C	273	1/1	0.23	-0.52	135,135,135,135	0
32	MG	A	2928	1/1	0.22	-0.56	135,135,135,135	0
32	MG	A	2904	1/1	0.18	-0.60	206,206,206,206	0
32	MG	A	2982	1/1	0.23	-0.63	148,148,148,148	0
32	MG	A	3013	1/1	0.22	-0.68	219,219,219,219	0
32	MG	A	2930	1/1	0.24	-0.71	171,171,171,171	0
32	MG	A	2936	1/1	0.20	-0.79	162,162,162,162	0
32	MG	A	2918	1/1	0.21	-0.86	164,164,164,164	0
33	ZN	4	781	1/1	0.28	-1.02	99,99,99,99	0
32	MG	A	2943	1/1	0.24	-1.08	171,171,171,171	0
32	MG	A	3021	1/1	0.23	-1.18	181,181,181,181	0
32	MG	A	2985	1/1	0.10	-1.21	220,220,220,220	0
32	MG	B	119	1/1	0.16	-1.22	224,224,224,224	0
32	MG	A	3014	1/1	0.24	-1.24	160,160,160,160	0
32	MG	A	3034	1/1	0.19	-1.27	170,170,170,170	0
32	MG	A	2993	1/1	0.18	-1.27	200,200,200,200	0
32	MG	C	274	1/1	0.21	-1.28	140,140,140,140	0
32	MG	A	2986	1/1	0.14	-1.29	303,303,303,303	0
32	MG	A	2945	1/1	0.20	-1.33	179,179,179,179	0
32	MG	A	2995	1/1	0.15	-1.35	198,198,198,198	0
32	MG	A	2946	1/1	0.14	-1.36	208,208,208,208	0
32	MG	A	2979	1/1	0.18	-1.36	145,145,145,145	0
32	MG	A	2965	1/1	0.31	-1.37	160,160,160,160	0
32	MG	A	2916	1/1	0.22	-1.47	165,165,165,165	0
32	MG	A	3016	1/1	0.12	-1.52	182,182,182,182	0
32	MG	A	3028	1/1	0.16	-1.52	187,187,187,187	0
32	MG	A	2972	1/1	0.17	-1.58	139,139,139,139	0
32	MG	A	2987	1/1	0.15	-1.64	214,214,214,214	0
32	MG	A	3010	1/1	0.18	-1.68	137,137,137,137	0
32	MG	A	2950	1/1	0.15	-1.69	208,208,208,208	0
32	MG	A	2952	1/1	0.07	-1.70	249,249,249,249	0
32	MG	A	2951	1/1	0.16	-1.72	203,203,203,203	0
32	MG	A	2934	1/1	0.14	-1.75	159,159,159,159	0
32	MG	A	3027	1/1	0.13	-1.82	168,168,168,168	0
32	MG	A	3035	1/1	0.22	-1.85	181,181,181,181	0
32	MG	A	2944	1/1	0.21	-1.89	176,176,176,176	0
32	MG	A	2996	1/1	0.16	-1.93	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3020	1/1	0.18	-2.10	170,170,170,170	0
32	MG	A	2970	1/1	0.20	-2.12	147,147,147,147	0
32	MG	A	2971	1/1	0.14	-2.18	143,143,143,143	0
32	MG	A	3029	1/1	0.08	-2.22	199,199,199,199	0
32	MG	A	2924	1/1	0.20	-2.25	151,151,151,151	0
32	MG	A	2920	1/1	0.14	-2.34	187,187,187,187	0
32	MG	A	3007	1/1	0.14	-2.45	142,142,142,142	0
32	MG	A	2907	1/1	0.12	-2.56	206,206,206,206	0
32	MG	A	2927	1/1	0.13	-2.57	162,162,162,162	0
32	MG	A	3018	1/1	0.14	-2.61	154,154,154,154	0
32	MG	A	2954	1/1	0.14	-2.65	160,160,160,160	0
32	MG	A	2938	1/1	0.16	-2.84	155,155,155,155	0
32	MG	A	2959	1/1	0.20	-2.88	141,141,141,141	0
32	MG	A	2964	1/1	0.09	-2.96	134,134,134,134	0
32	MG	A	2992	1/1	0.14	-2.99	179,179,179,179	0
32	MG	A	2926	1/1	0.12	-3.08	148,148,148,148	0
32	MG	A	2975	1/1	0.17	-3.35	182,182,182,182	0
32	MG	A	3002	1/1	0.14	-3.49	211,211,211,211	0
32	MG	A	2994	1/1	0.17	-3.51	174,174,174,174	0
32	MG	A	2947	1/1	0.09	-3.57	210,210,210,210	0
32	MG	A	2941	1/1	0.14	-3.67	197,197,197,197	0
32	MG	A	2973	1/1	0.07	-3.68	147,147,147,147	0
32	MG	A	2939	1/1	0.18	-3.70	212,212,212,212	0
32	MG	A	2915	1/1	0.12	-3.91	168,168,168,168	0
32	MG	A	2968	1/1	0.15	-4.14	152,152,152,152	0
32	MG	A	2919	1/1	0.17	-4.36	175,175,175,175	0
32	MG	A	2991	1/1	0.21	-4.69	180,180,180,180	0
32	MG	A	2957	1/1	0.13	-4.69	155,155,155,155	0
32	MG	A	2977	1/1	0.13	-4.86	187,187,187,187	0
32	MG	A	2988	1/1	0.14	-5.23	167,167,167,167	0
32	MG	A	2969	1/1	0.10	-5.36	150,150,150,150	0
32	MG	A	2910	1/1	0.09	-5.58	250,250,250,250	0
32	MG	A	2978	1/1	0.10	-5.80	155,155,155,155	0
32	MG	A	2925	1/1	0.19	-6.11	152,152,152,152	0
32	MG	A	2922	1/1	0.08	-6.16	245,245,245,245	0
32	MG	A	2976	1/1	0.10	-6.74	312,312,312,312	0
32	MG	J	143	1/1	0.33	-8.58	183,183,183,183	0
32	MG	A	2980	1/1	0.08	-10.62	162,162,162,162	0
32	MG	A	2962	1/1	0.06	-11.91	136,136,136,136	0
32	MG	A	2906	1/1	0.23	-	229,229,229,229	0
32	MG	A	2913	1/1	0.24	-	210,210,210,210	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.