



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3J5S
EMDB ID: : EMD-5784
Title : EttA binds to ribosome exit site and regulates translation by restricting ribosome and tRNA dynamics
Authors : Hashem, Y.
Deposited on : 2013-11-15
Resolution : 7.50 Å(reported)
Based on PDB ID : 3R8O, 3R8T, 2WDG, 4FIN

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

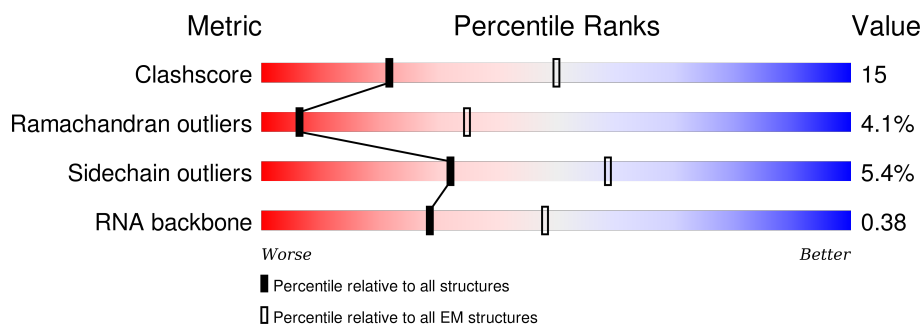
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	101	12% 13% 7% 68%
2	A	360	16% 19% 14% 52%
3	E	77	40% 43% 17%
4	D	561	65% 25% 8% .
5	F	234	64% 29% 6% .
6	G	178	71% 22% 7%
7	H	50	74% 18% 8%
8	I	151	61% 30% 7% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	32	Total	C	N	O	P	0	0
			687	306	126	223	32		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	174	Total	C	N	O	P	0	0
			3731	1663	674	1220	174		

- Molecule 3 is a RNA chain called P-site tRNA FMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 4 is a protein called Energy-dependent translational throttle A (EttA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	554	Total	C	N	O	S	0	0
			4393	2764	781	837	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-4	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-3	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-2	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-1	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	0	HIS	-	EXPRESSION TAG	UNP P0A9W3

- Molecule 5 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

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

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

- Molecule 7 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

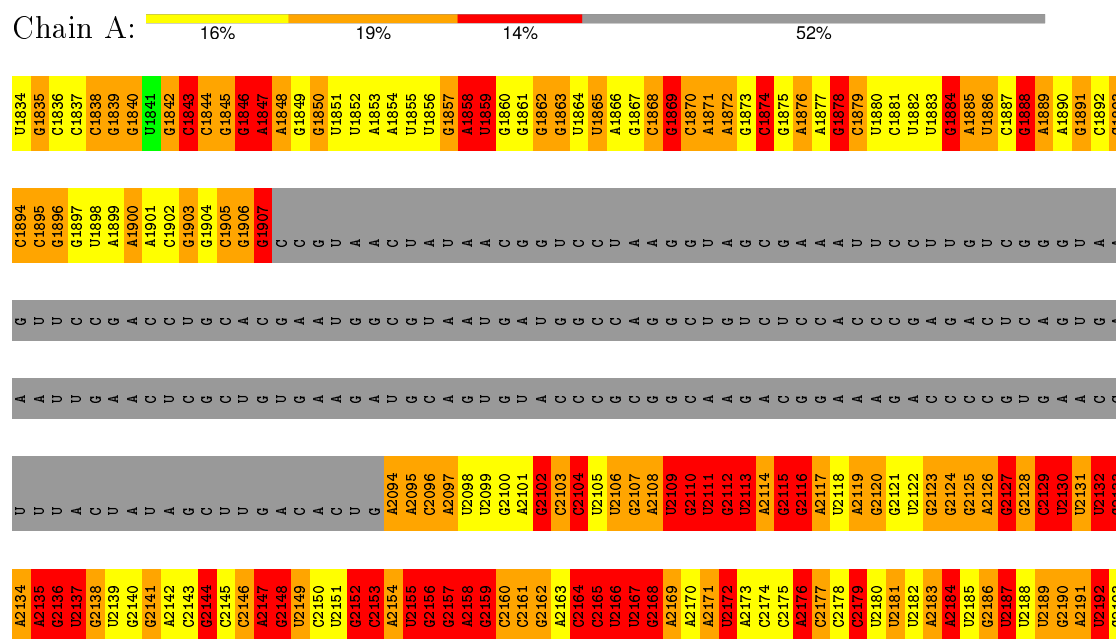
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

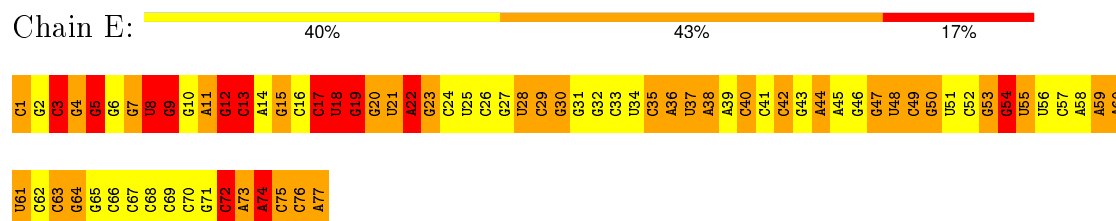
• Molecule 1: 16S ribosomal RNA



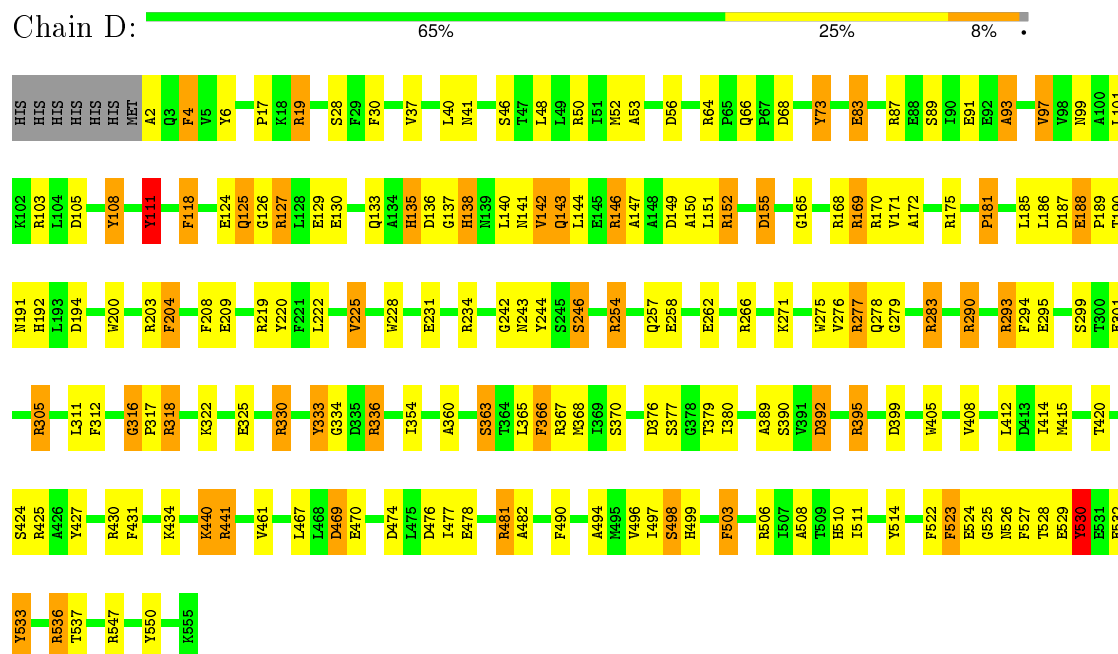
• Molecule 2: 23S ribosomal RNA



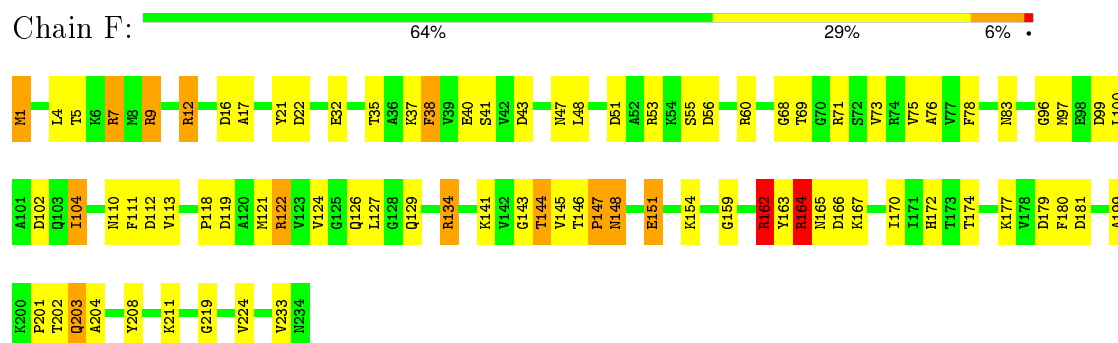
• Molecule 3: P-site tRNA FMet



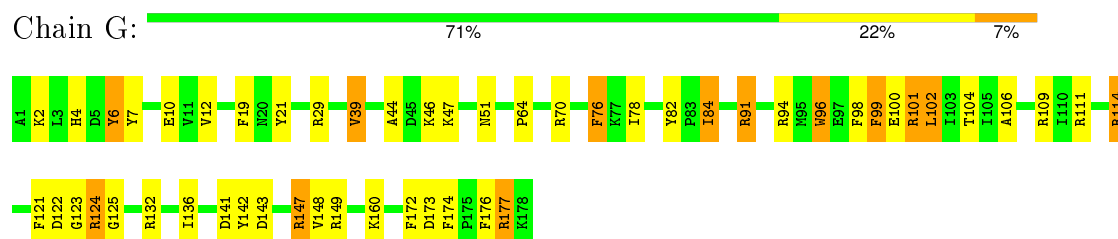
- Molecule 4: Energy-dependent translational throttle A (EttA)



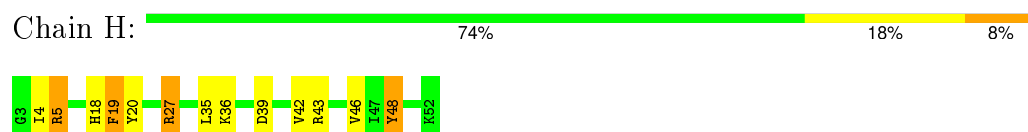
- Molecule 5: 50S ribosomal protein L1



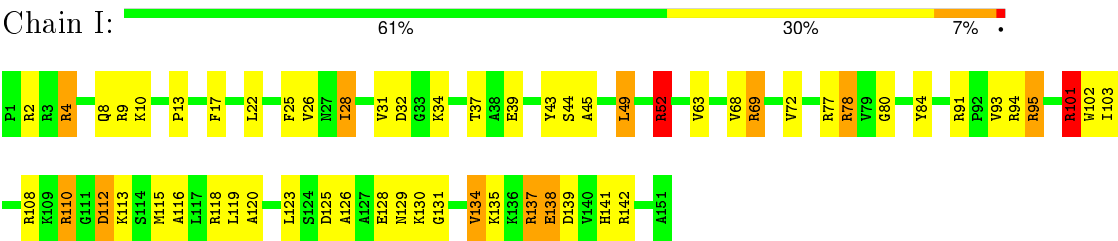
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L33



● Molecule 8: 30S ribosomal protein S7



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	39316	Depositor
Resolution determination method	gold standard FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	80000	Depositor
Image detector	GATAN UltraScan 4000 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	B	3.33	96/766 (12.5%)	3.35	147/1188 (12.4%)
2	A	3.17	486/4174 (11.6%)	3.15	702/6507 (10.8%)
3	E	3.23	213/1832 (11.6%)	3.28	351/2855 (12.3%)
4	D	1.58	22/4474 (0.5%)	2.04	130/6034 (2.2%)
5	F	1.52	5/1748 (0.3%)	1.97	49/2355 (2.1%)
6	G	1.65	8/1444 (0.6%)	2.08	40/1937 (2.1%)
7	H	1.63	2/417 (0.5%)	2.02	11/554 (2.0%)
8	I	1.61	6/1196 (0.5%)	2.31	50/1602 (3.1%)
All	All	2.41	838/16051 (5.2%)	2.65	1480/23032 (6.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	12
2	A	0	84
3	E	0	34
4	D	0	23
5	F	0	9
6	G	0	6
7	H	0	4
8	I	0	6
All	All	0	178

All (838) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	36	A	N9-C4	-18.05	1.27	1.37
1	B	1297	G	N9-C8	15.82	1.49	1.37
2	A	1879	C	N1-C6	14.46	1.45	1.37
1	B	1242	G	C8-N7	-13.58	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1236	A	C5-C4	13.00	1.47	1.38
3	E	19	G	N7-C5	12.89	1.47	1.39
2	A	2126	A	N3-C4	-12.71	1.27	1.34
3	E	74	A	N3-C4	12.13	1.42	1.34
2	A	2140	G	N7-C5	11.96	1.46	1.39
3	E	10	G	C8-N7	11.82	1.38	1.30
2	A	1895	C	N1-C6	11.80	1.44	1.37
3	E	9	G	N7-C5	11.66	1.46	1.39
2	A	2179	C	C2-N3	11.44	1.45	1.35
3	E	52	C	N1-C6	11.44	1.44	1.37
3	E	2	G	N9-C8	11.41	1.45	1.37
2	A	2186	G	N3-C4	11.28	1.43	1.35
1	B	1305	G	N7-C5	11.16	1.46	1.39
1	B	1334	G	C5-C4	11.09	1.46	1.38
2	A	2097	A	N9-C4	-11.05	1.31	1.37
2	A	2114	A	C8-N7	10.97	1.39	1.31
1	B	1290	G	N7-C5	10.84	1.45	1.39
2	A	2095	A	N7-C5	-10.82	1.32	1.39
3	E	36	A	N7-C5	-10.76	1.32	1.39
2	A	2115	G	P-O5'	-10.74	1.49	1.59
3	E	58	A	C6-N1	10.73	1.43	1.35
2	A	2096	C	N1-C6	10.71	1.43	1.37
3	E	55	U	P-O5'	-10.70	1.49	1.59
3	E	46	G	N7-C5	-10.64	1.32	1.39
3	E	68	C	N1-C2	-10.48	1.29	1.40
2	A	1886	U	C5'-C4'	10.42	1.63	1.51
2	A	2100	G	N3-C4	10.32	1.42	1.35
3	E	6	G	C6-N1	10.23	1.46	1.39
3	E	10	G	N7-C5	-10.20	1.33	1.39
3	E	30	G	N1-C2	-10.17	1.29	1.37
2	A	2183	A	N9-C4	-10.15	1.31	1.37
1	B	1299	A	C6-N1	-10.04	1.28	1.35
3	E	57	C	N1-C6	10.02	1.43	1.37
3	E	28	U	C4-C5	-9.98	1.34	1.43
2	A	2124	G	N9-C4	-9.98	1.29	1.38
1	B	1332	A	N9-C4	9.95	1.43	1.37
2	A	1849	G	C5-C4	9.90	1.45	1.38
2	A	2140	G	C5-C4	9.89	1.45	1.38
2	A	1872	A	N9-C4	-9.84	1.31	1.37
2	A	2115	G	C5'-C4'	9.84	1.63	1.51
2	A	2094	A	C5-C4	9.83	1.45	1.38
2	A	2110	G	C4'-C3'	9.82	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1897	G	N9-C4	-9.80	1.30	1.38
2	A	2180	U	N1-C6	9.73	1.46	1.38
2	A	2158	A	C5'-C4'	9.70	1.62	1.51
1	B	1298	U	C2'-C1'	-9.69	1.42	1.53
2	A	2161	C	C5'-C4'	9.64	1.62	1.51
2	A	2161	C	P-O5'	-9.62	1.50	1.59
2	A	1869	G	C6-N1	-9.61	1.32	1.39
2	A	1852	U	N3-C4	-9.58	1.29	1.38
2	A	1893	C	N3-C4	-9.57	1.27	1.33
2	A	2153	C	C2-N3	9.53	1.43	1.35
1	B	1305	G	C2'-C1'	-9.50	1.43	1.53
2	A	2170	A	N3-C4	-9.47	1.29	1.34
2	A	2173	A	O3'-P	-9.43	1.49	1.61
3	E	22	A	N7-C5	9.43	1.45	1.39
2	A	2144	G	N7-C5	9.38	1.44	1.39
2	A	2122	U	O3'-P	-9.35	1.50	1.61
2	A	2166	U	C5'-C4'	9.30	1.62	1.51
2	A	2111	U	C5'-C4'	9.30	1.62	1.51
1	B	1239	A	O3'-P	-9.28	1.50	1.61
3	E	20	G	C4'-O4'	-9.28	1.33	1.45
2	A	2123	G	C6-N1	-9.25	1.33	1.39
3	E	35	C	O3'-P	-9.25	1.50	1.61
3	E	5	G	C8-N7	9.23	1.36	1.30
1	B	1290	G	N9-C4	9.19	1.45	1.38
2	A	1885	A	N7-C5	-9.18	1.33	1.39
3	E	59	A	C8-N7	9.16	1.38	1.31
2	A	1873	G	C6-N1	9.16	1.46	1.39
1	B	1303	C	P-O5'	-9.15	1.50	1.59
2	A	1835	G	C8-N7	9.13	1.36	1.30
2	A	1847	A	O3'-P	-9.13	1.50	1.61
3	E	12	G	C6-N1	9.12	1.46	1.39
2	A	1838	C	C5'-C4'	9.11	1.62	1.51
3	E	66	C	N1-C6	9.09	1.42	1.37
2	A	1857	G	N9-C4	-9.07	1.30	1.38
2	A	2112	G	C5'-C4'	9.04	1.62	1.51
3	E	2	G	N7-C5	9.04	1.44	1.39
1	B	1333	A	N7-C5	9.04	1.44	1.39
3	E	33	C	C2-N3	-9.04	1.28	1.35
2	A	1888	G	P-O5'	-8.95	1.50	1.59
3	E	48	U	O3'-P	-8.95	1.50	1.61
1	B	1290	G	C4'-C3'	8.93	1.62	1.53
2	A	2116	G	N9-C8	-8.93	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	75	C	C4'-C3'	8.91	1.62	1.53
3	E	26	C	O3'-P	8.90	1.71	1.61
2	A	1901	A	N9-C4	8.90	1.43	1.37
2	A	2101	A	C5-C4	8.90	1.45	1.38
2	A	2158	A	O3'-P	-8.89	1.50	1.61
2	A	1835	G	P-O5'	-8.81	1.50	1.59
2	A	2107	G	P-O5'	-8.80	1.50	1.59
2	A	1890	A	N7-C5	-8.80	1.33	1.39
2	A	2136	G	C2'-C1'	-8.80	1.43	1.53
2	A	1845	G	N7-C5	8.79	1.44	1.39
3	E	24	C	C5'-C4'	8.77	1.61	1.51
2	A	1849	G	N3-C4	-8.71	1.29	1.35
2	A	2119	A	C6-N6	8.69	1.41	1.33
3	E	25	U	C2'-C1'	8.69	1.62	1.53
3	E	34	U	C2-N3	8.67	1.43	1.37
2	A	2146	C	C5'-C4'	8.67	1.61	1.51
3	E	69	C	C5'-C4'	8.66	1.61	1.51
2	A	1849	G	N1-C2	-8.62	1.30	1.37
1	B	1245	C	N3-C4	8.61	1.40	1.33
1	B	1304	G	N9-C8	8.61	1.43	1.37
1	B	1299	A	N9-C4	-8.60	1.32	1.37
1	B	1294	G	C3'-C2'	-8.58	1.43	1.52
2	A	1852	U	O3'-P	-8.57	1.50	1.61
2	A	2142	A	O3'-P	-8.57	1.50	1.61
3	E	74	A	P-O5'	-8.57	1.51	1.59
3	E	30	G	N7-C5	8.53	1.44	1.39
2	A	1862	G	C6-N1	-8.53	1.33	1.39
2	A	2164	C	N1-C6	8.52	1.42	1.37
2	A	1866	A	C2'-C1'	-8.48	1.44	1.53
2	A	1835	G	N3-C4	-8.47	1.29	1.35
2	A	1867	G	O3'-P	-8.47	1.50	1.61
2	A	1839	G	O4'-C1'	8.47	1.52	1.41
2	A	1837	C	C1'-N1	8.45	1.61	1.48
2	A	2171	A	N7-C5	8.44	1.44	1.39
2	A	1840	G	N3-C4	-8.39	1.29	1.35
2	A	2124	G	P-O5'	-8.36	1.51	1.59
2	A	2167	U	C4'-O4'	8.35	1.56	1.45
3	E	23	G	N1-C2	8.33	1.44	1.37
2	A	1874	C	C5'-C4'	8.29	1.61	1.51
2	A	2146	C	C4-N4	-8.28	1.26	1.33
2	A	2168	G	N7-C5	-8.28	1.34	1.39
1	B	1297	G	C2-N2	-8.27	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1334	G	N7-C5	-8.24	1.34	1.39
3	E	38	A	C5-C4	8.24	1.44	1.38
2	A	2114	A	N9-C4	8.22	1.42	1.37
3	E	26	C	N1-C6	8.22	1.42	1.37
2	A	1878	G	C8-N7	8.22	1.35	1.30
2	A	2171	A	O3'-P	-8.22	1.51	1.61
2	A	1902	C	C3'-C2'	-8.21	1.43	1.52
4	D	244	TYR	CE2-CZ	8.18	1.49	1.38
1	B	1301	U	P-O5'	-8.18	1.51	1.59
3	E	69	C	C2'-C1'	-8.17	1.44	1.53
1	B	1289	A	C5'-C4'	8.15	1.61	1.51
2	A	1844	C	N1-C6	8.15	1.42	1.37
3	E	47	G	C3'-O3'	8.12	1.53	1.42
3	E	63	C	N1-C6	8.09	1.42	1.37
2	A	2097	A	N7-C5	-8.09	1.34	1.39
1	B	1239	A	N9-C4	8.06	1.42	1.37
3	E	39	A	C3'-C2'	-8.05	1.43	1.52
3	E	5	G	C2-N2	-8.02	1.26	1.34
3	E	44	A	C5-C4	8.01	1.44	1.38
1	B	1295	U	C4'-C3'	-7.99	1.44	1.53
2	A	2120	G	C8-N7	-7.98	1.26	1.30
1	B	1297	G	N7-C5	7.93	1.44	1.39
2	A	2105	U	C4-C5	7.92	1.50	1.43
1	B	1237	C	N3-C4	-7.89	1.28	1.33
2	A	1873	G	P-O5'	-7.89	1.51	1.59
2	A	1837	C	C4-C5	7.88	1.49	1.43
2	A	1878	G	C4'-C3'	7.88	1.61	1.53
2	A	1898	U	C4-C5	7.87	1.50	1.43
2	A	2101	A	C6-N1	7.86	1.41	1.35
3	E	39	A	C2-N3	-7.86	1.26	1.33
2	A	2161	C	C2-N3	-7.85	1.29	1.35
3	E	66	C	N3-C4	7.85	1.39	1.33
3	E	18	U	C4'-C3'	-7.83	1.44	1.53
2	A	2165	C	P-O5'	-7.83	1.51	1.59
2	A	1870	C	C5'-C4'	7.82	1.60	1.51
2	A	2170	A	N9-C4	7.82	1.42	1.37
2	A	2119	A	N7-C5	-7.81	1.34	1.39
2	A	2152	G	N7-C5	-7.80	1.34	1.39
2	A	2175	C	N1-C6	7.80	1.41	1.37
2	A	2176	A	P-O5'	7.80	1.67	1.59
2	A	1876	A	C5'-C4'	7.79	1.60	1.51
2	A	1855	U	C2-N3	-7.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2151	U	N3-C4	-7.77	1.31	1.38
3	E	60	A	C2-N3	7.77	1.40	1.33
2	A	2161	C	C4-C5	7.77	1.49	1.43
3	E	77	A	C4'-O4'	-7.73	1.35	1.45
2	A	2145	C	C3'-C2'	7.73	1.61	1.52
3	E	57	C	P-O5'	-7.73	1.52	1.59
2	A	2094	A	N3-C4	-7.72	1.30	1.34
2	A	2159	G	O3'-P	-7.72	1.51	1.61
2	A	2186	G	N9-C8	-7.72	1.32	1.37
3	E	4	G	N9-C4	-7.71	1.31	1.38
2	A	1844	C	C2'-C1'	-7.70	1.44	1.53
2	A	1874	C	O3'-P	-7.70	1.51	1.61
2	A	2150	C	C2-N3	-7.69	1.29	1.35
1	B	1301	U	C2-N3	7.67	1.43	1.37
3	E	46	G	C5-C4	7.65	1.43	1.38
2	A	1890	A	C6-N6	7.63	1.40	1.33
3	E	45	A	O3'-P	-7.61	1.52	1.61
3	E	42	C	P-O5'	-7.59	1.52	1.59
2	A	1874	C	N3-C4	7.58	1.39	1.33
3	E	15	G	C5-C4	7.58	1.43	1.38
2	A	2117	A	C5'-C4'	7.58	1.60	1.51
1	B	1335	U	C2-N3	7.57	1.43	1.37
3	E	55	U	C5'-C4'	7.57	1.60	1.51
2	A	2130	U	C2'-C1'	-7.56	1.45	1.53
4	D	334	GLY	CA-C	-7.55	1.39	1.51
1	B	1300	G	N9-C8	-7.54	1.32	1.37
2	A	1863	G	N9-C8	7.54	1.43	1.37
1	B	1238	A	N7-C5	7.53	1.43	1.39
3	E	13	C	N1-C6	7.53	1.41	1.37
2	A	2144	G	C5'-C4'	7.53	1.60	1.51
2	A	1867	G	N3-C4	7.52	1.40	1.35
2	A	2128	G	N9-C8	-7.50	1.32	1.37
2	A	2099	U	C3'-O3'	7.50	1.52	1.42
2	A	1847	A	N3-C4	-7.49	1.30	1.34
2	A	1850	G	P-O5'	-7.49	1.52	1.59
3	E	45	A	N9-C8	7.48	1.43	1.37
2	A	2189	U	C3'-O3'	7.47	1.52	1.42
2	A	2180	U	O3'-P	-7.47	1.52	1.61
2	A	2135	A	N3-C4	7.46	1.39	1.34
2	A	2165	C	C4-N4	-7.45	1.27	1.33
2	A	2181	U	P-O5'	-7.43	1.52	1.59
2	A	2187	U	C4'-C3'	7.42	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2107	G	C5-C4	-7.40	1.33	1.38
2	A	2128	G	C6-N1	7.39	1.44	1.39
2	A	1858	A	C6-N1	-7.39	1.30	1.35
4	D	470	GLU	CD-OE1	7.39	1.33	1.25
3	E	49	C	P-O5'	-7.36	1.52	1.59
3	E	30	G	P-O5'	-7.36	1.52	1.59
3	E	40	C	C2-N3	-7.35	1.29	1.35
2	A	2112	G	N9-C4	7.35	1.43	1.38
2	A	2100	G	P-O5'	-7.34	1.52	1.59
2	A	2119	A	N9-C8	7.34	1.43	1.37
2	A	1885	A	C5'-C4'	7.33	1.60	1.51
3	E	59	A	N9-C4	-7.33	1.33	1.37
2	A	2151	U	O3'-P	-7.32	1.52	1.61
2	A	2150	C	C2-O2	7.31	1.31	1.24
2	A	2099	U	O3'-P	-7.29	1.52	1.61
2	A	2133	G	N7-C5	-7.28	1.34	1.39
3	E	43	G	C5-C6	7.25	1.49	1.42
3	E	63	C	P-O5'	-7.25	1.52	1.59
3	E	27	G	C2-N2	-7.23	1.27	1.34
3	E	29	C	P-O5'	-7.23	1.52	1.59
3	E	36	A	N3-C4	-7.22	1.30	1.34
2	A	2178	C	C4-C5	-7.21	1.37	1.43
2	A	2099	U	C2'-C1'	-7.20	1.45	1.53
2	A	1881	C	C3'-O3'	7.18	1.52	1.42
1	B	1302	C	C4-N4	-7.17	1.27	1.33
2	A	1906	G	C4'-C3'	-7.17	1.45	1.53
2	A	2108	A	N9-C4	-7.17	1.33	1.37
2	A	1862	G	C5-C6	7.16	1.49	1.42
2	A	2173	A	C5-C6	7.16	1.47	1.41
2	A	1846	G	C5'-C4'	7.15	1.59	1.51
1	B	1299	A	N3-C4	7.14	1.39	1.34
2	A	2101	A	P-O5'	-7.14	1.52	1.59
2	A	2182	U	O3'-P	-7.14	1.52	1.61
2	A	2170	A	P-O5'	-7.13	1.52	1.59
1	B	1334	G	O3'-P	-7.12	1.52	1.61
3	E	55	U	C2'-C1'	-7.11	1.45	1.53
2	A	1867	G	C6-O6	7.11	1.30	1.24
2	A	2136	G	C5'-C4'	7.11	1.59	1.51
3	E	31	G	N3-C4	7.11	1.40	1.35
2	A	2111	U	C3'-O3'	7.10	1.52	1.42
2	A	1894	C	N3-C4	7.09	1.39	1.33
1	B	1297	G	N9-C4	7.08	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1305	G	C6-N1	-7.07	1.34	1.39
2	A	2124	G	C6-O6	-7.05	1.17	1.24
3	E	43	G	N3-C4	-7.04	1.30	1.35
2	A	1906	G	N3-C4	-7.03	1.30	1.35
2	A	1893	C	P-O5'	-7.03	1.52	1.59
1	B	1334	G	N3-C4	-7.02	1.30	1.35
3	E	47	G	C8-N7	7.02	1.35	1.30
2	A	2170	A	C5-C6	-7.01	1.34	1.41
2	A	2175	C	C5'-C4'	6.99	1.59	1.51
3	E	3	C	N1-C2	6.98	1.47	1.40
3	E	11	A	N7-C5	-6.98	1.35	1.39
3	E	36	A	C5-C4	6.98	1.43	1.38
2	A	1888	G	O3'-P	-6.97	1.52	1.61
3	E	10	G	C2-N2	6.96	1.41	1.34
2	A	2158	A	N7-C5	-6.96	1.35	1.39
2	A	1863	G	O3'-P	-6.94	1.52	1.61
2	A	2160	C	C4'-O4'	6.94	1.54	1.45
2	A	1848	A	C6-N1	6.93	1.40	1.35
2	A	2156	G	C2'-C1'	-6.93	1.45	1.53
2	A	2175	C	O4'-C1'	-6.93	1.32	1.41
2	A	2168	G	C6-N1	6.92	1.44	1.39
1	B	1303	C	N1-C6	6.92	1.41	1.37
2	A	1898	U	C5'-C4'	6.92	1.59	1.51
2	A	1892	C	N1-C6	6.92	1.41	1.37
2	A	2112	G	C2-N3	6.91	1.38	1.32
2	A	2173	A	C2'-C1'	6.91	1.60	1.53
2	A	1904	G	N7-C5	6.89	1.43	1.39
2	A	2159	G	C5'-C4'	6.89	1.59	1.51
3	E	30	G	C3'-C2'	6.88	1.60	1.52
3	E	54	G	N9-C8	-6.87	1.33	1.37
3	E	23	G	C2-N2	-6.87	1.27	1.34
3	E	70	C	C5'-C4'	6.86	1.59	1.51
2	A	2158	A	C8-N7	6.84	1.36	1.31
2	A	1866	A	C6-N1	6.84	1.40	1.35
3	E	1	C	N3-C4	6.83	1.38	1.33
3	E	42	C	C5'-C4'	6.83	1.59	1.51
2	A	2193	G	C6-N1	6.83	1.44	1.39
2	A	1865	U	O3'-P	-6.82	1.52	1.61
2	A	2192	U	N1-C6	-6.82	1.31	1.38
2	A	2193	G	C8-N7	6.82	1.35	1.30
3	E	23	G	C4'-C3'	6.81	1.60	1.53
2	A	2097	A	C8-N7	-6.81	1.26	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	50	G	N7-C5	-6.80	1.35	1.39
2	A	2143	C	C3'-C2'	6.79	1.60	1.52
3	E	45	A	C5'-C4'	6.78	1.59	1.51
2	A	1838	C	P-O5'	-6.77	1.52	1.59
3	E	10	G	O4'-C1'	6.77	1.50	1.41
2	A	1847	A	C4'-C3'	6.76	1.60	1.53
2	A	1872	A	C5-C4	6.75	1.43	1.38
2	A	2152	G	P-O5'	-6.74	1.53	1.59
1	B	1237	C	O3'-P	-6.74	1.53	1.61
2	A	2192	U	C5'-C4'	6.72	1.59	1.51
1	B	1243	C	N3-C4	6.71	1.38	1.33
3	E	52	C	O4'-C1'	-6.71	1.32	1.41
1	B	1292	G	O3'-P	-6.70	1.53	1.61
1	B	1245	C	C4'-C3'	6.67	1.60	1.53
2	A	1838	C	N3-C4	6.67	1.38	1.33
2	A	2133	G	C5'-C4'	6.67	1.59	1.51
2	A	2177	C	N3-C4	6.66	1.38	1.33
3	E	45	A	N1-C2	6.66	1.40	1.34
2	A	1834	U	O3'-P	-6.65	1.53	1.61
2	A	1866	A	N3-C4	6.64	1.38	1.34
1	B	1238	A	C6-N6	6.63	1.39	1.33
2	A	2186	G	C3'-O3'	6.62	1.51	1.42
2	A	2184	A	C6-N1	-6.60	1.30	1.35
3	E	39	A	N3-C4	-6.60	1.30	1.34
3	E	28	U	C4'-C3'	6.59	1.60	1.53
1	B	1297	G	C8-N7	6.58	1.34	1.30
2	A	2108	A	C6-N1	6.58	1.40	1.35
2	A	2143	C	P-O5'	-6.57	1.53	1.59
2	A	2186	G	C2-N2	-6.56	1.27	1.34
2	A	2125	G	C2-N2	-6.55	1.28	1.34
2	A	2140	G	C2'-C1'	-6.55	1.46	1.53
3	E	49	C	C2-N3	6.55	1.41	1.35
2	A	2127	G	O4'-C1'	6.54	1.50	1.41
2	A	2129	C	C4-N4	-6.54	1.28	1.33
3	E	47	G	N7-C5	6.54	1.43	1.39
4	D	441	ARG	CD-NE	6.54	1.57	1.46
2	A	2119	A	N3-C4	-6.53	1.30	1.34
2	A	2174	C	C5'-C4'	6.53	1.59	1.51
3	E	30	G	C5-C4	-6.50	1.33	1.38
2	A	2124	G	C2-N3	-6.50	1.27	1.32
3	E	52	C	C2-N3	-6.50	1.30	1.35
2	A	2142	A	N1-C2	-6.50	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1903	G	C6-N1	-6.49	1.35	1.39
2	A	1843	C	C3'-C2'	-6.47	1.45	1.52
2	A	2133	G	N3-C4	-6.46	1.30	1.35
2	A	2153	C	C5'-C4'	6.45	1.59	1.51
2	A	1839	G	O3'-P	-6.45	1.53	1.61
1	B	1299	A	P-O5'	-6.45	1.53	1.59
2	A	1866	A	N9-C4	-6.45	1.33	1.37
2	A	2191	A	P-O5'	-6.45	1.53	1.59
2	A	2179	C	N1-C2	-6.44	1.33	1.40
3	E	64	G	N9-C8	6.44	1.42	1.37
3	E	43	G	O3'-P	-6.44	1.53	1.61
3	E	73	A	C5-C4	6.44	1.43	1.38
4	D	220	TYR	CG-CD2	6.42	1.47	1.39
2	A	1872	A	N3-C4	-6.42	1.30	1.34
2	A	2104	C	C2'-C1'	-6.42	1.46	1.53
2	A	2129	C	C5-C6	-6.42	1.29	1.34
2	A	2142	A	C6-N1	6.42	1.40	1.35
2	A	2170	A	C6-N6	6.42	1.39	1.33
1	B	1335	U	C4-C5	6.41	1.49	1.43
2	A	2170	A	N9-C8	6.41	1.42	1.37
3	E	38	A	C2'-C1'	6.40	1.60	1.53
2	A	1859	U	N1-C6	-6.40	1.32	1.38
2	A	2164	C	C5-C6	-6.40	1.29	1.34
3	E	58	A	C2-N3	6.39	1.39	1.33
2	A	1879	C	C5'-C4'	6.39	1.59	1.51
2	A	2151	U	C4'-C3'	6.38	1.60	1.53
3	E	4	G	C5-C4	-6.38	1.33	1.38
2	A	1869	G	C2-N3	-6.37	1.27	1.32
2	A	2169	A	N9-C4	-6.37	1.34	1.37
3	E	50	G	C2'-C1'	-6.36	1.46	1.53
2	A	1834	U	C2-N3	6.36	1.42	1.37
2	A	2095	A	C3'-O3'	6.36	1.51	1.42
2	A	2105	U	C2'-C1'	-6.36	1.46	1.53
2	A	2136	G	C6-N1	6.33	1.44	1.39
2	A	1862	G	C2-N2	-6.33	1.28	1.34
3	E	6	G	C5'-C4'	6.32	1.58	1.51
2	A	1835	G	N9-C8	6.31	1.42	1.37
2	A	2147	A	N3-C4	-6.31	1.31	1.34
3	E	25	U	C4-C5	-6.30	1.37	1.43
2	A	2149	U	C5'-C4'	6.30	1.58	1.51
2	A	2174	C	N3-C4	6.30	1.38	1.33
2	A	2138	G	N1-C2	6.29	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2172	U	O3'-P	-6.29	1.53	1.61
2	A	2178	C	O3'-P	-6.28	1.53	1.61
2	A	1853	A	C6-N6	-6.28	1.28	1.33
2	A	2188	U	O3'-P	-6.27	1.53	1.61
3	E	7	G	N9-C4	6.24	1.43	1.38
3	E	26	C	C2-N3	-6.24	1.30	1.35
1	B	1304	G	C4'-O4'	6.24	1.53	1.45
2	A	1877	A	C6-N1	6.23	1.40	1.35
1	B	1292	G	N9-C8	6.23	1.42	1.37
2	A	2175	C	O5'-C5'	6.22	1.54	1.44
2	A	2112	G	C6-O6	6.22	1.29	1.24
2	A	2174	C	C5-C6	6.21	1.39	1.34
2	A	1856	U	C4-C5	-6.21	1.38	1.43
2	A	2152	G	C5-C4	-6.21	1.34	1.38
2	A	2119	A	O3'-P	-6.20	1.53	1.61
4	D	124	GLU	CB-CG	6.20	1.64	1.52
2	A	1901	A	O3'-P	-6.19	1.53	1.61
1	B	1336	C	C4'-C3'	6.19	1.59	1.53
3	E	42	C	N1-C6	6.19	1.40	1.37
3	E	29	C	C4-C5	-6.19	1.38	1.43
2	A	1840	G	C6-N1	-6.19	1.35	1.39
2	A	2184	A	N9-C4	-6.18	1.34	1.37
2	A	1851	U	C5'-C4'	6.18	1.58	1.51
2	A	1860	G	N3-C4	-6.18	1.31	1.35
2	A	1902	C	C4'-C3'	6.18	1.59	1.53
2	A	2127	G	N9-C8	6.18	1.42	1.37
3	E	13	C	C4-C5	6.17	1.47	1.43
2	A	2128	G	C2-N2	-6.17	1.28	1.34
3	E	30	G	C6-O6	-6.16	1.18	1.24
3	E	9	G	C6-N1	6.16	1.43	1.39
2	A	2133	G	C6-N1	6.16	1.43	1.39
2	A	2127	G	N7-C5	-6.15	1.35	1.39
2	A	1884	G	C6-N1	6.15	1.43	1.39
2	A	2112	G	C2-N2	-6.15	1.28	1.34
1	B	1241	G	N3-C4	-6.14	1.31	1.35
2	A	1879	C	C2-N3	6.14	1.40	1.35
2	A	2147	A	C2'-C1'	-6.14	1.46	1.53
3	E	64	G	C5'-C4'	6.14	1.58	1.51
2	A	2157	G	P-O5'	-6.13	1.53	1.59
2	A	2116	G	C8-N7	6.13	1.34	1.30
1	B	1239	A	C1'-N9	-6.13	1.38	1.46
2	A	2176	A	N7-C5	6.12	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	29	C	N1-C6	6.12	1.40	1.37
2	A	2175	C	C3'-C2'	-6.12	1.46	1.52
3	E	13	C	C2-N3	-6.12	1.30	1.35
3	E	19	G	N3-C4	6.12	1.39	1.35
2	A	1834	U	P-O5'	-6.12	1.53	1.59
3	E	33	C	C4'-C3'	-6.11	1.46	1.53
1	B	1305	G	C4'-O4'	-6.11	1.37	1.45
2	A	2133	G	O3'-P	-6.11	1.53	1.61
2	A	2149	U	N3-C4	6.10	1.44	1.38
2	A	2158	A	C4'-C3'	6.10	1.59	1.53
3	E	48	U	N1-C6	-6.10	1.32	1.38
2	A	1895	C	C2-O2	-6.10	1.19	1.24
6	G	174	PHE	CE2-CZ	6.10	1.49	1.37
2	A	1896	G	C2'-C1'	-6.10	1.46	1.53
3	E	21	U	C2'-O2'	6.10	1.49	1.41
2	A	2149	U	C4'-O4'	-6.09	1.37	1.45
2	A	2154	A	C5'-C4'	-6.09	1.44	1.51
1	B	1298	U	N3-C4	-6.09	1.32	1.38
2	A	2101	A	C5'-C4'	6.08	1.58	1.51
3	E	49	C	N1-C6	-6.08	1.33	1.37
3	E	14	A	N3-C4	-6.08	1.31	1.34
1	B	1294	G	N9-C8	6.07	1.42	1.37
2	A	2192	U	C2-N3	-6.07	1.33	1.37
1	B	1295	U	C2-N3	6.07	1.42	1.37
2	A	1848	A	P-O5'	-6.07	1.53	1.59
2	A	1875	G	O3'-P	-6.07	1.53	1.61
2	A	2186	G	C6-N1	-6.07	1.35	1.39
1	B	1243	C	C5'-C4'	6.06	1.58	1.51
2	A	2155	U	C3'-O3'	6.06	1.50	1.42
2	A	1907	G	C6-N1	6.05	1.43	1.39
1	B	1294	G	P-O5'	-6.05	1.53	1.59
1	B	1304	G	O3'-P	-6.05	1.53	1.61
3	E	42	C	C1'-N1	6.05	1.57	1.48
3	E	61	U	P-O5'	-6.05	1.53	1.59
1	B	1291	U	C2'-C1'	-6.04	1.46	1.53
2	A	1846	G	C2-N3	6.03	1.37	1.32
3	E	69	C	N1-C6	-6.03	1.33	1.37
2	A	2104	C	C4'-C3'	6.03	1.59	1.53
3	E	19	G	P-O5'	-6.03	1.53	1.59
2	A	1877	A	C4'-C3'	-6.02	1.46	1.53
3	E	64	G	C2'-C1'	-6.02	1.46	1.53
3	E	69	C	C3'-C2'	-6.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1241	G	N7-C5	-6.01	1.35	1.39
2	A	1896	G	P-O5'	-6.01	1.53	1.59
1	B	1238	A	C6-N1	6.00	1.39	1.35
3	E	49	C	O3'-P	-6.00	1.53	1.61
1	B	1244	G	O3'-P	-6.00	1.53	1.61
3	E	2	G	C2-N2	-6.00	1.28	1.34
2	A	1901	A	N1-C2	-6.00	1.28	1.34
2	A	2119	A	N9-C4	-6.00	1.34	1.37
3	E	77	A	C8-N7	-6.00	1.27	1.31
2	A	2114	A	C4'-C3'	6.00	1.59	1.53
3	E	42	C	C2-N3	-5.99	1.30	1.35
2	A	1871	A	C2'-C1'	-5.99	1.46	1.53
2	A	1869	G	N9-C4	-5.98	1.33	1.38
2	A	2171	A	N3-C4	-5.98	1.31	1.34
2	A	1884	G	C2'-C1'	5.98	1.59	1.53
2	A	1907	G	C2-N3	5.98	1.37	1.32
3	E	44	A	N3-C4	5.97	1.38	1.34
2	A	1875	G	N1-C2	5.97	1.42	1.37
2	A	1893	C	N1-C2	5.97	1.46	1.40
3	E	34	U	C3'-C2'	-5.97	1.46	1.52
2	A	1856	U	N3-C4	5.96	1.43	1.38
3	E	43	G	C4'-C3'	5.96	1.59	1.53
2	A	2170	A	N7-C5	5.95	1.42	1.39
3	E	72	C	C4'-C3'	5.95	1.59	1.53
2	A	2099	U	C4-O4	-5.94	1.18	1.23
1	B	1292	G	C5'-C4'	5.94	1.58	1.51
2	A	2137	U	C4'-O4'	5.94	1.53	1.45
2	A	2111	U	N3-C4	-5.93	1.33	1.38
3	E	12	G	C5'-C4'	5.93	1.58	1.51
2	A	1857	G	C6-N1	-5.92	1.35	1.39
3	E	73	A	N9-C8	5.92	1.42	1.37
5	F	32	GLU	CA-CB	5.92	1.67	1.53
4	D	189	PRO	N-CD	-5.90	1.39	1.47
2	A	1888	G	C6-N1	5.90	1.43	1.39
2	A	2172	U	C2'-C1'	5.90	1.59	1.53
2	A	2176	A	C5-C4	-5.90	1.34	1.38
2	A	2182	U	O4'-C1'	5.90	1.49	1.41
2	A	1885	A	C5-C4	5.90	1.42	1.38
8	I	2	ARG	CD-NE	5.90	1.56	1.46
6	G	132	ARG	CZ-NH1	5.89	1.40	1.33
2	A	2142	A	N9-C4	5.89	1.41	1.37
3	E	20	G	N9-C8	-5.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1245	C	C2'-C1'	-5.88	1.46	1.53
2	A	2119	A	C8-N7	-5.88	1.27	1.31
2	A	1835	G	N1-C2	-5.88	1.33	1.37
2	A	1891	G	N9-C8	-5.88	1.33	1.37
2	A	2181	U	N3-C4	5.88	1.43	1.38
2	A	1848	A	C5'-C4'	5.87	1.58	1.51
2	A	2134	A	C8-N7	-5.87	1.27	1.31
3	E	13	C	C2'-C1'	-5.87	1.46	1.53
1	B	1299	A	N7-C5	5.87	1.42	1.39
2	A	1846	G	C4'-C3'	5.87	1.59	1.53
2	A	1904	G	P-O5'	-5.87	1.53	1.59
2	A	1848	A	C3'-C2'	-5.87	1.46	1.52
2	A	2122	U	N1-C2	-5.86	1.33	1.38
2	A	2154	A	N9-C4	-5.86	1.34	1.37
3	E	26	C	N3-C4	5.86	1.38	1.33
1	B	1332	A	P-O5'	-5.85	1.53	1.59
2	A	2111	U	O3'-P	-5.85	1.54	1.61
2	A	2117	A	N1-C2	-5.84	1.29	1.34
2	A	2095	A	C5-C6	5.84	1.46	1.41
2	A	1868	C	C2-N3	-5.83	1.31	1.35
2	A	1838	C	C2-N3	5.83	1.40	1.35
2	A	2155	U	P-O5'	-5.83	1.53	1.59
2	A	2119	A	C4'-O4'	5.82	1.53	1.45
2	A	2191	A	C2-N3	-5.82	1.28	1.33
2	A	1893	C	C3'-C2'	5.82	1.59	1.52
2	A	2144	G	C2-N2	-5.81	1.28	1.34
8	I	138	GLU	CD-OE1	-5.81	1.19	1.25
2	A	2171	A	P-O5'	-5.81	1.53	1.59
8	I	4	ARG	CD-NE	5.80	1.56	1.46
2	A	2181	U	C2-N3	-5.79	1.33	1.37
1	B	1293	C	C4-N4	-5.78	1.28	1.33
2	A	1850	G	C8-N7	5.78	1.34	1.30
2	A	2127	G	C2-N3	5.78	1.37	1.32
2	A	1850	G	C5-C4	-5.76	1.34	1.38
2	A	2190	G	N9-C8	5.75	1.41	1.37
2	A	1835	G	C2-N3	5.75	1.37	1.32
2	A	1895	C	O3'-P	-5.75	1.54	1.61
3	E	11	A	C5-C6	-5.75	1.35	1.41
2	A	2134	A	C5-C6	5.75	1.46	1.41
2	A	2136	G	C5-C4	-5.75	1.34	1.38
3	E	48	U	P-O5'	5.74	1.65	1.59
3	E	4	G	N1-C2	-5.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1845	G	C5'-C4'	5.74	1.58	1.51
2	A	2115	G	O4'-C1'	5.73	1.49	1.41
2	A	2098	U	C2'-C1'	-5.72	1.47	1.53
2	A	2181	U	N1-C6	-5.72	1.32	1.38
2	A	2131	U	C4-C5	5.71	1.48	1.43
2	A	1835	G	C5-C4	5.71	1.42	1.38
2	A	1884	G	P-O5'	-5.71	1.54	1.59
3	E	9	G	C4'-O4'	-5.71	1.38	1.45
1	B	1242	G	N7-C5	-5.70	1.35	1.39
2	A	1857	G	C2'-C1'	-5.70	1.47	1.53
2	A	2117	A	C4'-C3'	5.70	1.59	1.53
2	A	1881	C	C4-N4	-5.70	1.28	1.33
7	H	27	ARG	CD-NE	5.69	1.56	1.46
2	A	1895	C	C4'-C3'	-5.68	1.46	1.52
1	B	1294	G	C5-C6	5.68	1.48	1.42
1	B	1243	C	O3'-P	-5.68	1.54	1.61
2	A	2117	A	C2-N3	-5.68	1.28	1.33
2	A	2139	U	P-O5'	-5.68	1.54	1.59
2	A	2103	C	C4-C5	-5.68	1.38	1.43
3	E	13	C	N3-C4	5.67	1.38	1.33
1	B	1298	U	O3'-P	-5.66	1.54	1.61
3	E	23	G	C3'-C2'	-5.66	1.46	1.52
2	A	1847	A	C6-N1	-5.65	1.31	1.35
2	A	2112	G	C5-C4	-5.65	1.34	1.38
2	A	2144	G	C3'-O3'	5.65	1.50	1.42
6	G	123	GLY	N-CA	5.65	1.54	1.46
2	A	2170	A	C5-C4	5.65	1.42	1.38
2	A	2098	U	N1-C2	-5.65	1.33	1.38
3	E	23	G	O3'-P	-5.65	1.54	1.61
2	A	2147	A	O3'-P	-5.65	1.54	1.61
2	A	2106	U	P-O5'	-5.64	1.54	1.59
1	B	1239	A	N9-C8	5.64	1.42	1.37
2	A	1898	U	P-O5'	-5.64	1.54	1.59
3	E	35	C	C2-O2	5.64	1.29	1.24
2	A	1852	U	C1'-N1	-5.64	1.39	1.46
3	E	70	C	P-O5'	-5.63	1.54	1.59
2	A	2130	U	C4'-C3'	5.63	1.59	1.53
2	A	1897	G	O4'-C1'	5.60	1.49	1.41
2	A	1892	C	N3-C4	5.60	1.37	1.33
2	A	2163	A	N9-C8	5.60	1.42	1.37
2	A	2189	U	O3'-P	-5.60	1.54	1.61
2	A	2118	U	C2-N3	5.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2164	C	O3'-P	-5.60	1.54	1.61
2	A	2183	A	N9-C8	-5.60	1.33	1.37
3	E	33	C	P-O5'	-5.60	1.54	1.59
2	A	2126	A	C5-C4	-5.59	1.34	1.38
2	A	1906	G	C2-N2	-5.58	1.28	1.34
2	A	2120	G	C3'-O3'	5.58	1.50	1.42
3	E	28	U	N3-C4	5.58	1.43	1.38
2	A	2134	A	N1-C2	5.57	1.39	1.34
2	A	2125	G	C3'-C2'	-5.57	1.46	1.52
3	E	70	C	N1-C6	-5.56	1.33	1.37
2	A	2117	A	C2'-C1'	-5.56	1.47	1.53
2	A	2192	U	C4'-O4'	5.56	1.52	1.45
4	D	89	SER	CA-CB	5.56	1.61	1.52
6	G	10	GLU	CB-CG	5.55	1.62	1.52
2	A	1881	C	C2'-C1'	-5.55	1.47	1.53
2	A	1834	U	C4-C5	5.55	1.48	1.43
3	E	10	G	C2-N3	5.54	1.37	1.32
2	A	2123	G	N7-C5	5.54	1.42	1.39
2	A	2175	C	C2-N3	-5.54	1.31	1.35
1	B	1237	C	N1-C6	-5.54	1.33	1.37
3	E	7	G	C8-N7	-5.54	1.27	1.30
3	E	22	A	O3'-P	-5.54	1.54	1.61
2	A	2134	A	C6-N1	5.53	1.39	1.35
2	A	2182	U	C1'-N1	5.52	1.57	1.48
3	E	48	U	C4'-O4'	5.52	1.52	1.45
2	A	1850	G	C1'-N9	5.52	1.57	1.48
2	A	1877	A	N7-C5	5.52	1.42	1.39
2	A	2179	C	C2'-O2'	5.51	1.48	1.41
1	B	1237	C	C5'-C4'	5.51	1.57	1.51
3	E	5	G	N1-C2	5.51	1.42	1.37
5	F	68	GLY	N-CA	-5.50	1.37	1.46
4	D	37	VAL	CB-CG1	5.50	1.64	1.52
1	B	1237	C	C4'-C3'	5.50	1.59	1.53
2	A	2127	G	N3-C4	-5.50	1.31	1.35
2	A	2131	U	C4'-C3'	5.50	1.59	1.53
2	A	1889	A	C6-N1	-5.49	1.31	1.35
2	A	2099	U	C5-C6	5.49	1.39	1.34
2	A	2183	A	C8-N7	-5.49	1.27	1.31
1	B	1238	A	N3-C4	-5.49	1.31	1.34
2	A	2112	G	N9-C8	5.49	1.41	1.37
2	A	2130	U	C2-N3	-5.48	1.33	1.37
2	A	2114	A	C3'-C2'	-5.48	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1294	G	C5-C4	-5.48	1.34	1.38
2	A	2171	A	N1-C2	-5.48	1.29	1.34
5	F	151	GLU	CD-OE1	5.47	1.31	1.25
2	A	1863	G	C5-C4	5.47	1.42	1.38
2	A	1907	G	C5-C4	-5.47	1.34	1.38
3	E	54	G	N1-C2	-5.47	1.33	1.37
4	D	188	GLU	CD-OE1	5.47	1.31	1.25
3	E	4	G	P-O5'	-5.46	1.54	1.59
2	A	2147	A	C4'-C3'	-5.46	1.47	1.52
2	A	1850	G	C3'-C2'	-5.46	1.46	1.52
2	A	1844	C	O3'-P	-5.46	1.54	1.61
2	A	1886	U	C2'-C1'	-5.46	1.47	1.53
3	E	74	A	N7-C5	-5.46	1.35	1.39
1	B	1336	C	C3'-O3'	5.45	1.49	1.42
3	E	11	A	N9-C8	5.45	1.42	1.37
8	I	102	TRP	CZ3-CH2	5.45	1.48	1.40
2	A	2106	U	C3'-O3'	5.45	1.49	1.42
1	B	1239	A	C3'-O3'	5.44	1.49	1.42
4	D	316	GLY	N-CA	5.44	1.54	1.46
3	E	8	U	C5'-C4'	5.44	1.57	1.51
3	E	38	A	C8-N7	-5.43	1.27	1.31
2	A	1858	A	C3'-O3'	5.43	1.49	1.42
2	A	1857	G	O3'-P	-5.43	1.54	1.61
3	E	2	G	N9-C4	-5.43	1.33	1.38
3	E	18	U	C3'-C2'	5.43	1.58	1.52
4	D	271	LYS	CD-CE	5.43	1.64	1.51
1	B	1301	U	O3'-P	-5.42	1.54	1.61
2	A	2177	C	P-O5'	-5.42	1.54	1.59
2	A	1838	C	C4'-C3'	5.42	1.59	1.53
1	B	1236	A	C8-N7	-5.42	1.27	1.31
3	E	5	G	C5'-C4'	5.41	1.57	1.51
3	E	58	A	C5'-C4'	5.41	1.57	1.51
2	A	1845	G	C2-N2	-5.40	1.29	1.34
3	E	16	C	C4'-O4'	5.40	1.52	1.45
3	E	59	A	N9-C8	5.39	1.42	1.37
2	A	1892	C	C5-C6	-5.39	1.30	1.34
3	E	25	U	C4'-O4'	5.39	1.52	1.45
3	E	77	A	C6-N1	5.39	1.39	1.35
2	A	2188	U	C2-N3	5.39	1.41	1.37
2	A	1866	A	N7-C5	5.38	1.42	1.39
2	A	2188	U	N3-C4	-5.38	1.33	1.38
2	A	1853	A	N7-C5	-5.37	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	176	PHE	CG-CD2	5.37	1.46	1.38
1	B	1297	G	C2-N3	5.37	1.37	1.32
3	E	51	U	C1'-N1	5.37	1.56	1.48
1	B	1334	G	C6-N1	5.36	1.43	1.39
2	A	1899	A	C5-C4	-5.36	1.34	1.38
3	E	34	U	N3-C4	-5.36	1.33	1.38
2	A	2113	U	C5'-C4'	5.36	1.57	1.51
1	B	1241	G	C2-N3	-5.35	1.28	1.32
2	A	1870	C	N1-C6	-5.35	1.33	1.37
2	A	1900	A	N3-C4	-5.35	1.31	1.34
3	E	49	C	N3-C4	5.35	1.37	1.33
1	B	1302	C	C2'-C1'	-5.35	1.47	1.53
2	A	2116	G	N7-C5	5.35	1.42	1.39
2	A	2141	G	N9-C8	5.35	1.41	1.37
3	E	47	G	C4'-C3'	5.35	1.59	1.53
4	D	242	GLY	CA-C	-5.35	1.43	1.51
2	A	2107	G	O3'-P	-5.35	1.54	1.61
2	A	1871	A	N1-C2	5.34	1.39	1.34
2	A	2135	A	C5-C4	-5.34	1.35	1.38
3	E	4	G	C4'-C3'	5.34	1.59	1.53
2	A	1856	U	C2-N3	5.34	1.41	1.37
2	A	1905	C	C5'-C4'	5.33	1.57	1.51
4	D	30	PHE	CE1-CZ	5.33	1.47	1.37
1	B	1295	U	C4'-O4'	5.33	1.52	1.45
2	A	2119	A	C4'-C3'	5.33	1.59	1.53
3	E	68	C	C4-N4	5.32	1.38	1.33
2	A	2173	A	O4'-C1'	5.31	1.48	1.41
2	A	2138	G	N7-C5	5.31	1.42	1.39
2	A	2171	A	C5-C4	-5.30	1.35	1.38
2	A	1856	U	C2'-O2'	5.30	1.48	1.41
2	A	2142	A	C5'-C4'	5.30	1.57	1.51
3	E	24	C	C4'-O4'	5.30	1.52	1.45
3	E	61	U	C4'-C3'	5.30	1.58	1.53
3	E	43	G	N9-C4	-5.30	1.33	1.38
6	G	98	PHE	CA-CB	5.29	1.65	1.53
2	A	1839	G	N9-C8	5.29	1.41	1.37
2	A	2103	C	O3'-P	-5.29	1.54	1.61
2	A	2162	G	C3'-C2'	-5.29	1.47	1.52
3	E	29	C	C1'-N1	5.29	1.56	1.48
2	A	1866	A	C3'-O3'	5.29	1.49	1.42
3	E	77	A	C4'-C3'	5.28	1.58	1.53
2	A	2105	U	C3'-C2'	5.27	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	231	GLU	CG-CD	-5.27	1.44	1.51
3	E	62	C	N1-C6	5.27	1.40	1.37
2	A	1898	U	C2'-C1'	5.27	1.59	1.53
3	E	10	G	C2'-C1'	-5.27	1.47	1.53
2	A	2106	U	C5'-C4'	5.26	1.57	1.51
1	B	1332	A	N7-C5	-5.26	1.36	1.39
2	A	2160	C	C3'-C2'	5.26	1.58	1.52
3	E	44	A	N7-C5	-5.26	1.36	1.39
2	A	1886	U	C2-N3	-5.25	1.34	1.37
2	A	1840	G	C1'-N9	-5.24	1.39	1.46
2	A	1873	G	N3-C4	5.24	1.39	1.35
3	E	32	G	C4'-O4'	5.23	1.52	1.45
2	A	2141	G	C3'-O3'	5.23	1.49	1.42
2	A	1834	U	C3'-C2'	5.23	1.58	1.52
4	D	56	ASP	CA-CB	5.23	1.65	1.53
2	A	1865	U	C5-C6	-5.23	1.29	1.34
2	A	2152	G	C8-N7	-5.22	1.27	1.30
3	E	21	U	N1-C2	-5.22	1.33	1.38
3	E	51	U	C3'-O3'	5.22	1.49	1.42
2	A	2146	C	N1-C6	5.22	1.40	1.37
3	E	20	G	C2'-C1'	-5.21	1.47	1.53
2	A	1858	A	N9-C8	-5.21	1.33	1.37
2	A	2112	G	C3'-C2'	-5.21	1.47	1.52
3	E	66	C	C4-C5	5.21	1.47	1.43
8	I	128	GLU	CD-OE1	5.21	1.31	1.25
2	A	2128	G	N3-C4	5.20	1.39	1.35
3	E	58	A	N9-C4	-5.19	1.34	1.37
1	B	1240	U	C3'-C2'	5.19	1.58	1.52
2	A	1883	U	C2'-C1'	-5.19	1.47	1.53
2	A	1838	C	C2'-C1'	-5.19	1.47	1.53
3	E	53	G	C6-O6	-5.19	1.19	1.24
2	A	1866	A	C4'-C3'	-5.19	1.47	1.52
1	B	1298	U	P-O5'	-5.19	1.54	1.59
2	A	1904	G	C5'-C4'	5.19	1.57	1.51
3	E	46	G	N3-C4	-5.19	1.31	1.35
2	A	2138	G	C2-N2	-5.18	1.29	1.34
2	A	1876	A	N1-C2	5.18	1.39	1.34
2	A	2163	A	C4'-O4'	5.18	1.52	1.45
3	E	66	C	C3'-C2'	-5.18	1.47	1.52
3	E	6	G	C3'-O3'	5.18	1.49	1.42
3	E	23	G	C2-N3	-5.17	1.28	1.32
2	A	2107	G	C2-N2	-5.17	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1334	G	N9-C8	5.17	1.41	1.37
3	E	16	C	C2'-C1'	-5.16	1.47	1.53
2	A	2176	A	O3'-P	-5.16	1.54	1.61
2	A	2166	U	C4'-C3'	5.16	1.58	1.53
2	A	2123	G	C4'-C3'	5.16	1.58	1.53
2	A	1901	A	N3-C4	-5.15	1.31	1.34
2	A	2188	U	C3'-O3'	5.14	1.49	1.42
2	A	2186	G	N9-C4	5.14	1.42	1.38
2	A	2119	A	N1-C2	5.14	1.39	1.34
2	A	2157	G	N7-C5	5.13	1.42	1.39
2	A	2191	A	C5'-C4'	5.13	1.57	1.51
2	A	2193	G	C3'-O3'	5.13	1.49	1.42
2	A	2173	A	N1-C2	5.12	1.39	1.34
3	E	44	A	N9-C4	-5.12	1.34	1.37
3	E	77	A	C2-N3	-5.12	1.28	1.33
2	A	1860	G	N9-C4	5.12	1.42	1.38
2	A	2096	C	C4-C5	-5.12	1.38	1.43
2	A	1837	C	C5-C6	-5.11	1.30	1.34
2	A	2129	C	C4'-C3'	5.11	1.58	1.53
2	A	2158	A	C5-C6	-5.11	1.36	1.41
1	B	1236	A	N7-C5	-5.10	1.36	1.39
2	A	1853	A	O3'-P	-5.10	1.55	1.61
2	A	2148	G	N9-C4	5.10	1.42	1.38
4	D	73	TYR	CZ-OH	5.10	1.46	1.37
4	D	127	ARG	CD-NE	5.10	1.55	1.46
2	A	1895	C	N3-C4	5.09	1.37	1.33
2	A	1903	G	C2-N2	-5.09	1.29	1.34
2	A	2182	U	C4'-O4'	-5.09	1.39	1.45
3	E	33	C	C5'-C4'	5.09	1.57	1.51
4	D	370	SER	CB-OG	5.09	1.48	1.42
3	E	51	U	C2-N3	-5.09	1.34	1.37
2	A	2125	G	C5'-C4'	-5.08	1.45	1.51
3	E	19	G	O3'-P	-5.08	1.55	1.61
3	E	45	A	C6-N6	5.08	1.38	1.33
1	B	1289	A	C5-C6	5.07	1.45	1.41
1	B	1244	G	P-O5'	-5.07	1.54	1.59
2	A	1872	A	C6-N1	5.07	1.39	1.35
2	A	2104	C	N3-C4	-5.07	1.30	1.33
1	B	1244	G	C2-N3	5.06	1.36	1.32
2	A	2171	A	C4'-C3'	5.06	1.58	1.53
2	A	1849	G	C2'-C1'	-5.06	1.47	1.53
2	A	2159	G	C1'-N9	5.06	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	96	GLY	N-CA	5.06	1.53	1.46
3	E	58	A	N3-C4	-5.05	1.31	1.34
2	A	2162	G	C6-N1	5.05	1.43	1.39
2	A	1893	C	C2-N3	5.05	1.39	1.35
2	A	2105	U	N1-C2	-5.05	1.34	1.38
3	E	5	G	N3-C4	5.05	1.39	1.35
3	E	72	C	C5'-C4'	-5.05	1.45	1.51
6	G	160	LYS	N-CA	-5.05	1.36	1.46
2	A	1891	G	N3-C4	5.04	1.39	1.35
2	A	1869	G	C2-N2	-5.04	1.29	1.34
3	E	36	A	N9-C8	5.04	1.41	1.37
4	D	514	TYR	CG-CD2	5.04	1.45	1.39
3	E	17	C	N1-C2	5.04	1.45	1.40
3	E	40	C	C3'-C2'	5.04	1.58	1.52
2	A	1901	A	N9-C8	-5.03	1.33	1.37
3	E	42	C	C4-N4	5.03	1.38	1.33
6	G	132	ARG	CD-NE	5.03	1.54	1.46
3	E	26	C	C3'-O3'	5.03	1.49	1.42
2	A	2149	U	O3'-P	-5.03	1.55	1.61
3	E	22	A	N1-C2	5.03	1.38	1.34
2	A	2178	C	C2-N3	5.02	1.39	1.35
3	E	8	U	C3'-O3'	5.02	1.49	1.42
4	D	64	ARG	CD-NE	5.02	1.54	1.46
5	F	53	ARG	CD-NE	5.02	1.54	1.46
8	I	44	SER	CA-CB	5.02	1.60	1.52
1	B	1302	C	C4-C5	-5.02	1.39	1.43
1	B	1299	A	C1'-N9	5.02	1.56	1.48
2	A	2138	G	C2-N3	5.01	1.36	1.32
3	E	7	G	N7-C5	5.01	1.42	1.39
2	A	2126	A	C8-N7	-5.01	1.28	1.31
4	D	46	SER	CA-CB	5.01	1.60	1.52
2	A	2100	G	C2-N2	-5.01	1.29	1.34
7	H	48	TYR	N-CA	-5.01	1.36	1.46
3	E	45	A	C2'-C1'	-5.00	1.47	1.53
2	A	2165	C	C5'-C4'	5.00	1.57	1.51
3	E	40	C	C2'-C1'	-5.00	1.47	1.53

All (1480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	91	ARG	NE-CZ-NH2	-25.82	107.39	120.30
4	D	430	ARG	NE-CZ-NH1	23.11	131.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1236	A	N1-C6-N6	19.82	130.49	118.60
1	B	1334	G	C5-C6-O6	-18.89	117.27	128.60
1	B	1334	G	N1-C6-O6	17.55	130.43	119.90
2	A	1871	A	P-O3'-C3'	17.40	140.58	119.70
3	E	20	G	C5-C6-O6	-16.97	118.42	128.60
2	A	2123	G	C5-C6-O6	-16.71	118.57	128.60
8	I	137	ARG	NE-CZ-NH1	16.70	128.65	120.30
3	E	20	G	N1-C6-O6	16.07	129.54	119.90
8	I	43	TYR	CB-CG-CD1	15.88	130.53	121.00
8	I	95	ARG	NE-CZ-NH1	15.41	128.00	120.30
3	E	59	A	N9-C4-C5	15.24	111.89	105.80
3	E	10	G	C5-C6-O6	-15.12	119.53	128.60
4	D	283	ARG	NE-CZ-NH1	14.93	127.77	120.30
2	A	1903	G	N1-C6-O6	14.91	128.85	119.90
2	A	1904	G	C5-C6-O6	-14.80	119.72	128.60
2	A	2103	C	N3-C4-C5	14.69	127.78	121.90
3	E	10	G	N1-C6-O6	14.60	128.66	119.90
2	A	2158	A	P-O3'-C3'	14.51	137.11	119.70
6	G	94	ARG	NE-CZ-NH2	-14.35	113.12	120.30
2	A	1869	G	C5-C6-O6	-14.28	120.03	128.60
3	E	2	G	N1-C6-O6	14.27	128.46	119.90
4	D	168	ARG	NE-CZ-NH1	14.24	127.42	120.30
2	A	1860	G	C5-C6-O6	-13.94	120.24	128.60
4	D	19	ARG	NE-CZ-NH2	-13.92	113.34	120.30
4	D	87	ARG	NE-CZ-NH1	13.86	127.23	120.30
4	D	108	TYR	CB-CG-CD2	-13.78	112.73	121.00
4	D	152	ARG	NE-CZ-NH2	-13.62	113.49	120.30
2	A	1906	G	N1-C6-O6	13.56	128.04	119.90
2	A	2153	C	C6-N1-C2	-13.54	114.88	120.30
4	D	481	ARG	NE-CZ-NH1	13.53	127.06	120.30
2	A	2175	C	C6-N1-C2	-13.48	114.91	120.30
2	A	2118	U	N1-C2-O2	13.47	132.23	122.80
3	E	30	G	C4-C5-N7	13.44	116.18	110.80
3	E	57	C	C6-N1-C2	-13.44	114.92	120.30
3	E	3	C	C6-N1-C2	-13.42	114.93	120.30
8	I	52	ARG	NE-CZ-NH1	13.41	127.00	120.30
8	I	4	ARG	NE-CZ-NH2	-13.34	113.63	120.30
2	A	1891	G	C2-N3-C4	-13.22	105.29	111.90
2	A	1892	C	O4'-C1'-N1	13.21	118.77	108.20
2	A	2148	G	N1-C6-O6	13.13	127.78	119.90
2	A	2130	U	C5-C6-N1	13.12	129.26	122.70
2	A	2187	U	O4'-C1'-N1	13.06	118.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1904	G	N1-C6-O6	12.99	127.69	119.90
8	I	91	ARG	NE-CZ-NH1	12.90	126.75	120.30
2	A	2128	G	C5-C6-O6	-12.75	120.95	128.60
3	E	48	U	P-O3'-C3'	12.68	134.91	119.70
3	E	65	G	N1-C6-O6	12.67	127.50	119.90
4	D	395	ARG	NE-CZ-NH2	-12.61	113.99	120.30
2	A	1860	G	N1-C6-O6	12.54	127.42	119.90
1	B	1241	G	N1-C6-O6	12.31	127.28	119.90
1	B	1236	A	C5-C6-N6	-12.27	113.88	123.70
2	A	2169	A	O4'-C1'-N9	12.20	117.96	108.20
2	A	2109	U	O4'-C1'-N1	12.08	117.86	108.20
3	E	52	C	N3-C4-N4	-11.98	109.61	118.00
4	D	152	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	B	1290	G	O4'-C1'-N9	11.81	117.65	108.20
3	E	64	G	N1-C6-O6	-11.77	112.84	119.90
2	A	2110	G	C4-C5-N7	11.76	115.50	110.80
2	A	2110	G	C5-C6-N1	11.76	117.38	111.50
6	G	91	ARG	NE-CZ-NH1	-11.75	114.42	120.30
1	B	1333	A	N9-C4-C5	11.69	110.47	105.80
2	A	2102	G	N1-C6-O6	11.68	126.91	119.90
3	E	17	C	C6-N1-C2	-11.63	115.65	120.30
8	I	137	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	B	1238	A	N1-C6-N6	-11.57	111.66	118.60
2	A	1874	C	O4'-C1'-N1	11.55	117.44	108.20
3	E	32	G	N1-C6-O6	11.46	126.77	119.90
2	A	2107	G	C6-N1-C2	-11.44	118.23	125.10
2	A	2135	A	N1-C6-N6	-11.39	111.77	118.60
3	E	22	A	C8-N9-C4	11.36	110.35	105.80
2	A	2177	C	O4'-C1'-N1	11.36	117.28	108.20
3	E	69	C	C6-N1-C2	-11.34	115.76	120.30
1	B	1290	G	C4-C5-N7	-11.32	106.27	110.80
2	A	2164	C	N3-C4-C5	11.32	126.43	121.90
3	E	41	C	C6-N1-C2	-11.19	115.83	120.30
2	A	1907	G	N1-C6-O6	-11.15	113.21	119.90
2	A	2178	C	P-O3'-C3'	11.15	133.08	119.70
4	D	506	ARG	NE-CZ-NH2	-11.11	114.75	120.30
3	E	49	C	C5-C6-N1	11.06	126.53	121.00
6	G	29	ARG	NE-CZ-NH1	11.02	125.81	120.30
4	D	175	ARG	NE-CZ-NH2	-10.94	114.83	120.30
3	E	38	A	C4-C5-N7	-10.89	105.25	110.70
1	B	1302	C	C6-N1-C2	-10.89	115.94	120.30
2	A	2101	A	N1-C6-N6	10.87	125.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2120	G	C5-C6-O6	-10.87	122.08	128.60
2	A	1906	G	C5-C6-O6	-10.86	122.08	128.60
2	A	2115	G	O4'-C1'-N9	10.86	116.89	108.20
2	A	1843	C	O4'-C1'-N1	10.82	116.86	108.20
5	F	7	ARG	NE-CZ-NH2	-10.81	114.89	120.30
4	D	530	TYR	CB-CG-CD2	-10.81	114.52	121.00
2	A	2094	A	C8-N9-C4	10.80	110.12	105.80
6	G	109	ARG	NE-CZ-NH1	-10.79	114.91	120.30
3	E	65	G	C5-C6-O6	-10.77	122.14	128.60
2	A	1861	G	C5-C6-O6	-10.75	122.15	128.60
3	E	43	G	C5-C6-O6	10.75	135.05	128.60
2	A	1860	G	O4'-C1'-N9	10.74	116.79	108.20
2	A	2120	G	N3-C4-C5	-10.72	123.24	128.60
2	A	1850	G	N7-C8-N9	-10.71	107.74	113.10
5	F	9	ARG	NE-CZ-NH1	10.69	125.64	120.30
2	A	2101	A	N9-C4-C5	-10.68	101.53	105.80
1	B	1294	G	N1-C6-O6	10.68	126.31	119.90
4	D	108	TYR	CB-CG-CD1	10.65	127.39	121.00
1	B	1333	A	C4-C5-N7	-10.64	105.38	110.70
2	A	2110	G	C5-N7-C8	-10.62	98.99	104.30
2	A	1901	A	N1-C6-N6	-10.62	112.23	118.60
6	G	94	ARG	NE-CZ-NH1	10.58	125.59	120.30
4	D	506	ARG	NE-CZ-NH1	10.58	125.59	120.30
3	E	10	G	N7-C8-N9	-10.54	107.83	113.10
2	A	2165	C	O4'-C1'-N1	10.54	116.63	108.20
4	D	514	TYR	CB-CG-CD2	-10.54	114.68	121.00
2	A	2126	A	N1-C6-N6	10.50	124.90	118.60
4	D	522	PHE	CB-CG-CD2	-10.48	113.47	120.80
2	A	1873	G	N9-C4-C5	-10.46	101.22	105.40
3	E	27	G	N1-C6-O6	10.43	126.16	119.90
2	A	2103	C	C2-N3-C4	-10.42	114.69	119.90
5	F	53	ARG	NE-CZ-NH2	-10.39	115.11	120.30
2	A	2183	A	O4'-C1'-N9	10.39	116.51	108.20
3	E	35	C	C1'-O4'-C4'	10.35	118.18	109.90
2	A	2110	G	C4-C5-C6	-10.32	112.61	118.80
2	A	2153	C	O4'-C1'-N1	10.29	116.43	108.20
2	A	2095	A	C5-C6-N1	-10.28	112.56	117.70
3	E	68	C	N3-C4-C5	-10.24	117.81	121.90
2	A	2123	G	C5-C6-N1	10.21	116.61	111.50
2	A	2169	A	C5-C6-N1	10.20	122.80	117.70
8	I	77	ARG	NE-CZ-NH1	10.19	125.40	120.30
8	I	110	ARG	NE-CZ-NH2	10.19	125.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1881	C	O4'-C1'-N1	10.16	116.33	108.20
3	E	44	A	O4'-C1'-N9	10.16	116.33	108.20
4	D	395	ARG	NE-CZ-NH1	10.14	125.37	120.30
5	F	180	PHE	CB-CG-CD2	-10.14	113.70	120.80
2	A	1877	A	C5-C6-N1	-10.10	112.65	117.70
2	A	2190	G	O4'-C1'-N9	10.08	116.27	108.20
2	A	1851	U	O4'-C1'-N1	10.08	116.26	108.20
3	E	2	G	C8-N9-C4	10.08	110.43	106.40
2	A	2122	U	O4'-C1'-N1	10.07	116.25	108.20
1	B	1297	G	N1-C6-O6	10.06	125.94	119.90
2	A	2164	C	C4-C5-C6	-10.04	112.38	117.40
2	A	2181	U	O4'-C1'-N1	10.02	116.22	108.20
1	B	1292	G	N9-C4-C5	-10.02	101.39	105.40
2	A	2139	U	O4'-C1'-N1	10.01	116.21	108.20
3	E	25	U	N3-C4-O4	10.01	126.41	119.40
2	A	2157	G	P-O3'-C3'	9.99	131.69	119.70
3	E	16	C	C6-N1-C2	9.99	124.30	120.30
2	A	1906	G	C2-N3-C4	9.89	116.85	111.90
1	B	1297	G	C6-C5-N7	-9.85	124.49	130.40
3	E	69	C	C5-C6-N1	9.85	125.92	121.00
2	A	2128	G	O4'-C1'-N9	9.84	116.08	108.20
2	A	2190	G	C5-C6-O6	-9.84	122.70	128.60
3	E	77	A	C8-N9-C4	-9.83	101.87	105.80
1	B	1333	A	C2-N3-C4	9.80	115.50	110.60
4	D	50	ARG	NE-CZ-NH1	9.79	125.19	120.30
4	D	254	ARG	NE-CZ-NH1	9.77	125.19	120.30
2	A	2144	G	N3-C2-N2	-9.76	113.07	119.90
3	E	3	C	C5-C6-N1	9.75	125.88	121.00
4	D	219	ARG	NE-CZ-NH2	9.75	125.18	120.30
1	B	1298	U	C5-C4-O4	-9.74	120.05	125.90
7	H	19	PHE	CB-CG-CD2	9.73	127.61	120.80
2	A	1860	G	N3-C2-N2	9.73	126.71	119.90
8	I	4	ARG	NE-CZ-NH1	9.73	125.16	120.30
3	E	7	G	N1-C6-O6	9.72	125.73	119.90
4	D	234	ARG	NE-CZ-NH1	9.72	125.16	120.30
2	A	1844	C	N3-C4-C5	9.72	125.79	121.90
3	E	2	G	C5-C6-O6	-9.70	122.78	128.60
2	A	1844	C	C4-C5-C6	-9.68	112.56	117.40
2	A	1903	G	C5-C6-O6	-9.68	122.79	128.60
2	A	2144	G	N1-C6-O6	9.67	125.70	119.90
3	E	72	C	N3-C4-C5	-9.67	118.03	121.90
2	A	1887	C	C5-C6-N1	-9.66	116.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1242	G	N3-C4-C5	9.66	133.43	128.60
1	B	1304	G	C5-C6-O6	-9.61	122.83	128.60
2	A	2154	A	N1-C6-N6	-9.57	112.86	118.60
2	A	2136	G	N9-C4-C5	9.56	109.22	105.40
4	D	6	TYR	CB-CG-CD2	9.56	126.73	121.00
3	E	42	C	O4'-C1'-N1	9.54	115.83	108.20
7	H	43	ARG	NE-CZ-NH2	9.54	125.07	120.30
3	E	23	G	N3-C4-C5	9.54	133.37	128.60
2	A	2179	C	O4'-C1'-N1	9.53	115.82	108.20
2	A	2191	A	C5-N7-C8	-9.52	99.14	103.90
4	D	136	ASP	CB-CG-OD1	9.52	126.87	118.30
2	A	1872	A	N1-C2-N3	9.51	134.05	129.30
2	A	2136	G	C8-N9-C4	-9.50	102.60	106.40
3	E	1	C	C4-C5-C6	9.49	122.15	117.40
2	A	2095	A	C8-N9-C4	-9.48	102.01	105.80
2	A	2167	U	P-O5'-C5'	9.47	136.06	120.90
2	A	1884	G	O4'-C1'-N9	9.47	115.78	108.20
2	A	2180	U	O4'-C1'-N1	9.46	115.77	108.20
4	D	425	ARG	NE-CZ-NH2	-9.46	115.57	120.30
2	A	2112	G	O4'-C1'-N9	9.45	115.76	108.20
3	E	30	G	C5-N7-C8	-9.45	99.58	104.30
2	A	2167	U	O4'-C1'-N1	9.44	115.75	108.20
2	A	2110	G	P-O3'-C3'	9.44	131.03	119.70
4	D	136	ASP	CB-CG-OD2	-9.44	109.81	118.30
3	E	17	C	C2-N1-C1'	9.44	129.18	118.80
1	B	1245	C	O4'-C1'-N1	9.43	115.74	108.20
2	A	2144	G	C5-C6-O6	-9.42	122.95	128.60
3	E	77	A	N9-C4-C5	9.41	109.57	105.80
1	B	1292	G	O4'-C1'-N9	9.39	115.71	108.20
2	A	2180	U	C5-C6-N1	-9.38	118.01	122.70
6	G	173	ASP	CB-CG-OD2	9.38	126.74	118.30
3	E	64	G	C5-C6-O6	9.37	134.22	128.60
8	I	9	ARG	NE-CZ-NH2	-9.36	115.62	120.30
2	A	2126	A	N1-C2-N3	-9.35	124.62	129.30
2	A	2148	G	C5-C6-O6	-9.35	122.99	128.60
2	A	2152	G	P-O3'-C3'	9.34	130.91	119.70
3	E	11	A	C2-N3-C4	-9.33	105.93	110.60
2	A	2137	U	N3-C4-C5	-9.33	109.00	114.60
2	A	2105	U	C4'-C3'-C2'	-9.33	93.27	102.60
2	A	2097	A	C8-N9-C4	-9.33	102.07	105.80
2	A	2116	G	C5-C6-N1	-9.32	106.84	111.50
2	A	1861	G	N1-C6-O6	9.32	125.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	G	C6-N1-C2	9.31	130.69	125.10
4	D	430	ARG	NE-CZ-NH2	-9.30	115.65	120.30
3	E	76	C	P-O3'-C3'	9.30	130.86	119.70
3	E	56	U	N1-C2-N3	9.29	120.48	114.90
3	E	70	C	N3-C4-C5	9.29	125.61	121.90
3	E	63	C	O4'-C1'-N1	9.28	115.63	108.20
2	A	1894	C	N3-C4-C5	-9.28	118.19	121.90
3	E	36	A	C4-C5-C6	-9.26	112.37	117.00
2	A	2133	G	C4-C5-N7	9.25	114.50	110.80
2	A	1846	G	O4'-C1'-N9	9.25	115.60	108.20
2	A	2124	G	C8-N9-C4	9.22	110.09	106.40
2	A	2189	U	N3-C4-O4	9.19	125.83	119.40
2	A	1836	C	C5-C6-N1	-9.16	116.42	121.00
3	E	31	G	C5-C6-N1	9.16	116.08	111.50
8	I	43	TYR	CB-CG-CD2	-9.15	115.51	121.00
3	E	9	G	N1-C6-O6	9.12	125.37	119.90
2	A	1868	C	C6-N1-C2	-9.11	116.66	120.30
2	A	2105	U	O4'-C1'-N1	9.11	115.49	108.20
2	A	1872	A	P-O3'-C3'	9.10	130.62	119.70
3	E	54	G	O4'-C1'-N9	9.05	115.44	108.20
6	G	6	TYR	CB-CG-CD1	9.04	126.42	121.00
3	E	59	A	C8-N9-C4	-9.03	102.19	105.80
3	E	58	A	C1'-O4'-C4'	-9.02	102.69	109.90
2	A	2123	G	C4'-C3'-C2'	-9.01	93.59	102.60
3	E	33	C	C5-C4-N4	-9.00	113.90	120.20
2	A	2128	G	N1-C6-O6	8.99	125.29	119.90
5	F	75	VAL	CG1-CB-CG2	-8.95	96.59	110.90
3	E	9	G	O4'-C1'-N9	8.94	115.35	108.20
1	B	1294	G	C5-C6-O6	-8.94	123.24	128.60
3	E	22	A	N9-C4-C5	-8.92	102.23	105.80
2	A	2150	C	C6-N1-C2	-8.90	116.74	120.30
3	E	74	A	N1-C6-N6	-8.89	113.26	118.60
2	A	2160	C	C6-N1-C1'	-8.88	110.14	120.80
3	E	72	C	C4-C5-C6	8.88	121.84	117.40
2	A	2178	C	O4'-C1'-N1	8.88	115.30	108.20
3	E	47	G	C4'-C3'-C2'	-8.87	93.73	102.60
2	A	2157	G	C2'-C3'-O3'	8.87	129.01	109.50
2	A	2106	U	C5-C6-N1	8.87	127.13	122.70
3	E	17	C	O4'-C1'-N1	8.85	115.28	108.20
3	E	69	C	N3-C4-C5	-8.85	118.36	121.90
6	G	91	ARG	NE-CZ-NH2	8.85	124.72	120.30
2	A	2101	A	C8-N9-C4	8.84	109.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1332	A	C8-N9-C4	-8.81	102.28	105.80
2	A	2156	G	N1-C6-O6	8.81	125.19	119.90
8	I	101	ARG	NE-CZ-NH2	-8.80	115.90	120.30
3	E	6	G	N3-C4-C5	8.79	133.00	128.60
2	A	2132	U	N3-C4-O4	8.77	125.54	119.40
2	A	1848	A	C5-C6-N1	-8.74	113.33	117.70
3	E	23	G	O4'-C1'-N9	8.72	115.17	108.20
2	A	2172	U	N3-C4-O4	8.70	125.49	119.40
2	A	1901	A	C5-C6-N6	8.68	130.64	123.70
6	G	109	ARG	NE-CZ-NH2	8.67	124.63	120.30
3	E	66	C	N3-C4-C5	-8.65	118.44	121.90
2	A	2163	A	N1-C2-N3	8.65	133.62	129.30
2	A	2183	A	C4-C5-N7	-8.65	106.38	110.70
3	E	34	U	C1'-O4'-C4'	-8.64	102.99	109.90
5	F	1	MET	CG-SD-CE	-8.64	86.37	100.20
2	A	2123	G	N7-C8-N9	8.64	117.42	113.10
3	E	33	C	O4'-C1'-N1	8.62	115.10	108.20
4	D	4	PHE	CB-CG-CD2	8.60	126.82	120.80
1	B	1296	C	C5-C6-N1	-8.60	116.70	121.00
2	A	1847	A	N1-C6-N6	8.60	123.76	118.60
2	A	2143	C	O4'-C1'-N1	8.59	115.07	108.20
5	F	208	TYR	CB-CG-CD1	-8.59	115.85	121.00
2	A	2193	G	N1-C6-O6	8.58	125.05	119.90
3	E	2	G	N7-C8-N9	-8.57	108.81	113.10
2	A	1878	G	C8-N9-C4	-8.56	102.98	106.40
2	A	2132	U	C5-C4-O4	-8.56	120.77	125.90
3	E	37	U	N1-C2-O2	-8.54	116.82	122.80
2	A	1891	G	O4'-C1'-N9	8.53	115.02	108.20
3	E	26	C	N3-C4-C5	-8.52	118.49	121.90
4	D	441	ARG	NE-CZ-NH2	8.52	124.56	120.30
5	F	180	PHE	CB-CG-CD1	8.49	126.75	120.80
3	E	43	G	C8-N9-C4	8.48	109.79	106.40
3	E	71	G	N3-C4-C5	-8.48	124.36	128.60
3	E	31	G	N1-C6-O6	-8.46	114.83	119.90
2	A	2164	C	P-O3'-C3'	8.45	129.84	119.70
6	G	19	PHE	CB-CG-CD1	-8.45	114.89	120.80
2	A	2152	G	N1-C2-N3	-8.44	118.84	123.90
3	E	30	G	N9-C4-C5	-8.44	102.03	105.40
2	A	2103	C	O4'-C1'-N1	8.43	114.94	108.20
2	A	2128	G	C8-N9-C4	8.42	109.77	106.40
3	E	74	A	C5-C6-N1	8.41	121.91	117.70
1	B	1289	A	N1-C2-N3	-8.41	125.10	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1332	A	N1-C6-N6	8.41	123.64	118.60
3	E	58	A	O4'-C1'-N9	8.41	114.93	108.20
2	A	2109	U	C5'-C4'-O4'	8.40	119.19	109.10
2	A	2186	G	C2-N3-C4	-8.38	107.71	111.90
3	E	70	C	O4'-C1'-N1	8.38	114.91	108.20
2	A	1899	A	C5-N7-C8	-8.38	99.71	103.90
2	A	1869	G	N1-C6-O6	8.36	124.92	119.90
6	G	99	PHE	CB-CG-CD2	-8.35	114.95	120.80
2	A	2141	G	C5-N7-C8	8.35	108.47	104.30
2	A	1842	G	C4-C5-N7	-8.34	107.46	110.80
2	A	2133	G	O4'-C1'-N9	8.33	114.86	108.20
4	D	146	ARG	NE-CZ-NH1	8.33	124.47	120.30
2	A	2145	C	P-O3'-C3'	-8.32	109.72	119.70
5	F	134	ARG	NE-CZ-NH2	8.32	124.46	120.30
2	A	2145	C	C4'-C3'-C2'	-8.31	94.29	102.60
3	E	9	G	C5-C6-O6	-8.31	123.61	128.60
2	A	1840	G	N1-C6-O6	8.31	124.89	119.90
2	A	2108	A	N1-C6-N6	8.30	123.58	118.60
2	A	2120	G	N3-C2-N2	-8.30	114.09	119.90
3	E	38	A	C2-N3-C4	-8.30	106.45	110.60
2	A	1849	G	N9-C4-C5	-8.29	102.08	105.40
2	A	2129	C	C2-N1-C1'	8.29	127.92	118.80
2	A	2182	U	C5-C6-N1	-8.29	118.56	122.70
1	B	1295	U	N1-C2-O2	-8.28	117.01	122.80
5	F	71	ARG	NE-CZ-NH1	8.27	124.44	120.30
3	E	21	U	C5-C6-N1	8.27	126.83	122.70
3	E	32	G	C5-C6-O6	-8.26	123.64	128.60
3	E	57	C	N3-C4-C5	8.24	125.20	121.90
1	B	1242	G	C5-C6-O6	-8.23	123.66	128.60
2	A	2189	U	O4'-C1'-N1	8.23	114.78	108.20
7	H	5	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	A	2190	G	C8-N9-C4	-8.21	103.11	106.40
4	D	496	VAL	CG1-CB-CG2	-8.21	97.76	110.90
3	E	39	A	C2-N3-C4	8.21	114.70	110.60
3	E	41	C	C5-C6-N1	8.20	125.10	121.00
3	E	7	G	C5-C6-O6	-8.19	123.69	128.60
3	E	49	C	C6-N1-C2	-8.18	117.03	120.30
2	A	2120	G	C6-N1-C2	-8.17	120.20	125.10
1	B	1332	A	C4-C5-C6	8.16	121.08	117.00
2	A	1858	A	C2-N3-C4	-8.16	106.52	110.60
1	B	1299	A	N9-C4-C5	8.15	109.06	105.80
2	A	2162	G	C2-N3-C4	8.15	115.98	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1895	C	N1-C2-O2	8.15	123.79	118.90
2	A	1867	G	N3-C2-N2	8.14	125.60	119.90
2	A	2110	G	C6-N1-C2	-8.14	120.22	125.10
2	A	2133	G	N9-C4-C5	-8.12	102.15	105.40
2	A	2171	A	N9-C4-C5	8.12	109.05	105.80
4	D	441	ARG	NE-CZ-NH1	8.11	124.35	120.30
3	E	73	A	C3'-C2'-C1'	8.10	107.98	101.50
2	A	1846	G	C5-N7-C8	-8.10	100.25	104.30
2	A	1852	U	C6-N1-C2	-8.10	116.14	121.00
3	E	62	C	O4'-C1'-N1	8.09	114.67	108.20
6	G	19	PHE	CB-CG-CD2	8.08	126.46	120.80
3	E	58	A	N1-C2-N3	-8.08	125.26	129.30
2	A	2120	G	N1-C6-O6	8.07	124.74	119.90
2	A	2161	C	O4'-C1'-N1	8.05	114.64	108.20
2	A	1859	U	O4'-C1'-N1	8.04	114.63	108.20
2	A	1850	G	O4'-C1'-N9	8.02	114.62	108.20
3	E	31	G	C4-C5-N7	8.02	114.01	110.80
6	G	177	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	A	1876	A	C6-N1-C2	-8.02	113.79	118.60
3	E	5	G	N1-C6-O6	8.01	124.71	119.90
1	B	1292	G	C4-C5-N7	8.00	114.00	110.80
2	A	2102	G	C5-C6-N1	-8.00	107.50	111.50
2	A	1855	U	N1-C2-O2	7.99	128.40	122.80
3	E	23	G	N1-C6-O6	7.99	124.69	119.90
1	B	1243	C	C5-C4-N4	-7.96	114.62	120.20
3	E	57	C	N1-C2-O2	-7.95	114.13	118.90
2	A	2123	G	N1-C6-O6	7.94	124.67	119.90
2	A	2172	U	N1-C2-O2	-7.94	117.24	122.80
2	A	2095	A	N1-C6-N6	7.94	123.36	118.60
2	A	1838	C	N1-C2-O2	-7.93	114.14	118.90
2	A	1867	G	O4'-C1'-N9	7.92	114.54	108.20
2	A	1901	A	N1-C2-N3	7.91	133.25	129.30
2	A	2176	A	C1'-O4'-C4'	7.90	116.22	109.90
2	A	1847	A	N1-C2-N3	7.89	133.25	129.30
3	E	29	C	C6-N1-C2	-7.89	117.14	120.30
1	B	1304	G	C4-C5-N7	7.88	113.95	110.80
1	B	1245	C	C5-C6-N1	7.88	124.94	121.00
3	E	69	C	O4'-C1'-N1	7.88	114.50	108.20
2	A	2144	G	N1-C2-N2	7.87	123.29	116.20
2	A	1905	C	O4'-C1'-N1	7.87	114.49	108.20
2	A	1845	G	C4-C5-N7	-7.85	107.66	110.80
2	A	2168	G	N9-C4-C5	-7.85	102.26	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	367	ARG	NE-CZ-NH1	7.83	124.21	120.30
5	F	37	LYS	CB-CA-C	7.83	126.05	110.40
2	A	1894	C	N3-C4-N4	7.81	123.47	118.00
1	B	1238	A	C5-C6-N6	7.81	129.95	123.70
3	E	52	C	C5-C4-N4	7.81	125.67	120.20
3	E	15	G	C6-C5-N7	7.81	135.08	130.40
2	A	1883	U	C5-C6-N1	7.80	126.60	122.70
4	D	441	ARG	NH1-CZ-NH2	-7.78	110.84	119.40
3	E	6	G	C4-C5-C6	-7.78	114.13	118.80
2	A	1835	G	P-O5'-C5'	7.77	133.34	120.90
3	E	62	C	P-O3'-C3'	-7.77	110.37	119.70
2	A	2103	C	N3-C4-N4	-7.76	112.56	118.00
3	E	3	C	N3-C4-C5	-7.76	118.80	121.90
2	A	2154	A	O4'-C1'-N9	7.76	114.41	108.20
2	A	1838	C	C2-N3-C4	-7.75	116.02	119.90
1	B	1243	C	C6-N1-C2	7.74	123.40	120.30
3	E	57	C	C5-C6-N1	7.74	124.87	121.00
2	A	2102	G	C4-C5-N7	-7.74	107.70	110.80
2	A	2152	G	C4-C5-N7	7.74	113.89	110.80
2	A	1850	G	C8-N9-C4	7.73	109.49	106.40
2	A	1868	C	C5-C4-N4	7.72	125.61	120.20
2	A	2178	C	N3-C4-C5	7.72	124.99	121.90
2	A	1896	G	C2-N3-C4	7.72	115.76	111.90
2	A	1906	G	N3-C4-C5	-7.72	124.74	128.60
2	A	2130	U	C6-N1-C2	-7.72	116.37	121.00
1	B	1304	G	P-O3'-C3'	7.71	128.96	119.70
1	B	1242	G	N9-C4-C5	-7.71	102.32	105.40
1	B	1245	C	C2-N3-C4	7.71	123.75	119.90
2	A	2126	A	P-O3'-C3'	7.69	128.93	119.70
5	F	97	MET	CG-SD-CE	-7.68	87.91	100.20
3	E	66	C	C6-N1-C2	-7.67	117.23	120.30
1	B	1290	G	N9-C4-C5	7.67	108.47	105.40
2	A	2127	G	C4-C5-N7	7.67	113.87	110.80
1	B	1245	C	C4-C5-C6	-7.67	113.57	117.40
3	E	57	C	N1-C2-N3	7.67	124.57	119.20
2	A	1854	A	N1-C2-N3	7.65	133.12	129.30
2	A	2166	U	C4'-C3'-C2'	-7.64	94.96	102.60
2	A	2193	G	C5-C6-N1	-7.63	107.68	111.50
2	A	2169	A	C4-C5-C6	-7.63	113.18	117.00
2	A	2135	A	O4'-C1'-N9	7.63	114.30	108.20
8	I	22	LEU	CB-CG-CD2	7.62	123.95	111.00
3	E	15	G	N3-C2-N2	7.62	125.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2124	G	N7-C8-N9	-7.61	109.30	113.10
3	E	29	C	C2-N3-C4	-7.60	116.10	119.90
3	E	76	C	C5-C4-N4	-7.60	114.88	120.20
4	D	405	TRP	CB-CG-CD1	7.60	136.87	127.00
2	A	2131	U	P-O3'-C3'	7.59	128.81	119.70
6	G	101	ARG	NE-CZ-NH1	-7.59	116.50	120.30
2	A	1868	C	O4'-C1'-N1	7.58	114.27	108.20
2	A	2145	C	C1'-O4'-C4'	-7.58	103.83	109.90
2	A	2191	A	N1-C6-N6	7.58	123.15	118.60
3	E	49	C	P-O3'-C3'	7.58	128.80	119.70
3	E	75	C	C4-C5-C6	7.58	121.19	117.40
2	A	2133	G	P-O3'-C3'	7.58	128.79	119.70
5	F	99	ASP	CB-CG-OD2	7.57	125.12	118.30
2	A	1883	U	C4-C5-C6	-7.57	115.16	119.70
2	A	2130	U	P-O3'-C3'	-7.57	110.62	119.70
1	B	1332	A	O4'-C1'-N9	7.56	114.25	108.20
3	E	37	U	C4-C5-C6	7.56	124.23	119.70
1	B	1333	A	N3-C4-C5	-7.55	121.51	126.80
2	A	2120	G	N3-C4-N9	7.55	130.53	126.00
2	A	2155	U	O4'-C1'-N1	7.55	114.24	108.20
1	B	1292	G	P-O3'-C3'	7.54	128.75	119.70
2	A	2141	G	C3'-C2'-C1'	-7.53	95.48	101.50
2	A	1907	G	C5-C6-N1	7.51	115.26	111.50
8	I	110	ARG	NH1-CZ-NH2	-7.51	111.14	119.40
2	A	2147	A	O4'-C1'-N9	7.50	114.20	108.20
6	G	6	TYR	CB-CG-CD2	-7.50	116.50	121.00
2	A	2110	G	C3'-C2'-C1'	-7.49	95.51	101.50
7	H	43	ARG	NE-CZ-NH1	-7.48	116.56	120.30
4	D	390	SER	N-CA-CB	7.47	121.71	110.50
2	A	2192	U	O4'-C1'-N1	7.47	114.18	108.20
1	B	1244	G	C4-C5-N7	7.46	113.78	110.80
2	A	1892	C	C5-C6-N1	7.44	124.72	121.00
2	A	2168	G	C4-C5-N7	7.43	113.77	110.80
1	B	1290	G	C4-C5-C6	7.43	123.26	118.80
2	A	1906	G	C6-C5-N7	-7.43	125.94	130.40
4	D	220	TYR	CB-CG-CD2	7.42	125.45	121.00
2	A	2108	A	C5-C6-N6	-7.41	117.77	123.70
1	B	1238	A	C6-N1-C2	-7.41	114.16	118.60
2	A	2111	U	O3'-P-O5'	-7.41	89.93	104.00
2	A	2178	C	OP1-P-OP2	-7.41	108.49	119.60
2	A	2144	G	C4-C5-N7	-7.40	107.84	110.80
2	A	2118	U	N3-C2-O2	-7.39	117.03	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1304	G	N1-C6-O6	7.38	124.33	119.90
1	B	1292	G	C8-N9-C4	7.38	109.35	106.40
2	A	1893	C	O4'-C1'-N1	7.37	114.10	108.20
3	E	76	C	N3-C4-N4	7.37	123.16	118.00
1	B	1305	G	C8-N9-C4	7.36	109.34	106.40
3	E	4	G	C5-N7-C8	-7.36	100.62	104.30
3	E	6	G	C5-C6-O6	-7.35	124.19	128.60
4	D	200	TRP	CH2-CZ2-CE2	7.35	124.75	117.40
2	A	2148	G	P-O3'-C3'	7.34	128.51	119.70
3	E	35	C	O4'-C1'-N1	7.34	114.08	108.20
6	G	172	PHE	CB-CG-CD2	-7.34	115.66	120.80
2	A	1865	U	C4-C5-C6	7.34	124.10	119.70
3	E	43	G	C1'-O4'-C4'	-7.33	104.03	109.90
2	A	2180	U	C2-N3-C4	7.33	131.40	127.00
3	E	30	G	O4'-C1'-N9	7.33	114.06	108.20
5	F	162	ARG	CA-CB-CG	7.32	129.51	113.40
5	F	9	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	A	2162	G	P-O3'-C3'	-7.31	110.93	119.70
2	A	1899	A	N1-C6-N6	-7.30	114.22	118.60
2	A	1855	U	C2-N3-C4	7.30	131.38	127.00
2	A	2110	G	N9-C4-C5	-7.29	102.48	105.40
2	A	2174	C	C6-N1-C2	7.29	123.22	120.30
2	A	1878	G	C2-N3-C4	-7.29	108.25	111.90
3	E	11	A	C8-N9-C4	-7.29	102.89	105.80
3	E	40	C	O4'-C1'-N1	7.28	114.03	108.20
2	A	2127	G	O4'-C1'-N9	7.28	114.02	108.20
2	A	2168	G	O4'-C1'-N9	7.26	114.01	108.20
8	I	17	PHE	CB-CG-CD1	-7.25	115.72	120.80
3	E	9	G	C5-N7-C8	-7.25	100.67	104.30
2	A	1840	G	N9-C4-C5	7.25	108.30	105.40
2	A	1861	G	C4-C5-N7	-7.25	107.90	110.80
3	E	29	C	N3-C4-C5	7.25	124.80	121.90
2	A	2161	C	C2-N3-C4	-7.24	116.28	119.90
3	E	17	C	N3-C2-O2	-7.24	116.83	121.90
2	A	2141	G	C4-C5-N7	-7.24	107.91	110.80
2	A	1847	A	C6-N1-C2	-7.22	114.27	118.60
2	A	2113	U	N1-C2-N3	7.22	119.23	114.90
3	E	66	C	N3-C4-N4	7.22	123.06	118.00
2	A	1900	A	C6-C5-N7	7.19	137.33	132.30
2	A	1836	C	N3-C2-O2	-7.16	116.89	121.90
2	A	2112	G	C8-N9-C4	-7.16	103.54	106.40
3	E	44	A	N1-C6-N6	7.16	122.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	99	PHE	CB-CG-CD1	7.16	125.81	120.80
2	A	2137	U	N1-C2-N3	-7.15	110.61	114.90
2	A	1863	G	N1-C6-O6	-7.15	115.61	119.90
1	B	1305	G	N1-C6-O6	-7.13	115.62	119.90
1	B	1298	U	C2-N1-C1'	7.13	126.26	117.70
2	A	2147	A	C5-C6-N1	-7.13	114.14	117.70
1	B	1297	G	C5-C6-O6	-7.13	124.33	128.60
3	E	71	G	N3-C4-N9	7.12	130.28	126.00
3	E	33	C	N3-C4-N4	7.12	122.99	118.00
3	E	59	A	P-O5'-C5'	7.12	132.30	120.90
2	A	1869	G	O4'-C1'-N9	7.12	113.89	108.20
2	A	2160	C	C2-N3-C4	-7.12	116.34	119.90
2	A	1896	G	N3-C4-N9	7.12	130.27	126.00
3	E	69	C	N3-C4-N4	7.11	122.98	118.00
1	B	1237	C	C2-N3-C4	7.10	123.45	119.90
2	A	2114	A	P-O3'-C3'	-7.09	111.19	119.70
4	D	547	ARG	NE-CZ-NH1	7.09	123.84	120.30
4	D	469	ASP	CB-CG-OD1	7.08	124.67	118.30
2	A	1891	G	N1-C2-N3	7.08	128.15	123.90
1	B	1241	G	C5-C6-N1	-7.07	107.96	111.50
2	A	2102	G	C6-N1-C2	7.06	129.34	125.10
3	E	25	U	N3-C4-C5	-7.06	110.36	114.60
3	E	58	A	C5-C6-N1	-7.06	114.17	117.70
4	D	514	TYR	CB-CG-CD1	7.06	125.23	121.00
2	A	2173	A	C5-N7-C8	7.05	107.43	103.90
3	E	34	U	C5-C6-N1	-7.05	119.17	122.70
3	E	74	A	N9-C4-C5	-7.05	102.98	105.80
3	E	46	G	C5-C6-O6	-7.04	124.37	128.60
2	A	2176	A	C4'-C3'-C2'	7.04	109.64	102.60
3	E	46	G	C5-C6-N1	7.03	115.02	111.50
2	A	2172	U	N3-C4-C5	-7.03	110.38	114.60
3	E	57	C	C2-N3-C4	-7.03	116.39	119.90
2	A	2121	G	N1-C6-O6	7.02	124.11	119.90
2	A	1847	A	C4-C5-N7	-7.02	107.19	110.70
2	A	2110	G	C5-C6-O6	-7.01	124.39	128.60
3	E	43	G	N7-C8-N9	-7.01	109.59	113.10
2	A	2186	G	N1-C6-O6	-7.01	115.69	119.90
2	A	1836	C	C4-C5-C6	7.01	120.90	117.40
4	D	530	TYR	CB-CG-CD1	7.00	125.20	121.00
4	D	481	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
2	A	1900	A	O4'-C1'-N9	-6.99	102.61	108.20
2	A	1897	G	O4'-C1'-N9	6.97	113.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	127	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	A	1863	G	C5-C6-O6	6.97	132.78	128.60
4	D	144	LEU	CB-CG-CD1	6.96	122.84	111.00
1	B	1242	G	N1-C2-N3	-6.96	119.72	123.90
4	D	336	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	1336	C	C4-C5-C6	6.96	120.88	117.40
3	E	54	G	N3-C2-N2	6.96	124.77	119.90
3	E	43	G	C5-C6-N1	-6.95	108.02	111.50
3	E	25	U	C2-N3-C4	6.95	131.17	127.00
2	A	1889	A	N1-C6-N6	-6.95	114.43	118.60
3	E	4	G	O4'-C1'-N9	6.94	113.75	108.20
3	E	37	U	C6-N1-C2	-6.94	116.84	121.00
2	A	2171	A	C6-C5-N7	6.94	137.16	132.30
2	A	2118	U	N1-C2-N3	-6.94	110.74	114.90
2	A	2119	A	N1-C2-N3	-6.94	125.83	129.30
4	D	244	TYR	CB-CG-CD2	-6.93	116.84	121.00
2	A	2125	G	C5-C6-O6	6.93	132.76	128.60
1	B	1241	G	C5-C6-O6	-6.93	124.44	128.60
2	A	1901	A	C2-N3-C4	-6.92	107.14	110.60
2	A	2172	U	N1-C2-N3	6.92	119.05	114.90
2	A	2161	C	C5-C6-N1	-6.92	117.54	121.00
3	E	58	A	C2-N3-C4	6.91	114.06	110.60
2	A	2110	G	N7-C8-N9	6.91	116.55	113.10
1	B	1332	A	C5-C6-N1	-6.90	114.25	117.70
2	A	2139	U	C5-C4-O4	-6.90	121.76	125.90
2	A	2119	A	C5'-C4'-C3'	6.90	127.03	116.00
5	F	164	ARG	NE-CZ-NH2	6.90	123.75	120.30
2	A	1847	A	C5-C6-N6	-6.89	118.19	123.70
2	A	1899	A	C5-C6-N6	6.89	129.21	123.70
6	G	82	TYR	CB-CG-CD1	-6.89	116.86	121.00
3	E	19	G	C3'-C2'-C1'	6.89	107.01	101.50
3	E	16	C	C5-C6-N1	-6.88	117.56	121.00
2	A	2141	G	N7-C8-N9	-6.88	109.66	113.10
8	I	26	VAL	CA-CB-CG2	6.88	121.22	110.90
2	A	1839	G	N3-C4-C5	-6.88	125.16	128.60
2	A	1878	G	C5-N7-C8	-6.88	100.86	104.30
2	A	2123	G	C4-C5-C6	-6.88	114.67	118.80
2	A	2172	U	C4-C5-C6	6.87	123.82	119.70
3	E	54	G	C5-C6-O6	-6.87	124.48	128.60
7	H	48	TYR	CB-CG-CD1	-6.87	116.88	121.00
2	A	1888	G	N3-C2-N2	6.87	124.70	119.90
1	B	1335	U	C5'-C4'-O4'	6.86	117.33	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2133	G	N3-C4-C5	6.86	132.03	128.60
3	E	24	C	N3-C4-C5	-6.86	119.16	121.90
2	A	2173	A	N1-C6-N6	-6.85	114.49	118.60
4	D	405	TRP	CB-CG-CD2	-6.85	117.69	126.60
2	A	1889	A	C5-C6-N6	6.85	129.18	123.70
2	A	2153	C	C5'-C4'-C3'	-6.85	105.04	116.00
3	E	5	G	C8-N9-C4	6.85	109.14	106.40
2	A	1904	G	O4'-C1'-N9	6.84	113.67	108.20
2	A	1868	C	N3-C2-O2	-6.84	117.11	121.90
3	E	38	A	C4-N9-C1'	6.84	138.60	126.30
5	F	38	PHE	CB-CG-CD2	-6.83	116.02	120.80
2	A	2151	U	N3-C2-O2	-6.83	117.42	122.20
2	A	2175	C	C2-N1-C1'	6.83	126.31	118.80
3	E	59	A	O5'-P-OP2	-6.83	99.56	105.70
3	E	19	G	O4'-C4'-C3'	6.83	111.56	106.10
1	B	1242	G	O4'-C1'-N9	6.83	113.66	108.20
2	A	1866	A	C8-N9-C4	-6.83	103.07	105.80
1	B	1304	G	C2-N3-C4	-6.82	108.49	111.90
3	E	10	G	N3-C4-C5	6.82	132.01	128.60
1	B	1297	G	N7-C8-N9	-6.82	109.69	113.10
1	B	1334	G	N9-C4-C5	-6.82	102.67	105.40
2	A	2112	G	C5-C6-O6	-6.81	124.51	128.60
3	E	72	C	C1'-O4'-C4'	-6.81	104.45	109.90
1	B	1295	U	C5-C4-O4	-6.81	121.81	125.90
4	D	399	ASP	CB-CG-OD2	6.81	124.43	118.30
2	A	2137	U	O4'-C1'-N1	6.81	113.65	108.20
4	D	476	ASP	CB-CG-OD2	6.80	124.42	118.30
3	E	70	C	C2-N3-C4	-6.80	116.50	119.90
2	A	2173	A	C5-C6-N6	6.80	129.14	123.70
3	E	36	A	C6-C5-N7	6.79	137.06	132.30
1	B	1296	C	O4'-C1'-N1	6.79	113.63	108.20
3	E	30	G	C5-C6-O6	-6.79	124.53	128.60
2	A	1869	G	C5-N7-C8	-6.79	100.91	104.30
2	A	2158	A	N9-C4-C5	6.79	108.52	105.80
3	E	49	C	O4'-C1'-N1	6.78	113.62	108.20
3	E	57	C	C4-C5-C6	-6.77	114.01	117.40
2	A	1878	G	N9-C4-C5	6.77	108.11	105.40
4	D	333	TYR	CG-CD2-CE2	6.77	126.72	121.30
2	A	2104	C	C5-C4-N4	-6.76	115.47	120.20
2	A	2129	C	C6-N1-C1'	-6.75	112.69	120.80
2	A	2138	G	N1-C2-N3	-6.74	119.85	123.90
3	E	74	A	P-O3'-C3'	6.74	127.79	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1849	G	N3-C4-N9	6.74	130.04	126.00
4	D	425	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	A	2136	G	C2-N3-C4	6.72	115.26	111.90
2	A	1852	U	N3-C4-C5	6.72	118.63	114.60
1	B	1295	U	N3-C2-O2	6.72	126.90	122.20
3	E	50	G	C6-C5-N7	6.72	134.43	130.40
5	F	179	ASP	CB-CG-OD2	6.71	124.34	118.30
2	A	1877	A	C5-C6-N6	6.71	129.07	123.70
2	A	2158	A	N1-C6-N6	-6.71	114.57	118.60
2	A	2157	G	O4'-C1'-N9	6.70	113.56	108.20
2	A	1851	U	C3'-C2'-C1'	-6.70	96.14	101.50
2	A	2131	U	C3'-C2'-C1'	-6.70	96.14	101.50
2	A	2146	C	O4'-C1'-N1	6.70	113.56	108.20
1	B	1290	G	C8-N9-C4	-6.69	103.72	106.40
3	E	43	G	C4'-C3'-C2'	-6.69	95.91	102.60
6	G	7	TYR	CB-CG-CD1	-6.68	116.99	121.00
4	D	103	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	A	2147	A	P-O3'-C3'	6.68	127.72	119.70
2	A	2161	C	C6-N1-C2	6.67	122.97	120.30
2	A	2116	G	C4'-C3'-C2'	-6.67	95.94	102.60
2	A	1897	G	C5-N7-C8	-6.66	100.97	104.30
6	G	29	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	A	1900	A	C6-N1-C2	-6.65	114.61	118.60
3	E	75	C	O4'-C1'-N1	6.65	113.52	108.20
1	B	1241	G	C2-N3-C4	6.65	115.22	111.90
2	A	2118	U	O4'-C1'-N1	6.64	113.52	108.20
8	I	84	TYR	CB-CG-CD2	-6.64	117.02	121.00
2	A	2160	C	C5-C4-N4	-6.64	115.55	120.20
3	E	30	G	C4-C5-C6	-6.64	114.82	118.80
5	F	99	ASP	CB-CG-OD1	-6.63	112.33	118.30
2	A	1864	U	N1-C2-O2	6.63	127.44	122.80
4	D	50	ARG	NE-CZ-NH2	-6.63	116.99	120.30
4	D	258	GLU	O-C-N	-6.63	112.09	122.70
2	A	2183	A	C5-C6-N1	-6.62	114.39	117.70
2	A	2191	A	N7-C8-N9	6.62	117.11	113.80
2	A	2174	C	C5'-C4'-C3'	-6.62	105.41	116.00
2	A	2104	C	O4'-C1'-N1	6.61	113.49	108.20
2	A	2183	A	C5'-C4'-O4'	6.61	117.03	109.10
2	A	2190	G	N3-C2-N2	6.60	124.52	119.90
4	D	2	ALA	N-CA-CB	-6.60	100.86	110.10
2	A	2175	C	P-O3'-C3'	6.60	127.62	119.70
1	B	1294	G	C8-N9-C4	-6.60	103.76	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1840	G	C5-C6-O6	-6.60	124.64	128.60
2	A	2101	A	C4'-C3'-C2'	-6.59	96.01	102.60
2	A	2100	G	N9-C1'-C2'	-6.59	104.75	112.00
3	E	74	A	N1-C2-N3	6.58	132.59	129.30
2	A	2121	G	C4-C5-N7	-6.58	108.17	110.80
2	A	2136	G	C4'-C3'-C2'	-6.58	96.02	102.60
2	A	2191	A	C5-C6-N6	-6.58	118.43	123.70
2	A	2171	A	C6-N1-C2	-6.57	114.66	118.60
4	D	4	PHE	CB-CG-CD1	-6.57	116.20	120.80
2	A	1859	U	N3-C2-O2	6.57	126.80	122.20
3	E	7	G	P-O5'-C5'	6.56	131.40	120.90
1	B	1296	C	N1-C2-N3	-6.56	114.61	119.20
2	A	2095	A	C6-N1-C2	6.55	122.53	118.60
2	A	2131	U	C5-C4-O4	-6.55	121.97	125.90
8	I	2	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	E	74	A	O4'-C1'-N9	6.55	113.44	108.20
2	A	2171	A	C1'-O4'-C4'	-6.55	104.66	109.90
2	A	1878	G	N3-C4-N9	-6.54	122.07	126.00
2	A	2160	C	O4'-C1'-N1	6.54	113.43	108.20
2	A	2110	G	N3-C2-N2	-6.54	115.32	119.90
3	E	24	C	C4-C5-C6	6.54	120.67	117.40
1	B	1296	C	N3-C2-O2	6.53	126.47	121.90
2	A	1872	A	N1-C6-N6	-6.53	114.68	118.60
1	B	1289	A	C2-N3-C4	6.53	113.86	110.60
2	A	1878	G	N7-C8-N9	6.53	116.37	113.10
2	A	2116	G	P-O5'-C5'	6.53	131.35	120.90
2	A	1868	C	C3'-C2'-C1'	-6.53	96.28	101.50
2	A	2101	A	O4'-C1'-N9	6.53	113.42	108.20
2	A	1896	G	C5-C6-N1	-6.52	108.24	111.50
5	F	119	ASP	O-C-N	-6.52	112.26	122.70
2	A	2128	G	C6-C5-N7	6.52	134.31	130.40
3	E	23	G	N1-C2-N2	6.52	122.07	116.20
3	E	73	A	N1-C2-N3	-6.51	126.04	129.30
3	E	71	G	P-O3'-C3'	6.51	127.51	119.70
6	G	124	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	A	2106	U	C6-N1-C2	-6.51	117.10	121.00
2	A	2125	G	OP2-P-O3'	6.51	119.52	105.20
3	E	34	U	C4-C5-C6	6.51	123.60	119.70
2	A	2131	U	C6-N1-C2	6.50	124.90	121.00
3	E	15	G	C1'-O4'-C4'	6.50	115.10	109.90
5	F	202	THR	CA-CB-CG2	-6.50	103.30	112.40
2	A	2128	G	C4-C5-C6	-6.50	114.90	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2164	C	O5'-C5'-C4'	-6.50	99.36	111.70
2	A	1896	G	C6-N1-C2	6.50	129.00	125.10
3	E	64	G	C8-N9-C4	-6.49	103.81	106.40
4	D	366	PHE	CB-CG-CD1	6.49	125.34	120.80
3	E	2	G	P-O3'-C3'	-6.48	111.92	119.70
4	D	536	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	A	1840	G	N7-C8-N9	6.47	116.34	113.10
3	E	37	U	N3-C4-C5	-6.46	110.72	114.60
2	A	1836	C	N1-C2-O2	6.46	122.78	118.90
2	A	2151	U	O5'-P-OP1	-6.46	99.89	105.70
2	A	1857	G	P-O3'-C3'	6.45	127.44	119.70
5	F	41	SER	N-CA-CB	6.45	120.17	110.50
1	B	1290	G	N3-C4-C5	-6.44	125.38	128.60
3	E	5	G	C2-N3-C4	-6.44	108.68	111.90
1	B	1304	G	C5'-C4'-O4'	6.44	116.82	109.10
2	A	2164	C	C3'-C2'-C1'	6.43	106.65	101.50
3	E	4	G	N3-C4-C5	-6.43	125.39	128.60
3	E	52	C	N3-C4-C5	6.43	124.47	121.90
2	A	1865	U	C6-N1-C2	-6.42	117.15	121.00
2	A	1894	C	O4'-C1'-N1	6.42	113.34	108.20
3	E	46	G	C4-C5-C6	-6.42	114.95	118.80
8	I	25	PHE	CB-CG-CD1	6.42	125.29	120.80
3	E	31	G	C4-C5-C6	-6.42	114.95	118.80
1	B	1336	C	C2-N1-C1'	6.41	125.85	118.80
2	A	2168	G	C6-C5-N7	-6.41	126.55	130.40
2	A	2163	A	C6-N1-C2	-6.41	114.75	118.60
2	A	2190	G	C4-C5-N7	-6.41	108.23	110.80
4	D	430	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
2	A	2141	G	P-O3'-C3'	-6.41	112.01	119.70
2	A	1859	U	C2-N3-C4	-6.40	123.16	127.00
2	A	1869	G	C4-C5-C6	-6.40	114.96	118.80
2	A	1866	A	N7-C8-N9	6.39	117.00	113.80
3	E	16	C	C6-N1-C1'	-6.39	113.13	120.80
2	A	1853	A	O4'-C1'-N9	6.39	113.31	108.20
2	A	1861	G	C4'-C3'-C2'	-6.38	96.22	102.60
3	E	31	G	C5-N7-C8	-6.38	101.11	104.30
3	E	42	C	C5-C6-N1	-6.38	117.81	121.00
2	A	1842	G	C5-C6-O6	6.38	132.43	128.60
2	A	2109	U	C4'-C3'-C2'	-6.38	96.22	102.60
2	A	2189	U	N3-C4-C5	-6.37	110.78	114.60
2	A	1883	U	P-O3'-C3'	6.37	127.34	119.70
2	A	2121	G	N3-C4-N9	-6.37	122.18	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2176	A	OP1-P-OP2	-6.37	110.05	119.60
2	A	2126	A	C5-C6-N1	-6.36	114.52	117.70
3	E	42	C	N3-C4-C5	-6.36	119.36	121.90
3	E	74	A	C6-N1-C2	-6.36	114.78	118.60
2	A	1888	G	C3'-C2'-C1'	-6.36	96.41	101.50
3	E	8	U	N1-C2-N3	6.36	118.72	114.90
3	E	14	A	C4-C5-N7	6.36	113.88	110.70
3	E	32	G	N9-C4-C5	6.35	107.94	105.40
5	F	51	ASP	CB-CG-OD1	6.35	124.02	118.30
3	E	1	C	C5-C6-N1	-6.35	117.83	121.00
1	B	1298	U	P-O3'-C3'	6.34	127.31	119.70
2	A	2191	A	C3'-C2'-C1'	6.34	106.57	101.50
2	A	2116	G	C5-C6-O6	6.34	132.40	128.60
3	E	20	G	C5'-C4'-C3'	-6.34	105.86	116.00
5	F	144	THR	CA-CB-CG2	6.34	121.27	112.40
4	D	19	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	A	1895	C	N3-C2-O2	-6.33	117.47	121.90
2	A	1835	G	C2-N3-C4	6.33	115.06	111.90
2	A	2186	G	N3-C2-N2	6.33	124.33	119.90
2	A	2156	G	C5-C6-N1	-6.32	108.34	111.50
3	E	6	G	O4'-C1'-N9	6.32	113.26	108.20
2	A	1877	A	N7-C8-N9	6.32	116.96	113.80
8	I	110	ARG	NE-CZ-NH1	6.32	123.46	120.30
3	E	46	G	N9-C4-C5	-6.32	102.87	105.40
4	D	187	ASP	CB-CG-OD2	-6.32	112.62	118.30
2	A	2096	C	C6-N1-C2	-6.31	117.78	120.30
2	A	2123	G	C5-N7-C8	-6.31	101.14	104.30
2	A	2162	G	N1-C2-N3	-6.31	120.11	123.90
1	B	1305	G	N9-C4-C5	-6.31	102.88	105.40
2	A	2183	A	C4-C5-C6	6.31	120.15	117.00
2	A	2113	U	C6-N1-C2	-6.30	117.22	121.00
3	E	77	A	N1-C2-N3	6.30	132.45	129.30
2	A	2158	A	C5-C6-N1	6.29	120.84	117.70
3	E	6	G	C5-C6-N1	6.29	114.64	111.50
1	B	1305	G	C5-C6-N1	6.28	114.64	111.50
2	A	1857	G	C4'-C3'-C2'	-6.28	96.32	102.60
2	A	1903	G	C5-C6-N1	-6.28	108.36	111.50
6	G	21	TYR	CB-CG-CD1	6.28	124.77	121.00
3	E	12	G	N1-C6-O6	6.28	123.67	119.90
3	E	72	C	C5'-C4'-O4'	-6.28	101.57	109.10
3	E	77	A	C4-C5-N7	-6.27	107.56	110.70
3	E	77	A	C6-N1-C2	-6.27	114.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2190	G	C5'-C4'-C3'	-6.27	105.97	116.00
3	E	63	C	C5-C4-N4	-6.27	115.81	120.20
2	A	2158	A	C6-N1-C2	-6.27	114.84	118.60
4	D	168	ARG	NE-CZ-NH2	-6.27	117.17	120.30
5	F	122	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	1300	G	C4-C5-N7	-6.26	108.30	110.80
3	E	11	A	N1-C2-N3	6.26	132.43	129.30
2	A	2174	C	C2-N1-C1'	-6.25	111.92	118.80
2	A	2121	G	P-O3'-C3'	-6.25	112.20	119.70
1	B	1240	U	C5'-C4'-C3'	-6.25	106.00	116.00
5	F	174	THR	CA-CB-CG2	-6.25	103.66	112.40
2	A	2117	A	C2-N3-C4	6.24	113.72	110.60
3	E	59	A	N1-C2-N3	-6.24	126.18	129.30
3	E	2	G	N3-C2-N2	6.23	124.26	119.90
2	A	1888	G	C8-N9-C1'	6.23	135.10	127.00
2	A	2131	U	N1-C2-N3	-6.23	111.16	114.90
1	B	1240	U	C5-C4-O4	-6.22	122.17	125.90
3	E	6	G	N9-C4-C5	-6.22	102.91	105.40
3	E	50	G	C5-C6-N1	6.22	114.61	111.50
8	I	108	ARG	CG-CD-NE	-6.22	98.73	111.80
3	E	59	A	C5-C6-N1	6.22	120.81	117.70
8	I	95	ARG	CD-NE-CZ	6.22	132.31	123.60
2	A	1897	G	N1-C2-N2	-6.21	110.61	116.20
2	A	1901	A	C8-N9-C4	6.21	108.28	105.80
2	A	2165	C	C6-N1-C2	-6.20	117.82	120.30
3	E	38	A	N1-C2-N3	6.20	132.40	129.30
1	B	1296	C	C6-N1-C2	6.20	122.78	120.30
4	D	536	ARG	NE-CZ-NH2	-6.19	117.20	120.30
8	I	95	ARG	NH1-CZ-NH2	-6.19	112.59	119.40
2	A	2117	A	C5'-C4'-C3'	6.19	125.90	116.00
2	A	2118	U	C6-N1-C1'	-6.19	112.54	121.20
2	A	2185	U	O4'-C1'-N1	6.19	113.15	108.20
2	A	2137	U	C2-N3-C4	6.19	130.71	127.00
4	D	363	SER	N-CA-CB	6.19	119.78	110.50
6	G	114	ARG	NE-CZ-NH1	-6.19	117.21	120.30
2	A	1905	C	C3'-C2'-C1'	6.18	106.45	101.50
2	A	2176	A	C5-C6-N6	-6.18	118.75	123.70
3	E	73	A	C6-N1-C2	6.18	122.31	118.60
2	A	1901	A	N9-C4-C5	-6.18	103.33	105.80
2	A	1867	G	N1-C2-N2	-6.17	110.65	116.20
1	B	1241	G	C8-N9-C4	-6.17	103.93	106.40
2	A	1906	G	P-O5'-C5'	-6.17	111.03	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	38	A	C6-C5-N7	6.16	136.62	132.30
2	A	1885	A	C5-N7-C8	6.16	106.98	103.90
2	A	1866	A	C5-N7-C8	-6.16	100.82	103.90
2	A	1887	C	N3-C4-C5	6.16	124.36	121.90
7	H	39	ASP	O-C-N	-6.16	109.41	121.10
2	A	2148	G	C4-C5-N7	6.15	113.26	110.80
5	F	7	ARG	CB-CA-C	-6.15	98.10	110.40
5	F	208	TYR	CG-CD2-CE2	-6.15	116.38	121.30
1	B	1242	G	C4-C5-C6	-6.15	115.11	118.80
2	A	2184	A	O4'-C1'-N9	6.15	113.12	108.20
3	E	73	A	N9-C4-C5	-6.15	103.34	105.80
2	A	1899	A	N7-C8-N9	6.15	116.87	113.80
2	A	1895	C	O4'-C1'-N1	6.14	113.11	108.20
3	E	47	G	C5-N7-C8	-6.14	101.23	104.30
4	D	68	ASP	CB-CG-OD2	6.14	123.83	118.30
2	A	2112	G	C5'-C4'-C3'	-6.14	106.18	116.00
2	A	2156	G	N1-C2-N3	-6.14	120.22	123.90
2	A	2167	U	C2-N3-C4	6.13	130.68	127.00
2	A	2146	C	N1-C2-O2	6.13	122.58	118.90
2	A	2171	A	N7-C8-N9	-6.13	110.74	113.80
3	E	38	A	N7-C8-N9	6.13	116.86	113.80
5	F	17	ALA	N-CA-CB	-6.13	101.52	110.10
2	A	2125	G	C1'-O4'-C4'	-6.12	105.00	109.90
2	A	2102	G	C5-C6-O6	-6.12	124.93	128.60
2	A	1880	U	O4'-C1'-N1	6.12	113.09	108.20
2	A	1900	A	C4-C5-C6	-6.12	113.94	117.00
1	B	1242	G	N1-C6-O6	6.12	123.57	119.90
2	A	1847	A	P-O3'-C3'	6.12	127.04	119.70
1	B	1291	U	C3'-C2'-C1'	6.11	106.39	101.50
2	A	1837	C	P-O5'-C5'	-6.11	111.12	120.90
4	D	111	TYR	CB-CG-CD1	-6.11	117.33	121.00
3	E	5	G	N7-C8-N9	-6.11	110.05	113.10
2	A	2169	A	C5-C6-N6	-6.10	118.82	123.70
8	I	94	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	A	2101	A	C5-C6-N6	-6.10	118.82	123.70
3	E	34	U	O4'-C1'-N1	6.10	113.08	108.20
3	E	64	G	O4'-C1'-N9	6.10	113.08	108.20
2	A	2100	G	OP1-P-OP2	-6.09	110.46	119.60
3	E	24	C	N3-C4-N4	6.09	122.26	118.00
2	A	2128	G	N9-C4-C5	-6.09	102.96	105.40
1	B	1241	G	C4-N9-C1'	6.09	134.41	126.50
2	A	2116	G	C8-N9-C4	6.09	108.83	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	14	A	C8-N9-C1'	-6.08	116.75	127.70
3	E	31	G	N9-C4-C5	-6.08	102.97	105.40
2	A	1884	G	P-O5'-C5'	6.08	130.63	120.90
3	E	4	G	N1-C6-O6	-6.07	116.26	119.90
2	A	1869	G	C5-C6-N1	6.07	114.53	111.50
3	E	48	U	O4'-C1'-N1	6.07	113.06	108.20
2	A	2103	C	C6-N1-C2	-6.07	117.87	120.30
2	A	1858	A	C4-C5-N7	-6.06	107.67	110.70
3	E	69	C	C4'-C3'-C2'	-6.06	96.54	102.60
5	F	21	TYR	CB-CG-CD1	-6.06	117.37	121.00
2	A	1844	C	C5-C4-N4	-6.05	115.96	120.20
2	A	1840	G	O4'-C1'-N9	6.05	113.04	108.20
2	A	2140	G	C5-N7-C8	-6.05	101.28	104.30
2	A	2161	C	C5-C4-N4	-6.05	115.97	120.20
2	A	1907	G	C6-N1-C2	-6.05	121.47	125.10
1	B	1290	G	C5-N7-C8	6.04	107.32	104.30
1	B	1298	U	N3-C4-O4	6.04	123.63	119.40
3	E	66	C	C4-C5-C6	6.03	120.42	117.40
3	E	23	G	C5-C6-O6	-6.03	124.98	128.60
3	E	16	C	C3'-C2'-C1'	6.03	106.32	101.50
2	A	1899	A	C6-C5-N7	-6.03	128.08	132.30
4	D	360	ALA	N-CA-CB	-6.03	101.66	110.10
2	A	2157	G	C5-C6-O6	-6.03	124.98	128.60
2	A	2160	C	N3-C4-C5	6.03	124.31	121.90
1	B	1244	G	C5-N7-C8	-6.02	101.29	104.30
5	F	68	GLY	C-N-CA	6.02	136.75	121.70
4	D	395	ARG	CG-CD-NE	-6.02	99.16	111.80
3	E	21	U	C4-C5-C6	-6.01	116.09	119.70
4	D	293	ARG	N-CA-CB	6.01	121.42	110.60
2	A	2177	C	C5'-C4'-O4'	6.01	116.31	109.10
3	E	26	C	C5-C4-N4	6.01	124.41	120.20
2	A	2140	G	N1-C2-N3	-6.01	120.30	123.90
3	E	4	G	C5-C6-O6	6.01	132.20	128.60
2	A	2135	A	N7-C8-N9	-6.00	110.80	113.80
2	A	1849	G	O4'-C1'-N9	6.00	113.00	108.20
3	E	14	A	P-O3'-C3'	-5.99	112.51	119.70
3	E	39	A	N1-C6-N6	5.99	122.20	118.60
2	A	2121	G	O4'-C1'-N9	5.99	112.99	108.20
3	E	62	C	C5-C4-N4	-5.99	116.01	120.20
3	E	60	A	C5-C6-N1	5.99	120.69	117.70
2	A	2097	A	N9-C4-C5	5.99	108.19	105.80
2	A	1859	U	C5'-C4'-C3'	-5.98	106.43	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1896	G	N1-C2-N3	-5.98	120.31	123.90
3	E	50	G	O4'-C1'-N9	5.98	112.99	108.20
2	A	1840	G	P-O3'-C3'	5.98	126.88	119.70
2	A	1905	C	C2-N3-C4	-5.98	116.91	119.90
2	A	1862	G	C5'-C4'-C3'	-5.97	106.44	116.00
2	A	1886	U	O4'-C1'-C2'	-5.97	99.83	105.80
3	E	5	G	C5-C6-O6	-5.97	125.02	128.60
2	A	2159	G	C4-C5-N7	5.97	113.19	110.80
2	A	2165	C	C2-N1-C1'	5.97	125.36	118.80
3	E	39	A	N7-C8-N9	5.97	116.78	113.80
2	A	1903	G	O4'-C1'-N9	5.96	112.97	108.20
7	H	48	TYR	CG-CD2-CE2	-5.96	116.53	121.30
4	D	170	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	A	2119	A	N9-C1'-C2'	-5.95	105.46	112.00
2	A	2157	G	C5'-C4'-O4'	5.95	116.24	109.10
4	D	149	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	1293	C	O4'-C1'-N1	5.95	112.96	108.20
4	D	440	LYS	CB-CG-CD	5.94	127.05	111.60
3	E	60	A	C6-N1-C2	-5.94	115.04	118.60
2	A	2140	G	C4'-C3'-C2'	-5.94	96.66	102.60
4	D	151	LEU	C-N-CA	5.94	136.54	121.70
2	A	2169	A	C6-N1-C2	-5.93	115.04	118.60
4	D	290	ARG	NE-CZ-NH1	-5.93	117.33	120.30
2	A	1904	G	C6-C5-N7	5.93	133.96	130.40
1	B	1239	A	C4-C5-N7	5.92	113.66	110.70
4	D	28	SER	O-C-N	-5.92	113.22	122.70
6	G	96	TRP	CH2-CZ2-CE2	5.92	123.33	117.40
3	E	45	A	C8-N9-C4	-5.92	103.43	105.80
1	B	1243	C	O4'-C1'-N1	5.92	112.93	108.20
2	A	2120	G	C6-C5-N7	-5.92	126.85	130.40
2	A	1873	G	C1'-O4'-C4'	-5.91	105.17	109.90
2	A	2144	G	O4'-C1'-N9	5.91	112.93	108.20
2	A	2118	U	OP1-P-OP2	-5.91	110.73	119.60
2	A	2110	G	O4'-C1'-N9	5.91	112.93	108.20
2	A	2152	G	O4'-C1'-N9	5.91	112.93	108.20
4	D	527	PHE	CB-CG-CD2	-5.91	116.66	120.80
4	D	294	PHE	CD1-CE1-CZ	5.91	127.19	120.10
2	A	2148	G	C4'-C3'-C2'	-5.91	96.69	102.60
3	E	54	G	N1-C2-N2	-5.90	110.89	116.20
5	F	201	PRO	N-CA-CB	5.90	110.38	103.30
8	I	108	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	1236	A	C2-N3-C4	-5.89	107.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2128	G	N7-C8-N9	-5.88	110.16	113.10
3	E	53	G	N9-C4-C5	-5.88	103.05	105.40
3	E	59	A	O4'-C1'-N9	5.88	112.90	108.20
2	A	2127	G	C5-C6-O6	-5.87	125.08	128.60
2	A	2172	U	C5'-C4'-O4'	-5.87	102.05	109.10
2	A	1877	A	C6-N1-C2	5.87	122.12	118.60
2	A	2106	U	C5'-C4'-O4'	5.87	116.15	109.10
3	E	37	U	N1-C2-N3	5.87	118.42	114.90
1	B	1289	A	C3'-C2'-C1'	-5.87	96.81	101.50
1	B	1303	C	C6-N1-C1'	-5.87	113.76	120.80
2	A	2191	A	C4-C5-C6	-5.87	114.07	117.00
8	I	108	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	A	2130	U	C4-C5-C6	-5.87	116.18	119.70
3	E	54	G	N1-C6-O6	5.87	123.42	119.90
2	A	2141	G	C5-C6-O6	5.86	132.12	128.60
2	A	1901	A	O4'-C1'-N9	5.86	112.89	108.20
8	I	91	ARG	NH1-CZ-NH2	5.86	125.84	119.40
3	E	23	G	N3-C4-N9	-5.86	122.48	126.00
1	B	1241	G	O4'-C1'-N9	5.86	112.89	108.20
1	B	1303	C	C5-C6-N1	-5.86	118.07	121.00
2	A	1842	G	C2-N3-C4	5.86	114.83	111.90
2	A	1881	C	C2-N1-C1'	5.86	125.24	118.80
3	E	29	C	N1-C2-N3	5.85	123.29	119.20
2	A	1837	C	O4'-C1'-N1	5.85	112.88	108.20
3	E	10	G	C4-C5-N7	5.84	113.14	110.80
2	A	2127	G	OP1-P-OP2	-5.84	110.84	119.60
2	A	1890	A	P-O3'-C3'	-5.84	112.69	119.70
3	E	68	C	C2-N3-C4	5.83	122.82	119.90
4	D	234	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
3	E	4	G	C6-C5-N7	-5.83	126.90	130.40
3	E	62	C	N3-C2-O2	5.83	125.98	121.90
2	A	2134	A	O4'-C1'-N9	5.83	112.86	108.20
2	A	2129	C	N3-C4-C5	-5.83	119.57	121.90
3	E	3	C	C5'-C4'-C3'	-5.83	106.67	116.00
4	D	87	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
2	A	1852	U	C4-C5-C6	-5.83	116.20	119.70
3	E	67	C	O4'-C1'-N1	5.83	112.86	108.20
4	D	490	PHE	CG-CD2-CE2	-5.82	114.40	120.80
2	A	2099	U	C6-N1-C2	-5.82	117.51	121.00
2	A	2164	C	C5'-C4'-O4'	-5.82	102.12	109.10
3	E	6	G	C4-C5-N7	5.82	113.13	110.80
2	A	2169	A	C2-N3-C4	5.82	113.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	169	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	A	2127	G	N9-C1'-C2'	-5.82	105.60	112.00
1	B	1294	G	P-O5'-C5'	5.81	130.20	120.90
2	A	1878	G	O4'-C1'-N9	5.81	112.85	108.20
3	E	27	G	C5-C6-O6	-5.81	125.12	128.60
4	D	155	ASP	O-C-N	-5.81	113.41	122.70
3	E	5	G	P-O3'-C3'	-5.80	112.74	119.70
2	A	1896	G	N9-C4-C5	-5.80	103.08	105.40
4	D	135	HIS	CA-CB-CG	-5.80	103.74	113.60
6	G	70	ARG	O-C-N	-5.80	113.42	122.70
4	D	503	PHE	CB-CG-CD1	-5.80	116.74	120.80
2	A	2102	G	N9-C4-C5	5.79	107.72	105.40
2	A	1848	A	O4'-C1'-N9	5.79	112.83	108.20
2	A	2094	A	P-O5'-C5'	5.79	130.17	120.90
3	E	10	G	C2-N3-C4	-5.79	109.00	111.90
1	B	1236	A	C3'-C2'-C1'	-5.79	96.87	101.50
2	A	2111	U	OP2-P-O3'	5.79	117.93	105.20
2	A	1884	G	N1-C6-O6	5.79	123.37	119.90
3	E	59	A	N3-C4-N9	-5.78	122.77	127.40
2	A	2154	A	C5-C6-N1	5.78	120.59	117.70
2	A	2147	A	C5-C6-N6	5.78	128.32	123.70
6	G	141	ASP	CB-CG-OD1	5.77	123.50	118.30
2	A	2186	G	C5-C6-N1	5.77	114.39	111.50
3	E	2	G	C5-C6-N1	-5.77	108.61	111.50
2	A	2189	U	C6-N1-C2	-5.77	117.54	121.00
2	A	2153	C	C5-C6-N1	5.77	123.89	121.00
2	A	1901	A	OP1-P-OP2	-5.77	110.95	119.60
4	D	431	PHE	CB-CG-CD2	5.77	124.84	120.80
1	B	1336	C	C5-C6-N1	-5.76	118.12	121.00
3	E	38	A	P-O5'-C5'	-5.76	111.68	120.90
2	A	1907	G	C4-C5-N7	5.76	113.11	110.80
1	B	1296	C	N3-C4-C5	-5.76	119.60	121.90
3	E	55	U	O4'-C1'-N1	5.76	112.81	108.20
2	A	1880	U	C6-N1-C2	-5.76	117.55	121.00
5	F	102	ASP	CB-CG-OD2	5.76	123.48	118.30
2	A	2171	A	C4-C5-N7	-5.75	107.82	110.70
6	G	148	VAL	CA-CB-CG1	5.75	119.53	110.90
1	B	1300	G	N1-C2-N2	5.75	121.38	116.20
3	E	15	G	C5-C6-O6	-5.75	125.15	128.60
2	A	1888	G	P-O5'-C5'	5.74	130.09	120.90
4	D	204	PHE	CB-CG-CD2	5.74	124.82	120.80
2	A	2163	A	N9-C1'-C2'	-5.74	105.69	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2144	G	C8-N9-C1'	-5.74	119.54	127.00
2	A	2152	G	C5-C6-O6	-5.74	125.16	128.60
2	A	2186	G	N1-C2-N2	-5.73	111.04	116.20
2	A	2119	A	O4'-C1'-N9	5.73	112.78	108.20
1	B	1241	G	C6-N1-C2	5.73	128.54	125.10
2	A	1861	G	C5-N7-C8	5.73	107.16	104.30
2	A	1902	C	O4'-C1'-N1	5.73	112.78	108.20
2	A	2123	G	O4'-C1'-N9	5.73	112.78	108.20
2	A	2190	G	C5-C6-N1	5.73	114.36	111.50
4	D	522	PHE	CB-CG-CD1	5.72	124.80	120.80
2	A	1888	G	N3-C4-C5	-5.72	125.74	128.60
3	E	19	G	N1-C2-N2	-5.72	111.05	116.20
2	A	1850	G	N3-C4-C5	5.72	131.46	128.60
2	A	1891	G	P-O3'-C3'	-5.71	112.84	119.70
6	G	136	ILE	O-C-N	-5.71	113.56	122.70
2	A	1902	C	C4'-C3'-C2'	-5.71	96.89	102.60
3	E	27	G	C5-C6-N1	-5.71	108.65	111.50
1	B	1333	A	N1-C2-N3	-5.70	126.45	129.30
2	A	2153	C	C2-N3-C4	-5.70	117.05	119.90
2	A	1859	U	N1-C2-O2	-5.69	118.82	122.80
2	A	1866	A	N9-C4-C5	5.69	108.08	105.80
3	E	46	G	C2-N3-C4	5.69	114.75	111.90
5	F	199	ALA	N-CA-CB	-5.69	102.13	110.10
2	A	1847	A	N9-C4-C5	5.69	108.08	105.80
2	A	1855	U	C1'-O4'-C4'	5.69	114.45	109.90
2	A	1881	C	P-O5'-C5'	5.68	129.99	120.90
2	A	1906	G	N1-C2-N3	-5.68	120.49	123.90
2	A	2098	U	N3-C4-C5	-5.68	111.19	114.60
2	A	1840	G	C8-N9-C4	-5.68	104.13	106.40
2	A	1860	G	N3-C4-C5	5.68	131.44	128.60
2	A	2121	G	C5-C6-O6	-5.68	125.19	128.60
8	I	9	ARG	NE-CZ-NH1	5.67	123.14	120.30
6	G	12	VAL	CG1-CB-CG2	-5.67	101.83	110.90
2	A	2107	G	N1-C2-N3	5.67	127.30	123.90
3	E	38	A	C5'-C4'-O4'	5.66	115.89	109.10
2	A	2128	G	C5-N7-C8	5.66	107.13	104.30
2	A	2164	C	C5-C6-N1	5.66	123.83	121.00
1	B	1297	G	C4-C5-C6	5.66	122.19	118.80
2	A	2193	G	C4-C5-N7	-5.66	108.54	110.80
5	F	56	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	B	1242	G	C4'-C3'-C2'	-5.66	96.94	102.60
2	A	1834	U	P-O5'-C5'	5.66	129.95	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1872	A	C5-N7-C8	-5.66	101.07	103.90
3	E	44	A	N9-C4-C5	-5.66	103.54	105.80
3	E	3	C	C5-C4-N4	5.65	124.16	120.20
3	E	36	A	N3-C4-N9	-5.65	122.88	127.40
2	A	1871	A	P-O5'-C5'	-5.65	111.86	120.90
2	A	2190	G	C5-N7-C8	5.65	107.13	104.30
4	D	257	GLN	O-C-N	-5.65	113.66	122.70
6	G	121	PHE	CB-CG-CD1	-5.64	116.85	120.80
2	A	2158	A	N7-C8-N9	-5.64	110.98	113.80
3	E	8	U	OP1-P-OP2	-5.64	111.14	119.60
1	B	1237	C	N3-C4-C5	-5.63	119.65	121.90
1	B	1237	C	C6-N1-C2	5.63	122.55	120.30
1	B	1291	U	O4'-C1'-N1	5.63	112.70	108.20
5	F	219	GLY	N-CA-C	-5.63	99.03	113.10
5	F	78	PHE	CB-CG-CD1	-5.63	116.86	120.80
2	A	2156	G	C6-N1-C2	5.62	128.47	125.10
3	E	38	A	C8-N9-C4	-5.62	103.55	105.80
1	B	1292	G	N3-C4-N9	5.62	129.37	126.00
4	D	4	PHE	CB-CA-C	-5.62	99.16	110.40
3	E	72	C	C5-C6-N1	-5.62	118.19	121.00
2	A	2165	C	P-O3'-C3'	-5.61	112.96	119.70
4	D	219	ARG	NH1-CZ-NH2	-5.61	113.22	119.40
2	A	2149	U	N3-C4-O4	-5.61	115.47	119.40
3	E	48	U	C4-C5-C6	-5.61	116.33	119.70
2	A	2126	A	OP1-P-OP2	-5.61	111.19	119.60
2	A	2164	C	OP1-P-OP2	-5.61	111.19	119.60
1	B	1336	C	O4'-C1'-N1	5.61	112.69	108.20
8	I	78	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	A	1897	G	C3'-C2'-C1'	-5.60	97.02	101.50
2	A	1864	U	P-O3'-C3'	5.60	126.42	119.70
2	A	1849	G	C4-C5-N7	5.59	113.04	110.80
2	A	2144	G	N3-C4-C5	-5.59	125.80	128.60
5	F	12	ARG	NE-CZ-NH2	-5.59	117.50	120.30
3	E	61	U	C5'-C4'-O4'	5.59	115.81	109.10
1	B	1245	C	N3-C4-N4	5.59	121.91	118.00
2	A	2135	A	C4-C5-C6	-5.59	114.21	117.00
2	A	2173	A	N7-C8-N9	-5.59	111.01	113.80
3	E	41	C	N3-C4-C5	5.59	124.13	121.90
4	D	333	TYR	CB-CG-CD1	-5.58	117.65	121.00
7	H	36	LYS	O-C-N	-5.57	113.79	122.70
6	G	82	TYR	CG-CD1-CE1	-5.57	116.85	121.30
2	A	2138	G	N7-C8-N9	5.56	115.88	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	51	ASP	CB-CG-OD2	-5.56	113.29	118.30
4	D	172	ALA	CB-CA-C	-5.56	101.76	110.10
8	I	108	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
3	E	16	C	N1-C2-N3	-5.56	115.31	119.20
5	F	177	LYS	N-CA-CB	-5.56	100.59	110.60
3	E	14	A	O4'-C1'-N9	5.55	112.64	108.20
2	A	2174	C	C5'-C4'-O4'	5.55	115.76	109.10
1	B	1332	A	C6-C5-N7	-5.55	128.42	132.30
3	E	50	G	N9-C4-C5	5.55	107.62	105.40
2	A	1856	U	C4-C5-C6	5.54	123.03	119.70
2	A	2159	G	C5'-C4'-O4'	5.54	115.75	109.10
2	A	2176	A	C5-C6-N1	5.54	120.47	117.70
2	A	2111	U	N3-C2-O2	5.53	126.07	122.20
2	A	2143	C	N3-C4-C5	-5.53	119.69	121.90
4	D	408	VAL	O-C-N	-5.53	113.86	122.70
1	B	1244	G	C6-C5-N7	-5.52	127.09	130.40
2	A	1852	U	O4'-C1'-N1	5.52	112.62	108.20
4	D	547	ARG	CD-NE-CZ	5.52	131.33	123.60
8	I	101	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	1300	G	C1'-O4'-C4'	-5.52	105.49	109.90
3	E	5	G	C4'-C3'-C2'	-5.52	97.08	102.60
2	A	1872	A	C6-N1-C2	-5.51	115.29	118.60
3	E	38	A	C8-N9-C1'	-5.51	117.78	127.70
1	B	1244	G	N1-C6-O6	-5.51	116.59	119.90
3	E	30	G	C3'-C2'-C1'	-5.51	97.09	101.50
1	B	1303	C	O4'-C1'-N1	5.51	112.61	108.20
2	A	2145	C	C2'-C3'-O3'	5.50	122.51	113.70
3	E	68	C	N3-C4-N4	5.50	121.85	118.00
1	B	1334	G	C5-N7-C8	5.50	107.05	104.30
2	A	2137	U	N1-C2-O2	5.50	126.65	122.80
2	A	1897	G	N3-C4-C5	-5.50	125.85	128.60
2	A	2152	G	C5'-C4'-O4'	5.50	115.70	109.10
2	A	1878	G	C3'-C2'-C1'	-5.50	97.10	101.50
2	A	2171	A	C3'-C2'-C1'	-5.50	97.10	101.50
4	D	209	GLU	C-N-CA	5.50	133.84	122.30
8	I	116	ALA	CB-CA-C	-5.50	101.86	110.10
2	A	1903	G	C5-N7-C8	5.49	107.05	104.30
3	E	18	U	C5-C6-N1	-5.49	119.95	122.70
2	A	2179	C	C2-N3-C4	-5.49	117.16	119.90
2	A	1904	G	C4-C5-N7	-5.48	108.61	110.80
8	I	63	VAL	O-C-N	-5.48	113.93	122.70
2	A	2185	U	C6-N1-C2	-5.48	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2159	G	C5'-C4'-C3'	-5.48	107.24	116.00
2	A	2186	G	O4'-C1'-N9	5.48	112.58	108.20
1	B	1305	G	C4-C5-C6	-5.47	115.52	118.80
4	D	333	TYR	N-CA-CB	5.47	120.45	110.60
3	E	12	G	O4'-C1'-N9	5.47	112.57	108.20
2	A	1875	G	C5-C6-N1	-5.46	108.77	111.50
2	A	2159	G	C6-N1-C2	-5.46	121.82	125.10
2	A	2126	A	C2-N3-C4	5.46	113.33	110.60
4	D	467	LEU	O-C-N	-5.46	113.96	122.70
6	G	111	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	E	2	G	N1-C2-N3	-5.46	120.63	123.90
3	E	24	C	N3-C2-O2	-5.45	118.08	121.90
4	D	83	GLU	O-C-N	-5.45	113.98	122.70
6	G	143	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	1295	U	N3-C4-O4	5.45	123.21	119.40
4	D	262	GLU	CA-CB-CG	5.44	125.38	113.40
2	A	1863	G	C2-N3-C4	5.44	114.62	111.90
3	E	19	G	C4-C5-N7	-5.44	108.62	110.80
3	E	23	G	P-O5'-C5'	5.44	129.60	120.90
4	D	200	TRP	CZ3-CH2-CZ2	-5.43	115.08	121.60
2	A	1880	U	C5-C6-N1	5.43	125.42	122.70
4	D	283	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
1	B	1300	G	N1-C6-O6	5.43	123.16	119.90
3	E	8	U	C5-C4-O4	-5.43	122.64	125.90
2	A	2125	G	C5-C6-N1	-5.43	108.79	111.50
3	E	39	A	C5-N7-C8	-5.43	101.19	103.90
3	E	1	C	N3-C4-C5	-5.42	119.73	121.90
2	A	1885	A	C8-N9-C4	5.42	107.97	105.80
3	E	38	A	N9-C4-C5	5.42	107.97	105.80
1	B	1300	G	P-O5'-C5'	5.42	129.57	120.90
2	A	1887	C	C2-N3-C4	-5.42	117.19	119.90
2	A	2096	C	N3-C4-C5	5.42	124.07	121.90
2	A	2121	G	N3-C2-N2	5.42	123.69	119.90
2	A	2190	G	C6-C5-N7	5.41	133.65	130.40
8	I	108	ARG	CD-NE-CZ	-5.41	116.02	123.60
2	A	2135	A	C5-C6-N1	5.41	120.40	117.70
3	E	48	U	N1-C2-O2	5.41	126.58	122.80
2	A	1854	A	C6-N1-C2	-5.40	115.36	118.60
3	E	48	U	C2'-C3'-O3'	5.40	122.34	113.70
3	E	52	C	P-O5'-C5'	-5.40	112.26	120.90
5	F	181	ASP	CB-CG-OD2	-5.40	113.44	118.30
4	D	52	MET	CG-SD-CE	-5.40	91.57	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2153	C	N3-C2-O2	-5.39	118.12	121.90
2	A	1849	G	C5-N7-C8	-5.39	101.60	104.30
3	E	15	G	P-O3'-C3'	5.39	126.17	119.70
7	H	42	VAL	C-N-CA	5.39	135.18	121.70
2	A	2171	A	O4'-C1'-N9	5.39	112.51	108.20
3	E	75	C	C5-C6-N1	-5.39	118.31	121.00
4	D	389	ALA	CB-CA-C	5.39	118.18	110.10
8	I	52	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
3	E	48	U	N3-C4-C5	5.38	117.83	114.60
6	G	76	PHE	CB-CG-CD1	-5.38	117.03	120.80
2	A	1893	C	N1-C1'-C2'	-5.38	106.08	112.00
3	E	40	C	C5-C4-N4	-5.38	116.43	120.20
3	E	48	U	C2-N3-C4	-5.38	123.77	127.00
2	A	1854	A	C2-N3-C4	-5.38	107.91	110.60
3	E	24	C	C1'-O4'-C4'	-5.38	105.60	109.90
2	A	2140	G	C2-N3-C4	5.37	114.59	111.90
3	E	59	A	P-O3'-C3'	-5.37	113.25	119.70
4	D	68	ASP	CB-CG-OD1	-5.37	113.47	118.30
4	D	175	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	E	23	G	C4-C5-C6	-5.37	115.58	118.80
8	I	25	PHE	CD1-CG-CD2	-5.36	111.33	118.30
2	A	2106	U	O4'-C1'-N1	5.36	112.49	108.20
2	A	2176	A	N9-C4-C5	5.36	107.94	105.80
8	I	32	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	1243	C	OP1-P-O3'	5.36	116.98	105.20
3	E	62	C	N3-C4-N4	5.36	121.75	118.00
2	A	1850	G	N1-C2-N3	-5.35	120.69	123.90
3	E	74	A	C4-C5-N7	5.35	113.38	110.70
1	B	1300	G	C5'-C4'-C3'	-5.35	107.44	116.00
2	A	1899	A	C4-C5-N7	5.35	113.37	110.70
1	B	1236	A	N7-C8-N9	5.35	116.47	113.80
2	A	1851	U	N1-C2-O2	5.35	126.54	122.80
2	A	1857	G	C5-N7-C8	-5.34	101.63	104.30
2	A	2102	G	C5-N7-C8	5.34	106.97	104.30
8	I	17	PHE	CB-CG-CD2	5.34	124.54	120.80
2	A	1873	G	C4-C5-N7	5.34	112.94	110.80
2	A	1872	A	N9-C1'-C2'	-5.34	106.13	112.00
1	B	1245	C	C4'-C3'-C2'	-5.34	97.26	102.60
2	A	1881	C	N3-C2-O2	-5.33	118.17	121.90
1	B	1303	C	C2-N1-C1'	5.33	124.66	118.80
3	E	5	G	P-O5'-C5'	-5.33	112.38	120.90
2	A	1888	G	N1-C2-N2	-5.33	111.41	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	21	U	C6-N1-C2	-5.33	117.80	121.00
2	A	2147	A	N7-C8-N9	5.32	116.46	113.80
3	E	15	G	C2-N3-C4	5.32	114.56	111.90
4	D	228	TRP	CE2-CD2-CG	-5.32	103.04	107.30
3	E	56	U	N1-C2-O2	-5.32	119.08	122.80
2	A	2138	G	C2-N3-C4	5.32	114.56	111.90
2	A	1857	G	N9-C4-C5	5.31	107.53	105.40
2	A	1884	G	C5-C6-O6	-5.31	125.41	128.60
4	D	73	TYR	CG-CD2-CE2	-5.31	117.05	121.30
6	G	147	ARG	CG-CD-NE	-5.31	100.65	111.80
1	B	1239	A	C4-C5-C6	-5.31	114.35	117.00
3	E	4	G	P-O3'-C3'	5.31	126.07	119.70
5	F	22	ASP	CB-CG-OD1	5.31	123.08	118.30
2	A	2112	G	N3-C2-N2	-5.30	116.19	119.90
2	A	2173	A	C4-C5-N7	-5.30	108.05	110.70
2	A	2188	U	C5-C6-N1	5.30	125.35	122.70
3	E	31	G	N1-C2-N3	-5.30	120.72	123.90
2	A	2109	U	C3'-C2'-C1'	5.30	105.74	101.50
1	B	1237	C	P-O3'-C3'	5.30	126.06	119.70
2	A	1884	G	C4-C5-N7	-5.30	108.68	110.80
2	A	1906	G	C8-N9-C4	-5.30	104.28	106.40
3	E	8	U	C6-N1-C2	-5.30	117.82	121.00
3	E	43	G	N1-C6-O6	-5.30	116.72	119.90
3	E	66	C	N3-C2-O2	-5.30	118.19	121.90
3	E	70	C	C5-C4-N4	-5.30	116.49	120.20
2	A	1866	A	N1-C6-N6	5.29	121.77	118.60
2	A	1890	A	N1-C2-N3	-5.29	126.66	129.30
2	A	1856	U	C2-N3-C4	-5.29	123.83	127.00
3	E	27	G	N3-C2-N2	5.29	123.60	119.90
3	E	47	G	C5-C6-N1	5.28	114.14	111.50
3	E	17	C	O5'-C5'-C4'	5.28	121.73	111.70
2	A	2123	G	C8-N9-C4	-5.28	104.29	106.40
2	A	2142	A	P-O5'-C5'	-5.28	112.45	120.90
3	E	15	G	C4-C5-C6	-5.28	115.63	118.80
4	D	461	VAL	CB-CA-C	-5.28	101.38	111.40
1	B	1298	U	C6-N1-C1'	-5.27	113.82	121.20
2	A	2160	C	C5-C6-N1	-5.27	118.36	121.00
3	E	52	C	N1-C2-N3	-5.27	115.51	119.20
8	I	69	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	A	1903	G	C6-N1-C2	5.26	128.26	125.10
2	A	2189	U	C1'-O4'-C4'	5.26	114.11	109.90
3	E	17	C	N3-C4-N4	5.26	121.68	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2186	G	N7-C8-N9	5.26	115.73	113.10
2	A	2113	U	N3-C2-O2	-5.26	118.52	122.20
4	D	99	ASN	CA-CB-CG	-5.26	101.83	113.40
1	B	1302	C	C2-N1-C1'	5.26	124.58	118.80
1	B	1237	C	C5-C6-N1	-5.25	118.37	121.00
6	G	132	ARG	NE-CZ-NH2	5.25	122.93	120.30
2	A	1905	C	C5'-C4'-O4'	5.25	115.40	109.10
5	F	112	ASP	CB-CG-OD1	5.25	123.03	118.30
2	A	2127	G	C6-N1-C2	-5.25	121.95	125.10
2	A	1867	G	C4'-C3'-C2'	-5.25	97.35	102.60
3	E	63	C	C4-C5-C6	-5.25	114.78	117.40
2	A	1887	C	OP2-P-O3'	5.24	116.74	105.20
6	G	122	ASP	O-C-N	-5.24	114.29	123.20
2	A	1845	G	N9-C4-C5	5.24	107.50	105.40
2	A	2132	U	C5-C6-N1	-5.24	120.08	122.70
5	F	151	GLU	CB-CA-C	-5.23	99.93	110.40
2	A	2166	U	C1'-O4'-C4'	-5.23	105.71	109.90
3	E	26	C	C2-N3-C4	5.23	122.52	119.90
2	A	1853	A	O3'-P-O5'	5.23	113.94	104.00
2	A	1868	C	N3-C4-N4	-5.23	114.34	118.00
2	A	2127	G	C6-C5-N7	-5.23	127.26	130.40
4	D	434	LYS	O-C-N	-5.23	114.31	123.20
2	A	1840	G	N3-C4-N9	-5.23	122.86	126.00
2	A	1866	A	O5'-P-OP1	-5.23	101.00	105.70
2	A	2188	U	C4'-C3'-C2'	5.23	107.83	102.60
1	B	1303	C	P-O5'-C5'	5.22	129.26	120.90
3	E	14	A	N9-C4-C5	-5.22	103.71	105.80
1	B	1332	A	N1-C2-N3	-5.22	126.69	129.30
2	A	1857	G	OP1-P-OP2	-5.22	111.77	119.60
4	D	376	ASP	CB-CG-OD2	5.22	123.00	118.30
8	I	115	MET	O-C-N	-5.22	114.35	122.70
3	E	11	A	C5-C6-N6	-5.22	119.53	123.70
5	F	122	ARG	CD-NE-CZ	5.22	130.90	123.60
2	A	2120	G	C2-N3-C4	5.21	114.51	111.90
2	A	2121	G	C6-C5-N7	5.21	133.53	130.40
4	D	66	GLN	CG-CD-OE1	-5.21	111.17	121.60
3	E	10	G	C5-N7-C8	5.21	106.91	104.30
3	E	52	C	O4'-C1'-N1	5.21	112.37	108.20
4	D	53	ALA	O-C-N	-5.21	114.34	123.20
2	A	2171	A	N1-C2-N3	5.21	131.90	129.30
4	D	498	SER	CA-C-O	5.21	131.03	120.10
2	A	2112	G	C2-N3-C4	-5.21	109.30	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	494	ALA	N-CA-CB	-5.21	102.81	110.10
2	A	1842	G	C6-C5-N7	5.20	133.52	130.40
2	A	1900	A	C4-C5-N7	-5.20	108.10	110.70
2	A	2159	G	N3-C2-N2	-5.20	116.26	119.90
2	A	1861	G	C6-N1-C2	-5.20	121.98	125.10
2	A	1864	U	OP1-P-OP2	-5.20	111.80	119.60
2	A	1902	C	C1'-O4'-C4'	-5.20	105.74	109.90
1	B	1237	C	O4'-C1'-N1	5.19	112.35	108.20
3	E	19	G	C4-C5-C6	5.19	121.91	118.80
5	F	7	ARG	CG-CD-NE	-5.19	100.91	111.80
3	E	17	C	C5-C4-N4	-5.18	116.57	120.20
2	A	1866	A	C4-C5-C6	5.18	119.59	117.00
7	H	35	LEU	CB-CA-C	-5.18	100.35	110.20
2	A	2118	U	N3-C4-O4	5.18	123.03	119.40
2	A	2144	G	C4-N9-C1'	5.17	133.22	126.50
2	A	2161	C	N3-C2-O2	-5.17	118.28	121.90
4	D	365	LEU	CB-CG-CD2	-5.17	102.21	111.00
2	A	2185	U	C5-C4-O4	-5.17	122.80	125.90
3	E	22	A	C5'-C4'-C3'	-5.17	107.73	116.00
4	D	392	ASP	O-C-N	-5.17	114.43	122.70
2	A	1895	C	N3-C4-C5	-5.16	119.83	121.90
2	A	2120	G	P-O3'-C3'	5.16	125.89	119.70
3	E	74	A	N3-C4-N9	5.16	131.53	127.40
4	D	2	ALA	CB-CA-C	5.16	117.83	110.10
2	A	2162	G	OP2-P-O3'	5.16	116.54	105.20
4	D	246	SER	O-C-N	-5.16	114.45	122.70
1	B	1243	C	C2-N3-C4	-5.15	117.32	119.90
2	A	1851	U	N3-C4-C5	5.15	117.69	114.60
2	A	2144	G	C5-N7-C8	5.15	106.88	104.30
2	A	2190	G	N1-C2-N3	-5.15	120.81	123.90
4	D	138	HIS	N-CA-CB	5.15	119.87	110.60
2	A	2104	C	C3'-C2'-C1'	5.14	105.62	101.50
2	A	1888	G	O4'-C1'-N9	5.14	112.31	108.20
2	A	2094	A	N9-C4-C5	-5.14	103.74	105.80
2	A	2107	G	N1-C6-O6	-5.14	116.82	119.90
2	A	1902	C	N1-C2-O2	5.13	121.98	118.90
2	A	2104	C	C2-N3-C4	-5.13	117.33	119.90
3	E	19	G	N9-C4-C5	5.13	107.45	105.40
4	D	171	VAL	CB-CA-C	-5.13	101.65	111.40
8	I	80	GLY	N-CA-C	-5.13	100.27	113.10
2	A	1899	A	C8-N9-C4	-5.13	103.75	105.80
1	B	1297	G	C4-C5-N7	5.12	112.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2177	C	O5'-C5'-C4'	-5.12	101.96	111.70
3	E	22	A	N7-C8-N9	-5.12	111.24	113.80
2	A	2101	A	N1-C2-N3	5.12	131.86	129.30
3	E	16	C	OP1-P-OP2	-5.12	111.92	119.60
3	E	44	A	N3-C4-N9	5.12	131.50	127.40
2	A	1871	A	N1-C6-N6	5.12	121.67	118.60
2	A	1891	G	N1-C2-N2	-5.12	111.59	116.20
2	A	2126	A	C3'-C2'-C1'	5.12	105.59	101.50
3	E	26	C	N1-C1'-C2'	-5.12	106.37	112.00
3	E	53	G	P-O3'-C3'	5.11	125.83	119.70
1	B	1294	G	O4'-C1'-N9	5.11	112.29	108.20
2	A	1880	U	C2'-C3'-O3'	5.11	121.87	113.70
2	A	2167	U	N1-C2-N3	-5.11	111.84	114.90
7	H	42	VAL	O-C-N	-5.11	114.53	122.70
1	B	1301	U	O4'-C1'-N1	5.10	112.28	108.20
2	A	2129	C	C1'-O4'-C4'	-5.10	105.82	109.90
3	E	18	U	C4-C5-C6	5.10	122.76	119.70
3	E	50	G	C4-C5-N7	-5.10	108.76	110.80
1	B	1302	C	C5-C6-N1	5.10	123.55	121.00
2	A	1835	G	N3-C2-N2	5.10	123.47	119.90
3	E	17	C	C6-N1-C1'	-5.10	114.68	120.80
2	A	1897	G	N3-C2-N2	5.10	123.47	119.90
4	D	6	TYR	CB-CG-CD1	-5.10	117.94	121.00
3	E	18	U	N3-C4-C5	-5.09	111.54	114.60
2	A	1885	A	C5-C6-N1	-5.09	115.15	117.70
4	D	496	VAL	CA-CB-CG2	5.09	118.54	110.90
2	A	1852	U	N3-C4-O4	-5.09	115.84	119.40
3	E	31	G	N3-C4-C5	5.09	131.15	128.60
2	A	2107	G	OP2-P-O3'	5.09	116.39	105.20
1	B	1297	G	C4'-C3'-C2'	5.09	107.69	102.60
2	A	2119	A	OP2-P-O3'	5.08	116.38	105.20
4	D	200	TRP	CD1-NE1-CE2	-5.08	104.42	109.00
2	A	2173	A	C4'-C3'-C2'	5.08	107.68	102.60
6	G	96	TRP	CG-CD2-CE3	-5.08	129.33	133.90
8	I	115	MET	CG-SD-CE	-5.08	92.07	100.20
1	B	1244	G	O4'-C1'-C2'	5.08	112.17	107.60
3	E	50	G	C8-N9-C4	-5.08	104.37	106.40
4	D	275	TRP	CZ3-CH2-CZ2	-5.08	115.51	121.60
2	A	1867	G	N7-C8-N9	-5.08	110.56	113.10
2	A	2135	A	N1-C2-N3	-5.07	126.76	129.30
4	D	379	THR	N-CA-CB	5.07	119.94	110.30
8	I	118	ARG	NE-CZ-NH2	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1289	A	C8-N9-C4	-5.07	103.77	105.80
2	A	1858	A	C4'-C3'-C2'	-5.07	97.53	102.60
3	E	47	G	P-O3'-C3'	-5.07	113.61	119.70
2	A	2109	U	C5'-C4'-C3'	-5.07	107.89	116.00
5	F	181	ASP	CB-CG-OD1	5.07	122.86	118.30
6	G	47	LYS	O-C-N	-5.07	114.60	122.70
6	G	7	TYR	CG-CD2-CE2	-5.06	117.25	121.30
2	A	2133	G	C8-N9-C4	5.06	108.42	106.40
2	A	2182	U	O4'-C1'-N1	5.06	112.25	108.20
3	E	12	G	C5-C6-O6	-5.06	125.56	128.60
3	E	74	A	C3'-C2'-C1'	5.06	105.55	101.50
3	E	27	G	C8-N9-C4	-5.06	104.38	106.40
3	E	14	A	C4-N9-C1'	5.05	135.40	126.30
4	D	93	ALA	N-CA-CB	5.05	117.18	110.10
4	D	294	PHE	CG-CD1-CE1	-5.05	115.24	120.80
5	F	148	ASN	N-CA-C	-5.05	97.36	111.00
2	A	1850	G	C6-N1-C2	5.05	128.13	125.10
5	F	119	ASP	CA-C-O	5.05	130.70	120.10
3	E	7	G	N3-C4-C5	-5.05	126.08	128.60
1	B	1333	A	C5-N7-C8	5.04	106.42	103.90
3	E	4	G	N3-C4-N9	5.04	129.03	126.00
2	A	1836	C	O4'-C1'-N1	5.04	112.23	108.20
3	E	50	G	OP1-P-OP2	-5.04	112.04	119.60
8	I	94	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	A	1835	G	C5-C6-O6	-5.04	125.58	128.60
2	A	1875	G	N1-C2-N3	-5.04	120.88	123.90
2	A	2119	A	N7-C8-N9	-5.04	111.28	113.80
3	E	27	G	C4-C5-N7	5.04	112.81	110.80
3	E	42	C	C4'-C3'-C2'	-5.04	97.56	102.60
2	A	2175	C	N1-C2-N3	5.04	122.73	119.20
3	E	25	U	N3-C2-O2	5.04	125.73	122.20
3	E	49	C	C2-N3-C4	-5.04	117.38	119.90
8	I	134	VAL	CA-CB-CG2	-5.04	103.35	110.90
1	B	1303	C	C3'-C2'-C1'	-5.03	97.47	101.50
2	A	1860	G	C4'-C3'-C2'	-5.03	97.57	102.60
2	A	1901	A	C5'-C4'-O4'	5.03	115.14	109.10
2	A	2190	G	N1-C6-O6	5.03	122.92	119.90
2	A	1897	G	P-O5'-C5'	-5.03	112.86	120.90
2	A	1857	G	N1-C6-O6	5.02	122.91	119.90
2	A	1870	C	C1'-O4'-C4'	-5.02	105.88	109.90
8	I	49	LEU	CB-CA-C	5.02	119.74	110.20
8	I	25	PHE	CG-CD1-CE1	5.02	126.32	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2189	U	N1-C2-O2	-5.02	119.29	122.80
4	D	420	THR	CB-CA-C	-5.01	98.06	111.60
8	I	25	PHE	CG-CD2-CE2	5.01	126.31	120.80
2	A	2153	C	N3-C4-C5	-5.01	119.90	121.90
2	A	2174	C	OP1-P-OP2	-5.01	112.09	119.60
3	E	22	A	P-O3'-C3'	5.01	125.71	119.70
3	E	1	C	O4'-C1'-N1	5.00	112.20	108.20
3	E	60	A	C5-N7-C8	5.00	106.40	103.90

There are no chirality outliers.

All (178) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1835	G	Sidechain
2	A	1838	C	Sidechain
2	A	1839	G	Sidechain
2	A	1840	G	Sidechain
2	A	1842	G	Sidechain
2	A	1843	C	Sidechain
2	A	1845	G	Sidechain
2	A	1846	G	Sidechain
2	A	1850	G	Sidechain
2	A	1857	G	Sidechain
2	A	1858	A	Sidechain
2	A	1859	U	Sidechain
2	A	1862	G	Sidechain
2	A	1863	G	Sidechain
2	A	1865	U	Sidechain
2	A	1868	C	Sidechain
2	A	1869	G	Sidechain
2	A	1874	C	Sidechain
2	A	1876	A	Sidechain
2	A	1878	G	Sidechain
2	A	1882	U	Sidechain
2	A	1884	G	Sidechain
2	A	1886	U	Sidechain
2	A	1888	G	Sidechain
2	A	1889	A	Sidechain
2	A	1891	G	Sidechain
2	A	1894	C	Sidechain
2	A	1895	C	Sidechain
2	A	1896	G	Sidechain

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Mol	Chain	Res	Type	Group
2	A	1900	A	Sidechain
2	A	2094	A	Sidechain
2	A	2095	A	Sidechain
2	A	2102	G	Sidechain
2	A	2103	C	Sidechain
2	A	2104	C	Sidechain
2	A	2106	U	Sidechain
2	A	2109	U	Sidechain
2	A	2110	G	Sidechain
2	A	2111	U	Sidechain
2	A	2112	G	Sidechain
2	A	2114	A	Sidechain
2	A	2115	G	Sidechain
2	A	2116	G	Sidechain
2	A	2120	G	Sidechain
2	A	2123	G	Sidechain
2	A	2124	G	Sidechain
2	A	2125	G	Sidechain
2	A	2127	G	Sidechain
2	A	2128	G	Sidechain
2	A	2129	C	Sidechain
2	A	2130	U	Sidechain
2	A	2132	U	Sidechain
2	A	2133	G	Sidechain
2	A	2135	A	Sidechain
2	A	2136	G	Sidechain
2	A	2137	U	Sidechain
2	A	2138	G	Sidechain
2	A	2141	G	Sidechain
2	A	2144	G	Sidechain
2	A	2147	A	Sidechain
2	A	2148	G	Sidechain
2	A	2152	G	Sidechain
2	A	2153	C	Sidechain
2	A	2154	A	Sidechain
2	A	2156	G	Sidechain
2	A	2157	G	Sidechain
2	A	2158	A	Sidechain
2	A	2159	G	Sidechain
2	A	2160	C	Sidechain
2	A	2161	C	Sidechain
2	A	2164	C	Sidechain

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Mol	Chain	Res	Type	Group
2	A	2165	C	Sidechain
2	A	2166	U	Sidechain
2	A	2168	G	Sidechain
2	A	2176	A	Sidechain
2	A	2177	C	Sidechain
2	A	2179	C	Sidechain
2	A	2184	A	Sidechain
2	A	2186	G	Sidechain
2	A	2187	U	Sidechain
2	A	2189	U	Sidechain
2	A	2190	G	Sidechain
2	A	2191	A	Sidechain
2	A	2192	U	Sidechain
1	B	1239	A	Sidechain
1	B	1242	G	Sidechain
1	B	1243	C	Sidechain
1	B	1290	G	Sidechain
1	B	1295	U	Sidechain
1	B	1296	C	Sidechain
1	B	1301	U	Sidechain
1	B	1302	C	Sidechain
1	B	1304	G	Sidechain
1	B	1332	A	Sidechain
1	B	1334	G	Sidechain
1	B	1336	C	Sidechain
4	D	111	TYR	Sidechain
4	D	181	PRO	Peptide
4	D	186	LEU	Peptide
4	D	19	ARG	Sidechain
4	D	225	VAL	Peptide
4	D	254	ARG	Sidechain
4	D	290	ARG	Sidechain
4	D	293	ARG	Sidechain
4	D	316	GLY	Peptide
4	D	318	ARG	Sidechain
4	D	330	ARG	Sidechain
4	D	333	TYR	Sidechain
4	D	336	ARG	Sidechain
4	D	366	PHE	Sidechain
4	D	392	ASP	Peptide
4	D	395	ARG	Sidechain
4	D	427	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	D	441	ARG	Sidechain
4	D	481	ARG	Sidechain
4	D	503	PHE	Sidechain
4	D	508	ALA	Peptide
4	D	530	TYR	Sidechain
4	D	550	TYR	Sidechain
3	E	1	C	Sidechain
3	E	11	A	Sidechain
3	E	12	G	Sidechain
3	E	13	C	Sidechain
3	E	15	G	Sidechain
3	E	18	U	Sidechain
3	E	19	G	Sidechain
3	E	22	A	Sidechain
3	E	23	G	Sidechain
3	E	28	U	Sidechain
3	E	29	C	Sidechain
3	E	3	C	Sidechain
3	E	30	G	Sidechain
3	E	35	C	Sidechain
3	E	36	A	Sidechain
3	E	37	U	Sidechain
3	E	38	A	Sidechain
3	E	4	G	Sidechain
3	E	40	C	Sidechain
3	E	42	C	Sidechain
3	E	44	A	Sidechain
3	E	47	G	Sidechain
3	E	5	G	Sidechain
3	E	53	G	Sidechain
3	E	59	A	Sidechain
3	E	60	A	Sidechain
3	E	61	U	Sidechain
3	E	63	C	Sidechain
3	E	64	G	Sidechain
3	E	7	G	Sidechain
3	E	73	A	Sidechain
3	E	74	A	Sidechain
3	E	8	U	Sidechain
3	E	9	G	Sidechain
5	F	12	ARG	Sidechain
5	F	124	VAL	Peptide

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Mol	Chain	Res	Type	Group
5	F	134	ARG	Sidechain
5	F	162	ARG	Sidechain
5	F	163	TYR	Sidechain
5	F	164	ARG	Sidechain
5	F	203	GLN	Peptide
5	F	35	THR	Peptide
5	F	7	ARG	Sidechain
6	G	124	ARG	Sidechain
6	G	149	ARG	Sidechain
6	G	177	ARG	Sidechain
6	G	6	TYR	Sidechain
6	G	76	PHE	Sidechain
6	G	91	ARG	Sidechain
7	H	20	TYR	Sidechain
7	H	27	ARG	Sidechain
7	H	48	TYR	Sidechain
7	H	5	ARG	Sidechain
8	I	101	ARG	Sidechain
8	I	4	ARG	Sidechain
8	I	52	ARG	Sidechain
8	I	69	ARG	Sidechain
8	I	78	ARG	Sidechain
8	I	95	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	687	0	342	24	0
2	A	3731	0	1828	67	0
3	E	1640	0	827	29	0
4	D	4393	0	4377	333	0
5	F	1733	0	1824	152	0
6	G	1420	0	1460	10	0
7	H	410	0	440	1	0
8	I	1182	0	1240	124	0
All	All	15196	0	12338	421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:U:C4	8:I:31:VAL:HG12	1.20	1.68
4:D:108:TYR:HA	5:F:118:PRO:CB	1.17	1.59
4:D:108:TYR:CA	5:F:118:PRO:HB2	1.27	1.57
4:D:108:TYR:CE2	5:F:121:MET:HB3	1.34	1.57
4:D:523:PHE:CD1	8:I:130:LYS:HB2	1.37	1.57
2:A:2169:A:C2	4:D:141:ASN:HB2	1.40	1.55
4:D:111:TYR:CD1	5:F:147:PRO:HA	1.42	1.53
4:D:536:ARG:NH1	8:I:137:ARG:NH2	1.65	1.44
4:D:133:GLN:HG2	5:F:60:ARG:CD	1.44	1.42
1:B:1240:U:C4	8:I:31:VAL:CG1	2.11	1.34
4:D:536:ARG:NH1	8:I:137:ARG:HH22	0.83	1.31
2:A:2113:U:C4'	4:D:147:ALA:HA	1.63	1.29
4:D:108:TYR:CA	5:F:118:PRO:CB	1.94	1.28
4:D:108:TYR:HB3	5:F:118:PRO:O	1.29	1.28
4:D:322:LYS:CG	8:I:113:LYS:HZ3	1.45	1.27
4:D:523:PHE:HD1	8:I:130:LYS:CB	1.45	1.27
1:B:1240:U:C1'	8:I:37:THR:HG21	1.64	1.27
4:D:129:GLU:OE1	5:F:143:GLY:HA3	1.18	1.27
4:D:108:TYR:OH	5:F:121:MET:HG2	1.34	1.26
4:D:533:TYR:HB2	8:I:129:ASN:O	1.08	1.26
4:D:108:TYR:C	5:F:118:PRO:HB2	1.57	1.25
2:A:2169:A:H2	4:D:141:ASN:CB	1.49	1.23
4:D:322:LYS:HG3	8:I:113:LYS:NZ	1.51	1.23
4:D:536:ARG:HH12	8:I:137:ARG:NH2	1.24	1.22
4:D:108:TYR:CE2	5:F:121:MET:CB	2.22	1.21
4:D:133:GLN:CG	5:F:60:ARG:HD2	1.70	1.21
4:D:140:LEU:HD21	5:F:129:GLN:CG	1.69	1.20
4:D:133:GLN:CG	5:F:60:ARG:CD	2.20	1.19
4:D:111:TYR:CB	5:F:118:PRO:HG3	1.73	1.18
4:D:125:GLN:NE2	5:F:144:THR:HG23	1.59	1.18
4:D:108:TYR:CE1	5:F:145:VAL:HG11	1.79	1.17
4:D:111:TYR:HB2	5:F:118:PRO:CG	1.74	1.17
4:D:532:GLU:HG3	8:I:138:GLU:OE1	1.47	1.14
2:A:2113:U:H1'	4:D:146:ARG:HG3	1.30	1.14
4:D:536:ARG:HH22	8:I:137:ARG:NH1	1.43	1.13
4:D:412:LEU:HD21	6:G:46:LYS:H	1.07	1.13
4:D:533:TYR:CB	8:I:129:ASN:O	1.96	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2113:U:C5'	4:D:147:ALA:HA	1.80	1.12
2:A:2169:A:C2	4:D:141:ASN:CB	2.25	1.11
4:D:137:GLY:HA2	5:F:129:GLN:HE21	1.16	1.11
4:D:130:GLU:HB3	5:F:55:SER:HB3	1.22	1.10
4:D:523:PHE:HB2	8:I:130:LYS:HD2	1.31	1.10
1:B:1240:U:C2	8:I:37:THR:CG2	2.35	1.10
2:A:2113:U:C2	4:D:143:GLN:OE1	2.03	1.10
4:D:111:TYR:CE1	5:F:147:PRO:HA	1.86	1.09
4:D:111:TYR:CD1	5:F:147:PRO:CA	2.36	1.08
2:A:2113:U:H1'	4:D:146:ARG:CG	1.84	1.08
2:A:2113:U:C1'	4:D:146:ARG:HG3	1.81	1.08
1:B:1240:U:O2	8:I:37:THR:CG2	2.03	1.07
4:D:108:TYR:HB3	5:F:118:PRO:C	1.74	1.07
2:A:2113:U:C6	4:D:143:GLN:NE2	2.21	1.07
4:D:536:ARG:NH2	8:I:137:ARG:HH12	1.50	1.06
4:D:129:GLU:OE1	5:F:143:GLY:CA	2.03	1.05
3:E:3:C:H1'	4:D:277:ARG:NH2	1.72	1.05
4:D:140:LEU:CD2	5:F:129:GLN:HG3	1.87	1.04
1:B:1240:U:O4	8:I:31:VAL:HG12	1.58	1.03
3:E:17:C:OP2	3:E:18:U:C5	2.11	1.03
4:D:111:TYR:HE1	5:F:147:PRO:HB3	1.23	1.02
1:B:1240:U:C5	8:I:31:VAL:CG1	2.43	1.02
2:A:2113:U:C5	4:D:143:GLN:NE2	2.28	1.02
4:D:111:TYR:CE1	5:F:147:PRO:CA	2.43	1.01
4:D:133:GLN:OE1	5:F:141:LYS:HB3	1.60	1.01
4:D:536:ARG:CZ	8:I:137:ARG:HH22	1.73	1.01
1:B:1240:U:C5	8:I:31:VAL:HG12	1.96	1.01
4:D:108:TYR:O	5:F:118:PRO:HB2	1.59	1.00
4:D:111:TYR:CE2	5:F:145:VAL:HG23	1.96	0.99
4:D:108:TYR:CG	5:F:118:PRO:HA	1.97	0.99
4:D:108:TYR:HA	5:F:118:PRO:HB3	0.99	0.98
4:D:523:PHE:CD1	8:I:130:LYS:CB	2.28	0.98
3:E:3:C:C1'	4:D:277:ARG:HH21	1.77	0.98
4:D:108:TYR:CB	5:F:118:PRO:O	2.10	0.97
2:A:2113:U:H5'	4:D:147:ALA:HA	1.43	0.97
4:D:412:LEU:HD21	6:G:46:LYS:N	1.80	0.97
4:D:108:TYR:CE1	5:F:145:VAL:CG1	2.48	0.97
4:D:140:LEU:HD21	5:F:129:GLN:HG3	0.99	0.96
2:A:2169:A:N3	4:D:141:ASN:OD1	1.97	0.96
4:D:141:ASN:OD1	5:F:127:LEU:HD13	1.65	0.95
1:B:1240:U:C2	8:I:37:THR:HG23	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:TYR:HB2	5:F:118:PRO:HG3	0.95	0.94
2:A:2113:U:C2'	4:D:146:ARG:HG3	1.97	0.94
2:A:2113:U:O2'	4:D:146:ARG:HG3	1.67	0.94
2:A:2113:U:H4'	4:D:147:ALA:HA	1.47	0.93
4:D:118:PHE:CE2	5:F:148:ASN:ND2	2.37	0.93
1:B:1240:U:H1'	8:I:37:THR:HG21	1.49	0.92
5:F:60:ARG:HH12	5:F:164:ARG:NE	1.67	0.92
4:D:533:TYR:O	4:D:533:TYR:HD1	1.53	0.91
2:A:2169:A:C2	4:D:141:ASN:OD1	2.23	0.91
4:D:111:TYR:HE2	5:F:145:VAL:HG23	1.36	0.90
4:D:108:TYR:CZ	5:F:121:MET:HB3	2.07	0.90
4:D:322:LYS:CG	8:I:113:LYS:NZ	2.21	0.90
4:D:108:TYR:HE2	5:F:121:MET:HB3	1.32	0.89
4:D:130:GLU:HB3	5:F:55:SER:CB	2.03	0.89
4:D:130:GLU:O	5:F:55:SER:OG	1.90	0.89
4:D:111:TYR:HD1	5:F:147:PRO:HA	1.21	0.89
4:D:118:PHE:H	4:D:118:PHE:HD1	1.21	0.89
3:E:72:C:O2'	4:D:278:GLN:O	1.89	0.88
4:D:529:GLU:CD	8:I:135:LYS:HD2	1.93	0.88
2:A:2113:U:C4'	4:D:147:ALA:CA	2.51	0.87
8:I:125:ASP:OD1	8:I:130:LYS:HE2	1.75	0.87
2:A:2113:U:O2	4:D:146:ARG:NE	2.08	0.87
4:D:524:GLU:CB	8:I:110:ARG:NE	2.37	0.87
4:D:111:TYR:HB3	5:F:83:ASN:ND2	1.90	0.86
1:B:1240:U:O4'	8:I:37:THR:HG21	1.75	0.86
4:D:133:GLN:OE1	5:F:141:LYS:CB	2.23	0.86
4:D:524:GLU:OE1	8:I:110:ARG:HG3	1.75	0.86
1:B:1240:U:O2	8:I:37:THR:HG22	1.75	0.86
2:A:1907:G:N2	3:E:12:G:O3'	2.08	0.86
4:D:108:TYR:CD1	5:F:145:VAL:HG21	2.11	0.85
4:D:108:TYR:CD1	5:F:118:PRO:HA	2.10	0.85
4:D:523:PHE:CE1	8:I:130:LYS:HB2	2.11	0.85
4:D:111:TYR:CE1	5:F:147:PRO:HB3	2.12	0.85
4:D:524:GLU:CG	8:I:110:ARG:NE	2.41	0.84
4:D:118:PHE:HE2	5:F:148:ASN:ND2	1.74	0.84
5:F:60:ARG:NH1	5:F:164:ARG:CD	2.41	0.84
4:D:140:LEU:HD21	5:F:129:GLN:CB	2.08	0.83
4:D:528:THR:HB	8:I:142:ARG:CZ	2.08	0.83
4:D:524:GLU:CG	8:I:110:ARG:HE	1.92	0.83
4:D:125:GLN:CD	5:F:144:THR:HA	1.99	0.83
3:E:72:C:C5'	4:D:278:GLN:HE21	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:533:TYR:HD2	8:I:130:LYS:HB3	1.43	0.82
4:D:526:ASN:HB2	4:D:529:GLU:OE2	1.79	0.82
4:D:322:LYS:CB	8:I:113:LYS:NZ	2.42	0.82
4:D:108:TYR:CZ	5:F:121:MET:HG2	2.14	0.82
3:E:17:C:OP2	3:E:18:U:C6	2.33	0.82
4:D:528:THR:HB	8:I:142:ARG:NH2	1.94	0.82
2:A:2113:U:H5'	4:D:147:ALA:CA	2.10	0.81
4:D:108:TYR:O	5:F:118:PRO:CB	2.29	0.81
4:D:533:TYR:CE2	8:I:130:LYS:HD3	2.16	0.81
4:D:111:TYR:HE1	5:F:147:PRO:CB	1.94	0.81
4:D:133:GLN:HG2	5:F:60:ARG:HD3	1.62	0.81
4:D:524:GLU:HG2	8:I:110:ARG:CD	2.09	0.81
4:D:526:ASN:N	4:D:529:GLU:OE2	2.13	0.80
4:D:533:TYR:C	4:D:533:TYR:CD1	2.51	0.80
4:D:533:TYR:C	4:D:533:TYR:HD1	1.86	0.80
4:D:108:TYR:HH	5:F:121:MET:HG2	1.43	0.80
4:D:108:TYR:CB	5:F:118:PRO:CB	2.59	0.80
4:D:108:TYR:CB	5:F:118:PRO:HB2	2.11	0.80
4:D:111:TYR:CE1	5:F:147:PRO:CB	2.66	0.79
4:D:529:GLU:CG	8:I:135:LYS:HG3	2.13	0.79
5:F:60:ARG:HH12	5:F:164:ARG:CZ	1.96	0.78
1:B:1240:U:N1	8:I:37:THR:HG21	1.97	0.78
4:D:108:TYR:CG	5:F:118:PRO:CA	2.65	0.78
4:D:532:GLU:CG	8:I:138:GLU:OE1	2.29	0.78
3:E:3:C:C2'	4:D:277:ARG:HH21	1.95	0.78
4:D:322:LYS:HG3	8:I:113:LYS:HZ3	0.66	0.78
4:D:129:GLU:CD	5:F:143:GLY:HA3	2.03	0.77
4:D:108:TYR:CD2	5:F:121:MET:HB3	2.17	0.77
4:D:111:TYR:HB3	5:F:83:ASN:HD21	1.47	0.77
2:A:1907:G:H21	3:E:13:C:P	2.07	0.77
4:D:529:GLU:CD	8:I:135:LYS:CD	2.53	0.77
4:D:108:TYR:CE2	5:F:121:MET:CG	2.68	0.77
4:D:529:GLU:CD	8:I:135:LYS:CG	2.53	0.77
4:D:533:TYR:HE2	8:I:130:LYS:HD3	1.50	0.77
4:D:412:LEU:CD2	6:G:46:LYS:H	1.94	0.76
4:D:108:TYR:CZ	5:F:121:MET:CB	2.66	0.76
4:D:105:ASP:OD2	5:F:122:ARG:HB3	1.86	0.76
4:D:529:GLU:OE1	8:I:135:LYS:HD2	1.87	0.75
4:D:133:GLN:HG2	5:F:60:ARG:HD2	0.77	0.75
4:D:524:GLU:HB3	8:I:110:ARG:CZ	2.16	0.74
4:D:108:TYR:CB	5:F:118:PRO:CA	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:524:GLU:CB	8:I:110:ARG:CZ	2.64	0.74
4:D:108:TYR:CZ	5:F:145:VAL:HG11	2.20	0.74
4:D:133:GLN:CG	5:F:60:ARG:HD3	2.16	0.73
4:D:529:GLU:OE1	8:I:135:LYS:HB2	1.88	0.73
4:D:524:GLU:HG2	8:I:110:ARG:HG3	1.71	0.73
4:D:133:GLN:CD	5:F:60:ARG:HD3	2.09	0.73
4:D:138:HIS:CE1	4:D:140:LEU:HD23	2.24	0.73
4:D:412:LEU:HD21	6:G:46:LYS:HB2	1.71	0.73
4:D:524:GLU:CD	8:I:110:ARG:HG3	2.09	0.73
4:D:529:GLU:HG2	8:I:135:LYS:HG3	1.71	0.73
4:D:529:GLU:OE2	8:I:135:LYS:NZ	2.18	0.72
4:D:322:LYS:HB3	8:I:113:LYS:HZ1	1.55	0.72
4:D:141:ASN:OD1	5:F:127:LEU:CD1	2.38	0.72
4:D:536:ARG:HH12	8:I:137:ARG:CZ	2.01	0.72
4:D:529:GLU:CD	8:I:135:LYS:HG3	2.10	0.72
5:F:60:ARG:NH1	5:F:164:ARG:NE	2.36	0.72
4:D:137:GLY:HA2	5:F:129:GLN:NE2	1.98	0.72
4:D:322:LYS:CB	8:I:113:LYS:HZ1	2.00	0.72
2:A:2169:A:C2	4:D:141:ASN:CG	2.64	0.71
4:D:108:TYR:OH	5:F:121:MET:CG	2.28	0.71
4:D:111:TYR:CD2	5:F:118:PRO:HG3	2.25	0.71
4:D:533:TYR:HB2	8:I:129:ASN:C	2.08	0.71
4:D:125:GLN:HE22	5:F:144:THR:HG23	1.51	0.70
4:D:108:TYR:CD2	5:F:118:PRO:O	2.45	0.70
4:D:111:TYR:CG	5:F:118:PRO:HG3	2.26	0.70
2:A:2113:U:O2'	4:D:146:ARG:CG	2.40	0.70
1:B:1240:U:C2	8:I:37:THR:HG21	2.16	0.69
2:A:2113:U:H5''	4:D:150:ALA:HB3	1.74	0.69
4:D:536:ARG:HH12	8:I:137:ARG:HH22	0.79	0.69
4:D:524:GLU:HG2	8:I:110:ARG:CG	2.23	0.69
4:D:108:TYR:O	5:F:118:PRO:CG	2.40	0.69
3:E:3:C:O2	4:D:277:ARG:NH2	2.27	0.68
4:D:532:GLU:HB3	8:I:138:GLU:CD	2.13	0.68
3:E:3:C:C1'	4:D:277:ARG:NH2	2.40	0.68
3:E:17:C:OP2	3:E:18:U:H5	1.70	0.68
4:D:105:ASP:OD2	5:F:122:ARG:CB	2.42	0.68
4:D:524:GLU:HG2	8:I:110:ARG:NE	2.07	0.68
4:D:510:HIS:NE2	4:D:524:GLU:CD	2.48	0.67
1:B:1240:U:N1	8:I:37:THR:CG2	2.55	0.67
4:D:108:TYR:CZ	5:F:121:MET:CG	2.78	0.67
4:D:524:GLU:CG	8:I:110:ARG:HG3	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:U:O2	8:I:34:LYS:HB2	1.95	0.66
4:D:108:TYR:CB	5:F:118:PRO:C	2.57	0.66
2:A:2113:U:O4'	4:D:147:ALA:CA	2.44	0.66
4:D:526:ASN:CB	4:D:529:GLU:OE2	2.44	0.66
1:B:1240:U:N3	8:I:31:VAL:HG12	2.00	0.66
3:E:3:C:H1'	4:D:277:ARG:HH22	1.58	0.66
4:D:133:GLN:HE22	5:F:141:LYS:HD3	1.61	0.65
5:F:60:ARG:NH1	5:F:164:ARG:CG	2.59	0.65
4:D:133:GLN:HE22	5:F:141:LYS:CD	2.09	0.65
4:D:524:GLU:HB2	8:I:110:ARG:NH2	2.12	0.65
4:D:108:TYR:HD1	5:F:145:VAL:HG21	1.57	0.65
4:D:322:LYS:HD2	8:I:113:LYS:HE2	1.79	0.65
2:A:1907:G:N2	3:E:13:C:OP1	2.27	0.65
3:E:54:G:H2'	3:E:55:U:C6	2.32	0.65
4:D:524:GLU:CB	8:I:110:ARG:HE	2.06	0.64
2:A:2113:U:O4'	4:D:147:ALA:HB2	1.97	0.64
3:E:17:C:P	3:E:18:U:H5	2.21	0.64
4:D:322:LYS:HG3	8:I:113:LYS:CE	2.28	0.64
1:B:1240:U:C1'	8:I:37:THR:CG2	2.58	0.63
4:D:108:TYR:HB3	5:F:118:PRO:CA	2.28	0.63
2:A:2113:U:H1'	4:D:146:ARG:HG2	1.78	0.63
4:D:130:GLU:CB	5:F:55:SER:HB3	2.13	0.63
4:D:108:TYR:CG	5:F:118:PRO:O	2.52	0.62
2:A:2113:U:O4'	4:D:147:ALA:HA	1.98	0.62
4:D:118:PHE:N	4:D:118:PHE:HD1	1.93	0.62
4:D:108:TYR:O	5:F:118:PRO:HG2	1.99	0.62
4:D:536:ARG:CZ	8:I:138:GLU:OE2	2.47	0.62
4:D:510:HIS:HE2	4:D:524:GLU:CD	2.02	0.62
2:A:2113:U:O2	4:D:146:ARG:CZ	2.48	0.62
2:A:2113:U:N3	4:D:143:GLN:OE1	2.32	0.62
4:D:108:TYR:CA	5:F:118:PRO:HB3	1.94	0.61
4:D:192:HIS:H	4:D:499:HIS:CE1	2.17	0.61
4:D:108:TYR:CE1	5:F:145:VAL:HG21	2.35	0.61
5:F:60:ARG:NH1	5:F:164:ARG:HD2	2.14	0.61
4:D:137:GLY:CA	5:F:129:GLN:HE21	2.02	0.61
3:E:72:C:H4'	4:D:278:GLN:HG3	1.82	0.61
1:B:1240:U:O4'	8:I:37:THR:CG2	2.47	0.61
4:D:101:LEU:HD22	5:F:126:GLN:HE21	1.66	0.61
4:D:533:TYR:HD2	8:I:130:LYS:CB	2.13	0.61
4:D:525:GLY:HA3	4:D:529:GLU:OE1	2.00	0.60
4:D:322:LYS:HE3	8:I:112:ASP:C	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:524:GLU:CD	8:I:110:ARG:HE	2.03	0.60
4:D:111:TYR:CG	5:F:146:THR:O	2.55	0.60
2:A:2169:A:H2	4:D:141:ASN:HB2	0.60	0.60
4:D:133:GLN:OE1	5:F:60:ARG:HD3	2.02	0.60
5:F:60:ARG:NH1	5:F:164:ARG:HG2	2.17	0.59
4:D:118:PHE:CD1	4:D:118:PHE:N	2.65	0.59
4:D:532:GLU:CB	8:I:138:GLU:CD	2.71	0.59
4:D:536:ARG:NH2	8:I:137:ARG:NH1	2.24	0.59
4:D:129:GLU:OE1	5:F:144:THR:N	2.35	0.59
1:B:1240:U:H3	8:I:31:VAL:H	1.49	0.59
4:D:469:ASP:HA	4:D:497:ILE:HD12	1.85	0.59
2:A:2113:U:C5'	4:D:150:ALA:HB3	2.33	0.58
4:D:510:HIS:CD2	4:D:524:GLU:OE2	2.57	0.58
2:A:1907:G:N2	3:E:13:C:P	2.75	0.58
5:F:60:ARG:HH12	5:F:164:ARG:CD	2.12	0.57
4:D:142:VAL:HG13	4:D:146:ARG:CZ	2.34	0.57
4:D:311:LEU:HG	4:D:312:PHE:H	1.69	0.57
2:A:2113:U:C2	4:D:143:GLN:CD	2.78	0.57
2:A:1847:A:H62	2:A:1893:C:H41	1.52	0.57
4:D:111:TYR:HE2	5:F:145:VAL:CG2	2.14	0.57
8:I:125:ASP:OD1	8:I:130:LYS:CE	2.49	0.57
2:A:2113:U:N1	4:D:143:GLN:NE2	2.52	0.57
2:A:2113:U:H4'	4:D:147:ALA:CA	2.26	0.57
4:D:536:ARG:HH22	8:I:137:ARG:HH12	0.68	0.57
4:D:133:GLN:CG	5:F:60:ARG:NE	2.68	0.56
2:A:2113:U:O4'	4:D:147:ALA:CB	2.53	0.56
4:D:510:HIS:CD2	4:D:524:GLU:CD	2.78	0.56
4:D:533:TYR:CD2	8:I:130:LYS:HB3	2.34	0.56
4:D:524:GLU:HB2	8:I:110:ARG:CZ	2.35	0.56
4:D:133:GLN:CD	5:F:60:ARG:CD	2.70	0.56
4:D:533:TYR:O	4:D:533:TYR:CD1	2.44	0.56
4:D:412:LEU:CD2	6:G:46:LYS:HB2	2.36	0.56
4:D:108:TYR:HE1	5:F:145:VAL:CG1	2.14	0.56
3:E:3:C:O2	4:D:277:ARG:NE	2.38	0.55
2:A:1843:C:H2'	2:A:1844:C:C6	2.41	0.55
3:E:3:C:O2	4:D:277:ARG:CZ	2.53	0.55
1:B:1240:U:C5	8:I:31:VAL:HG11	2.36	0.55
7:H:18:HIS:CE1	7:H:19:PHE:CZ	2.94	0.55
1:B:1240:U:O4'	8:I:37:THR:OG1	2.23	0.55
4:D:108:TYR:CE1	5:F:145:VAL:CG2	2.90	0.55
4:D:533:TYR:CA	8:I:129:ASN:O	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:524:GLU:HB2	8:I:110:ARG:HH21	1.70	0.54
4:D:529:GLU:HG2	8:I:135:LYS:CB	2.37	0.54
4:D:529:GLU:HG2	8:I:135:LYS:CG	2.37	0.54
4:D:108:TYR:HE2	5:F:121:MET:CB	1.94	0.53
4:D:524:GLU:HB3	8:I:110:ARG:NE	2.13	0.53
4:D:138:HIS:CD2	4:D:140:LEU:H	2.26	0.53
4:D:529:GLU:OE2	8:I:135:LYS:HD2	2.09	0.53
2:A:2113:U:H5'	4:D:150:ALA:CB	2.39	0.53
4:D:140:LEU:CD2	5:F:129:GLN:CB	2.83	0.53
4:D:526:ASN:H	4:D:529:GLU:CD	2.11	0.52
3:E:72:C:H5'	4:D:278:GLN:HE21	1.69	0.52
4:D:108:TYR:CE2	5:F:121:MET:HG2	2.43	0.52
1:B:1240:U:O2	8:I:37:THR:HG21	1.98	0.52
4:D:125:GLN:CG	5:F:144:THR:HA	2.39	0.51
4:D:510:HIS:NE2	4:D:524:GLU:OE1	2.36	0.51
4:D:108:TYR:CD1	5:F:118:PRO:CA	2.88	0.51
2:A:2113:U:O2	4:D:143:GLN:OE1	2.28	0.51
4:D:130:GLU:C	5:F:55:SER:HG	2.07	0.51
4:D:118:PHE:CD2	5:F:148:ASN:ND2	2.78	0.51
4:D:118:PHE:CD2	5:F:147:PRO:HB2	2.46	0.51
3:E:3:C:C2'	4:D:277:ARG:NH2	2.69	0.51
4:D:125:GLN:CD	5:F:144:THR:HG23	2.27	0.51
4:D:125:GLN:HG2	4:D:126:GLY:N	2.26	0.50
5:F:170:ILE:HG23	5:F:172:HIS:CE1	2.47	0.50
4:D:368:MET:HB3	4:D:380:ILE:HD12	1.92	0.50
8:I:119:LEU:HD13	8:I:123:LEU:HG	1.94	0.50
6:G:39:VAL:HG22	6:G:39:VAL:O	2.11	0.50
3:E:72:C:O5'	4:D:278:GLN:NE2	2.45	0.50
2:A:2166:U:C5	2:A:2167:U:C4	3.00	0.49
4:D:111:TYR:HD2	5:F:118:PRO:HB3	1.78	0.49
4:D:532:GLU:HB3	8:I:138:GLU:OE2	2.11	0.49
4:D:322:LYS:CE	8:I:112:ASP:O	2.60	0.49
4:D:97:VAL:HG21	4:D:135:HIS:CD2	2.47	0.49
8:I:28:ILE:HG21	8:I:101:ARG:HA	1.93	0.49
4:D:111:TYR:HD2	5:F:118:PRO:CG	2.26	0.49
4:D:108:TYR:HE2	5:F:121:MET:CG	2.16	0.49
2:A:1843:C:H2'	2:A:1844:C:H6	1.79	0.48
2:A:2113:U:C5'	4:D:147:ALA:CA	2.69	0.48
3:E:72:C:H4'	4:D:278:GLN:CG	2.43	0.48
2:A:2164:C:C2	2:A:2172:U:C5	3.02	0.48
5:F:166:ASP:CG	5:F:170:ILE:HG22	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:104:ILE:H	5:F:104:ILE:HD13	1.79	0.48
8:I:137:ARG:O	8:I:141:HIS:CD2	2.67	0.48
4:D:414:ILE:HB	6:G:44:ALA:HA	1.96	0.48
4:D:111:TYR:CD2	5:F:118:PRO:CG	2.96	0.47
4:D:129:GLU:OE1	5:F:143:GLY:C	2.50	0.47
4:D:111:TYR:CD1	5:F:146:THR:O	2.67	0.47
2:A:2169:A:N3	4:D:141:ASN:CG	2.65	0.47
2:A:1878:G:C6	2:A:1879:C:C4	3.02	0.47
5:F:60:ARG:HH11	5:F:164:ARG:HD2	1.80	0.47
3:E:17:C:P	3:E:18:U:C5	3.01	0.47
3:E:72:C:H6	3:E:72:C:H5'	1.78	0.47
4:D:529:GLU:CG	8:I:135:LYS:CG	2.86	0.47
4:D:105:ASP:OD2	5:F:122:ARG:HD3	2.15	0.47
2:A:2107:G:C6	2:A:2183:A:C2	3.03	0.47
2:A:2115:G:H3'	2:A:2116:G:C5'	2.45	0.47
4:D:111:TYR:CD2	5:F:146:THR:O	2.68	0.47
5:F:151:GLU:HA	5:F:154:LYS:HE3	1.97	0.47
4:D:125:GLN:HG3	5:F:144:THR:HA	1.96	0.47
4:D:412:LEU:CD2	6:G:46:LYS:N	2.63	0.46
1:B:1242:G:C6	1:B:1243:C:C4	3.03	0.46
4:D:523:PHE:HB2	8:I:130:LYS:CD	2.22	0.46
6:G:102:LEU:HA	6:G:106:ALA:HB3	1.97	0.46
4:D:533:TYR:HE1	4:D:537:THR:HG1	1.63	0.46
2:A:2183:A:H2'	2:A:2184:A:C8	2.50	0.46
2:A:2107:G:C5	2:A:2183:A:C2	3.04	0.46
2:A:2155:U:C5	2:A:2156:G:C5	3.04	0.46
4:D:118:PHE:HB3	5:F:147:PRO:HB2	1.98	0.46
4:D:523:PHE:CE2	4:D:525:GLY:O	2.69	0.46
8:I:125:ASP:HB3	8:I:131:GLY:CA	2.45	0.45
3:E:72:C:C4'	4:D:278:GLN:HE21	2.28	0.45
3:E:72:C:C5'	4:D:278:GLN:NE2	2.72	0.45
4:D:322:LYS:HE2	8:I:112:ASP:O	2.16	0.45
4:D:125:GLN:OE1	5:F:144:THR:HA	2.15	0.45
4:D:524:GLU:CB	8:I:110:ARG:NH2	2.76	0.45
4:D:526:ASN:HB2	8:I:135:LYS:HZ3	1.81	0.45
4:D:301:GLU:OE1	4:D:305:ARG:NH2	2.50	0.45
5:F:60:ARG:NH2	5:F:165:ASN:O	2.50	0.45
4:D:311:LEU:HB2	4:D:482:ALA:HB1	1.98	0.45
4:D:511:ILE:HB	4:D:523:PHE:CD2	2.52	0.44
4:D:529:GLU:OE2	8:I:135:LYS:CD	2.65	0.44
4:D:533:TYR:CD2	8:I:130:LYS:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:325:GLU:OE1	8:I:113:LYS:HE3	2.17	0.44
4:D:368:MET:CB	4:D:380:ILE:HD12	2.48	0.44
4:D:510:HIS:HD2	4:D:524:GLU:OE2	1.99	0.44
4:D:415:MET:HG3	4:D:424:SER:HB3	1.99	0.43
8:I:129:ASN:HA	8:I:134:VAL:HG21	1.99	0.43
2:A:2113:U:C4	4:D:143:GLN:NE2	2.79	0.43
4:D:536:ARG:NH1	8:I:137:ARG:CZ	2.66	0.43
4:D:529:GLU:HG2	8:I:135:LYS:HA	2.00	0.43
2:A:2167:U:C4	2:A:2168:G:C5	3.07	0.43
4:D:524:GLU:HB2	8:I:110:ARG:NE	2.27	0.43
8:I:125:ASP:HB3	8:I:131:GLY:HA2	2.00	0.43
4:D:322:LYS:HE3	8:I:112:ASP:CA	2.49	0.43
4:D:511:ILE:HB	4:D:523:PHE:HD2	1.84	0.43
2:A:2113:U:C2	4:D:143:GLN:NE2	2.87	0.42
4:D:528:THR:CB	8:I:142:ARG:NH2	2.77	0.42
5:F:104:ILE:CD1	5:F:104:ILE:H	2.32	0.42
5:F:76:ALA:HB2	5:F:111:PHE:CE2	2.53	0.42
3:E:17:C:O5'	3:E:18:U:H5	2.03	0.42
4:D:111:TYR:HB2	5:F:118:PRO:HG2	1.88	0.42
4:D:133:GLN:CD	5:F:60:ARG:HH11	2.23	0.42
2:A:2113:U:H4'	4:D:146:ARG:O	2.20	0.42
2:A:1885:A:O4'	4:D:4:PHE:HZ	2.03	0.42
4:D:533:TYR:HE1	4:D:537:THR:OG1	2.03	0.42
4:D:523:PHE:CB	8:I:130:LYS:HD2	2.23	0.42
5:F:104:ILE:HD13	5:F:104:ILE:N	2.35	0.42
2:A:2108:A:C2	2:A:2109:U:C5	3.08	0.42
4:D:523:PHE:CZ	4:D:530:TYR:HB2	2.54	0.42
4:D:532:GLU:CB	8:I:138:GLU:OE1	2.67	0.42
4:D:105:ASP:OD2	5:F:122:ARG:CD	2.67	0.42
4:D:133:GLN:OE1	5:F:141:LYS:CG	2.68	0.41
2:A:2168:G:N2	2:A:2171:A:C8	2.88	0.41
2:A:2096:C:H2'	2:A:2097:A:C8	2.55	0.41
8:I:45:ALA:HA	8:I:120:ALA:HB2	2.01	0.41
4:D:322:LYS:HB3	8:I:113:LYS:NZ	2.22	0.41
2:A:2115:G:H3'	2:A:2116:G:H5"	2.01	0.41
4:D:108:TYR:CE1	5:F:145:VAL:HG13	2.48	0.41
4:D:330:ARG:HB3	4:D:377:SER:HB3	2.03	0.41
4:D:133:GLN:OE1	5:F:141:LYS:CA	2.69	0.41
2:A:1846:G:H3'	2:A:1847:A:H5"	2.02	0.41
2:A:1878:G:C5	2:A:1879:C:C5	3.08	0.41
4:D:111:TYR:CE2	5:F:145:VAL:CG2	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:HIS:HE1	5:F:129:GLN:HB2	1.86	0.41
8:I:68:VAL:HG11	8:I:103:ILE:HG13	2.02	0.41
5:F:5:THR:O	5:F:9:ARG:HG3	2.20	0.41
5:F:47:ASN:HB2	5:F:211:LYS:O	2.21	0.41
2:A:1846:G:C6	2:A:1847:A:C6	3.09	0.41
4:D:111:TYR:CE1	5:F:147:PRO:N	2.88	0.40
4:D:73:TYR:HA	4:D:185:LEU:O	2.20	0.40
5:F:60:ARG:CZ	5:F:164:ARG:HG2	2.51	0.40
2:A:2113:U:H5'	4:D:147:ALA:O	2.21	0.40
4:D:108:TYR:CZ	5:F:145:VAL:CG1	2.95	0.40
4:D:533:TYR:CD2	8:I:130:LYS:CG	3.04	0.40
4:D:322:LYS:HE3	8:I:112:ASP:O	2.21	0.40
4:D:412:LEU:HD21	6:G:46:LYS:CB	2.44	0.40
4:D:354:ILE:HB	4:D:497:ILE:HG12	2.04	0.40
4:D:222:LEU:HA	4:D:222:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	552/561 (98%)	508 (92%)	27 (5%)	17 (3%)	5	42
5	F	232/234 (99%)	199 (86%)	23 (10%)	10 (4%)	3	34
6	G	176/178 (99%)	138 (78%)	26 (15%)	12 (7%)	1	23
7	H	48/50 (96%)	38 (79%)	9 (19%)	1 (2%)	9	50
8	I	149/151 (99%)	119 (80%)	23 (15%)	7 (5%)	3	32
All	All	1157/1174 (99%)	1002 (87%)	108 (9%)	47 (4%)	6	35

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	83	GLU
4	D	91	GLU
4	D	143	GLN
4	D	317	PRO
6	G	102	LEU
4	D	165	GLY
4	D	194	ASP
4	D	283	ARG
4	D	295	GLU
5	F	4	LEU
5	F	167	LYS
5	F	203	GLN
6	G	78	ILE
6	G	84	ILE
6	G	100	GLU
6	G	104	THR
8	I	13	PRO
8	I	126	ALA
8	I	139	ASP
4	D	155	ASP
4	D	208	PHE
4	D	243	ASN
5	F	100	LEU
5	F	159	GLY
5	F	204	ALA
6	G	2	LYS
6	G	96	TRP
8	I	112	ASP
4	D	93	ALA
4	D	299	SER
5	F	110	ASN
6	G	51	ASN
6	G	101	ARG
7	H	4	ILE
8	I	52	ARG
4	D	181	PRO
6	G	125	GLY
8	I	10	LYS
6	G	4	HIS
6	G	39	VAL
4	D	142	VAL
4	D	279	GLY
8	I	28	ILE

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Mol	Chain	Res	Type
4	D	225	VAL
5	F	73	VAL
5	F	147	PRO
5	F	233	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	465/472 (98%)	436 (94%)	29 (6%)	23	60
5	F	181/181 (100%)	170 (94%)	11 (6%)	23	60
6	G	149/149 (100%)	143 (96%)	6 (4%)	38	71
7	H	45/45 (100%)	44 (98%)	1 (2%)	60	83
8	I	124/124 (100%)	119 (96%)	5 (4%)	38	71
All	All	964/971 (99%)	912 (95%)	52 (5%)	32	64

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	17	PRO
4	D	40	LEU
4	D	41	ASN
4	D	48	LEU
4	D	97	VAL
4	D	118	PHE
4	D	125	GLN
4	D	127	ARG
4	D	152	ARG
4	D	169	ARG
4	D	188	GLU
4	D	190	THR
4	D	191	ASN
4	D	203	ARG
4	D	204	PHE

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Mol	Chain	Res	Type
4	D	246	SER
4	D	266	ARG
4	D	276	VAL
4	D	277	ARG
4	D	305	ARG
4	D	318	ARG
4	D	363	SER
4	D	440	LYS
4	D	474	ASP
4	D	477	ILE
4	D	478	GLU
4	D	498	SER
4	D	523	PHE
4	D	533	TYR
5	F	1	MET
5	F	16	ASP
5	F	38	PHE
5	F	40	GLU
5	F	43	ASP
5	F	48	LEU
5	F	69	THR
5	F	104	ILE
5	F	113	VAL
5	F	162	ARG
5	F	224	VAL
6	G	64	PRO
6	G	84	ILE
6	G	99	PHE
6	G	114	ARG
6	G	142	TYR
6	G	147	ARG
7	H	46	VAL
8	I	8	GLN
8	I	39	GLU
8	I	49	LEU
8	I	72	VAL
8	I	93	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	76	GLN

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Mol	Chain	Res	Type
4	D	138	HIS
4	D	162	ASN
4	D	257	GLN
4	D	278	GLN
5	F	126	GLN
5	F	129	GLN
5	F	172	HIS
7	H	18	HIS
8	I	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	30/101 (29%)	12 (40%)	3 (10%)
2	A	172/360 (47%)	53 (30%)	9 (5%)
3	E	76/77 (98%)	19 (25%)	1 (1%)
All	All	278/538 (51%)	84 (30%)	13 (4%)

All (84) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	1238	A
1	B	1240	U
1	B	1243	C
1	B	1292	G
1	B	1293	C
1	B	1299	A
1	B	1300	G
1	B	1302	C
1	B	1304	G
1	B	1305	G
1	B	1335	U
1	B	1336	C
2	A	1846	G
2	A	1847	A
2	A	1848	A
2	A	1858	A
2	A	1859	U
2	A	1869	G
2	A	1870	C
2	A	1871	A

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Mol	Chain	Res	Type
2	A	1872	A
2	A	1874	C
2	A	1884	G
2	A	1888	G
2	A	1903	G
2	A	1905	C
2	A	1906	G
2	A	1907	G
2	A	2102	G
2	A	2104	C
2	A	2110	G
2	A	2111	U
2	A	2112	G
2	A	2113	U
2	A	2117	A
2	A	2119	A
2	A	2127	G
2	A	2130	U
2	A	2131	U
2	A	2132	U
2	A	2133	G
2	A	2134	A
2	A	2135	A
2	A	2136	G
2	A	2137	U
2	A	2144	G
2	A	2146	C
2	A	2147	A
2	A	2148	G
2	A	2149	U
2	A	2152	G
2	A	2153	C
2	A	2155	U
2	A	2157	G
2	A	2158	A
2	A	2159	G
2	A	2162	G
2	A	2164	C
2	A	2165	C
2	A	2167	U
2	A	2176	A
2	A	2179	C

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Mol	Chain	Res	Type
2	A	2181	U
2	A	2187	U
2	A	2192	U
3	E	5	G
3	E	8	U
3	E	9	G
3	E	13	C
3	E	17	C
3	E	18	U
3	E	19	G
3	E	20	G
3	E	21	U
3	E	22	A
3	E	48	U
3	E	49	C
3	E	50	G
3	E	54	G
3	E	72	C
3	E	74	A
3	E	75	C
3	E	76	C
3	E	77	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	1299	A
1	B	1332	A
1	B	1335	U
2	A	1871	A
2	A	2110	G
2	A	2126	A
2	A	2129	C
2	A	2152	G
2	A	2157	G
2	A	2158	A
2	A	2159	G
2	A	2172	U
3	E	9	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.