Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 09:58 PM EST

PDB ID	:	3J46
EMDB ID	:	EMD-5693
Title	:	Structure of the SecY protein translocation channel in action
Authors	:	Akey, C.W.; Park, E.; Menetret, J.F.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.; Rapoport, T.A.
Deposited on	:	2013-06-18
Resolution	:	10.10 Å(reported)
Based on initial models	:	3I8G, 2I2P, 3J01

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

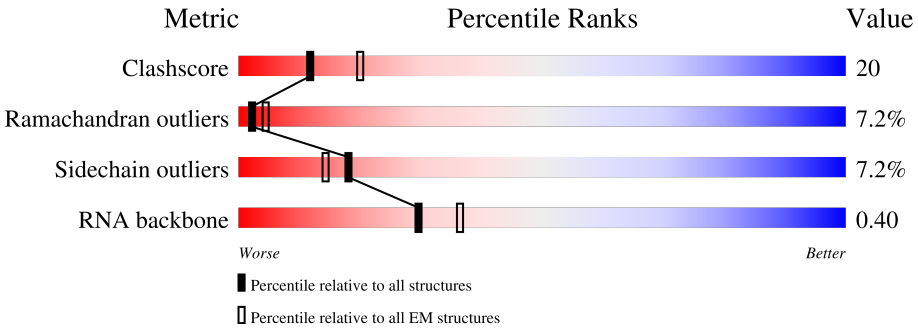
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 10.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	y	437	13% 73% 20% 5%
2	E	56	23% 46% 48% 5%
3	G	67	10% 58% 31% 7%
4	n	101	44% 59% 30% 6% 5%
5	p	76	16% 45% 50% 5%
6	a	76	25% 61% 36%
7	5	234	14% 75% 22%

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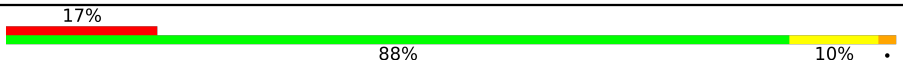
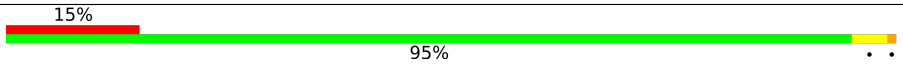
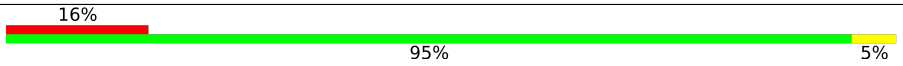
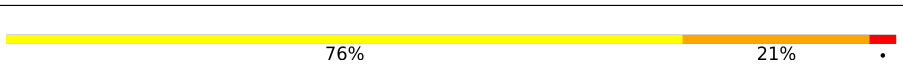
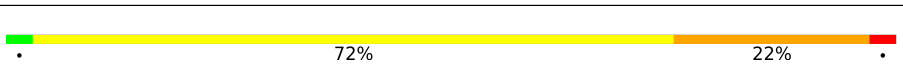
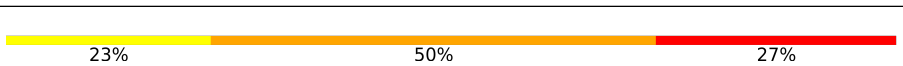
Mol	Chain	Length	Quality of chain
8	T	100	
9	U	103	
10	Y	63	
11	1	63	
12	2	36	
13	3	44	
14	4	109	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 17478 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
			Total	C	N	O	S		
1	y	437	3361	2220	554	569	18	0	1

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	ACETYLATION	UNP P0AGA2
y	68	CYS	SER	ENGINEERED MUTATION	UNP P0AGA2
y	441	NH2	-	AMIDATION	UNP P0AGA2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	56	433	283	76	73	1	0	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
			Total	C	N	O	S		
3	G	67	461	301	74	82	4	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	ACE	-	ACETYLATION	UNP P0AG99
G	74	NH2	-	AMIDATION	UNP P0AG99

- Molecule 4 is a protein called NC100.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	101	Total	C	N	O	S	0	0
			760	480	132	146	2		

- Molecule 5 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 6 is a RNA chain called A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

- Molecule 7 is a protein called 50S ribosomal protein L1.

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

- Molecule 8 is a protein called 50S ribosomal protein L23P.

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

- Molecule 9 is a protein called 50S ribosomal protein L24P.

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

- Molecule 10 is a protein called 50S ribosomal protein L29P.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 12 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 13 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	44	Total	C	N	O	P	0	0
			948	423	180	301	44		

- Molecule 14 is a RNA chain called 23S ribosomal RNA.

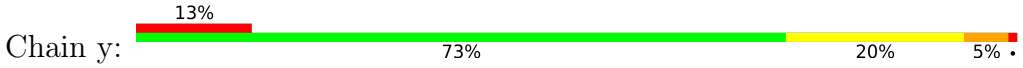
Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	109	Total	C	N	O	P	0	0
			2325	1038	409	769	109		

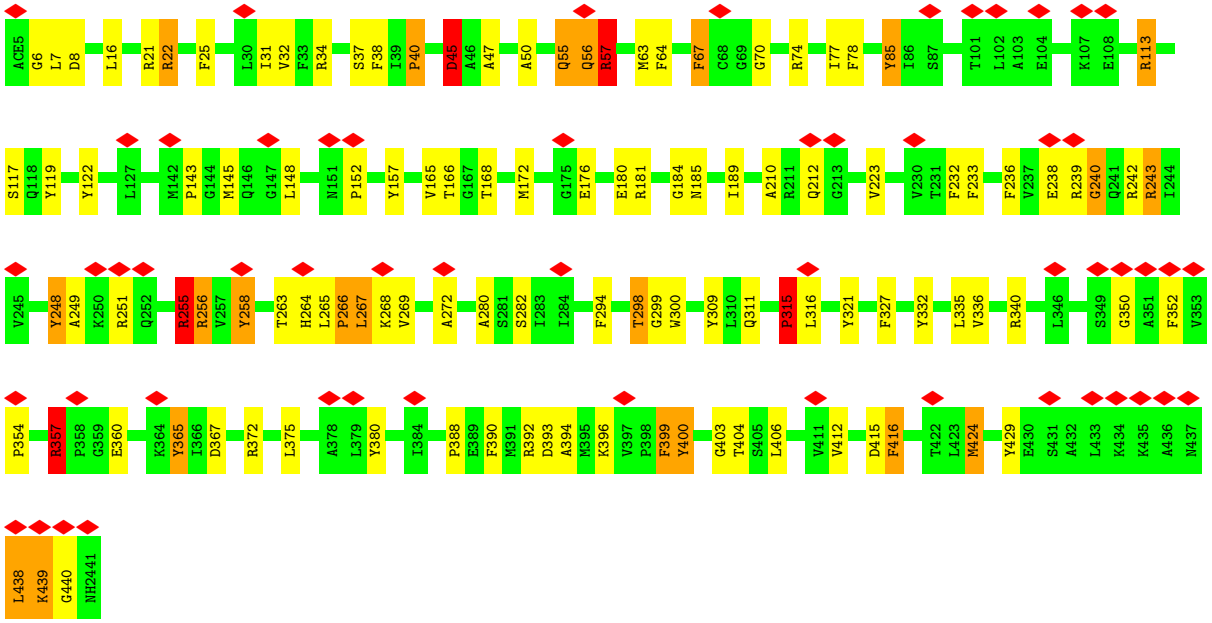
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

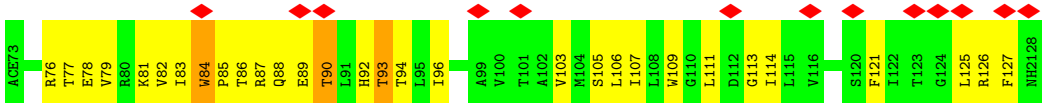
Chain y:





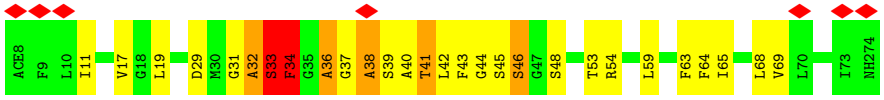
• Molecule 2: Preprotein translocase subunit SecE

Chain E:



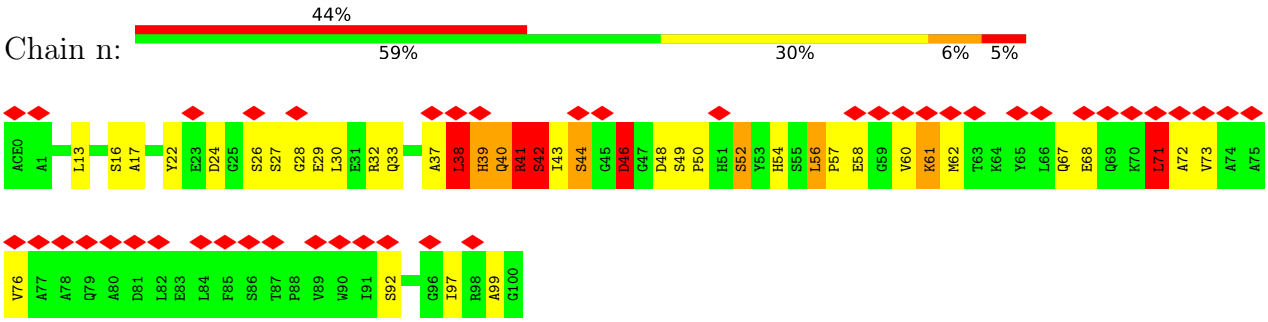
• Molecule 3: Protein-export membrane protein SecG

Chain G:



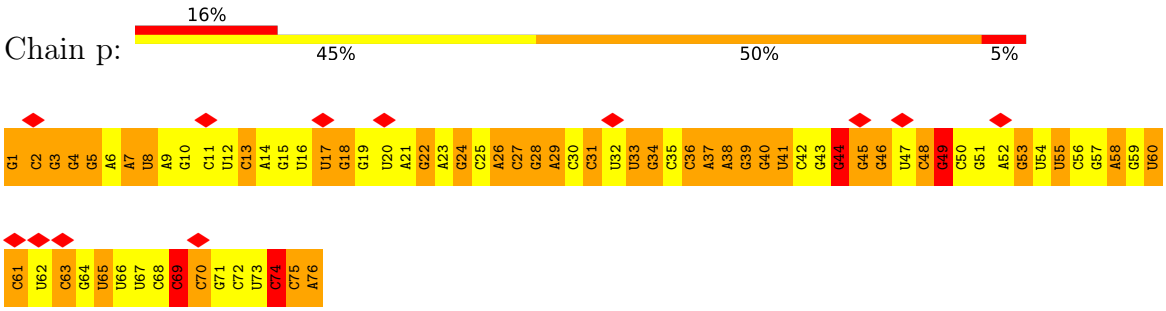
• Molecule 4: NC100

Chain n:



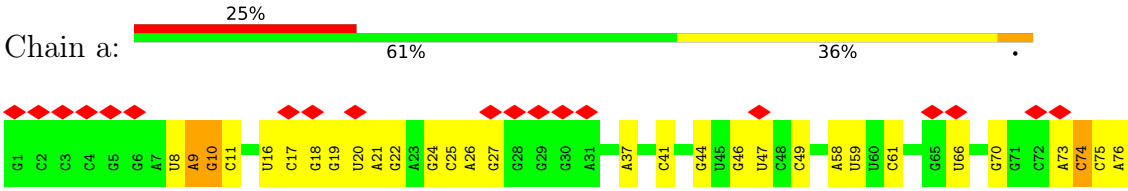
• Molecule 5: P-tRNA

Chain p:



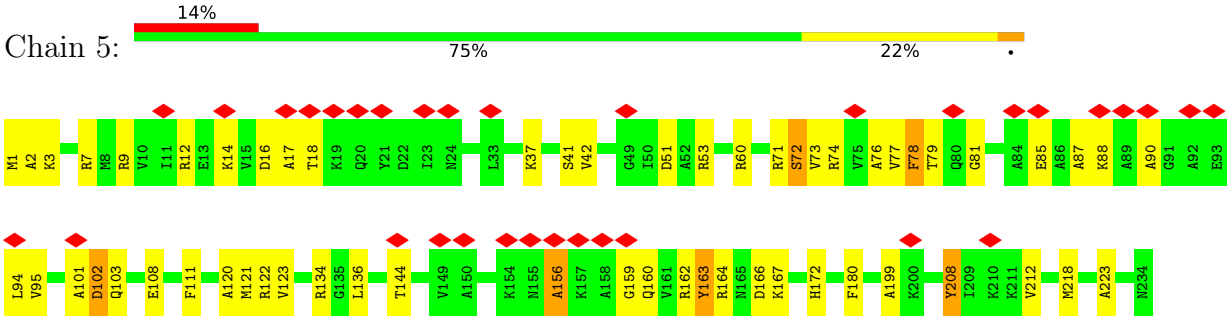
• Molecule 6: A-tRNA

Chain a:



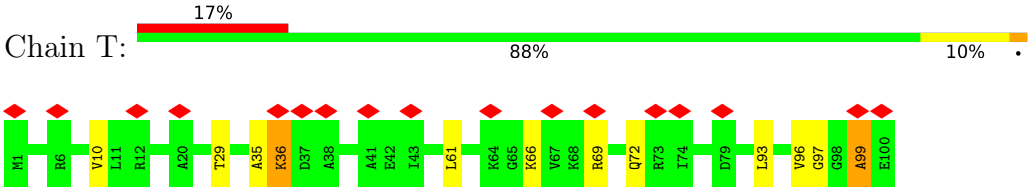
• Molecule 7: 50S ribosomal protein L1

Chain 5:



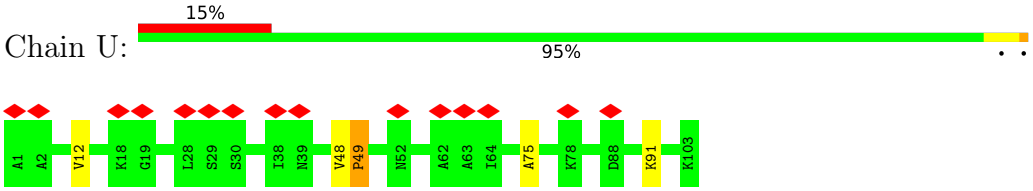
• Molecule 8: 50S ribosomal protein L23P

Chain T:



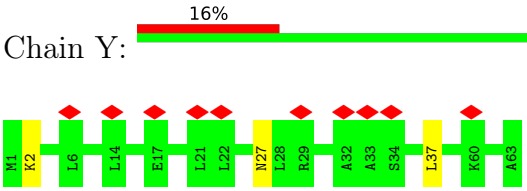
• Molecule 9: 50S ribosomal protein L24P

Chain U:



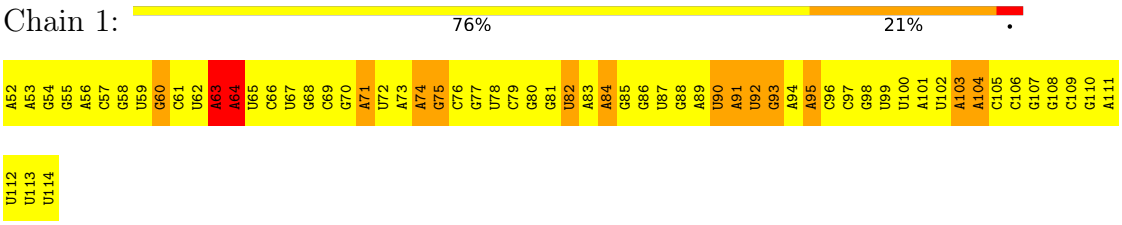
• Molecule 10: 50S ribosomal protein L29P

Chain Y:



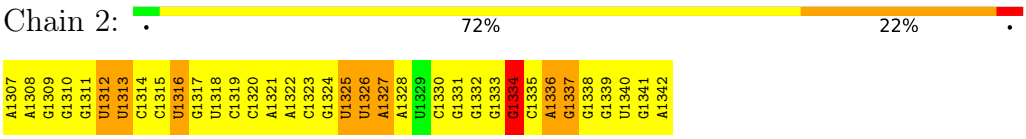
• Molecule 11: 23S ribosomal RNA

Chain 1:



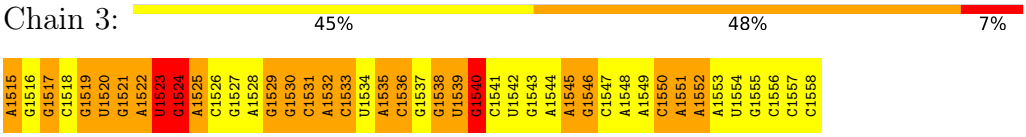
• Molecule 12: 23S ribosomal RNA

Chain 2:



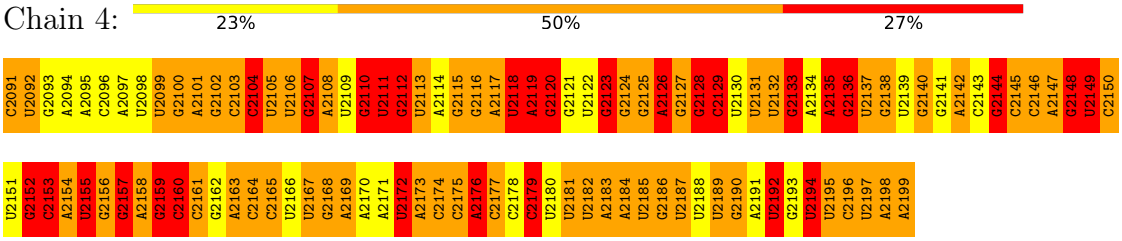
• Molecule 13: 23S ribosomal RNA

Chain 3:



• Molecule 14: 23S ribosomal RNA

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	42000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	3.245	Depositor
Minimum map value	-0.464	Depositor
Average map value	0.072	Depositor
Map value standard deviation	0.294	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.12, 2.12, 2.12	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	y	1.71	27/3434 (0.8%)	2.07	97/4657 (2.1%)
2	E	1.70	3/437 (0.7%)	2.26	24/596 (4.0%)
3	G	1.65	3/463 (0.6%)	2.12	17/622 (2.7%)
4	n	1.63	2/774 (0.3%)	1.60	14/1048 (1.3%)
5	p	3.30	222/1810 (12.3%)	3.82	397/2820 (14.1%)
6	a	0.35	0/1783	0.77	4/2776 (0.1%)
7	5	1.66	11/1748 (0.6%)	1.92	30/2355 (1.3%)
8	T	0.98	0/794	1.09	1/1060 (0.1%)
9	U	0.96	0/797	1.04	0/1062
10	Y	1.00	0/510	0.90	0/677
11	1	1.62	1/1511 (0.1%)	2.50	178/2354 (7.6%)
12	2	1.63	1/867 (0.1%)	2.45	97/1351 (7.2%)
13	3	3.35	127/1062 (12.0%)	3.85	256/1655 (15.5%)
14	4	3.46	373/2599 (14.4%)	3.88	636/4049 (15.7%)
All	All	2.21	770/18589 (4.1%)	2.66	1751/27082 (6.5%)

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	2	18
2	E	0	2
3	G	0	1
4	n	3	0
5	p	0	29
6	a	0	1
7	5	0	3
9	U	0	1
11	1	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	2	0	2
13	3	0	19
14	4	0	63
All	All	5	141

All (770) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	n	99	ALA	C-N	31.42	1.89	1.33
13	3	1516	G	O3'-P	25.56	1.91	1.61
4	n	22	TYR	C-N	22.00	1.84	1.34
13	3	1551	A	O3'-P	17.96	1.82	1.61
14	4	2098	U	C2-N3	14.56	1.48	1.37
13	3	1522	A	N7-C5	-14.50	1.30	1.39
14	4	2141	G	C2-N3	13.51	1.43	1.32
13	3	1528	A	N7-C5	-13.18	1.31	1.39
13	3	1548	A	N7-C5	-13.14	1.31	1.39
14	4	2156	G	N9-C8	13.06	1.47	1.37
14	4	2126	A	C6-N6	12.97	1.44	1.33
13	3	1551	A	N7-C5	-12.74	1.31	1.39
5	p	64	G	C8-N7	12.72	1.38	1.30
5	p	11	C	N3-C4	12.71	1.42	1.33
14	4	2148	G	N1-C2	12.63	1.47	1.37
5	p	51	G	C6-N1	12.37	1.48	1.39
14	4	2157	G	C6-N1	12.36	1.48	1.39
5	p	21	A	N9-C8	12.34	1.47	1.37
13	3	1519	G	C6-N1	12.33	1.48	1.39
14	4	2121	G	N9-C8	12.24	1.46	1.37
14	4	2198	A	C6-N6	12.23	1.43	1.33
14	4	2094	A	N9-C4	12.19	1.45	1.37
14	4	2141	G	N1-C2	12.07	1.47	1.37
5	p	6	A	N7-C5	-12.07	1.32	1.39
14	4	2161	C	N1-C6	12.03	1.44	1.37
14	4	2148	G	C2-N3	11.90	1.42	1.32
5	p	5	G	C6-N1	11.90	1.47	1.39
14	4	2101	A	N7-C5	-11.90	1.32	1.39
14	4	2183	A	C5-C4	11.67	1.47	1.38
14	4	2168	G	N7-C5	-11.66	1.32	1.39
14	4	2137	U	C2-N3	11.65	1.46	1.37
14	4	2127	G	C2-N3	11.61	1.42	1.32
13	3	1538	G	C6-N1	11.38	1.47	1.39
5	p	15	G	C6-N1	11.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	58	A	C2'-C1'	-11.33	1.40	1.53
13	3	1540	G	N9-C8	11.31	1.45	1.37
5	p	59	G	N7-C5	-11.08	1.32	1.39
13	3	1519	G	N1-C2	11.06	1.46	1.37
5	p	7	A	C6-N6	11.03	1.42	1.33
13	3	1543	G	C2-N3	10.96	1.41	1.32
14	4	2101	A	C6-N1	10.95	1.43	1.35
5	p	40	G	N7-C5	10.84	1.45	1.39
13	3	1549	A	C6-N6	10.77	1.42	1.33
14	4	2130	U	C4-C5	10.65	1.53	1.43
5	p	15	G	N7-C5	-10.57	1.32	1.39
14	4	2168	G	C5-C4	-10.47	1.31	1.38
5	p	21	A	N9-C4	10.46	1.44	1.37
5	p	68	C	N3-C4	10.43	1.41	1.33
14	4	2190	G	C6-N1	10.43	1.46	1.39
13	3	1531	C	C4-N4	10.41	1.43	1.33
5	p	65	U	N1-C2	10.37	1.47	1.38
14	4	2093	G	C6-N1	10.34	1.46	1.39
5	p	53	G	C6-N1	10.27	1.46	1.39
14	4	2125	G	N7-C5	-10.22	1.33	1.39
5	p	44	G	N9-C8	-10.19	1.30	1.37
5	p	13	C	C4-N4	10.16	1.43	1.33
14	4	2134	A	N7-C5	-10.13	1.33	1.39
5	p	1	G	N9-C4	10.09	1.46	1.38
14	4	2095	A	C6-N6	10.01	1.42	1.33
5	p	40	G	C2-N3	10.00	1.40	1.32
14	4	2097	A	C6-N6	9.97	1.42	1.33
14	4	2187	U	P-O5'	9.92	1.69	1.59
14	4	2178	C	N3-C4	9.89	1.40	1.33
13	3	1531	C	N3-C4	9.80	1.40	1.33
14	4	2145	C	C4-N4	9.79	1.42	1.33
13	3	1545	A	N7-C5	-9.75	1.33	1.39
14	4	2159	G	C2-N3	9.74	1.40	1.32
14	4	2117	A	C5-C4	9.71	1.45	1.38
5	p	39	G	C2-N3	9.65	1.40	1.32
14	4	2193	G	N9-C8	9.59	1.44	1.37
14	4	2096	C	N3-C4	9.57	1.40	1.33
13	3	1547	C	N1-C6	9.56	1.42	1.37
14	4	2148	G	C8-N7	-9.56	1.25	1.30
14	4	2163	A	N7-C5	-9.44	1.33	1.39
14	4	2160	C	N3-C4	9.43	1.40	1.33
14	4	2124	G	N7-C5	-9.43	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	52	A	C6-N6	9.42	1.41	1.33
14	4	2156	G	C6-N1	9.38	1.46	1.39
14	4	2157	G	N7-C5	-9.37	1.33	1.39
5	p	10	G	N7-C5	-9.35	1.33	1.39
5	p	5	G	N7-C5	-9.35	1.33	1.39
14	4	2164	C	C2-N3	9.32	1.43	1.35
13	3	1543	G	C2'-C1'	-9.30	1.43	1.53
14	4	2120	G	C5-C4	-9.30	1.31	1.38
5	p	72	C	N1-C2	-9.30	1.30	1.40
13	3	1530	G	N9-C4	9.29	1.45	1.38
13	3	1530	G	N1-C2	9.28	1.45	1.37
14	4	2091	C	N3-C4	9.27	1.40	1.33
14	4	2169	A	N7-C5	-9.24	1.33	1.39
5	p	57	G	C6-N1	9.22	1.46	1.39
13	3	1523	U	C2-N3	9.21	1.44	1.37
14	4	2170	A	C2-N3	9.16	1.41	1.33
14	4	2131	U	C4-C5	-9.16	1.35	1.43
5	p	37	A	C5-C4	9.15	1.45	1.38
14	4	2104	C	P-O5'	-9.10	1.50	1.59
14	4	2190	G	N7-C5	9.10	1.44	1.39
14	4	2096	C	N1-C6	9.07	1.42	1.37
5	p	51	G	C2-N2	9.05	1.43	1.34
14	4	2101	A	C6-N6	9.05	1.41	1.33
14	4	2192	U	N1-C2	9.00	1.46	1.38
14	4	2123	G	N1-C2	8.96	1.45	1.37
14	4	2108	A	N7-C5	-8.93	1.33	1.39
5	p	30	C	P-O5'	-8.93	1.50	1.59
14	4	2143	C	C5'-C4'	8.89	1.62	1.51
5	p	7	A	C6-N1	8.88	1.41	1.35
14	4	2125	G	C8-N7	-8.85	1.25	1.30
14	4	2176	A	N7-C5	-8.81	1.33	1.39
14	4	2110	G	C2-N3	8.79	1.39	1.32
13	3	1542	U	C2-N3	-8.79	1.31	1.37
14	4	2093	G	N3-C4	-8.76	1.29	1.35
5	p	56	C	N1-C6	-8.74	1.31	1.37
5	p	53	G	C2-N3	8.69	1.39	1.32
14	4	2169	A	N9-C4	8.65	1.43	1.37
14	4	2099	U	N3-C4	8.60	1.46	1.38
5	p	47	U	N3-C4	8.59	1.46	1.38
5	p	15	G	N9-C8	-8.58	1.31	1.37
14	4	2095	A	N7-C5	-8.58	1.34	1.39
14	4	2149	U	C2-N3	8.56	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	1527	G	C2-N2	8.55	1.43	1.34
14	4	2146	C	C4-N4	8.53	1.41	1.33
14	4	2159	G	C6-N1	8.52	1.45	1.39
14	4	2119	A	N9-C4	8.51	1.43	1.37
14	4	2112	G	C8-N7	-8.50	1.25	1.30
14	4	2132	U	C2-N3	8.47	1.43	1.37
14	4	2167	U	C2-N3	8.46	1.43	1.37
5	p	64	G	N9-C4	8.44	1.44	1.38
5	p	57	G	N7-C5	-8.43	1.34	1.39
14	4	2117	A	N7-C5	-8.43	1.34	1.39
5	p	9	A	N9-C4	8.42	1.42	1.37
14	4	2128	G	C6-N1	8.41	1.45	1.39
14	4	2141	G	C8-N7	-8.41	1.25	1.30
14	4	2101	A	C8-N7	-8.41	1.25	1.31
14	4	2150	C	C4-N4	8.39	1.41	1.33
14	4	2099	U	C2-N3	8.39	1.43	1.37
5	p	24	G	C4'-C3'	8.39	1.62	1.53
14	4	2147	A	N7-C5	-8.39	1.34	1.39
14	4	2189	U	O4'-C1'	8.39	1.52	1.41
14	4	2199	A	C8-N7	-8.38	1.25	1.31
14	4	2140	G	C5-C6	-8.38	1.33	1.42
5	p	40	G	C5-C4	8.36	1.44	1.38
14	4	2156	G	C5-C4	8.36	1.44	1.38
14	4	2189	U	C3'-C2'	-8.35	1.43	1.52
14	4	2147	A	C5-C4	8.35	1.44	1.38
14	4	2126	A	C5-C4	8.35	1.44	1.38
14	4	2091	C	N1-C6	-8.34	1.32	1.37
5	p	22	G	N1-C2	8.34	1.44	1.37
14	4	2112	G	C5'-C4'	8.33	1.61	1.51
5	p	18	G	N1-C2	8.32	1.44	1.37
14	4	2179	C	N3-C4	8.31	1.39	1.33
14	4	2186	G	C2-N3	8.29	1.39	1.32
5	p	1	G	C2-N2	8.29	1.42	1.34
14	4	2113	U	N3-C4	8.27	1.45	1.38
5	p	56	C	C2-N3	8.23	1.42	1.35
13	3	1546	G	N1-C2	8.23	1.44	1.37
5	p	64	G	C2-N3	8.23	1.39	1.32
14	4	2153	C	C4-C5	8.23	1.49	1.43
5	p	3	G	N7-C5	-8.22	1.34	1.39
5	p	16	U	N3-C4	8.20	1.45	1.38
5	p	57	G	C5-C6	-8.19	1.34	1.42
5	p	62	U	C2-N3	8.18	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2139	U	P-O5'	-8.14	1.51	1.59
14	4	2196	C	N1-C6	8.14	1.42	1.37
13	3	1536	C	C4-N4	8.13	1.41	1.33
7	5	60	ARG	CD-NE	8.13	1.60	1.46
14	4	2169	A	C6-N1	8.12	1.41	1.35
5	p	9	A	N7-C5	-8.11	1.34	1.39
14	4	2143	C	C4'-C3'	-8.10	1.44	1.53
5	p	60	U	C2-N3	8.08	1.43	1.37
5	p	9	A	C4'-C3'	8.06	1.62	1.53
5	p	50	C	C4-N4	8.06	1.41	1.33
5	p	10	G	N1-C2	8.06	1.44	1.37
14	4	2097	A	C6-N1	8.02	1.41	1.35
14	4	2123	G	N7-C5	-8.01	1.34	1.39
14	4	2100	G	C2-N3	7.99	1.39	1.32
14	4	2169	A	N3-C4	7.99	1.39	1.34
13	3	1547	C	N3-C4	7.99	1.39	1.33
5	p	12	U	C2-N3	7.98	1.43	1.37
14	4	2155	U	C5'-C4'	7.98	1.60	1.51
14	4	2106	U	C2-N3	7.98	1.43	1.37
14	4	2136	G	N1-C2	7.98	1.44	1.37
14	4	2123	G	C2-N3	7.96	1.39	1.32
14	4	2183	A	N9-C4	-7.96	1.33	1.37
14	4	2176	A	C5-C4	7.95	1.44	1.38
5	p	70	C	N3-C4	7.93	1.39	1.33
5	p	15	G	N3-C4	7.90	1.41	1.35
14	4	2093	G	C2'-C1'	-7.90	1.44	1.53
14	4	2172	U	C2'-C1'	-7.89	1.44	1.53
5	p	45	G	C2-N3	7.88	1.39	1.32
14	4	2128	G	C2-N3	7.88	1.39	1.32
5	p	66	U	C2-N3	7.85	1.43	1.37
5	p	28	G	C6-N1	7.82	1.45	1.39
13	3	1521	G	C2-N3	7.82	1.39	1.32
5	p	32	U	N3-C4	7.81	1.45	1.38
5	p	57	G	C2-N2	7.81	1.42	1.34
13	3	1522	A	N9-C4	-7.80	1.33	1.37
13	3	1527	G	C6-N1	7.80	1.45	1.39
5	p	34	G	C2-N3	7.76	1.39	1.32
14	4	2114	A	C4'-C3'	7.76	1.61	1.53
5	p	35	C	N3-C4	7.75	1.39	1.33
5	p	52	A	C1'-N9	7.75	1.60	1.48
5	p	1	G	N1-C2	7.74	1.44	1.37
5	p	13	C	C4-C5	7.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	29	A	N7-C5	-7.73	1.34	1.39
14	4	2197	U	N1-C6	7.72	1.44	1.38
5	p	48	C	N3-C4	7.72	1.39	1.33
5	p	19	G	N9-C8	-7.71	1.32	1.37
5	p	31	C	C2-N3	7.69	1.42	1.35
14	4	2172	U	C4'-C3'	7.69	1.61	1.53
14	4	2188	U	C2-N3	7.68	1.43	1.37
14	4	2121	G	C2-N2	7.68	1.42	1.34
5	p	24	G	C6-N1	7.67	1.45	1.39
13	3	1518	C	P-O5'	-7.67	1.52	1.59
5	p	75	C	C4-N4	7.65	1.40	1.33
14	4	2114	A	P-O5'	-7.65	1.52	1.59
14	4	2145	C	C4-C5	7.63	1.49	1.43
5	p	57	G	O3'-P	-7.62	1.52	1.61
14	4	2135	A	P-O5'	7.59	1.67	1.59
13	3	1536	C	N3-C4	7.59	1.39	1.33
14	4	2128	G	N1-C2	7.58	1.43	1.37
14	4	2190	G	N3-C4	7.57	1.40	1.35
14	4	2160	C	N1-C6	7.56	1.41	1.37
5	p	64	G	C5-C4	7.54	1.43	1.38
5	p	2	C	C5'-C4'	7.54	1.60	1.51
13	3	1539	U	C4'-C3'	-7.52	1.44	1.53
14	4	2176	A	C6-N6	7.52	1.40	1.33
14	4	2147	A	C6-N1	7.51	1.40	1.35
5	p	45	G	C8-N7	7.50	1.35	1.30
14	4	2183	A	C6-N1	7.50	1.40	1.35
14	4	2143	C	N3-C4	7.50	1.39	1.33
14	4	2116	G	N9-C8	-7.49	1.32	1.37
14	4	2171	A	C4'-C3'	7.49	1.61	1.53
14	4	2132	U	N3-C4	7.48	1.45	1.38
5	p	71	G	O3'-P	-7.42	1.52	1.61
14	4	2157	G	C8-N7	7.42	1.35	1.30
13	3	1525	A	N7-C5	-7.42	1.34	1.39
14	4	2135	A	C2-N3	7.40	1.40	1.33
14	4	2140	G	C6-N1	7.40	1.44	1.39
14	4	2113	U	C5'-C4'	7.38	1.60	1.51
14	4	2092	U	N3-C4	7.37	1.45	1.38
14	4	2194	U	C2-N3	7.37	1.43	1.37
13	3	1545	A	N3-C4	-7.35	1.30	1.34
14	4	2182	U	N3-C4	7.35	1.45	1.38
13	3	1531	C	P-O5'	-7.35	1.52	1.59
5	p	15	G	N1-C2	7.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	70	C	C5'-C4'	7.33	1.60	1.51
14	4	2111	U	N1-C2	7.33	1.45	1.38
5	p	53	G	C5-C4	7.32	1.43	1.38
13	3	1542	U	C4-C5	7.32	1.50	1.43
13	3	1540	G	C5-C6	-7.31	1.35	1.42
13	3	1548	A	N9-C4	7.30	1.42	1.37
14	4	2187	U	C4-C5	7.28	1.50	1.43
5	p	50	C	N3-C4	7.28	1.39	1.33
14	4	2175	C	N3-C4	7.27	1.39	1.33
14	4	2126	A	C8-N7	-7.26	1.26	1.31
13	3	1538	G	N1-C2	7.26	1.43	1.37
14	4	2199	A	C6-N1	7.24	1.40	1.35
14	4	2134	A	C2'-C1'	-7.24	1.45	1.53
14	4	2150	C	N3-C4	7.24	1.39	1.33
5	p	17	U	C2-N3	7.24	1.42	1.37
5	p	56	C	C4-C5	7.24	1.48	1.43
13	3	1530	G	C5'-C4'	7.23	1.60	1.51
14	4	2170	A	N9-C8	7.20	1.43	1.37
14	4	2163	A	C6-N6	7.20	1.39	1.33
5	p	61	C	C4-C5	7.19	1.48	1.43
13	3	1543	G	C5'-C4'	7.18	1.59	1.51
7	5	74	ARG	CD-NE	7.18	1.58	1.46
5	p	22	G	N7-C5	-7.17	1.34	1.39
14	4	2156	G	O3'-P	-7.16	1.52	1.61
5	p	36	C	N3-C4	7.16	1.39	1.33
13	3	1522	A	C6-N1	-7.16	1.30	1.35
5	p	49	G	N7-C5	7.16	1.43	1.39
13	3	1537	G	C8-N7	7.15	1.35	1.30
5	p	62	U	C5'-C4'	7.12	1.59	1.51
14	4	2124	G	C2-N3	7.12	1.38	1.32
14	4	2120	G	P-O5'	-7.10	1.52	1.59
14	4	2128	G	C5-C4	7.10	1.43	1.38
13	3	1527	G	C5-C6	-7.09	1.35	1.42
13	3	1551	A	C5-C4	-7.08	1.33	1.38
1	y	181	ARG	NE-CZ	7.07	1.42	1.33
14	4	2093	G	N7-C5	-7.05	1.35	1.39
13	3	1541	C	N3-C4	7.04	1.38	1.33
13	3	1543	G	C3'-C2'	7.04	1.60	1.52
5	p	53	G	N7-C5	-7.03	1.35	1.39
14	4	2125	G	N1-C2	7.03	1.43	1.37
5	p	34	G	N9-C4	7.02	1.43	1.38
14	4	2179	C	N1-C6	7.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2109	U	C2-O2	7.01	1.28	1.22
14	4	2167	U	P-O5'	-7.01	1.52	1.59
14	4	2144	G	C6-N1	7.00	1.44	1.39
5	p	10	G	C6-N1	7.00	1.44	1.39
14	4	2190	G	C6-O6	7.00	1.30	1.24
14	4	2184	A	C6-N1	7.00	1.40	1.35
14	4	2149	U	N1-C6	-6.99	1.31	1.38
5	p	3	G	C4'-C3'	6.99	1.60	1.53
14	4	2186	G	C5-C4	-6.99	1.33	1.38
14	4	2169	A	C6-N6	6.96	1.39	1.33
14	4	2182	U	C2'-C1'	-6.96	1.45	1.53
13	3	1522	A	N9-C8	-6.96	1.32	1.37
14	4	2119	A	N9-C8	-6.96	1.32	1.37
14	4	2108	A	C6-N6	6.95	1.39	1.33
13	3	1547	C	C4-N4	6.94	1.40	1.33
5	p	7	A	N9-C8	-6.92	1.32	1.37
14	4	2120	G	C6-O6	6.91	1.30	1.24
13	3	1521	G	C2'-C1'	-6.90	1.45	1.53
5	p	20	U	C2-N3	6.89	1.42	1.37
13	3	1533	C	N3-C4	6.88	1.38	1.33
14	4	2191	A	C5'-C4'	6.87	1.59	1.51
14	4	2119	A	N7-C5	6.86	1.43	1.39
14	4	2156	G	C2'-C1'	-6.86	1.45	1.53
7	5	162	ARG	CZ-NH1	6.85	1.42	1.33
5	p	23	A	N7-C5	-6.84	1.35	1.39
13	3	1530	G	P-O5'	-6.84	1.52	1.59
14	4	2163	A	N9-C8	-6.84	1.32	1.37
14	4	2110	G	O3'-P	-6.84	1.52	1.61
14	4	2184	A	C6-N6	6.84	1.39	1.33
5	p	48	C	C4-N4	6.83	1.40	1.33
5	p	3	G	C5-C6	6.82	1.49	1.42
5	p	32	U	N1-C2	6.82	1.44	1.38
14	4	2199	A	C1'-N9	6.82	1.58	1.48
5	p	37	A	C6-N1	6.81	1.40	1.35
5	p	54	U	C2-O2	6.79	1.28	1.22
14	4	2146	C	C4'-C3'	-6.78	1.45	1.53
14	4	2197	U	P-O5'	-6.78	1.52	1.59
1	y	157	TYR	CG-CD1	6.78	1.48	1.39
13	3	1521	G	O4'-C1'	6.78	1.50	1.41
5	p	51	G	C4'-C3'	6.77	1.60	1.53
13	3	1539	U	N1-C6	6.76	1.44	1.38
14	4	2152	G	N1-C2	6.75	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	1536	C	C4'-C3'	6.75	1.60	1.53
14	4	2121	G	C8-N7	6.73	1.34	1.30
14	4	2135	A	N9-C4	6.73	1.41	1.37
14	4	2137	U	C4-C5	-6.71	1.37	1.43
5	p	73	U	N1-C2	-6.70	1.32	1.38
14	4	2135	A	C5-C4	6.70	1.43	1.38
14	4	2109	U	N3-C4	6.69	1.44	1.38
13	3	1547	C	C2-N3	6.68	1.41	1.35
14	4	2181	U	C4-C5	6.68	1.49	1.43
5	p	3	G	C2-N3	6.67	1.38	1.32
5	p	20	U	C1'-N1	6.67	1.58	1.48
1	y	372	ARG	NE-CZ	6.67	1.41	1.33
14	4	2143	C	C4-C5	6.67	1.48	1.43
13	3	1524	G	P-O5'	-6.65	1.53	1.59
5	p	73	U	C5-C6	6.65	1.40	1.34
13	3	1539	U	N3-C4	6.64	1.44	1.38
14	4	2155	U	C3'-C2'	-6.64	1.45	1.52
14	4	2104	C	C1'-N1	6.64	1.58	1.48
14	4	2144	G	C3'-C2'	6.63	1.60	1.52
5	p	42	C	N3-C4	6.62	1.38	1.33
14	4	2120	G	C6-N1	6.62	1.44	1.39
5	p	32	U	C2-N3	6.61	1.42	1.37
5	p	58	A	C3'-O3'	6.61	1.51	1.42
13	3	1522	A	P-O5'	-6.61	1.53	1.59
5	p	58	A	O3'-P	-6.61	1.53	1.61
14	4	2139	U	C5'-C4'	6.60	1.59	1.51
1	y	74	ARG	CD-NE	6.59	1.57	1.46
5	p	61	C	C2-N3	6.59	1.41	1.35
14	4	2146	C	C2-O2	6.59	1.30	1.24
5	p	37	A	N9-C4	6.58	1.41	1.37
14	4	2172	U	N1-C2	6.58	1.44	1.38
5	p	71	G	C2'-C1'	-6.57	1.46	1.53
14	4	2113	U	C4'-C3'	6.57	1.60	1.53
5	p	68	C	O3'-P	-6.55	1.53	1.61
14	4	2190	G	C2-N3	6.55	1.38	1.32
14	4	2199	A	C6-N6	6.54	1.39	1.33
13	3	1529	G	C2-N3	6.54	1.38	1.32
13	3	1533	C	P-O5'	-6.53	1.53	1.59
5	p	64	G	N1-C2	6.53	1.43	1.37
5	p	44	G	C6-N1	6.52	1.44	1.39
5	p	29	A	C6-N6	6.51	1.39	1.33
5	p	25	C	N3-C4	6.50	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2173	A	C6-N1	-6.50	1.30	1.35
14	4	2165	C	C2-N3	6.50	1.41	1.35
13	3	1527	G	N3-C4	6.49	1.40	1.35
5	p	37	A	C6-N6	6.49	1.39	1.33
13	3	1524	G	C5'-C4'	6.49	1.59	1.51
14	4	2146	C	N1-C6	6.48	1.41	1.37
14	4	2179	C	C4-C5	-6.48	1.37	1.43
14	4	2092	U	O3'-P	-6.47	1.53	1.61
5	p	38	A	C5-C4	-6.46	1.34	1.38
14	4	2168	G	P-O5'	6.46	1.66	1.59
5	p	2	C	C1'-N1	6.46	1.58	1.48
5	p	60	U	O3'-P	-6.46	1.53	1.61
5	p	59	G	N3-C4	-6.46	1.30	1.35
14	4	2100	G	N9-C8	6.45	1.42	1.37
5	p	16	U	C3'-C2'	6.45	1.60	1.52
14	4	2143	C	C5-C6	6.45	1.39	1.34
14	4	2184	A	C8-N7	6.45	1.36	1.31
5	p	43	G	N7-C5	-6.45	1.35	1.39
14	4	2135	A	C2'-C1'	-6.45	1.46	1.53
5	p	20	U	P-O5'	6.44	1.66	1.59
5	p	26	A	C2'-C1'	-6.44	1.46	1.53
5	p	58	A	N3-C4	-6.44	1.30	1.34
13	3	1522	A	C6-N6	6.42	1.39	1.33
14	4	2168	G	C8-N7	6.42	1.34	1.30
14	4	2152	G	O4'-C1'	6.42	1.50	1.41
5	p	56	C	C5'-C4'	6.41	1.59	1.51
13	3	1533	C	N1-C6	6.41	1.41	1.37
13	3	1530	G	N3-C4	-6.40	1.30	1.35
5	p	51	G	C2-N3	6.39	1.37	1.32
13	3	1547	C	C3'-C2'	-6.39	1.45	1.52
14	4	2141	G	N7-C5	6.39	1.43	1.39
14	4	2107	G	N3-C4	6.37	1.40	1.35
5	p	59	G	C5-C4	6.37	1.42	1.38
14	4	2105	U	N1-C6	-6.36	1.32	1.38
14	4	2142	A	C6-N6	6.36	1.39	1.33
14	4	2111	U	C2-N3	6.35	1.42	1.37
14	4	2136	G	C2'-C1'	-6.35	1.46	1.53
14	4	2097	A	C5'-C4'	6.34	1.58	1.51
5	p	29	A	C6-N1	6.33	1.40	1.35
14	4	2120	G	O3'-P	-6.32	1.53	1.61
14	4	2155	U	C2-N3	6.32	1.42	1.37
1	y	400	TYR	CZ-OH	6.30	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2144	G	C5-C6	-6.30	1.36	1.42
14	4	2170	A	C6-N1	6.29	1.40	1.35
13	3	1530	G	C6-N1	6.28	1.44	1.39
14	4	2138	G	C6-N1	6.28	1.44	1.39
14	4	2102	G	P-O5'	-6.28	1.53	1.59
14	4	2199	A	N9-C8	-6.28	1.32	1.37
13	3	1532	A	C5'-C4'	6.28	1.58	1.51
14	4	2152	G	N7-C5	-6.26	1.35	1.39
5	p	37	A	N7-C5	-6.25	1.35	1.39
5	p	1	G	N9-C8	6.24	1.42	1.37
5	p	40	G	O3'-P	-6.24	1.53	1.61
5	p	43	G	C8-N7	6.24	1.34	1.30
14	4	2173	A	N1-C2	6.24	1.40	1.34
14	4	2095	A	C6-N1	-6.23	1.31	1.35
14	4	2162	G	C5-C6	6.23	1.48	1.42
14	4	2135	A	C5'-C4'	6.23	1.58	1.51
14	4	2110	G	N3-C4	6.23	1.39	1.35
5	p	51	G	P-O5'	-6.23	1.53	1.59
14	4	2096	C	O3'-P	-6.22	1.53	1.61
14	4	2121	G	C6-N1	-6.21	1.35	1.39
14	4	2145	C	C5'-C4'	6.21	1.58	1.51
13	3	1524	G	C2-N2	6.20	1.40	1.34
5	p	25	C	C3'-C2'	-6.20	1.46	1.52
5	p	75	C	N3-C4	-6.20	1.29	1.33
5	p	40	G	N1-C2	6.19	1.42	1.37
14	4	2092	U	P-O5'	6.19	1.66	1.59
14	4	2198	A	N9-C4	6.19	1.41	1.37
13	3	1536	C	C2'-C1'	-6.19	1.46	1.53
5	p	34	G	N7-C5	-6.19	1.35	1.39
14	4	2104	C	N3-C4	6.19	1.38	1.33
13	3	1519	G	N7-C5	-6.18	1.35	1.39
14	4	2127	G	N9-C4	6.18	1.42	1.38
14	4	2101	A	C2'-C1'	-6.18	1.46	1.53
14	4	2108	A	N9-C8	-6.18	1.32	1.37
14	4	2116	G	N9-C4	6.18	1.42	1.38
5	p	36	C	C4-N4	6.18	1.39	1.33
5	p	25	C	C5'-C4'	6.17	1.58	1.51
5	p	7	A	N7-C5	-6.16	1.35	1.39
1	y	37	SER	CA-CB	6.16	1.62	1.52
13	3	1525	A	C5-C4	6.15	1.43	1.38
14	4	2133	G	C6-N1	6.15	1.43	1.39
13	3	1529	G	N7-C5	-6.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2127	G	N3-C4	-6.14	1.31	1.35
14	4	2198	A	C1'-N9	-6.14	1.38	1.46
5	p	15	G	C2-N2	6.14	1.40	1.34
5	p	31	C	C5'-C4'	6.14	1.58	1.51
7	5	9	ARG	NE-CZ	6.13	1.41	1.33
5	p	26	A	N7-C5	-6.13	1.35	1.39
5	p	40	G	N9-C4	6.13	1.42	1.38
1	y	233	PHE	CG-CD1	6.12	1.48	1.38
14	4	2180	U	C4'-C3'	6.11	1.59	1.53
5	p	53	G	N3-C4	-6.10	1.31	1.35
7	5	2	ALA	CA-CB	6.10	1.65	1.52
14	4	2131	U	O3'-P	-6.10	1.53	1.61
3	G	19	LEU	N-CA	-6.10	1.34	1.46
14	4	2103	C	C4-C5	6.10	1.47	1.43
5	p	3	G	N9-C4	6.09	1.42	1.38
5	p	55	U	C5'-C4'	-6.09	1.44	1.51
5	p	10	G	C2-N3	6.09	1.37	1.32
13	3	1526	C	P-O5'	-6.09	1.53	1.59
1	y	350	GLY	CA-C	-6.08	1.42	1.51
14	4	2127	G	C8-N7	6.06	1.34	1.30
14	4	2148	G	C5-C4	-6.06	1.34	1.38
14	4	2101	A	C5'-C4'	6.05	1.58	1.51
14	4	2102	G	C2-N2	6.05	1.40	1.34
14	4	2170	A	C5-C4	6.05	1.43	1.38
5	p	65	U	C2-N3	6.04	1.42	1.37
1	y	360	GLU	CB-CG	6.04	1.63	1.52
14	4	2189	U	C5'-C4'	6.03	1.58	1.51
1	y	242	ARG	CD-NE	6.03	1.56	1.46
14	4	2149	U	N1-C2	6.02	1.44	1.38
5	p	11	C	O4'-C1'	6.02	1.49	1.41
5	p	74	C	C4'-C3'	-6.02	1.46	1.53
7	5	218	MET	C-N	6.01	1.43	1.33
14	4	2105	U	N1-C2	6.01	1.44	1.38
14	4	2121	G	N3-C4	6.00	1.39	1.35
14	4	2191	A	N9-C4	-6.00	1.34	1.37
5	p	13	C	C2-N3	5.99	1.40	1.35
13	3	1537	G	N1-C2	5.99	1.42	1.37
14	4	2181	U	C4'-C3'	5.99	1.59	1.53
14	4	2111	U	C1'-N1	5.99	1.57	1.48
5	p	23	A	N9-C8	5.98	1.42	1.37
14	4	2148	G	N3-C4	5.98	1.39	1.35
14	4	2100	G	N1-C2	5.97	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2129	C	C3'-C2'	5.97	1.59	1.52
13	3	1537	G	N3-C4	-5.96	1.31	1.35
14	4	2182	U	N1-C2	-5.95	1.33	1.38
5	p	20	U	C4'-O4'	5.94	1.53	1.45
13	3	1518	C	O3'-P	-5.94	1.54	1.61
14	4	2100	G	N7-C5	5.94	1.42	1.39
13	3	1518	C	C4'-O4'	-5.92	1.37	1.45
13	3	1544	A	C8-N7	5.92	1.35	1.31
14	4	2178	C	C4-N4	5.91	1.39	1.33
5	p	76	A	C5-C6	5.91	1.46	1.41
14	4	2104	C	N1-C2	5.91	1.46	1.40
14	4	2094	A	C2'-C1'	-5.90	1.46	1.53
5	p	67	U	C4'-C3'	-5.90	1.46	1.52
14	4	2132	U	C2-O2	5.90	1.27	1.22
14	4	2094	A	C6-N6	5.90	1.38	1.33
14	4	2194	U	N1-C6	-5.89	1.32	1.38
14	4	2136	G	C6-N1	5.89	1.43	1.39
14	4	2180	U	P-O5'	-5.89	1.53	1.59
1	y	248	TYR	CZ-OH	5.88	1.47	1.37
14	4	2127	G	P-O5'	5.87	1.65	1.59
14	4	2100	G	C4'-O4'	5.86	1.53	1.45
14	4	2144	G	C8-N7	5.86	1.34	1.30
13	3	1526	C	C4-N4	5.86	1.39	1.33
5	p	64	G	C5-C6	5.86	1.48	1.42
13	3	1546	G	C2'-C1'	-5.86	1.47	1.53
2	E	79	VAL	CB-CG2	5.85	1.65	1.52
14	4	2185	U	C2-N3	5.84	1.41	1.37
5	p	2	C	N3-C4	5.84	1.38	1.33
7	5	71	ARG	CZ-NH2	5.83	1.40	1.33
14	4	2101	A	N3-C4	-5.83	1.31	1.34
14	4	2103	C	N3-C4	5.83	1.38	1.33
5	p	46	G	O3'-P	-5.83	1.54	1.61
14	4	2112	G	O5'-C5'	5.82	1.53	1.44
14	4	2127	G	C4'-C3'	5.82	1.59	1.53
13	3	1536	C	C5-C6	-5.82	1.29	1.34
13	3	1540	G	C2-N3	5.82	1.37	1.32
14	4	2160	C	C4-N4	5.81	1.39	1.33
14	4	2107	G	P-O5'	-5.81	1.53	1.59
14	4	2092	U	C5-C6	-5.81	1.28	1.34
13	3	1528	A	C6-N1	5.80	1.39	1.35
1	y	357	ARG	CZ-NH2	5.80	1.40	1.33
14	4	2114	A	N7-C5	-5.79	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	52	A	N7-C5	-5.79	1.35	1.39
13	3	1526	C	C2-N3	5.79	1.40	1.35
7	5	41	SER	CA-CB	5.78	1.61	1.52
14	4	2188	U	C5-C6	5.78	1.39	1.34
14	4	2195	U	N1-C2	5.78	1.43	1.38
5	p	1	G	C2-N3	5.78	1.37	1.32
14	4	2112	G	C2-N2	5.78	1.40	1.34
13	3	1517	G	C2-N2	5.77	1.40	1.34
13	3	1522	A	C5-C4	5.77	1.42	1.38
5	p	54	U	C2-N3	5.76	1.41	1.37
1	y	242	ARG	CZ-NH1	5.76	1.40	1.33
5	p	27	C	C4'-C3'	-5.73	1.46	1.52
13	3	1537	G	C6-N1	5.73	1.43	1.39
14	4	2112	G	P-O5'	-5.72	1.54	1.59
14	4	2142	A	C2'-C1'	-5.72	1.47	1.53
14	4	2126	A	N9-C4	5.71	1.41	1.37
13	3	1540	G	C2'-C1'	5.71	1.59	1.53
5	p	38	A	C6-N1	5.70	1.39	1.35
1	y	233	PHE	CB-CG	5.69	1.61	1.51
13	3	1517	G	N9-C8	-5.69	1.33	1.37
14	4	2198	A	C6-N1	5.69	1.39	1.35
5	p	19	G	C5-C6	5.68	1.48	1.42
5	p	32	U	O4'-C1'	5.67	1.49	1.41
14	4	2178	C	C4'-C3'	-5.67	1.46	1.52
14	4	2186	G	C8-N7	5.67	1.34	1.30
14	4	2130	U	C4'-O4'	5.67	1.52	1.45
14	4	2181	U	N3-C4	5.67	1.43	1.38
5	p	27	C	N1-C6	5.67	1.40	1.37
14	4	2198	A	N7-C5	-5.66	1.35	1.39
14	4	2151	U	O4'-C1'	5.65	1.49	1.41
5	p	68	C	C4-C5	5.65	1.47	1.43
2	E	96	ILE	N-CA	5.65	1.57	1.46
14	4	2120	G	N9-C4	-5.65	1.33	1.38
14	4	2176	A	C5'-C4'	5.65	1.58	1.51
13	3	1549	A	N1-C2	5.64	1.39	1.34
14	4	2171	A	N7-C5	-5.64	1.35	1.39
5	p	15	G	C4'-C3'	-5.64	1.47	1.52
14	4	2183	A	C2-N3	5.63	1.38	1.33
14	4	2133	G	N1-C2	5.62	1.42	1.37
14	4	2134	A	C4'-C3'	5.62	1.59	1.53
14	4	2098	U	C1'-N1	5.62	1.57	1.48
14	4	2101	A	C5-C4	5.61	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2177	C	N1-C2	-5.61	1.34	1.40
5	p	42	C	N1-C2	5.60	1.45	1.40
14	4	2128	G	N7-C5	-5.59	1.35	1.39
5	p	7	A	P-O5'	-5.59	1.54	1.59
5	p	55	U	C3'-C2'	-5.59	1.46	1.52
14	4	2194	U	C3'-C2'	5.58	1.59	1.52
5	p	76	A	C6-N1	5.58	1.39	1.35
14	4	2191	A	C6-N6	5.58	1.38	1.33
5	p	8	U	C2-O2	5.57	1.27	1.22
14	4	2177	C	C4-N4	5.57	1.39	1.33
5	p	36	C	N1-C2	-5.57	1.34	1.40
5	p	27	C	O4'-C1'	5.56	1.48	1.41
1	y	380	TYR	CE2-CZ	5.55	1.45	1.38
1	y	70	GLY	CA-C	-5.55	1.43	1.51
14	4	2124	G	N9-C4	-5.54	1.33	1.38
14	4	2162	G	C3'-C2'	-5.54	1.46	1.52
5	p	60	U	C4'-C3'	5.54	1.59	1.53
1	y	255	ARG	CZ-NH2	5.53	1.40	1.33
5	p	13	C	C5-C6	-5.53	1.29	1.34
13	3	1534	U	N1-C6	-5.53	1.32	1.38
14	4	2137	U	C5'-C4'	5.52	1.57	1.51
5	p	22	G	C6-N1	5.51	1.43	1.39
14	4	2164	C	C3'-C2'	-5.51	1.46	1.52
13	3	1551	A	C6-N1	-5.51	1.31	1.35
13	3	1547	C	P-O5'	-5.50	1.54	1.59
14	4	2195	U	O3'-P	-5.50	1.54	1.61
13	3	1526	C	C2'-O2'	-5.50	1.34	1.41
13	3	1529	G	C3'-O3'	-5.49	1.34	1.42
13	3	1519	G	C2-N2	5.48	1.40	1.34
14	4	2144	G	C4'-C3'	5.47	1.59	1.53
14	4	2150	C	O5'-C5'	5.47	1.53	1.44
5	p	6	A	C6-N1	5.47	1.39	1.35
13	3	1548	A	C3'-C2'	5.47	1.58	1.52
13	3	1529	G	N9-C4	-5.46	1.33	1.38
13	3	1548	A	C8-N7	-5.46	1.27	1.31
14	4	2164	C	O4'-C1'	5.46	1.48	1.41
14	4	2147	A	N9-C8	5.46	1.42	1.37
5	p	5	G	C5-C6	5.45	1.47	1.42
5	p	19	G	O4'-C1'	5.45	1.48	1.41
5	p	53	G	C8-N7	-5.45	1.27	1.30
14	4	2143	C	N1-C2	5.45	1.45	1.40
14	4	2174	C	C4'-C3'	5.45	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	62	U	C4-O4	5.44	1.28	1.23
14	4	2130	U	C1'-N1	5.43	1.56	1.48
5	p	65	U	O4'-C1'	5.43	1.48	1.41
14	4	2146	C	C2'-C1'	-5.42	1.47	1.53
14	4	2169	A	C2'-C1'	-5.42	1.47	1.53
5	p	57	G	N9-C8	5.42	1.41	1.37
13	3	1540	G	N1-C2	5.42	1.42	1.37
14	4	2172	U	C5'-C4'	5.41	1.57	1.51
14	4	2187	U	C2-N3	5.41	1.41	1.37
5	p	64	G	N9-C8	-5.40	1.34	1.37
14	4	2174	C	C5-C6	-5.40	1.30	1.34
5	p	67	U	C4-C5	5.40	1.48	1.43
5	p	69	C	O3'-P	-5.40	1.54	1.61
5	p	6	A	N9-C4	-5.40	1.34	1.37
5	p	11	C	C5-C6	-5.39	1.30	1.34
5	p	5	G	C2-N3	5.39	1.37	1.32
5	p	48	C	C2-N3	5.39	1.40	1.35
13	3	1522	A	O3'-P	-5.38	1.54	1.61
5	p	15	G	C8-N7	5.38	1.34	1.30
5	p	75	C	C4-C5	-5.38	1.38	1.43
14	4	2098	U	N3-C4	5.38	1.43	1.38
5	p	8	U	C3'-C2'	-5.37	1.46	1.52
1	y	240	GLY	N-CA	-5.37	1.38	1.46
14	4	2153	C	N3-C4	5.36	1.37	1.33
13	3	1530	G	O3'-P	-5.36	1.54	1.61
14	4	2176	A	C2'-C1'	-5.36	1.47	1.53
14	4	2193	G	N1-C2	5.35	1.42	1.37
14	4	2171	A	C3'-C2'	5.35	1.58	1.52
5	p	43	G	C2-N2	5.35	1.39	1.34
14	4	2159	G	C8-N7	-5.35	1.27	1.30
14	4	2093	G	C5-C4	5.34	1.42	1.38
14	4	2126	A	C6-N1	5.34	1.39	1.35
14	4	2148	G	C6-N1	5.34	1.43	1.39
13	3	1535	A	C6-N6	5.34	1.38	1.33
14	4	2146	C	N3-C4	5.34	1.37	1.33
14	4	2168	G	N1-C2	5.34	1.42	1.37
5	p	22	G	N9-C4	5.33	1.42	1.38
13	3	1529	G	C5-C6	5.33	1.47	1.42
14	4	2144	G	C5'-C4'	5.33	1.57	1.51
2	E	103	VAL	CB-CG1	5.32	1.64	1.52
5	p	53	G	C2-N2	-5.32	1.29	1.34
13	3	1548	A	C6-N1	5.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	1551	A	C4'-C3'	-5.32	1.47	1.52
14	4	2143	C	N1-C6	5.32	1.40	1.37
13	3	1533	C	C2'-C1'	-5.30	1.47	1.53
13	3	1532	A	N1-C2	5.30	1.39	1.34
13	3	1523	U	N3-C4	5.30	1.43	1.38
14	4	2164	C	C4-N4	5.29	1.38	1.33
5	p	31	C	N1-C6	-5.29	1.33	1.37
14	4	2123	G	C5-C6	-5.29	1.37	1.42
13	3	1549	A	C6-N1	5.29	1.39	1.35
1	y	340	ARG	CD-NE	5.28	1.55	1.46
5	p	11	C	N1-C6	-5.28	1.33	1.37
14	4	2190	G	C5'-C4'	5.28	1.57	1.51
3	G	46	SER	CA-CB	5.28	1.60	1.52
14	4	2152	G	N9-C4	-5.27	1.33	1.38
13	3	1550	C	P-O5'	-5.26	1.54	1.59
13	3	1522	A	C4'-C3'	5.26	1.58	1.53
14	4	2171	A	N9-C4	-5.26	1.34	1.37
13	3	1544	A	C6-N6	5.25	1.38	1.33
5	p	76	A	C2-N3	5.25	1.38	1.33
14	4	2114	A	N1-C2	5.25	1.39	1.34
5	p	75	C	C1'-N1	5.25	1.56	1.48
14	4	2136	G	C8-N7	-5.25	1.27	1.30
14	4	2140	G	N7-C5	-5.24	1.36	1.39
13	3	1522	A	C2'-C1'	-5.24	1.47	1.53
14	4	2125	G	C3'-C2'	-5.23	1.47	1.52
5	p	64	G	P-O5'	5.23	1.65	1.59
14	4	2186	G	N9-C8	-5.23	1.34	1.37
13	3	1551	A	N1-C2	-5.23	1.29	1.34
14	4	2108	A	N9-C4	5.22	1.41	1.37
5	p	69	C	N1-C6	5.22	1.40	1.37
14	4	2172	U	N3-C4	5.22	1.43	1.38
14	4	2121	G	P-O5'	-5.21	1.54	1.59
14	4	2139	U	C2-N3	5.21	1.41	1.37
1	y	380	TYR	CA-CB	5.21	1.65	1.53
13	3	1529	G	C2'-C1'	-5.21	1.47	1.53
14	4	2189	U	C2'-C1'	-5.21	1.47	1.53
5	p	55	U	O4'-C1'	5.20	1.48	1.41
14	4	2151	U	O3'-P	-5.20	1.54	1.61
1	y	440	GLY	CA-C	5.20	1.60	1.51
14	4	2159	G	C2'-C1'	-5.20	1.47	1.53
14	4	2094	A	C5'-C4'	5.20	1.57	1.51
14	4	2097	A	N9-C8	5.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2116	G	C6-N1	5.20	1.43	1.39
14	4	2154	A	C6-N1	5.19	1.39	1.35
13	3	1523	U	C4'-C3'	5.19	1.58	1.53
5	p	24	G	C2-N3	5.19	1.36	1.32
14	4	2091	C	N1-C2	5.18	1.45	1.40
14	4	2165	C	O3'-P	-5.18	1.54	1.61
14	4	2186	G	C2-N2	5.17	1.39	1.34
14	4	2104	C	C4'-O4'	-5.17	1.38	1.45
13	3	1517	G	N3-C4	5.16	1.39	1.35
5	p	49	G	C2-N2	5.16	1.39	1.34
14	4	2093	G	O4'-C1'	5.15	1.48	1.41
14	4	2161	C	C4'-C3'	5.15	1.58	1.53
14	4	2162	G	N7-C5	-5.15	1.36	1.39
1	y	282	SER	CA-CB	5.14	1.60	1.52
14	4	2183	A	C2'-C1'	-5.14	1.47	1.53
7	5	74	ARG	NE-CZ	5.14	1.39	1.33
13	3	1547	C	O4'-C1'	5.14	1.48	1.41
13	3	1543	G	C6-N1	5.14	1.43	1.39
12	2	1340	U	C2-N3	5.14	1.41	1.37
1	y	294	PHE	CG-CD2	5.13	1.46	1.38
14	4	2111	U	C5'-C4'	5.13	1.57	1.51
1	y	25	PHE	CE1-CZ	5.13	1.47	1.37
1	y	399	PHE	CE2-CZ	5.12	1.47	1.37
5	p	16	U	C4'-C3'	5.12	1.58	1.53
7	5	180	PHE	CG-CD1	5.12	1.46	1.38
14	4	2136	G	C2-N2	5.12	1.39	1.34
14	4	2105	U	C5'-C4'	5.12	1.57	1.51
5	p	21	A	N1-C2	5.12	1.39	1.34
14	4	2185	U	C4'-C3'	-5.12	1.47	1.52
5	p	34	G	C5-C4	5.11	1.42	1.38
13	3	1519	G	C5'-C4'	5.10	1.57	1.51
14	4	2140	G	P-O5'	-5.10	1.54	1.59
7	5	134	ARG	NE-CZ	5.10	1.39	1.33
5	p	20	U	C4-O4	5.10	1.27	1.23
14	4	2158	A	C4'-C3'	5.10	1.58	1.53
5	p	40	G	N3-C4	-5.09	1.31	1.35
5	p	7	A	O3'-P	-5.09	1.55	1.61
13	3	1551	A	C4'-O4'	5.09	1.52	1.45
14	4	2122	U	C2-N3	5.08	1.41	1.37
3	G	46	SER	C-N	5.08	1.42	1.33
14	4	2186	G	N7-C5	-5.08	1.36	1.39
5	p	11	C	C3'-O3'	5.08	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2165	C	C5-C6	-5.08	1.30	1.34
14	4	2188	U	N3-C4	5.08	1.43	1.38
5	p	71	G	C2'-O2'	-5.07	1.35	1.41
5	p	26	A	C6-N6	5.07	1.38	1.33
14	4	2160	C	C2'-C1'	-5.06	1.47	1.53
1	y	16	LEU	C-N	5.06	1.42	1.33
13	3	1542	U	C3'-C2'	5.06	1.58	1.52
5	p	44	G	C3'-O3'	5.05	1.49	1.42
13	3	1541	C	C4-N4	5.05	1.38	1.33
13	3	1537	G	C2'-O2'	-5.05	1.35	1.41
5	p	69	C	C4-N4	5.04	1.38	1.33
5	p	24	G	N3-C4	5.04	1.39	1.35
14	4	2151	U	C4'-C3'	5.04	1.58	1.53
14	4	2107	G	C5'-C4'	5.04	1.57	1.51
13	3	1540	G	C3'-C2'	-5.03	1.47	1.52
14	4	2094	A	C5-C6	-5.03	1.36	1.41
1	y	294	PHE	CG-CD1	5.03	1.46	1.38
14	4	2131	U	C4-O4	-5.03	1.19	1.23
14	4	2117	A	N9-C4	-5.02	1.34	1.37
14	4	2168	G	C6-N1	5.02	1.43	1.39
14	4	2107	G	C2-N3	5.01	1.36	1.32
14	4	2171	A	P-O5'	-5.00	1.54	1.59

All (1751) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	19	G	N1-C6-O6	24.02	134.31	119.90
14	4	2108	A	N1-C6-N6	22.36	132.01	118.60
5	p	18	G	N1-C6-O6	20.82	132.39	119.90
5	p	37	A	N1-C6-N6	20.71	131.02	118.60
13	3	1535	A	N1-C6-N6	20.48	130.89	118.60
14	4	2154	A	N1-C6-N6	20.03	130.62	118.60
13	3	1525	A	N1-C6-N6	18.96	129.97	118.60
14	4	2102	G	N1-C6-O6	18.95	131.27	119.90
1	y	56	GLN	N-CA-CB	18.88	144.58	110.60
14	4	2174	C	C6-N1-C2	-18.33	112.97	120.30
5	p	21	A	N1-C6-N6	18.26	129.56	118.60
13	3	1551	A	P-O3'-C3'	18.10	141.42	119.70
5	p	29	A	N1-C6-N6	18.04	129.42	118.60
13	3	1538	G	N1-C6-O6	17.98	130.69	119.90
5	p	40	G	N1-C6-O6	17.97	130.68	119.90
5	p	7	A	N1-C6-N6	17.84	129.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1549	A	N1-C6-N6	17.83	129.30	118.60
5	p	58	A	N1-C6-N6	17.36	129.02	118.60
5	p	27	C	C6-N1-C2	-17.23	113.41	120.30
5	p	49	G	C5-C6-O6	-17.02	118.39	128.60
5	p	5	G	N1-C6-O6	16.93	130.06	119.90
5	p	5	G	C5-C6-O6	-16.87	118.48	128.60
5	p	7	A	C5-C6-N1	-16.78	109.31	117.70
13	3	1548	A	C5-C6-N1	-16.71	109.34	117.70
5	p	19	G	C5-C6-O6	-16.68	118.59	128.60
14	4	2158	A	N1-C6-N6	16.67	128.60	118.60
14	4	2094	A	C4-C5-C6	16.48	125.24	117.00
4	n	41	ARG	N-CA-CB	16.38	140.09	110.60
14	4	2117	A	N1-C6-N6	16.24	128.34	118.60
5	p	49	G	N1-C6-O6	16.23	129.64	119.90
14	4	2110	G	N1-C6-O6	16.21	129.63	119.90
5	p	11	C	N3-C4-N4	16.15	129.31	118.00
5	p	58	A	C4-C5-C6	16.06	125.03	117.00
4	n	46	ASP	N-CA-CB	16.04	139.47	110.60
14	4	2136	G	N1-C6-O6	16.00	129.50	119.90
1	y	119	TYR	CB-CG-CD1	15.90	130.54	121.00
14	4	2178	C	N3-C4-C5	-15.87	115.55	121.90
5	p	44	G	N7-C8-N9	15.81	121.00	113.10
14	4	2190	G	C5-C6-O6	-15.77	119.14	128.60
1	y	403	GLY	N-CA-C	15.74	152.45	113.10
13	3	1545	A	N1-C6-N6	15.68	128.01	118.60
14	4	2126	A	N1-C6-N6	15.53	127.92	118.60
13	3	1546	G	N1-C6-O6	15.51	129.20	119.90
14	4	2147	A	C5-C6-N1	-15.43	109.99	117.70
14	4	2097	A	N1-C6-N6	15.33	127.80	118.60
4	n	41	ARG	CB-CA-C	-15.17	80.06	110.40
5	p	63	C	O4'-C1'-N1	15.11	120.29	108.20
14	4	2136	G	C5-C6-O6	-15.02	119.59	128.60
13	3	1517	G	C5-C6-N1	-15.01	104.00	111.50
14	4	2170	A	C8-N9-C4	-14.83	99.87	105.80
5	p	59	G	C5-C6-O6	-14.78	119.73	128.60
5	p	26	A	N1-C6-N6	14.73	127.44	118.60
5	p	58	A	C5-C6-N1	-14.58	110.41	117.70
13	3	1549	A	C5-C6-N1	-14.54	110.43	117.70
14	4	2134	A	N1-C6-N6	14.53	127.32	118.60
5	p	76	A	N1-C6-N6	14.46	127.28	118.60
13	3	1529	G	N1-C6-O6	14.46	128.58	119.90
1	y	57	ARG	NE-CZ-NH2	14.35	127.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2159	G	N1-C6-O6	14.34	128.50	119.90
5	p	61	C	N3-C4-C5	-14.34	116.16	121.90
14	4	2141	G	C5-C6-O6	-14.22	120.06	128.60
14	4	2159	G	C4-C5-N7	-14.16	105.14	110.80
14	4	2114	A	N1-C6-N6	14.16	127.10	118.60
13	3	1518	C	N3-C4-N4	14.16	127.91	118.00
5	p	40	G	C5-C6-O6	-14.06	120.16	128.60
14	4	2114	A	C5-C6-N1	-14.02	110.69	117.70
14	4	2179	C	C5-C4-N4	-13.98	110.41	120.20
13	3	1541	C	O4'-C1'-N1	13.92	119.34	108.20
14	4	2169	A	C5-N7-C8	13.92	110.86	103.90
13	3	1551	A	OP2-P-O3'	-13.88	74.65	105.20
4	n	40	GLN	CB-CA-C	13.88	138.16	110.40
13	3	1524	G	N1-C6-O6	13.81	128.19	119.90
2	E	127	PHE	CB-CG-CD2	13.80	130.46	120.80
14	4	2147	A	N1-C6-N6	13.75	126.85	118.60
14	4	2162	G	C2-N3-C4	13.74	118.77	111.90
1	y	365	TYR	CB-CG-CD1	13.69	129.22	121.00
7	5	78	PHE	CB-CG-CD2	13.64	130.35	120.80
5	p	52	A	N1-C6-N6	13.61	126.77	118.60
14	4	2173	A	N9-C4-C5	13.57	111.23	105.80
5	p	19	G	C2-N3-C4	13.53	118.67	111.90
14	4	2135	A	N1-C6-N6	13.53	126.72	118.60
14	4	2179	C	N3-C4-N4	13.49	127.45	118.00
7	5	78	PHE	CB-CG-CD1	-13.41	111.42	120.80
1	y	119	TYR	CB-CG-CD2	-13.40	112.96	121.00
14	4	2190	G	N1-C6-O6	13.35	127.91	119.90
14	4	2170	A	C4-C5-C6	13.29	123.64	117.00
14	4	2107	G	C5-C6-O6	-13.28	120.63	128.60
11	1	56	A	N1-C6-N6	13.27	126.56	118.60
13	3	1530	G	C8-N9-C4	-13.26	101.10	106.40
5	p	6	A	N1-C6-N6	13.24	126.54	118.60
14	4	2097	A	C8-N9-C4	-13.20	100.52	105.80
13	3	1517	G	N1-C6-O6	13.19	127.81	119.90
14	4	2174	C	C5-C6-N1	13.18	127.59	121.00
14	4	2127	G	C5-C6-O6	-13.16	120.70	128.60
4	n	40	GLN	N-CA-CB	13.15	134.28	110.60
13	3	1519	G	N1-C6-O6	13.14	127.79	119.90
14	4	2144	G	N3-C2-N2	13.13	129.09	119.90
14	4	2158	A	N1-C2-N3	13.13	135.87	129.30
14	4	2169	A	C4-C5-C6	13.10	123.55	117.00
5	p	18	G	C5-C6-O6	-13.09	120.75	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2192	U	C5-C4-O4	-13.08	118.05	125.90
14	4	2112	G	N1-C6-O6	13.05	127.73	119.90
5	p	64	G	O4'-C1'-N9	13.04	118.63	108.20
14	4	2094	A	C5-N7-C8	13.01	110.40	103.90
11	1	104	A	N1-C6-N6	12.98	126.39	118.60
5	p	38	A	N1-C6-N6	12.92	126.35	118.60
14	4	2133	G	N1-C6-O6	12.90	127.64	119.90
13	3	1543	G	N1-C6-O6	12.80	127.58	119.90
14	4	2167	U	O4'-C1'-N1	12.79	118.43	108.20
14	4	2097	A	C5-C6-N1	-12.79	111.31	117.70
5	p	11	C	N3-C4-C5	-12.75	116.80	121.90
5	p	24	G	O4'-C1'-N9	12.73	118.39	108.20
14	4	2173	A	N1-C6-N6	12.67	126.20	118.60
5	p	44	G	C8-N9-C4	-12.66	101.34	106.40
14	4	2094	A	N1-C6-N6	12.66	126.19	118.60
13	3	1548	A	C5-N7-C8	12.65	110.22	103.90
14	4	2120	G	N1-C6-O6	12.62	127.47	119.90
14	4	2103	C	N3-C4-N4	12.62	126.83	118.00
5	p	21	A	C5-C6-N6	-12.60	113.62	123.70
14	4	2175	C	P-O3'-C3'	12.58	134.79	119.70
14	4	2148	G	N1-C6-O6	12.57	127.44	119.90
14	4	2114	A	C4-C5-C6	12.55	123.28	117.00
1	y	113	ARG	NE-CZ-NH1	12.53	126.57	120.30
11	1	83	A	N1-C6-N6	12.51	126.11	118.60
7	5	71	ARG	NE-CZ-NH2	-12.49	114.06	120.30
14	4	2108	A	C5-C6-N1	-12.49	111.45	117.70
11	1	95	A	N1-C6-N6	12.49	126.09	118.60
5	p	38	A	C4-C5-C6	12.46	123.23	117.00
14	4	2102	G	C5-C6-O6	-12.44	121.14	128.60
13	3	1520	U	O4'-C1'-N1	12.39	118.11	108.20
11	1	89	A	N1-C6-N6	12.37	126.02	118.60
11	1	111	A	N1-C6-N6	12.36	126.02	118.60
5	p	14	A	N1-C6-N6	12.35	126.01	118.60
1	y	340	ARG	NE-CZ-NH2	12.34	126.47	120.30
11	1	84	A	N1-C6-N6	12.32	125.99	118.60
5	p	1	G	N1-C6-O6	12.31	127.28	119.90
14	4	2123	G	C5-C6-O6	-12.28	121.23	128.60
1	y	255	ARG	NE-CZ-NH1	12.28	126.44	120.30
5	p	59	G	N1-C6-O6	12.28	127.27	119.90
5	p	76	A	C5-C6-N1	-12.26	111.57	117.70
5	p	74	C	N3-C4-C5	-12.26	117.00	121.90
14	4	2128	G	C5-C6-O6	-12.25	121.25	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1517	G	C6-N1-C2	12.25	132.45	125.10
5	p	34	G	O4'-C1'-N9	12.24	117.99	108.20
11	1	91	A	N1-C6-N6	12.23	125.94	118.60
1	y	404	THR	N-CA-CB	-12.23	87.06	110.30
11	1	53	A	N1-C6-N6	12.20	125.92	118.60
14	4	2184	A	N1-C6-N6	12.19	125.92	118.60
14	4	2126	A	C5-C6-N1	-12.15	111.62	117.70
14	4	2189	U	O4'-C1'-N1	12.15	117.92	108.20
1	y	365	TYR	CB-CG-CD2	-12.13	113.72	121.00
14	4	2178	C	O4'-C1'-N1	12.13	117.90	108.20
14	4	2105	U	O4'-C1'-N1	12.07	117.86	108.20
5	p	35	C	C6-N1-C2	-12.06	115.47	120.30
14	4	2127	G	N1-C6-O6	12.06	127.13	119.90
14	4	2196	C	O4'-C1'-N1	12.06	117.84	108.20
11	1	52	A	N1-C6-N6	12.05	125.83	118.60
13	3	1548	A	N1-C6-N6	12.04	125.83	118.60
5	p	28	G	N1-C6-O6	12.03	127.12	119.90
13	3	1536	C	N3-C4-C5	-12.02	117.09	121.90
14	4	2158	A	C5-C6-N6	-11.99	114.11	123.70
14	4	2138	G	C4-C5-C6	11.97	125.98	118.80
14	4	2095	A	N1-C6-N6	11.94	125.76	118.60
13	3	1529	G	C5-C6-O6	-11.92	121.45	128.60
12	2	1327	A	N1-C6-N6	11.90	125.74	118.60
5	p	48	C	N3-C4-N4	11.89	126.32	118.00
14	4	2124	G	C6-C5-N7	-11.88	123.27	130.40
12	2	1328	A	N1-C6-N6	11.88	125.73	118.60
14	4	2191	A	C4-C5-C6	11.86	122.93	117.00
13	3	1528	A	C2-N3-C4	-11.85	104.68	110.60
12	2	1322	A	N1-C6-N6	11.82	125.69	118.60
11	1	101	A	N1-C6-N6	11.80	125.68	118.60
14	4	2167	U	N3-C4-O4	11.78	127.64	119.40
5	p	56	C	N3-C4-C5	-11.75	117.20	121.90
14	4	2148	G	C4-C5-C6	11.74	125.84	118.80
11	1	73	A	N1-C6-N6	11.73	125.64	118.60
4	n	42	SER	N-CA-CB	11.71	128.07	110.50
5	p	39	G	N3-C2-N2	11.71	128.09	119.90
14	4	2176	A	N1-C6-N6	11.69	125.61	118.60
5	p	26	A	C8-N9-C4	-11.69	101.12	105.80
14	4	2094	A	C8-N9-C4	-11.67	101.13	105.80
5	p	25	C	N3-C4-N4	11.66	126.16	118.00
14	4	2096	C	N3-C4-N4	11.66	126.16	118.00
5	p	37	A	C5-C6-N6	-11.64	114.39	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1537	G	P-O3'-C3'	11.60	133.62	119.70
11	1	71	A	N1-C6-N6	11.59	125.55	118.60
14	4	2161	C	P-O3'-C3'	11.58	133.59	119.70
14	4	2120	G	C5-C6-O6	-11.57	121.66	128.60
5	p	51	G	N1-C6-O6	11.57	126.84	119.90
12	2	1336	A	N1-C6-N6	11.55	125.53	118.60
5	p	15	G	N1-C6-O6	11.53	126.82	119.90
14	4	2154	A	C5-C6-N1	-11.51	111.94	117.70
14	4	2094	A	C5-C6-N1	-11.49	111.96	117.70
5	p	13	C	N3-C4-C5	-11.48	117.31	121.90
14	4	2144	G	C5-C6-O6	-11.48	121.71	128.60
13	3	1517	G	C4-C5-C6	11.48	125.69	118.80
11	1	64	A	N1-C6-N6	11.47	125.48	118.60
11	1	74	A	N1-C6-N6	11.46	125.47	118.60
1	y	233	PHE	CB-CG-CD2	-11.45	112.78	120.80
14	4	2173	A	C4-C5-N7	-11.43	104.98	110.70
12	2	1321	A	N1-C6-N6	11.43	125.46	118.60
5	p	7	A	C4-C5-C6	11.42	122.71	117.00
14	4	2146	C	N3-C4-C5	-11.40	117.34	121.90
13	3	1545	A	C4-C5-C6	11.40	122.70	117.00
14	4	2141	G	N1-C6-O6	11.38	126.73	119.90
14	4	2124	G	C4-C5-N7	11.34	115.34	110.80
5	p	27	C	C5-C6-N1	11.33	126.67	121.00
14	4	2156	G	N1-C6-O6	11.33	126.70	119.90
14	4	2120	G	N9-C4-C5	11.31	109.93	105.40
1	y	242	ARG	NE-CZ-NH2	11.30	125.95	120.30
11	1	94	A	N1-C6-N6	11.28	125.37	118.60
11	1	63	A	N1-C6-N6	11.28	125.37	118.60
5	p	45	G	N1-C6-O6	11.27	126.66	119.90
5	p	74	C	C5-C4-N4	11.26	128.08	120.20
14	4	2177	C	O4'-C1'-N1	11.21	117.17	108.20
12	2	1315	C	P-O3'-C3'	11.20	133.14	119.70
12	2	1307	A	N1-C6-N6	11.19	125.31	118.60
5	p	13	C	N3-C4-N4	11.19	125.83	118.00
13	3	1544	A	N1-C6-N6	11.19	125.31	118.60
5	p	58	A	N9-C4-C5	11.18	110.27	105.80
5	p	1	G	C5-C6-O6	-11.13	121.92	128.60
5	p	58	A	C8-N9-C4	-11.11	101.36	105.80
14	4	2107	G	C5-C6-N1	11.10	117.05	111.50
13	3	1546	G	C5-C6-O6	-11.08	121.95	128.60
14	4	2104	C	C5-C6-N1	11.07	126.54	121.00
14	4	2138	G	C6-C5-N7	-11.07	123.76	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2162	G	N3-C4-C5	-11.06	123.07	128.60
14	4	2159	G	C5-N7-C8	11.06	109.83	104.30
5	p	61	C	N3-C4-N4	11.05	125.74	118.00
5	p	31	C	O4'-C1'-N1	11.05	117.04	108.20
14	4	2162	G	O4'-C1'-N9	11.02	117.01	108.20
5	p	69	C	N3-C4-N4	11.01	125.71	118.00
14	4	2091	C	O4'-C1'-N1	11.01	117.01	108.20
14	4	2104	C	N3-C4-N4	11.01	125.70	118.00
5	p	76	A	O4'-C1'-N9	11.00	117.00	108.20
14	4	2168	G	N1-C2-N3	-10.97	117.32	123.90
5	p	35	C	C5-C6-N1	10.96	126.48	121.00
14	4	2091	C	N3-C4-N4	10.95	125.67	118.00
5	p	61	C	O4'-C1'-N1	10.93	116.94	108.20
14	4	2105	U	C5-C4-O4	10.93	132.46	125.90
5	p	9	A	C4-C5-C6	10.89	122.45	117.00
13	3	1537	G	N1-C6-O6	10.86	126.41	119.90
5	p	23	A	C4-C5-C6	10.83	122.42	117.00
13	3	1552	A	N1-C6-N6	10.82	125.09	118.60
13	3	1528	A	N1-C2-N3	10.81	134.71	129.30
5	p	68	C	N3-C4-C5	-10.81	117.58	121.90
14	4	2150	C	N3-C4-C5	10.75	126.20	121.90
13	3	1536	C	N3-C4-N4	10.74	125.52	118.00
14	4	2092	U	C5-C6-N1	10.74	128.07	122.70
14	4	2144	G	N1-C6-O6	10.71	126.33	119.90
14	4	2094	A	C4-C5-N7	-10.67	105.37	110.70
13	3	1530	G	O4'-C1'-N9	10.64	116.71	108.20
13	3	1518	C	C5-C4-N4	-10.63	112.76	120.20
14	4	2146	C	C2-N3-C4	10.59	125.19	119.90
14	4	2199	A	C4-C5-C6	10.51	122.25	117.00
13	3	1553	A	N1-C6-N6	10.50	124.90	118.60
11	1	103	A	N1-C6-N6	10.49	124.90	118.60
12	2	1342	A	N1-C6-N6	10.49	124.89	118.60
1	y	416	PHE	CB-CG-CD2	10.47	128.13	120.80
14	4	2138	G	C5-C6-N1	-10.47	106.27	111.50
14	4	2155	U	C5-C4-O4	-10.46	119.63	125.90
14	4	2137	U	C5-C6-N1	10.45	127.92	122.70
5	p	51	G	C5-C6-O6	-10.43	122.34	128.60
14	4	2104	C	O4'-C1'-N1	10.42	116.54	108.20
13	3	1535	A	C5-C6-N1	-10.42	112.49	117.70
14	4	2151	U	O4'-C1'-N1	10.42	116.53	108.20
5	p	6	A	C4-C5-C6	10.39	122.19	117.00
13	3	1537	G	C2-N3-C4	10.39	117.09	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1546	G	C4-C5-N7	-10.38	106.65	110.80
14	4	2091	C	N3-C4-C5	-10.38	117.75	121.90
14	4	2154	A	O4'-C1'-N9	10.38	116.50	108.20
14	4	2162	G	N1-C6-O6	10.37	126.12	119.90
13	3	1550	C	N3-C4-C5	-10.36	117.76	121.90
5	p	23	A	N1-C6-N6	10.34	124.81	118.60
5	p	19	G	N1-C2-N3	-10.32	117.71	123.90
5	p	69	C	C6-N1-C2	-10.30	116.18	120.30
13	3	1538	G	C5-C6-O6	-10.28	122.43	128.60
13	3	1533	C	C6-N1-C2	-10.28	116.19	120.30
5	p	10	G	C6-C5-N7	-10.27	124.24	130.40
5	p	18	G	N3-C2-N2	10.26	127.08	119.90
5	p	29	A	C5-C6-N6	-10.24	115.50	123.70
14	4	2160	C	O4'-C1'-N1	10.23	116.39	108.20
14	4	2157	G	N1-C6-O6	10.23	126.04	119.90
14	4	2162	G	C5-C6-O6	-10.20	122.48	128.60
4	n	71	LEU	N-CA-C	10.17	138.45	111.00
13	3	1535	A	O4'-C1'-N9	10.15	116.32	108.20
14	4	2120	G	C8-N9-C4	-10.15	102.34	106.40
14	4	2169	A	O4'-C1'-N9	10.13	116.31	108.20
13	3	1550	C	N3-C4-N4	10.12	125.08	118.00
14	4	2170	A	N1-C6-N6	10.12	124.67	118.60
14	4	2117	A	C5-C6-N1	-10.10	112.65	117.70
14	4	2170	A	N9-C4-C5	10.09	109.84	105.80
14	4	2098	U	C5-C6-N1	10.09	127.75	122.70
14	4	2097	A	C4-C5-C6	10.09	122.04	117.00
13	3	1519	G	C6-C5-N7	-10.08	124.35	130.40
13	3	1548	A	C4-C5-C6	10.08	122.04	117.00
14	4	2158	A	C2-N3-C4	-10.07	105.56	110.60
13	3	1532	A	N1-C6-N6	10.07	124.64	118.60
14	4	2101	A	O4'-C1'-N9	10.07	116.26	108.20
13	3	1528	A	N1-C6-N6	10.04	124.62	118.60
14	4	2124	G	O4'-C1'-N9	10.03	116.22	108.20
5	p	76	A	C4-C5-C6	10.03	122.01	117.00
14	4	2128	G	N1-C2-N3	-10.02	117.89	123.90
11	1	81	G	N1-C6-O6	10.01	125.90	119.90
14	4	2152	G	C5-C6-O6	-10.01	122.60	128.60
14	4	2199	A	N1-C6-N6	10.00	124.60	118.60
14	4	2119	A	C4-C5-C6	10.00	122.00	117.00
14	4	2184	A	C5-C6-N6	-10.00	115.70	123.70
12	2	1338	G	N1-C6-O6	9.99	125.90	119.90
5	p	67	U	O4'-C1'-N1	9.97	116.18	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	108	G	N1-C6-O6	9.97	125.88	119.90
14	4	2133	G	C5-C6-O6	-9.96	122.63	128.60
13	3	1515	A	O4'-C1'-N9	9.95	116.16	108.20
14	4	2110	G	C5-C6-O6	-9.95	122.63	128.60
14	4	2192	U	O4'-C1'-N1	9.94	116.15	108.20
14	4	2192	U	N3-C4-O4	9.94	126.36	119.40
13	3	1527	G	N1-C6-O6	9.93	125.86	119.90
3	G	54	ARG	NE-CZ-NH2	-9.91	115.34	120.30
7	5	208	TYR	CB-CG-CD1	-9.91	115.06	121.00
5	p	70	C	N3-C4-C5	-9.90	117.94	121.90
14	4	2092	U	C2-N3-C4	-9.90	121.06	127.00
11	1	86	G	N1-C6-O6	9.89	125.84	119.90
14	4	2093	G	N1-C6-O6	9.87	125.82	119.90
14	4	2198	A	O4'-C1'-N9	9.87	116.09	108.20
5	p	18	G	C5-C6-N1	-9.87	106.57	111.50
5	p	65	U	C5-C4-O4	-9.86	119.99	125.90
5	p	49	G	O4'-C1'-N9	9.84	116.07	108.20
14	4	2168	G	C6-C5-N7	-9.84	124.50	130.40
14	4	2093	G	C5-C6-O6	-9.83	122.70	128.60
7	5	74	ARG	NE-CZ-NH1	9.83	125.22	120.30
14	4	2148	G	C5-C6-O6	-9.83	122.70	128.60
14	4	2097	A	O4'-C1'-N9	9.82	116.06	108.20
5	p	43	G	O4'-C1'-N9	9.81	116.05	108.20
5	p	68	C	C6-N1-C2	9.80	124.22	120.30
14	4	2097	A	C6-C5-N7	-9.79	125.45	132.30
14	4	2142	A	N1-C6-N6	9.79	124.47	118.60
13	3	1516	G	O3'-P-O5'	9.77	122.57	104.00
13	3	1525	A	C5-C6-N1	-9.77	112.82	117.70
12	2	1308	A	N1-C6-N6	9.75	124.45	118.60
5	p	38	A	C5-C6-N1	-9.75	112.83	117.70
14	4	2161	C	C6-N1-C2	-9.73	116.41	120.30
13	3	1549	A	O4'-C1'-N9	9.71	115.97	108.20
5	p	26	A	C4-C5-C6	9.70	121.85	117.00
14	4	2154	A	C4-C5-C6	9.70	121.85	117.00
14	4	2193	G	C8-N9-C4	-9.69	102.52	106.40
14	4	2099	U	O4'-C1'-N1	9.68	115.94	108.20
14	4	2176	A	C5-C6-N6	-9.67	115.96	123.70
14	4	2190	G	O4'-C1'-N9	9.66	115.93	108.20
14	4	2157	G	C5-C6-O6	-9.64	122.81	128.60
11	1	107	G	N1-C6-O6	9.63	125.68	119.90
13	3	1544	A	C4-C5-C6	9.63	121.81	117.00
13	3	1551	A	N1-C6-N6	9.62	124.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	48	C	O4'-C1'-N1	9.61	115.89	108.20
5	p	9	A	C8-N9-C4	-9.59	101.97	105.80
5	p	63	C	N1-C2-N3	-9.58	112.49	119.20
14	4	2141	G	N1-C2-N3	-9.57	118.16	123.90
4	n	39	HIS	N-CA-CB	9.57	127.82	110.60
5	p	58	A	C4-C5-N7	-9.57	105.92	110.70
11	1	70	G	N1-C6-O6	9.55	125.63	119.90
13	3	1535	A	C4-C5-C6	9.54	121.77	117.00
12	2	1309	G	N1-C6-O6	9.53	125.61	119.90
5	p	66	U	O4'-C1'-N1	9.52	115.82	108.20
12	2	1310	G	N1-C6-O6	9.52	125.61	119.90
14	4	2152	G	C2-N3-C4	9.49	116.64	111.90
5	p	46	G	P-O3'-C3'	9.48	131.08	119.70
5	p	72	C	O4'-C1'-N1	9.48	115.78	108.20
14	4	2104	C	N3-C4-C5	-9.47	118.11	121.90
13	3	1543	G	N3-C2-N2	9.47	126.53	119.90
14	4	2117	A	C4-C5-N7	-9.47	105.97	110.70
13	3	1538	G	C6-C5-N7	-9.46	124.72	130.40
13	3	1546	G	N9-C4-C5	9.45	109.18	105.40
7	5	163	TYR	CB-CG-CD1	-9.42	115.35	121.00
5	p	27	C	N3-C4-N4	9.42	124.59	118.00
5	p	3	G	P-O3'-C3'	9.42	131.00	119.70
11	1	77	G	N1-C6-O6	9.38	125.53	119.90
14	4	2174	C	N3-C4-N4	9.37	124.56	118.00
11	1	75	G	N1-C6-O6	9.35	125.51	119.90
1	y	25	PHE	CB-CG-CD1	-9.35	114.26	120.80
14	4	2124	G	N1-C6-O6	9.34	125.50	119.90
13	3	1532	A	C4-C5-C6	9.33	121.66	117.00
1	y	55	GLN	N-CA-C	9.32	136.16	111.00
14	4	2174	C	N3-C4-C5	-9.31	118.17	121.90
13	3	1518	C	O4'-C1'-N1	9.31	115.64	108.20
14	4	2124	G	C5-C6-O6	-9.30	123.02	128.60
14	4	2178	C	C6-N1-C1'	-9.30	109.64	120.80
14	4	2122	U	O4'-C1'-N1	9.29	115.63	108.20
13	3	1538	G	C5-C6-N1	-9.28	106.86	111.50
14	4	2117	A	C5-N7-C8	9.27	108.54	103.90
14	4	2168	G	C2-N3-C4	9.27	116.54	111.90
5	p	18	G	C8-N9-C4	9.26	110.10	106.40
5	p	69	C	C5-C4-N4	-9.24	113.73	120.20
14	4	2148	G	C5-N7-C8	9.24	108.92	104.30
5	p	3	G	O4'-C1'-N9	9.24	115.59	108.20
14	4	2104	C	C6-N1-C2	-9.24	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2175	C	O4'-C1'-N1	9.24	115.59	108.20
5	p	57	G	N1-C6-O6	9.23	125.44	119.90
5	p	6	A	N1-C2-N3	9.22	133.91	129.30
13	3	1548	A	N7-C8-N9	-9.22	109.19	113.80
5	p	9	A	N1-C6-N6	9.21	124.13	118.60
14	4	2170	A	C6-C5-N7	-9.21	125.85	132.30
5	p	23	A	C6-C5-N7	-9.20	125.86	132.30
14	4	2115	G	O4'-C1'-N9	9.19	115.55	108.20
4	n	41	ARG	N-CA-C	9.17	135.77	111.00
11	1	85	G	N1-C6-O6	9.17	125.40	119.90
11	1	99	U	O4'-C1'-N1	9.17	115.53	108.20
5	p	9	A	O4'-C1'-N9	9.15	115.52	108.20
5	p	17	U	C1'-O4'-C4'	-9.15	102.58	109.90
14	4	2170	A	N1-C2-N3	9.14	133.87	129.30
14	4	2145	C	O4'-C1'-N1	9.13	115.50	108.20
13	3	1544	A	C5-C6-N1	-9.12	113.14	117.70
13	3	1525	A	C5-N7-C8	9.12	108.46	103.90
12	2	1337	G	N1-C6-O6	9.11	125.37	119.90
13	3	1551	A	C5-N7-C8	9.12	108.46	103.90
13	3	1522	A	N1-C2-N3	9.10	133.85	129.30
14	4	2131	U	O4'-C1'-N1	9.10	115.48	108.20
5	p	11	C	C5-C4-N4	-9.08	113.85	120.20
13	3	1530	G	N1-C2-N3	-9.07	118.46	123.90
5	p	62	U	O4'-C1'-N1	9.06	115.45	108.20
14	4	2154	A	N1-C2-N3	9.06	133.83	129.30
12	2	1332	G	N1-C6-O6	9.05	125.33	119.90
5	p	26	A	N9-C4-C5	9.05	109.42	105.80
14	4	2165	C	O4'-C1'-N1	9.05	115.44	108.20
13	3	1521	G	N3-C2-N2	9.05	126.23	119.90
5	p	64	G	C5-C6-N1	-9.04	106.98	111.50
13	3	1549	A	C4-C5-C6	9.04	121.52	117.00
5	p	14	A	O4'-C1'-N9	9.03	115.43	108.20
11	1	110	G	N1-C6-O6	9.03	125.32	119.90
13	3	1546	G	C4-C5-C6	9.03	124.22	118.80
14	4	2191	A	N1-C6-N6	9.03	124.02	118.60
14	4	2155	U	O4'-C1'-N1	9.01	115.41	108.20
14	4	2156	G	C5-C6-N1	-9.01	106.99	111.50
14	4	2167	U	C5-C4-O4	-9.01	120.49	125.90
3	G	36	ALA	CB-CA-C	-9.00	96.61	110.10
14	4	2184	A	N9-C4-C5	9.00	109.40	105.80
12	2	1324	G	N1-C6-O6	8.99	125.30	119.90
11	1	92	U	O4'-C1'-N1	8.98	115.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2173	A	C5-N7-C8	8.98	108.39	103.90
5	p	59	G	O4'-C1'-N9	8.97	115.38	108.20
5	p	69	C	O4'-C1'-N1	8.97	115.38	108.20
13	3	1527	G	C5-C6-O6	-8.97	123.22	128.60
14	4	2149	U	O4'-C1'-N1	8.97	115.38	108.20
12	2	1333	G	P-O3'-C3'	8.96	130.46	119.70
14	4	2108	A	C5-C6-N6	-8.96	116.53	123.70
13	3	1551	A	OP1-P-O3'	8.96	124.91	105.20
14	4	2150	C	C4-C5-C6	-8.96	112.92	117.40
13	3	1521	G	O4'-C1'-N9	8.96	115.36	108.20
5	p	19	G	C5-C6-N1	-8.95	107.02	111.50
14	4	2150	C	C5-C4-N4	-8.95	113.94	120.20
14	4	2111	U	O4'-C1'-N1	8.94	115.35	108.20
14	4	2150	C	C2-N3-C4	-8.94	115.43	119.90
14	4	2183	A	N1-C6-N6	8.93	123.96	118.60
13	3	1555	G	N1-C6-O6	8.93	125.26	119.90
14	4	2153	C	P-O5'-C5'	-8.93	106.61	120.90
13	3	1516	G	N1-C6-O6	8.92	125.25	119.90
14	4	2176	A	C8-N9-C4	-8.92	102.23	105.80
14	4	2182	U	O4'-C1'-N1	8.92	115.33	108.20
14	4	2146	C	N3-C4-N4	8.91	124.24	118.00
5	p	44	G	N3-C4-C5	-8.90	124.15	128.60
11	1	57	C	O4'-C1'-N1	8.90	115.32	108.20
11	1	60	G	N1-C6-O6	8.89	125.23	119.90
13	3	1535	A	C5-C6-N6	-8.89	116.59	123.70
14	4	2103	C	N3-C4-C5	-8.89	118.34	121.90
14	4	2123	G	N1-C6-O6	8.89	125.23	119.90
5	p	26	A	O4'-C1'-N9	8.88	115.30	108.20
14	4	2118	U	N3-C4-C5	-8.87	109.28	114.60
14	4	2135	A	C6-N1-C2	8.86	123.92	118.60
13	3	1519	G	C5-C6-O6	-8.86	123.28	128.60
11	1	80	G	N1-C6-O6	8.86	125.22	119.90
12	2	1334	G	N1-C6-O6	8.84	125.20	119.90
14	4	2111	U	C6-N1-C2	-8.84	115.70	121.00
2	E	126	ARG	NE-CZ-NH2	-8.84	115.88	120.30
14	4	2128	G	C2-N3-C4	8.84	116.32	111.90
14	4	2125	G	N1-C6-O6	8.82	125.19	119.90
14	4	2199	A	C4-C5-N7	-8.82	106.29	110.70
11	1	86	G	C5-C6-O6	-8.80	123.32	128.60
5	p	56	C	N1-C2-O2	8.79	124.17	118.90
14	4	2109	U	O4'-C1'-N1	8.79	115.23	108.20
5	p	34	G	N9-C4-C5	-8.78	101.89	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2125	G	N3-C2-N2	8.78	126.04	119.90
13	3	1519	G	N1-C2-N3	-8.77	118.64	123.90
11	1	69	C	O4'-C1'-N1	8.77	115.22	108.20
14	4	2168	G	N9-C4-C5	8.77	108.91	105.40
13	3	1540	G	N3-C2-N2	8.76	126.03	119.90
5	p	25	C	C6-N1-C2	-8.76	116.80	120.30
14	4	2193	G	C2-N3-C4	8.76	116.28	111.90
14	4	2147	A	O4'-C1'-N9	8.76	115.21	108.20
11	1	58	G	N1-C6-O6	8.74	125.15	119.90
13	3	1548	A	C6-N1-C2	8.74	123.84	118.60
7	5	208	TYR	CB-CG-CD2	8.74	126.24	121.00
11	1	98	G	N1-C6-O6	8.72	125.14	119.90
13	3	1530	G	N7-C8-N9	8.71	117.46	113.10
5	p	11	C	C4-C5-C6	8.71	121.76	117.40
5	p	14	A	C5-C6-N6	-8.71	116.73	123.70
11	1	68	G	N1-C6-O6	8.71	125.12	119.90
5	p	63	C	N3-C2-O2	8.70	127.99	121.90
12	2	1311	G	N1-C6-O6	8.70	125.12	119.90
5	p	12	U	P-O5'-C5'	8.69	134.81	120.90
13	3	1517	G	C6-C5-N7	-8.69	125.18	130.40
4	n	40	GLN	N-CA-C	-8.69	87.54	111.00
14	4	2098	U	N1-C2-N3	-8.68	109.69	114.90
12	2	1333	G	N1-C6-O6	8.68	125.11	119.90
13	3	1544	A	C8-N9-C4	-8.67	102.33	105.80
13	3	1539	U	O4'-C1'-N1	8.67	115.14	108.20
14	4	2139	U	O4'-C1'-N1	8.67	115.13	108.20
5	p	53	G	O4'-C1'-N9	8.66	115.13	108.20
12	2	1339	G	N1-C6-O6	8.64	125.09	119.90
14	4	2173	A	C8-N9-C4	-8.64	102.34	105.80
14	4	2184	A	C4-C5-N7	-8.62	106.39	110.70
14	4	2133	G	O4'-C1'-N9	8.62	115.10	108.20
14	4	2094	A	N9-C4-C5	8.62	109.25	105.80
13	3	1521	G	N1-C6-O6	8.62	125.07	119.90
14	4	2128	G	N1-C6-O6	8.59	125.05	119.90
1	y	256	ARG	NE-CZ-NH1	8.57	124.58	120.30
14	4	2125	G	N1-C2-N3	-8.56	118.76	123.90
11	1	55	G	N1-C6-O6	8.55	125.03	119.90
5	p	53	G	N7-C8-N9	8.54	117.37	113.10
13	3	1545	A	C5-C6-N1	-8.54	113.43	117.70
5	p	65	U	O4'-C1'-N1	8.54	115.03	108.20
5	p	2	C	O4'-C1'-N1	8.54	115.03	108.20
5	p	45	G	O4'-C1'-N9	8.54	115.03	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	93	G	N1-C6-O6	8.53	125.02	119.90
14	4	2125	G	C5-C6-O6	-8.52	123.49	128.60
14	4	2123	G	N3-C2-N2	8.52	125.86	119.90
13	3	1542	U	C4-C5-C6	-8.52	114.59	119.70
14	4	2104	C	C2-N3-C4	8.51	124.15	119.90
12	2	1315	C	O4'-C1'-N1	8.50	115.00	108.20
13	3	1544	A	N7-C8-N9	8.49	118.05	113.80
14	4	2119	A	N1-C6-N6	8.49	123.69	118.60
14	4	2164	C	C6-N1-C2	8.49	123.69	120.30
14	4	2193	G	C5'-C4'-O4'	8.48	119.28	109.10
13	3	1533	C	N3-C4-C5	-8.47	118.51	121.90
13	3	1542	U	O4'-C1'-N1	8.47	114.98	108.20
5	p	45	G	C6-N1-C2	8.46	130.18	125.10
13	3	1519	G	C2-N3-C4	8.46	116.13	111.90
14	4	2150	C	C5-C6-N1	8.45	125.22	121.00
14	4	2191	A	C6-C5-N7	-8.45	126.38	132.30
13	3	1550	C	O4'-C1'-N1	8.44	114.95	108.20
5	p	57	G	C5-C6-O6	-8.44	123.54	128.60
14	4	2100	G	C6-C5-N7	-8.43	125.34	130.40
13	3	1515	A	N1-C6-N6	8.41	123.65	118.60
14	4	2170	A	N7-C8-N9	8.41	118.01	113.80
14	4	2181	U	C5'-C4'-O4'	8.41	119.19	109.10
5	p	25	C	C5-C4-N4	-8.40	114.32	120.20
5	p	52	A	C8-N9-C4	-8.40	102.44	105.80
13	3	1527	G	N1-C2-N3	-8.39	118.86	123.90
14	4	2168	G	O4'-C1'-N9	8.38	114.90	108.20
1	y	248	TYR	CB-CG-CD1	-8.38	115.97	121.00
13	3	1529	G	C8-N9-C4	-8.37	103.05	106.40
12	2	1331	G	N1-C6-O6	8.37	124.92	119.90
13	3	1551	A	O3'-P-O5'	8.37	119.90	104.00
13	3	1548	A	N9-C4-C5	-8.35	102.46	105.80
14	4	2178	C	C2-N3-C4	8.35	124.07	119.90
14	4	2112	G	C5-C6-O6	-8.34	123.59	128.60
14	4	2186	G	N7-C8-N9	-8.34	108.93	113.10
7	5	71	ARG	NE-CZ-NH1	8.34	124.47	120.30
11	1	112	U	O4'-C1'-N1	8.33	114.86	108.20
1	y	367	ASP	CB-CG-OD1	8.33	125.79	118.30
14	4	2116	G	C2-N3-C4	-8.33	107.74	111.90
5	p	36	C	O4'-C1'-N1	8.32	114.86	108.20
5	p	30	C	O4'-C1'-N1	8.32	114.86	108.20
5	p	16	U	P-O3'-C3'	8.31	129.67	119.70
11	1	97	C	O4'-C1'-N1	8.31	114.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	10	G	C4-C5-C6	8.30	123.78	118.80
14	4	2105	U	C4-C5-C6	8.29	124.67	119.70
5	p	57	G	P-O3'-C3'	8.26	129.61	119.70
14	4	2159	G	C5-C6-O6	-8.26	123.64	128.60
14	4	2147	A	C4-C5-C6	8.26	121.13	117.00
13	3	1523	U	C5-C6-N1	8.26	126.83	122.70
5	p	63	C	C2-N3-C4	8.25	124.03	119.90
11	1	109	C	O4'-C1'-N1	8.25	114.80	108.20
14	4	2153	C	N3-C4-C5	-8.24	118.60	121.90
13	3	1531	C	C6-N1-C2	-8.24	117.00	120.30
14	4	2178	C	C6-N1-C2	8.24	123.59	120.30
14	4	2156	G	C5-N7-C8	8.24	108.42	104.30
5	p	28	G	C8-N9-C4	-8.23	103.11	106.40
11	1	54	G	N1-C6-O6	8.23	124.84	119.90
11	1	81	G	C5-C6-O6	-8.22	123.67	128.60
11	1	105	C	O4'-C1'-N1	8.22	114.77	108.20
14	4	2155	U	N3-C4-O4	8.21	125.14	119.40
11	1	88	G	N1-C6-O6	8.20	124.82	119.90
5	p	11	C	C6-N1-C2	8.19	123.58	120.30
5	p	8	U	O4'-C1'-N1	8.19	114.75	108.20
14	4	2111	U	N3-C4-C5	-8.18	109.69	114.60
14	4	2115	G	N1-C2-N3	-8.17	119.00	123.90
14	4	2145	C	N3-C4-N4	8.16	123.71	118.00
5	p	64	G	C6-N1-C2	8.15	129.99	125.10
12	2	1341	G	N1-C6-O6	8.14	124.78	119.90
13	3	1531	C	O4'-C1'-N1	8.14	114.71	108.20
14	4	2199	A	C5-N7-C8	8.12	107.96	103.90
13	3	1525	A	C5-C6-N6	-8.12	117.21	123.70
14	4	2173	A	C5-C6-N1	-8.12	113.64	117.70
14	4	2149	U	N1-C2-O2	8.11	128.48	122.80
14	4	2152	G	N1-C2-N3	-8.10	119.04	123.90
5	p	12	U	O4'-C1'-N1	8.10	114.68	108.20
5	p	73	U	O4'-C1'-N1	8.10	114.68	108.20
14	4	2165	C	C3'-C2'-C1'	8.10	107.98	101.50
13	3	1540	G	C5-C6-O6	-8.08	123.75	128.60
14	4	2179	C	N1-C2-N3	-8.07	113.55	119.20
14	4	2183	A	C4-C5-C6	8.07	121.03	117.00
12	2	1319	C	O4'-C1'-N1	8.07	114.66	108.20
5	p	46	G	N1-C6-O6	8.06	124.74	119.90
2	E	127	PHE	CB-CG-CD1	-8.05	115.17	120.80
13	3	1549	A	C5-N7-C8	8.04	107.92	103.90
14	4	2116	G	N3-C4-C5	8.03	132.61	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	2	1338	G	C5-C6-O6	-8.03	123.78	128.60
1	y	233	PHE	CB-CG-CD1	8.02	126.41	120.80
5	p	6	A	C5-N7-C8	8.01	107.91	103.90
14	4	2118	U	N3-C4-O4	8.01	125.01	119.40
5	p	64	G	N1-C6-O6	8.01	124.70	119.90
14	4	2134	A	C5-C6-N6	-8.01	117.30	123.70
11	1	66	C	O4'-C1'-N1	8.00	114.60	108.20
5	p	56	C	O4'-C1'-N1	8.00	114.60	108.20
14	4	2169	A	N1-C6-N6	7.99	123.40	118.60
14	4	2117	A	N9-C4-C5	7.99	109.00	105.80
14	4	2118	U	C6-N1-C2	-7.99	116.21	121.00
14	4	2105	U	O4'-C4'-C3'	-7.98	96.02	104.00
11	1	77	G	C5-C6-O6	-7.98	123.81	128.60
13	3	1544	A	O4'-C1'-N9	7.98	114.58	108.20
14	4	2092	U	O4'-C1'-N1	7.97	114.58	108.20
14	4	2163	A	C5-N7-C8	7.97	107.89	103.90
13	3	1529	G	C5-N7-C8	-7.96	100.32	104.30
14	4	2168	G	N7-C8-N9	-7.96	109.12	113.10
11	1	106	C	O4'-C1'-N1	7.96	114.57	108.20
5	p	4	G	C5-C6-O6	-7.96	123.83	128.60
13	3	1517	G	O4'-C1'-N9	7.96	114.56	108.20
14	4	2102	G	C4-C5-C6	7.95	123.57	118.80
14	4	2159	G	C4-C5-C6	7.95	123.57	118.80
14	4	2179	C	O4'-C1'-N1	7.95	114.56	108.20
5	p	9	A	C5-N7-C8	7.95	107.87	103.90
5	p	54	U	O4'-C1'-N1	7.95	114.56	108.20
14	4	2110	G	C2-N3-C4	-7.94	107.93	111.90
14	4	2097	A	N7-C8-N9	7.93	117.76	113.80
14	4	2102	G	C5-C6-N1	-7.92	107.54	111.50
14	4	2103	C	C5-C4-N4	-7.92	114.66	120.20
5	p	27	C	N1-C2-O2	-7.92	114.15	118.90
5	p	52	A	N9-C4-C5	7.91	108.97	105.80
14	4	2135	A	C5-C6-N1	-7.91	113.75	117.70
5	p	60	U	O4'-C1'-N1	7.89	114.51	108.20
5	p	75	C	O4'-C1'-N1	7.89	114.51	108.20
14	4	2162	G	N3-C4-N9	7.89	130.73	126.00
14	4	2167	U	C4-C5-C6	7.88	124.43	119.70
13	3	1548	A	C6-C5-N7	-7.88	126.78	132.30
5	p	48	C	N3-C4-C5	-7.88	118.75	121.90
5	p	36	C	N3-C4-N4	7.88	123.51	118.00
14	4	2148	G	C4-C5-N7	-7.87	107.65	110.80
14	4	2105	U	N3-C4-C5	-7.87	109.88	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2183	A	C2-N3-C4	7.86	114.53	110.60
5	p	48	C	C6-N1-C2	-7.85	117.16	120.30
5	p	25	C	O4'-C1'-N1	7.84	114.47	108.20
14	4	2154	A	C5-C6-N6	-7.84	117.43	123.70
14	4	2107	G	C8-N9-C4	-7.84	103.27	106.40
5	p	53	G	C8-N9-C4	-7.83	103.27	106.40
1	y	67	PHE	CB-CG-CD1	-7.83	115.32	120.80
13	3	1549	A	C6-N1-C2	7.83	123.30	118.60
12	2	1323	C	O4'-C1'-N1	7.83	114.46	108.20
14	4	2108	A	C2-N3-C4	-7.82	106.69	110.60
1	y	64	PHE	CB-CG-CD2	-7.82	115.33	120.80
5	p	73	U	C2-N1-C1'	7.82	127.08	117.70
14	4	2173	A	C4-C5-C6	7.82	120.91	117.00
11	1	61	C	O4'-C1'-N1	7.81	114.45	108.20
5	p	26	A	N3-C4-C5	-7.81	121.33	126.80
14	4	2173	A	N1-C2-N3	-7.81	125.39	129.30
14	4	2193	G	N1-C2-N3	-7.81	119.21	123.90
11	1	108	G	C5-C6-O6	-7.81	123.92	128.60
14	4	2096	C	N3-C4-C5	-7.81	118.78	121.90
14	4	2126	A	C5-N7-C8	7.81	107.80	103.90
11	1	85	G	C5-C6-O6	-7.80	123.92	128.60
14	4	2097	A	C5-N7-C8	-7.80	100.00	103.90
5	p	69	C	P-O3'-C3'	7.79	129.05	119.70
5	p	28	G	C5-C6-O6	-7.79	123.92	128.60
13	3	1524	G	C5-C6-N1	-7.79	107.60	111.50
5	p	48	C	C5-C4-N4	-7.79	114.75	120.20
5	p	40	G	C4-C5-N7	-7.78	107.69	110.80
14	4	2183	A	N3-C4-C5	-7.78	121.36	126.80
14	4	2133	G	C1'-O4'-C4'	-7.76	103.69	109.90
1	y	294	PHE	CB-CG-CD2	-7.76	115.37	120.80
5	p	51	G	C8-N9-C4	7.76	109.50	106.40
14	4	2193	G	O4'-C1'-N9	7.76	114.41	108.20
14	4	2092	U	N1-C2-N3	7.76	119.55	114.90
14	4	2140	G	C5-C6-O6	-7.75	123.95	128.60
14	4	2104	C	C2-N1-C1'	7.75	127.33	118.80
14	4	2137	U	C5'-C4'-O4'	7.75	118.40	109.10
5	p	10	G	C8-N9-C4	-7.75	103.30	106.40
14	4	2160	C	N3-C4-C5	-7.75	118.80	121.90
5	p	24	G	C4-C5-N7	-7.74	107.70	110.80
13	3	1545	A	O4'-C1'-N9	7.74	114.39	108.20
2	E	96	ILE	CB-CA-C	-7.72	96.16	111.60
5	p	19	G	P-O3'-C3'	7.71	128.95	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1529	G	C6-C5-N7	-7.71	125.78	130.40
5	p	13	C	O4'-C1'-N1	7.71	114.36	108.20
14	4	2151	U	C5-C6-N1	-7.70	118.85	122.70
5	p	66	U	C2-N3-C4	-7.70	122.38	127.00
12	2	1317	G	N1-C6-O6	7.69	124.52	119.90
14	4	2180	U	N3-C2-O2	-7.68	116.82	122.20
14	4	2197	U	C2-N3-C4	7.68	131.61	127.00
5	p	6	A	C5-C6-N1	-7.67	113.86	117.70
5	p	64	G	P-O3'-C3'	-7.67	110.50	119.70
14	4	2145	C	C6-N1-C2	7.67	123.37	120.30
11	1	79	C	O4'-C1'-N1	7.65	114.32	108.20
14	4	2167	U	N3-C2-O2	7.65	127.56	122.20
14	4	2111	U	N3-C4-O4	7.64	124.75	119.40
13	3	1551	A	N7-C8-N9	-7.63	109.98	113.80
5	p	27	C	N3-C4-C5	-7.62	118.85	121.90
14	4	2138	G	O4'-C1'-N9	7.62	114.30	108.20
14	4	2146	C	N1-C2-O2	7.62	123.47	118.90
5	p	49	G	N3-C2-N2	7.62	125.23	119.90
13	3	1541	C	C6-N1-C2	7.62	123.35	120.30
14	4	2138	G	N3-C4-C5	-7.61	124.79	128.60
11	1	110	G	C5-C6-O6	-7.61	124.04	128.60
14	4	2110	G	C5-C6-N1	-7.60	107.70	111.50
5	p	37	A	O4'-C1'-N9	7.59	114.27	108.20
14	4	2127	G	C5'-C4'-O4'	7.59	118.21	109.10
14	4	2097	A	N9-C4-C5	7.58	108.83	105.80
14	4	2151	U	N3-C4-C5	-7.57	110.06	114.60
13	3	1530	G	N3-C2-N2	7.57	125.20	119.90
14	4	2138	G	C4'-C3'-C2'	-7.57	95.03	102.60
2	E	92	HIS	C-N-CA	7.57	140.62	121.70
12	2	1330	C	O4'-C1'-N1	7.57	114.25	108.20
5	p	42	C	O4'-C4'-C3'	-7.57	96.44	104.00
5	p	76	A	C6-C5-N7	-7.57	127.00	132.30
13	3	1537	G	N1-C2-N3	-7.57	119.36	123.90
13	3	1530	G	N3-C4-C5	7.56	132.38	128.60
14	4	2095	A	O4'-C1'-N9	7.56	114.25	108.20
3	G	34	PHE	N-CA-CB	7.55	124.20	110.60
5	p	45	G	C5-C6-N1	-7.55	107.72	111.50
5	p	32	U	N1-C2-N3	7.55	119.43	114.90
5	p	25	C	C5-C6-N1	7.55	124.78	121.00
14	4	2147	A	C5-N7-C8	7.55	107.67	103.90
14	4	2158	A	C4-C5-C6	7.55	120.78	117.00
14	4	2147	A	C6-N1-C2	7.54	123.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1521	G	C5-C6-O6	-7.54	124.08	128.60
14	4	2106	U	C4-C5-C6	7.54	124.22	119.70
14	4	2181	U	N3-C2-O2	7.53	127.47	122.20
5	p	55	U	O4'-C1'-N1	7.52	114.22	108.20
12	2	1337	G	C5-C6-O6	-7.52	124.09	128.60
14	4	2096	C	O4'-C1'-N1	7.52	114.22	108.20
5	p	68	C	C5'-C4'-O4'	7.52	118.12	109.10
5	p	53	G	C5-C6-O6	-7.51	124.09	128.60
5	p	50	C	C6-N1-C2	7.51	123.31	120.30
14	4	2164	C	C1'-O4'-C4'	-7.51	103.89	109.90
3	G	41	THR	CA-CB-CG2	-7.50	101.90	112.40
13	3	1543	G	C5-C6-N1	-7.50	107.75	111.50
5	p	17	U	N3-C2-O2	7.50	127.45	122.20
14	4	2114	A	C8-N9-C4	-7.50	102.80	105.80
5	p	38	A	N7-C8-N9	-7.49	110.05	113.80
14	4	2193	G	N1-C6-O6	7.49	124.40	119.90
14	4	2098	U	C2-N3-C4	7.49	131.50	127.00
13	3	1555	G	C5-C6-O6	-7.49	124.11	128.60
5	p	32	U	C2-N3-C4	-7.48	122.51	127.00
14	4	2093	G	C4'-C3'-C2'	-7.48	95.12	102.60
14	4	2187	U	O4'-C1'-N1	7.48	114.18	108.20
11	1	82	U	O4'-C1'-N1	7.48	114.18	108.20
14	4	2183	A	C4-C5-N7	-7.48	106.96	110.70
14	4	2194	U	O4'-C1'-N1	7.48	114.18	108.20
13	3	1550	C	C5-C6-N1	7.48	124.74	121.00
14	4	2163	A	O4'-C1'-N9	7.47	114.18	108.20
5	p	38	A	O4'-C1'-N9	7.46	114.17	108.20
2	E	86	THR	N-CA-CB	7.46	124.48	110.30
5	p	17	U	O4'-C1'-C2'	7.46	114.31	107.60
11	1	60	G	C5-C6-O6	-7.46	124.13	128.60
14	4	2096	C	C5-C4-N4	-7.45	114.98	120.20
13	3	1550	C	N3-C2-O2	7.45	127.11	121.90
4	n	99	ALA	C-N-CA	-7.44	106.67	122.30
11	1	76	C	O4'-C1'-N1	7.44	114.16	108.20
7	5	72	SER	N-CA-CB	7.44	121.66	110.50
12	2	1335	C	O4'-C1'-N1	7.44	114.15	108.20
11	1	80	G	C5-C6-O6	-7.44	124.14	128.60
13	3	1526	C	N3-C4-N4	7.43	123.20	118.00
5	p	19	G	C6-N1-C2	7.42	129.55	125.10
14	4	2144	G	N1-C2-N3	-7.42	119.45	123.90
5	p	26	A	C5-C6-N1	-7.41	114.00	117.70
11	1	70	G	C5-C6-O6	-7.40	124.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	5	G	C4-C5-N7	7.39	113.75	110.80
14	4	2190	G	N1-C2-N3	-7.39	119.47	123.90
14	4	2121	G	C5-C6-O6	-7.38	124.17	128.60
5	p	69	C	C5-C6-N1	7.38	124.69	121.00
5	p	18	G	C6-N1-C2	7.37	129.52	125.10
14	4	2116	G	C1'-O4'-C4'	-7.36	104.02	109.90
13	3	1531	C	C2-N3-C4	-7.35	116.22	119.90
1	y	251	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	y	300	TRP	CB-CG-CD2	7.34	136.14	126.60
5	p	20	U	N3-C4-O4	7.34	124.54	119.40
14	4	2117	A	C4-C5-C6	7.34	120.67	117.00
14	4	2184	A	C2-N3-C4	7.34	114.27	110.60
12	2	1336	A	O4'-C1'-N9	7.33	114.07	108.20
1	y	255	ARG	N-CA-CB	7.33	123.80	110.60
5	p	11	C	O4'-C1'-N1	7.33	114.07	108.20
7	5	1	MET	CG-SD-CE	-7.33	88.47	100.20
14	4	2118	U	O4'-C1'-N1	7.33	114.06	108.20
13	3	1524	G	C5-C6-O6	-7.33	124.20	128.60
14	4	2177	C	N3-C4-C5	-7.33	118.97	121.90
14	4	2130	U	C5'-C4'-O4'	7.32	117.88	109.10
13	3	1528	A	C5-C6-N6	-7.32	117.85	123.70
13	3	1533	C	C2-N3-C4	7.32	123.56	119.90
14	4	2159	G	C5-C6-N1	-7.30	107.85	111.50
14	4	2149	U	N1-C2-N3	-7.30	110.52	114.90
14	4	2108	A	C6-N1-C2	7.29	122.97	118.60
14	4	2164	C	N1-C2-O2	7.29	123.27	118.90
14	4	2190	G	C4-N9-C1'	-7.29	117.03	126.50
14	4	2148	G	P-O3'-C3'	7.29	128.44	119.70
14	4	2146	C	C3'-C2'-C1'	7.28	107.32	101.50
5	p	48	C	C5-C6-N1	7.26	124.63	121.00
14	4	2174	C	O4'-C1'-N1	7.25	114.00	108.20
5	p	13	C	P-O3'-C3'	-7.25	111.00	119.70
11	1	52	A	C4-C5-C6	7.24	120.62	117.00
14	4	2178	C	C2-N1-C1'	7.23	126.76	118.80
13	3	1523	U	O4'-C1'-N1	7.22	113.98	108.20
14	4	2156	G	C6-N1-C2	7.22	129.43	125.10
14	4	2116	G	N3-C2-N2	7.22	124.95	119.90
12	2	1310	G	C5-C6-O6	-7.21	124.28	128.60
14	4	2114	A	C6-C5-N7	-7.20	127.26	132.30
13	3	1523	U	C3'-C2'-C1'	7.20	107.26	101.50
12	2	1324	G	C5-C6-O6	-7.19	124.28	128.60
5	p	5	G	N3-C4-C5	7.19	132.20	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1545	A	C6-C5-N7	-7.19	127.27	132.30
5	p	39	G	P-O3'-C3'	-7.19	111.07	119.70
14	4	2145	C	P-O5'-C5'	7.18	132.40	120.90
5	p	7	A	C6-N1-C2	7.18	122.91	118.60
5	p	56	C	N3-C4-N4	7.18	123.02	118.00
7	5	101	ALA	CB-CA-C	-7.18	99.33	110.10
11	1	107	G	C5-C6-O6	-7.18	124.29	128.60
14	4	2140	G	C5-C6-N1	7.17	115.09	111.50
11	1	96	C	O4'-C1'-N1	7.16	113.93	108.20
7	5	74	ARG	NE-CZ-NH2	-7.16	116.72	120.30
14	4	2142	A	P-O5'-C5'	-7.15	109.47	120.90
5	p	51	G	N1-C2-N3	-7.14	119.61	123.90
13	3	1545	A	C5-C6-N6	-7.14	117.99	123.70
11	1	89	A	O4'-C1'-N9	7.14	113.91	108.20
14	4	2181	U	C6-N1-C2	7.13	125.28	121.00
14	4	2193	G	N9-C4-C5	7.13	108.25	105.40
14	4	2127	G	C6-C5-N7	-7.12	126.13	130.40
14	4	2168	G	C8-N9-C4	-7.12	103.55	106.40
5	p	58	A	N3-C4-C5	-7.12	121.82	126.80
14	4	2173	A	N3-C4-C5	-7.11	121.82	126.80
13	3	1551	A	C2-N3-C4	-7.10	107.05	110.60
12	2	1309	G	C5-C6-O6	-7.10	124.34	128.60
14	4	2132	U	C1'-O4'-C4'	-7.10	104.22	109.90
2	E	105	SER	N-CA-CB	7.09	121.14	110.50
14	4	2152	G	C8-N9-C4	-7.09	103.57	106.40
5	p	52	A	C4-C5-C6	7.08	120.54	117.00
5	p	61	C	C6-N1-C2	-7.08	117.47	120.30
13	3	1532	A	C5-C6-N6	-7.08	118.03	123.70
14	4	2180	U	C4'-C3'-C2'	-7.08	95.52	102.60
5	p	72	C	C5-C6-N1	7.07	124.54	121.00
12	2	1332	G	C5-C6-O6	-7.07	124.36	128.60
5	p	6	A	P-O3'-C3'	7.07	128.18	119.70
14	4	2158	A	O4'-C1'-N9	7.07	113.85	108.20
5	p	50	C	O4'-C1'-N1	7.07	113.85	108.20
11	1	59	U	O4'-C1'-N1	7.07	113.85	108.20
14	4	2092	U	C6-N1-C2	-7.06	116.76	121.00
5	p	43	G	C5-C6-O6	-7.06	124.37	128.60
13	3	1540	G	N1-C2-N3	-7.06	119.67	123.90
13	3	1524	G	O4'-C1'-N9	7.05	113.84	108.20
11	1	90	U	O4'-C1'-N1	7.05	113.84	108.20
1	y	352	PHE	CB-CG-CD1	-7.04	115.87	120.80
4	n	99	ALA	CA-C-N	-7.04	102.12	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	78	U	O4'-C1'-N1	7.04	113.83	108.20
13	3	1524	G	C6-N1-C2	7.04	129.32	125.10
14	4	2161	C	N3-C4-N4	7.04	122.92	118.00
14	4	2100	G	N7-C8-N9	7.03	116.61	113.10
14	4	2126	A	C6-N1-C2	7.02	122.81	118.60
13	3	1525	A	C4-C5-N7	-7.01	107.19	110.70
14	4	2100	G	P-O5'-C5'	-7.01	109.67	120.90
5	p	26	A	C5-C6-N6	-7.01	118.09	123.70
13	3	1516	G	C5-C6-O6	-7.01	124.39	128.60
5	p	51	G	N7-C8-N9	-7.01	109.59	113.10
14	4	2106	U	N3-C4-C5	-7.01	110.39	114.60
5	p	9	A	N3-C4-C5	-7.00	121.90	126.80
14	4	2107	G	C4-C5-C6	-7.00	114.60	118.80
14	4	2164	C	P-O3'-C3'	7.00	128.10	119.70
1	y	22	ARG	NE-CZ-NH1	6.98	123.79	120.30
14	4	2191	A	N3-C4-C5	-6.97	121.92	126.80
14	4	2115	G	C2-N3-C4	6.97	115.39	111.90
5	p	53	G	N1-C6-O6	6.97	124.08	119.90
5	p	50	C	C1'-O4'-C4'	6.96	115.47	109.90
14	4	2152	G	N3-C2-N2	6.95	124.77	119.90
5	p	32	U	C6-N1-C2	-6.95	116.83	121.00
14	4	2142	A	C5-C6-N1	-6.95	114.22	117.70
14	4	2123	G	N1-C2-N3	-6.95	119.73	123.90
12	2	1322	A	O4'-C1'-N9	6.93	113.75	108.20
5	p	29	A	C6-C5-N7	-6.93	127.45	132.30
5	p	17	U	N1-C2-N3	-6.92	110.75	114.90
7	5	7	ARG	NE-CZ-NH2	-6.92	116.84	120.30
13	3	1520	U	N1-C2-O2	-6.91	117.96	122.80
14	4	2199	A	N1-C2-N3	6.90	132.75	129.30
1	y	47	ALA	N-CA-CB	6.90	119.76	110.10
14	4	2156	G	N3-C2-N2	6.90	124.73	119.90
4	n	38	LEU	N-CA-C	6.90	129.62	111.00
13	3	1516	G	O4'-C1'-N9	6.89	113.72	108.20
13	3	1530	G	N3-C4-N9	-6.89	121.86	126.00
13	3	1556	C	O4'-C1'-N1	6.89	113.72	108.20
14	4	2095	A	C5-C6-N1	-6.89	114.25	117.70
1	y	298	THR	N-CA-CB	6.89	123.39	110.30
1	y	315	PRO	C-N-CA	6.89	138.92	121.70
5	p	10	G	N1-C6-O6	6.89	124.03	119.90
11	1	67	U	O4'-C1'-N1	6.89	113.71	108.20
11	1	75	G	C5-C6-O6	-6.88	124.47	128.60
14	4	2141	G	C5'-C4'-O4'	6.88	117.36	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	1527	G	N9-C4-C5	6.88	108.15	105.40
13	3	1525	A	C4-C5-C6	6.88	120.44	117.00
5	p	44	G	C5'-C4'-O4'	6.88	117.35	109.10
13	3	1543	G	C6-C5-N7	-6.87	126.28	130.40
1	y	47	ALA	CB-CA-C	-6.87	99.79	110.10
13	3	1537	G	C5-C6-N1	-6.87	108.06	111.50
5	p	12	U	N1-C2-N3	-6.87	110.78	114.90
14	4	2107	G	N7-C8-N9	6.87	116.53	113.10
13	3	1529	G	O4'-C1'-N9	6.85	113.68	108.20
13	3	1538	G	N1-C2-N3	-6.84	119.80	123.90
14	4	2186	G	O4'-C1'-N9	6.84	113.67	108.20
5	p	54	U	N3-C2-O2	6.84	126.99	122.20
13	3	1542	U	N1-C2-O2	-6.84	118.01	122.80
13	3	1519	G	C4-C5-C6	6.83	122.90	118.80
1	y	327	PHE	CB-CG-CD2	6.83	125.58	120.80
1	y	380	TYR	CG-CD2-CE2	6.83	126.76	121.30
14	4	2101	A	N1-C2-N3	6.82	132.71	129.30
14	4	2138	G	N1-C6-O6	6.82	123.99	119.90
3	G	48	SER	N-CA-CB	6.82	120.73	110.50
5	p	29	A	C8-N9-C4	-6.81	103.08	105.80
14	4	2142	A	C4-C5-C6	6.81	120.40	117.00
14	4	2095	A	C6-C5-N7	-6.80	127.54	132.30
5	p	31	C	N3-C4-C5	-6.80	119.18	121.90
13	3	1549	A	C4-C5-N7	-6.79	107.30	110.70
13	3	1517	G	N3-C2-N2	6.79	124.65	119.90
14	4	2171	A	P-O5'-C5'	6.79	131.76	120.90
1	y	440	GLY	CA-C-O	-6.78	108.39	120.60
11	1	98	G	C5-C6-O6	-6.78	124.53	128.60
12	2	1311	G	C5-C6-O6	-6.78	124.53	128.60
13	3	1552	A	C4-C5-C6	6.78	120.39	117.00
1	y	45	ASP	N-CA-CB	6.77	122.79	110.60
14	4	2120	G	C5-N7-C8	-6.77	100.91	104.30
5	p	5	G	N9-C4-C5	-6.77	102.69	105.40
12	2	1333	G	C5-C6-O6	-6.77	124.54	128.60
14	4	2140	G	C8-N9-C4	-6.77	103.69	106.40
13	3	1540	G	P-O3'-C3'	-6.76	111.58	119.70
14	4	2170	A	N3-C4-C5	-6.76	122.07	126.80
13	3	1538	G	N3-C2-N2	6.76	124.63	119.90
14	4	2169	A	C5-C6-N1	-6.76	114.32	117.70
14	4	2133	G	C6-C5-N7	-6.76	126.34	130.40
14	4	2127	G	C6-N1-C2	-6.75	121.05	125.10
14	4	2146	C	O4'-C1'-N1	6.75	113.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	15	G	C5-C6-N1	-6.75	108.12	111.50
12	2	1339	G	C5-C6-O6	-6.75	124.55	128.60
11	1	56	A	C5-C6-N6	-6.75	118.30	123.70
14	4	2152	G	C5'-C4'-O4'	6.75	117.20	109.10
14	4	2195	U	O4'-C1'-N1	6.74	113.59	108.20
14	4	2094	A	N3-C4-C5	-6.72	122.10	126.80
14	4	2185	U	N3-C4-O4	-6.72	114.70	119.40
3	G	34	PHE	CB-CG-CD2	-6.72	116.10	120.80
14	4	2102	G	O4'-C1'-N9	6.71	113.57	108.20
14	4	2108	A	O4'-C1'-N9	6.71	113.57	108.20
14	4	2164	C	O4'-C1'-N1	6.71	113.57	108.20
11	1	96	C	N3-C4-N4	6.71	122.70	118.00
14	4	2179	C	C2-N3-C4	6.71	123.25	119.90
12	2	1313	U	C2-N1-C1'	6.71	125.75	117.70
14	4	2163	A	N1-C6-N6	6.70	122.62	118.60
14	4	2108	A	N1-C2-N3	-6.70	125.95	129.30
5	p	47	U	C4-C5-C6	6.69	123.71	119.70
14	4	2169	A	C4-C5-N7	-6.69	107.36	110.70
5	p	12	U	N3-C4-O4	6.69	124.08	119.40
14	4	2100	G	C8-N9-C4	-6.68	103.73	106.40
1	y	424	MET	N-CA-CB	6.68	122.62	110.60
5	p	57	G	N1-C2-N3	-6.68	119.89	123.90
13	3	1527	G	C8-N9-C4	-6.68	103.73	106.40
12	2	1310	G	O4'-C1'-N9	6.68	113.54	108.20
14	4	2153	C	O4'-C1'-N1	6.68	113.54	108.20
14	4	2104	C	C5-C4-N4	-6.67	115.53	120.20
2	E	89	GLU	N-CA-CB	6.66	122.58	110.60
11	1	99	U	C2-N1-C1'	6.66	125.69	117.70
13	3	1546	G	N3-C4-C5	-6.65	125.28	128.60
14	4	2164	C	C6-N1-C1'	-6.65	112.82	120.80
14	4	2113	U	O4'-C1'-N1	6.65	113.52	108.20
14	4	2178	C	C4-C5-C6	6.64	120.72	117.40
5	p	39	G	N1-C2-N2	-6.64	110.23	116.20
13	3	1529	G	N7-C8-N9	6.64	116.42	113.10
3	G	63	PHE	CB-CG-CD1	6.62	125.44	120.80
5	p	19	G	N3-C4-C5	-6.62	125.29	128.60
5	p	1	G	C4'-C3'-C2'	-6.62	95.98	102.60
14	4	2183	A	N7-C8-N9	6.62	117.11	113.80
5	p	70	C	N1-C2-O2	6.62	122.87	118.90
14	4	2186	G	N1-C2-N2	6.62	122.16	116.20
5	p	71	G	C4-C5-N7	6.62	113.45	110.80
14	4	2101	A	N1-C6-N6	6.61	122.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2146	C	C6-N1-C2	6.61	122.95	120.30
4	n	17	ALA	N-CA-CB	6.61	119.35	110.10
5	p	52	A	C5-C6-N6	-6.61	118.41	123.70
12	2	1326	U	O4'-C1'-N1	6.61	113.48	108.20
5	p	73	U	C6-N1-C1'	-6.60	111.96	121.20
13	3	1533	C	C5-C4-N4	6.60	124.82	120.20
13	3	1534	U	O4'-C1'-N1	6.60	113.48	108.20
13	3	1543	G	C5-C6-O6	-6.60	124.64	128.60
5	p	23	A	N1-C2-N3	6.60	132.60	129.30
13	3	1529	G	N3-C4-C5	-6.60	125.30	128.60
14	4	2165	C	P-O3'-C3'	6.60	127.62	119.70
13	3	1517	G	N7-C8-N9	6.59	116.40	113.10
5	p	46	G	C5-C6-O6	-6.59	124.64	128.60
5	p	32	U	C4-C5-C6	6.58	123.65	119.70
14	4	2162	G	N1-C2-N3	-6.58	119.95	123.90
5	p	63	C	O5'-P-OP2	-6.56	99.79	105.70
1	y	8	ASP	CB-CA-C	6.56	123.52	110.40
14	4	2185	U	C5-C6-N1	6.56	125.98	122.70
5	p	27	C	N3-C2-O2	6.56	126.49	121.90
5	p	20	U	C5-C4-O4	-6.55	121.97	125.90
1	y	236	PHE	CG-CD1-CE1	-6.54	113.61	120.80
5	p	18	G	N7-C8-N9	-6.53	109.84	113.10
14	4	2190	G	C8-N9-C1'	6.53	135.48	127.00
1	y	243	ARG	NE-CZ-NH2	6.52	123.56	120.30
12	2	1314	C	O4'-C1'-N1	6.52	113.42	108.20
13	3	1518	C	N3-C4-C5	-6.52	119.29	121.90
5	p	29	A	C4-C5-C6	6.52	120.26	117.00
5	p	4	G	N1-C6-O6	6.52	123.81	119.90
13	3	1547	C	O4'-C1'-N1	6.52	113.42	108.20
13	3	1549	A	C2-N3-C4	-6.52	107.34	110.60
2	E	83	ILE	CB-CA-C	-6.51	98.57	111.60
5	p	49	G	N3-C4-C5	-6.51	125.34	128.60
5	p	73	U	N3-C4-C5	-6.51	110.69	114.60
1	y	300	TRP	CB-CG-CD1	-6.51	118.54	127.00
11	1	53	A	C4-C5-C6	6.51	120.25	117.00
11	1	93	G	C5-C6-O6	-6.51	124.69	128.60
14	4	2127	G	C4-C5-C6	6.51	122.70	118.80
11	1	58	G	C5-C6-O6	-6.51	124.70	128.60
11	1	95	A	C5-C6-N6	-6.50	118.50	123.70
14	4	2148	G	C6-C5-N7	-6.50	126.50	130.40
2	E	114	ILE	CB-CA-C	6.49	124.59	111.60
11	1	74	A	C4-C5-C6	6.49	120.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	94	LEU	N-CA-CB	6.49	123.38	110.40
14	4	2102	G	C6-C5-N7	-6.49	126.51	130.40
14	4	2096	C	C4-C5-C6	6.49	120.64	117.40
11	1	113	U	O4'-C1'-N1	6.49	113.39	108.20
14	4	2114	A	C6-N1-C2	6.49	122.49	118.60
5	p	21	A	O4'-C1'-N9	6.48	113.39	108.20
14	4	2120	G	N3-C4-N9	-6.47	122.12	126.00
14	4	2154	A	P-O3'-C3'	6.47	127.47	119.70
14	4	2098	U	N3-C4-C5	-6.47	110.72	114.60
11	1	95	A	C4-C5-C6	6.47	120.23	117.00
14	4	2158	A	C6-N1-C2	-6.47	114.72	118.60
5	p	65	U	N3-C4-O4	6.46	123.92	119.40
13	3	1544	A	N9-C4-C5	6.46	108.39	105.80
11	1	54	G	C5-C6-O6	-6.46	124.72	128.60
1	y	22	ARG	NE-CZ-NH2	6.46	123.53	120.30
11	1	110	G	O4'-C1'-N9	6.45	113.36	108.20
12	2	1334	G	C5-C6-O6	-6.45	124.73	128.60
14	4	2180	U	N1-C2-N3	6.45	118.77	114.90
1	y	22	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
5	p	5	G	O4'-C1'-N9	6.44	113.35	108.20
14	4	2136	G	C8-N9-C4	-6.43	103.83	106.40
11	1	114	U	O4'-C1'-N1	6.43	113.34	108.20
14	4	2144	G	N1-C2-N2	-6.43	110.41	116.20
11	1	105	C	N3-C4-N4	6.42	122.50	118.00
12	2	1309	G	O4'-C1'-N9	6.42	113.34	108.20
5	p	75	C	N3-C4-N4	6.41	122.49	118.00
11	1	55	G	C5-C6-O6	-6.41	124.75	128.60
14	4	2127	G	C8-N9-C4	-6.41	103.84	106.40
11	1	104	A	C5-C6-N6	-6.40	118.58	123.70
1	y	390	PHE	CB-CG-CD2	6.40	125.28	120.80
13	3	1557	C	O4'-C1'-N1	6.40	113.32	108.20
1	y	340	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
5	p	59	G	N3-C2-N2	6.39	124.38	119.90
12	2	1315	C	N3-C4-N4	6.39	122.47	118.00
12	2	1317	G	O4'-C1'-N9	6.39	113.31	108.20
14	4	2143	C	C5-C4-N4	-6.39	115.73	120.20
14	4	2157	G	C5'-C4'-O4'	6.38	116.76	109.10
14	4	2183	A	O4'-C1'-N9	6.38	113.31	108.20
14	4	2113	U	N3-C4-O4	6.38	123.87	119.40
11	1	64	A	C5-C6-N1	-6.38	114.51	117.70
13	3	1545	A	N3-C4-C5	-6.38	122.33	126.80
11	1	107	G	O4'-C1'-N9	6.38	113.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	101	A	C4-C5-C6	6.38	120.19	117.00
1	y	238	GLU	N-CA-CB	6.37	122.06	110.60
14	4	2130	U	C5-C4-O4	-6.37	122.08	125.90
14	4	2185	U	P-O5'-C5'	-6.36	110.72	120.90
14	4	2148	G	O4'-C1'-N9	6.36	113.29	108.20
14	4	2163	A	N7-C8-N9	-6.36	110.62	113.80
5	p	23	A	C5-C6-N6	-6.36	118.62	123.70
5	p	25	C	N3-C4-C5	-6.35	119.36	121.90
11	1	87	U	O4'-C1'-N1	6.35	113.28	108.20
11	1	91	A	C4-C5-C6	6.35	120.17	117.00
14	4	2123	G	C5'-C4'-O4'	6.34	116.71	109.10
14	4	2117	A	C5-C6-N6	-6.34	118.63	123.70
12	2	1341	G	C5-C6-O6	-6.33	124.80	128.60
14	4	2135	A	N7-C8-N9	6.33	116.97	113.80
14	4	2176	A	C4-C5-N7	-6.33	107.53	110.70
5	p	30	C	C1'-O4'-C4'	6.33	114.96	109.90
5	p	1	G	C5-N7-C8	6.32	107.46	104.30
11	1	54	G	O4'-C1'-N9	6.32	113.26	108.20
14	4	2167	U	P-O5'-C5'	6.32	131.01	120.90
14	4	2198	A	C5-N7-C8	6.32	107.06	103.90
5	p	13	C	N1-C2-N3	-6.31	114.78	119.20
14	4	2101	A	C5-N7-C8	6.31	107.05	103.90
11	1	52	A	C5-C6-N1	-6.30	114.55	117.70
5	p	37	A	C5-C6-N1	-6.30	114.55	117.70
14	4	2189	U	N3-C4-O4	6.30	123.81	119.40
13	3	1521	G	C4-C5-N7	-6.29	108.28	110.80
11	1	111	A	C4-C5-C6	6.29	120.14	117.00
5	p	34	G	C5-C6-O6	-6.28	124.83	128.60
14	4	2179	C	N3-C2-O2	6.28	126.30	121.90
7	5	60	ARG	NE-CZ-NH1	6.28	123.44	120.30
13	3	1517	G	N1-C2-N3	-6.28	120.13	123.90
13	3	1521	G	N1-C2-N3	-6.28	120.13	123.90
14	4	2165	C	N3-C4-C5	-6.28	119.39	121.90
5	p	74	C	C4-C5-C6	6.28	120.54	117.40
14	4	2141	G	O4'-C1'-N9	6.27	113.22	108.20
5	p	42	C	C3'-C2'-C1'	-6.27	96.48	101.50
14	4	2132	U	O4'-C1'-N1	6.27	113.22	108.20
11	1	77	G	O4'-C1'-N9	6.26	113.21	108.20
14	4	2144	G	C8-N9-C1'	-6.26	118.86	127.00
11	1	111	A	O4'-C1'-N9	6.25	113.20	108.20
13	3	1537	G	C5-C6-O6	-6.25	124.85	128.60
14	4	2110	G	C6-N1-C2	6.25	128.85	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	10	G	C5-C6-N1	-6.25	108.38	111.50
5	p	6	A	C4-C5-N7	-6.24	107.58	110.70
14	4	2126	A	C4-C5-C6	6.24	120.12	117.00
14	4	2144	G	N9-C4-C5	-6.24	102.90	105.40
12	2	1331	G	C5-C6-O6	-6.24	124.86	128.60
13	3	1544	A	C6-C5-N7	-6.24	127.94	132.30
14	4	2133	G	C2-N3-C4	-6.24	108.78	111.90
12	2	1316	U	O4'-C1'-N1	6.23	113.19	108.20
5	p	18	G	N1-C2-N3	-6.23	120.16	123.90
5	p	3	G	N3-C2-N2	6.22	124.25	119.90
14	4	2143	C	P-O3'-C3'	6.22	127.16	119.70
1	y	166	THR	N-CA-CB	6.22	122.11	110.30
1	y	429	TYR	CG-CD2-CE2	-6.22	116.33	121.30
5	p	61	C	C4-C5-C6	6.22	120.51	117.40
14	4	2186	G	N1-C2-N3	-6.21	120.17	123.90
12	2	1317	G	C5-C6-O6	-6.21	124.88	128.60
14	4	2191	A	N3-C4-N9	6.20	132.36	127.40
14	4	2129	C	O4'-C1'-N1	6.20	113.16	108.20
13	3	1557	C	N3-C4-N4	6.19	122.33	118.00
12	2	1307	A	O4'-C1'-N9	6.19	113.15	108.20
5	p	10	G	O4'-C1'-N9	6.18	113.14	108.20
14	4	2093	G	P-O3'-C3'	-6.18	112.28	119.70
5	p	22	G	C5-N7-C8	6.18	107.39	104.30
11	1	109	C	N3-C4-N4	6.17	122.32	118.00
14	4	2174	C	C2-N3-C4	6.17	122.99	119.90
11	1	93	G	O4'-C1'-N9	6.17	113.14	108.20
13	3	1528	A	O4'-C1'-N9	6.17	113.14	108.20
7	5	208	TYR	CZ-CE2-CD2	6.17	125.35	119.80
13	3	1517	G	O5'-P-OP2	-6.17	100.15	105.70
5	p	45	G	C5-C6-O6	-6.17	124.90	128.60
11	1	68	G	O4'-C1'-N9	6.17	113.13	108.20
14	4	2196	C	N3-C4-C5	-6.17	119.43	121.90
14	4	2095	A	N7-C8-N9	-6.17	110.72	113.80
5	p	19	G	C3'-C2'-C1'	-6.16	96.57	101.50
13	3	1523	U	C4-C5-C6	-6.16	116.00	119.70
14	4	2103	C	O4'-C1'-N1	6.16	113.12	108.20
1	y	399	PHE	CB-CG-CD2	6.16	125.11	120.80
11	1	71	A	C4-C5-C6	6.15	120.08	117.00
5	p	75	C	C4-C5-C6	6.15	120.48	117.40
14	4	2167	U	N3-C4-C5	-6.15	110.91	114.60
7	5	102	ASP	CB-CG-OD1	-6.15	112.77	118.30
12	2	1321	A	C4-C5-C6	6.15	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	3	G	N9-C4-C5	-6.15	102.94	105.40
13	3	1544	A	C5-N7-C8	-6.14	100.83	103.90
14	4	2167	U	N1-C1'-C2'	-6.14	105.24	112.00
1	y	113	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	E	121	PHE	CB-CG-CD2	-6.14	116.50	120.80
14	4	2123	G	C4'-C3'-C2'	-6.14	96.46	102.60
13	3	1550	C	C2-N3-C4	6.13	122.97	119.90
11	1	94	A	O4'-C1'-N9	6.13	113.10	108.20
1	y	438	LEU	N-CA-CB	6.13	122.66	110.40
5	p	36	C	C5-C4-N4	-6.13	115.91	120.20
1	y	168	THR	CA-CB-CG2	6.13	120.98	112.40
13	3	1526	C	C2-N3-C4	6.12	122.96	119.90
11	1	94	A	C4-C5-C6	6.12	120.06	117.00
1	y	272	ALA	CB-CA-C	-6.11	100.93	110.10
14	4	2102	G	C8-N9-C4	-6.11	103.95	106.40
2	E	82	VAL	CA-CB-CG2	-6.11	101.74	110.90
3	G	64	PHE	CB-CG-CD1	-6.11	116.52	120.80
11	1	73	A	O4'-C1'-N9	6.11	113.09	108.20
5	p	2	C	N1-C1'-C2'	-6.10	105.28	112.00
7	5	164	ARG	NE-CZ-NH1	6.10	123.35	120.30
14	4	2167	U	N1-C2-O2	-6.10	118.53	122.80
14	4	2144	G	O4'-C1'-N9	6.10	113.08	108.20
11	1	65	U	O4'-C1'-N1	6.09	113.07	108.20
14	4	2111	U	C4-C5-C6	6.09	123.35	119.70
5	p	30	C	C2-N3-C4	-6.09	116.86	119.90
14	4	2180	U	C5-C4-O4	-6.08	122.25	125.90
12	2	1318	U	O4'-C1'-N1	6.08	113.06	108.20
5	p	12	U	C6-N1-C2	6.07	124.64	121.00
13	3	1541	C	N3-C4-N4	6.07	122.25	118.00
5	p	59	G	N7-C8-N9	-6.07	110.07	113.10
13	3	1535	A	C6-C5-N7	-6.07	128.05	132.30
14	4	2131	U	P-O3'-C3'	6.07	126.98	119.70
14	4	2188	U	N3-C4-C5	-6.05	110.97	114.60
5	p	57	G	C5-N7-C8	6.05	107.33	104.30
5	p	4	G	C8-N9-C4	-6.05	103.98	106.40
5	p	13	C	C4-C5-C6	6.04	120.42	117.40
14	4	2148	G	N1-C2-N3	-6.04	120.28	123.90
12	2	1336	A	C5-C6-N6	-6.03	118.87	123.70
5	p	63	C	C6-N1-C2	6.03	122.71	120.30
1	y	40	PRO	N-CD-CG	6.02	112.24	103.20
11	1	102	U	O4'-C1'-N1	6.02	113.02	108.20
5	p	53	G	C1'-O4'-C4'	-6.02	105.08	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2171	A	O4'-C1'-N9	6.02	113.02	108.20
1	y	242	ARG	NE-CZ-NH1	-6.02	117.29	120.30
11	1	73	A	C4-C5-C6	6.02	120.01	117.00
5	p	75	C	N1-C2-O2	6.02	122.51	118.90
11	1	108	G	O4'-C1'-N9	6.02	113.01	108.20
3	G	34	PHE	CB-CG-CD1	6.01	125.01	120.80
12	2	1314	C	N3-C4-N4	6.01	122.21	118.00
14	4	2199	A	C6-N1-C2	-6.01	114.99	118.60
14	4	2182	U	N3-C4-O4	6.01	123.61	119.40
14	4	2197	U	P-O3'-C3'	6.01	126.91	119.70
11	1	56	A	C4-C5-C6	6.00	120.00	117.00
14	4	2152	G	N1-C6-O6	6.00	123.50	119.90
14	4	2194	U	N1-C2-N3	-6.00	111.30	114.90
11	1	89	A	C5-C6-N1	-6.00	114.70	117.70
2	E	88	GLN	N-CA-CB	5.99	121.39	110.60
14	4	2192	U	C5-C6-N1	5.99	125.70	122.70
5	p	24	G	C5-C6-O6	5.99	132.19	128.60
11	1	103	A	O4'-C1'-N9	5.99	112.99	108.20
13	3	1544	A	C5'-C4'-O4'	5.99	116.28	109.10
5	p	44	G	C2-N3-C4	5.99	114.89	111.90
14	4	2169	A	N1-C2-N3	5.98	132.29	129.30
14	4	2110	G	C6-C5-N7	-5.98	126.81	130.40
5	p	29	A	O4'-C1'-N9	5.97	112.98	108.20
11	1	89	A	C4-C5-C6	5.97	119.99	117.00
12	2	1336	A	C4-C5-C6	5.97	119.98	117.00
5	p	15	G	C4-C5-C6	5.96	122.38	118.80
5	p	10	G	P-O5'-C5'	-5.96	111.36	120.90
12	2	1342	A	C4-C5-C6	5.96	119.98	117.00
14	4	2151	U	C2-N3-C4	5.96	130.58	127.00
13	3	1556	C	N3-C4-C5	-5.96	119.52	121.90
3	G	33	SER	C-N-CA	5.96	136.59	121.70
5	p	13	C	C6-N1-C2	5.96	122.68	120.30
5	p	15	G	P-O3'-C3'	5.96	126.85	119.70
5	p	70	C	N3-C4-N4	5.96	122.17	118.00
14	4	2120	G	N1-C2-N3	-5.96	120.33	123.90
14	4	2157	G	P-O3'-C3'	5.96	126.85	119.70
11	1	104	A	C4-C5-C6	5.95	119.98	117.00
13	3	1546	G	N1-C2-N3	-5.95	120.33	123.90
1	y	248	TYR	CG-CD2-CE2	-5.95	116.54	121.30
13	3	1523	U	N1-C2-N3	-5.95	111.33	114.90
11	1	68	G	C5-C6-O6	-5.94	125.03	128.60
11	1	83	A	C5-C6-N6	-5.94	118.95	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	29	A	P-O3'-C3'	5.94	126.83	119.70
11	1	83	A	C4-C5-C6	5.92	119.96	117.00
7	5	162	ARG	NE-CZ-NH2	-5.92	117.34	120.30
13	3	1541	C	C5-C4-N4	-5.92	116.06	120.20
11	1	60	G	O4'-C1'-N9	5.92	112.94	108.20
5	p	13	C	C5'-C4'-C3'	-5.92	106.53	116.00
5	p	45	G	N7-C8-N9	-5.92	110.14	113.10
14	4	2161	C	N3-C4-C5	-5.92	119.53	121.90
5	p	44	G	C4-C5-N7	-5.91	108.44	110.80
11	1	84	A	C5-C6-N6	-5.91	118.97	123.70
14	4	2120	G	N3-C2-N2	5.91	124.04	119.90
5	p	15	G	C5-C6-O6	-5.91	125.06	128.60
7	5	134	ARG	NE-CZ-NH1	5.91	123.25	120.30
13	3	1545	A	C8-N9-C4	-5.91	103.44	105.80
5	p	43	G	C6-N1-C2	-5.90	121.56	125.10
11	1	84	A	C4-C5-C6	5.90	119.95	117.00
11	1	97	C	N3-C4-N4	5.90	122.13	118.00
11	1	53	A	C5-C6-N6	-5.90	118.98	123.70
5	p	17	U	O4'-C1'-N1	5.90	112.92	108.20
13	3	1553	A	C4-C5-C6	5.90	119.95	117.00
7	5	156	ALA	N-CA-CB	5.89	118.35	110.10
11	1	66	C	N3-C4-C5	-5.89	119.54	121.90
12	2	1325	U	O4'-C1'-N1	5.89	112.91	108.20
14	4	2172	U	C6-N1-C2	-5.89	117.47	121.00
14	4	2198	A	N1-C2-N3	5.89	132.25	129.30
14	4	2147	A	P-O3'-C3'	5.89	126.77	119.70
12	2	1334	G	O4'-C1'-N9	5.88	112.91	108.20
5	p	28	G	O4'-C1'-N9	5.88	112.90	108.20
5	p	22	G	O4'-C1'-N9	5.87	112.90	108.20
11	1	103	A	C4-C5-C6	5.87	119.94	117.00
11	1	111	A	C5-C6-N6	-5.87	119.00	123.70
14	4	2104	C	C6-N1-C1'	-5.87	113.76	120.80
14	4	2112	G	O4'-C1'-N9	5.86	112.89	108.20
5	p	30	C	C5'-C4'-O4'	5.86	116.13	109.10
2	E	109	TRP	NE1-CE2-CZ2	5.86	136.84	130.40
6	a	74	C	O4'-C1'-N1	5.86	112.89	108.20
14	4	2141	G	N3-C2-N2	5.86	124.00	119.90
14	4	2169	A	N3-C4-C5	-5.85	122.70	126.80
7	5	123	VAL	CG1-CB-CG2	5.85	120.26	110.90
8	T	99	ALA	N-CA-CB	5.85	118.29	110.10
14	4	2130	U	O4'-C1'-N1	5.85	112.88	108.20
14	4	2186	G	N1-C6-O6	5.85	123.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	125	LEU	CB-CG-CD2	5.85	120.94	111.00
13	3	1532	A	C6-N1-C2	-5.84	115.09	118.60
7	5	108	GLU	N-CA-CB	5.84	121.12	110.60
14	4	2178	C	N3-C4-N4	5.84	122.09	118.00
14	4	2151	U	O4'-C4'-C3'	-5.84	98.16	104.00
5	p	12	U	N1-C2-O2	5.83	126.88	122.80
5	p	70	C	C6-N1-C2	-5.83	117.97	120.30
13	3	1558	C	N3-C4-C5	-5.83	119.57	121.90
14	4	2110	G	C4-C5-C6	5.83	122.30	118.80
14	4	2111	U	C4'-C3'-C2'	-5.83	96.77	102.60
14	4	2132	U	P-O3'-C3'	5.83	126.69	119.70
5	p	59	G	N1-C2-N2	-5.83	110.96	116.20
5	p	74	C	N3-C4-N4	-5.83	113.92	118.00
11	1	98	G	O4'-C1'-N9	5.82	112.86	108.20
14	4	2121	G	C5-C6-N1	5.82	114.41	111.50
5	p	71	G	C1'-O4'-C4'	-5.82	105.25	109.90
12	2	1338	G	O4'-C1'-N9	5.82	112.85	108.20
3	G	17	VAL	CG1-CB-CG2	-5.82	101.59	110.90
14	4	2112	G	C5-C6-N1	-5.82	108.59	111.50
14	4	2197	U	O4'-C1'-N1	5.81	112.85	108.20
1	y	240	GLY	C-N-CA	5.80	136.21	121.70
14	4	2181	U	O4'-C1'-N1	5.80	112.84	108.20
5	p	57	G	C2-N3-C4	5.80	114.80	111.90
11	1	91	A	C5-C6-N1	-5.80	114.80	117.70
14	4	2188	U	O4'-C1'-N1	5.80	112.84	108.20
1	y	40	PRO	CA-N-CD	-5.80	103.39	111.50
11	1	75	G	O4'-C1'-N9	5.79	112.84	108.20
14	4	2177	C	C4'-C3'-C2'	-5.79	96.81	102.60
11	1	76	C	N3-C4-N4	5.79	122.05	118.00
13	3	1531	C	P-O3'-C3'	5.78	126.64	119.70
14	4	2099	U	C6-N1-C2	5.78	124.47	121.00
3	G	31	GLY	N-CA-C	5.78	127.55	113.10
11	1	79	C	N3-C4-N4	5.78	122.04	118.00
14	4	2139	U	C5'-C4'-O4'	5.78	116.03	109.10
5	p	52	A	C5-C6-N1	-5.78	114.81	117.70
13	3	1525	A	C6-N1-C2	5.78	122.07	118.60
14	4	2168	G	C5-C6-N1	-5.77	108.61	111.50
11	1	69	C	N3-C4-C5	-5.77	119.59	121.90
11	1	57	C	N3-C4-N4	5.77	122.04	118.00
5	p	7	A	C6-C5-N7	-5.77	128.26	132.30
5	p	14	A	C4'-C3'-C2'	-5.76	96.83	102.60
11	1	64	A	C4-C5-C6	5.76	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	223	VAL	CA-CB-CG1	5.76	119.54	110.90
14	4	2093	G	C8-N9-C4	-5.76	104.10	106.40
5	p	55	U	C2-N1-C1'	5.76	124.61	117.70
14	4	2162	G	N3-C2-N2	5.76	123.93	119.90
14	4	2146	C	N1-C2-N3	-5.75	115.17	119.20
14	4	2091	C	P-O3'-C3'	5.75	126.60	119.70
14	4	2180	U	C5'-C4'-C3'	-5.75	106.80	116.00
11	1	71	A	C5-C6-N1	-5.75	114.83	117.70
12	2	1339	G	O4'-C1'-N9	5.75	112.80	108.20
1	y	21	ARG	NE-CZ-NH2	5.75	123.17	120.30
13	3	1543	G	C5-N7-C8	-5.75	101.43	104.30
11	1	79	C	N3-C4-C5	-5.74	119.60	121.90
11	1	53	A	O4'-C1'-N9	5.74	112.79	108.20
1	y	352	PHE	CB-CG-CD2	5.73	124.81	120.80
5	p	43	G	N1-C6-O6	5.73	123.34	119.90
1	y	394	ALA	CB-CA-C	-5.73	101.51	110.10
13	3	1517	G	N3-C4-C5	-5.73	125.74	128.60
5	p	18	G	N9-C4-C5	-5.72	103.11	105.40
13	3	1531	C	N3-C4-N4	5.72	122.00	118.00
5	p	1	G	C6-C5-N7	-5.71	126.97	130.40
13	3	1537	G	O4'-C1'-N9	5.71	112.77	108.20
5	p	61	C	P-O5'-C5'	5.71	130.03	120.90
14	4	2091	C	C5-C4-N4	-5.71	116.21	120.20
5	p	30	C	N3-C2-O2	-5.70	117.91	121.90
14	4	2093	G	C6-C5-N7	-5.70	126.98	130.40
14	4	2184	A	N7-C8-N9	-5.70	110.95	113.80
11	1	101	A	O4'-C1'-N9	5.70	112.76	108.20
13	3	1538	G	C4-C5-N7	5.70	113.08	110.80
14	4	2143	C	C6-N1-C2	5.70	122.58	120.30
14	4	2173	A	C5'-C4'-C3'	5.70	125.12	116.00
14	4	2102	G	N7-C8-N9	5.70	115.95	113.10
5	p	1	G	N1-C2-N3	-5.69	120.48	123.90
13	3	1547	C	C1'-O4'-C4'	-5.69	105.34	109.90
13	3	1551	A	N9-C4-C5	5.69	108.08	105.80
14	4	2144	G	C8-N9-C4	5.69	108.68	106.40
14	4	2134	A	C4-C5-C6	5.69	119.85	117.00
13	3	1530	G	C3'-C2'-C1'	-5.69	96.95	101.50
6	a	9	A	C2'-C3'-O3'	5.69	122.80	113.70
1	y	393	ASP	CB-CG-OD2	-5.68	113.18	118.30
13	3	1558	C	N3-C4-N4	5.68	121.98	118.00
1	y	439	LYS	N-CA-CB	5.68	120.83	110.60
5	p	59	G	N9-C4-C5	-5.68	103.13	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2121	G	O4'-C1'-N9	5.68	112.74	108.20
11	1	88	G	C5-C6-O6	-5.68	125.19	128.60
12	2	1327	A	C5-C6-N6	-5.67	119.16	123.70
13	3	1551	A	C4-C5-C6	5.67	119.84	117.00
13	3	1534	U	C1'-O4'-C4'	5.67	114.44	109.90
14	4	2119	A	C6-C5-N7	-5.67	128.33	132.30
13	3	1547	C	C5-C4-N4	-5.67	116.23	120.20
14	4	2137	U	O4'-C1'-N1	5.67	112.73	108.20
14	4	2145	C	C2-N3-C4	5.67	122.73	119.90
12	2	1319	C	N3-C4-N4	5.66	121.96	118.00
14	4	2151	U	C6-N1-C2	5.66	124.40	121.00
14	4	2171	A	N1-C6-N6	5.66	122.00	118.60
14	4	2110	G	O4'-C1'-N9	5.66	112.73	108.20
14	4	2168	G	C4-C5-C6	5.66	122.20	118.80
14	4	2145	C	O4'-C1'-C2'	-5.66	100.14	105.80
12	2	1330	C	N3-C4-N4	5.65	121.95	118.00
14	4	2092	U	C2-N1-C1'	5.65	124.48	117.70
12	2	1327	A	C4-C5-C6	5.65	119.82	117.00
14	4	2165	C	C4'-C3'-C2'	-5.65	96.95	102.60
5	p	38	A	C5-N7-C8	5.64	106.72	103.90
5	p	38	A	C6-C5-N7	-5.64	128.35	132.30
12	2	1307	A	C4-C5-C6	5.64	119.82	117.00
14	4	2109	U	O5'-P-OP1	-5.64	100.62	105.70
5	p	46	G	N3-C2-N2	5.64	123.85	119.90
13	3	1546	G	C1'-O4'-C4'	-5.63	105.39	109.90
13	3	1557	C	N3-C4-C5	-5.63	119.65	121.90
1	y	122	TYR	CG-CD1-CE1	5.63	125.81	121.30
5	p	40	G	C8-N9-C4	5.63	108.65	106.40
5	p	74	C	C6-N1-C2	-5.63	118.05	120.30
5	p	13	C	C2-N3-C4	5.63	122.71	119.90
13	3	1527	G	N3-C4-N9	-5.63	122.62	126.00
12	2	1328	A	C5-C6-N6	-5.62	119.20	123.70
11	1	62	U	P-O3'-C3'	5.62	126.45	119.70
13	3	1526	C	N3-C4-C5	-5.62	119.65	121.90
3	G	11	ILE	CA-CB-CG2	-5.62	99.66	110.90
1	y	268	LYS	CB-CG-CD	5.62	126.20	111.60
14	4	2182	U	C4'-C3'-C2'	-5.62	96.98	102.60
5	p	23	A	C5-N7-C8	5.61	106.71	103.90
14	4	2188	U	O4'-C4'-C3'	-5.61	98.39	104.00
5	p	20	U	C5'-C4'-C3'	-5.61	107.02	116.00
5	p	52	A	O4'-C1'-N9	5.61	112.69	108.20
11	1	63	A	C4-C5-C6	5.61	119.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	28	G	N9-C4-C5	5.61	107.64	105.40
14	4	2150	C	O4'-C1'-N1	5.61	112.69	108.20
5	p	26	A	C6-C5-N7	-5.61	128.38	132.30
3	G	39	SER	N-CA-CB	-5.60	102.09	110.50
5	p	45	G	N1-C2-N3	-5.60	120.54	123.90
11	1	101	A	C5-C6-N6	-5.60	119.22	123.70
13	3	1528	A	C8-N9-C4	-5.60	103.56	105.80
14	4	2151	U	C4-C5-C6	5.60	123.06	119.70
13	3	1529	G	C2-N3-C4	5.59	114.70	111.90
12	2	1323	C	N3-C4-N4	5.59	121.91	118.00
14	4	2093	G	C4-C5-N7	5.59	113.03	110.80
14	4	2135	A	N1-C2-N3	-5.59	126.51	129.30
12	2	1322	A	C5-C6-N1	-5.58	114.91	117.70
5	p	37	A	N9-C4-C5	-5.58	103.57	105.80
14	4	2107	G	C6-C5-N7	5.58	133.75	130.40
14	4	2115	G	C1'-O4'-C4'	-5.58	105.44	109.90
14	4	2115	G	C5-C6-O6	-5.58	125.25	128.60
14	4	2191	A	C5-C6-N1	-5.58	114.91	117.70
12	2	1330	C	N3-C4-C5	-5.58	119.67	121.90
12	2	1313	U	O4'-C1'-N1	5.57	112.66	108.20
14	4	2112	G	C4-C5-N7	-5.57	108.57	110.80
14	4	2135	A	O4'-C1'-N9	5.57	112.66	108.20
13	3	1517	G	C8-N9-C4	-5.57	104.17	106.40
5	p	36	C	N1-C2-O2	5.56	122.24	118.90
5	p	40	G	C4-N9-C1'	-5.56	119.27	126.50
13	3	1552	A	P-O5'-C5'	5.56	129.80	120.90
14	4	2114	A	P-O3'-C3'	5.56	126.37	119.70
1	y	258	TYR	CB-CG-CD1	-5.55	117.67	121.00
3	G	63	PHE	CB-CG-CD2	-5.55	116.91	120.80
5	p	74	C	O4'-C1'-N1	5.55	112.64	108.20
11	1	91	A	C5-C6-N6	-5.55	119.26	123.70
5	p	33	U	O4'-C1'-N1	5.55	112.64	108.20
7	5	164	ARG	CG-CD-NE	-5.54	100.16	111.80
13	3	1552	A	O4'-C1'-N9	5.54	112.63	108.20
12	2	1328	A	C4-C5-C6	5.54	119.77	117.00
1	y	335	LEU	O-C-N	5.54	131.56	122.70
13	3	1529	G	N9-C1'-C2'	-5.53	105.92	112.00
11	1	89	A	C5-C6-N6	-5.53	119.28	123.70
14	4	2168	G	C4-N9-C1'	5.53	133.69	126.50
5	p	59	G	P-O3'-C3'	5.53	126.33	119.70
7	5	208	TYR	N-CA-CB	5.53	120.55	110.60
14	4	2141	G	N7-C8-N9	5.52	115.86	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2136	G	C4'-C3'-C2'	-5.52	97.08	102.60
5	p	72	C	C2-N3-C4	-5.51	117.14	119.90
12	2	1321	A	O4'-C1'-N9	5.51	112.61	108.20
5	p	52	A	N3-C4-N9	-5.51	122.99	127.40
11	1	56	A	O4'-C1'-N9	5.51	112.61	108.20
11	1	83	A	C5-C6-N1	-5.51	114.94	117.70
14	4	2137	U	N1-C2-N3	-5.51	111.59	114.90
14	4	2180	U	O4'-C1'-N1	5.51	112.61	108.20
5	p	11	C	N1-C2-N3	-5.51	115.34	119.20
12	2	1308	A	C4-C5-C6	5.51	119.75	117.00
13	3	1546	G	C5-C6-N1	-5.51	108.75	111.50
13	3	1535	A	N3-C4-C5	-5.50	122.95	126.80
13	3	1538	G	C4-C5-C6	5.50	122.10	118.80
13	3	1549	A	O5'-C5'-C4'	-5.50	101.24	111.70
13	3	1552	A	C5-C6-N1	-5.50	114.95	117.70
14	4	2176	A	N3-C4-C5	-5.50	122.95	126.80
1	y	85	TYR	CB-CG-CD1	-5.50	117.70	121.00
5	p	4	G	N9-C4-C5	5.50	107.60	105.40
14	4	2170	A	C6-N1-C2	-5.50	115.30	118.60
13	3	1536	C	O4'-C1'-N1	5.50	112.60	108.20
5	p	28	G	N7-C8-N9	5.50	115.85	113.10
13	3	1556	C	N3-C4-N4	5.50	121.85	118.00
5	p	6	A	C2-N3-C4	-5.49	107.85	110.60
5	p	31	C	N3-C4-N4	5.49	121.84	118.00
14	4	2100	G	C4-C5-C6	5.49	122.09	118.80
2	E	84	TRP	CD1-CG-CD2	-5.48	101.91	106.30
5	p	15	G	C8-N9-C4	-5.48	104.21	106.40
12	2	1332	G	O4'-C1'-N9	5.48	112.58	108.20
13	3	1537	G	N3-C2-N2	5.48	123.74	119.90
13	3	1532	A	N3-C4-C5	-5.48	122.97	126.80
5	p	53	G	C3'-C2'-C1'	-5.48	97.12	101.50
5	p	12	U	C5-C4-O4	-5.48	122.61	125.90
5	p	14	A	O5'-C5'-C4'	-5.48	101.30	111.70
14	4	2134	A	C6-C5-N7	-5.47	128.47	132.30
14	4	2168	G	N3-C2-N2	5.47	123.73	119.90
13	3	1536	C	N1-C2-O2	5.47	122.18	118.90
5	p	29	A	C5-C6-N1	-5.47	114.97	117.70
1	y	249	ALA	CB-CA-C	5.46	118.30	110.10
1	y	412	VAL	CA-CB-CG1	5.46	119.09	110.90
2	E	113	GLY	N-CA-C	5.46	126.75	113.10
14	4	2183	A	N9-C4-C5	5.46	107.98	105.80
5	p	27	C	C2-N3-C4	5.46	122.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2165	C	C5-C6-N1	5.46	123.73	121.00
2	E	106	LEU	CB-CG-CD2	5.45	120.27	111.00
12	2	1320	C	N3-C4-C5	-5.45	119.72	121.90
14	4	2104	C	C5'-C4'-O4'	5.45	115.64	109.10
1	y	243	ARG	CB-CA-C	5.45	121.29	110.40
14	4	2198	A	N1-C6-N6	5.45	121.87	118.60
11	1	111	A	C5-C6-N1	-5.45	114.98	117.70
14	4	2140	G	O4'-C1'-N9	5.44	112.56	108.20
1	y	50	ALA	N-CA-CB	5.44	117.71	110.10
13	3	1527	G	O4'-C1'-N9	5.44	112.55	108.20
14	4	2131	U	C5-C4-O4	-5.43	122.64	125.90
12	2	1307	A	C5-C6-N6	-5.43	119.36	123.70
14	4	2095	A	C5-C6-N6	-5.43	119.36	123.70
11	1	69	C	N3-C4-N4	5.43	121.80	118.00
14	4	2129	C	C6-N1-C1'	5.43	127.31	120.80
12	2	1313	U	C6-N1-C1'	-5.43	113.60	121.20
13	3	1543	G	N3-C4-C5	5.43	131.31	128.60
11	1	61	C	N3-C4-N4	5.42	121.80	118.00
11	1	73	A	C5-C6-N6	-5.42	119.36	123.70
14	4	2199	A	C5-C6-N6	-5.42	119.36	123.70
1	y	165	VAL	CA-CB-CG1	5.42	119.03	110.90
7	5	51	ASP	CB-CG-OD2	-5.42	113.42	118.30
13	3	1518	C	C5'-C4'-C3'	5.41	124.66	116.00
1	y	392	ARG	NE-CZ-NH1	-5.41	117.59	120.30
14	4	2196	C	N3-C4-N4	5.41	121.79	118.00
14	4	2198	A	OP1-P-OP2	-5.41	111.48	119.60
5	p	9	A	C5-C6-N6	-5.41	119.38	123.70
5	p	51	G	P-O3'-C3'	5.40	126.18	119.70
11	1	73	A	C5-C6-N1	-5.40	115.00	117.70
13	3	1536	C	C4-C5-C6	5.40	120.10	117.40
14	4	2100	G	O4'-C1'-N9	5.40	112.52	108.20
2	E	127	PHE	CG-CD1-CE1	5.40	126.74	120.80
11	1	63	A	O4'-C1'-N9	5.40	112.52	108.20
5	p	6	A	C5-C6-N6	-5.40	119.38	123.70
5	p	55	U	O4'-C4'-C3'	-5.39	98.61	104.00
1	y	258	TYR	N-CA-CB	5.39	120.31	110.60
14	4	2092	U	C5'-C4'-C3'	-5.39	107.37	116.00
1	y	25	PHE	CB-CG-CD2	5.39	124.57	120.80
11	1	94	A	C5-C6-N1	-5.39	115.00	117.70
13	3	1537	G	C4-C5-C6	5.39	122.03	118.80
1	y	390	PHE	CB-CG-CD1	-5.39	117.03	120.80
14	4	2093	G	N3-C2-N2	-5.39	116.13	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	6	A	P-O5'-C5'	-5.39	112.28	120.90
1	y	263	THR	CA-CB-CG2	-5.38	104.86	112.40
12	2	1322	A	C5-C6-N6	-5.38	119.39	123.70
14	4	2141	G	C4-C5-C6	5.38	122.03	118.80
5	p	44	G	C5-N7-C8	-5.38	101.61	104.30
14	4	2107	G	C5-N7-C8	-5.38	101.61	104.30
14	4	2177	C	N3-C4-N4	5.38	121.77	118.00
5	p	49	G	C2-N3-C4	5.38	114.59	111.90
14	4	2114	A	O4'-C1'-N9	5.37	112.50	108.20
14	4	2184	A	N9-C1'-C2'	-5.36	106.10	112.00
13	3	1554	U	O4'-C1'-N1	5.36	112.49	108.20
14	4	2143	C	O4'-C1'-N1	5.36	112.49	108.20
5	p	40	G	N9-C1'-C2'	-5.36	106.10	112.00
14	4	2147	A	C2-N3-C4	-5.36	107.92	110.60
5	p	65	U	C5-C6-N1	-5.36	120.02	122.70
14	4	2129	C	C3'-C2'-C1'	5.35	105.78	101.50
5	p	49	G	N1-C2-N3	-5.34	120.69	123.90
12	2	1335	C	N3-C4-N4	5.34	121.74	118.00
5	p	12	U	C5-C6-N1	-5.34	120.03	122.70
5	p	58	A	P-O3'-C3'	5.34	126.11	119.70
13	3	1529	G	C4-C5-N7	5.34	112.94	110.80
13	3	1553	A	O4'-C1'-N9	5.34	112.47	108.20
2	E	96	ILE	CA-CB-CG1	5.33	121.14	111.00
12	2	1322	A	C4-C5-C6	5.33	119.67	117.00
14	4	2142	A	C6-C5-N7	-5.33	128.56	132.30
11	1	84	A	C5-C6-N1	-5.33	115.03	117.70
14	4	2145	C	N3-C4-C5	-5.33	119.77	121.90
11	1	104	A	C5-C6-N1	-5.33	115.04	117.70
5	p	23	A	P-O3'-C3'	5.33	126.09	119.70
5	p	70	C	C5-C6-N1	5.33	123.66	121.00
11	1	74	A	C5-C6-N6	-5.33	119.44	123.70
14	4	2168	G	O5'-P-OP2	-5.32	100.91	105.70
3	G	32	ALA	CA-C-N	-5.32	105.50	117.20
12	2	1321	A	C5-C6-N6	-5.32	119.45	123.70
1	y	406	LEU	CB-CG-CD2	5.32	120.03	111.00
11	1	63	A	C5-C6-N6	-5.32	119.45	123.70
12	2	1342	A	C5-C6-N1	-5.31	115.04	117.70
14	4	2126	A	C5-C6-N6	-5.31	119.45	123.70
5	p	13	C	C5'-C4'-O4'	5.31	115.47	109.10
12	2	1314	C	N3-C4-C5	-5.30	119.78	121.90
13	3	1530	G	N1-C6-O6	5.30	123.08	119.90
12	2	1327	A	C5-C6-N1	-5.30	115.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2151	U	C1'-O4'-C4'	5.30	114.14	109.90
11	1	106	C	N3-C4-N4	5.30	121.71	118.00
14	4	2101	A	C3'-C2'-C1'	-5.30	97.26	101.50
14	4	2126	A	N9-C4-C5	-5.30	103.68	105.80
5	p	72	C	N1-C2-N3	5.30	122.91	119.20
11	1	57	C	N3-C4-C5	-5.30	119.78	121.90
14	4	2170	A	O4'-C1'-C2'	5.29	112.37	107.60
13	3	1522	A	C2-N3-C4	-5.29	107.95	110.60
5	p	71	G	N3-C2-N2	5.28	123.60	119.90
14	4	2144	G	C5'-C4'-O4'	5.28	115.44	109.10
14	4	2177	C	C2-N3-C4	5.28	122.54	119.90
5	p	27	C	C5-C4-N4	-5.28	116.50	120.20
5	p	32	U	O4'-C1'-N1	5.28	112.42	108.20
11	1	52	A	O4'-C1'-N9	5.28	112.42	108.20
13	3	1538	G	C8-N9-C4	-5.28	104.29	106.40
14	4	2095	A	C5'-C4'-O4'	5.28	115.44	109.10
14	4	2184	A	C5-N7-C8	5.28	106.54	103.90
11	1	86	G	O4'-C1'-N9	5.28	112.42	108.20
5	p	63	C	C6-N1-C1'	-5.28	114.47	120.80
5	p	7	A	C5-N7-C8	5.27	106.54	103.90
14	4	2141	G	C2-N3-C4	5.27	114.54	111.90
14	4	2132	U	C5-C6-N1	5.27	125.34	122.70
14	4	2145	C	C5-C4-N4	-5.27	116.51	120.20
5	p	21	A	OP1-P-OP2	-5.26	111.70	119.60
14	4	2153	C	N3-C4-N4	5.26	121.69	118.00
13	3	1555	G	O4'-C1'-N9	5.26	112.41	108.20
6	a	10	G	C2'-C3'-O3'	5.26	122.12	113.70
1	y	157	TYR	CG-CD1-CE1	-5.26	117.09	121.30
14	4	2099	U	P-O5'-C5'	-5.26	112.49	120.90
14	4	2109	U	C5-C4-O4	-5.26	122.75	125.90
14	4	2134	A	C2-N3-C4	-5.26	107.97	110.60
12	2	1324	G	C5'-C4'-C3'	-5.26	107.59	116.00
14	4	2119	A	C5-C6-N1	-5.26	115.07	117.70
14	4	2176	A	C5-N7-C8	5.26	106.53	103.90
5	p	15	G	C4-C5-N7	-5.26	108.70	110.80
12	2	1328	A	C5-C6-N1	-5.26	115.07	117.70
13	3	1536	C	N3-C2-O2	-5.25	118.22	121.90
14	4	2113	U	C1'-O4'-C4'	5.25	114.10	109.90
1	y	57	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
5	p	26	A	N7-C8-N9	5.25	116.42	113.80
12	2	1327	A	O4'-C1'-N9	5.25	112.40	108.20
14	4	2113	U	N3-C4-C5	-5.25	111.45	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	50	C	C2-N3-C4	-5.24	117.28	119.90
6	a	74	C	C1'-O4'-C4'	-5.24	105.71	109.90
13	3	1543	G	P-O3'-C3'	5.24	125.99	119.70
5	p	56	C	C5-C6-N1	5.24	123.62	121.00
14	4	2163	A	C8-N9-C4	5.24	107.89	105.80
12	2	1337	G	O4'-C1'-N9	5.24	112.39	108.20
14	4	2135	A	C5-C6-N6	-5.24	119.51	123.70
14	4	2150	C	P-O5'-C5'	-5.24	112.52	120.90
14	4	2169	A	C6-C5-N7	-5.23	128.64	132.30
14	4	2180	U	C3'-C2'-C1'	5.23	105.69	101.50
1	y	311	GLN	CA-C-N	5.23	131.74	117.10
11	1	74	A	C5-C6-N1	-5.23	115.09	117.70
12	2	1323	C	N3-C4-C5	-5.23	119.81	121.90
5	p	40	G	C2'-C3'-O3'	5.22	122.06	113.70
14	4	2156	G	N7-C8-N9	-5.22	110.49	113.10
5	p	17	U	C5'-C4'-O4'	5.22	115.36	109.10
14	4	2193	G	C5-C6-O6	-5.22	125.47	128.60
14	4	2135	A	C6-C5-N7	-5.21	128.65	132.30
11	1	53	A	C5-C6-N1	-5.21	115.09	117.70
11	1	99	U	C6-N1-C1'	-5.21	113.91	121.20
11	1	101	A	C5-C6-N1	-5.21	115.10	117.70
12	2	1321	A	C5-C6-N1	-5.21	115.10	117.70
11	1	66	C	N3-C4-N4	5.20	121.64	118.00
13	3	1534	U	C2-N3-C4	-5.20	123.88	127.00
14	4	2133	G	C4-C5-C6	5.20	121.92	118.80
7	5	71	ARG	CD-NE-CZ	-5.19	116.33	123.60
14	4	2149	U	N3-C4-O4	5.19	123.03	119.40
14	4	2152	G	N9-C4-C5	5.19	107.48	105.40
14	4	2126	A	P-O3'-C3'	5.19	125.93	119.70
7	5	111	PHE	CB-CG-CD2	5.19	124.43	120.80
12	2	1315	C	N3-C4-C5	-5.19	119.83	121.90
13	3	1553	A	C5-C6-N1	-5.18	115.11	117.70
14	4	2169	A	N7-C8-N9	-5.18	111.21	113.80
5	p	71	G	N9-C4-C5	-5.18	103.33	105.40
14	4	2135	A	C8-N9-C4	-5.18	103.73	105.80
14	4	2180	U	C2-N3-C4	-5.18	123.89	127.00
14	4	2100	G	C5-N7-C8	-5.17	101.71	104.30
14	4	2173	A	C6-N1-C2	5.17	121.70	118.60
13	3	1548	A	N3-C4-N9	5.17	131.54	127.40
14	4	2186	G	C5-N7-C8	5.17	106.89	104.30
5	p	11	C	N1-C2-O2	5.17	122.00	118.90
14	4	2130	U	C2-N3-C4	-5.16	123.90	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	2178	C	C1'-O4'-C4'	5.16	114.03	109.90
5	p	28	G	C5-C6-N1	-5.16	108.92	111.50
13	3	1535	A	O4'-C1'-C2'	-5.16	100.64	105.80
13	3	1540	G	N1-C6-O6	5.16	123.00	119.90
14	4	2127	G	N9-C4-C5	5.16	107.46	105.40
14	4	2143	C	N1-C2-O2	5.16	122.00	118.90
14	4	2187	U	OP1-P-OP2	-5.16	111.86	119.60
14	4	2170	A	C5-C6-N1	-5.15	115.12	117.70
14	4	2093	G	N7-C8-N9	5.15	115.67	113.10
1	y	236	PHE	CB-CG-CD1	-5.15	117.20	120.80
5	p	58	A	C6-C5-N7	-5.15	128.70	132.30
11	1	76	C	N3-C4-C5	-5.15	119.84	121.90
14	4	2190	G	N9-C4-C5	-5.15	103.34	105.40
11	1	85	G	O4'-C1'-N9	5.14	112.32	108.20
13	3	1519	G	C5-C6-N1	-5.14	108.93	111.50
5	p	55	U	N3-C2-O2	-5.14	118.60	122.20
1	y	122	TYR	CG-CD2-CE2	-5.14	117.19	121.30
2	E	121	PHE	CZ-CE2-CD2	-5.14	113.93	120.10
1	y	267	LEU	CB-CA-C	5.14	119.96	110.20
14	4	2092	U	N1-C2-O2	-5.14	119.20	122.80
1	y	354	PRO	CA-C-N	5.13	126.47	116.20
2	E	76	ARG	NE-CZ-NH2	-5.13	117.73	120.30
13	3	1531	C	C5-C4-N4	-5.13	116.61	120.20
2	E	90	THR	CA-CB-CG2	-5.13	105.22	112.40
14	4	2095	A	C4-C5-C6	5.13	119.57	117.00
1	y	394	ALA	N-CA-CB	5.13	117.28	110.10
5	p	26	A	C4-C5-N7	-5.13	108.14	110.70
11	1	52	A	C5-C6-N6	-5.13	119.60	123.70
13	3	1544	A	N3-C4-C5	-5.13	123.21	126.80
11	1	56	A	C5-C6-N1	-5.13	115.14	117.70
14	4	2164	C	P-O5'-C5'	-5.13	112.70	120.90
11	1	91	A	O4'-C1'-N9	5.12	112.30	108.20
1	y	184	GLY	C-N-CA	5.11	134.49	121.70
11	1	63	A	C5-C6-N1	-5.11	115.14	117.70
14	4	2143	C	C1'-O4'-C4'	-5.11	105.81	109.90
5	p	68	C	N3-C4-N4	5.11	121.58	118.00
14	4	2111	U	C2-N3-C4	5.11	130.06	127.00
13	3	1521	G	C5-N7-C8	5.11	106.85	104.30
13	3	1551	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	y	57	ARG	N-CA-CB	5.11	119.79	110.60
13	3	1546	G	O5'-C5'-C4'	-5.11	102.00	111.70
11	1	94	A	C5-C6-N6	-5.10	119.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	117	SER	N-CA-CB	5.10	118.15	110.50
11	1	70	G	O4'-C1'-N9	5.10	112.28	108.20
11	1	74	A	O4'-C1'-N9	5.10	112.28	108.20
11	1	106	C	N3-C4-C5	-5.10	119.86	121.90
14	4	2144	G	C4-C5-N7	5.10	112.84	110.80
14	4	2193	G	P-O3'-C3'	5.10	125.82	119.70
11	1	71	A	C5-C6-N6	-5.10	119.62	123.70
14	4	2120	G	C5'-C4'-C3'	5.10	124.16	116.00
12	2	1308	A	O4'-C1'-N9	5.09	112.28	108.20
1	y	166	THR	CA-CB-CG2	-5.09	105.27	112.40
1	y	269	VAL	CA-CB-CG1	-5.09	103.27	110.90
14	4	2120	G	C2-N3-C4	5.09	114.44	111.90
1	y	340	ARG	N-CA-C	-5.09	97.27	111.00
14	4	2105	U	C5-C6-N1	-5.08	120.16	122.70
14	4	2125	G	C2-N3-C4	5.08	114.44	111.90
14	4	2195	U	N3-C4-O4	5.08	122.95	119.40
5	p	4	G	P-O5'-C5'	5.08	129.02	120.90
7	5	42	VAL	CA-CB-CG2	-5.07	103.29	110.90
11	1	103	A	C5-C6-N6	-5.07	119.64	123.70
5	p	75	C	N3-C4-C5	-5.07	119.87	121.90
14	4	2185	U	C1'-O4'-C4'	-5.07	105.84	109.90
11	1	104	A	O4'-C1'-N9	5.07	112.25	108.20
12	2	1336	A	C5'-C4'-O4'	5.06	115.18	109.10
5	p	41	U	OP1-P-OP2	-5.06	112.00	119.60
5	p	44	G	N9-C4-C5	5.06	107.42	105.40
14	4	2155	U	O5'-C5'-C4'	5.06	121.32	111.70
1	y	239	ARG	NE-CZ-NH1	-5.06	117.77	120.30
14	4	2194	U	C3'-C2'-C1'	-5.06	97.45	101.50
5	p	16	U	N3-C2-O2	5.06	125.74	122.20
14	4	2095	A	C5'-C4'-C3'	-5.06	107.91	116.00
14	4	2192	U	C4-C5-C6	-5.05	116.67	119.70
14	4	2118	U	C4'-C3'-C2'	5.05	107.65	102.60
14	4	2180	U	OP1-P-OP2	-5.05	112.02	119.60
5	p	21	A	N7-C8-N9	-5.05	111.28	113.80
5	p	57	G	C8-N9-C4	-5.05	104.38	106.40
13	3	1524	G	C6-C5-N7	-5.04	127.38	130.40
11	1	61	C	N3-C4-C5	-5.04	119.89	121.90
2	E	93	THR	C-N-CA	5.03	134.28	121.70
5	p	24	G	C4'-C3'-C2'	-5.03	97.57	102.60
5	p	35	C	N1-C2-O2	-5.03	115.88	118.90
14	4	2121	G	N1-C2-N3	-5.03	120.88	123.90
7	5	199	ALA	N-CA-CB	5.03	117.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	97	C	N3-C4-C5	-5.03	119.89	121.90
14	4	2130	U	N1-C2-N3	5.03	117.92	114.90
14	4	2181	U	N1-C2-N3	-5.02	111.89	114.90
1	y	64	PHE	N-CA-CB	-5.02	101.57	110.60
5	p	68	C	C2-N1-C1'	-5.02	113.28	118.80
12	2	1335	C	N3-C4-C5	-5.01	119.89	121.90
5	p	13	C	N1-C2-O2	5.01	121.91	118.90
13	3	1528	A	C6-N1-C2	-5.01	115.59	118.60
3	G	34	PHE	N-CA-C	-5.01	97.47	111.00
11	1	109	C	N3-C4-C5	-5.01	119.89	121.90
1	y	280	ALA	N-CA-CB	5.01	117.11	110.10
12	2	1312	U	O4'-C1'-N1	5.00	112.20	108.20
13	3	1522	A	N9-C4-C5	-5.00	103.80	105.80

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	y	55	GLN	CA
1	y	56	GLN	CA
4	n	38	LEU	CA
4	n	39	HIS	CA
4	n	40	GLN	CA

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1	60	G	Sidechain
11	1	72	U	Sidechain
12	2	1327	A	Sidechain
12	2	1334	G	Sidechain
13	3	1515	A	Sidechain
13	3	1517	G	Sidechain
13	3	1519	G	Sidechain
13	3	1520	U	Sidechain
13	3	1521	G	Sidechain
13	3	1522	A	Sidechain
13	3	1523	U	Sidechain
13	3	1524	G	Sidechain
13	3	1525	A	Sidechain
13	3	1529	G	Sidechain
13	3	1530	G	Sidechain
13	3	1531	C	Sidechain

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Mol	Chain	Res	Type	Group
13	3	1533	C	Sidechain
13	3	1536	C	Sidechain
13	3	1539	U	Sidechain
13	3	1540	G	Sidechain
13	3	1545	A	Sidechain
13	3	1546	G	Sidechain
13	3	1550	C	Sidechain
14	4	2099	U	Sidechain
14	4	2100	G	Sidechain
14	4	2101	A	Sidechain
14	4	2104	C	Sidechain
14	4	2105	U	Sidechain
14	4	2106	U	Sidechain
14	4	2107	G	Sidechain
14	4	2108	A	Sidechain
14	4	2110	G	Sidechain
14	4	2112	G	Sidechain
14	4	2113	U	Sidechain
14	4	2115	G	Sidechain
14	4	2116	G	Sidechain
14	4	2118	U	Sidechain
14	4	2119	A	Sidechain
14	4	2120	G	Sidechain
14	4	2123	G	Sidechain
14	4	2124	G	Sidechain
14	4	2125	G	Sidechain
14	4	2126	A	Sidechain
14	4	2127	G	Sidechain
14	4	2128	G	Sidechain
14	4	2129	C	Sidechain
14	4	2133	G	Sidechain
14	4	2135	A	Sidechain
14	4	2136	G	Sidechain
14	4	2140	G	Sidechain
14	4	2142	A	Sidechain
14	4	2144	G	Sidechain
14	4	2148	G	Sidechain
14	4	2149	U	Sidechain
14	4	2150	C	Sidechain
14	4	2152	G	Sidechain
14	4	2153	C	Sidechain
14	4	2154	A	Sidechain

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Mol	Chain	Res	Type	Group
14	4	2155	U	Sidechain
14	4	2156	G	Sidechain
14	4	2157	G	Sidechain
14	4	2159	G	Sidechain
14	4	2160	C	Sidechain
14	4	2161	C	Sidechain
14	4	2167	U	Sidechain
14	4	2168	G	Sidechain
14	4	2169	A	Sidechain
14	4	2172	U	Sidechain
14	4	2173	A	Sidechain
14	4	2174	C	Sidechain
14	4	2175	C	Sidechain
14	4	2176	A	Sidechain
14	4	2177	C	Sidechain
14	4	2179	C	Sidechain
14	4	2182	U	Sidechain
14	4	2183	A	Sidechain
14	4	2184	A	Sidechain
14	4	2185	U	Sidechain
14	4	2186	G	Sidechain
14	4	2187	U	Sidechain
14	4	2189	U	Sidechain
14	4	2190	G	Sidechain
14	4	2192	U	Sidechain
14	4	2194	U	Sidechain
14	4	2196	C	Sidechain
14	4	2197	U	Sidechain
7	5	122	ARG	Sidechain
7	5	163	TYR	Sidechain
7	5	208	TYR	Sidechain
2	E	87	ARG	Sidechain
2	E	93	THR	Mainchain
3	G	41	THR	Peptide
9	U	48	VAL	Peptide
6	a	66	U	Sidechain
5	p	1	G	Sidechain
5	p	13	C	Sidechain
5	p	24	G	Sidechain
5	p	26	A	Sidechain
5	p	27	C	Sidechain
5	p	28	G	Sidechain

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Mol	Chain	Res	Type	Group
5	p	29	A	Sidechain
5	p	3	G	Sidechain
5	p	31	C	Sidechain
5	p	33	U	Sidechain
5	p	34	G	Sidechain
5	p	36	C	Sidechain
5	p	38	A	Sidechain
5	p	39	G	Sidechain
5	p	40	G	Sidechain
5	p	41	U	Sidechain
5	p	44	G	Sidechain
5	p	45	G	Sidechain
5	p	48	C	Sidechain
5	p	49	G	Sidechain
5	p	53	G	Sidechain
5	p	55	U	Sidechain
5	p	58	A	Sidechain
5	p	63	C	Sidechain
5	p	65	U	Sidechain
5	p	69	C	Sidechain
5	p	70	C	Sidechain
5	p	74	C	Sidechain
5	p	76	A	Sidechain
1	y	22	ARG	Sidechain
1	y	232	PHE	Sidechain
1	y	243	ARG	Sidechain
1	y	248	TYR	Sidechain
1	y	265	LEU	Peptide
1	y	266	PRO	Mainchain
1	y	309	TYR	Sidechain
1	y	321	TYR	Sidechain
1	y	332	TYR	Sidechain
1	y	34	ARG	Sidechain
1	y	357	ARG	Sidechain
1	y	365	TYR	Sidechain
1	y	38	PHE	Sidechain
1	y	424	MET	Mainchain
1	y	45	ASP	Sidechain
1	y	57	ARG	Sidechain
1	y	67	PHE	Sidechain
1	y	85	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	22	0
3	G	461	0	485	7	0
4	n	760	0	742	0	0
5	p	1621	0	818	0	0
6	a	1626	0	833	0	0
7	5	1733	0	1824	8	0
8	T	787	0	844	20	0
9	U	789	0	847	0	0
10	Y	509	0	543	0	0
11	1	1350	0	678	2	0
12	2	775	0	389	0	0
13	3	948	0	478	0	0
14	4	2325	0	1168	8	0
All	All	17478	0	13629	45	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 20.

All (45) 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:81:LYS:HD2	8:T:93:LEU:CD1	1.30	1.62
2:E:81:LYS:CD	8:T:93:LEU:HD12	1.04	1.51
2:E:81:LYS:CD	8:T:93:LEU:CD1	1.94	1.21
2:E:81:LYS:HZ3	8:T:93:LEU:CG	1.57	1.17
2:E:81:LYS:CE	8:T:93:LEU:HD12	1.77	1.13
2:E:81:LYS:NZ	8:T:93:LEU:HG	1.65	1.12
2:E:81:LYS:NZ	8:T:93:LEU:CD1	2.13	1.11
2:E:81:LYS:HD3	8:T:93:LEU:HB2	1.26	1.10
2:E:81:LYS:HZ2	8:T:93:LEU:CD1	1.71	1.03
2:E:81:LYS:HD3	8:T:93:LEU:CB	1.91	1.01
2:E:81:LYS:NZ	8:T:93:LEU:CG	2.22	0.98
2:E:81:LYS:HZ3	8:T:93:LEU:HG	0.81	0.96
2:E:81:LYS:HZ2	8:T:93:LEU:HD11	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:LYS:HD3	8:T:93:LEU:HD12	1.50	0.93
2:E:81:LYS:HD2	8:T:93:LEU:HD13	1.55	0.85
2:E:81:LYS:HD3	8:T:93:LEU:CD1	2.05	0.82
2:E:78:GLU:HA	8:T:93:LEU:HD13	1.64	0.78
2:E:81:LYS:CD	8:T:93:LEU:CG	2.67	0.73
3:G:34:PHE:CD1	3:G:36:ALA:HB3	2.22	0.73
2:E:81:LYS:HD3	8:T:93:LEU:CG	2.22	0.68
3:G:36:ALA:HB1	3:G:40:ALA:HB3	1.85	0.59
2:E:81:LYS:HD2	8:T:93:LEU:HD12	0.59	0.58
3:G:29:ASP:O	3:G:33:SER:HB2	2.06	0.55
14:4:2103:C:C5	14:4:2104:C:C6	2.97	0.53
3:G:36:ALA:HB1	3:G:40:ALA:CB	2.42	0.50
14:4:2103:C:C5	14:4:2104:C:C5	3.01	0.49
14:4:2111:U:H3'	14:4:2112:G:H5'	1.94	0.48
7:5:172:HIS:CD2	14:4:2123:G:H21	2.32	0.48
7:5:53:ARG:HB3	7:5:167:LYS:HA	1.95	0.47
11:1:82:U:H3	11:1:104:A:H61	1.62	0.47
14:4:2091:C:H3'	14:4:2092:U:H5"	1.97	0.46
2:E:84:TRP:HB2	2:E:85:PRO:HD3	1.97	0.46
14:4:2110:G:H3'	14:4:2111:U:H5'	1.98	0.46
11:1:63:A:H2'	11:1:64:A:C8	2.51	0.46
2:E:107:ILE:O	2:E:111:LEU:HD12	2.16	0.45
7:5:212:VAL:O	7:5:223:ALA:HB1	2.16	0.45
3:G:37:GLY:O	3:G:38:ALA:HB2	2.17	0.45
3:G:68:LEU:HG	3:G:69:VAL:N	2.33	0.44
3:G:32:ALA:HB3	3:G:53:THR:HG21	1.99	0.44
7:5:156:ALA:HA	7:5:160:GLN:HB3	2.00	0.43
7:5:79:THR:HB	7:5:81:GLY:H	1.84	0.43
7:5:14:LYS:HB2	7:5:17:ALA:HB2	2.00	0.43
7:5:12:ARG:HE	14:4:2107:G:H4'	1.84	0.41
7:5:76:ALA:HB1	7:5:103:GLN:NE2	2.36	0.41
14:4:2194:U:H2'	14:4:2195:U:C6	2.57	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%)	392 (90%)	18 (4%)	25 (6%)	1 18
2	E	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	8 38
3	G	65/67 (97%)	57 (88%)	4 (6%)	4 (6%)	1 17
4	n	99/101 (98%)	42 (42%)	26 (26%)	31 (31%)	0 0
7	5	232/234 (99%)	198 (85%)	25 (11%)	9 (4%)	3 23
8	T	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1 14
9	U	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	4 28
10	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4 26
All	All	1145/1161 (99%)	941 (82%)	122 (11%)	82 (7%)	2 14

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	45	ASP
1	y	56	GLN
1	y	258	TYR
1	y	266	PRO
1	y	298	THR
1	y	315	PRO
1	y	316	LEU
1	y	396	LYS
3	G	34	PHE
3	G	38	ALA
4	n	16	SER
4	n	24	ASP
4	n	26	SER
4	n	27	SER
4	n	30	LEU
4	n	33	GLN
4	n	37	ALA
4	n	38	LEU
4	n	39	HIS
4	n	40	GLN
4	n	43	ILE
4	n	44	SER
4	n	46	ASP

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Mol	Chain	Res	Type
4	n	48	ASP
4	n	52	SER
4	n	60	VAL
4	n	62	MET
4	n	68	GLU
4	n	71	LEU
4	n	72	ALA
7	5	18	THR
7	5	37	LYS
7	5	120	ALA
8	T	35	ALA
8	T	36	LYS
8	T	99	ALA
9	U	49	PRO
1	y	148	LEU
1	y	210	ALA
1	y	212	GLN
1	y	399	PHE
1	y	438	LEU
1	y	439	LYS
4	n	29	GLU
4	n	41	ARG
4	n	42	SER
4	n	73	VAL
4	n	76	VAL
7	5	16	ASP
7	5	159	GLY
8	T	72	GLN
10	Y	2	LYS
10	Y	37	LEU
1	y	40	PRO
1	y	400	TYR
2	E	90	THR
4	n	61	LYS
7	5	87	ALA
7	5	88	LYS
7	5	90	ALA
8	T	97	GLY
1	y	185	ASN
3	G	45	SER
4	n	57	PRO
9	U	12	VAL

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Mol	Chain	Res	Type
9	U	75	ALA
1	y	55	GLN
1	y	78	PHE
1	y	255	ARG
4	n	50	PRO
7	5	72	SER
8	T	10	VAL
1	y	256	ARG
4	n	49	SER
8	T	29	THR
3	G	44	GLY
1	y	299	GLY
4	n	28	GLY
1	y	143	PRO
4	n	56	LEU
1	y	6	GLY
1	y	240	GLY

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%)	330 (94%)	23 (6%)	17 42
2	E	47/47 (100%)	45 (96%)	2 (4%)	29 53
3	G	46/46 (100%)	39 (85%)	7 (15%)	3 14
4	n	77/77 (100%)	61 (79%)	16 (21%)	1 6
7	5	181/181 (100%)	170 (94%)	11 (6%)	18 44
8	T	84/84 (100%)	79 (94%)	5 (6%)	19 44
9	U	84/84 (100%)	82 (98%)	2 (2%)	49 69
10	Y	55/55 (100%)	54 (98%)	1 (2%)	59 77
All	All	927/927 (100%)	860 (93%)	67 (7%)	18 39

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	7	LEU
1	y	31	ILE
1	y	32	VAL
1	y	57	ARG
1	y	63	MET
1	y	77	ILE
1	y	113	ARG
1	y	145	MET
1	y	152	PRO
1	y	172	MET
1	y	176	GLU
1	y	180	GLU
1	y	189	ILE
1	y	255	ARG
1	y	264	HIS
1	y	267	LEU
1	y	315	PRO
1	y	336	VAL
1	y	357	ARG
1	y	375	LEU
1	y	388	PRO
1	y	415	ASP
1	y	416	PHE
2	E	77	THR
2	E	94	THR
3	G	33	SER
3	G	34	PHE
3	G	42	LEU
3	G	43	PHE
3	G	46	SER
3	G	59	LEU
3	G	65	ILE
4	n	13	LEU
4	n	32	ARG
4	n	38	LEU
4	n	41	ARG
4	n	42	SER
4	n	44	SER
4	n	46	ASP
4	n	52	SER
4	n	54	HIS
4	n	56	LEU
4	n	58	GLU

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Mol	Chain	Res	Type
4	n	61	LYS
4	n	67	GLN
4	n	71	LEU
4	n	92	SER
4	n	97	ILE
7	5	3	LYS
7	5	73	VAL
7	5	77	VAL
7	5	78	PHE
7	5	85	GLU
7	5	95	VAL
7	5	102	ASP
7	5	121	MET
7	5	136	LEU
7	5	144	THR
7	5	166	ASP
8	T	36	LYS
8	T	61	LEU
8	T	66	LYS
8	T	69	ARG
8	T	96	VAL
9	U	49	PRO
9	U	91	LYS
10	Y	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	252	GLN
1	y	345	ASN
1	y	419	GLN
4	n	33	GLN
4	n	39	HIS
4	n	40	GLN
7	5	103	GLN
7	5	165	ASN
7	5	168	ASN
8	T	70	HIS
9	U	52	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	1	62/63 (98%)	13 (20%)	1 (1%)
12	2	35/36 (97%)	8 (22%)	1 (2%)
13	3	43/44 (97%)	7 (16%)	2 (4%)
14	4	108/109 (99%)	39 (36%)	8 (7%)
5	p	75/76 (98%)	17 (22%)	0
6	a	74/76 (97%)	28 (37%)	0
All	All	397/404 (98%)	112 (28%)	12 (3%)

All (112) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	p	2	C
5	p	4	G
5	p	5	G
5	p	7	A
5	p	8	U
5	p	17	U
5	p	18	G
5	p	22	G
5	p	37	A
5	p	44	G
5	p	46	G
5	p	49	G
5	p	60	U
5	p	61	C
5	p	69	C
5	p	74	C
5	p	75	C
6	a	8	U
6	a	9	A
6	a	10	G
6	a	11	C
6	a	16	U
6	a	17	C
6	a	18	G
6	a	19	G
6	a	20	U
6	a	21	A
6	a	22	G
6	a	24	G
6	a	25	C
6	a	26	A
6	a	27	G

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Mol	Chain	Res	Type
6	a	41	C
6	a	44	G
6	a	46	G
6	a	47	U
6	a	49	C
6	a	58	A
6	a	59	U
6	a	61	C
6	a	70	G
6	a	73	A
6	a	74	C
6	a	75	C
6	a	76	A
11	1	63	A
11	1	64	A
11	1	71	A
11	1	74	A
11	1	75	G
11	1	84	A
11	1	90	U
11	1	91	A
11	1	92	U
11	1	93	G
11	1	95	A
11	1	100	U
11	1	103	A
12	2	1312	U
12	2	1313	U
12	2	1316	U
12	2	1325	U
12	2	1326	U
12	2	1334	G
12	2	1336	A
12	2	1337	G
13	3	1523	U
13	3	1524	G
13	3	1532	A
13	3	1535	A
13	3	1538	G
13	3	1540	G
13	3	1552	A
14	4	2102	G

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Mol	Chain	Res	Type
14	4	2104	C
14	4	2111	U
14	4	2117	A
14	4	2118	U
14	4	2119	A
14	4	2120	G
14	4	2126	A
14	4	2128	G
14	4	2129	C
14	4	2131	U
14	4	2132	U
14	4	2133	G
14	4	2135	A
14	4	2136	G
14	4	2137	U
14	4	2138	G
14	4	2144	G
14	4	2145	C
14	4	2146	C
14	4	2147	A
14	4	2148	G
14	4	2149	U
14	4	2152	G
14	4	2153	C
14	4	2155	U
14	4	2158	A
14	4	2159	G
14	4	2160	C
14	4	2163	A
14	4	2164	C
14	4	2165	C
14	4	2166	U
14	4	2176	A
14	4	2179	C
14	4	2181	U
14	4	2192	U
14	4	2198	A
14	4	2199	A

All (12) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
11	1	91	A
12	2	1312	U
13	3	1535	A
13	3	1551	A
14	4	2132	U
14	4	2144	G
14	4	2145	C
14	4	2147	A
14	4	2152	G
14	4	2157	G
14	4	2163	A
14	4	2172	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MIA	a	37	6	24,31,32	1.85	4 (16%)	26,44,47	3.11	6 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MIA	a	37	6	-	2/11/33/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	37	MIA	C13-C14	6.42	1.50	1.32
6	a	37	MIA	C2-S10	4.22	1.79	1.75
6	a	37	MIA	C12-C13	-2.87	1.35	1.48
6	a	37	MIA	C8-N7	-2.06	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	a	37	MIA	C11-S10-C2	10.57	110.16	102.27
6	a	37	MIA	C12-N6-C6	-8.85	109.44	122.55
6	a	37	MIA	C5-C6-N1	-3.69	117.74	120.81
6	a	37	MIA	C2-N3-C4	-3.30	110.78	115.32
6	a	37	MIA	C12-C13-C14	-3.28	120.76	127.14
6	a	37	MIA	C16-C14-C15	2.59	120.33	114.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	37	MIA	N6-C12-C13-C14
6	a	37	MIA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	3	2
4	n	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	1516:G	O3'	1517:G	P	1.91
1	n	99:ALA	C	100:GLY	N	1.89
1	n	22:TYR	C	23:GLU	N	1.84
1	3	1551:A	O3'	1552:A	P	1.82

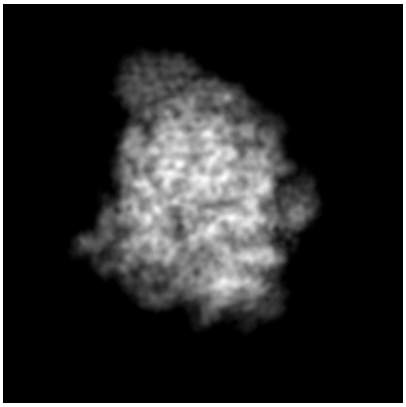
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5693. These allow visual inspection of the internal detail of the map and identification of artifacts.

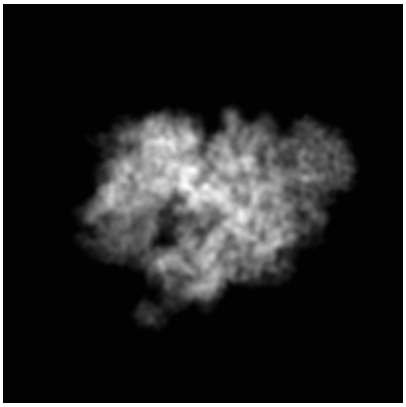
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

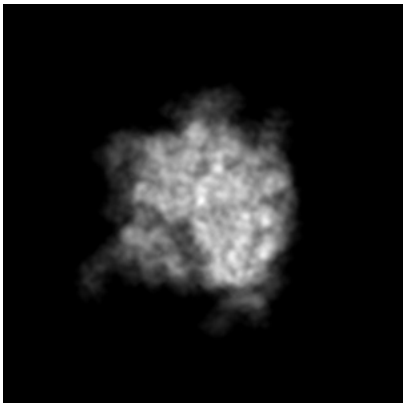
6.1.1 Primary map



X



Y

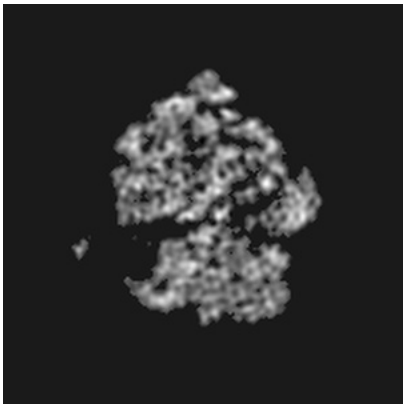


Z

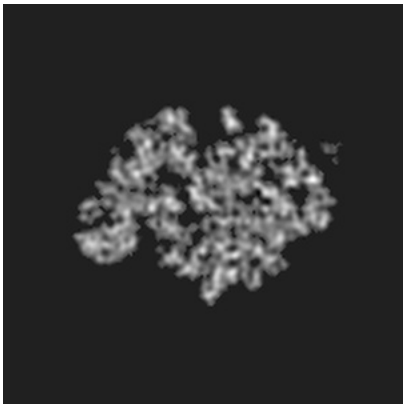
The images above show the map projected in three orthogonal directions.

6.2 Central slices

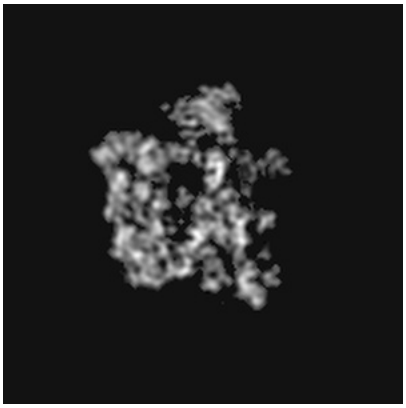
6.2.1 Primary map



X Index: 96



Y Index: 96

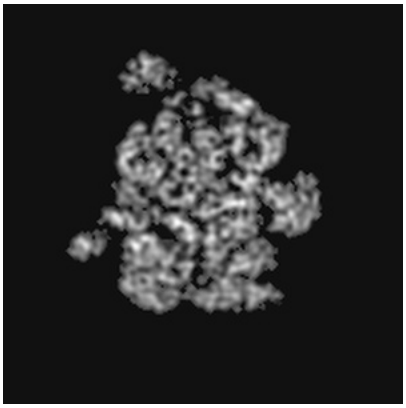


Z Index: 96

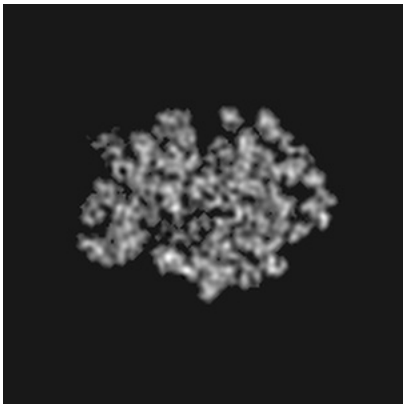
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

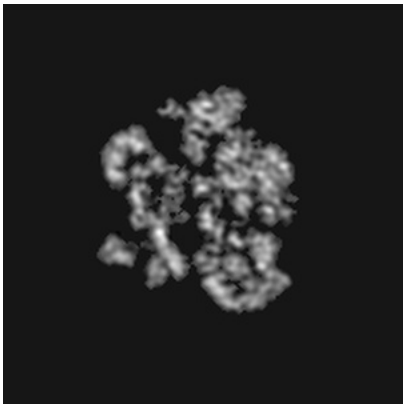
6.3.1 Primary map



X Index: 103



Y Index: 99

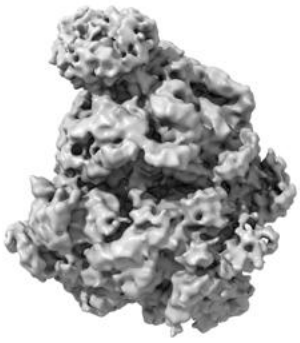


Z Index: 89

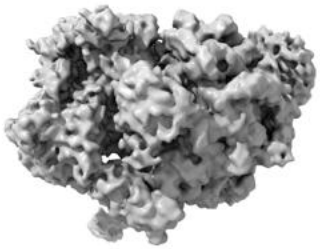
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

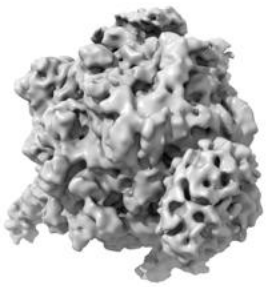
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

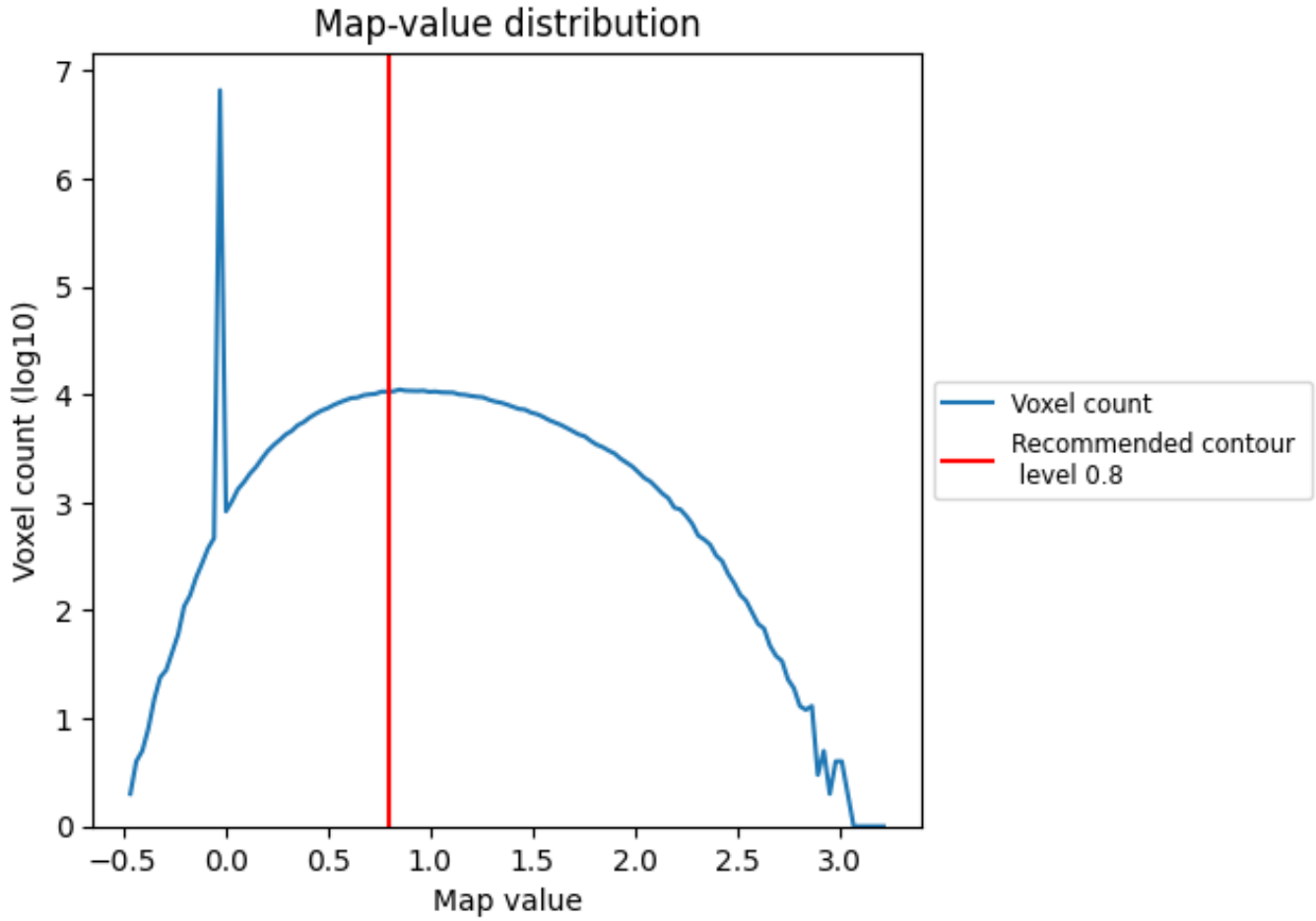
6.5 Mask visualisation (i)

This section was not generated.

7 Map analysis

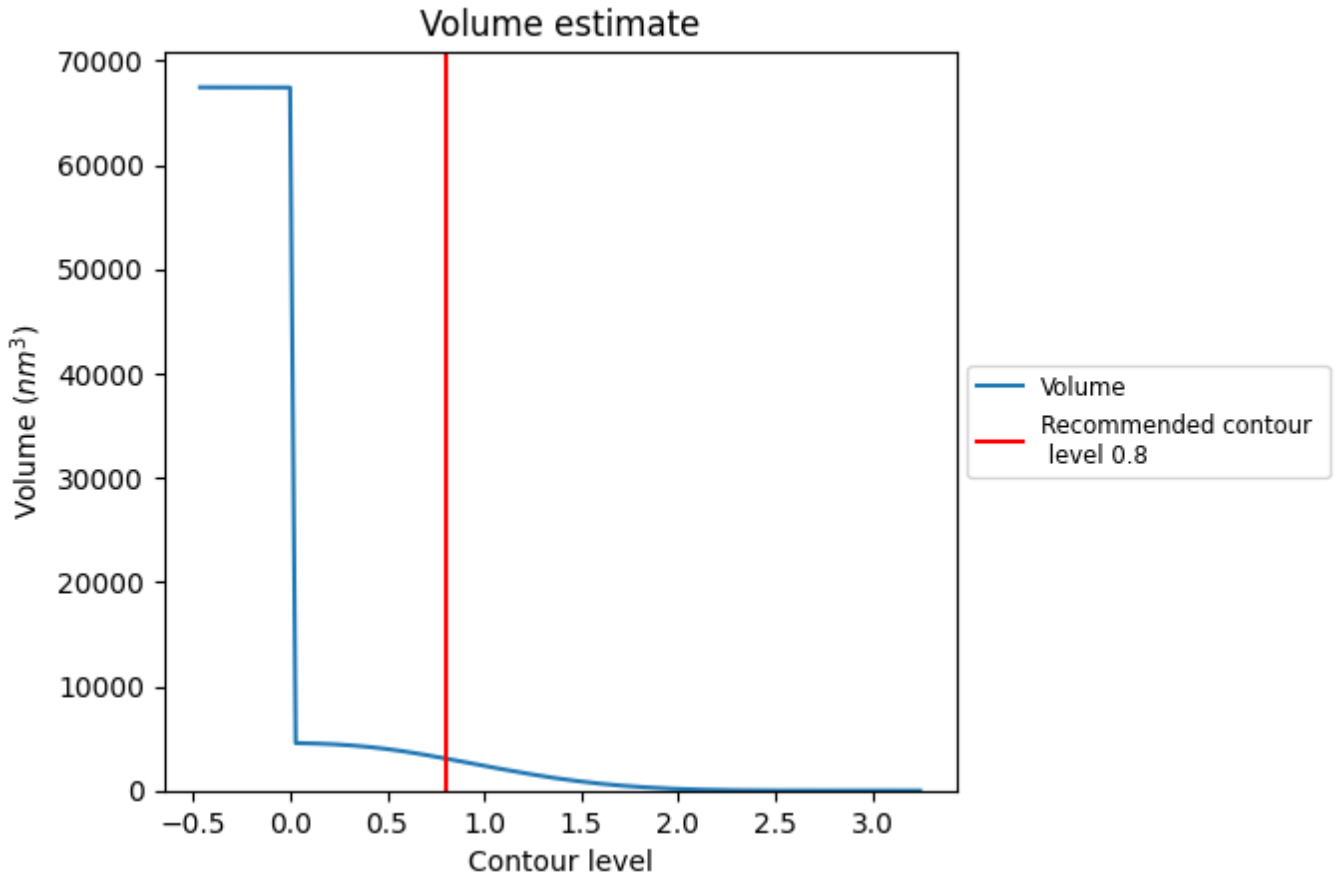
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

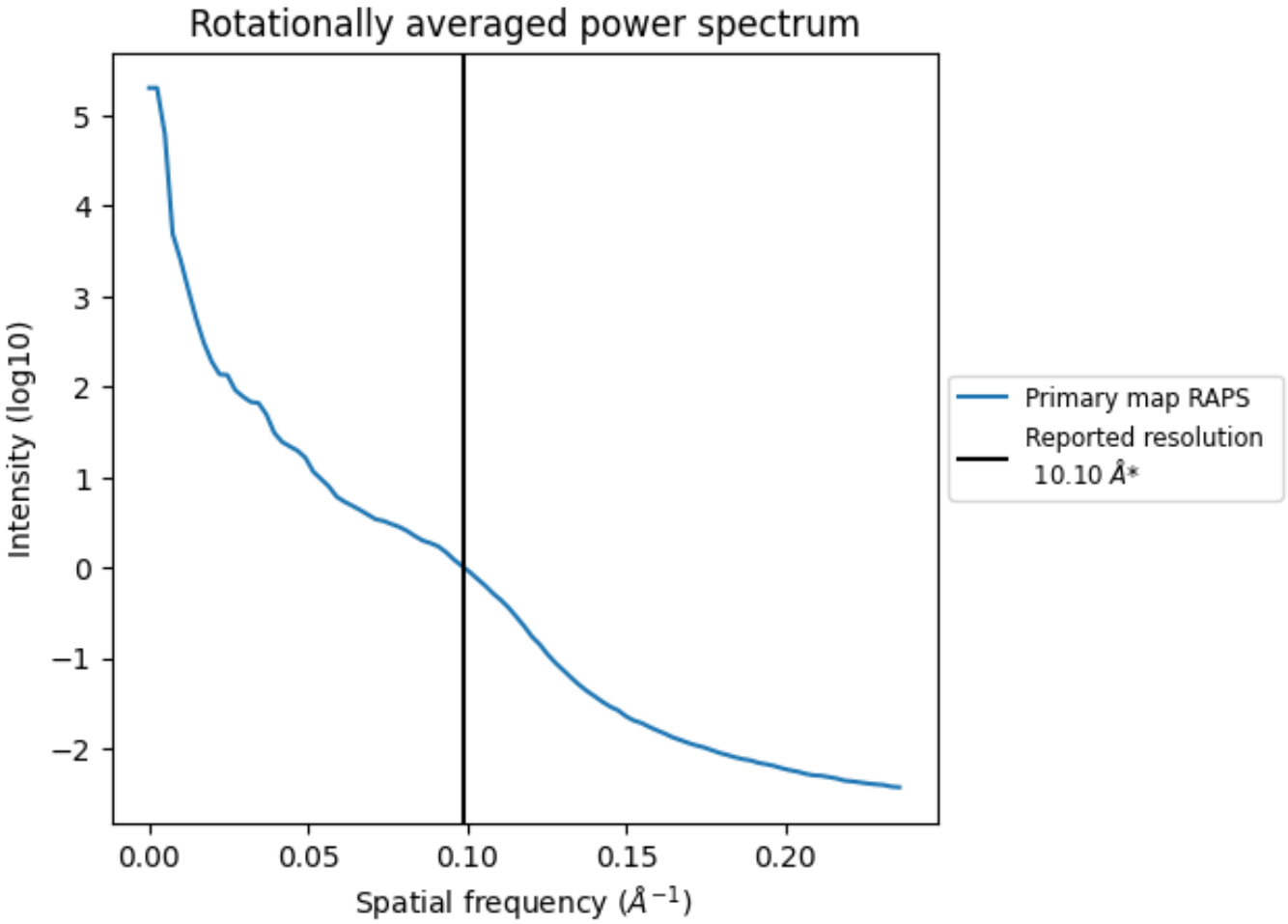
7.2 Volume estimate



The volume at the recommended contour level is 3075 nm^3; this corresponds to an approximate mass of 2778 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.099 $Å^{-1}$

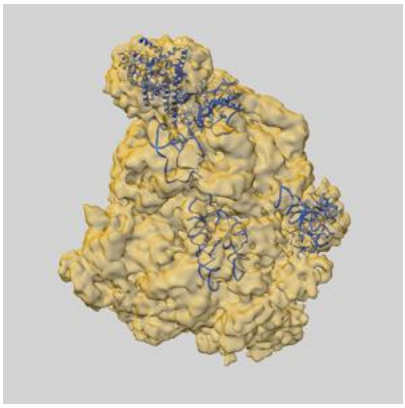
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

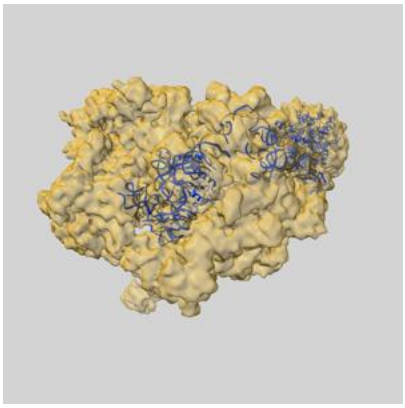
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5693 and PDB model 3J46. Per-residue inclusion information can be found in section 3 on page 7.

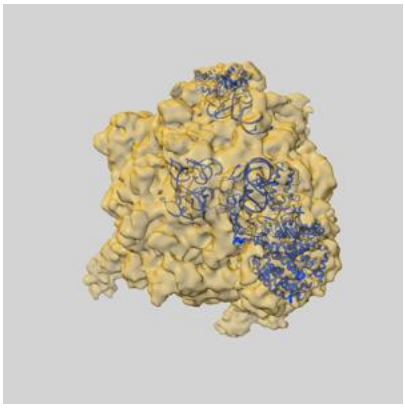
9.1 Map-model overlay



X



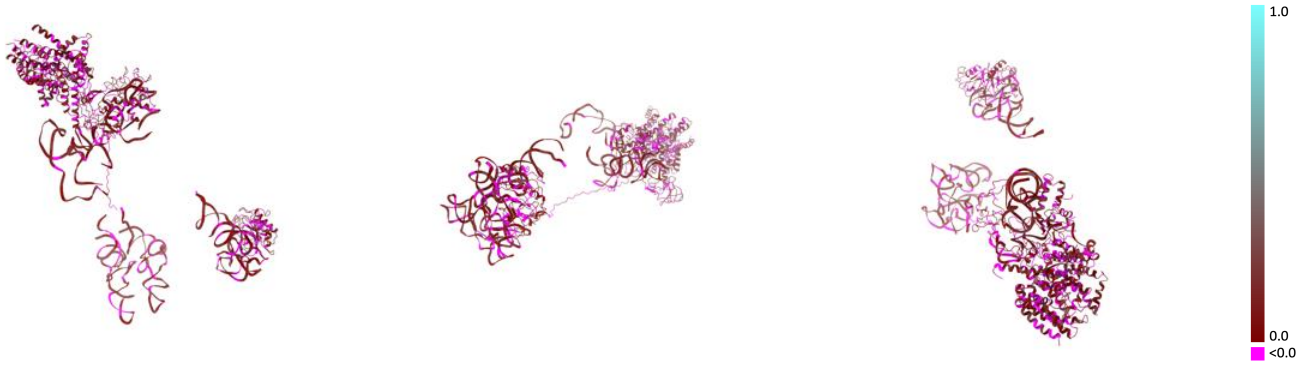
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

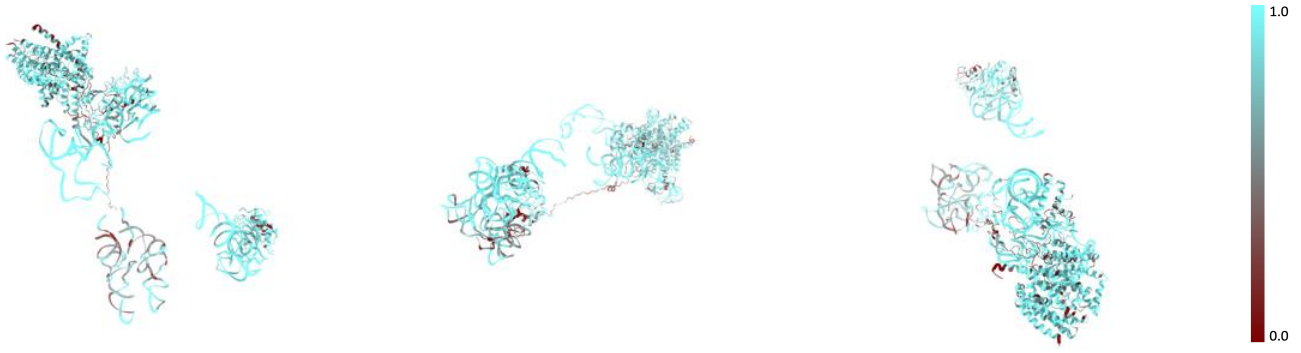
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

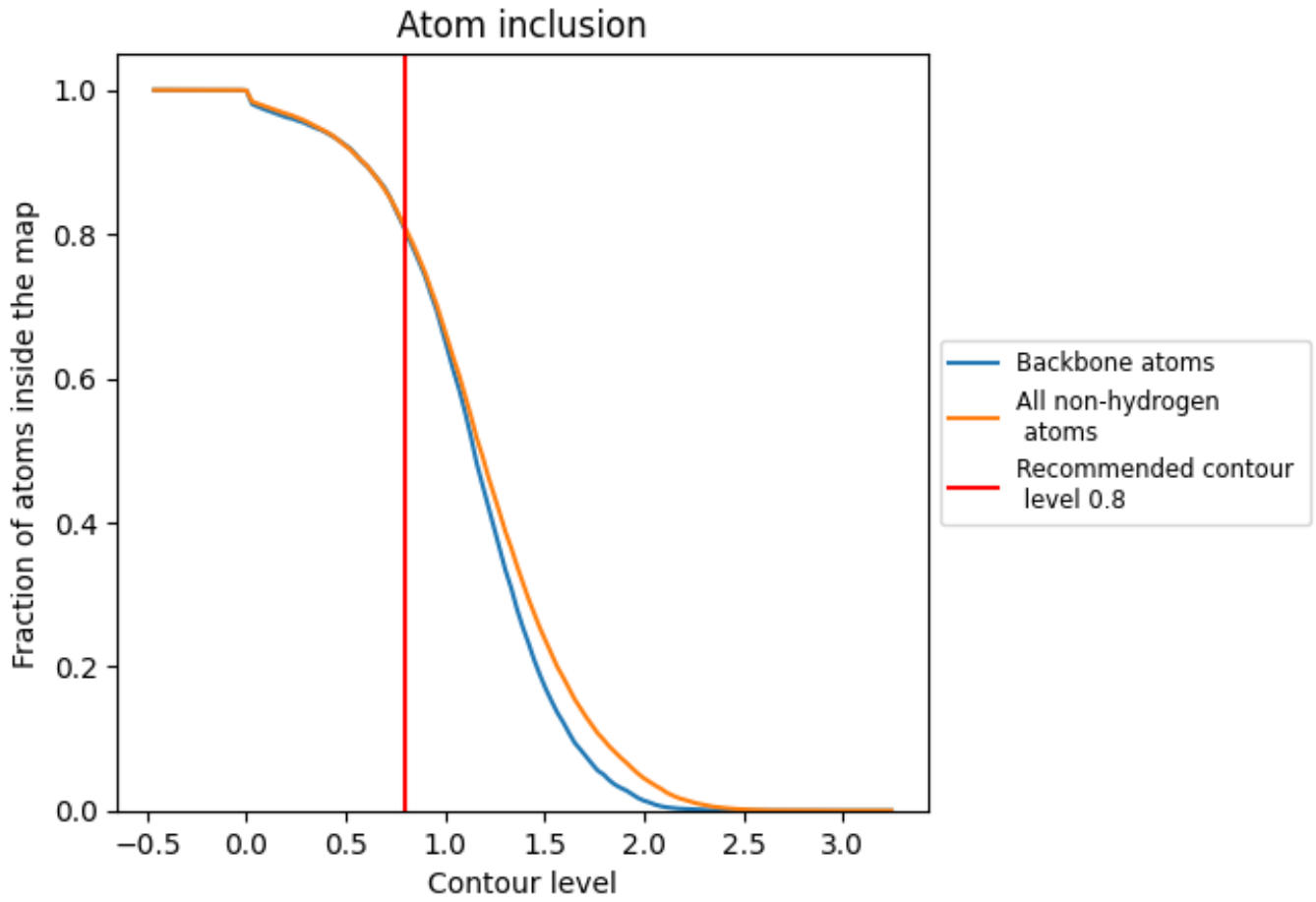
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8085	0.0790
1	0.9526	0.1260
2	0.9548	0.1000
3	0.9589	0.1440
4	0.9630	0.0950
5	0.8074	0.0590
E	0.7238	0.0410
G	0.8581	0.0510
T	0.7276	0.0700
U	0.8108	0.0750
Y	0.7907	0.0870
a	0.6292	0.0690
n	0.5294	-0.0090
p	0.6582	0.0960
y	0.8141	0.0630