wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:50 PM BST

PDB ID	:	3J45
EMDB ID:	:	EMD-5692
Title	:	Structure of a non-translocating SecY protein channel with the 70S ribosome
Authors	:	Menetret, J.F.; Park, E.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.; Rapoport, T.A.; Akey, C.W.
Deposited on	:	2013-06-18
Resolution	:	9.50 Å(reported)
Based on PDB ID	:	2I2P, 3J01

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

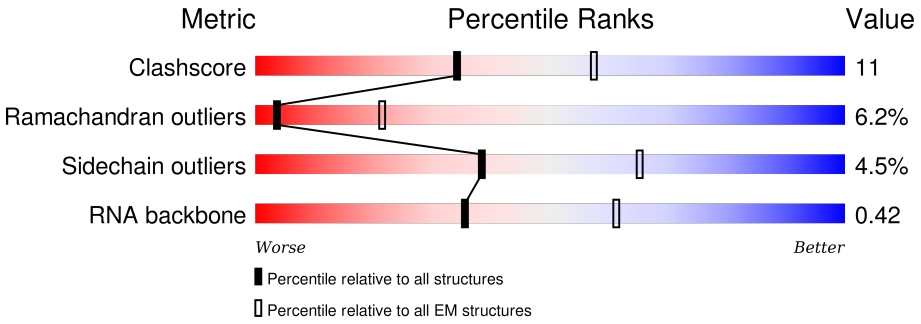
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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 <=5%

Mol	Chain	Length	Quality of chain
1	y	437	74% 21% .
2	E	56	64% 32% .
3	G	65	51% 34% 12% .
4	T	100	67% 26% 7%
5	U	103	68% 22% 9% .
6	Y	63	71% 25% .
7	1	63	46% 38% 16%
8	2	36	50% 36% 14%

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Mol	Chain	Length	Quality of chain
9	3	18	33% 50% 17%
10	4	61	56% 43%
11	5	108	27% 55% 19%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	437	Total	C	N	O	S	0	1
			3361	2220	554	570	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	ACETYLATION	UNP P0AGA2
y	441	NH2	-	AMIDATION	UNP P0AGA2

- Molecule 2 is a protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	56	Total	C	N	O	S	0	1
			433	283	76	73	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	ACE	-	ACETYLATION	UNP P0AG96
E	128	NH2	-	AMIDATION	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	65	Total	C	N	O	S	0	0
			457	299	73	81	4		

- Molecule 4 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 5 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 6 is a protein called 50S ribosomal protein L29.

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

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	18	Total	C	N	O	P	0	0
			387	172	71	126	18		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	61	Total	C	N	O	P	0	0
			1312	584	240	427	61		

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

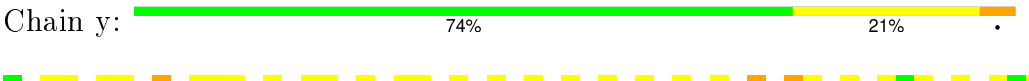
Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	108	Total	C	N	O	P	0	0
			2305	1029	406	762	108		

3 Residue-property plots (i)

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

- Molecule 1: Protein translocase subunit SecY

Chain y:



- Molecule 2: Preprotein translocase subunit SecE

Chain E:

- Molecule 3: Protein-export membrane protein SecG

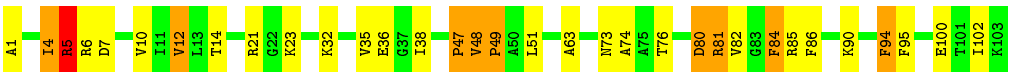
Chain G:

- Molecule 4: 50S ribosomal protein L23

Chain T:

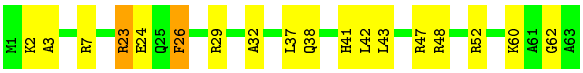
- Molecule 5: 50S ribosomal protein L24

Chain U:



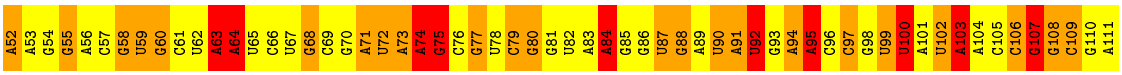
- Molecule 6: 50S ribosomal protein L29

Chain Y:



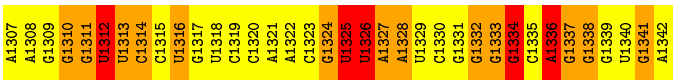
- Molecule 7: 23S ribosomal RNA

Chain 1:



- Molecule 8: 23S ribosomal RNA

Chain 2:

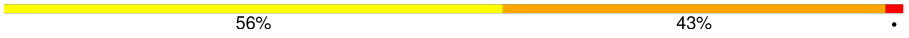


- Molecule 9: 23S ribosomal RNA

Chain 3:

- Molecule 10: 23S ribosomal RNA

Chain 4:



- Molecule 11: 23S ribosomal RNA

Chain 5:


G2152
C2153
A2154
U2155
G2156
G2157
A2158
G2159
C2160
C2161
G2162
A2163
C2164
C2165
U2166
U2167
G2168
A2169
A2170
A2171
U2172
A2173
C2174
C2175
A2176
C2177
C2178
C2179
U2180
U2181
U2182
A2183
A2184
U2185
G2186
U2187
U2188
U2189
G2190
A2191
U2192
G2193
U2194
U2195
C2196
U2197
A2198
A2199

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	39000	Depositor
Resolution determination method	Comparison of 3D map with calculated map of docked ribosomal components, with the second map made with EMAN at 7 Angstrom resolution	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	y	1.70	23/3434 (0.7%)	2.02	104/4657 (2.2%)
10	4	3.59	206/1468 (14.0%)	3.69	312/2289 (13.6%)
11	5	3.40	375/2577 (14.6%)	3.71	573/4015 (14.3%)
2	E	1.79	5/437 (1.1%)	2.35	17/596 (2.9%)
3	G	0.27	0/462	1.57	12/620 (1.9%)
4	T	1.64	7/794 (0.9%)	1.92	16/1060 (1.5%)
5	U	1.71	7/797 (0.9%)	1.95	20/1062 (1.9%)
6	Y	1.80	5/510 (1.0%)	1.93	13/677 (1.9%)
7	1	3.51	207/1511 (13.7%)	3.45	299/2354 (12.7%)
8	2	3.40	117/867 (13.5%)	3.56	188/1351 (13.9%)
9	3	3.68	75/432 (17.4%)	3.86	100/672 (14.9%)
All	All	2.75	1027/13289 (7.7%)	3.01	1654/19353 (8.5%)

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	y	0	6
10	4	0	20
11	5	0	54
2	E	0	1
3	G	3	0
4	T	0	1
5	U	0	3
6	Y	0	1
7	1	0	30
8	2	0	15
9	3	0	10
All	All	3	141

All (1027) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1892	C	N1-C6	18.20	1.48	1.37
7	1	114	U	C2-N3	16.37	1.49	1.37
9	3	1532	A	N3-C4	-15.69	1.25	1.34
10	4	1854	A	N9-C4	-15.56	1.28	1.37
10	4	1850	G	N7-C5	-15.20	1.30	1.39
8	2	1322	A	N7-C5	-14.95	1.30	1.39
7	1	91	A	C6-N6	14.35	1.45	1.33
11	5	2183	A	N7-C5	-13.92	1.30	1.39
10	4	1849	G	C6-N1	13.75	1.49	1.39
10	4	1843	C	N1-C6	-13.60	1.28	1.37
11	5	2179	C	N1-C6	13.39	1.45	1.37
7	1	73	A	N7-C5	-13.33	1.31	1.39
7	1	53	A	N7-C5	13.26	1.47	1.39
11	5	2162	G	N7-C5	-13.21	1.31	1.39
11	5	2125	G	N9-C8	-13.11	1.28	1.37
7	1	84	A	C6-N1	13.05	1.44	1.35
11	5	2112	G	N9-C4	12.97	1.48	1.38
11	5	2178	C	N1-C6	12.91	1.44	1.37
7	1	71	A	N9-C4	12.87	1.45	1.37
10	4	1868	C	N3-C4	12.62	1.42	1.33
7	1	69	C	N1-C6	12.57	1.44	1.37
11	5	2198	A	C6-N1	12.46	1.44	1.35
8	2	1324	G	N1-C2	12.38	1.47	1.37
11	5	2098	U	N3-C4	12.35	1.49	1.38
7	1	66	C	N1-C6	12.22	1.44	1.37
7	1	104	A	N7-C5	-12.17	1.31	1.39
10	4	1877	A	N7-C5	-12.11	1.31	1.39
10	4	1866	A	N7-C5	-11.98	1.32	1.39
10	4	1844	C	P-O5'	-11.61	1.48	1.59
10	4	1857	G	C2-N3	11.54	1.42	1.32
11	5	2103	C	N3-C4	11.53	1.42	1.33
11	5	2099	U	C2-N3	11.50	1.45	1.37
7	1	76	C	N3-C4	11.44	1.42	1.33
7	1	75	G	C5-C4	11.44	1.46	1.38
10	4	1878	G	C6-N1	11.29	1.47	1.39
11	5	2141	G	N1-C2	11.25	1.46	1.37
7	1	109	C	N1-C6	11.18	1.43	1.37
11	5	2199	A	C6-N6	11.16	1.42	1.33
10	4	1861	G	N7-C5	-11.13	1.32	1.39
7	1	77	G	C5'-C4'	11.12	1.64	1.51
7	1	86	G	C2-N3	11.09	1.41	1.32
10	4	1853	A	N7-C5	-11.04	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1333	G	C8-N7	11.04	1.37	1.30
7	1	86	G	N1-C2	10.95	1.46	1.37
11	5	2104	C	N1-C6	10.93	1.43	1.37
10	4	1890	A	N7-C5	-10.81	1.32	1.39
11	5	2129	C	C4-N4	10.80	1.43	1.33
10	4	1846	G	N1-C2	10.78	1.46	1.37
10	4	1889	A	C6-N6	10.78	1.42	1.33
7	1	58	G	N9-C8	10.73	1.45	1.37
10	4	1871	A	C5-C4	10.71	1.46	1.38
10	4	1894	C	C4-C5	10.64	1.51	1.43
7	1	90	U	N3-C4	10.63	1.48	1.38
8	2	1342	A	C6-N6	10.59	1.42	1.33
11	5	2147	A	C6-N6	10.58	1.42	1.33
11	5	2148	G	C8-N7	10.56	1.37	1.30
10	4	1884	G	C6-N1	10.48	1.46	1.39
11	5	2172	U	C2'-C1'	-10.41	1.41	1.53
10	4	1867	G	N1-C2	10.40	1.46	1.37
7	1	53	A	N9-C4	10.36	1.44	1.37
7	1	80	G	N9-C4	-10.30	1.29	1.38
8	2	1318	U	C2-N3	10.29	1.45	1.37
7	1	85	G	P-O5'	-10.23	1.49	1.59
7	1	82	U	C4-C5	10.19	1.52	1.43
7	1	96	C	C2-N3	10.18	1.43	1.35
11	5	2152	G	N9-C8	10.15	1.45	1.37
7	1	85	G	C8-N7	-10.13	1.24	1.30
10	4	1867	G	N9-C8	-10.07	1.30	1.37
10	4	1894	C	C4-N4	10.06	1.43	1.33
10	4	1848	A	N3-C4	-10.06	1.28	1.34
9	3	1538	G	N1-C2	10.05	1.45	1.37
11	5	2132	U	C2-N3	10.02	1.44	1.37
11	5	2190	G	C5'-C4'	10.02	1.63	1.51
7	1	70	G	N9-C8	-9.98	1.30	1.37
11	5	2147	A	C6-N1	9.96	1.42	1.35
9	3	1542	U	C2-N3	9.90	1.44	1.37
7	1	55	G	N3-C4	-9.88	1.28	1.35
11	5	2154	A	N7-C5	-9.82	1.33	1.39
8	2	1315	C	N1-C6	9.79	1.43	1.37
10	4	1872	A	N9-C4	9.78	1.43	1.37
7	1	66	C	N3-C4	9.77	1.40	1.33
7	1	85	G	C2-N3	9.77	1.40	1.32
8	2	1328	A	N3-C4	-9.77	1.28	1.34
8	2	1339	G	N9-C4	-9.74	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2104	C	N3-C4	9.71	1.40	1.33
7	1	74	A	C8-N7	9.71	1.38	1.31
7	1	92	U	C5'-C4'	9.67	1.62	1.51
7	1	97	C	C2-N3	9.66	1.43	1.35
11	5	2111	U	N3-C4	9.64	1.47	1.38
11	5	2168	G	C5-C4	9.58	1.45	1.38
7	1	80	G	N9-C8	9.56	1.44	1.37
11	5	2191	A	N7-C5	-9.56	1.33	1.39
7	1	112	U	C2-N3	9.52	1.44	1.37
8	2	1341	G	C5-C6	-9.49	1.32	1.42
9	3	1529	G	C6-N1	9.46	1.46	1.39
11	5	2129	C	N1-C6	9.46	1.42	1.37
7	1	92	U	C2-N3	9.39	1.44	1.37
11	5	2117	A	N7-C5	-9.35	1.33	1.39
10	4	1895	C	C2-N3	9.34	1.43	1.35
10	4	1866	A	C8-N7	-9.33	1.25	1.31
7	1	76	C	N1-C6	9.33	1.42	1.37
11	5	2109	U	C2-N3	9.31	1.44	1.37
10	4	1888	G	C5-C4	9.30	1.44	1.38
10	4	1862	G	C2-N2	9.29	1.43	1.34
9	3	1539	U	C2-N3	9.28	1.44	1.37
8	2	1339	G	N1-C2	9.28	1.45	1.37
7	1	58	G	N7-C5	9.21	1.44	1.39
7	1	75	G	C6-N1	9.21	1.46	1.39
7	1	59	U	C2-N3	9.20	1.44	1.37
11	5	2112	G	C2-N3	9.15	1.40	1.32
7	1	75	G	N1-C2	9.15	1.45	1.37
8	2	1341	G	C5-C4	9.13	1.44	1.38
10	4	1896	G	N7-C5	-9.11	1.33	1.39
11	5	2159	G	N1-C2	9.09	1.45	1.37
11	5	2181	U	N1-C6	9.07	1.46	1.38
10	4	1860	G	C2-N2	9.06	1.43	1.34
11	5	2158	A	N9-C8	9.05	1.45	1.37
11	5	2173	A	N7-C5	-9.03	1.33	1.39
7	1	83	A	N3-C4	-9.02	1.29	1.34
7	1	54	G	C5-C6	-9.02	1.33	1.42
11	5	2194	U	C2-N3	9.01	1.44	1.37
7	1	62	U	C4-C5	9.01	1.51	1.43
9	3	1537	G	N7-C5	-9.00	1.33	1.39
10	4	1845	G	N7-C5	-8.98	1.33	1.39
11	5	2101	A	C5-C4	-8.98	1.32	1.38
9	3	1535	A	C6-N1	8.98	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1897	G	C6-N1	8.95	1.45	1.39
10	4	1841	U	C2-N3	8.95	1.44	1.37
7	1	76	C	C2-N3	8.94	1.42	1.35
7	1	96	C	C4-C5	8.94	1.50	1.43
11	5	2152	G	N9-C4	-8.93	1.30	1.38
8	2	1330	C	N3-C4	8.91	1.40	1.33
11	5	2120	G	C2-N3	8.90	1.39	1.32
11	5	2112	G	N1-C2	8.88	1.44	1.37
10	4	1884	G	C2-N3	8.87	1.39	1.32
7	1	97	C	C4-N4	8.87	1.42	1.33
10	4	1854	A	C2'-C1'	-8.82	1.43	1.53
10	4	1858	A	N7-C5	-8.81	1.33	1.39
7	1	74	A	C2'-C1'	-8.81	1.43	1.53
9	3	1526	C	C4-N4	8.77	1.41	1.33
7	1	84	A	C4'-C3'	8.76	1.62	1.53
10	4	1847	A	C5'-C4'	8.76	1.61	1.51
9	3	1543	G	N3-C4	8.76	1.41	1.35
10	4	1881	C	C2-N3	8.74	1.42	1.35
1	y	85	TYR	CE1-CZ	8.73	1.50	1.38
7	1	104	A	C6-N1	8.72	1.41	1.35
8	2	1323	C	C5'-C4'	8.71	1.61	1.51
11	5	2094	A	C5-C6	-8.70	1.33	1.41
11	5	2100	G	N7-C5	-8.69	1.34	1.39
8	2	1320	C	N1-C6	-8.68	1.31	1.37
11	5	2147	A	C2'-C1'	8.68	1.62	1.53
11	5	2118	U	C2-N3	8.65	1.43	1.37
9	3	1535	A	N9-C4	8.63	1.43	1.37
9	3	1542	U	C4-C5	8.60	1.51	1.43
7	1	103	A	N3-C4	-8.58	1.29	1.34
10	4	1889	A	C5-C6	8.57	1.48	1.41
10	4	1846	G	C5-C4	8.55	1.44	1.38
10	4	1847	A	N7-C5	-8.52	1.34	1.39
8	2	1331	G	C2-N2	8.52	1.43	1.34
7	1	62	U	P-O5'	-8.50	1.51	1.59
11	5	2142	A	N3-C4	8.50	1.40	1.34
8	2	1334	G	C2-N3	8.50	1.39	1.32
10	4	1882	U	N1-C6	8.49	1.45	1.38
11	5	2148	G	O3'-P	-8.49	1.50	1.61
8	2	1336	A	C2-N3	8.47	1.41	1.33
9	3	1529	G	N7-C5	-8.45	1.34	1.39
10	4	1843	C	C5'-C4'	8.45	1.61	1.51
11	5	2134	A	N7-C5	-8.45	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	3	1532	A	C6-N6	8.44	1.40	1.33
8	2	1334	G	N9-C8	8.43	1.43	1.37
10	4	1842	G	N7-C5	-8.43	1.34	1.39
10	4	1898	U	C2-N3	8.43	1.43	1.37
7	1	58	G	O3'-P	-8.41	1.51	1.61
7	1	103	A	C8-N7	-8.40	1.25	1.31
10	4	1897	G	C2-N3	8.39	1.39	1.32
10	4	1848	A	C6-N1	8.38	1.41	1.35
11	5	2136	G	C2-N3	8.37	1.39	1.32
11	5	2144	G	C2-N3	8.35	1.39	1.32
10	4	1843	C	C4-C5	8.34	1.49	1.43
9	3	1529	G	N9-C4	8.34	1.44	1.38
8	2	1337	G	N3-C4	8.32	1.41	1.35
9	3	1538	G	N7-C5	-8.31	1.34	1.39
8	2	1310	G	N9-C8	8.31	1.43	1.37
8	2	1312	U	C4-C5	8.31	1.51	1.43
10	4	1852	U	C3'-C2'	-8.30	1.43	1.52
11	5	2122	U	P-O5'	-8.28	1.51	1.59
11	5	2191	A	C6-N6	8.24	1.40	1.33
9	3	1529	G	C4'-C3'	-8.22	1.44	1.53
11	5	2107	G	N3-C4	-8.21	1.29	1.35
10	4	1862	G	N9-C4	-8.19	1.31	1.38
11	5	2107	G	C8-N7	-8.18	1.26	1.30
10	4	1850	G	C2-N3	8.17	1.39	1.32
7	1	111	A	C6-N6	8.17	1.40	1.33
8	2	1312	U	C2-N3	8.16	1.43	1.37
11	5	2170	A	N9-C8	-8.13	1.31	1.37
8	2	1307	A	C5-C4	8.12	1.44	1.38
10	4	1884	G	N9-C8	-8.12	1.32	1.37
11	5	2098	U	C2-N3	8.11	1.43	1.37
11	5	2154	A	C6-N1	8.11	1.41	1.35
10	4	1855	U	C2-N3	8.11	1.43	1.37
10	4	1858	A	N9-C4	-8.08	1.32	1.37
11	5	2096	C	P-O5'	-8.07	1.51	1.59
10	4	1845	G	N1-C2	8.05	1.44	1.37
9	3	1531	C	C4-N4	8.04	1.41	1.33
10	4	1896	G	C2'-C1'	-8.03	1.44	1.53
11	5	2141	G	C5'-C4'	8.03	1.60	1.51
11	5	2162	G	N9-C8	8.03	1.43	1.37
10	4	1869	G	N9-C8	8.02	1.43	1.37
11	5	2123	G	N1-C2	7.99	1.44	1.37
7	1	93	G	C6-N1	7.97	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2099	U	C2'-C1'	-7.97	1.44	1.53
11	5	2183	A	C6-N1	7.97	1.41	1.35
7	1	103	A	N7-C5	-7.96	1.34	1.39
7	1	67	U	N1-C2	7.96	1.45	1.38
11	5	2144	G	C5'-C4'	7.95	1.60	1.51
10	4	1878	G	C5-C4	7.94	1.44	1.38
11	5	2146	C	C5'-C4'	7.94	1.60	1.51
7	1	104	A	C5-C4	7.94	1.44	1.38
10	4	1884	G	N3-C4	-7.93	1.29	1.35
9	3	1543	G	C5-C4	-7.92	1.32	1.38
10	4	1868	C	C4-N4	7.92	1.41	1.33
10	4	1889	A	C4'-C3'	7.91	1.61	1.53
11	5	2159	G	N7-C5	-7.90	1.34	1.39
11	5	2182	U	C2-N3	7.88	1.43	1.37
8	2	1314	C	O4'-C1'	7.85	1.51	1.41
8	2	1331	G	C6-N1	-7.85	1.34	1.39
8	2	1310	G	N1-C2	7.84	1.44	1.37
7	1	113	U	N3-C4	7.81	1.45	1.38
10	4	1860	G	P-O5'	7.80	1.67	1.59
11	5	2173	A	C5-C4	7.80	1.44	1.38
8	2	1328	A	C6-N1	7.80	1.41	1.35
10	4	1838	C	N1-C2	-7.79	1.32	1.40
11	5	2128	G	P-O5'	-7.79	1.51	1.59
11	5	2138	G	C2-N3	7.77	1.39	1.32
8	2	1308	A	C2-N3	7.77	1.40	1.33
11	5	2130	U	O3'-P	-7.76	1.51	1.61
11	5	2186	G	C2-N2	7.76	1.42	1.34
8	2	1334	G	N3-C4	-7.75	1.30	1.35
10	4	1870	C	N1-C2	7.75	1.47	1.40
1	y	430	GLU	CD-OE1	7.75	1.34	1.25
7	1	60	G	N9-C8	-7.73	1.32	1.37
7	1	57	C	C2-N3	7.73	1.42	1.35
10	4	1846	G	N7-C5	-7.72	1.34	1.39
7	1	104	A	N9-C4	-7.71	1.33	1.37
7	1	72	U	C2-N3	7.71	1.43	1.37
11	5	2093	G	C6-N1	7.71	1.45	1.39
7	1	87	U	C2-N3	7.70	1.43	1.37
11	5	2104	C	P-O5'	7.70	1.67	1.59
9	3	1529	G	N3-C4	-7.69	1.30	1.35
10	4	1852	U	C5'-C4'	7.69	1.60	1.51
8	2	1317	G	P-O5'	-7.68	1.52	1.59
11	5	2133	G	C4'-C3'	7.65	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1839	G	N7-C5	-7.64	1.34	1.39
8	2	1336	A	N7-C5	-7.63	1.34	1.39
11	5	2137	U	C2'-C1'	7.62	1.61	1.53
7	1	73	A	C6-N1	7.62	1.40	1.35
9	3	1526	C	N3-C4	7.62	1.39	1.33
10	4	1863	G	C8-N7	7.62	1.35	1.30
7	1	63	A	N7-C5	7.61	1.43	1.39
8	2	1314	C	C4-C5	7.61	1.49	1.43
11	5	2172	U	N1-C6	7.61	1.44	1.38
7	1	74	A	N9-C4	7.60	1.42	1.37
11	5	2153	C	C5'-C4'	7.60	1.60	1.51
10	4	1892	C	N3-C4	7.59	1.39	1.33
11	5	2164	C	C4-N4	7.58	1.40	1.33
11	5	2199	A	N1-C2	7.58	1.41	1.34
7	1	54	G	C8-N7	7.58	1.35	1.30
9	3	1543	G	C5'-C4'	7.55	1.60	1.51
8	2	1334	G	N7-C5	-7.54	1.34	1.39
8	2	1332	G	N9-C8	7.54	1.43	1.37
11	5	2120	G	C2'-C1'	-7.52	1.45	1.53
8	2	1320	C	C4-N4	7.51	1.40	1.33
11	5	2121	G	N1-C2	7.51	1.43	1.37
11	5	2102	G	C2-N3	7.50	1.38	1.32
7	1	91	A	N7-C5	-7.50	1.34	1.39
11	5	2163	A	N3-C4	7.49	1.39	1.34
11	5	2116	G	C2-N3	7.49	1.38	1.32
11	5	2107	G	C2-N3	7.48	1.38	1.32
8	2	1326	U	C2-N3	7.47	1.43	1.37
11	5	2126	A	C4'-C3'	7.47	1.61	1.53
11	5	2180	U	C4-C5	7.47	1.50	1.43
7	1	74	A	P-O5'	-7.47	1.52	1.59
11	5	2153	C	C2'-C1'	-7.45	1.45	1.53
11	5	2155	U	N1-C2	7.45	1.45	1.38
11	5	2097	A	C6-N6	7.45	1.40	1.33
9	3	1534	U	C2-N3	7.44	1.43	1.37
9	3	1539	U	C1'-N1	7.44	1.59	1.48
9	3	1528	A	N9-C4	7.44	1.42	1.37
8	2	1339	G	C5'-C4'	7.43	1.60	1.51
7	1	89	A	C4'-C3'	7.43	1.61	1.53
1	y	380	TYR	CG-CD1	7.42	1.48	1.39
7	1	68	G	C3'-C2'	7.42	1.61	1.52
9	3	1543	G	N7-C5	-7.42	1.34	1.39
11	5	2107	G	C5-C4	7.41	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2113	U	O4'-C1'	7.41	1.51	1.41
8	2	1328	A	C8-N7	-7.40	1.26	1.31
10	4	1876	A	P-O5'	-7.40	1.52	1.59
11	5	2097	A	C5-C4	7.40	1.44	1.38
11	5	2132	U	C4'-O4'	7.39	1.55	1.45
11	5	2173	A	C5'-C4'	7.39	1.60	1.51
8	2	1311	G	C2-N2	7.37	1.42	1.34
10	4	1849	G	C5-C4	7.35	1.43	1.38
7	1	55	G	C8-N7	-7.35	1.26	1.30
7	1	63	A	C2'-C1'	-7.35	1.45	1.53
7	1	112	U	C4'-C3'	7.34	1.61	1.53
8	2	1328	A	N7-C5	-7.34	1.34	1.39
9	3	1541	C	P-O5'	-7.34	1.52	1.59
8	2	1328	A	C6-N6	7.33	1.39	1.33
11	5	2113	U	C2-N3	7.33	1.42	1.37
11	5	2158	A	C5-C4	7.33	1.43	1.38
11	5	2127	G	N9-C4	-7.32	1.32	1.38
9	3	1538	G	C5-C4	-7.32	1.33	1.38
8	2	1333	G	N1-C2	7.32	1.43	1.37
11	5	2124	G	C2-N3	7.32	1.38	1.32
11	5	2149	U	C5'-C4'	7.31	1.60	1.51
7	1	58	G	N9-C4	7.30	1.43	1.38
10	4	1878	G	N1-C2	7.30	1.43	1.37
7	1	70	G	C6-N1	7.30	1.44	1.39
9	3	1539	U	C2'-C1'	-7.29	1.45	1.53
8	2	1340	U	C3'-O3'	7.29	1.52	1.42
8	2	1316	U	C2'-C1'	-7.29	1.45	1.53
11	5	2112	G	N3-C4	-7.29	1.30	1.35
8	2	1311	G	C8-N7	7.28	1.35	1.30
11	5	2193	G	N9-C4	-7.28	1.32	1.38
7	1	93	G	O4'-C1'	7.27	1.51	1.41
1	y	239	ARG	NE-CZ	7.25	1.42	1.33
9	3	1534	U	C4'-C3'	-7.24	1.45	1.53
10	4	1844	C	C3'-C2'	-7.24	1.44	1.52
10	4	1859	U	C5-C6	7.23	1.40	1.34
9	3	1539	U	C3'-C2'	7.22	1.60	1.52
7	1	60	G	C5'-C4'	7.22	1.60	1.51
10	4	1890	A	O3'-P	7.21	1.69	1.61
9	3	1537	G	C2-N3	7.21	1.38	1.32
11	5	2102	G	C8-N7	-7.21	1.26	1.30
9	3	1541	C	N3-C4	7.20	1.39	1.33
9	3	1538	G	C2-N3	7.19	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1895	C	N3-C4	7.18	1.39	1.33
11	5	2096	C	N1-C2	7.17	1.47	1.40
11	5	2130	U	C2-N3	7.17	1.42	1.37
7	1	76	C	C2'-C1'	-7.17	1.45	1.53
10	4	1860	G	C2'-C1'	-7.14	1.45	1.53
9	3	1530	G	C5-C4	-7.13	1.33	1.38
10	4	1863	G	C2-N3	7.13	1.38	1.32
8	2	1336	A	N3-C4	7.12	1.39	1.34
11	5	2126	A	N7-C5	7.11	1.43	1.39
11	5	2157	G	C5-C6	-7.11	1.35	1.42
10	4	1881	C	C4-N4	7.11	1.40	1.33
11	5	2132	U	C4'-C3'	7.09	1.60	1.53
8	2	1338	G	N1-C2	7.02	1.43	1.37
11	5	2104	C	C5'-C4'	7.01	1.59	1.51
11	5	2181	U	C5-C6	-7.01	1.27	1.34
8	2	1324	G	N3-C4	7.01	1.40	1.35
9	3	1541	C	N1-C6	7.01	1.41	1.37
8	2	1333	G	N9-C8	7.00	1.42	1.37
9	3	1533	C	N1-C6	6.99	1.41	1.37
11	5	2112	G	N9-C8	6.99	1.42	1.37
11	5	2142	A	C5-C6	6.99	1.47	1.41
11	5	2166	U	C2-N3	6.99	1.42	1.37
7	1	70	G	P-O5'	-6.98	1.52	1.59
10	4	1881	C	N3-C4	6.98	1.38	1.33
11	5	2100	G	C6-N1	6.98	1.44	1.39
7	1	84	A	C5-C4	6.97	1.43	1.38
8	2	1330	C	C4'-C3'	-6.96	1.45	1.53
10	4	1865	U	O3'-P	-6.96	1.52	1.61
9	3	1540	G	C2-N3	6.95	1.38	1.32
7	1	71	A	P-O5'	-6.95	1.52	1.59
10	4	1860	G	N7-C5	-6.95	1.35	1.39
11	5	2144	G	C8-N7	-6.94	1.26	1.30
11	5	2173	A	N9-C4	6.94	1.42	1.37
11	5	2119	A	C6-N1	6.94	1.40	1.35
7	1	81	G	N1-C2	6.93	1.43	1.37
7	1	65	U	N3-C4	6.93	1.44	1.38
11	5	2107	G	N1-C2	6.93	1.43	1.37
8	2	1317	G	C2-N3	6.92	1.38	1.32
10	4	1873	G	C2-N3	6.92	1.38	1.32
10	4	1868	C	C2'-C1'	-6.91	1.45	1.53
7	1	88	G	C6-N1	6.90	1.44	1.39
11	5	2121	G	C2-N2	6.88	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2170	A	C5-C4	6.87	1.43	1.38
10	4	1885	A	N7-C5	-6.86	1.35	1.39
11	5	2114	A	N9-C8	6.86	1.43	1.37
11	5	2096	C	C2'-C1'	-6.86	1.45	1.53
11	5	2136	G	C2-N2	6.86	1.41	1.34
11	5	2105	U	N1-C6	-6.86	1.31	1.38
11	5	2144	G	C2-N2	6.86	1.41	1.34
10	4	1886	U	C4-C5	6.85	1.49	1.43
11	5	2154	A	C5-C4	-6.85	1.33	1.38
8	2	1311	G	N3-C4	-6.85	1.30	1.35
11	5	2159	G	P-O5'	-6.85	1.52	1.59
8	2	1325	U	C2'-C1'	-6.84	1.45	1.53
11	5	2143	C	P-O5'	-6.84	1.52	1.59
9	3	1526	C	N1-C2	6.83	1.47	1.40
10	4	1888	G	C6-N1	6.83	1.44	1.39
11	5	2187	U	N3-C4	6.83	1.44	1.38
7	1	70	G	N1-C2	6.82	1.43	1.37
9	3	1537	G	C5-C6	6.82	1.49	1.42
10	4	1843	C	P-O5'	-6.82	1.52	1.59
7	1	80	G	C2-N3	6.82	1.38	1.32
7	1	86	G	C5-C4	6.80	1.43	1.38
8	2	1321	A	P-O5'	-6.80	1.52	1.59
7	1	91	A	N9-C4	6.80	1.42	1.37
10	4	1848	A	C6-N6	6.80	1.39	1.33
10	4	1878	G	N3-C4	6.79	1.40	1.35
11	5	2134	A	N9-C8	6.79	1.43	1.37
8	2	1334	G	C6-N1	6.78	1.44	1.39
11	5	2106	U	N3-C4	6.78	1.44	1.38
11	5	2158	A	N7-C5	-6.78	1.35	1.39
8	2	1311	G	N7-C5	-6.76	1.35	1.39
10	4	1885	A	N9-C8	-6.76	1.32	1.37
11	5	2094	A	N7-C5	-6.76	1.35	1.39
11	5	2117	A	C8-N7	6.75	1.36	1.31
10	4	1891	G	C2-N3	6.75	1.38	1.32
11	5	2176	A	C6-N1	6.75	1.40	1.35
1	y	383	PHE	CG-CD2	6.74	1.48	1.38
11	5	2114	A	C6-N6	6.74	1.39	1.33
10	4	1854	A	C6-N6	6.74	1.39	1.33
11	5	2183	A	C4'-O4'	-6.74	1.36	1.45
10	4	1867	G	C5-C4	6.73	1.43	1.38
10	4	1870	C	C3'-C2'	6.73	1.60	1.52
11	5	2124	G	C2-N2	6.73	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1337	G	C5-C4	6.73	1.43	1.38
7	1	55	G	C2-N3	6.73	1.38	1.32
7	1	56	A	C4'-C3'	6.73	1.60	1.53
11	5	2194	U	N3-C4	6.73	1.44	1.38
9	3	1543	G	C4'-O4'	6.72	1.54	1.45
8	2	1312	U	C2'-C1'	-6.72	1.46	1.53
4	T	3	ARG	NE-CZ	6.71	1.41	1.33
7	1	73	A	P-O5'	-6.71	1.53	1.59
10	4	1863	G	N1-C2	6.71	1.43	1.37
10	4	1867	G	O3'-P	-6.70	1.53	1.61
11	5	2149	U	N3-C4	6.69	1.44	1.38
7	1	80	G	C5-C4	6.69	1.43	1.38
11	5	2156	G	C8-N7	-6.69	1.26	1.30
8	2	1313	U	N3-C4	6.67	1.44	1.38
8	2	1327	A	N9-C8	6.67	1.43	1.37
11	5	2167	U	N3-C4	6.67	1.44	1.38
10	4	1891	G	C6-N1	6.66	1.44	1.39
7	1	106	C	C4'-C3'	-6.66	1.45	1.53
8	2	1324	G	C8-N7	-6.66	1.26	1.30
10	4	1864	U	N3-C4	6.65	1.44	1.38
7	1	93	G	C3'-O3'	6.64	1.51	1.42
11	5	2103	C	C4'-O4'	-6.64	1.36	1.45
11	5	2175	C	C5'-C4'	6.64	1.59	1.51
9	3	1530	G	C8-N7	-6.64	1.26	1.30
10	4	1887	C	C2-N3	6.64	1.41	1.35
11	5	2159	G	C5'-C4'	6.63	1.59	1.51
11	5	2094	A	O3'-P	-6.62	1.53	1.61
8	2	1324	G	C5-C4	6.62	1.43	1.38
6	Y	52	ARG	CZ-NH1	6.61	1.41	1.33
8	2	1339	G	C5-C4	6.61	1.43	1.38
7	1	106	C	C2-N3	6.61	1.41	1.35
11	5	2114	A	P-O5'	-6.60	1.53	1.59
11	5	2162	G	O3'-P	-6.60	1.53	1.61
8	2	1337	G	N7-C5	-6.60	1.35	1.39
7	1	70	G	N3-C4	6.59	1.40	1.35
10	4	1890	A	C6-N6	6.59	1.39	1.33
11	5	2184	A	C1'-N9	6.59	1.58	1.48
7	1	77	G	C5-C4	6.58	1.43	1.38
10	4	1871	A	C8-N7	6.58	1.36	1.31
11	5	2197	U	N3-C4	6.56	1.44	1.38
4	T	77	ARG	NE-CZ	6.55	1.41	1.33
11	5	2153	C	C4-N4	6.55	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	3	ARG	CZ-NH1	6.54	1.41	1.33
8	2	1332	G	C2'-O2'	6.54	1.50	1.41
11	5	2119	A	C5'-C4'	6.53	1.59	1.51
11	5	2154	A	N9-C4	6.53	1.41	1.37
7	1	81	G	C6-N1	6.53	1.44	1.39
7	1	94	A	P-O5'	-6.52	1.53	1.59
7	1	113	U	C4-C5	6.52	1.49	1.43
11	5	2160	C	C4-C5	6.52	1.48	1.43
11	5	2156	G	N9-C8	6.51	1.42	1.37
10	4	1863	G	C6-N1	6.51	1.44	1.39
11	5	2112	G	C6-N1	6.51	1.44	1.39
7	1	67	U	C2-O2	6.50	1.28	1.22
7	1	78	U	C2-N3	6.50	1.42	1.37
11	5	2114	A	N9-C4	-6.49	1.33	1.37
10	4	1891	G	O3'-P	6.49	1.69	1.61
10	4	1850	G	C6-N1	6.49	1.44	1.39
11	5	2115	G	C3'-C2'	-6.48	1.45	1.52
11	5	2152	G	N7-C5	-6.48	1.35	1.39
10	4	1868	C	C4-C5	-6.47	1.37	1.43
7	1	105	C	C2'-C1'	-6.47	1.46	1.53
11	5	2133	G	N1-C2	6.47	1.43	1.37
10	4	1842	G	C5-C4	6.46	1.42	1.38
7	1	52	A	C6-N6	6.46	1.39	1.33
7	1	54	G	C2-N3	6.46	1.38	1.32
10	4	1896	G	C5'-C4'	6.46	1.59	1.51
11	5	2199	A	C5'-C4'	6.46	1.59	1.51
10	4	1842	G	N1-C2	6.46	1.43	1.37
11	5	2103	C	C2'-C1'	-6.46	1.46	1.53
11	5	2127	G	C2'-C1'	-6.46	1.46	1.53
11	5	2184	A	N7-C5	-6.46	1.35	1.39
7	1	70	G	C8-N7	6.46	1.34	1.30
11	5	2164	C	N1-C6	6.45	1.41	1.37
11	5	2102	G	N9-C8	-6.44	1.33	1.37
7	1	56	A	N7-C5	-6.44	1.35	1.39
7	1	75	G	C4'-C3'	6.44	1.60	1.53
10	4	1883	U	C2-N3	6.44	1.42	1.37
11	5	2183	A	C5-C4	6.43	1.43	1.38
11	5	2143	C	C4-N4	6.43	1.39	1.33
7	1	63	A	C2-N3	6.42	1.39	1.33
11	5	2104	C	N1-C2	6.42	1.46	1.40
1	y	388	PRO	N-CD	6.41	1.56	1.47
11	5	2185	U	N1-C6	6.41	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	90	U	O3'-P	-6.41	1.53	1.61
7	1	61	C	C4-C5	6.40	1.48	1.43
9	3	1526	C	C4'-C3'	6.40	1.60	1.53
10	4	1877	A	N3-C4	6.40	1.38	1.34
7	1	60	G	N9-C4	-6.39	1.32	1.38
8	2	1324	G	C2'-C1'	6.38	1.60	1.53
10	4	1898	U	C4-C5	6.38	1.49	1.43
7	1	114	U	C1'-N1	6.37	1.58	1.48
11	5	2121	G	N9-C8	6.36	1.42	1.37
8	2	1337	G	C3'-C2'	-6.35	1.45	1.52
10	4	1854	A	N7-C5	-6.35	1.35	1.39
10	4	1858	A	C3'-O3'	6.34	1.51	1.42
7	1	98	G	N9-C4	-6.33	1.32	1.38
11	5	2134	A	C6-N1	6.33	1.40	1.35
10	4	1896	G	C2-N3	6.33	1.37	1.32
7	1	52	A	N7-C5	-6.33	1.35	1.39
2	E	112	ASP	C-N	6.33	1.44	1.33
7	1	95	A	C3'-C2'	-6.32	1.45	1.52
1	y	122	TYR	CG-CD2	6.32	1.47	1.39
2	E	124	GLY	CA-C	-6.31	1.41	1.51
11	5	2139	U	C2-N3	6.30	1.42	1.37
11	5	2141	G	C8-N7	-6.29	1.27	1.30
10	4	1850	G	C3'-O3'	6.29	1.50	1.42
11	5	2094	A	C3'-O3'	6.29	1.50	1.42
8	2	1308	A	N9-C8	-6.29	1.32	1.37
11	5	2110	G	C5'-C4'	6.29	1.58	1.51
11	5	2099	U	N1-C2	6.28	1.44	1.38
11	5	2113	U	C4-C5	6.27	1.49	1.43
10	4	1876	A	C6-N1	-6.27	1.31	1.35
7	1	102	U	C4-C5	6.26	1.49	1.43
11	5	2152	G	N3-C4	6.25	1.39	1.35
10	4	1847	A	N1-C2	-6.25	1.28	1.34
11	5	2173	A	N1-C2	6.25	1.40	1.34
11	5	2182	U	C4-C5	6.25	1.49	1.43
9	3	1533	C	C2-N3	6.25	1.40	1.35
11	5	2120	G	C6-N1	6.25	1.44	1.39
11	5	2192	U	C5'-C4'	6.25	1.58	1.51
10	4	1896	G	C8-N7	-6.25	1.27	1.30
11	5	2136	G	C8-N7	6.25	1.34	1.30
11	5	2192	U	C4-C5	6.25	1.49	1.43
8	2	1322	A	C2'-C1'	-6.24	1.46	1.53
9	3	1532	A	C5-C4	6.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	76	C	C4-C5	-6.24	1.38	1.43
11	5	2115	G	N1-C2	6.24	1.42	1.37
11	5	2135	A	N7-C5	-6.24	1.35	1.39
11	5	2173	A	C4'-C3'	-6.24	1.46	1.53
11	5	2184	A	N3-C4	6.24	1.38	1.34
7	1	88	G	C8-N7	-6.23	1.27	1.30
11	5	2114	A	N7-C5	-6.23	1.35	1.39
7	1	91	A	C5'-C4'	6.22	1.58	1.51
7	1	91	A	C5-C4	6.22	1.43	1.38
9	3	1540	G	C2'-C1'	-6.22	1.46	1.53
11	5	2134	A	C8-N7	-6.22	1.27	1.31
7	1	55	G	N1-C2	6.22	1.42	1.37
10	4	1856	U	C4-C5	6.22	1.49	1.43
7	1	71	A	C4'-C3'	6.21	1.59	1.53
10	4	1838	C	P-O5'	-6.20	1.53	1.59
11	5	2191	A	O4'-C1'	6.20	1.49	1.41
7	1	88	G	O3'-P	-6.20	1.53	1.61
1	y	242	ARG	CD-NE	6.20	1.56	1.46
7	1	67	U	C2-N3	6.18	1.42	1.37
11	5	2192	U	C4'-C3'	6.18	1.59	1.53
10	4	1857	G	C5'-C4'	6.18	1.58	1.51
11	5	2095	A	C6-N6	6.17	1.38	1.33
7	1	85	G	C1'-N9	6.17	1.58	1.48
10	4	1890	A	P-O5'	-6.17	1.53	1.59
7	1	88	G	C6-O6	6.16	1.29	1.24
7	1	103	A	N9-C4	-6.16	1.34	1.37
10	4	1889	A	C6-N1	6.16	1.39	1.35
7	1	81	G	N3-C4	-6.16	1.31	1.35
11	5	2185	U	C2-N3	6.15	1.42	1.37
9	3	1527	G	C6-N1	6.15	1.43	1.39
11	5	2130	U	N3-C4	6.15	1.44	1.38
11	5	2199	A	N9-C4	6.15	1.41	1.37
7	1	91	A	C3'-O3'	6.15	1.50	1.42
10	4	1862	G	O3'-P	-6.14	1.53	1.61
10	4	1843	C	N3-C4	6.14	1.38	1.33
11	5	2153	C	C3'-C2'	-6.14	1.46	1.52
11	5	2131	U	C4-O4	-6.14	1.18	1.23
11	5	2184	A	N1-C2	6.13	1.39	1.34
11	5	2183	A	P-O5'	-6.13	1.53	1.59
8	2	1309	G	C6-N1	6.13	1.43	1.39
11	5	2135	A	C5'-C4'	6.13	1.58	1.51
10	4	1838	C	C4-N4	6.12	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2166	U	P-O5'	-6.12	1.53	1.59
10	4	1846	G	C5'-C4'	6.12	1.58	1.51
11	5	2163	A	N9-C8	6.11	1.42	1.37
7	1	68	G	C5'-C4'	6.11	1.58	1.51
7	1	113	U	C5'-C4'	6.11	1.58	1.51
10	4	1897	G	C8-N7	6.11	1.34	1.30
8	2	1342	A	C2'-C1'	-6.11	1.46	1.53
7	1	63	A	C5'-C4'	6.10	1.58	1.51
9	3	1537	G	P-O5'	-6.10	1.53	1.59
9	3	1541	C	C4-N4	6.10	1.39	1.33
5	U	95	PHE	CG-CD1	6.10	1.47	1.38
7	1	99	U	C4-C5	6.10	1.49	1.43
8	2	1328	A	N9-C4	-6.09	1.34	1.37
11	5	2142	A	C2'-C1'	-6.09	1.46	1.53
10	4	1861	G	C2-N3	6.09	1.37	1.32
11	5	2101	A	C4'-C3'	6.09	1.59	1.53
11	5	2190	G	N3-C4	6.09	1.39	1.35
7	1	52	A	N3-C4	-6.08	1.31	1.34
10	4	1873	G	C6-N1	6.08	1.43	1.39
11	5	2149	U	C4'-C3'	-6.08	1.46	1.53
7	1	87	U	C5-C6	-6.08	1.28	1.34
8	2	1332	G	N3-C4	6.08	1.39	1.35
10	4	1894	C	O3'-P	-6.07	1.53	1.61
11	5	2128	G	C8-N7	-6.07	1.27	1.30
10	4	1858	A	C2'-C1'	-6.07	1.46	1.53
7	1	74	A	C6-N6	6.07	1.38	1.33
8	2	1342	A	N3-C4	6.07	1.38	1.34
11	5	2105	U	C2-N3	6.06	1.42	1.37
7	1	71	A	C6-N6	6.06	1.38	1.33
11	5	2156	G	C2-N3	6.06	1.37	1.32
11	5	2187	U	C2-N3	6.05	1.42	1.37
11	5	2140	G	N7-C5	-6.04	1.35	1.39
7	1	100	U	N1-C6	-6.04	1.32	1.38
9	3	1537	G	C8-N7	-6.03	1.27	1.30
11	5	2125	G	C3'-C2'	-6.03	1.46	1.52
8	2	1323	C	C2'-C1'	-6.02	1.46	1.53
11	5	2156	G	N1-C2	6.02	1.42	1.37
10	4	1862	G	C2-N3	6.02	1.37	1.32
9	3	1533	C	O3'-P	-6.02	1.53	1.61
11	5	2152	G	C3'-O3'	6.02	1.50	1.42
11	5	2120	G	N9-C4	-6.02	1.33	1.38
11	5	2144	G	C4'-O4'	-6.01	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1876	A	C8-N7	-6.01	1.27	1.31
11	5	2144	G	C5-C6	-6.01	1.36	1.42
9	3	1529	G	N9-C8	-6.01	1.33	1.37
10	4	1863	G	P-O5'	6.01	1.65	1.59
8	2	1322	A	N9-C8	-6.00	1.32	1.37
11	5	2139	U	C2'-C1'	-6.00	1.46	1.53
10	4	1893	C	C5'-C4'	6.00	1.58	1.51
10	4	1860	G	N9-C8	6.00	1.42	1.37
11	5	2157	G	C5-C4	6.00	1.42	1.38
8	2	1322	A	C6-N6	5.99	1.38	1.33
8	2	1327	A	C6-N6	5.99	1.38	1.33
11	5	2160	C	C2'-C1'	-5.98	1.46	1.53
11	5	2175	C	C4-C5	-5.98	1.38	1.43
11	5	2123	G	N3-C4	5.98	1.39	1.35
7	1	107	G	C2'-C1'	-5.98	1.46	1.53
11	5	2145	C	N3-C4	5.97	1.38	1.33
10	4	1884	G	C5-C4	5.96	1.42	1.38
11	5	2125	G	N9-C4	-5.96	1.33	1.38
7	1	52	A	C5'-C4'	5.95	1.58	1.51
10	4	1864	U	C2-N3	5.95	1.42	1.37
11	5	2145	C	N1-C6	5.95	1.40	1.37
8	2	1308	A	C8-N7	5.94	1.35	1.31
10	4	1870	C	C4'-C3'	5.94	1.59	1.53
11	5	2172	U	C3'-C2'	-5.94	1.46	1.52
8	2	1326	U	C4'-O4'	-5.94	1.37	1.45
10	4	1861	G	C2'-C1'	-5.94	1.46	1.53
10	4	1896	G	N9-C4	-5.94	1.33	1.38
1	y	176	GLU	N-CA	-5.94	1.34	1.46
11	5	2161	C	C4-N4	5.94	1.39	1.33
11	5	2100	G	C2-N3	5.93	1.37	1.32
11	5	2142	A	C4'-C3'	5.92	1.59	1.53
7	1	78	U	C2-O2	5.91	1.27	1.22
9	3	1536	C	C2'-C1'	-5.91	1.46	1.53
1	y	357	ARG	CD-NE	5.91	1.56	1.46
10	4	1840	G	N1-C2	5.91	1.42	1.37
10	4	1840	G	N7-C5	-5.90	1.35	1.39
8	2	1333	G	C2'-C1'	-5.90	1.46	1.53
11	5	2092	U	N3-C4	5.90	1.43	1.38
11	5	2103	C	N1-C6	-5.90	1.33	1.37
11	5	2142	A	O3'-P	-5.90	1.54	1.61
11	5	2176	A	N9-C4	5.90	1.41	1.37
10	4	1845	G	C5'-C4'	5.88	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1317	G	C8-N7	5.88	1.34	1.30
7	1	88	G	N9-C8	-5.88	1.33	1.37
7	1	97	C	C4-C5	5.87	1.47	1.43
7	1	100	U	P-O5'	5.87	1.65	1.59
11	5	2163	A	N7-C5	5.86	1.42	1.39
11	5	2168	G	C8-N7	-5.86	1.27	1.30
11	5	2094	A	N9-C8	-5.86	1.33	1.37
11	5	2156	G	P-O5'	-5.86	1.53	1.59
11	5	2194	U	N1-C2	5.85	1.43	1.38
10	4	1854	A	P-O5'	-5.85	1.53	1.59
11	5	2127	G	C8-N7	-5.85	1.27	1.30
1	y	248	TYR	CZ-OH	5.84	1.47	1.37
8	2	1341	G	C2-N2	5.84	1.40	1.34
1	y	74	ARG	CZ-NH2	5.84	1.40	1.33
11	5	2139	U	N1-C2	5.84	1.43	1.38
11	5	2150	C	O3'-P	-5.84	1.54	1.61
11	5	2136	G	N7-C5	-5.84	1.35	1.39
11	5	2160	C	C4-N4	5.84	1.39	1.33
8	2	1334	G	C2-N2	5.84	1.40	1.34
11	5	2124	G	N3-C4	-5.83	1.31	1.35
11	5	2163	A	C6-N6	5.83	1.38	1.33
7	1	78	U	P-O5'	-5.82	1.53	1.59
7	1	100	U	C3'-C2'	-5.82	1.46	1.52
11	5	2146	C	N3-C4	5.82	1.38	1.33
11	5	2151	U	C4-C5	5.82	1.48	1.43
8	2	1322	A	C5-C4	-5.82	1.34	1.38
7	1	107	G	N7-C5	5.82	1.42	1.39
11	5	2170	A	O4'-C1'	5.82	1.49	1.41
10	4	1852	U	C5-C6	5.82	1.39	1.34
11	5	2193	G	C4'-C3'	-5.81	1.46	1.52
7	1	73	A	N3-C4	5.81	1.38	1.34
11	5	2167	U	N1-C6	-5.81	1.32	1.38
7	1	88	G	N1-C2	5.80	1.42	1.37
9	3	1531	C	O3'-P	-5.79	1.54	1.61
11	5	2128	G	O3'-P	-5.79	1.54	1.61
8	2	1321	A	C3'-O3'	5.79	1.50	1.42
10	4	1859	U	C1'-N1	5.79	1.57	1.48
10	4	1862	G	C6-N1	5.78	1.43	1.39
11	5	2199	A	N3-C4	5.78	1.38	1.34
11	5	2122	U	O3'-P	-5.77	1.54	1.61
11	5	2185	U	C2'-C1'	-5.77	1.47	1.53
7	1	94	A	C6-N1	5.77	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2128	G	N7-C5	-5.77	1.35	1.39
10	4	1873	G	C2-N2	5.77	1.40	1.34
10	4	1846	G	C2'-C1'	-5.76	1.47	1.53
5	U	5	ARG	CD-NE	5.76	1.56	1.46
6	Y	23	ARG	NE-CZ	5.75	1.40	1.33
11	5	2117	A	C4'-C3'	5.75	1.59	1.53
7	1	112	U	C2'-C1'	-5.75	1.47	1.53
8	2	1342	A	N7-C5	5.75	1.42	1.39
9	3	1540	G	C2-N2	5.75	1.40	1.34
11	5	2193	G	C8-N7	-5.74	1.27	1.30
7	1	68	G	N7-C5	5.74	1.42	1.39
11	5	2119	A	C5-C6	5.74	1.46	1.41
7	1	101	A	N9-C4	-5.74	1.34	1.37
7	1	77	G	N9-C4	-5.74	1.33	1.38
9	3	1540	G	N1-C2	5.74	1.42	1.37
11	5	2153	C	O3'-P	-5.74	1.54	1.61
10	4	1872	A	C6-N6	5.73	1.38	1.33
10	4	1873	G	C2'-C1'	-5.73	1.47	1.53
10	4	1896	G	N9-C8	-5.73	1.33	1.37
10	4	1885	A	N9-C4	5.73	1.41	1.37
7	1	57	C	O4'-C1'	-5.72	1.34	1.41
11	5	2102	G	C6-N1	5.72	1.43	1.39
11	5	2185	U	O3'-P	-5.72	1.54	1.61
11	5	2186	G	C4'-C3'	5.72	1.59	1.53
7	1	113	U	C4'-C3'	-5.72	1.46	1.52
10	4	1847	A	C8-N7	-5.72	1.27	1.31
7	1	85	G	C6-N1	5.72	1.43	1.39
11	5	2171	A	N1-C2	5.71	1.39	1.34
11	5	2147	A	C5'-C4'	5.71	1.58	1.51
11	5	2182	U	N1-C2	-5.71	1.33	1.38
11	5	2171	A	N3-C4	-5.71	1.31	1.34
11	5	2127	G	N9-C8	5.70	1.41	1.37
10	4	1877	A	C6-N6	5.70	1.38	1.33
10	4	1852	U	C2'-C1'	-5.70	1.47	1.53
11	5	2131	U	N1-C2	5.70	1.43	1.38
10	4	1867	G	C2'-C1'	-5.70	1.47	1.53
11	5	2100	G	C2-N2	5.70	1.40	1.34
7	1	56	A	C6-N1	-5.69	1.31	1.35
11	5	2161	C	C4-C5	5.69	1.47	1.43
11	5	2180	U	O3'-P	-5.68	1.54	1.61
11	5	2174	C	C2'-O2'	-5.68	1.34	1.41
7	1	102	U	P-O5'	5.68	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2181	U	C4-C5	5.68	1.48	1.43
10	4	1851	U	O3'-P	-5.67	1.54	1.61
7	1	89	A	N9-C4	5.66	1.41	1.37
10	4	1869	G	N1-C2	5.66	1.42	1.37
11	5	2116	G	C4'-C3'	-5.66	1.46	1.52
7	1	73	A	C3'-C2'	5.66	1.59	1.52
11	5	2160	C	C1'-N1	5.66	1.57	1.48
10	4	1862	G	N1-C2	5.66	1.42	1.37
7	1	62	U	C5'-C4'	5.65	1.58	1.51
8	2	1341	G	C6-N1	5.64	1.43	1.39
8	2	1341	G	C2-N3	5.64	1.37	1.32
11	5	2121	G	O3'-P	-5.63	1.54	1.61
11	5	2165	C	C1'-N1	5.63	1.57	1.48
11	5	2171	A	C5'-C4'	5.63	1.58	1.51
2	E	84	TRP	NE1-CE2	5.63	1.44	1.37
10	4	1858	A	C4'-O4'	-5.63	1.38	1.45
7	1	114	U	N3-C4	5.63	1.43	1.38
7	1	60	G	C2'-C1'	-5.62	1.47	1.53
11	5	2131	U	C5-C6	5.62	1.39	1.34
9	3	1534	U	C5'-C4'	5.62	1.58	1.51
5	U	85	ARG	NE-CZ	5.62	1.40	1.33
11	5	2100	G	P-O5'	5.61	1.65	1.59
11	5	2150	C	C4'-C3'	5.61	1.59	1.53
11	5	2170	A	C2'-C1'	-5.61	1.47	1.53
9	3	1527	G	C5-C4	5.61	1.42	1.38
11	5	2159	G	C6-O6	5.61	1.29	1.24
7	1	93	G	N3-C4	5.61	1.39	1.35
10	4	1849	G	C5-C6	-5.61	1.36	1.42
10	4	1860	G	C6-N1	5.60	1.43	1.39
11	5	2138	G	C6-N1	5.60	1.43	1.39
11	5	2162	G	N1-C2	5.60	1.42	1.37
11	5	2141	G	N3-C4	5.60	1.39	1.35
11	5	2186	G	C2-N3	5.60	1.37	1.32
11	5	2133	G	N9-C4	-5.60	1.33	1.38
11	5	2134	A	N3-C4	5.59	1.38	1.34
11	5	2179	C	N3-C4	5.59	1.37	1.33
10	4	1881	C	N1-C6	5.59	1.40	1.37
7	1	107	G	N3-C4	5.58	1.39	1.35
10	4	1891	G	C5-C4	5.58	1.42	1.38
11	5	2112	G	N7-C5	-5.58	1.35	1.39
8	2	1309	G	P-O5'	-5.58	1.54	1.59
11	5	2161	C	O3'-P	-5.58	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	56	A	N9-C4	5.57	1.41	1.37
7	1	80	G	N1-C2	5.57	1.42	1.37
9	3	1529	G	C2-N2	5.57	1.40	1.34
10	4	1871	A	C6-N6	5.57	1.38	1.33
7	1	69	C	N3-C4	5.56	1.37	1.33
11	5	2168	G	P-O5'	5.56	1.65	1.59
11	5	2158	A	N3-C4	5.56	1.38	1.34
9	3	1543	G	C2-N2	5.56	1.40	1.34
10	4	1878	G	C8-N7	5.55	1.34	1.30
1	y	255	ARG	CZ-NH2	5.55	1.40	1.33
7	1	108	G	C8-N7	-5.55	1.27	1.30
6	Y	7	ARG	NE-CZ	5.54	1.40	1.33
11	5	2196	C	O4'-C1'	5.54	1.48	1.41
1	y	389	GLU	CB-CG	5.54	1.62	1.52
11	5	2178	C	C4-C5	5.54	1.47	1.43
11	5	2191	A	C2'-C1'	-5.53	1.47	1.53
10	4	1889	A	C5-C4	5.53	1.42	1.38
10	4	1848	A	C8-N7	-5.53	1.27	1.31
11	5	2155	U	C4'-C3'	5.52	1.59	1.53
11	5	2140	G	C2-N3	5.52	1.37	1.32
11	5	2132	U	C2'-C1'	-5.51	1.47	1.53
11	5	2159	G	C2'-O2'	5.51	1.48	1.41
7	1	68	G	C6-N1	5.51	1.43	1.39
9	3	1527	G	N1-C2	5.50	1.42	1.37
11	5	2113	U	C2'-O2'	-5.50	1.34	1.41
11	5	2185	U	C5'-C4'	5.50	1.57	1.51
9	3	1533	C	C4-C5	-5.50	1.38	1.43
11	5	2135	A	C6-N6	5.50	1.38	1.33
7	1	81	G	C2-N3	5.49	1.37	1.32
11	5	2176	A	C5'-C4'	5.49	1.57	1.51
8	2	1331	G	C3'-C2'	5.48	1.58	1.52
10	4	1882	U	C5'-C4'	-5.48	1.44	1.51
10	4	1882	U	N1-C2	5.48	1.43	1.38
8	2	1320	C	P-O5'	5.47	1.65	1.59
10	4	1856	U	C1'-N1	5.47	1.56	1.48
7	1	90	U	C4-O4	5.47	1.28	1.23
8	2	1310	G	C2-N2	-5.47	1.29	1.34
8	2	1324	G	N9-C8	-5.47	1.34	1.37
10	4	1860	G	N9-C4	-5.47	1.33	1.38
5	U	5	ARG	CZ-NH1	5.46	1.40	1.33
7	1	53	A	C5'-C4'	5.46	1.57	1.51
10	4	1840	G	O4'-C1'	5.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	67	U	C4'-C3'	5.46	1.59	1.53
7	1	111	A	O4'-C1'	5.46	1.48	1.41
7	1	100	U	C2-N3	5.45	1.41	1.37
10	4	1869	G	C5-C6	-5.44	1.36	1.42
11	5	2097	A	C2'-C1'	-5.44	1.47	1.53
11	5	2126	A	O3'-P	-5.43	1.54	1.61
8	2	1309	G	N9-C4	-5.43	1.33	1.38
10	4	1876	A	C5-C6	5.42	1.46	1.41
10	4	1847	A	N3-C4	-5.42	1.31	1.34
11	5	2116	G	O4'-C1'	5.42	1.48	1.41
11	5	2179	C	C3'-C2'	-5.42	1.46	1.52
7	1	57	C	C4-N4	-5.41	1.29	1.33
1	y	10	GLN	CA-CB	5.40	1.65	1.53
11	5	2138	G	C3'-O3'	5.40	1.49	1.42
11	5	2158	A	C6-N1	5.39	1.39	1.35
7	1	110	G	C2'-C1'	-5.39	1.47	1.53
7	1	59	U	O3'-P	-5.39	1.54	1.61
11	5	2155	U	O3'-P	-5.39	1.54	1.61
9	3	1539	U	C3'-O3'	-5.39	1.34	1.42
11	5	2155	U	N3-C4	5.39	1.43	1.38
11	5	2180	U	P-O5'	-5.39	1.54	1.59
9	3	1541	C	C4'-O4'	5.38	1.52	1.45
9	3	1530	G	N9-C8	-5.38	1.34	1.37
4	T	56	GLU	CG-CD	5.38	1.60	1.51
10	4	1893	C	C5-C6	-5.38	1.30	1.34
5	U	82	VAL	CB-CG1	-5.37	1.41	1.52
9	3	1532	A	C4'-O4'	5.37	1.52	1.45
11	5	2156	G	C2'-C1'	-5.37	1.47	1.53
10	4	1851	U	N1-C2	5.36	1.43	1.38
7	1	106	C	C5'-C4'	5.36	1.57	1.51
6	Y	52	ARG	CD-NE	5.36	1.55	1.46
8	2	1328	A	C5-C4	-5.36	1.35	1.38
11	5	2173	A	C2-N3	5.36	1.38	1.33
9	3	1527	G	P-O5'	-5.35	1.54	1.59
11	5	2137	U	N1-C6	-5.35	1.33	1.38
7	1	94	A	C2-N3	5.35	1.38	1.33
10	4	1887	C	N1-C6	5.35	1.40	1.37
8	2	1338	G	C6-N1	5.34	1.43	1.39
8	2	1314	C	C4'-O4'	-5.34	1.38	1.45
7	1	85	G	C2'-C1'	-5.34	1.47	1.53
11	5	2162	G	P-O5'	-5.34	1.54	1.59
10	4	1848	A	O4'-C1'	-5.34	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	56	A	C5'-C4'	5.34	1.57	1.51
4	T	21	SER	CA-CB	5.33	1.60	1.52
7	1	67	U	C5-C6	-5.33	1.29	1.34
11	5	2110	G	C4'-C3'	5.33	1.59	1.53
2	E	117	ARG	CZ-NH2	5.33	1.40	1.33
7	1	85	G	O3'-P	-5.32	1.54	1.61
11	5	2093	G	C5'-C4'	5.32	1.57	1.51
11	5	2160	C	N1-C2	5.32	1.45	1.40
2	E	113	GLY	N-CA	5.32	1.54	1.46
11	5	2100	G	O3'-P	-5.31	1.54	1.61
7	1	56	A	C8-N7	-5.31	1.27	1.31
9	3	1533	C	C4-N4	5.31	1.38	1.33
11	5	2114	A	C2'-C1'	-5.31	1.47	1.53
11	5	2146	C	C4'-C3'	-5.31	1.47	1.52
10	4	1854	A	C4'-C3'	-5.31	1.47	1.52
1	y	365	TYR	CD2-CE2	5.31	1.47	1.39
10	4	1892	C	C5-C6	-5.31	1.30	1.34
8	2	1329	U	P-O5'	-5.30	1.54	1.59
11	5	2157	G	C2-N3	5.30	1.36	1.32
11	5	2126	A	C8-N7	5.30	1.35	1.31
11	5	2194	U	C5-C6	5.30	1.39	1.34
4	T	26	LYS	CA-CB	5.29	1.65	1.53
10	4	1874	C	N3-C4	5.29	1.37	1.33
11	5	2151	U	C2-N3	5.29	1.41	1.37
7	1	87	U	C1'-N1	5.29	1.56	1.48
11	5	2136	G	N9-C8	5.29	1.41	1.37
8	2	1322	A	C6-N1	5.29	1.39	1.35
11	5	2117	A	O4'-C1'	5.29	1.48	1.41
11	5	2136	G	O3'-P	-5.28	1.54	1.61
8	2	1312	U	C5'-C4'	5.28	1.57	1.51
11	5	2142	A	C6-N6	5.28	1.38	1.33
11	5	2176	A	P-O5'	-5.28	1.54	1.59
1	y	321	TYR	CG-CD2	5.27	1.46	1.39
9	3	1538	G	N3-C4	-5.27	1.31	1.35
6	Y	48	ARG	CZ-NH1	5.27	1.39	1.33
10	4	1838	C	C2-N3	5.26	1.40	1.35
7	1	87	U	N3-C4	5.26	1.43	1.38
7	1	70	G	O4'-C1'	5.25	1.48	1.41
11	5	2161	C	C3'-C2'	5.25	1.58	1.52
8	2	1311	G	C5-C4	5.24	1.42	1.38
11	5	2133	G	C8-N7	-5.24	1.27	1.30
11	5	2157	G	C6-N1	5.24	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	100	U	C2'-C1'	5.24	1.59	1.53
8	2	1310	G	C3'-O3'	5.24	1.49	1.42
10	4	1845	G	C5-C4	5.24	1.42	1.38
11	5	2186	G	C5-C6	-5.24	1.37	1.42
7	1	59	U	N1-C2	-5.24	1.33	1.38
8	2	1310	G	P-O5'	-5.23	1.54	1.59
10	4	1843	C	C4-N4	5.23	1.38	1.33
11	5	2136	G	C5-C4	5.23	1.42	1.38
10	4	1870	C	C4-N4	5.22	1.38	1.33
5	U	94	PHE	CG-CD1	5.22	1.46	1.38
10	4	1888	G	N7-C5	5.21	1.42	1.39
1	y	293	TRP	CG-CD2	5.21	1.52	1.43
10	4	1874	C	C3'-O3'	5.20	1.49	1.42
1	y	22	ARG	NE-CZ	5.20	1.39	1.33
8	2	1341	G	N3-C4	-5.20	1.31	1.35
9	3	1536	C	P-O5'	-5.20	1.54	1.59
10	4	1847	A	N9-C4	5.20	1.41	1.37
10	4	1883	U	C4-C5	5.20	1.48	1.43
10	4	1844	C	C5'-C4'	5.19	1.57	1.51
7	1	52	A	C4'-O4'	5.19	1.52	1.45
11	5	2188	U	O5'-C5'	5.19	1.52	1.44
10	4	1890	A	C1'-N9	5.18	1.56	1.48
8	2	1326	U	C2-O2	5.18	1.27	1.22
1	y	110	GLU	CB-CG	5.18	1.61	1.52
1	y	286	PHE	CG-CD2	5.18	1.46	1.38
8	2	1338	G	C4'-C3'	5.18	1.58	1.53
11	5	2163	A	O3'-P	-5.18	1.54	1.61
11	5	2167	U	C2'-C1'	-5.18	1.47	1.53
11	5	2177	C	N1-C6	5.18	1.40	1.37
11	5	2178	C	P-O5'	-5.18	1.54	1.59
7	1	92	U	O3'-P	-5.17	1.54	1.61
10	4	1885	A	C5-C4	5.17	1.42	1.38
11	5	2127	G	C4'-O4'	-5.17	1.38	1.45
11	5	2199	A	C2'-C1'	-5.17	1.47	1.53
10	4	1865	U	C5'-C4'	5.16	1.57	1.51
11	5	2153	C	N3-C4	5.16	1.37	1.33
9	3	1542	U	O3'-P	-5.15	1.54	1.61
11	5	2140	G	C5'-C4'	5.15	1.57	1.51
7	1	88	G	N7-C5	-5.15	1.36	1.39
8	2	1341	G	N9-C4	-5.15	1.33	1.38
8	2	1308	A	C6-N1	5.14	1.39	1.35
11	5	2154	A	P-O5'	5.14	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2112	G	C1'-N9	5.14	1.56	1.48
7	1	110	G	C3'-C2'	5.13	1.58	1.52
8	2	1327	A	C5-C6	5.13	1.45	1.41
9	3	1527	G	N7-C5	-5.13	1.36	1.39
1	y	68	SER	C-N	5.13	1.42	1.33
10	4	1888	G	C1'-N9	5.13	1.56	1.48
11	5	2149	U	N1-C2	-5.13	1.33	1.38
11	5	2128	G	C3'-C2'	5.13	1.58	1.52
11	5	2147	A	N9-C4	5.13	1.41	1.37
11	5	2165	C	N1-C6	5.13	1.40	1.37
11	5	2173	A	C6-N6	5.13	1.38	1.33
11	5	2105	U	C2'-C1'	-5.12	1.47	1.53
4	T	68	LYS	N-CA	-5.12	1.36	1.46
11	5	2190	G	N9-C4	-5.12	1.33	1.38
11	5	2180	U	C5'-C4'	5.12	1.57	1.51
1	y	181	ARG	CD-NE	5.12	1.55	1.46
11	5	2102	G	C5'-C4'	5.12	1.57	1.51
7	1	66	C	C4-N4	5.11	1.38	1.33
11	5	2188	U	C3'-C2'	-5.11	1.47	1.52
7	1	72	U	C1'-N1	-5.11	1.39	1.46
9	3	1528	A	C6-N1	5.11	1.39	1.35
8	2	1311	G	C4'-O4'	5.11	1.52	1.45
11	5	2118	U	C3'-O3'	5.10	1.49	1.42
8	2	1309	G	N3-C4	5.10	1.39	1.35
8	2	1340	U	C5-C6	5.09	1.38	1.34
7	1	74	A	C6-N1	5.09	1.39	1.35
7	1	54	G	O4'-C1'	-5.09	1.35	1.41
10	4	1866	A	C5-C4	5.09	1.42	1.38
8	2	1340	U	C2-N3	5.08	1.41	1.37
11	5	2156	G	C4'-C3'	5.08	1.58	1.53
11	5	2185	U	C5-C6	5.08	1.38	1.34
7	1	84	A	N7-C5	-5.08	1.36	1.39
9	3	1538	G	C4'-O4'	5.08	1.52	1.45
10	4	1898	U	C5-C6	5.08	1.38	1.34
10	4	1866	A	C5-C6	5.07	1.45	1.41
7	1	74	A	C5-C4	5.07	1.42	1.38
11	5	2123	G	P-O5'	-5.07	1.54	1.59
7	1	99	U	N1-C2	5.07	1.43	1.38
10	4	1888	G	N9-C4	-5.06	1.33	1.38
11	5	2114	A	C5-C6	-5.06	1.36	1.41
8	2	1332	G	C5-C4	5.05	1.41	1.38
11	5	2194	U	C3'-O3'	5.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1338	G	C6-O6	5.04	1.28	1.24
8	2	1326	U	O4'-C1'	5.04	1.48	1.41
11	5	2147	A	C8-N7	-5.04	1.28	1.31
7	1	55	G	C5-C4	5.04	1.41	1.38
9	3	1543	G	C6-N1	5.04	1.43	1.39
11	5	2189	U	C3'-C2'	-5.04	1.47	1.52
11	5	2184	A	N9-C8	-5.03	1.33	1.37
10	4	1882	U	C2-N3	-5.03	1.34	1.37
5	U	21	ARG	CZ-NH2	5.03	1.39	1.33
11	5	2136	G	N1-C2	5.03	1.41	1.37
11	5	2191	A	C5-C4	5.03	1.42	1.38
11	5	2163	A	C8-N7	5.03	1.35	1.31
10	4	1838	C	C4-C5	-5.02	1.39	1.43
11	5	2165	C	C2'-C1'	5.01	1.58	1.53
9	3	1534	U	C3'-C2'	5.01	1.58	1.52
7	1	61	C	P-O5'	-5.01	1.54	1.59
11	5	2162	G	C2-N3	5.00	1.36	1.32
7	1	100	U	C5'-C4'	5.00	1.57	1.51
11	5	2174	C	N1-C6	5.00	1.40	1.37

All (1654) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	1540	G	N1-C6-O6	26.41	135.75	119.90
11	5	2198	A	N1-C6-N6	26.09	134.26	118.60
10	4	1857	G	N1-C6-O6	24.56	134.64	119.90
10	4	1857	G	C5-C6-O6	-22.03	115.38	128.60
11	5	2171	A	N1-C6-N6	21.65	131.59	118.60
7	1	73	A	N1-C6-N6	21.64	131.58	118.60
2	E	80	ARG	NE-CZ-NH2	-21.35	109.62	120.30
9	3	1540	G	C5-C6-O6	-20.64	116.22	128.60
11	5	2097	A	N1-C6-N6	20.50	130.90	118.60
10	4	1850	G	N1-C6-O6	19.55	131.63	119.90
11	5	2115	G	N1-C6-O6	19.17	131.40	119.90
7	1	70	G	N1-C6-O6	18.82	131.19	119.90
7	1	91	A	N1-C6-N6	18.77	129.87	118.60
11	5	2101	A	N1-C6-N6	18.38	129.62	118.60
10	4	1871	A	N1-C6-N6	18.17	129.50	118.60
8	2	1334	G	N1-C6-O6	18.15	130.79	119.90
10	4	1842	G	N1-C6-O6	18.13	130.78	119.90
11	5	2135	A	N1-C6-N6	18.12	129.47	118.60
7	1	73	A	C5-C6-N6	-17.64	109.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Y	48	ARG	NE-CZ-NH2	17.29	128.95	120.30
3	G	52	MET	N-CA-CB	17.12	141.41	110.60
1	y	243	ARG	NE-CZ-NH2	-17.09	111.75	120.30
2	E	80	ARG	NE-CZ-NH1	17.00	128.80	120.30
10	4	1873	G	N1-C6-O6	16.96	130.07	119.90
7	1	74	A	N1-C6-N6	16.88	128.73	118.60
11	5	2097	A	C5-C6-N6	-16.85	110.22	123.70
11	5	2193	G	C5-C6-O6	-16.74	118.56	128.60
10	4	1877	A	C8-N9-C4	-16.59	99.16	105.80
11	5	2144	G	C5-C6-O6	-16.33	118.80	128.60
11	5	2161	C	N3-C4-C5	-16.33	115.37	121.90
11	5	2137	U	O4'-C1'-N1	15.88	120.91	108.20
1	y	85	TYR	CB-CG-CD1	-15.71	111.57	121.00
8	2	1327	A	N1-C6-N6	15.60	127.96	118.60
11	5	2156	G	N1-C6-O6	15.44	129.16	119.90
10	4	1850	G	C5-C6-O6	-15.17	119.50	128.60
10	4	1854	A	C4-C5-C6	15.16	124.58	117.00
9	3	1538	G	C2-N3-C4	15.16	119.48	111.90
11	5	2199	A	N1-C6-N6	15.15	127.69	118.60
11	5	2173	A	N1-C6-N6	15.11	127.67	118.60
3	G	46	SER	N-CA-CB	-15.09	87.87	110.50
10	4	1890	A	N1-C6-N6	15.07	127.64	118.60
10	4	1866	A	N1-C6-N6	14.98	127.59	118.60
11	5	2186	G	C5-C6-O6	-14.96	119.62	128.60
10	4	1876	A	C4-C5-C6	14.92	124.46	117.00
7	1	70	G	C5-C6-O6	-14.88	119.67	128.60
7	1	52	A	N1-C6-N6	14.87	127.52	118.60
10	4	1889	A	N1-C6-N6	14.83	127.50	118.60
11	5	2156	G	C5-C6-O6	-14.74	119.76	128.60
10	4	1860	G	C5-C6-O6	-14.64	119.81	128.60
7	1	88	G	C4-C5-N7	-14.61	104.95	110.80
11	5	2124	G	N1-C6-O6	14.60	128.66	119.90
11	5	2193	G	N1-C6-O6	14.59	128.66	119.90
7	1	89	A	N1-C6-N6	14.57	127.34	118.60
11	5	2127	G	N1-C6-O6	14.55	128.63	119.90
11	5	2144	G	N1-C6-O6	14.49	128.59	119.90
9	3	1537	G	N1-C6-O6	14.44	128.56	119.90
11	5	2095	A	N1-C6-N6	14.36	127.22	118.60
11	5	2173	A	C5-C6-N6	-14.36	112.21	123.70
11	5	2121	G	N1-C6-O6	14.32	128.49	119.90
10	4	1873	G	C5-C6-O6	-14.32	120.01	128.60
10	4	1871	A	C5-C6-N1	-14.31	110.55	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1839	G	N1-C6-O6	14.27	128.46	119.90
10	4	1842	G	C6-N1-C2	14.10	133.56	125.10
10	4	1854	A	N9-C4-C5	14.10	111.44	105.80
7	1	57	C	O4'-C1'-N1	14.09	119.47	108.20
8	2	1338	G	N1-C6-O6	14.09	128.35	119.90
9	3	1543	G	C5-C6-O6	-13.99	120.20	128.60
10	4	1874	C	O4'-C1'-N1	13.92	119.34	108.20
11	5	2186	G	N1-C6-O6	13.85	128.21	119.90
11	5	2119	A	O4'-C1'-N9	13.85	119.28	108.20
11	5	2115	G	C5-C6-O6	-13.83	120.30	128.60
1	y	21	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	y	74	ARG	NE-CZ-NH2	-13.79	113.40	120.30
11	5	2142	A	N1-C6-N6	13.74	126.85	118.60
11	5	2176	A	C5-C6-N1	-13.73	110.84	117.70
1	y	243	ARG	NE-CZ-NH1	13.68	127.14	120.30
11	5	2158	A	N1-C6-N6	13.61	126.77	118.60
11	5	2184	A	C5-C6-N1	-13.61	110.89	117.70
5	U	86	PHE	CB-CG-CD1	13.52	130.27	120.80
11	5	2183	A	N1-C6-N6	13.52	126.71	118.60
11	5	2184	A	C4-C5-C6	13.38	123.69	117.00
7	1	103	A	N1-C6-N6	13.37	126.62	118.60
11	5	2176	A	N1-C6-N6	13.30	126.58	118.60
7	1	83	A	N1-C6-N6	13.28	126.57	118.60
11	5	2132	U	O4'-C1'-N1	13.26	118.81	108.20
8	2	1342	A	N1-C6-N6	13.24	126.54	118.60
8	2	1321	A	C8-N9-C4	-13.22	100.51	105.80
11	5	2147	A	P-O3'-C3'	13.17	135.50	119.70
10	4	1877	A	N1-C6-N6	13.15	126.49	118.60
11	5	2198	A	C5-C6-N1	-13.13	111.13	117.70
11	5	2174	C	N3-C4-C5	-13.11	116.66	121.90
11	5	2162	G	C4-C5-N7	13.09	116.04	110.80
10	4	1839	G	C5-C6-O6	-13.09	120.75	128.60
8	2	1315	C	P-O3'-C3'	13.05	135.37	119.70
3	G	51	PHE	N-CA-C	13.03	146.18	111.00
8	2	1341	G	C4-C5-N7	-13.00	105.60	110.80
3	G	44	GLY	N-CA-C	12.92	145.39	113.10
1	y	236	PHE	CB-CG-CD2	-12.90	111.77	120.80
10	4	1840	G	C8-N9-C4	-12.86	101.26	106.40
11	5	2171	A	C5-C6-N6	-12.85	113.42	123.70
7	1	79	C	O4'-C1'-N1	12.82	118.46	108.20
11	5	2174	C	O4'-C1'-N1	12.80	118.44	108.20
10	4	1852	U	O4'-C1'-N1	12.69	118.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1309	G	N1-C6-O6	12.67	127.50	119.90
9	3	1527	G	N1-C6-O6	12.65	127.49	119.90
9	3	1533	C	O4'-C1'-N1	12.62	118.30	108.20
10	4	1842	G	N1-C2-N3	-12.62	116.33	123.90
9	3	1531	C	N3-C4-C5	-12.61	116.86	121.90
7	1	68	G	N1-C6-O6	12.59	127.45	119.90
9	3	1537	G	C5-C6-O6	-12.56	121.06	128.60
7	1	91	A	C5-C6-N6	-12.56	113.65	123.70
11	5	2177	C	O4'-C1'-N1	12.54	118.23	108.20
7	1	111	A	O4'-C1'-N9	12.52	118.22	108.20
7	1	95	A	N1-C6-N6	12.46	126.08	118.60
8	2	1338	G	C5-C6-O6	-12.46	121.12	128.60
11	5	2168	G	N1-C6-O6	12.46	127.38	119.90
4	T	77	ARG	NE-CZ-NH2	-12.44	114.08	120.30
2	E	117	ARG	NE-CZ-NH2	-12.43	114.08	120.30
10	4	1861	G	C5-C6-O6	-12.43	121.14	128.60
11	5	2176	A	C6-C5-N7	-12.39	123.62	132.30
11	5	2102	G	O4'-C1'-N9	12.38	118.11	108.20
1	y	255	ARG	NE-CZ-NH1	12.33	126.46	120.30
11	5	2158	A	C8-N9-C4	-12.30	100.88	105.80
11	5	2121	G	C5-N7-C8	12.29	110.44	104.30
11	5	2146	C	O4'-C1'-N1	12.24	117.99	108.20
7	1	58	G	N1-C6-O6	12.14	127.18	119.90
11	5	2159	G	N1-C2-N3	-12.14	116.62	123.90
10	4	1861	G	O4'-C1'-N9	12.14	117.91	108.20
11	5	2124	G	C5-C6-O6	-12.12	121.33	128.60
7	1	88	G	N1-C6-O6	12.09	127.15	119.90
11	5	2155	U	C5-C4-O4	-12.09	118.65	125.90
11	5	2174	C	C6-N1-C2	-11.99	115.50	120.30
1	y	74	ARG	NE-CZ-NH1	11.97	126.29	120.30
11	5	2178	C	O4'-C1'-N1	11.97	117.77	108.20
9	3	1543	G	C4-C5-N7	11.95	115.58	110.80
9	3	1535	A	N1-C6-N6	11.95	125.77	118.60
1	y	372	ARG	NE-CZ-NH1	-11.93	114.34	120.30
8	2	1310	G	C6-C5-N7	-11.83	123.30	130.40
8	2	1322	A	N1-C6-N6	11.81	125.69	118.60
11	5	2121	G	N7-C8-N9	-11.81	107.20	113.10
7	1	56	A	O4'-C1'-N9	11.79	117.63	108.20
3	G	48	SER	CB-CA-C	11.77	132.47	110.10
8	2	1333	G	P-O3'-C3'	11.77	133.82	119.70
8	2	1333	G	C4-C5-N7	11.75	115.50	110.80
11	5	2167	U	O4'-C1'-N1	11.75	117.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1334	G	C5-C6-O6	-11.73	121.56	128.60
8	2	1321	A	C4-C5-C6	11.73	122.86	117.00
11	5	2148	G	N1-C6-O6	11.73	126.94	119.90
11	5	2159	G	N1-C6-O6	11.68	126.91	119.90
11	5	2125	G	N3-C2-N2	11.63	128.04	119.90
8	2	1308	A	C4-C5-C6	11.62	122.81	117.00
10	4	1855	U	C5-C6-N1	11.60	128.50	122.70
10	4	1845	G	O4'-C1'-N9	11.55	117.44	108.20
10	4	1847	A	N1-C6-N6	11.54	125.53	118.60
11	5	2199	A	C4-C5-C6	11.52	122.76	117.00
7	1	106	C	C6-N1-C2	-11.46	115.71	120.30
11	5	2177	C	N3-C4-N4	11.46	126.02	118.00
11	5	2199	A	C5-C6-N6	-11.40	114.58	123.70
7	1	97	C	O4'-C1'-N1	11.40	117.32	108.20
9	3	1538	G	N1-C2-N3	-11.38	117.07	123.90
10	4	1840	G	C4-C5-C6	11.38	125.63	118.80
11	5	2112	G	N1-C6-O6	11.38	126.72	119.90
11	5	2198	A	C5-C6-N6	-11.37	114.60	123.70
11	5	2120	G	N1-C6-O6	11.36	126.72	119.90
7	1	85	G	N1-C6-O6	11.34	126.70	119.90
11	5	2127	G	C5-C6-N1	-11.29	105.85	111.50
7	1	94	A	C5-C6-N1	-11.29	112.06	117.70
11	5	2137	U	C5-C4-O4	-11.28	119.13	125.90
10	4	1842	G	C5-C6-O6	-11.27	121.84	128.60
10	4	1893	C	O4'-C1'-N1	11.22	117.18	108.20
7	1	112	U	O4'-C1'-N1	11.21	117.17	108.20
10	4	1843	C	O4'-C1'-N1	11.21	117.17	108.20
11	5	2113	U	C5-C6-N1	11.21	128.30	122.70
8	2	1323	C	O4'-C1'-N1	11.17	117.14	108.20
1	y	321	TYR	CB-CG-CD1	11.13	127.68	121.00
10	4	1858	A	N9-C4-C5	11.13	110.25	105.80
7	1	88	G	C5-C6-O6	-11.08	121.95	128.60
7	1	100	U	C2-N3-C4	-11.08	120.35	127.00
7	1	63	A	O4'-C1'-N9	11.05	117.04	108.20
11	5	2122	U	C5-C6-N1	11.02	128.21	122.70
7	1	66	C	C2-N3-C4	11.00	125.40	119.90
1	y	34	ARG	NE-CZ-NH2	-11.00	114.80	120.30
11	5	2141	G	N3-C2-N2	11.00	127.60	119.90
7	1	90	U	O4'-C1'-N1	10.96	116.97	108.20
9	3	1543	G	N1-C6-O6	10.92	126.45	119.90
11	5	2193	G	O4'-C1'-N9	10.92	116.94	108.20
7	1	106	C	N3-C4-C5	-10.91	117.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1895	C	C5-C6-N1	10.90	126.45	121.00
7	1	64	A	N1-C6-N6	10.84	125.11	118.60
11	5	2101	A	C4-C5-C6	10.83	122.42	117.00
10	4	1870	C	O4'-C1'-N1	10.82	116.85	108.20
11	5	2093	G	N3-C4-C5	10.82	134.01	128.60
7	1	52	A	C5-C6-N1	-10.80	112.30	117.70
10	4	1866	A	C5-C6-N1	-10.80	112.30	117.70
8	2	1307	A	N1-C6-N6	10.78	125.07	118.60
5	U	86	PHE	CB-CG-CD2	-10.78	113.26	120.80
10	4	1840	G	N9-C4-C5	10.77	109.71	105.40
10	4	1873	G	N1-C2-N3	-10.77	117.44	123.90
11	5	2181	U	O4'-C1'-N1	10.76	116.81	108.20
8	2	1309	G	C5-C6-O6	-10.76	122.14	128.60
11	5	2170	A	C4-C5-C6	10.75	122.38	117.00
11	5	2148	G	P-O3'-C3'	10.75	132.60	119.70
7	1	53	A	N1-C6-N6	10.72	125.03	118.60
11	5	2108	A	N1-C6-N6	10.71	125.03	118.60
11	5	2123	G	O4'-C1'-N9	10.71	116.77	108.20
11	5	2157	G	N1-C6-O6	10.69	126.31	119.90
5	U	6	ARG	NE-CZ-NH1	10.68	125.64	120.30
10	4	1840	G	C5-C6-N1	-10.68	106.16	111.50
11	5	2148	G	C5-C6-O6	-10.67	122.20	128.60
11	5	2135	A	C4-C5-N7	-10.65	105.38	110.70
11	5	2139	U	O4'-C1'-N1	10.65	116.72	108.20
7	1	111	A	C5-C6-N6	-10.65	115.18	123.70
10	4	1858	A	N1-C6-N6	10.65	124.99	118.60
7	1	53	A	O4'-C1'-N9	10.59	116.67	108.20
11	5	2155	U	N3-C4-O4	10.59	126.81	119.40
8	2	1324	G	N7-C8-N9	10.58	118.39	113.10
10	4	1858	A	C4-C5-C6	10.58	122.29	117.00
7	1	86	G	N3-C2-N2	10.56	127.29	119.90
10	4	1871	A	C6-N1-C2	10.53	124.92	118.60
11	5	2133	G	C4-C5-N7	-10.52	106.59	110.80
7	1	58	G	C5-C6-O6	-10.51	122.29	128.60
10	4	1843	C	N3-C4-N4	10.51	125.35	118.00
10	4	1857	G	C2-N3-C4	-10.47	106.66	111.90
4	T	6	ARG	NE-CZ-NH2	-10.47	115.07	120.30
8	2	1332	G	C5-C6-O6	-10.47	122.32	128.60
7	1	101	A	O4'-C1'-N9	10.45	116.56	108.20
10	4	1888	G	C5-C6-N1	-10.45	106.27	111.50
11	5	2119	A	C5-C6-N1	-10.44	112.48	117.70
10	4	1849	G	C5-C6-O6	-10.43	122.34	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1863	G	N1-C6-O6	10.41	126.15	119.90
10	4	1861	G	N1-C6-O6	10.41	126.15	119.90
10	4	1872	A	O4'-C1'-N9	10.41	116.53	108.20
11	5	2163	A	N1-C6-N6	10.39	124.84	118.60
11	5	2184	A	O4'-C1'-N9	10.39	116.52	108.20
7	1	111	A	N1-C6-N6	10.37	124.82	118.60
11	5	2108	A	O4'-C1'-N9	10.37	116.50	108.20
10	4	1843	C	C6-N1-C2	10.36	124.44	120.30
9	3	1534	U	O4'-C1'-N1	10.34	116.47	108.20
11	5	2188	U	O4'-C1'-N1	10.32	116.46	108.20
11	5	2135	A	C5-N7-C8	10.31	109.05	103.90
11	5	2094	A	C4-C5-C6	10.29	122.14	117.00
4	T	95	PHE	CB-CG-CD2	10.29	128.00	120.80
1	y	340	ARG	NE-CZ-NH1	-10.28	115.16	120.30
7	1	88	G	C5-N7-C8	10.23	109.42	104.30
7	1	71	A	N1-C6-N6	10.23	124.74	118.60
9	3	1531	C	C2-N3-C4	10.23	125.01	119.90
8	2	1333	G	C4'-C3'-C2'	-10.22	92.38	102.60
8	2	1318	U	O4'-C1'-N1	10.20	116.36	108.20
7	1	73	A	C5-N7-C8	10.15	108.98	103.90
7	1	63	A	C5-C6-N1	-10.13	112.64	117.70
11	5	2158	A	C5-C6-N1	-10.13	112.64	117.70
8	2	1325	U	O4'-C1'-N1	10.12	116.30	108.20
11	5	2116	G	N1-C6-O6	10.12	125.97	119.90
9	3	1528	A	N1-C6-N6	10.11	124.67	118.60
9	3	1541	C	O4'-C1'-N1	10.10	116.28	108.20
8	2	1319	C	O4'-C1'-N1	10.09	116.27	108.20
11	5	2098	U	N3-C4-C5	-10.08	108.55	114.60
7	1	84	A	N1-C6-N6	10.07	124.64	118.60
9	3	1542	U	O4'-C1'-N1	10.06	116.25	108.20
7	1	68	G	C5-C6-O6	-10.05	122.57	128.60
10	4	1885	A	C5-C6-N1	-10.05	112.68	117.70
11	5	2125	G	C4-C5-N7	-10.05	106.78	110.80
10	4	1845	G	C5-C6-N1	-10.04	106.48	111.50
11	5	2171	A	O4'-C1'-N9	10.03	116.23	108.20
8	2	1325	U	N3-C4-O4	10.00	126.40	119.40
10	4	1875	G	C5-N7-C8	10.00	109.30	104.30
10	4	1847	A	O4'-C1'-N9	10.00	116.20	108.20
7	1	56	A	C5-N7-C8	9.99	108.90	103.90
11	5	2176	A	C4-C5-C6	9.99	122.00	117.00
10	4	1884	G	N1-C2-N3	-9.99	117.91	123.90
11	5	2155	U	O4'-C1'-N1	9.99	116.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	63	A	C4-C5-C6	9.98	121.99	117.00
9	3	1533	C	N3-C4-N4	9.97	124.98	118.00
8	2	1308	A	N1-C6-N6	9.96	124.57	118.60
10	4	1849	G	N1-C6-O6	9.96	125.87	119.90
7	1	61	C	N3-C4-C5	-9.94	117.93	121.90
1	y	211	ARG	NE-CZ-NH2	-9.93	115.33	120.30
11	5	2182	U	N1-C2-N3	9.92	120.85	114.90
8	2	1337	G	N9-C4-C5	-9.91	101.44	105.40
8	2	1309	G	N1-C2-N3	-9.89	117.96	123.90
11	5	2162	G	C6-C5-N7	-9.89	124.46	130.40
7	1	101	A	C4-C5-C6	9.89	121.94	117.00
8	2	1339	G	N1-C2-N3	-9.89	117.97	123.90
10	4	1879	C	O4'-C1'-N1	9.88	116.10	108.20
7	1	73	A	O4'-C1'-N9	9.87	116.09	108.20
11	5	2151	U	O4'-C1'-N1	9.85	116.08	108.20
7	1	94	A	C4-C5-C6	9.85	121.92	117.00
7	1	98	G	C5-C6-O6	-9.83	122.70	128.60
10	4	1888	G	N7-C8-N9	9.82	118.01	113.10
11	5	2190	G	N3-C2-N2	9.82	126.77	119.90
8	2	1335	C	C2-N3-C4	9.80	124.80	119.90
8	2	1324	G	N1-C6-O6	9.80	125.78	119.90
8	2	1329	U	C5-C4-O4	-9.79	120.03	125.90
7	1	54	G	C5-C6-O6	-9.77	122.74	128.60
9	3	1532	A	C5-C6-N1	-9.75	112.82	117.70
11	5	2159	G	N3-C4-C5	9.75	133.47	128.60
7	1	97	C	N3-C4-C5	-9.73	118.01	121.90
8	2	1327	A	C5-C6-N6	-9.70	115.94	123.70
11	5	2161	C	P-O3'-C3'	9.70	131.34	119.70
11	5	2179	C	O4'-C1'-N1	9.69	115.95	108.20
7	1	95	A	C4-C5-C6	9.69	121.84	117.00
11	5	2162	G	C5-C6-O6	-9.69	122.79	128.60
1	y	22	ARG	NE-CZ-NH2	-9.68	115.46	120.30
10	4	1880	U	N3-C4-O4	9.68	126.17	119.40
1	y	429	TYR	CB-CG-CD1	-9.67	115.20	121.00
11	5	2122	U	C4-C5-C6	-9.67	113.90	119.70
10	4	1849	G	O4'-C1'-N9	9.66	115.93	108.20
8	2	1335	C	N3-C4-N4	9.63	124.74	118.00
11	5	2172	U	C5-C4-O4	9.62	131.67	125.90
11	5	2129	C	O4'-C1'-N1	9.62	115.89	108.20
10	4	1845	G	N3-C4-C5	9.62	133.41	128.60
9	3	1539	U	N3-C4-O4	9.61	126.13	119.40
11	5	2159	G	C5-C6-O6	-9.57	122.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	1540	G	N3-C2-N2	9.56	126.59	119.90
11	5	2123	G	C5-C6-O6	-9.54	122.88	128.60
9	3	1528	A	C5-C6-N1	-9.51	112.94	117.70
11	5	2160	C	C5-C4-N4	-9.51	113.55	120.20
11	5	2182	U	O4'-C1'-N1	9.50	115.80	108.20
9	3	1529	G	C5-C6-N1	-9.50	106.75	111.50
11	5	2128	G	N1-C6-O6	9.48	125.59	119.90
1	y	38	PHE	CB-CG-CD1	9.48	127.44	120.80
7	1	82	U	O4'-C1'-N1	9.48	115.79	108.20
11	5	2095	A	C4-C5-C6	9.48	121.74	117.00
10	4	1889	A	C5-C6-N1	-9.48	112.96	117.70
10	4	1843	C	N3-C4-C5	-9.47	118.11	121.90
7	1	69	C	N3-C4-C5	-9.46	118.12	121.90
11	5	2142	A	C5-C6-N1	-9.45	112.97	117.70
10	4	1854	A	C4-C5-N7	-9.43	105.98	110.70
11	5	2177	C	C6-N1-C2	-9.42	116.53	120.30
10	4	1848	A	N1-C6-N6	9.42	124.25	118.60
11	5	2134	A	O4'-C1'-N9	9.42	115.73	108.20
10	4	1896	G	C5-C6-O6	-9.42	122.95	128.60
8	2	1321	A	C5-C6-N1	-9.41	113.00	117.70
1	y	317	TYR	CB-CG-CD1	9.39	126.63	121.00
11	5	2110	G	P-O3'-C3'	9.39	130.96	119.70
10	4	1871	A	C4-C5-C6	9.38	121.69	117.00
8	2	1310	G	C4-C5-C6	9.37	124.42	118.80
10	4	1888	G	N1-C6-O6	9.37	125.52	119.90
11	5	2176	A	O4'-C1'-N9	9.36	115.69	108.20
11	5	2107	G	N1-C6-O6	9.36	125.51	119.90
11	5	2103	C	N3-C4-C5	-9.35	118.16	121.90
8	2	1310	G	C5-C6-N1	-9.34	106.83	111.50
11	5	2162	G	N1-C6-O6	9.32	125.49	119.90
7	1	95	A	C5-C6-N1	-9.26	113.07	117.70
10	4	1842	G	C5-C6-N1	-9.24	106.88	111.50
8	2	1335	C	P-O3'-C3'	9.24	130.78	119.70
11	5	2133	G	N3-C2-N2	9.23	126.36	119.90
11	5	2122	U	O4'-C1'-N1	9.23	115.58	108.20
9	3	1527	G	P-O3'-C3'	9.21	130.76	119.70
8	2	1320	C	N3-C4-C5	-9.21	118.22	121.90
10	4	1892	C	O4'-C1'-N1	9.21	115.56	108.20
7	1	54	G	N9-C4-C5	9.19	109.08	105.40
9	3	1527	G	O4'-C1'-N9	9.19	115.55	108.20
11	5	2100	G	O4'-C1'-N9	9.17	115.53	108.20
8	2	1323	C	N3-C4-N4	9.16	124.41	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1870	C	C5'-C4'-O4'	9.16	120.09	109.10
11	5	2112	G	C8-N9-C4	-9.16	102.74	106.40
11	5	2095	A	C5-C6-N1	-9.15	113.12	117.70
11	5	2171	A	C3'-C2'-C1'	-9.14	94.18	101.50
9	3	1532	A	N1-C6-N6	9.14	124.08	118.60
9	3	1539	U	C5-C4-O4	-9.14	120.42	125.90
11	5	2115	G	N1-C2-N3	-9.13	118.42	123.90
1	y	317	TYR	CB-CG-CD2	-9.13	115.52	121.00
11	5	2118	U	N3-C2-O2	9.11	128.58	122.20
11	5	2155	U	N1-C2-N3	-9.11	109.44	114.90
7	1	59	U	O4'-C1'-N1	9.10	115.48	108.20
10	4	1887	C	N3-C4-N4	9.09	124.36	118.00
11	5	2169	A	C8-N9-C4	-9.09	102.16	105.80
10	4	1897	G	N9-C4-C5	-9.07	101.77	105.40
10	4	1858	A	C5-C6-N1	-9.07	113.17	117.70
11	5	2135	A	O4'-C1'-N9	9.07	115.45	108.20
11	5	2098	U	C5-C6-N1	9.06	127.23	122.70
11	5	2115	G	C4-C5-N7	9.04	114.42	110.80
7	1	88	G	C2-N3-C4	9.03	116.42	111.90
11	5	2137	U	N3-C4-O4	9.03	125.72	119.40
7	1	100	U	N1-C2-N3	9.02	120.31	114.90
8	2	1342	A	C5-C6-N6	-9.00	116.50	123.70
10	4	1882	U	O4'-C1'-N1	9.00	115.40	108.20
10	4	1897	G	C8-N9-C4	8.99	109.99	106.40
10	4	1885	A	C6-N1-C2	8.98	123.99	118.60
11	5	2128	G	O4'-C1'-N9	8.98	115.39	108.20
11	5	2169	A	C4-C5-N7	-8.98	106.21	110.70
11	5	2128	G	C5-C6-O6	-8.97	123.22	128.60
10	4	1876	A	C5-N7-C8	8.97	108.39	103.90
11	5	2101	A	C5-C6-N1	-8.96	113.22	117.70
8	2	1331	G	C8-N9-C4	-8.95	102.82	106.40
9	3	1543	G	N9-C4-C5	-8.94	101.82	105.40
7	1	88	G	C6-C5-N7	8.93	135.76	130.40
1	y	268	LYS	N-CA-C	8.93	135.10	111.00
10	4	1872	A	C8-N9-C4	-8.92	102.23	105.80
11	5	2119	A	N1-C6-N6	8.90	123.94	118.60
11	5	2123	G	N1-C6-O6	8.89	125.24	119.90
11	5	2156	G	N1-C2-N3	-8.88	118.57	123.90
11	5	2158	A	C4-C5-C6	8.88	121.44	117.00
11	5	2161	C	N3-C4-N4	8.88	124.22	118.00
10	4	1845	G	N1-C6-O6	8.85	125.21	119.90
11	5	2115	G	C5-C6-N1	-8.85	107.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1867	G	C4-C5-N7	-8.83	107.27	110.80
11	5	2145	C	N3-C4-N4	8.83	124.18	118.00
11	5	2112	G	C5-N7-C8	8.82	108.71	104.30
3	G	45	SER	N-CA-C	8.81	134.78	111.00
10	4	1847	A	N1-C2-N3	8.80	133.70	129.30
10	4	1870	C	C5'-C4'-C3'	-8.79	101.93	116.00
10	4	1890	A	C6-C5-N7	-8.79	126.15	132.30
11	5	2134	A	N1-C2-N3	8.79	133.70	129.30
1	y	157	TYR	CB-CG-CD1	8.79	126.27	121.00
11	5	2134	A	C2-N3-C4	-8.79	106.20	110.60
11	5	2144	G	O4'-C1'-N9	8.79	115.23	108.20
7	1	113	U	O4'-C1'-N1	8.78	115.22	108.20
10	4	1893	C	N3-C4-C5	-8.77	118.39	121.90
11	5	2198	A	C4-C5-C6	8.77	121.38	117.00
11	5	2147	A	C6-C5-N7	-8.76	126.17	132.30
10	4	1860	G	N1-C6-O6	8.76	125.16	119.90
6	Y	23	ARG	NE-CZ-NH1	8.76	124.68	120.30
11	5	2147	A	N1-C6-N6	8.76	123.85	118.60
11	5	2199	A	N1-C2-N3	8.76	133.68	129.30
11	5	2174	C	C2-N1-C1'	8.75	128.43	118.80
11	5	2111	U	P-O3'-C3'	8.74	130.19	119.70
8	2	1309	G	O4'-C1'-N9	8.74	115.19	108.20
7	1	99	U	O4'-C1'-N1	8.73	115.18	108.20
1	y	181	ARG	NE-CZ-NH1	-8.72	115.94	120.30
8	2	1339	G	C2-N3-C4	8.72	116.26	111.90
7	1	74	A	C2-N3-C4	-8.72	106.24	110.60
11	5	2177	C	C5-C4-N4	-8.72	114.10	120.20
7	1	74	A	C5-C6-N1	-8.71	113.34	117.70
2	E	121	PHE	CB-CG-CD1	8.71	126.90	120.80
1	y	321	TYR	CB-CG-CD2	-8.71	115.78	121.00
7	1	101	A	N1-C6-N6	8.70	123.82	118.60
8	2	1331	G	N3-C2-N2	8.70	125.99	119.90
7	1	91	A	O4'-C1'-N9	8.68	115.15	108.20
2	E	76	ARG	NE-CZ-NH2	-8.68	115.96	120.30
9	3	1531	C	P-O3'-C3'	8.68	130.12	119.70
7	1	81	G	C5-C6-N1	-8.68	107.16	111.50
11	5	2175	C	P-O3'-C3'	8.68	130.12	119.70
7	1	53	A	N9-C4-C5	-8.68	102.33	105.80
11	5	2097	A	O4'-C1'-N9	8.67	115.14	108.20
11	5	2129	C	C4-C5-C6	-8.66	113.07	117.40
11	5	2189	U	N1-C2-O2	-8.66	116.74	122.80
7	1	63	A	N1-C6-N6	8.66	123.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	110	G	N1-C6-O6	8.66	125.10	119.90
10	4	1876	A	N3-C4-C5	-8.66	120.74	126.80
8	2	1341	G	C5-N7-C8	8.65	108.62	104.30
1	y	429	TYR	CB-CG-CD2	8.64	126.18	121.00
11	5	2135	A	C5-C6-N6	-8.64	116.79	123.70
8	2	1321	A	N9-C4-C5	8.63	109.25	105.80
8	2	1335	C	N3-C4-C5	-8.63	118.45	121.90
11	5	2161	C	C4'-C3'-C2'	-8.63	93.97	102.60
9	3	1527	G	C5-C6-O6	-8.62	123.42	128.60
11	5	2162	G	C8-N9-C4	-8.61	102.95	106.40
11	5	2102	G	C2-N3-C4	-8.61	107.60	111.90
8	2	1308	A	C5-C6-N1	-8.60	113.40	117.70
8	2	1324	G	C5-C6-O6	-8.60	123.44	128.60
2	E	126	ARG	NE-CZ-NH1	8.57	124.59	120.30
7	1	76	C	C4-C5-C6	8.56	121.68	117.40
11	5	2143	C	C5-C4-N4	-8.56	114.20	120.20
1	y	256	ARG	NE-CZ-NH1	8.56	124.58	120.30
7	1	92	U	O4'-C1'-N1	8.56	115.05	108.20
10	4	1890	A	C4-C5-C6	8.56	121.28	117.00
2	E	117	ARG	N-CA-CB	8.55	125.99	110.60
7	1	105	C	O4'-C1'-N1	8.54	115.03	108.20
7	1	79	C	N3-C4-C5	-8.53	118.49	121.90
10	4	1846	G	N3-C2-N2	8.53	125.87	119.90
11	5	2114	A	C8-N9-C4	-8.53	102.39	105.80
10	4	1885	A	C4-C5-N7	-8.53	106.44	110.70
11	5	2184	A	N1-C6-N6	8.52	123.71	118.60
7	1	66	C	N3-C4-C5	-8.52	118.49	121.90
11	5	2189	U	N3-C2-O2	8.50	128.15	122.20
10	4	1848	A	C5-C6-N6	-8.49	116.91	123.70
8	2	1338	G	C2-N3-C4	8.48	116.14	111.90
10	4	1870	C	C2-N1-C1'	8.48	128.13	118.80
8	2	1322	A	O4'-C1'-N9	8.47	114.97	108.20
6	Y	52	ARG	NE-CZ-NH2	8.46	124.53	120.30
7	1	94	A	N1-C6-N6	8.44	123.66	118.60
8	2	1329	U	C2-N3-C4	-8.43	121.94	127.00
1	y	416	PHE	CB-CG-CD1	-8.43	114.90	120.80
8	2	1339	G	N1-C6-O6	8.43	124.96	119.90
11	5	2125	G	C4-C5-C6	8.43	123.86	118.80
10	4	1860	G	N3-C2-N2	8.43	125.80	119.90
8	2	1326	U	O4'-C1'-N1	8.41	114.93	108.20
11	5	2120	G	C5-C6-O6	-8.41	123.56	128.60
11	5	2171	A	C4-C5-C6	8.40	121.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	1533	C	C4-C5-C6	8.39	121.60	117.40
11	5	2098	U	O4'-C1'-N1	8.39	114.92	108.20
11	5	2121	G	N3-C2-N2	8.39	125.77	119.90
8	2	1336	A	O4'-C1'-N9	8.39	114.91	108.20
7	1	69	C	O4'-C1'-N1	8.38	114.91	108.20
7	1	58	G	C8-N9-C4	-8.36	103.06	106.40
9	3	1540	G	C5-C6-N1	-8.36	107.32	111.50
8	2	1331	G	N1-C2-N3	-8.36	118.89	123.90
11	5	2116	G	C1'-O4'-C4'	-8.35	103.22	109.90
10	4	1862	G	N3-C2-N2	8.35	125.74	119.90
11	5	2098	U	C5-C4-O4	8.34	130.91	125.90
7	1	114	U	C5-C6-N1	8.34	126.87	122.70
1	y	399	PHE	CB-CG-CD1	8.33	126.63	120.80
8	2	1308	A	O4'-C1'-N9	8.33	114.86	108.20
10	4	1840	G	C6-C5-N7	-8.33	125.40	130.40
7	1	56	A	N1-C6-N6	8.33	123.60	118.60
7	1	58	G	N1-C2-N3	-8.31	118.91	123.90
11	5	2199	A	C6-N1-C2	-8.31	113.61	118.60
11	5	2168	G	C5-C6-N1	-8.30	107.35	111.50
1	y	248	TYR	CB-CG-CD1	-8.29	116.02	121.00
1	y	113	ARG	NE-CZ-NH2	-8.29	116.15	120.30
11	5	2137	U	N3-C2-O2	8.29	128.00	122.20
8	2	1321	A	N3-C4-C5	-8.29	121.00	126.80
10	4	1842	G	N3-C2-N2	8.29	125.70	119.90
10	4	1876	A	O4'-C1'-N9	8.27	114.82	108.20
11	5	2159	G	C6-N1-C2	8.27	130.06	125.10
6	Y	47	ARG	NE-CZ-NH1	-8.27	116.17	120.30
10	4	1891	G	C2-N3-C4	-8.27	107.77	111.90
7	1	86	G	N1-C2-N3	-8.25	118.95	123.90
11	5	2115	G	C6-C5-N7	-8.25	125.45	130.40
11	5	2169	A	N9-C4-C5	8.24	109.10	105.80
8	2	1307	A	C4-C5-C6	8.23	121.12	117.00
10	4	1866	A	C8-N9-C4	-8.23	102.51	105.80
7	1	81	G	N3-C4-N9	-8.22	121.07	126.00
11	5	2101	A	C5-C6-N6	-8.22	117.12	123.70
10	4	1848	A	N7-C8-N9	8.22	117.91	113.80
11	5	2190	G	C5-C6-O6	-8.21	123.67	128.60
11	5	2121	G	C5-C6-O6	-8.21	123.68	128.60
7	1	99	U	C5-C6-N1	8.20	126.80	122.70
8	2	1316	U	O4'-C1'-N1	8.18	114.74	108.20
10	4	1858	A	C8-N9-C4	-8.17	102.53	105.80
11	5	2157	G	C5-C6-O6	-8.17	123.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2122	U	C5-C4-O4	-8.16	121.00	125.90
10	4	1870	C	C1'-O4'-C4'	8.16	116.42	109.90
11	5	2182	U	N1-C2-O2	-8.16	117.09	122.80
11	5	2174	C	C2-N3-C4	8.15	123.98	119.90
10	4	1871	A	C8-N9-C4	-8.15	102.54	105.80
10	4	1850	G	C6-N1-C2	8.14	129.98	125.10
10	4	1897	G	C5-C6-O6	-8.14	123.72	128.60
1	y	269	VAL	N-CA-CB	8.13	129.40	111.50
11	5	2127	G	C6-N1-C2	8.13	129.98	125.10
11	5	2154	A	N1-C6-N6	8.13	123.48	118.60
11	5	2166	U	N3-C2-O2	8.13	127.89	122.20
1	y	67	PHE	CB-CG-CD1	-8.13	115.11	120.80
11	5	2113	U	C6-N1-C2	-8.12	116.13	121.00
10	4	1850	G	N3-C4-C5	8.11	132.65	128.60
7	1	95	A	N1-C2-N3	-8.10	125.25	129.30
10	4	1844	C	C5-C4-N4	8.09	125.86	120.20
10	4	1847	A	C5-N7-C8	8.09	107.95	103.90
10	4	1848	A	C8-N9-C4	-8.09	102.56	105.80
7	1	83	A	N7-C8-N9	-8.09	109.76	113.80
8	2	1334	G	N7-C8-N9	-8.09	109.06	113.10
11	5	2092	U	N3-C4-O4	8.09	125.06	119.40
7	1	83	A	C4-C5-C6	8.07	121.03	117.00
8	2	1311	G	N1-C6-O6	8.07	124.74	119.90
10	4	1870	C	C2-N3-C4	8.07	123.94	119.90
10	4	1879	C	C6-N1-C2	-8.07	117.07	120.30
9	3	1543	G	C6-C5-N7	-8.05	125.57	130.40
10	4	1873	G	C2-N3-C4	8.05	115.92	111.90
11	5	2154	A	C6-N1-C2	-8.05	113.77	118.60
10	4	1885	A	O4'-C1'-N9	8.05	114.64	108.20
11	5	2147	A	C4-C5-C6	8.03	121.02	117.00
7	1	52	A	C4-C5-C6	8.03	121.01	117.00
7	1	104	A	N1-C6-N6	8.02	123.41	118.60
9	3	1527	G	N3-C2-N2	8.02	125.51	119.90
11	5	2114	A	C5-N7-C8	-8.02	99.89	103.90
11	5	2175	C	O4'-C1'-N1	8.00	114.60	108.20
7	1	57	C	C2-N3-C4	8.00	123.90	119.90
7	1	72	U	N3-C4-O4	8.00	125.00	119.40
11	5	2141	G	N1-C2-N2	-8.00	109.00	116.20
7	1	106	C	C5-C6-N1	7.99	125.00	121.00
8	2	1330	C	O4'-C1'-N1	7.99	114.59	108.20
1	y	400	TYR	CB-CG-CD2	7.99	125.79	121.00
11	5	2197	U	C6-N1-C2	7.99	125.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1840	G	N1-C6-O6	7.98	124.69	119.90
10	4	1867	G	C2-N3-C4	7.97	115.89	111.90
11	5	2121	G	C4-C5-C6	7.97	123.58	118.80
11	5	2129	C	C5-C6-N1	7.97	124.99	121.00
10	4	1843	C	C6-N1-C1'	-7.97	111.24	120.80
11	5	2103	C	C4-C5-C6	7.97	121.39	117.40
7	1	62	U	P-O3'-C3'	7.95	129.24	119.70
7	1	81	G	O4'-C1'-N9	7.95	114.56	108.20
8	2	1338	G	C8-N9-C4	-7.95	103.22	106.40
7	1	55	G	N1-C6-O6	7.94	124.67	119.90
10	4	1871	A	N7-C8-N9	7.94	117.77	113.80
7	1	95	A	N3-C4-C5	-7.94	121.24	126.80
10	4	1880	U	O4'-C1'-N1	7.94	114.55	108.20
11	5	2114	A	N1-C6-N6	7.94	123.36	118.60
10	4	1878	G	N1-C6-O6	7.93	124.66	119.90
11	5	2135	A	C5-C6-N1	-7.93	113.74	117.70
7	1	55	G	O4'-C1'-N9	7.92	114.54	108.20
11	5	2130	U	N1-C2-N3	-7.92	110.15	114.90
9	3	1541	C	C5-C6-N1	-7.92	117.04	121.00
7	1	110	G	C5-C6-O6	-7.91	123.85	128.60
10	4	1895	C	N3-C4-N4	7.91	123.53	118.00
10	4	1874	C	N1-C2-O2	-7.90	114.16	118.90
7	1	80	G	C5-C6-N1	-7.90	107.55	111.50
10	4	1862	G	O4'-C1'-N9	7.89	114.51	108.20
8	2	1333	G	C3'-C2'-C1'	7.89	107.81	101.50
7	1	89	A	C5-C6-N1	-7.87	113.76	117.70
7	1	73	A	N7-C8-N9	-7.87	109.87	113.80
7	1	57	C	C5-C6-N1	7.86	124.93	121.00
3	G	50	ASN	N-CA-CB	-7.86	96.46	110.60
10	4	1866	A	C4-C5-C6	7.84	120.92	117.00
8	2	1330	C	C5-C6-N1	7.83	124.92	121.00
9	3	1530	G	C8-N9-C4	-7.81	103.28	106.40
9	3	1530	G	N1-C2-N3	-7.81	119.22	123.90
11	5	2164	C	C2-N3-C4	7.81	123.80	119.90
7	1	84	A	C5-C6-N6	-7.79	117.47	123.70
10	4	1842	G	O4'-C1'-N9	7.79	114.43	108.20
8	2	1342	A	C4-C5-C6	7.76	120.88	117.00
10	4	1860	G	C2-N3-C4	7.76	115.78	111.90
10	4	1871	A	P-O3'-C3'	7.76	129.01	119.70
10	4	1891	G	O4'-C1'-N9	7.74	114.39	108.20
11	5	2120	G	N3-C2-N2	7.73	125.31	119.90
10	4	1884	G	C4-C5-N7	-7.72	107.71	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1334	G	C5-C6-N1	-7.72	107.64	111.50
11	5	2182	U	C6-N1-C2	-7.72	116.37	121.00
8	2	1333	G	C5-N7-C8	-7.72	100.44	104.30
11	5	2102	G	C6-N1-C2	-7.71	120.47	125.10
11	5	2113	U	N3-C4-O4	7.71	124.80	119.40
1	y	157	TYR	CB-CG-CD2	-7.70	116.38	121.00
8	2	1334	G	N1-C2-N3	-7.70	119.28	123.90
7	1	76	C	O4'-C1'-N1	7.70	114.36	108.20
11	5	2133	G	C5-C6-O6	-7.70	123.98	128.60
11	5	2152	G	O4'-C1'-N9	7.69	114.35	108.20
9	3	1539	U	N3-C2-O2	7.69	127.58	122.20
11	5	2101	A	C6-C5-N7	-7.68	126.92	132.30
11	5	2153	C	C5'-C4'-C3'	-7.68	103.71	116.00
11	5	2184	A	C2-N3-C4	-7.67	106.77	110.60
7	1	66	C	O4'-C1'-N1	7.66	114.33	108.20
11	5	2170	A	O4'-C1'-N9	7.66	114.33	108.20
7	1	53	A	C5-C6-N6	-7.66	117.57	123.70
7	1	98	G	O4'-C1'-N9	7.66	114.32	108.20
9	3	1538	G	C6-C5-N7	-7.65	125.81	130.40
11	5	2126	A	N1-C6-N6	7.65	123.19	118.60
11	5	2106	U	C2-N3-C4	-7.65	122.41	127.00
11	5	2154	A	N7-C8-N9	-7.65	109.98	113.80
11	5	2147	A	C5-C6-N1	-7.64	113.88	117.70
11	5	2109	U	N3-C4-O4	7.63	124.74	119.40
11	5	2118	U	P-O3'-C3'	-7.63	110.54	119.70
7	1	70	G	N1-C2-N3	-7.63	119.32	123.90
10	4	1844	C	N3-C4-C5	-7.63	118.85	121.90
11	5	2150	C	C5-C4-N4	-7.63	114.86	120.20
7	1	74	A	C5-C6-N6	-7.61	117.61	123.70
11	5	2093	G	C4-C5-N7	7.60	113.84	110.80
11	5	2116	G	C4'-C3'-C2'	7.60	110.20	102.60
8	2	1322	A	C5-C6-N6	-7.60	117.62	123.70
7	1	102	U	P-O3'-C3'	7.59	128.80	119.70
11	5	2163	A	C5-C6-N6	-7.58	117.63	123.70
11	5	2133	G	N1-C6-O6	7.58	124.45	119.90
11	5	2177	C	C5'-C4'-O4'	7.58	118.20	109.10
7	1	89	A	C4-C5-C6	7.58	120.79	117.00
11	5	2113	U	C5-C4-O4	-7.58	121.35	125.90
11	5	2114	A	C4-C5-N7	7.58	114.49	110.70
11	5	2109	U	O4'-C1'-N1	7.57	114.26	108.20
11	5	2167	U	C5-C6-N1	7.57	126.49	122.70
11	5	2157	G	O4'-C1'-N9	7.57	114.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1863	G	N9-C4-C5	7.57	108.43	105.40
10	4	1885	A	C5-N7-C8	7.56	107.68	103.90
8	2	1338	G	N1-C2-N3	-7.55	119.37	123.90
1	y	217	PHE	CB-CG-CD2	-7.55	115.52	120.80
11	5	2158	A	N9-C4-C5	7.55	108.82	105.80
11	5	2105	U	N3-C4-C5	-7.55	110.07	114.60
11	5	2127	G	C4-C5-C6	7.54	123.33	118.80
7	1	69	C	C2-N3-C4	7.54	123.67	119.90
10	4	1875	G	N7-C8-N9	-7.54	109.33	113.10
11	5	2146	C	N3-C4-N4	7.54	123.28	118.00
11	5	2111	U	O4'-C1'-N1	7.53	114.22	108.20
11	5	2101	A	O4'-C1'-N9	7.53	114.22	108.20
11	5	2136	G	C6-C5-N7	-7.53	125.88	130.40
10	4	1853	A	O4'-C1'-N9	7.52	114.22	108.20
11	5	2121	G	C5-C6-N1	-7.52	107.74	111.50
4	T	3	ARG	NE-CZ-NH1	7.51	124.06	120.30
10	4	1857	G	N3-C4-C5	7.51	132.36	128.60
4	T	25	GLU	OE1-CD-OE2	7.51	132.31	123.30
11	5	2095	A	C5-N7-C8	7.51	107.65	103.90
1	y	332	TYR	CB-CG-CD1	-7.50	116.50	121.00
7	1	71	A	O4'-C1'-N9	7.50	114.20	108.20
9	3	1530	G	C6-C5-N7	-7.48	125.91	130.40
9	3	1529	G	C5-N7-C8	7.48	108.04	104.30
7	1	96	C	N3-C4-C5	-7.48	118.91	121.90
11	5	2115	G	O4'-C1'-N9	7.48	114.18	108.20
11	5	2194	U	C5-C4-O4	-7.47	121.42	125.90
10	4	1890	A	C5-C6-N1	-7.47	113.96	117.70
2	E	117	ARG	NE-CZ-NH1	7.47	124.03	120.30
7	1	63	A	N7-C8-N9	7.47	117.53	113.80
10	4	1872	A	N7-C8-N9	7.46	117.53	113.80
11	5	2114	A	C6-C5-N7	-7.46	127.08	132.30
10	4	1845	G	N3-C4-N9	-7.46	121.52	126.00
10	4	1875	G	C4-C5-N7	-7.46	107.82	110.80
11	5	2164	C	C6-N1-C1'	-7.46	111.85	120.80
10	4	1845	G	C2-N3-C4	-7.46	108.17	111.90
11	5	2093	G	C5-C6-O6	-7.46	124.13	128.60
7	1	53	A	C8-N9-C4	7.45	108.78	105.80
11	5	2160	C	O4'-C1'-N1	7.44	114.15	108.20
11	5	2112	G	C5-C6-N1	-7.43	107.78	111.50
7	1	91	A	N9-C4-C5	-7.42	102.83	105.80
8	2	1329	U	N3-C4-C5	7.42	119.05	114.60
9	3	1538	G	N3-C4-C5	-7.42	124.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	93	G	C5-C6-O6	-7.42	124.15	128.60
8	2	1315	C	O4'-C1'-N1	7.42	114.14	108.20
11	5	2147	A	N9-C4-C5	-7.42	102.83	105.80
11	5	2160	C	N3-C4-N4	7.42	123.19	118.00
10	4	1868	C	C6-N1-C2	7.41	123.27	120.30
4	T	29	THR	CA-CB-CG2	-7.41	102.03	112.40
11	5	2116	G	C6-C5-N7	-7.41	125.96	130.40
7	1	85	G	C5-C6-O6	-7.40	124.16	128.60
10	4	1855	U	O4'-C1'-N1	7.40	114.12	108.20
10	4	1854	A	C5-C6-N1	-7.40	114.00	117.70
8	2	1342	A	C5'-C4'-O4'	7.39	117.97	109.10
8	2	1334	G	C5-N7-C8	7.39	107.99	104.30
9	3	1533	C	C5-C4-N4	-7.38	115.03	120.20
11	5	2191	A	C5-N7-C8	7.38	107.59	103.90
10	4	1895	C	C6-N1-C2	-7.37	117.35	120.30
9	3	1538	G	C5-N7-C8	7.37	107.99	104.30
9	3	1531	C	N3-C4-N4	7.37	123.16	118.00
11	5	2127	G	P-O3'-C3'	-7.37	110.86	119.70
8	2	1308	A	C2-N3-C4	-7.37	106.92	110.60
7	1	68	G	C4'-C3'-C2'	-7.36	95.24	102.60
11	5	2143	C	O4'-C1'-N1	7.36	114.09	108.20
7	1	106	C	N3-C4-N4	7.36	123.15	118.00
10	4	1869	G	C6-C5-N7	-7.36	125.99	130.40
10	4	1840	G	N3-C4-C5	-7.36	124.92	128.60
11	5	2169	A	C4-C5-C6	7.35	120.67	117.00
7	1	77	G	O4'-C1'-N9	7.34	114.07	108.20
9	3	1532	A	C4-C5-C6	7.34	120.67	117.00
10	4	1876	A	C5-C6-N1	-7.34	114.03	117.70
11	5	2099	U	C4'-C3'-C2'	-7.34	95.26	102.60
10	4	1875	G	C5-C6-O6	-7.34	124.20	128.60
9	3	1533	C	N1-C2-O2	7.33	123.30	118.90
10	4	1850	G	N1-C2-N3	-7.33	119.50	123.90
10	4	1886	U	N3-C4-O4	7.33	124.53	119.40
1	y	255	ARG	N-CA-CB	7.33	123.79	110.60
8	2	1342	A	C3'-C2'-C1'	-7.32	95.64	101.50
7	1	82	U	C5-C6-N1	7.32	126.36	122.70
7	1	101	A	C6-C5-N7	-7.32	127.18	132.30
8	2	1332	G	N9-C4-C5	-7.32	102.47	105.40
9	3	1543	G	C2-N3-C4	-7.31	108.25	111.90
11	5	2116	G	C4-C5-C6	7.31	123.19	118.80
10	4	1868	C	C5-C4-N4	-7.31	115.08	120.20
11	5	2105	U	N3-C4-O4	7.30	124.51	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2166	U	N1-C2-O2	-7.29	117.69	122.80
11	5	2107	G	C4-C5-N7	-7.29	107.88	110.80
9	3	1538	G	N7-C8-N9	-7.28	109.46	113.10
10	4	1863	G	C4-C5-C6	7.27	123.16	118.80
7	1	84	A	C5'-C4'-O4'	7.27	117.83	109.10
9	3	1529	G	O4'-C1'-N9	7.27	114.02	108.20
8	2	1312	U	C1'-O4'-C4'	-7.25	104.10	109.90
7	1	99	U	C2-N1-C1'	7.24	126.39	117.70
9	3	1540	G	N1-C2-N3	-7.24	119.56	123.90
11	5	2139	U	C5-C4-O4	-7.24	121.56	125.90
9	3	1528	A	C4-C5-C6	7.24	120.62	117.00
11	5	2160	C	C4-C5-C6	-7.23	113.78	117.40
11	5	2180	U	O4'-C1'-N1	7.23	113.98	108.20
8	2	1340	U	C5-C4-O4	-7.23	121.56	125.90
9	3	1540	G	O4'-C1'-N9	7.22	113.98	108.20
9	3	1537	G	P-O3'-C3'	7.22	128.36	119.70
11	5	2093	G	O4'-C1'-N9	7.22	113.97	108.20
11	5	2118	U	C2-N1-C1'	7.22	126.36	117.70
1	y	251	ARG	NE-CZ-NH2	-7.21	116.70	120.30
10	4	1888	G	C5-N7-C8	-7.20	100.70	104.30
9	3	1535	A	O4'-C1'-N9	7.20	113.96	108.20
11	5	2096	C	C4-C5-C6	7.19	121.00	117.40
7	1	103	A	O4'-C1'-N9	7.18	113.95	108.20
11	5	2133	G	N9-C4-C5	7.18	108.27	105.40
7	1	80	G	C6-N1-C2	7.18	129.41	125.10
8	2	1310	G	N1-C2-N3	-7.18	119.59	123.90
9	3	1537	G	N9-C4-C5	-7.17	102.53	105.40
11	5	2143	C	N3-C4-N4	7.17	123.02	118.00
1	y	192	PHE	CB-CG-CD2	-7.16	115.79	120.80
10	4	1839	G	N1-C2-N3	-7.16	119.60	123.90
11	5	2115	G	C6-N1-C2	7.16	129.39	125.10
8	2	1336	A	P-O5'-C5'	7.16	132.35	120.90
11	5	2169	A	C5-N7-C8	7.15	107.48	103.90
10	4	1870	C	C6-N1-C1'	-7.15	112.22	120.80
11	5	2159	G	N7-C8-N9	7.15	116.67	113.10
1	y	166	THR	CA-CB-CG2	7.14	122.40	112.40
8	2	1324	G	N3-C4-N9	7.14	130.28	126.00
3	G	45	SER	N-CA-CB	-7.13	99.80	110.50
11	5	2147	A	C3'-C2'-C1'	-7.13	95.80	101.50
9	3	1539	U	O4'-C1'-N1	7.13	113.90	108.20
10	4	1893	C	C4-C5-C6	7.13	120.97	117.40
10	4	1870	C	OP1-P-OP2	-7.12	108.92	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2154	A	C5-N7-C8	7.12	107.46	103.90
7	1	74	A	C6-C5-N7	-7.12	127.32	132.30
11	5	2142	A	C4-C5-C6	7.11	120.55	117.00
9	3	1534	U	N3-C2-O2	7.10	127.17	122.20
10	4	1842	G	N7-C8-N9	-7.10	109.55	113.10
11	5	2166	U	C4'-C3'-C2'	-7.10	95.50	102.60
6	Y	23	ARG	NE-CZ-NH2	-7.10	116.75	120.30
7	1	81	G	N1-C6-O6	7.09	124.16	119.90
11	5	2115	G	N3-C2-N2	7.09	124.86	119.90
10	4	1877	A	C6-N1-C2	7.08	122.85	118.60
11	5	2116	G	O4'-C1'-N9	7.08	113.87	108.20
11	5	2177	C	C4-C5-C6	7.08	120.94	117.40
11	5	2150	C	P-O3'-C3'	7.07	128.19	119.70
11	5	2181	U	C2-N3-C4	7.07	131.24	127.00
8	2	1311	G	N1-C2-N3	-7.07	119.66	123.90
8	2	1311	G	O4'-C1'-N9	7.07	113.85	108.20
11	5	2117	A	C8-N9-C4	-7.06	102.97	105.80
8	2	1308	A	N1-C2-N3	7.06	132.83	129.30
10	4	1866	A	C4-C5-N7	-7.05	107.17	110.70
11	5	2125	G	N3-C4-C5	-7.04	125.08	128.60
11	5	2166	U	N3-C4-O4	7.04	124.33	119.40
11	5	2096	C	O4'-C1'-N1	7.04	113.83	108.20
7	1	81	G	N3-C4-C5	7.03	132.12	128.60
11	5	2192	U	N3-C4-O4	7.02	124.32	119.40
1	y	383	PHE	CB-CG-CD2	7.01	125.71	120.80
8	2	1312	U	O4'-C1'-N1	7.01	113.81	108.20
11	5	2125	G	N9-C4-C5	7.01	108.20	105.40
11	5	2178	C	C2-N1-C1'	7.00	126.50	118.80
8	2	1339	G	N3-C2-N2	7.00	124.80	119.90
11	5	2170	A	N3-C4-N9	7.00	133.00	127.40
10	4	1895	C	N3-C4-C5	-6.99	119.10	121.90
11	5	2140	G	N3-C2-N2	6.99	124.79	119.90
10	4	1880	U	N3-C4-C5	-6.99	110.41	114.60
10	4	1888	G	O4'-C1'-N9	6.98	113.78	108.20
8	2	1309	G	N3-C2-N2	6.98	124.79	119.90
10	4	1838	C	N3-C4-C5	-6.97	119.11	121.90
8	2	1323	C	C5-C4-N4	-6.95	115.33	120.20
11	5	2164	C	C2-N1-C1'	6.95	126.45	118.80
7	1	86	G	O4'-C1'-N9	6.95	113.76	108.20
7	1	108	G	N1-C6-O6	6.95	124.07	119.90
9	3	1538	G	C4-C5-C6	6.94	122.97	118.80
11	5	2150	C	N1-C1'-C2'	-6.94	104.36	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2138	G	N7-C8-N9	-6.94	109.63	113.10
8	2	1315	C	N1-C2-O2	6.93	123.06	118.90
10	4	1896	G	N9-C4-C5	-6.93	102.63	105.40
11	5	2097	A	N3-C4-C5	-6.93	121.95	126.80
8	2	1307	A	N3-C4-C5	-6.92	121.95	126.80
10	4	1846	G	N7-C8-N9	6.91	116.56	113.10
9	3	1537	G	N3-C2-N2	6.90	124.73	119.90
11	5	2157	G	C4-C5-N7	-6.90	108.04	110.80
11	5	2112	G	O4'-C1'-N9	6.90	113.72	108.20
7	1	83	A	C5-C6-N6	-6.89	118.19	123.70
11	5	2095	A	C4-C5-N7	-6.89	107.25	110.70
11	5	2180	U	N1-C2-O2	6.89	127.62	122.80
11	5	2154	A	C4-C5-C6	6.89	120.45	117.00
10	4	1876	A	C6-C5-N7	-6.89	127.48	132.30
11	5	2120	G	P-O5'-C5'	-6.89	109.88	120.90
4	T	1	MET	CG-SD-CE	-6.89	89.18	100.20
7	1	93	G	N9-C4-C5	6.89	108.15	105.40
10	4	1859	U	N3-C4-C5	-6.89	110.47	114.60
11	5	2095	A	N9-C4-C5	6.88	108.55	105.80
8	2	1308	A	P-O3'-C3'	6.88	127.95	119.70
11	5	2127	G	C6-C5-N7	-6.88	126.27	130.40
10	4	1890	A	C5-C6-N6	-6.87	118.20	123.70
7	1	95	A	C6-N1-C2	6.87	122.72	118.60
7	1	68	G	C2-N3-C4	-6.85	108.47	111.90
9	3	1537	G	N3-C4-N9	6.85	130.11	126.00
7	1	80	G	N1-C6-O6	6.85	124.01	119.90
7	1	77	G	N7-C8-N9	6.84	116.52	113.10
8	2	1311	G	O3'-P-O5'	-6.84	91.01	104.00
11	5	2125	G	C1'-O4'-C4'	-6.84	104.43	109.90
7	1	55	G	N3-C2-N2	6.83	124.68	119.90
7	1	104	A	C5-C6-N1	-6.83	114.29	117.70
10	4	1868	C	N3-C4-N4	6.83	122.78	118.00
11	5	2195	U	O4'-C1'-N1	6.82	113.66	108.20
8	2	1337	G	N3-C4-N9	6.82	130.09	126.00
10	4	1856	U	C5-C4-O4	6.80	129.98	125.90
1	y	270	ASN	N-CA-CB	6.79	122.83	110.60
7	1	85	G	C6-C5-N7	-6.79	126.32	130.40
11	5	2170	A	N3-C4-C5	-6.79	122.05	126.80
1	y	282	SER	N-CA-CB	6.79	120.68	110.50
11	5	2138	G	C5-N7-C8	6.79	107.69	104.30
11	5	2154	A	O4'-C1'-N9	6.79	113.63	108.20
7	1	99	U	N3-C4-O4	6.78	124.15	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	72	U	C1'-O4'-C4'	-6.78	104.47	109.90
11	5	2183	A	C5-C6-N6	-6.78	118.28	123.70
9	3	1526	C	N3-C4-C5	-6.78	119.19	121.90
8	2	1322	A	C8-N9-C4	-6.78	103.09	105.80
11	5	2118	U	C6-N1-C1'	-6.77	111.72	121.20
10	4	1839	G	C6-N1-C2	6.76	129.16	125.10
10	4	1863	G	N1-C2-N3	-6.76	119.84	123.90
11	5	2125	G	C2-N3-C4	6.76	115.28	111.90
8	2	1339	G	C6-N1-C2	6.75	129.15	125.10
9	3	1528	A	O4'-C1'-N9	6.75	113.60	108.20
10	4	1876	A	N1-C6-N6	6.75	122.65	118.60
11	5	2154	A	N1-C2-N3	6.75	132.67	129.30
11	5	2152	G	C2-N3-C4	-6.75	108.53	111.90
7	1	98	G	N1-C6-O6	6.74	123.94	119.90
7	1	99	U	N3-C4-C5	-6.74	110.56	114.60
10	4	1869	G	N3-C2-N2	6.72	124.61	119.90
7	1	85	G	C4-C5-C6	6.72	122.83	118.80
7	1	103	A	C5-C6-N1	-6.72	114.34	117.70
2	E	126	ARG	NE-CZ-NH2	-6.71	116.94	120.30
11	5	2174	C	C5-C6-N1	6.71	124.36	121.00
11	5	2136	G	C4-C5-C6	6.71	122.83	118.80
7	1	89	A	O4'-C1'-N9	6.70	113.56	108.20
10	4	1886	U	O4'-C1'-N1	6.70	113.56	108.20
11	5	2107	G	C5-C6-O6	-6.70	124.58	128.60
7	1	54	G	C8-N9-C4	-6.70	103.72	106.40
11	5	2159	G	C4-C5-N7	6.69	113.48	110.80
10	4	1879	C	N1-C2-O2	-6.69	114.89	118.90
7	1	57	C	C1'-O4'-C4'	6.69	115.25	109.90
11	5	2095	A	P-O5'-C5'	-6.69	110.20	120.90
8	2	1325	U	N3-C4-C5	-6.68	110.59	114.60
11	5	2106	U	O4'-C1'-N1	6.68	113.55	108.20
7	1	80	G	C5-N7-C8	-6.68	100.96	104.30
11	5	2168	G	C5-C6-O6	-6.68	124.59	128.60
10	4	1894	C	O4'-C1'-N1	6.68	113.54	108.20
11	5	2175	C	C5-C4-N4	-6.68	115.53	120.20
10	4	1895	C	O4'-C1'-N1	6.67	113.54	108.20
11	5	2150	C	N3-C4-N4	6.67	122.67	118.00
7	1	86	G	P-O3'-C3'	6.67	127.70	119.70
7	1	74	A	C4-C5-C6	6.66	120.33	117.00
8	2	1331	G	O4'-C1'-N9	6.66	113.53	108.20
10	4	1861	G	N7-C8-N9	-6.66	109.77	113.10
11	5	2097	A	C4'-C3'-C2'	-6.64	95.96	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2102	G	N1-C2-N3	6.64	127.88	123.90
10	4	1878	G	O4'-C1'-N9	6.63	113.50	108.20
10	4	1845	G	C6-N1-C2	6.62	129.07	125.10
11	5	2121	G	C6-N1-C2	6.62	129.07	125.10
8	2	1339	G	C5-C6-O6	-6.62	124.63	128.60
11	5	2094	A	C6-C5-N7	-6.62	127.67	132.30
11	5	2194	U	N3-C4-O4	6.61	124.03	119.40
9	3	1529	G	C4-C5-N7	-6.60	108.16	110.80
3	G	45	SER	CB-CA-C	6.60	122.63	110.10
9	3	1540	G	C8-N9-C4	-6.59	103.76	106.40
8	2	1333	G	C5-C6-N1	6.59	114.80	111.50
8	2	1330	C	C6-N1-C2	-6.59	117.66	120.30
7	1	80	G	C6-C5-N7	-6.58	126.45	130.40
11	5	2141	G	N9-C4-C5	-6.58	102.77	105.40
11	5	2099	U	O4'-C1'-N1	6.57	113.45	108.20
11	5	2189	U	C5-C4-O4	-6.56	121.96	125.90
1	y	233	PHE	CB-CG-CD1	-6.56	116.21	120.80
11	5	2113	U	C4-C5-C6	-6.55	115.77	119.70
1	y	291	ALA	N-CA-CB	6.55	119.26	110.10
6	Y	48	ARG	NH1-CZ-NH2	-6.55	112.20	119.40
11	5	2176	A	C5'-C4'-C3'	-6.54	105.54	116.00
5	U	80	ASP	CB-CG-OD2	-6.54	112.42	118.30
9	3	1537	G	C8-N9-C1'	-6.53	118.51	127.00
8	2	1332	G	N3-C4-N9	6.53	129.92	126.00
11	5	2198	A	C8-N9-C4	-6.53	103.19	105.80
11	5	2152	G	C6-C5-N7	-6.53	126.48	130.40
7	1	71	A	P-O3'-C3'	6.53	127.53	119.70
11	5	2179	C	N3-C4-C5	6.53	124.51	121.90
1	y	380	TYR	CG-CD2-CE2	6.52	126.52	121.30
11	5	2153	C	N1-C2-O2	-6.52	114.99	118.90
11	5	2172	U	O4'-C1'-N1	6.51	113.41	108.20
1	y	95	LEU	N-CA-CB	6.51	123.42	110.40
7	1	109	C	C2-N3-C4	6.51	123.16	119.90
7	1	72	U	C5-C4-O4	-6.51	122.00	125.90
11	5	2169	A	O4'-C1'-N9	6.50	113.40	108.20
7	1	112	U	C1'-O4'-C4'	-6.50	104.70	109.90
10	4	1877	A	N9-C4-C5	6.50	108.40	105.80
10	4	1889	A	N1-C2-N3	6.50	132.55	129.30
11	5	2104	C	C5'-C4'-O4'	6.50	116.90	109.10
1	y	344	ASP	CB-CG-OD2	-6.49	112.46	118.30
11	5	2093	G	N1-C6-O6	6.48	123.79	119.90
11	5	2191	A	N1-C6-N6	6.48	122.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1887	C	C5-C4-N4	-6.48	115.67	120.20
9	3	1527	G	C5-C6-N1	-6.47	108.26	111.50
11	5	2111	U	P-O5'-C5'	6.47	131.26	120.90
1	y	429	TYR	CG-CD1-CE1	6.47	126.47	121.30
9	3	1534	U	N1-C2-O2	-6.47	118.27	122.80
10	4	1884	G	C2-N3-C4	6.47	115.13	111.90
11	5	2184	A	C4-C5-N7	-6.46	107.47	110.70
11	5	2193	G	N7-C8-N9	6.46	116.33	113.10
11	5	2181	U	C1'-O4'-C4'	-6.46	104.74	109.90
9	3	1535	A	C5-C6-N1	-6.45	114.47	117.70
8	2	1307	A	C5-C6-N1	-6.45	114.47	117.70
7	1	63	A	C5'-C4'-C3'	-6.45	105.68	116.00
10	4	1843	C	C5-C4-N4	-6.45	115.69	120.20
10	4	1863	G	C5-C6-O6	-6.45	124.73	128.60
9	3	1537	G	C6-N1-C2	6.43	128.96	125.10
10	4	1891	G	C5-C6-N1	-6.43	108.29	111.50
7	1	73	A	P-O3'-C3'	-6.43	111.99	119.70
5	U	6	ARG	NE-CZ-NH2	-6.42	117.09	120.30
7	1	54	G	N1-C2-N3	-6.42	120.05	123.90
1	y	288	ALA	CB-CA-C	-6.42	100.47	110.10
11	5	2114	A	O4'-C1'-N9	6.42	113.34	108.20
7	1	104	A	C3'-C2'-C1'	-6.42	96.36	101.50
10	4	1894	C	C6-N1-C2	6.41	122.86	120.30
7	1	57	C	N1-C2-N3	-6.40	114.72	119.20
11	5	2180	U	N1-C2-N3	-6.39	111.06	114.90
1	y	429	TYR	CG-CD2-CE2	-6.39	116.19	121.30
7	1	103	A	C5-C6-N6	-6.39	118.59	123.70
11	5	2121	G	C6-C5-N7	-6.39	126.57	130.40
11	5	2141	G	C5-C6-O6	-6.39	124.77	128.60
11	5	2140	G	C3'-C2'-C1'	6.38	106.61	101.50
10	4	1854	A	N3-C4-C5	-6.38	122.33	126.80
10	4	1877	A	C5-C6-N6	-6.38	118.60	123.70
11	5	2164	C	C3'-C2'-C1'	-6.37	96.40	101.50
11	5	2104	C	O4'-C1'-N1	6.37	113.29	108.20
9	3	1536	C	N3-C4-C5	-6.37	119.35	121.90
8	2	1337	G	C5-C6-O6	-6.36	124.78	128.60
11	5	2114	A	P-O3'-C3'	6.36	127.33	119.70
11	5	2115	G	P-O5'-C5'	-6.36	110.73	120.90
8	2	1330	C	N3-C4-N4	6.35	122.45	118.00
1	y	393	ASP	CB-CG-OD2	6.35	124.01	118.30
11	5	2183	A	C4'-C3'-C2'	-6.35	96.25	102.60
10	4	1862	G	C6-C5-N7	-6.35	126.59	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2120	G	N1-C2-N3	-6.35	120.09	123.90
11	5	2133	G	P-O3'-C3'	6.35	127.32	119.70
10	4	1867	G	N1-C2-N3	-6.35	120.09	123.90
5	U	81	ARG	NE-CZ-NH2	-6.34	117.13	120.30
8	2	1342	A	N9-C4-C5	6.34	108.34	105.80
11	5	2134	A	C6-N1-C2	-6.34	114.80	118.60
8	2	1333	G	C5-C6-O6	-6.34	124.80	128.60
11	5	2160	C	C3'-C2'-C1'	-6.34	96.43	101.50
10	4	1875	G	N1-C6-O6	6.33	123.70	119.90
11	5	2125	G	N1-C2-N3	-6.33	120.10	123.90
8	2	1341	G	N7-C8-N9	-6.33	109.94	113.10
8	2	1324	G	N3-C4-C5	-6.33	125.44	128.60
7	1	100	U	C6-N1-C2	-6.32	117.21	121.00
11	5	2124	G	C6-C5-N7	-6.32	126.61	130.40
7	1	97	C	C5-C6-N1	6.32	124.16	121.00
9	3	1536	C	C6-N1-C2	-6.32	117.77	120.30
11	5	2192	U	O4'-C1'-N1	6.32	113.25	108.20
11	5	2119	A	C4-C5-C6	6.31	120.16	117.00
11	5	2098	U	N3-C2-O2	6.31	126.62	122.20
11	5	2130	U	N3-C4-C5	-6.31	110.82	114.60
10	4	1891	G	C6-C5-N7	-6.31	126.62	130.40
7	1	93	G	N1-C6-O6	6.30	123.68	119.90
10	4	1862	G	C4-C5-N7	6.30	113.32	110.80
8	2	1309	G	C6-N1-C2	6.29	128.88	125.10
8	2	1338	G	C6-C5-N7	-6.29	126.63	130.40
11	5	2133	G	O4'-C1'-N9	6.28	113.23	108.20
7	1	54	G	O4'-C1'-N9	6.28	113.22	108.20
11	5	2154	A	C5-C6-N6	-6.28	118.68	123.70
7	1	74	A	N1-C2-N3	6.27	132.44	129.30
8	2	1324	G	P-O5'-C5'	-6.27	110.87	120.90
7	1	60	G	C1'-O4'-C4'	-6.26	104.89	109.90
10	4	1849	G	N7-C8-N9	6.26	116.23	113.10
7	1	92	U	C5-C4-O4	-6.26	122.15	125.90
10	4	1881	C	N3-C4-C5	-6.26	119.40	121.90
5	U	76	THR	CA-CB-CG2	-6.25	103.65	112.40
7	1	67	U	O4'-C1'-N1	6.25	113.20	108.20
7	1	69	C	N3-C4-N4	6.23	122.36	118.00
7	1	68	G	N7-C8-N9	6.23	116.21	113.10
10	4	1844	C	C2-N3-C4	6.23	123.01	119.90
11	5	2187	U	O4'-C1'-N1	6.23	113.18	108.20
10	4	1865	U	P-O3'-C3'	6.22	127.16	119.70
11	5	2097	A	N3-C4-N9	6.21	132.37	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2116	G	C5-C6-O6	-6.21	124.87	128.60
11	5	2192	U	N3-C4-C5	-6.21	110.88	114.60
8	2	1307	A	C8-N9-C4	-6.20	103.32	105.80
10	4	1886	U	N1-C2-O2	-6.20	118.46	122.80
7	1	79	C	N3-C4-N4	6.20	122.34	118.00
11	5	2092	U	O4'-C1'-N1	6.20	113.16	108.20
10	4	1898	U	P-O5'-C5'	6.20	130.81	120.90
1	y	414	MET	N-CA-CB	6.19	121.75	110.60
7	1	83	A	P-O5'-C5'	6.19	130.81	120.90
8	2	1311	G	C6-N1-C2	6.19	128.81	125.10
10	4	1884	G	C6-N1-C2	6.19	128.81	125.10
11	5	2134	A	N9-C4-C5	-6.19	103.32	105.80
10	4	1876	A	N3-C4-N9	6.18	132.35	127.40
2	E	84	TRP	CA-CB-CG	6.18	125.45	113.70
7	1	60	G	O4'-C1'-N9	6.18	113.15	108.20
7	1	71	A	C5-C6-N1	-6.18	114.61	117.70
7	1	63	A	P-O3'-C3'	6.18	127.11	119.70
5	U	48	VAL	CA-CB-CG2	-6.18	101.63	110.90
11	5	2188	U	P-O3'-C3'	-6.17	112.29	119.70
1	y	223	VAL	CG1-CB-CG2	6.17	120.78	110.90
7	1	77	G	C5-C6-O6	-6.17	124.90	128.60
10	4	1871	A	C4-C5-N7	-6.17	107.61	110.70
10	4	1886	U	N3-C2-O2	6.17	126.52	122.20
10	4	1888	G	P-O3'-C3'	6.17	127.10	119.70
10	4	1862	G	C8-N9-C4	6.17	108.87	106.40
10	4	1881	C	O4'-C1'-N1	6.16	113.13	108.20
11	5	2121	G	O4'-C1'-N9	6.16	113.13	108.20
11	5	2145	C	O4'-C1'-N1	6.16	113.13	108.20
7	1	89	A	C5-C6-N6	-6.15	118.78	123.70
8	2	1339	G	C4-N9-C1'	-6.15	118.50	126.50
10	4	1850	G	N3-C4-N9	-6.15	122.31	126.00
11	5	2146	C	C5-C4-N4	-6.15	115.89	120.20
11	5	2179	C	C5-C4-N4	-6.15	115.90	120.20
7	1	68	G	O4'-C1'-N9	6.14	113.12	108.20
7	1	95	A	C2-N3-C4	6.14	113.67	110.60
10	4	1874	C	C4'-C3'-C2'	-6.14	96.46	102.60
11	5	2150	C	O4'-C1'-N1	6.14	113.11	108.20
7	1	103	A	C4-C5-C6	6.13	120.07	117.00
1	y	161	VAL	CA-CB-CG2	-6.13	101.71	110.90
8	2	1331	G	N7-C8-N9	6.13	116.17	113.10
10	4	1848	A	C4'-C3'-C2'	-6.13	96.47	102.60
11	5	2154	A	C5'-C4'-O4'	6.13	116.45	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1336	A	C5-C6-N1	6.12	120.76	117.70
10	4	1857	G	N9-C4-C5	-6.12	102.95	105.40
11	5	2132	U	C6-N1-C1'	-6.12	112.63	121.20
11	5	2199	A	N3-C4-C5	-6.12	122.52	126.80
7	1	55	G	N1-C2-N3	-6.12	120.23	123.90
7	1	85	G	N3-C2-N2	6.12	124.18	119.90
10	4	1844	C	O4'-C1'-N1	6.12	113.09	108.20
7	1	99	U	C6-N1-C2	-6.11	117.33	121.00
8	2	1337	G	C4-C5-N7	6.11	113.25	110.80
10	4	1871	A	N9-C4-C5	6.11	108.25	105.80
10	4	1846	G	N1-C2-N3	-6.11	120.23	123.90
11	5	2114	A	N7-C8-N9	6.11	116.85	113.80
7	1	85	G	C5-C6-N1	-6.10	108.45	111.50
7	1	94	A	O4'-C1'-N9	6.09	113.08	108.20
11	5	2093	G	N9-C4-C5	-6.09	102.96	105.40
11	5	2166	U	O4'-C1'-N1	6.09	113.07	108.20
11	5	2100	G	C3'-C2'-C1'	-6.09	96.63	101.50
11	5	2120	G	O4'-C1'-N9	6.09	113.07	108.20
11	5	2188	U	C5-C6-N1	-6.09	119.66	122.70
11	5	2155	U	C5'-C4'-O4'	6.09	116.41	109.10
8	2	1324	G	C6-C5-N7	-6.08	126.75	130.40
10	4	1847	A	C5-C6-N6	-6.08	118.83	123.70
1	y	337	PHE	CB-CG-CD1	6.08	125.06	120.80
11	5	2168	G	P-O3'-C3'	-6.08	112.41	119.70
10	4	1861	G	C3'-C2'-C1'	-6.08	96.64	101.50
11	5	2197	U	N3-C4-O4	6.07	123.65	119.40
8	2	1336	A	C6-N1-C2	-6.07	114.96	118.60
10	4	1884	G	N1-C6-O6	6.06	123.54	119.90
2	E	116	VAL	CA-CB-CG2	-6.06	101.81	110.90
8	2	1334	G	O4'-C1'-N9	6.06	113.05	108.20
11	5	2192	U	C6-N1-C2	-6.06	117.37	121.00
11	5	2191	A	N1-C2-N3	6.05	132.33	129.30
11	5	2115	G	C5-N7-C8	-6.05	101.28	104.30
7	1	107	G	N1-C6-O6	6.05	123.53	119.90
8	2	1311	G	N3-C4-C5	6.05	131.62	128.60
8	2	1316	U	C5-C4-O4	6.04	129.53	125.90
7	1	52	A	P-O3'-C3'	-6.04	112.45	119.70
8	2	1330	C	C2-N3-C4	6.04	122.92	119.90
8	2	1313	U	C2-N1-C1'	6.04	124.95	117.70
11	5	2180	U	C2-N3-C4	6.04	130.62	127.00
8	2	1328	A	C2-N3-C4	6.02	113.61	110.60
10	4	1840	G	C4-C5-N7	-6.02	108.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1884	G	C5-C6-N1	-6.02	108.49	111.50
11	5	2109	U	N1-C2-N3	-6.02	111.29	114.90
11	5	2154	A	C6-C5-N7	-6.02	128.09	132.30
10	4	1888	G	C6-N1-C2	6.01	128.71	125.10
11	5	2175	C	C6-N1-C2	-6.01	117.89	120.30
8	2	1337	G	O4'-C1'-N9	6.00	113.00	108.20
9	3	1543	G	N7-C8-N9	-6.00	110.10	113.10
4	T	84	TYR	CB-CG-CD1	-6.00	117.40	121.00
8	2	1327	A	P-O5'-C5'	-6.00	111.30	120.90
11	5	2168	G	C4-C5-N7	-6.00	108.40	110.80
11	5	2092	U	N3-C4-C5	-6.00	111.00	114.60
11	5	2139	U	N3-C4-C5	5.99	118.20	114.60
11	5	2155	U	C6-N1-C2	5.99	124.59	121.00
11	5	2133	G	N1-C2-N3	-5.98	120.31	123.90
11	5	2194	U	O4'-C1'-N1	5.98	112.99	108.20
1	y	287	PRO	N-CA-CB	5.98	110.48	103.30
10	4	1850	G	O4'-C1'-N9	5.98	112.98	108.20
11	5	2125	G	C5-C6-N1	-5.98	108.51	111.50
1	y	85	TYR	CG-CD1-CE1	-5.98	116.52	121.30
11	5	2182	U	C5'-C4'-O4'	5.98	116.27	109.10
9	3	1539	U	C1'-O4'-C4'	5.97	114.68	109.90
11	5	2159	G	N3-C4-N9	-5.97	122.42	126.00
11	5	2174	C	C6-N1-C1'	-5.97	113.64	120.80
1	y	416	PHE	CB-CG-CD2	5.96	124.98	120.80
8	2	1332	G	C4-C5-N7	5.96	113.18	110.80
11	5	2137	U	C5-C6-N1	5.96	125.68	122.70
10	4	1855	U	C2-N1-C1'	5.96	124.85	117.70
7	1	111	A	C6-N1-C2	-5.95	115.03	118.60
11	5	2166	U	N3-C4-C5	-5.95	111.03	114.60
7	1	105	C	N3-C2-O2	5.95	126.06	121.90
10	4	1863	G	P-O5'-C5'	-5.95	111.39	120.90
11	5	2103	C	N3-C4-N4	5.95	122.16	118.00
11	5	2151	U	C5-C4-O4	-5.94	122.33	125.90
11	5	2111	U	N3-C4-O4	5.94	123.56	119.40
7	1	75	G	C1'-O4'-C4'	5.94	114.65	109.90
10	4	1892	C	N1-C2-O2	-5.94	115.34	118.90
11	5	2158	A	C4'-C3'-C2'	-5.94	96.66	102.60
10	4	1840	G	N3-C2-N2	5.94	124.06	119.90
7	1	63	A	C6-N1-C2	5.93	122.16	118.60
4	T	25	GLU	CG-CD-OE2	-5.93	106.44	118.30
7	1	91	A	N3-C4-N9	5.93	132.14	127.40
7	1	98	G	C2-N3-C4	5.93	114.86	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2117	A	O4'-C1'-N9	5.92	112.94	108.20
7	1	95	A	C8-N9-C4	-5.92	103.43	105.80
11	5	2118	U	N1-C2-O2	-5.92	118.65	122.80
10	4	1896	G	C8-N9-C4	5.92	108.77	106.40
11	5	2141	G	N1-C6-O6	5.91	123.45	119.90
10	4	1896	G	N1-C6-O6	5.91	123.45	119.90
11	5	2109	U	C5'-C4'-O4'	5.91	116.19	109.10
10	4	1866	A	C6-N1-C2	5.91	122.14	118.60
5	U	84	PHE	CB-CG-CD2	-5.91	116.67	120.80
10	4	1892	C	C6-N1-C2	-5.91	117.94	120.30
7	1	95	A	C6-C5-N7	-5.90	128.17	132.30
10	4	1866	A	C5-C6-N6	-5.90	118.98	123.70
10	4	1880	U	C5'-C4'-O4'	5.90	116.18	109.10
2	E	81	LYS	N-CA-CB	5.90	121.21	110.60
1	y	248	TYR	CG-CD2-CE2	-5.90	116.58	121.30
10	4	1897	G	C5-C6-N1	5.89	114.45	111.50
7	1	64	A	C5-C6-N6	-5.89	118.99	123.70
10	4	1866	A	N7-C8-N9	5.89	116.75	113.80
2	E	127	PHE	CG-CD1-CE1	-5.89	114.32	120.80
7	1	77	G	N1-C6-O6	5.89	123.43	119.90
1	y	370	MET	CG-SD-CE	-5.89	90.78	100.20
7	1	53	A	C3'-C2'-C1'	5.89	106.21	101.50
10	4	1876	A	N1-C2-N3	5.88	132.24	129.30
10	4	1848	A	C6-N1-C2	-5.88	115.07	118.60
11	5	2140	G	N9-C4-C5	-5.88	103.05	105.40
7	1	54	G	C5-C6-N1	5.87	114.44	111.50
7	1	79	C	C2-N1-C1'	5.87	125.26	118.80
10	4	1877	A	N3-C4-C5	-5.87	122.69	126.80
11	5	2122	U	C6-N1-C2	-5.87	117.48	121.00
7	1	110	G	O4'-C1'-N9	5.86	112.89	108.20
9	3	1535	A	C4-C5-C6	5.86	119.93	117.00
1	y	38	PHE	CG-CD2-CE2	5.85	127.24	120.80
9	3	1530	G	N7-C8-N9	5.85	116.03	113.10
11	5	2112	G	C6-C5-N7	-5.85	126.89	130.40
9	3	1541	C	C6-N1-C2	5.85	122.64	120.30
7	1	80	G	C4-C5-N7	5.85	113.14	110.80
7	1	83	A	O4'-C1'-N9	5.85	112.88	108.20
11	5	2197	U	N1-C2-N3	-5.84	111.39	114.90
7	1	101	A	N3-C4-N9	5.84	132.07	127.40
11	5	2130	U	C2-N3-C4	5.84	130.50	127.00
10	4	1859	U	N3-C2-O2	5.84	126.28	122.20
11	5	2176	A	C4-C5-N7	5.84	113.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	101	A	C8-N9-C4	5.83	108.13	105.80
8	2	1323	C	P-O3'-C3'	5.83	126.70	119.70
7	1	68	G	C4-C5-N7	-5.83	108.47	110.80
11	5	2094	A	C5-C6-N1	-5.83	114.78	117.70
9	3	1542	U	N1-C2-O2	-5.83	118.72	122.80
8	2	1330	C	N3-C4-C5	-5.83	119.57	121.90
9	3	1539	U	N1-C2-N3	-5.82	111.41	114.90
7	1	100	U	N3-C2-O2	-5.82	118.13	122.20
10	4	1889	A	C4-C5-C6	5.82	119.91	117.00
7	1	64	A	N9-C4-C5	-5.81	103.48	105.80
11	5	2170	A	C5-C6-N1	-5.81	114.80	117.70
11	5	2165	C	P-O3'-C3'	5.81	126.67	119.70
9	3	1530	G	O4'-C1'-N9	5.81	112.84	108.20
10	4	1858	A	N3-C4-N9	-5.80	122.76	127.40
11	5	2105	U	O4'-C1'-N1	5.80	112.84	108.20
1	y	85	TYR	CB-CG-CD2	5.80	124.48	121.00
7	1	84	A	O4'-C1'-N9	5.79	112.83	108.20
10	4	1891	G	C4-C5-C6	5.79	122.27	118.80
11	5	2145	C	C5-C4-N4	-5.79	116.15	120.20
8	2	1310	G	C6-N1-C2	5.78	128.57	125.10
11	5	2176	A	N9-C4-C5	-5.78	103.49	105.80
10	4	1895	C	C5-C4-N4	-5.78	116.16	120.20
11	5	2108	A	C5-C6-N6	-5.78	119.08	123.70
8	2	1310	G	N1-C6-O6	5.77	123.36	119.90
11	5	2167	U	P-O5'-C5'	5.77	130.13	120.90
6	Y	29	ARG	CG-CD-NE	-5.77	99.69	111.80
7	1	99	U	C2-N3-C4	5.77	130.46	127.00
11	5	2096	C	C6-N1-C2	-5.77	117.99	120.30
7	1	100	U	C3'-C2'-C1'	5.76	106.11	101.50
6	Y	3	ALA	N-CA-CB	5.76	118.16	110.10
11	5	2148	G	O4'-C1'-N9	5.76	112.81	108.20
10	4	1883	U	C5-C6-N1	5.75	125.58	122.70
10	4	1884	G	C3'-C2'-C1'	5.75	106.10	101.50
1	y	9	PHE	CB-CG-CD2	5.75	124.83	120.80
11	5	2134	A	C4-C5-N7	5.75	113.58	110.70
7	1	64	A	C6-C5-N7	-5.75	128.28	132.30
9	3	1541	C	C4-C5-C6	5.75	120.27	117.40
10	4	1891	G	N1-C6-O6	5.75	123.35	119.90
9	3	1531	C	O4'-C1'-N1	5.74	112.80	108.20
11	5	2186	G	C5-N7-C8	5.74	107.17	104.30
1	y	45	ASP	N-CA-CB	5.74	120.93	110.60
7	1	81	G	C4-N9-C1'	5.74	133.96	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1326	U	C5'-C4'-O4'	5.74	115.99	109.10
7	1	107	G	C5-C6-O6	-5.74	125.16	128.60
8	2	1307	A	N1-C2-N3	5.74	132.17	129.30
10	4	1877	A	C5-C6-N1	-5.73	114.83	117.70
11	5	2124	G	C3'-C2'-C1'	5.73	106.08	101.50
11	5	2180	U	C3'-C2'-C1'	-5.73	96.92	101.50
11	5	2193	G	C5-N7-C8	-5.73	101.44	104.30
11	5	2156	G	C2-N3-C4	5.73	114.76	111.90
7	1	87	U	C5-C6-N1	5.72	125.56	122.70
8	2	1335	C	O4'-C1'-N1	5.72	112.78	108.20
9	3	1542	U	C2-N3-C4	-5.72	123.56	127.00
1	y	113	ARG	NE-CZ-NH1	5.72	123.16	120.30
10	4	1846	G	C8-N9-C4	-5.72	104.11	106.40
7	1	101	A	C5-C6-N1	-5.72	114.84	117.70
4	T	66	LYS	N-CA-C	-5.71	95.57	111.00
10	4	1876	A	C4'-C3'-C2'	5.71	108.31	102.60
8	2	1340	U	N3-C4-O4	5.71	123.40	119.40
11	5	2106	U	C4'-C3'-C2'	-5.71	96.89	102.60
11	5	2177	C	N1-C2-O2	-5.71	115.47	118.90
6	Y	32	ALA	CB-CA-C	-5.71	101.53	110.10
8	2	1317	G	C5-C6-N1	-5.71	108.65	111.50
11	5	2105	U	P-O3'-C3'	5.71	126.55	119.70
10	4	1893	C	N3-C4-N4	5.71	121.99	118.00
11	5	2112	G	C4-C5-C6	5.70	122.22	118.80
7	1	106	C	N1-C2-O2	-5.70	115.48	118.90
11	5	2168	G	C2-N3-C4	-5.70	109.05	111.90
11	5	2196	C	C6-N1-C2	5.70	122.58	120.30
11	5	2167	U	N3-C4-O4	5.70	123.39	119.40
10	4	1860	G	N1-C2-N3	-5.69	120.48	123.90
8	2	1327	A	O4'-C1'-N9	5.69	112.75	108.20
8	2	1317	G	N1-C2-N3	-5.68	120.49	123.90
11	5	2159	G	C8-N9-C4	-5.67	104.13	106.40
11	5	2171	A	N1-C2-N3	-5.67	126.46	129.30
11	5	2118	U	C5-C6-N1	5.67	125.54	122.70
11	5	2171	A	C5-C6-N1	-5.67	114.86	117.70
8	2	1309	G	N3-C4-N9	-5.67	122.60	126.00
8	2	1325	U	O3'-P-O5'	-5.67	93.23	104.00
8	2	1337	G	P-O5'-C5'	-5.67	111.83	120.90
11	5	2145	C	N3-C4-C5	-5.66	119.63	121.90
1	y	119	TYR	CA-CB-CG	5.66	124.16	113.40
1	y	390	PHE	CB-CG-CD2	-5.66	116.84	120.80
9	3	1538	G	N3-C4-N9	5.66	129.39	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	77	ARG	NH1-CZ-NH2	5.65	125.62	119.40
4	T	12	ARG	NE-CZ-NH1	5.65	123.13	120.30
7	1	63	A	C6-C5-N7	-5.65	128.34	132.30
10	4	1898	U	O4'-C1'-N1	5.65	112.72	108.20
11	5	2169	A	N1-C6-N6	5.65	121.99	118.60
8	2	1324	G	C4-C5-C6	5.64	122.19	118.80
7	1	105	C	N3-C4-C5	-5.64	119.64	121.90
10	4	1846	G	C6-C5-N7	-5.64	127.02	130.40
10	4	1866	A	C5-N7-C8	5.64	106.72	103.90
8	2	1333	G	P-O5'-C5'	5.63	129.91	120.90
10	4	1860	G	C5-C6-N1	5.63	114.31	111.50
10	4	1842	G	C5-N7-C8	5.63	107.11	104.30
10	4	1884	G	O4'-C1'-N9	5.63	112.70	108.20
10	4	1863	G	C2-N3-C4	5.62	114.71	111.90
7	1	68	G	N3-C4-N9	-5.62	122.63	126.00
5	U	102	ILE	N-CA-C	-5.62	95.82	111.00
9	3	1528	A	C6-C5-N7	-5.62	128.37	132.30
11	5	2175	C	C5-C6-N1	5.62	123.81	121.00
8	2	1311	G	C5-C6-O6	-5.62	125.23	128.60
8	2	1332	G	N1-C6-O6	5.62	123.27	119.90
8	2	1313	U	C6-N1-C1'	-5.61	113.34	121.20
11	5	2119	A	C1'-O4'-C4'	5.61	114.39	109.90
11	5	2122	U	N3-C4-C5	5.61	117.96	114.60
11	5	2168	G	P-O5'-C5'	5.61	129.87	120.90
5	U	90	LYS	N-CA-CB	5.60	120.69	110.60
8	2	1334	G	N3-C4-N9	-5.60	122.64	126.00
10	4	1864	U	C5-C6-N1	5.60	125.50	122.70
3	G	52	MET	N-CA-C	-5.59	95.89	111.00
10	4	1859	U	C5'-C4'-O4'	5.59	115.81	109.10
1	y	35	ILE	CA-CB-CG1	-5.59	100.38	111.00
11	5	2161	C	OP1-P-O3'	5.59	117.50	105.20
1	y	139	LEU	CA-C-N	5.58	132.74	117.10
1	y	344	ASP	CB-CG-OD1	5.58	123.32	118.30
7	1	84	A	C5'-C4'-C3'	-5.58	107.07	116.00
7	1	87	U	C6-N1-C2	-5.58	117.65	121.00
7	1	55	G	N9-C4-C5	-5.58	103.17	105.40
7	1	64	A	O4'-C1'-N9	5.58	112.66	108.20
7	1	78	U	C5'-C4'-O4'	5.58	115.79	109.10
11	5	2157	G	N3-C2-N2	5.58	123.81	119.90
11	5	2142	A	C5-C6-N6	-5.58	119.24	123.70
11	5	2126	A	C5-C6-N6	-5.57	119.24	123.70
11	5	2126	A	P-O5'-C5'	-5.57	111.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	149	VAL	CA-CB-CG1	-5.56	102.56	110.90
7	1	74	A	O4'-C1'-N9	5.56	112.65	108.20
11	5	2134	A	P-O3'-C3'	5.56	126.38	119.70
8	2	1321	A	C4-C5-N7	-5.56	107.92	110.70
11	5	2147	A	P-O5'-C5'	5.56	129.80	120.90
7	1	86	G	N9-C4-C5	-5.56	103.18	105.40
7	1	83	A	C5-C6-N1	-5.56	114.92	117.70
10	4	1863	G	O4'-C1'-N9	5.56	112.65	108.20
7	1	83	A	C6-C5-N7	-5.55	128.41	132.30
11	5	2190	G	N1-C6-O6	5.55	123.23	119.90
8	2	1341	G	N1-C2-N3	-5.55	120.57	123.90
7	1	105	C	C4-C5-C6	5.54	120.17	117.40
9	3	1540	G	C6-N1-C2	5.54	128.43	125.10
11	5	2121	G	N1-C2-N3	-5.54	120.58	123.90
1	y	258	TYR	CB-CG-CD1	-5.54	117.68	121.00
2	E	121	PHE	C-N-CA	5.54	135.54	121.70
11	5	2188	U	C1'-O4'-C4'	-5.54	105.47	109.90
11	5	2196	C	N1-C2-O2	5.53	122.22	118.90
9	3	1535	A	C5-C6-N6	-5.53	119.28	123.70
11	5	2151	U	N3-C4-O4	5.53	123.27	119.40
8	2	1324	G	C5-N7-C8	-5.52	101.54	104.30
11	5	2101	A	P-O3'-C3'	-5.52	113.07	119.70
11	5	2140	G	O4'-C1'-N9	5.52	112.62	108.20
7	1	94	A	C6-C5-N7	-5.52	128.44	132.30
11	5	2173	A	OP1-P-OP2	-5.52	111.32	119.60
8	2	1310	G	N3-C2-N2	5.52	123.76	119.90
8	2	1339	G	C8-N9-C1'	5.52	134.18	127.00
10	4	1854	A	O4'-C1'-N9	5.52	112.62	108.20
11	5	2129	C	N3-C4-N4	-5.52	114.14	118.00
11	5	2181	U	C5'-C4'-O4'	5.52	115.72	109.10
7	1	79	C	C4-C5-C6	5.51	120.16	117.40
9	3	1529	G	C8-N9-C4	-5.51	104.19	106.40
11	5	2138	G	O4'-C1'-N9	5.51	112.61	108.20
11	5	2161	C	O4'-C1'-N1	5.51	112.61	108.20
1	y	46	ALA	CB-CA-C	-5.50	101.85	110.10
11	5	2165	C	N3-C4-N4	5.50	121.85	118.00
11	5	2189	U	N3-C4-O4	5.50	123.25	119.40
10	4	1873	G	C6-N1-C2	5.50	128.40	125.10
9	3	1532	A	C2-N3-C4	5.50	113.35	110.60
10	4	1850	G	C5-C6-N1	-5.50	108.75	111.50
11	5	2184	A	C5-N7-C8	5.50	106.65	103.90
8	2	1307	A	N9-C4-C5	5.49	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	57	C	O4'-C4'-C3'	-5.49	98.51	104.00
11	5	2171	A	C2-N3-C4	5.49	113.34	110.60
11	5	2177	C	OP1-P-O3'	5.49	117.28	105.20
1	y	122	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	y	400	TYR	CB-CG-CD1	-5.49	117.71	121.00
10	4	1882	U	N3-C2-O2	5.49	126.04	122.20
10	4	1897	G	C4-C5-N7	5.48	112.99	110.80
7	1	109	C	N3-C2-O2	5.48	125.74	121.90
8	2	1319	C	C1'-O4'-C4'	-5.48	105.51	109.90
4	T	95	PHE	CB-CG-CD1	-5.48	116.96	120.80
11	5	2113	U	C1'-O4'-C4'	-5.48	105.52	109.90
10	4	1853	A	N1-C6-N6	5.48	121.89	118.60
6	Y	3	ALA	CB-CA-C	-5.47	101.89	110.10
11	5	2116	G	N7-C8-N9	-5.47	110.36	113.10
11	5	2119	A	N7-C8-N9	-5.47	111.06	113.80
7	1	100	U	C5'-C4'-C3'	-5.47	107.24	116.00
11	5	2102	G	N7-C8-N9	5.47	115.83	113.10
11	5	2110	G	C4-N9-C1'	-5.47	119.39	126.50
8	2	1324	G	C5'-C4'-C3'	-5.47	107.25	116.00
7	1	70	G	C4-C5-C6	5.46	122.08	118.80
8	2	1308	A	C4-C5-N7	-5.46	107.97	110.70
1	y	249	ALA	CB-CA-C	5.46	118.29	110.10
7	1	103	A	C5-N7-C8	5.46	106.63	103.90
8	2	1327	A	C5-N7-C8	5.46	106.63	103.90
1	y	383	PHE	CB-CG-CD1	-5.46	116.98	120.80
5	U	5	ARG	NE-CZ-NH1	5.46	123.03	120.30
11	5	2167	U	C4-C5-C6	-5.46	116.43	119.70
1	y	192	PHE	CB-CG-CD1	5.45	124.62	120.80
11	5	2111	U	N3-C4-C5	-5.45	111.33	114.60
7	1	86	G	C8-N9-C4	5.45	108.58	106.40
11	5	2105	U	C5-C6-N1	5.45	125.42	122.70
8	2	1324	G	O4'-C4'-C3'	5.45	110.46	106.10
7	1	72	U	C4-C5-C6	5.44	122.97	119.70
8	2	1317	G	C6-N1-C2	5.44	128.37	125.10
11	5	2102	G	N9-C4-C5	-5.44	103.22	105.40
10	4	1870	C	N1-C2-N3	-5.43	115.40	119.20
11	5	2178	C	C6-N1-C2	-5.43	118.13	120.30
1	y	85	TYR	CD1-CG-CD2	5.42	123.86	117.90
7	1	101	A	N3-C4-C5	-5.42	123.01	126.80
11	5	2134	A	N1-C6-N6	5.42	121.85	118.60
8	2	1331	G	C4-N9-C1'	5.42	133.54	126.50
1	y	411	VAL	CA-CB-CG2	-5.41	102.78	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1885	A	C8-N9-C4	-5.41	103.64	105.80
11	5	2196	C	P-O3'-C3'	5.41	126.19	119.70
5	U	51	LEU	CB-CG-CD1	-5.40	101.83	111.00
11	5	2135	A	C6-C5-N7	5.40	136.08	132.30
1	y	294	PHE	CG-CD1-CE1	-5.39	114.87	120.80
11	5	2196	C	N3-C4-N4	5.39	121.78	118.00
8	2	1320	C	C4-C5-C6	5.39	120.09	117.40
11	5	2128	G	C2-N3-C4	5.39	114.59	111.90
7	1	111	A	C4-C5-C6	-5.38	114.31	117.00
11	5	2183	A	C5-C6-N1	-5.38	115.01	117.70
8	2	1310	G	N3-C4-C5	-5.38	125.91	128.60
10	4	1854	A	C5-C6-N6	5.38	128.00	123.70
10	4	1896	G	O4'-C1'-N9	5.38	112.50	108.20
7	1	75	G	N3-C4-C5	5.38	131.29	128.60
11	5	2176	A	C6-N1-C2	5.38	121.83	118.60
1	y	335	LEU	CB-CG-CD2	5.38	120.14	111.00
7	1	108	G	N3-C2-N2	5.37	123.66	119.90
11	5	2130	U	C4-C5-C6	5.37	122.92	119.70
10	4	1889	A	C5-C6-N6	-5.37	119.40	123.70
11	5	2163	A	C5'-C4'-O4'	5.37	115.55	109.10
7	1	113	U	N1-C2-O2	-5.37	119.04	122.80
1	y	258	TYR	N-CA-CB	5.37	120.26	110.60
7	1	83	A	C1'-O4'-C4'	5.37	114.19	109.90
8	2	1332	G	C5-C6-N1	5.37	114.18	111.50
10	4	1845	G	C5-N7-C8	5.37	106.98	104.30
11	5	2198	A	N7-C8-N9	5.36	116.48	113.80
8	2	1341	G	C6-C5-N7	5.36	133.62	130.40
5	U	36	GLU	CB-CA-C	-5.36	99.68	110.40
11	5	2190	G	N1-C2-N3	-5.36	120.69	123.90
7	1	93	G	C4-C5-N7	-5.36	108.66	110.80
11	5	2105	U	C6-N1-C2	-5.36	117.79	121.00
10	4	1854	A	C5'-C4'-O4'	5.35	115.53	109.10
11	5	2140	G	C6-N1-C2	5.35	128.31	125.10
11	5	2116	G	N1-C2-N3	-5.35	120.69	123.90
1	y	214	ASP	CB-CG-OD1	5.34	123.11	118.30
8	2	1309	G	N9-C4-C5	5.34	107.54	105.40
10	4	1876	A	C4-C5-N7	-5.34	108.03	110.70
8	2	1340	U	O4'-C1'-N1	5.34	112.47	108.20
11	5	2110	G	C8-N9-C1'	5.33	133.94	127.00
1	y	399	PHE	CB-CG-CD2	-5.33	117.07	120.80
10	4	1861	G	N9-C4-C5	-5.33	103.27	105.40
7	1	55	G	C5-C6-N1	-5.33	108.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2117	A	N1-C6-N6	5.33	121.80	118.60
2	E	118	LEU	N-CA-CB	5.33	121.06	110.40
8	2	1310	G	C8-N9-C4	-5.33	104.27	106.40
7	1	76	C	N3-C4-N4	5.33	121.73	118.00
7	1	94	A	C2-N3-C4	-5.33	107.94	110.60
11	5	2192	U	C5-C6-N1	5.32	125.36	122.70
1	y	317	TYR	N-CA-CB	5.32	120.18	110.60
9	3	1543	G	C6-N1-C2	-5.32	121.91	125.10
10	4	1861	G	C8-N9-C4	5.32	108.53	106.40
6	Y	24	GLU	O-C-N	-5.31	114.20	122.70
10	4	1874	C	N3-C4-N4	5.31	121.72	118.00
11	5	2179	C	C4-C5-C6	-5.31	114.75	117.40
11	5	2187	U	N3-C4-C5	-5.31	111.42	114.60
7	1	63	A	C8-N9-C4	-5.31	103.68	105.80
11	5	2135	A	N9-C4-C5	5.30	107.92	105.80
7	1	67	U	P-O3'-C3'	5.30	126.06	119.70
11	5	2139	U	N1-C1'-C2'	-5.30	106.17	112.00
11	5	2164	C	N3-C4-C5	-5.29	119.78	121.90
11	5	2173	A	C8-N9-C4	-5.29	103.68	105.80
11	5	2102	G	C5-C6-O6	-5.29	125.42	128.60
11	5	2144	G	N1-C2-N3	-5.29	120.72	123.90
1	y	163	SER	N-CA-CB	5.29	118.44	110.50
10	4	1859	U	N1-C2-O2	-5.29	119.10	122.80
11	5	2127	G	C5-C6-O6	-5.29	125.43	128.60
6	Y	7	ARG	NE-CZ-NH2	-5.29	117.66	120.30
8	2	1326	U	N3-C4-C5	5.29	117.77	114.60
11	5	2157	G	P-O3'-C3'	5.29	126.05	119.70
7	1	112	U	OP1-P-OP2	-5.29	111.67	119.60
5	U	10	VAL	CA-CB-CG1	5.28	118.82	110.90
7	1	99	U	O4'-C4'-C3'	-5.28	98.72	104.00
7	1	69	C	OP1-P-OP2	-5.28	111.68	119.60
9	3	1528	A	C4'-C3'-C2'	-5.28	97.32	102.60
1	y	328	PHE	CB-CG-CD1	-5.28	117.11	120.80
10	4	1842	G	P-O5'-C5'	-5.27	112.47	120.90
10	4	1847	A	C2-N3-C4	-5.27	107.97	110.60
11	5	2156	G	N3-C2-N2	5.27	123.59	119.90
7	1	55	G	N3-C4-C5	5.26	131.23	128.60
11	5	2106	U	N1-C2-O2	-5.26	119.12	122.80
11	5	2182	U	C5'-C4'-C3'	-5.26	107.59	116.00
7	1	97	C	C2-N3-C4	5.25	122.53	119.90
10	4	1855	U	C4-C5-C6	-5.25	116.55	119.70
11	5	2151	U	C4-C5-C6	-5.25	116.55	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	1321	A	N7-C8-N9	5.25	116.43	113.80
11	5	2171	A	C6-C5-N7	-5.25	128.62	132.30
11	5	2160	C	N1-C2-N3	-5.25	115.53	119.20
7	1	108	G	C5-C6-N1	-5.24	108.88	111.50
8	2	1307	A	C3'-C2'-C1'	-5.24	97.31	101.50
9	3	1528	A	C8-N9-C4	-5.24	103.70	105.80
11	5	2188	U	C5-C4-O4	5.24	129.05	125.90
11	5	2189	U	OP1-P-OP2	-5.24	111.74	119.60
5	U	100	GLU	CB-CG-CD	-5.24	100.05	114.20
7	1	93	G	C2-N3-C4	5.24	114.52	111.90
1	y	412	VAL	CA-CB-CG1	5.24	118.76	110.90
1	y	298	THR	CA-CB-CG2	-5.24	105.07	112.40
7	1	57	C	C4'-C3'-C2'	-5.24	97.36	102.60
8	2	1328	A	N1-C6-N6	5.24	121.74	118.60
11	5	2162	G	N1-C2-N3	-5.24	120.76	123.90
10	4	1876	A	N7-C8-N9	-5.23	111.18	113.80
11	5	2112	G	C5-C6-O6	-5.23	125.46	128.60
11	5	2131	U	O4'-C1'-N1	5.23	112.39	108.20
1	y	321	TYR	CD1-CE1-CZ	5.23	124.51	119.80
11	5	2109	U	N3-C4-C5	-5.23	111.46	114.60
10	4	1870	C	O4'-C4'-C3'	-5.23	98.77	104.00
7	1	58	G	O5'-P-OP1	5.22	116.97	110.70
7	1	61	C	C5'-C4'-O4'	5.22	115.36	109.10
7	1	58	G	N3-C4-C5	-5.22	125.99	128.60
1	y	25	PHE	CB-CG-CD1	5.21	124.45	120.80
7	1	73	A	N1-C2-N3	5.21	131.91	129.30
10	4	1850	G	N7-C8-N9	-5.21	110.49	113.10
11	5	2143	C	N1-C2-N3	-5.21	115.55	119.20
1	y	293	TRP	CE3-CZ3-CH2	-5.21	115.47	121.20
11	5	2176	A	C1'-O4'-C4'	5.21	114.07	109.90
7	1	71	A	C6-N1-C2	5.21	121.73	118.60
7	1	77	G	C4-C5-N7	-5.21	108.72	110.80
10	4	1853	A	C5-N7-C8	5.21	106.50	103.90
11	5	2108	A	N9-C4-C5	-5.21	103.72	105.80
10	4	1861	G	C5-N7-C8	5.21	106.90	104.30
10	4	1862	G	C4-N9-C1'	-5.21	119.73	126.50
11	5	2152	G	C4-C5-N7	5.20	112.88	110.80
11	5	2101	A	C4'-C3'-C2'	-5.19	97.41	102.60
11	5	2149	U	P-O3'-C3'	5.19	125.93	119.70
2	E	109	TRP	CE3-CZ3-CH2	-5.19	115.49	121.20
11	5	2185	U	C4-C5-C6	5.19	122.81	119.70
7	1	76	C	O5'-C5'-C4'	-5.19	101.84	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2196	C	O4'-C1'-N1	5.19	112.35	108.20
7	1	76	C	N3-C4-C5	-5.19	119.83	121.90
8	2	1317	G	N3-C2-N2	5.19	123.53	119.90
11	5	2161	C	C4-C5-C6	5.19	119.99	117.40
11	5	2178	C	P-O3'-C3'	5.19	125.92	119.70
4	T	92	ASN	N-CA-C	-5.19	97.00	111.00
10	4	1887	C	C4'-C3'-C2'	-5.18	97.42	102.60
1	y	417	MET	O-C-N	-5.18	114.41	122.70
3	G	29	ASP	CB-CG-OD2	5.18	122.96	118.30
10	4	1853	A	N9-C4-C5	-5.17	103.73	105.80
11	5	2092	U	C5-C6-N1	5.17	125.28	122.70
1	y	119	TYR	CB-CG-CD2	-5.17	117.90	121.00
8	2	1337	G	N1-C6-O6	5.17	123.00	119.90
7	1	91	A	C4-C5-C6	5.16	119.58	117.00
11	5	2113	U	O4'-C1'-N1	5.16	112.33	108.20
10	4	1885	A	N1-C6-N6	5.16	121.70	118.60
8	2	1317	G	C6-C5-N7	-5.16	127.30	130.40
7	1	63	A	C5-N7-C8	-5.16	101.32	103.90
10	4	1870	C	C4-C5-C6	5.16	119.98	117.40
10	4	1870	C	N3-C4-C5	-5.16	119.84	121.90
7	1	65	U	C1'-O4'-C4'	-5.15	105.78	109.90
1	y	215	LEU	N-CA-C	-5.15	97.09	111.00
5	U	47	PRO	N-CD-CG	5.15	110.93	103.20
10	4	1872	A	C6-C5-N7	-5.15	128.69	132.30
11	5	2137	U	N1-C2-O2	-5.15	119.19	122.80
8	2	1325	U	C5-C4-O4	-5.14	122.82	125.90
10	4	1874	C	O5'-P-OP2	-5.14	101.07	105.70
7	1	107	G	O4'-C1'-N9	5.14	112.31	108.20
5	U	36	GLU	N-CA-CB	5.14	119.85	110.60
11	5	2132	U	N1-C1'-C2'	-5.14	106.35	112.00
11	5	2100	G	N3-C4-N9	5.14	129.08	126.00
10	4	1877	A	C4-C5-C6	5.13	119.57	117.00
11	5	2106	U	N1-C2-N3	5.13	117.98	114.90
11	5	2116	G	C3'-C2'-C1'	-5.13	97.39	101.50
7	1	66	C	N1-C2-N3	-5.13	115.61	119.20
8	2	1328	A	P-O5'-C5'	5.13	129.11	120.90
11	5	2147	A	O4'-C1'-N9	5.13	112.31	108.20
7	1	55	G	C1'-O4'-C4'	-5.13	105.80	109.90
2	E	106	LEU	CB-CA-C	5.13	119.95	110.20
7	1	75	G	N7-C8-N9	5.13	115.67	113.10
10	4	1838	C	C4'-C3'-C2'	-5.13	97.47	102.60
7	1	57	C	N3-C4-C5	-5.13	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	62	U	N3-C4-O4	5.13	122.99	119.40
7	1	88	G	C3'-C2'-C1'	-5.13	97.40	101.50
1	y	53	LEU	CB-CG-CD1	-5.12	102.29	111.00
7	1	93	G	N1-C2-N3	-5.12	120.83	123.90
10	4	1860	G	P-O3'-C3'	-5.12	113.56	119.70
7	1	60	G	C8-N9-C4	5.11	108.44	106.40
7	1	104	A	C4-C5-C6	5.11	119.56	117.00
11	5	2130	U	O4'-C1'-N1	5.11	112.29	108.20
7	1	59	U	N3-C4-O4	5.11	122.97	119.40
10	4	1869	G	N1-C6-O6	5.11	122.96	119.90
7	1	55	G	C6-C5-N7	-5.11	127.34	130.40
8	2	1333	G	C6-C5-N7	-5.10	127.34	130.40
11	5	2160	C	C6-N1-C1'	-5.10	114.68	120.80
11	5	2184	A	C6-C5-N7	-5.10	128.73	132.30
7	1	53	A	C6-C5-N7	-5.10	128.73	132.30
9	3	1535	A	N1-C2-N3	5.10	131.85	129.30
6	Y	42	LEU	CB-CG-CD1	-5.09	102.35	111.00
8	2	1316	U	C5-C6-N1	5.09	125.25	122.70
11	5	2114	A	C6-N1-C2	5.09	121.65	118.60
7	1	68	G	N9-C4-C5	5.09	107.43	105.40
1	y	429	TYR	CD1-CE1-CZ	-5.08	115.22	119.80
11	5	2104	C	C4-C5-C6	5.08	119.94	117.40
9	3	1529	G	C5-C6-O6	5.08	131.65	128.60
1	y	181	ARG	NE-CZ-NH2	5.07	122.83	120.30
4	T	89	GLU	C-N-CA	5.07	132.95	122.30
11	5	2095	A	C5-C6-N6	-5.07	119.64	123.70
11	5	2152	G	N1-C6-O6	5.07	122.94	119.90
9	3	1543	G	N3-C4-C5	5.07	131.13	128.60
7	1	59	U	N3-C4-C5	-5.07	111.56	114.60
10	4	1859	U	N1-C1'-C2'	-5.06	106.43	112.00
11	5	2119	A	C5-N7-C8	5.06	106.43	103.90
5	U	4	ILE	CA-CB-CG1	5.06	120.62	111.00
10	4	1844	C	P-O5'-C5'	5.06	129.00	120.90
3	G	50	ASN	N-CA-C	-5.06	97.33	111.00
7	1	85	G	C4-C5-N7	-5.06	108.78	110.80
1	y	386	LEU	N-CA-CB	5.06	120.51	110.40
9	3	1537	G	C8-N9-C4	5.06	108.42	106.40
7	1	63	A	N9-C4-C5	5.05	107.82	105.80
10	4	1873	G	N3-C2-N2	5.05	123.44	119.90
11	5	2184	A	C6-N1-C2	5.05	121.63	118.60
11	5	2183	A	C6-N1-C2	5.05	121.63	118.60
10	4	1889	A	O4'-C1'-N9	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	1891	G	P-O5'-C5'	5.05	128.98	120.90
11	5	2177	C	N3-C4-C5	-5.05	119.88	121.90
10	4	1856	U	C1'-O4'-C4'	-5.04	105.86	109.90
11	5	2178	C	C6-N1-C1'	-5.04	114.75	120.80
11	5	2176	A	C3'-C2'-C1'	5.04	105.53	101.50
4	T	64	LYS	CB-CA-C	-5.03	100.33	110.40
9	3	1527	G	C5-N7-C8	5.03	106.82	104.30
11	5	2170	A	C6-C5-N7	-5.03	128.78	132.30
5	U	80	ASP	N-CA-CB	5.03	119.66	110.60
11	5	2144	G	C1'-O4'-C4'	-5.03	105.88	109.90
1	y	142	MET	CA-C-N	5.03	131.18	117.10
11	5	2137	U	N1-C1'-C2'	-5.03	106.47	112.00
9	3	1537	G	C4-N9-C1'	5.03	133.03	126.50
10	4	1842	G	N9-C4-C5	-5.03	103.39	105.40
11	5	2177	C	C5'-C4'-C3'	-5.03	107.96	116.00
7	1	64	A	C4-C5-N7	5.02	113.21	110.70
10	4	1881	C	C6-N1-C2	-5.02	118.29	120.30
1	y	409	VAL	CA-CB-CG1	5.02	118.43	110.90
9	3	1527	G	C4-C5-C6	5.02	121.81	118.80
8	2	1314	C	C5-C6-N1	5.02	123.51	121.00
11	5	2093	G	N3-C4-N9	-5.02	122.99	126.00
11	5	2159	G	C5-N7-C8	-5.02	101.79	104.30
1	y	33	PHE	CB-CG-CD1	-5.02	117.29	120.80
10	4	1876	A	P-O3'-C3'	-5.02	113.68	119.70
11	5	2124	G	C4'-C3'-C2'	-5.02	97.58	102.60
1	y	380	TYR	CD1-CE1-CZ	5.01	124.31	119.80
11	5	2186	G	N3-C4-N9	5.01	129.01	126.00
7	1	73	A	N9-C4-C5	-5.01	103.80	105.80
8	2	1309	G	P-O3'-C3'	-5.01	113.69	119.70
11	5	2153	C	O4'-C1'-N1	5.01	112.21	108.20
10	4	1898	U	C5-C4-O4	5.01	128.91	125.90
7	1	66	C	N3-C4-N4	5.01	121.50	118.00
11	5	2172	U	N3-C4-O4	-5.01	115.89	119.40
11	5	2176	A	C5-N7-C8	-5.00	101.40	103.90
8	2	1326	U	C5'-C4'-C3'	-5.00	108.00	116.00
10	4	1881	C	N3-C4-N4	5.00	121.50	118.00
1	y	150	ILE	N-CA-C	-5.00	97.50	111.00
8	2	1342	A	O4'-C1'-N9	5.00	112.20	108.20
11	5	2183	A	C8-N9-C4	-5.00	103.80	105.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	45	SER	CA
3	G	48	SER	CA
3	G	51	PHE	CA

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	1	100	U	Sidechain
7	1	103	A	Sidechain
7	1	106	C	Sidechain
7	1	107	G	Sidechain
7	1	108	G	Sidechain
7	1	109	C	Sidechain
7	1	113	U	Sidechain
7	1	52	A	Sidechain
7	1	55	G	Sidechain
7	1	58	G	Sidechain
7	1	59	U	Sidechain
7	1	60	G	Sidechain
7	1	63	A	Sidechain
7	1	64	A	Sidechain
7	1	68	G	Sidechain
7	1	72	U	Sidechain
7	1	73	A	Sidechain
7	1	74	A	Sidechain
7	1	75	G	Sidechain
7	1	77	G	Sidechain
7	1	79	C	Sidechain
7	1	84	A	Sidechain
7	1	87	U	Sidechain
7	1	88	G	Sidechain
7	1	91	A	Sidechain
7	1	92	U	Sidechain
7	1	94	A	Sidechain
7	1	95	A	Sidechain
7	1	97	C	Sidechain
7	1	99	U	Sidechain
8	2	1310	G	Sidechain
8	2	1311	G	Sidechain
8	2	1312	U	Sidechain
8	2	1314	C	Sidechain
8	2	1324	G	Sidechain
8	2	1325	U	Sidechain

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Mol	Chain	Res	Type	Group
8	2	1326	U	Sidechain
8	2	1327	A	Sidechain
8	2	1328	A	Sidechain
8	2	1333	G	Sidechain
8	2	1334	G	Sidechain
8	2	1336	A	Sidechain
8	2	1337	G	Sidechain
8	2	1338	G	Sidechain
8	2	1341	G	Sidechain
9	3	1527	G	Sidechain
9	3	1529	G	Sidechain
9	3	1530	G	Sidechain
9	3	1534	U	Sidechain
9	3	1535	A	Sidechain
9	3	1537	G	Sidechain
9	3	1538	G	Sidechain
9	3	1539	U	Sidechain
9	3	1540	G	Sidechain
9	3	1542	U	Sidechain
10	4	1838	C	Sidechain
10	4	1840	G	Sidechain
10	4	1841	U	Sidechain
10	4	1846	G	Sidechain
10	4	1857	G	Sidechain
10	4	1858	A	Sidechain
10	4	1859	U	Sidechain
10	4	1860	G	Sidechain
10	4	1862	G	Sidechain
10	4	1864	U	Sidechain
10	4	1877	A	Sidechain
10	4	1878	G	Sidechain
10	4	1880	U	Sidechain
10	4	1881	C	Sidechain
10	4	1886	U	Sidechain
10	4	1887	C	Sidechain
10	4	1890	A	Sidechain
10	4	1891	G	Sidechain
10	4	1895	C	Sidechain
10	4	1898	U	Sidechain
11	5	2094	A	Sidechain
11	5	2099	U	Sidechain
11	5	2100	G	Sidechain

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Mol	Chain	Res	Type	Group
11	5	2101	A	Sidechain
11	5	2104	C	Sidechain
11	5	2105	U	Sidechain
11	5	2107	G	Sidechain
11	5	2110	G	Sidechain
11	5	2111	U	Sidechain
11	5	2113	U	Sidechain
11	5	2117	A	Sidechain
11	5	2119	A	Sidechain
11	5	2121	G	Sidechain
11	5	2123	G	Sidechain
11	5	2124	G	Sidechain
11	5	2125	G	Sidechain
11	5	2126	A	Sidechain
11	5	2127	G	Sidechain
11	5	2129	C	Sidechain
11	5	2130	U	Sidechain
11	5	2133	G	Sidechain
11	5	2139	U	Sidechain
11	5	2140	G	Sidechain
11	5	2142	A	Sidechain
11	5	2143	C	Sidechain
11	5	2146	C	Sidechain
11	5	2147	A	Sidechain
11	5	2148	G	Sidechain
11	5	2150	C	Sidechain
11	5	2151	U	Sidechain
11	5	2153	C	Sidechain
11	5	2157	G	Sidechain
11	5	2159	G	Sidechain
11	5	2160	C	Sidechain
11	5	2161	C	Sidechain
11	5	2162	G	Sidechain
11	5	2165	C	Sidechain
11	5	2169	A	Sidechain
11	5	2170	A	Sidechain
11	5	2171	A	Sidechain
11	5	2172	U	Sidechain
11	5	2174	C	Sidechain
11	5	2175	C	Sidechain
11	5	2179	C	Sidechain
11	5	2180	U	Sidechain

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Mol	Chain	Res	Type	Group
11	5	2182	U	Sidechain
11	5	2184	A	Sidechain
11	5	2187	U	Sidechain
11	5	2188	U	Sidechain
11	5	2189	U	Sidechain
11	5	2190	G	Sidechain
11	5	2192	U	Sidechain
11	5	2193	G	Sidechain
11	5	2194	U	Sidechain
2	E	92	HIS	Sidechain
4	T	77	ARG	Sidechain
5	U	48	VAL	Peptide
5	U	5	ARG	Sidechain
5	U	94	PHE	Sidechain
6	Y	26	PHE	Sidechain
1	y	216	HIS	Sidechain
1	y	248	TYR	Sidechain
1	y	25	PHE	Sidechain
1	y	309	TYR	Sidechain
1	y	390	PHE	Sidechain
1	y	400	TYR	Sidechain

5.2 Too-close contacts (i)

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	y	3361	0	3514	0	0
2	E	433	0	466	24	0
3	G	457	0	481	63	0
4	T	787	0	846	5	0
5	U	789	0	847	4	0
6	Y	509	0	543	3	0
7	1	1350	0	676	1	0
8	2	775	0	385	0	0
9	3	387	0	196	0	0
10	4	1312	0	659	3	0
11	5	2305	0	1156	4	0
All	All	12465	0	9769	84	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 11.

All (84) 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)
2:E:126:ARG:HE	3:G:68:LEU:CD2	1.54	1.20
2:E:126:ARG:CB	3:G:68:LEU:HD21	1.73	1.18
2:E:126:ARG:NH2	3:G:65:ILE:HG12	1.68	1.08
2:E:126:ARG:HE	3:G:68:LEU:HD22	1.02	1.08
2:E:126:ARG:HB3	3:G:68:LEU:CD2	1.87	1.04
3:G:22:LEU:CG	3:G:26:LYS:HE3	1.91	1.00
3:G:28:ALA:O	3:G:32:ALA:CB	2.12	0.98
2:E:126:ARG:NE	3:G:68:LEU:HD22	1.79	0.95
2:E:126:ARG:HB3	3:G:68:LEU:HD21	0.95	0.95
3:G:55:MET:O	3:G:59:LEU:HG	1.65	0.94
3:G:62:LEU:O	3:G:66:ILE:HG13	1.69	0.93
3:G:29:ASP:OD1	3:G:30:MET:N	2.03	0.92
3:G:28:ALA:O	3:G:32:ALA:HB2	1.70	0.91
2:E:126:ARG:NE	3:G:68:LEU:CD2	2.33	0.87
3:G:22:LEU:HG	3:G:26:LYS:HE3	1.57	0.85
3:G:22:LEU:CD1	3:G:26:LYS:HE3	2.05	0.85
3:G:47:GLY:O	3:G:48:SER:HB3	1.76	0.85
3:G:50:ASN:OD1	3:G:54:ARG:NH1	2.11	0.84
3:G:18:GLY:HA2	3:G:63:PHE:CZ	2.14	0.82
3:G:22:LEU:HD11	3:G:26:LYS:HE3	1.62	0.81
2:E:126:ARG:CZ	3:G:65:ILE:HG12	2.11	0.79
2:E:126:ARG:HH22	3:G:65:ILE:HG12	1.43	0.79
3:G:28:ALA:O	3:G:32:ALA:HB3	1.83	0.78
3:G:53:THR:O	3:G:56:THR:OG1	2.03	0.75
3:G:73:ILE:HG22	3:G:73:ILE:O	1.88	0.71
3:G:47:GLY:O	3:G:48:SER:CB	2.38	0.71
2:E:126:ARG:CG	3:G:68:LEU:HD21	2.24	0.67
3:G:62:LEU:O	3:G:66:ILE:CG1	2.43	0.66
3:G:18:GLY:CA	3:G:63:PHE:CZ	2.78	0.65
3:G:22:LEU:HD21	3:G:26:LYS:NZ	2.12	0.64
2:E:126:ARG:NH2	3:G:65:ILE:CG1	2.54	0.64
3:G:26:LYS:O	3:G:29:ASP:OD1	2.16	0.64
2:E:126:ARG:CG	3:G:68:LEU:CD2	2.76	0.63
3:G:43:PHE:CD2	3:G:43:PHE:N	2.63	0.63
2:E:126:ARG:NH1	3:G:65:ILE:HG12	2.14	0.62
2:E:126:ARG:CB	3:G:68:LEU:CD2	2.63	0.62
3:G:22:LEU:CD2	3:G:26:LYS:HE3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:ARG:O	3:G:68:LEU:HD11	2.01	0.60
2:E:126:ARG:HE	3:G:68:LEU:HD23	1.56	0.59
3:G:43:PHE:HD2	3:G:43:PHE:N	1.99	0.59
3:G:22:LEU:HD11	3:G:26:LYS:CE	2.34	0.57
11:5:2162:G:H22	11:5:2164:C:H4'	1.69	0.57
3:G:65:ILE:O	3:G:68:LEU:HB3	2.04	0.57
3:G:43:PHE:H	3:G:43:PHE:HD2	1.53	0.56
3:G:17:VAL:HA	3:G:20:ILE:HD12	1.88	0.55
3:G:63:PHE:HA	3:G:66:ILE:HD12	1.88	0.55
5:U:12:VAL:HG12	5:U:14:THR:H	1.72	0.54
4:T:3:ARG:HE	4:T:42:GLU:HG2	1.73	0.54
3:G:22:LEU:HD21	3:G:26:LYS:CE	2.38	0.53
2:E:126:ARG:NH2	3:G:65:ILE:HA	2.24	0.53
3:G:35:GLY:HA2	3:G:42:LEU:HD12	1.92	0.52
3:G:22:LEU:HG	3:G:26:LYS:CE	2.37	0.52
3:G:58:LEU:O	3:G:62:LEU:HG	2.11	0.51
4:T:4:GLU:H	4:T:7:LEU:HD23	1.76	0.50
3:G:22:LEU:HD21	3:G:26:LYS:HE3	1.93	0.49
4:T:58:VAL:HG22	4:T:85:VAL:HG13	1.94	0.48
3:G:55:MET:O	3:G:59:LEU:CG	2.52	0.48
2:E:126:ARG:HH21	3:G:65:ILE:HA	1.78	0.48
3:G:26:LYS:O	3:G:30:MET:HG3	2.15	0.47
10:4:1885:A:C8	10:4:1886:U:C5	3.03	0.47
11:5:2104:C:OP1	11:5:2104:C:H4'	2.14	0.46
3:G:58:LEU:O	3:G:62:LEU:CG	2.64	0.46
11:5:2196:C:H2'	11:5:2197:U:C6	2.51	0.46
10:4:1865:U:C5	10:4:1875:G:C6	3.04	0.45
3:G:18:GLY:CA	3:G:63:PHE:HZ	2.28	0.45
11:5:2128:G:C6	11:5:2160:C:C5	3.05	0.45
7:1:80:G:C2	7:1:107:G:C2	3.05	0.45
3:G:22:LEU:O	3:G:26:LYS:HG3	2.16	0.45
4:T:61:LEU:HD23	4:T:61:LEU:N	2.32	0.44
2:E:95:LEU:HD12	2:E:95:LEU:H	1.82	0.44
2:E:126:ARG:HG2	3:G:68:LEU:CD2	2.48	0.43
2:E:126:ARG:HH22	3:G:65:ILE:CG1	2.22	0.43
6:Y:60:LYS:HG3	6:Y:62:GLY:O	2.20	0.42
3:G:29:ASP:HA	3:G:32:ALA:HB3	2.01	0.42
3:G:35:GLY:HA2	3:G:42:LEU:CD1	2.50	0.42
10:4:1873:G:C6	10:4:1874:C:C4	3.08	0.42
5:U:35:VAL:HB	5:U:38:ILE:HD11	2.02	0.41
6:Y:23:ARG:H	6:Y:26:PHE:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:1:ALA:HB3	5:U:84:PHE:CE1	2.55	0.41
5:U:32:LYS:HB3	5:U:63:ALA:HB1	2.03	0.41
2:E:126:ARG:NE	3:G:68:LEU:HD23	2.25	0.41
2:E:126:ARG:HG2	3:G:68:LEU:HD23	2.03	0.41
4:T:92:ASN:HD22	4:T:94:ASP:H	1.68	0.41
6:Y:38:GLN:HE21	6:Y:43:LEU:CD1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	y	435/437 (100%)	386 (89%)	27 (6%)	22 (5%)	2 30
2	E	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	4 38
3	G	63/65 (97%)	50 (79%)	7 (11%)	6 (10%)	1 15
4	T	98/100 (98%)	71 (72%)	18 (18%)	9 (9%)	1 17
5	U	101/103 (98%)	79 (78%)	13 (13%)	9 (9%)	1 17
6	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	5 40
All	All	812/824 (98%)	683 (84%)	79 (10%)	50 (6%)	4 26

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	142	MET
1	y	258	TYR
1	y	266	PRO
1	y	338	ASN
1	y	340	ARG
1	y	355	GLY

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Mol	Chain	Res	Type
1	y	356	ILE
3	G	44	GLY
3	G	48	SER
3	G	51	PHE
5	U	49	PRO
1	y	215	LEU
1	y	270	ASN
1	y	354	PRO
1	y	394	ALA
3	G	45	SER
3	G	52	MET
4	T	10	VAL
4	T	21	SER
5	U	12	VAL
5	U	47	PRO
1	y	313	GLY
2	E	89	GLU
2	E	125	LEU
3	G	35	GLY
4	T	18	GLU
4	T	52	GLU
4	T	86	THR
5	U	73	ASN
5	U	80	ASP
6	Y	2	LYS
6	Y	37	LEU
1	y	183	ILE
1	y	311	GLN
1	y	396	LYS
4	T	36	LYS
5	U	7	ASP
5	U	81	ARG
1	y	214	ASP
1	y	255	ARG
1	y	269	VAL
4	T	38	ALA
4	T	76	ARG
5	U	5	ARG
5	U	74	ALA
1	y	256	ARG
1	y	350	GLY
1	y	246	VAL

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Mol	Chain	Res	Type
4	T	74	ILE
1	y	274	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	y	353/353 (100%)	336 (95%)	17 (5%)	31 67
2	E	47/47 (100%)	45 (96%)	2 (4%)	35 70
3	G	46/46 (100%)	43 (94%)	3 (6%)	21 58
4	T	84/84 (100%)	80 (95%)	4 (5%)	31 67
5	U	84/84 (100%)	81 (96%)	3 (4%)	42 74
6	Y	55/55 (100%)	54 (98%)	1 (2%)	66 87
All	All	669/669 (100%)	639 (96%)	30 (4%)	38 69

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	149	VAL
1	y	174	LEU
1	y	223	VAL
1	y	244	ILE
1	y	255	ARG
1	y	264	HIS
1	y	265	LEU
1	y	267	LEU
1	y	268	LYS
1	y	269	VAL
1	y	298	THR
1	y	310	LEU
1	y	312	PRO
1	y	349	SER
1	y	370	MET
1	y	397	VAL

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Mol	Chain	Res	Type
1	y	409	VAL
2	E	76	ARG
2	E	90	THR
3	G	43	PHE
3	G	45	SER
3	G	46	SER
4	T	1	MET
4	T	10	VAL
4	T	61	LEU
4	T	73	ARG
5	U	4	ILE
5	U	23	LYS
5	U	49	PRO
6	Y	41	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	10	GLN
1	y	252	GLN
4	T	15	HIS
4	T	59	ASN
4	T	70	HIS
4	T	92	ASN
6	Y	38	GLN
6	Y	41	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	60/61 (98%)	2 (3%)	0
11	5	107/108 (99%)	37 (34%)	8 (7%)
7	1	62/63 (98%)	12 (19%)	0
8	2	35/36 (97%)	7 (20%)	2 (5%)
9	3	17/18 (94%)	5 (29%)	0
All	All	281/286 (98%)	63 (22%)	10 (3%)

All (63) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	1	63	A
7	1	64	A
7	1	71	A
7	1	74	A
7	1	75	G
7	1	84	A
7	1	90	U
7	1	92	U
7	1	95	A
7	1	100	U
7	1	102	U
7	1	103	A
8	2	1312	U
8	2	1313	U
8	2	1316	U
8	2	1325	U
8	2	1326	U
8	2	1334	G
8	2	1336	A
9	3	1532	A
9	3	1535	A
9	3	1536	C
9	3	1538	G
9	3	1540	G
10	4	1870	C
10	4	1896	G
11	5	2102	G
11	5	2104	C
11	5	2111	U
11	5	2116	G
11	5	2117	A
11	5	2118	U
11	5	2119	A
11	5	2120	G
11	5	2121	G
11	5	2126	A
11	5	2127	G
11	5	2128	G
11	5	2130	U
11	5	2132	U
11	5	2135	A
11	5	2136	G
11	5	2137	U

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Mol	Chain	Res	Type
11	5	2145	C
11	5	2146	C
11	5	2147	A
11	5	2148	G
11	5	2149	U
11	5	2153	C
11	5	2155	U
11	5	2158	A
11	5	2160	C
11	5	2163	A
11	5	2164	C
11	5	2165	C
11	5	2166	U
11	5	2167	U
11	5	2176	A
11	5	2179	C
11	5	2181	U
11	5	2192	U
11	5	2198	A
11	5	2199	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	2	1312	U
8	2	1332	G
11	5	2116	G
11	5	2120	G
11	5	2126	A
11	5	2144	G
11	5	2145	C
11	5	2152	G
11	5	2164	C
11	5	2172	U

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

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

5.5 Carbohydrates

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.