



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:24 am GMT

PDB ID : 6YLX
EMDB ID : EMD-10841
Title : pre-60S State NE1 (TAP-Flag-Nop53)
Authors : Kater, L.; Beckmann, R.
Deposited on : 2020-04-07
Resolution : 3.90 Å(reported)
Based on initial models : 6N8J, 3JCT, 6ELZ

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:

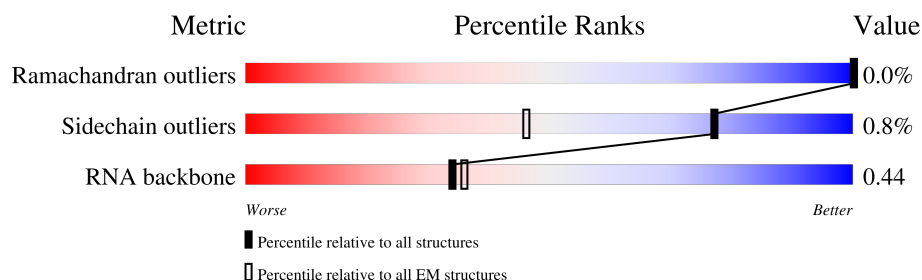
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.90 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.



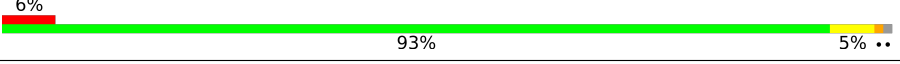

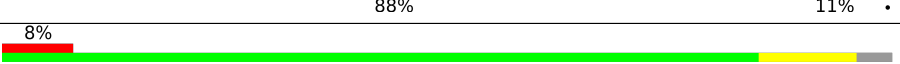
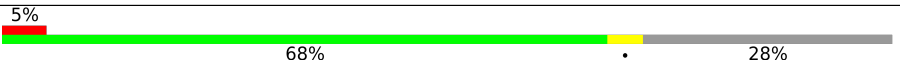

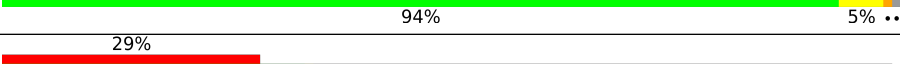
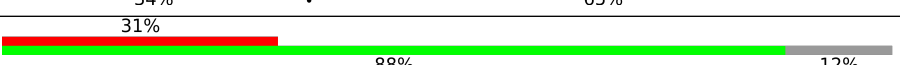
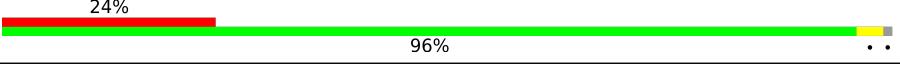
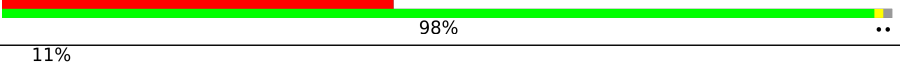
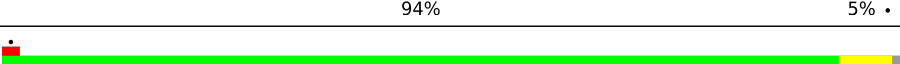
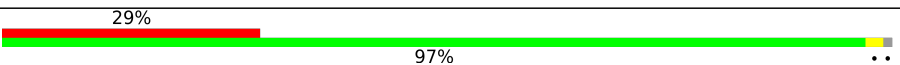

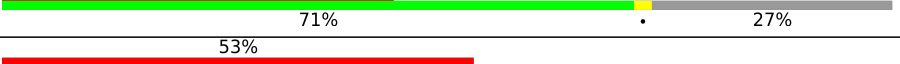
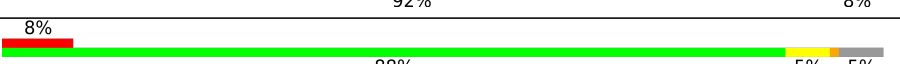

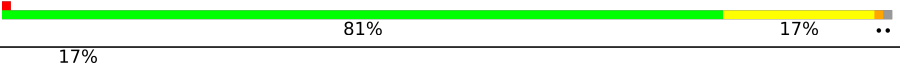

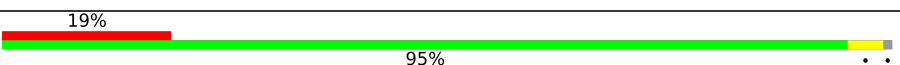

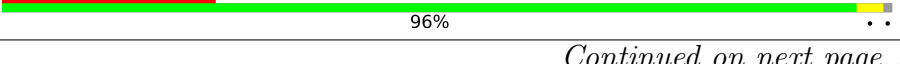



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	B	387	
2	C	362	
3	E	176	
4	F	244	
5	G	256	
6	H	191	
7	K	376	
8	L	199	

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Mol	Chain	Length	Quality of chain
9	M	138	
10	N	204	
11	O	199	
12	P	184	
13	Q	186	
14	R	189	
15	S	172	
16	T	160	
17	U	121	
18	V	137	
19	W	236	
20	X	142	
21	Y	127	
22	Z	136	
23	a	149	
24	b	647	
25	c	105	
26	d	113	
27	e	130	
28	f	107	
29	g	121	
30	h	120	
31	i	100	
32	j	88	
33	k	78	

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Mol	Chain	Length	Quality of chain
34	l	51	
35	n	605	
36	o	220	
37	q	455	
38	r	261	
39	s	520	
40	t	322	
41	u	199	
42	y	245	
43	z	106	
44	1	3396	
45	2	158	
46	6	232	
47	w	841	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 118882 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 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 2 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 3 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 4 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 5 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	192	Total	C	N	O	S	0	0
			1515	974	267	272	2		

- Molecule 6 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 7 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	256	Total	C	N	O	S	0	0
			2064	1332	342	387	3		

- Molecule 8 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	187	Total	C	N	O	S	0	0
			1499	934	307	258			

- Molecule 9 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 10 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	180	Total	C	N	O	S	0	0
			1543	968	325	249	1		

- Molecule 11 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	176	Total	C	N	O	S	0	0
			1397	868	279	250			

- Molecule 13 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 14 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 15 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 16 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	56	Total	C	N	O	S	0	0
			434	268	86	79	1		

- Molecule 17 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 18 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 19 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 20 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 21 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 22 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 23 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 24 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	470	Total	C	N	O	S	0	0
			3814	2424	663	709	18		

- Molecule 25 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 26 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 28 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 29 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 30 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 31 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 32 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 33 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 34 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 35 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 36 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	q	87	Total	C	N	O	S	0	0
			723	450	129	143	1		

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	r	217	Total	C	N	O	S	0	0
			1760	1110	334	309	7		

- Molecule 39 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 40 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 41 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	u	123	Total	C	N	O	S	0	0
			1040	652	211	168	9		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 43 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 44 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	2534	Total	C	N	O	P	0	0
			54232	24220	9799	17679	2534		

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 46 is a RNA chain called ITS2.

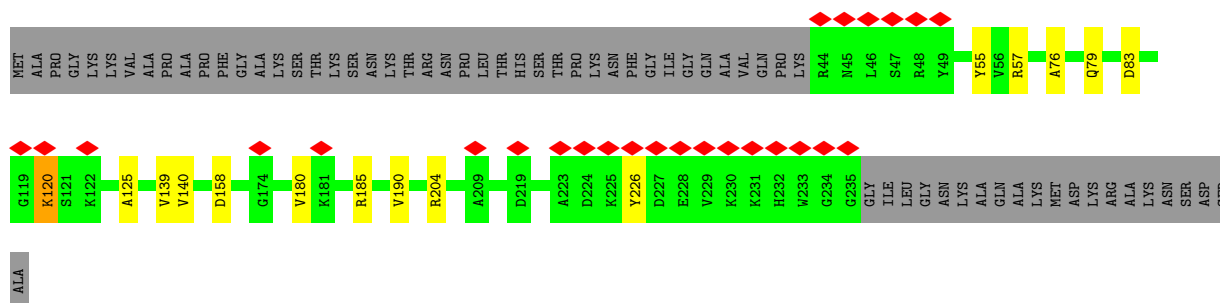
Mol	Chain	Residues	Atoms					AltConf	Trace
46	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 47 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

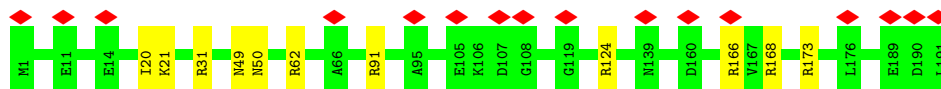
Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	360	Total	C	N	O	S	0	0
			2898	1860	507	516	15		



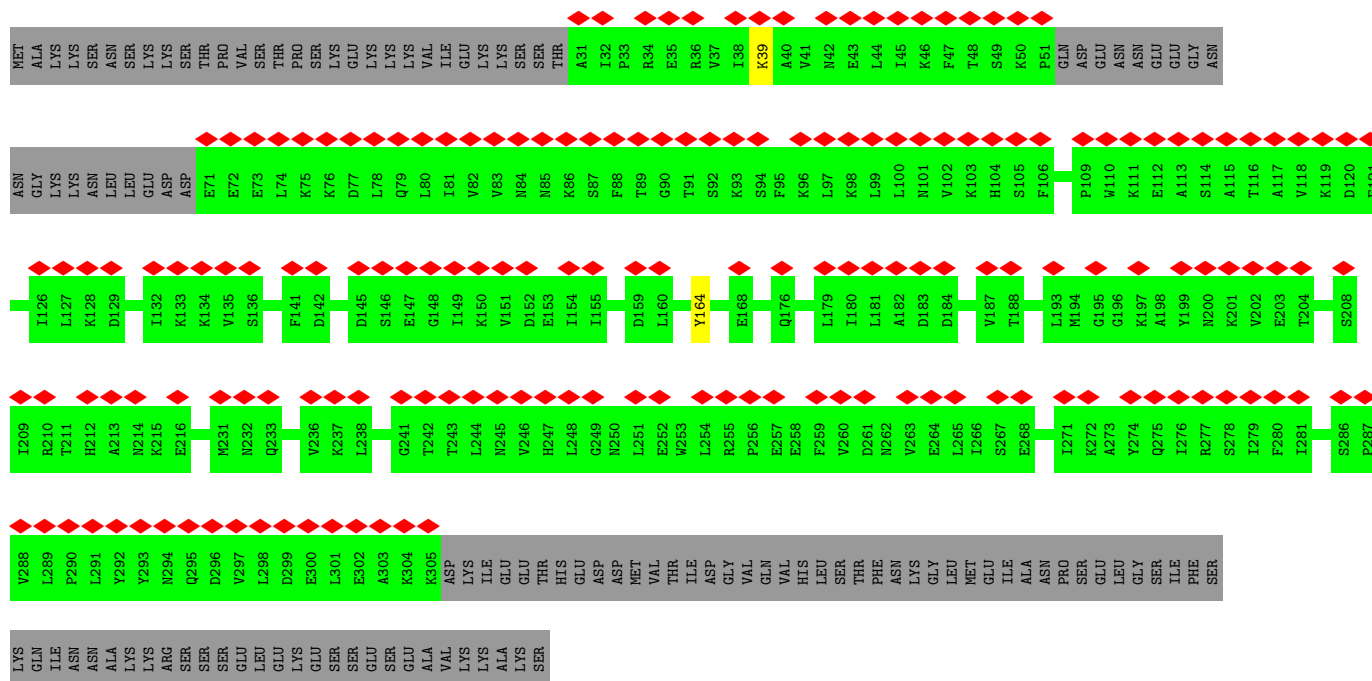
- Molecule 5: 60S ribosomal protein L8-A



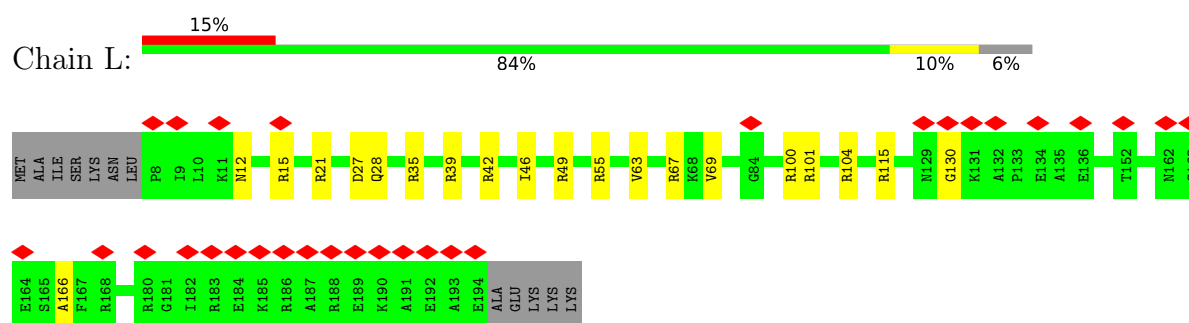
- Molecule 6: 60S ribosomal protein L9-A



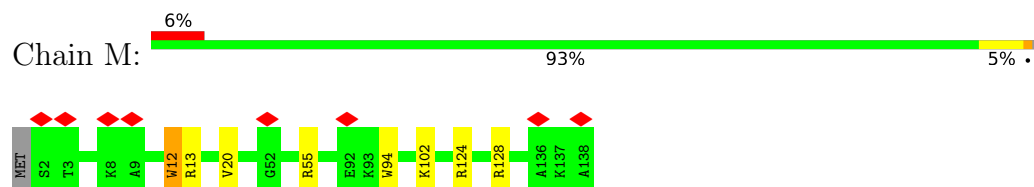
- Molecule 7: Proteasome-interacting protein CIC1



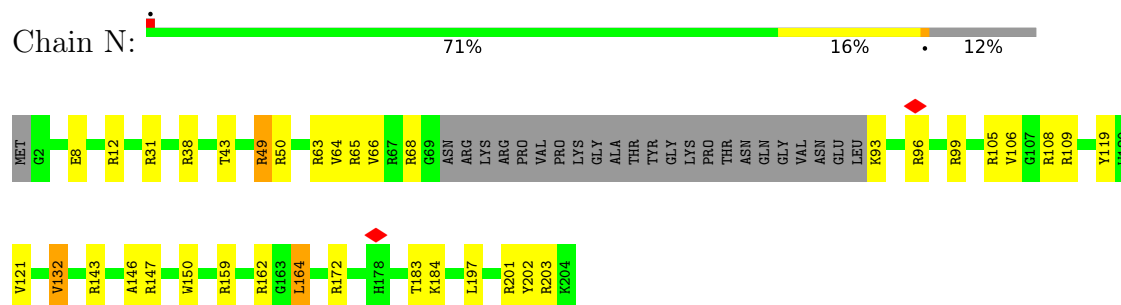
- Molecule 8: 60S ribosomal protein L13-A



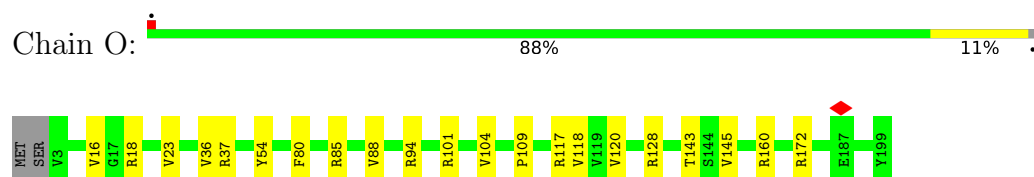
- Molecule 9: 60S ribosomal protein L14-A



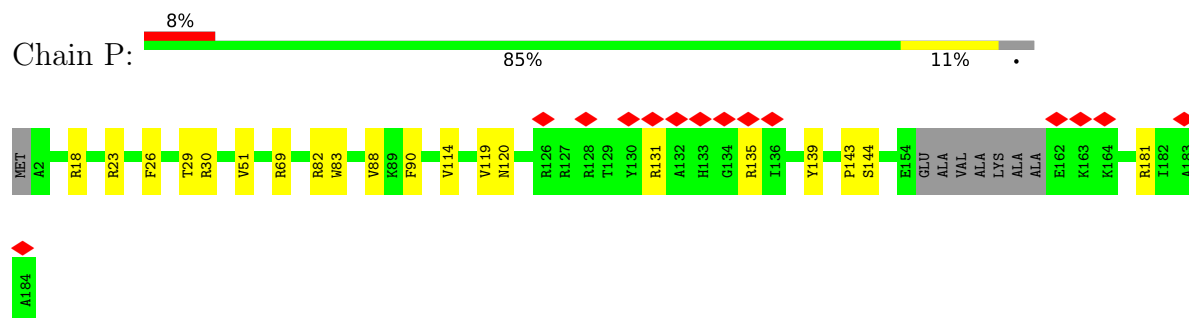
- Molecule 10: 60S ribosomal protein L15-A



- Molecule 11: 60S ribosomal protein L16-A



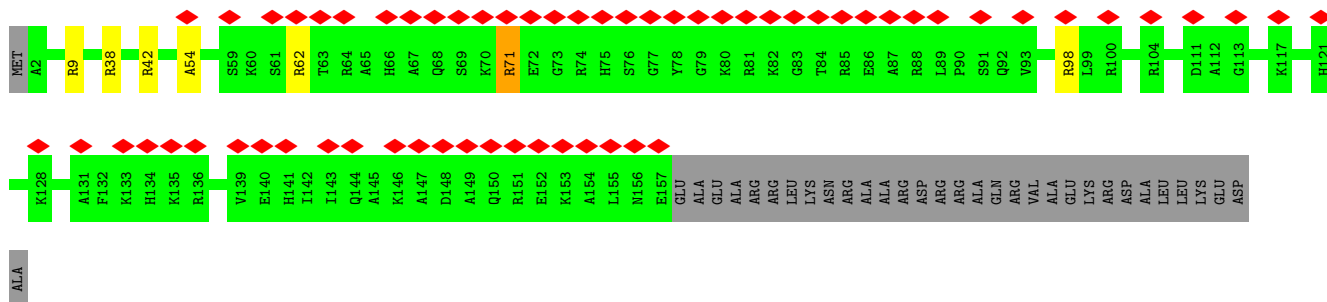
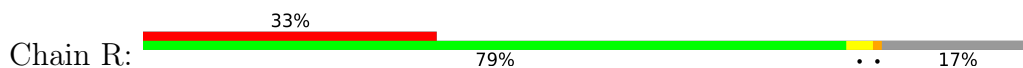
- Molecule 12: 60S ribosomal protein L17-A



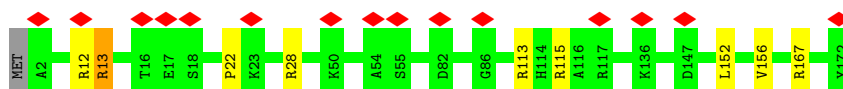
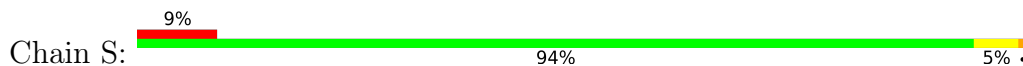
- Molecule 13: 60S ribosomal protein L18-A



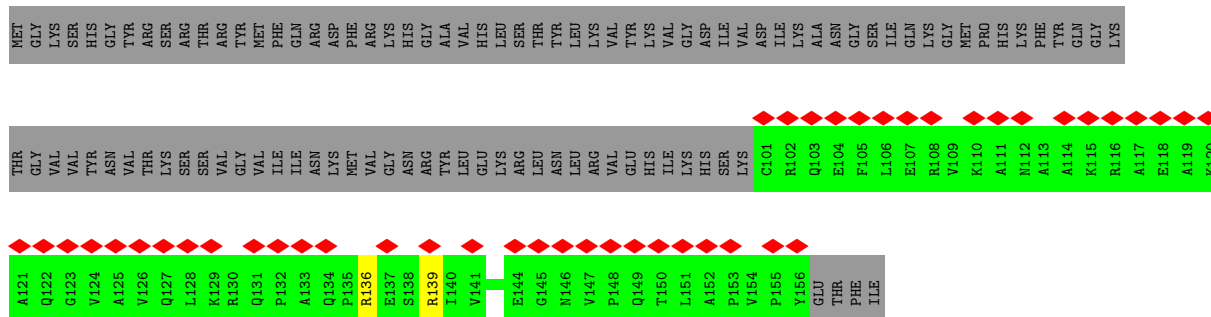
- Molecule 14: 60S ribosomal protein L19-A



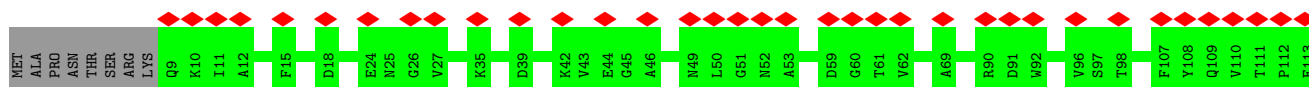
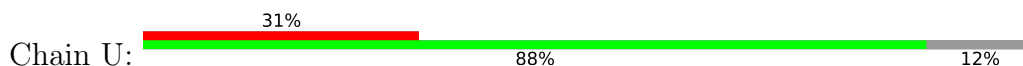
- Molecule 15: 60S ribosomal protein L20-A



- Molecule 16: 60S ribosomal protein L21-A

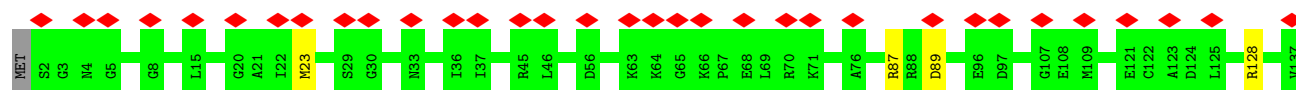


- Molecule 17: 60S ribosomal protein L22-A

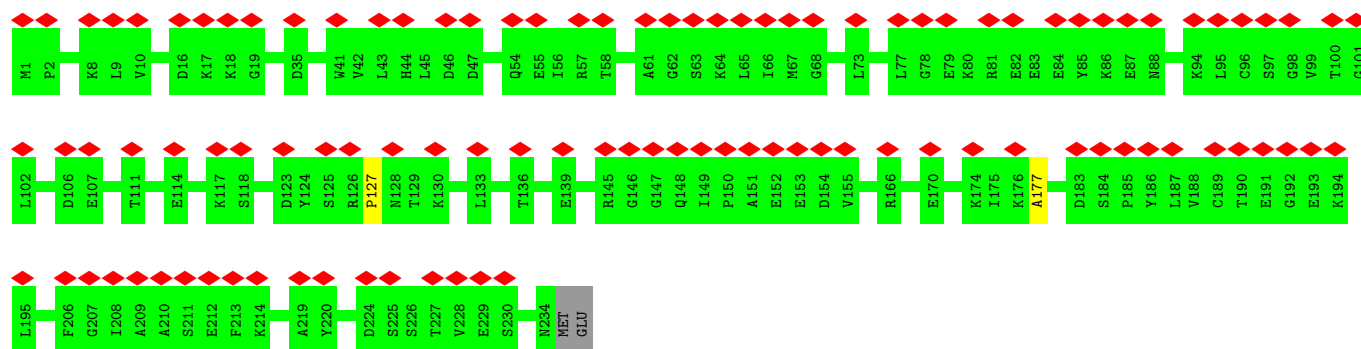
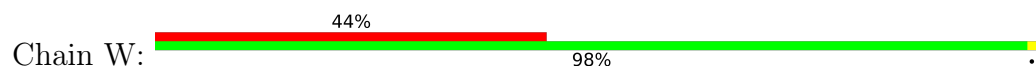




- Molecule 18: 60S ribosomal protein L23-A



- Molecule 19: Ribosome assembly factor MRT4



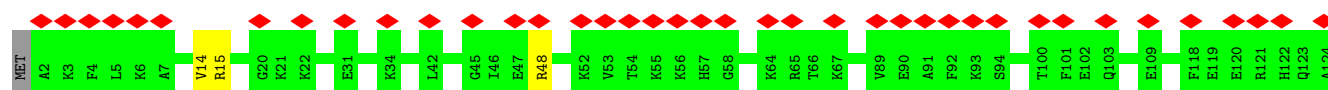
- Molecule 20: 60S ribosomal protein L25

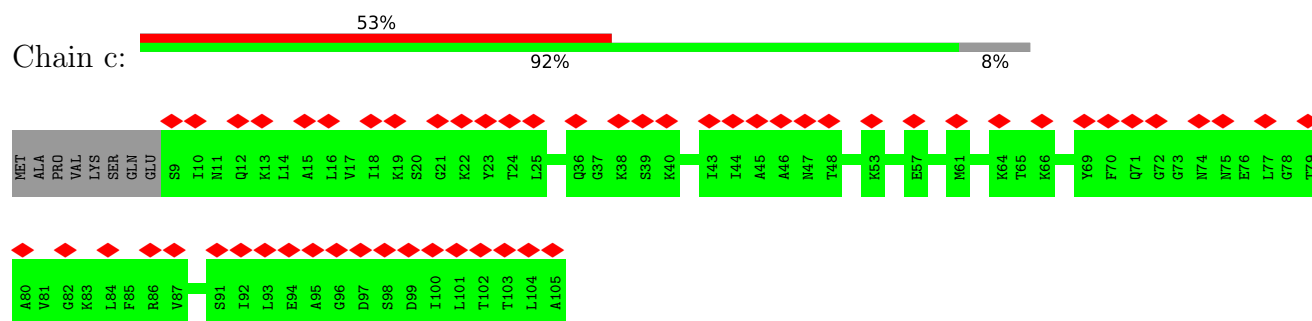


- Molecule 21: 60S ribosomal protein L26-A

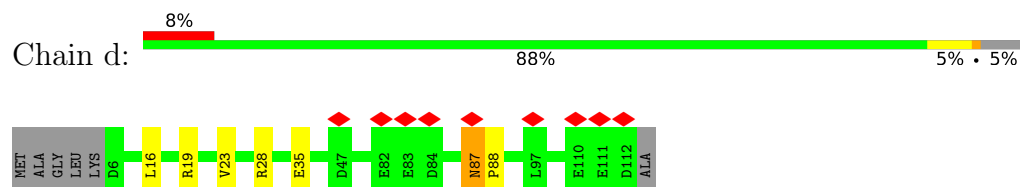


- Molecule 22: 60S ribosomal protein L27-A

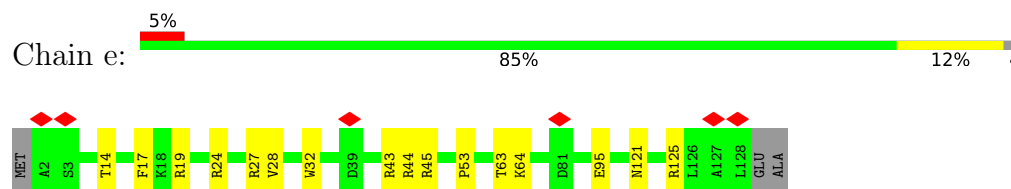




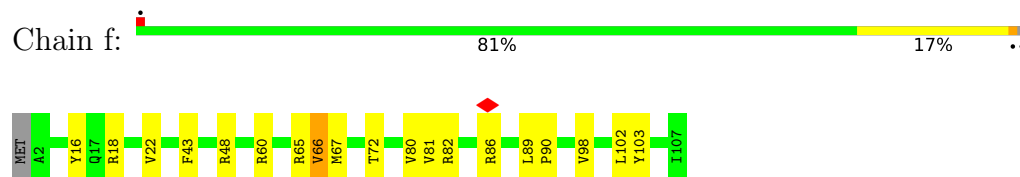
- Molecule 26: 60S ribosomal protein L31-A



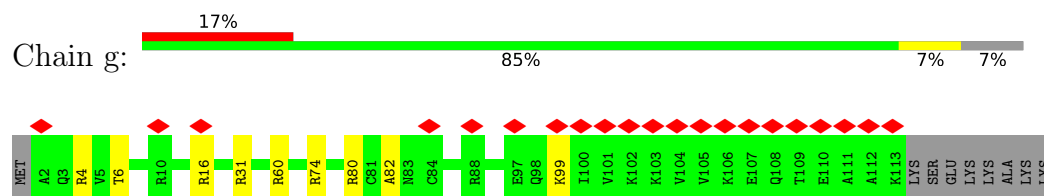
- Molecule 27: 60S ribosomal protein L32



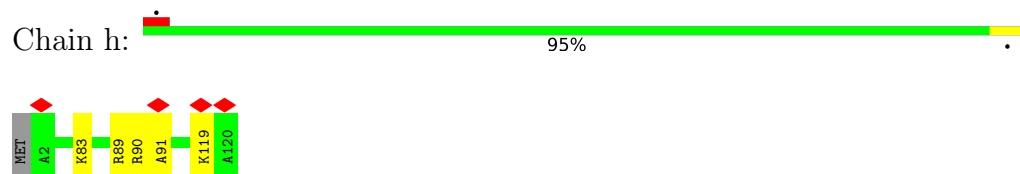
- Molecule 28: 60S ribosomal protein L33-A



- Molecule 29: 60S ribosomal protein L34-A



- Molecule 30: 60S ribosomal protein L35-A

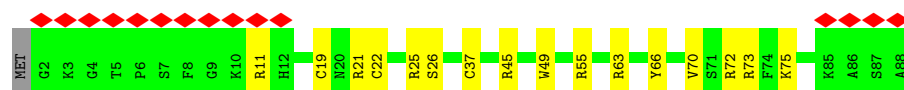
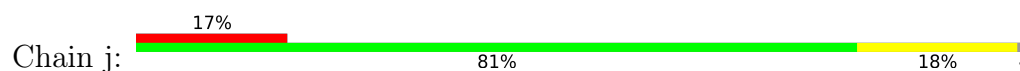


- Molecule 31: 60S ribosomal protein L36-A

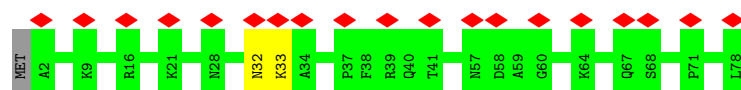




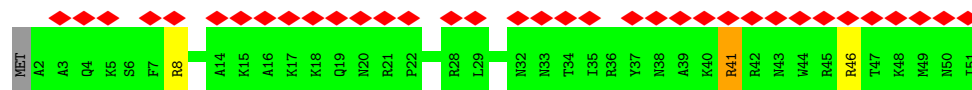
- Molecule 32: 60S ribosomal protein L37-A



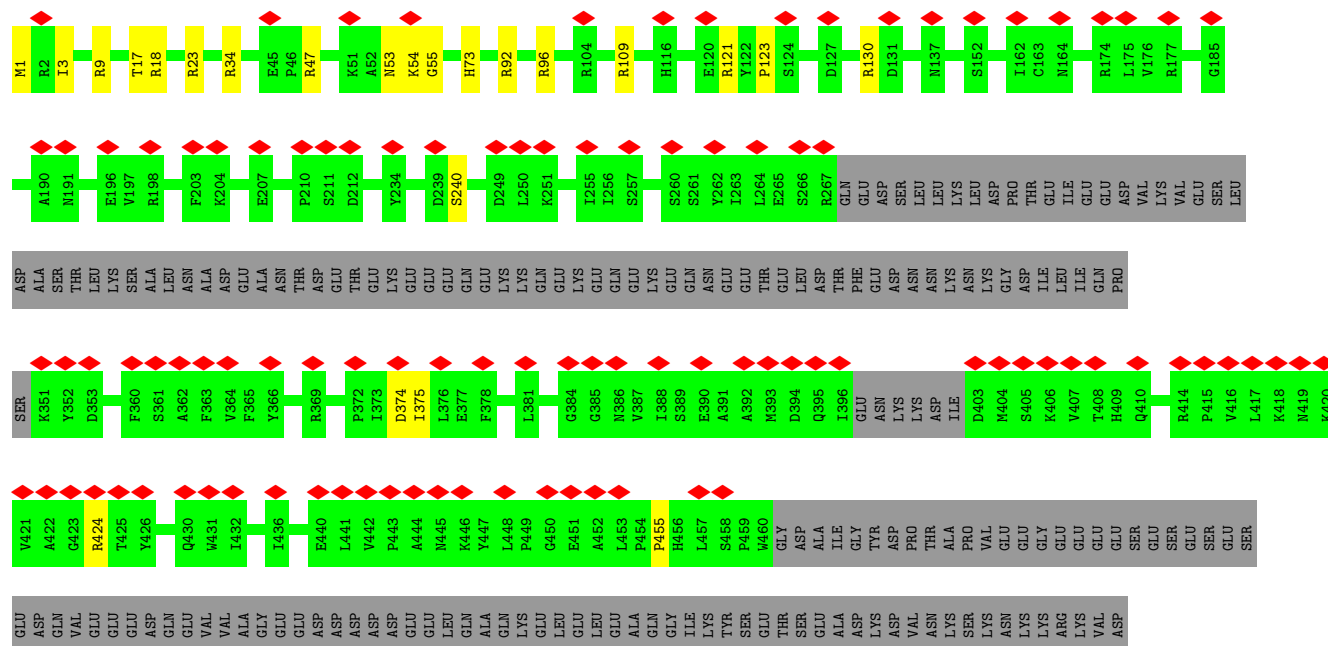
- Molecule 33: 60S ribosomal protein L38



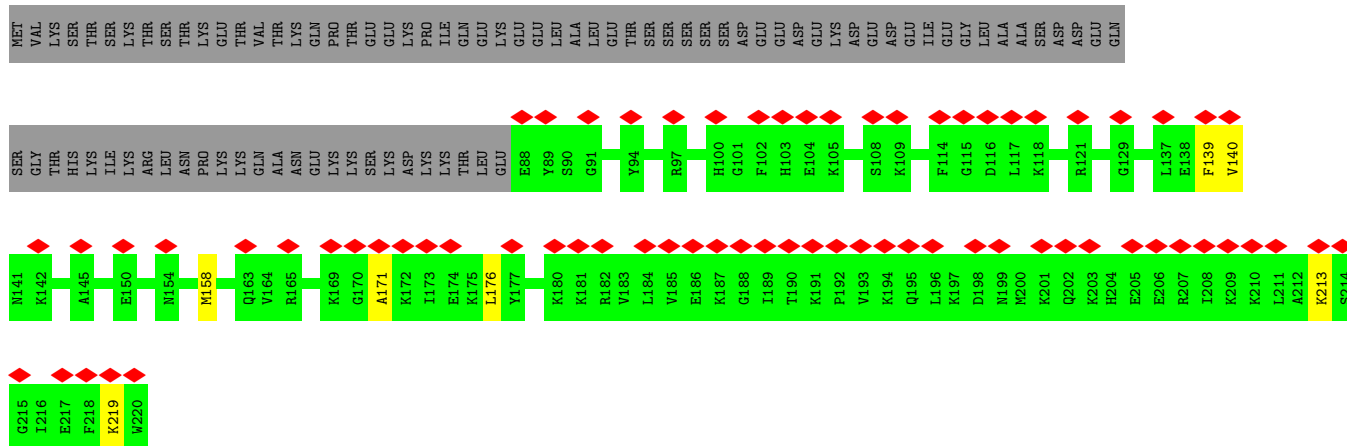
- Molecule 34: 60S ribosomal protein L39



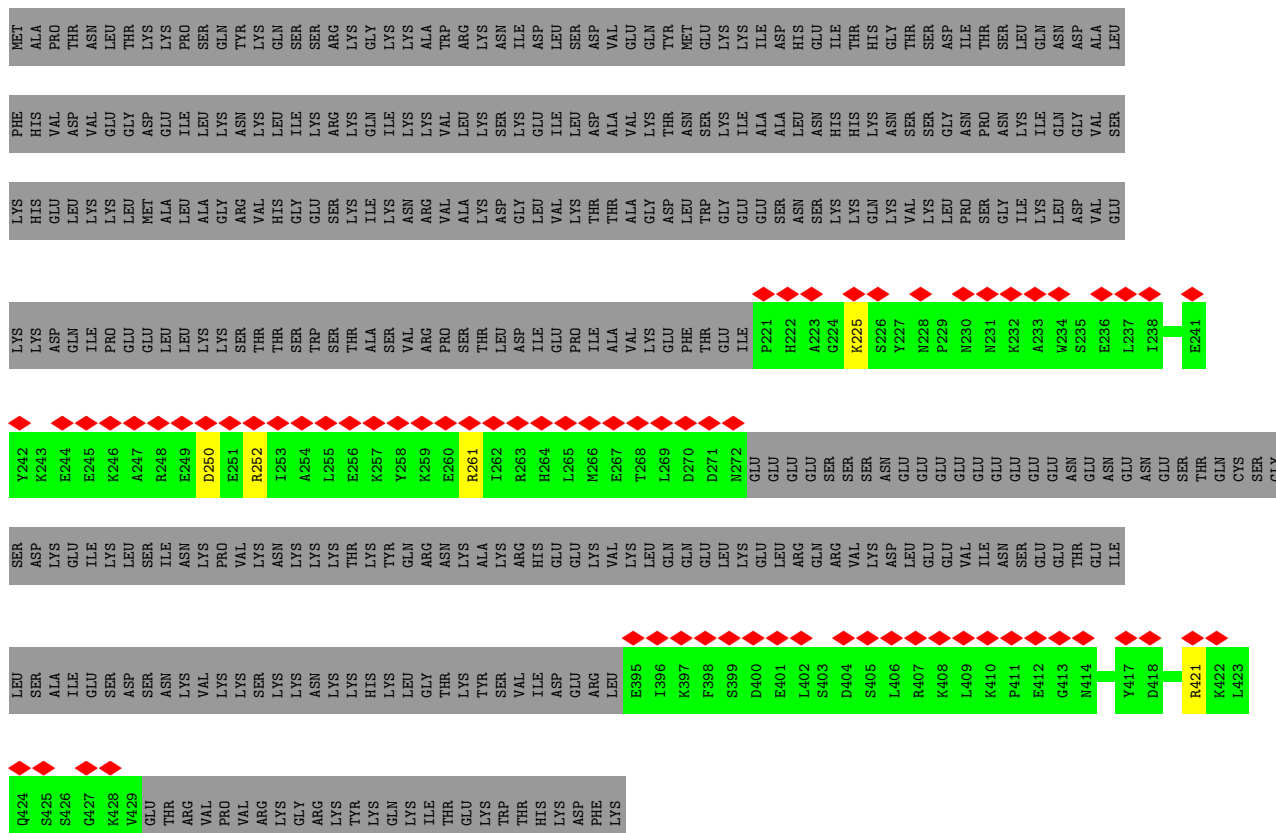
- Molecule 35: Pescadillo homolog



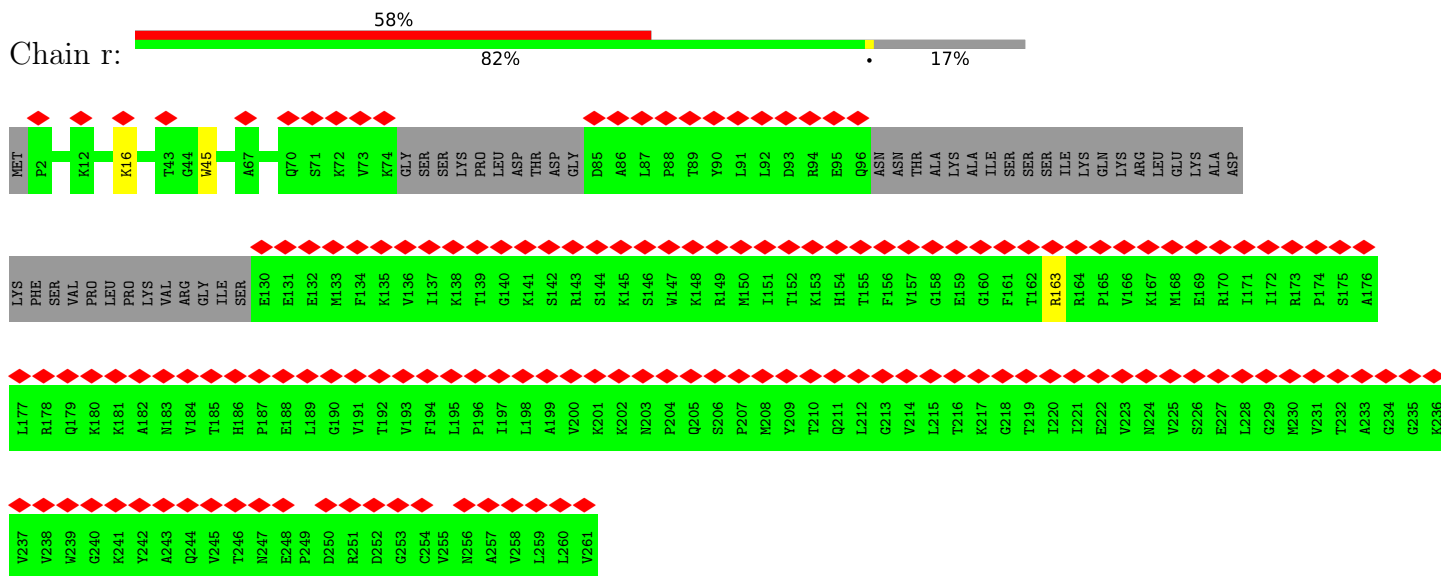
- Molecule 36: Ribosome biogenesis protein 15



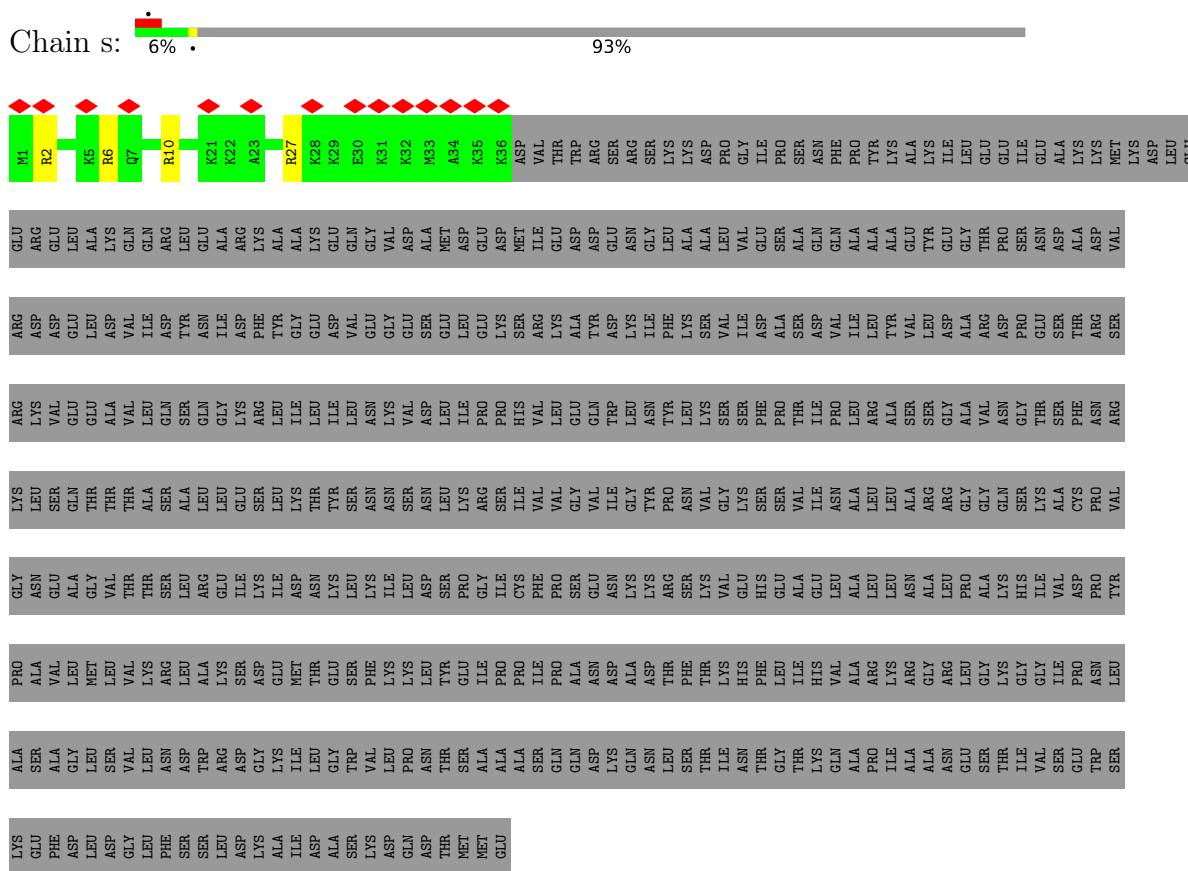
- Molecule 37: Ribosome biogenesis protein NOP53



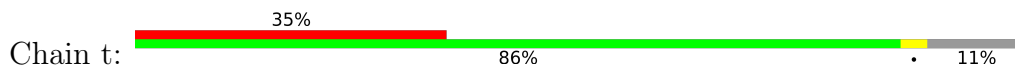
- Molecule 38: Ribosome biogenesis protein NSA2



- Molecule 39: Nuclear GTP-binding protein NUG1

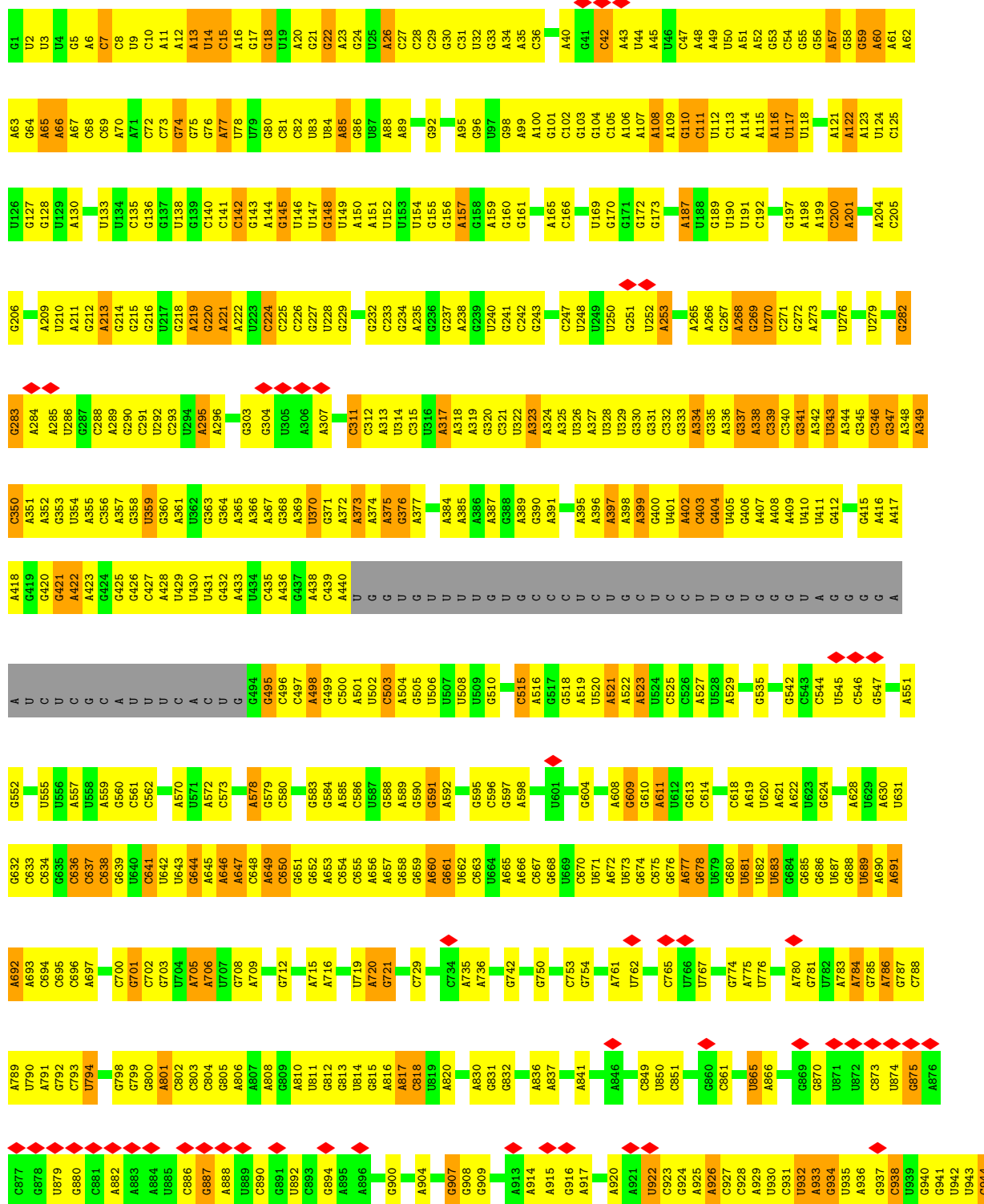
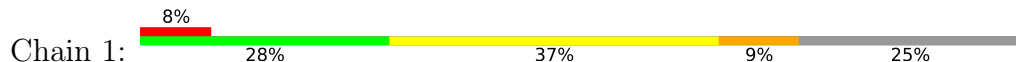


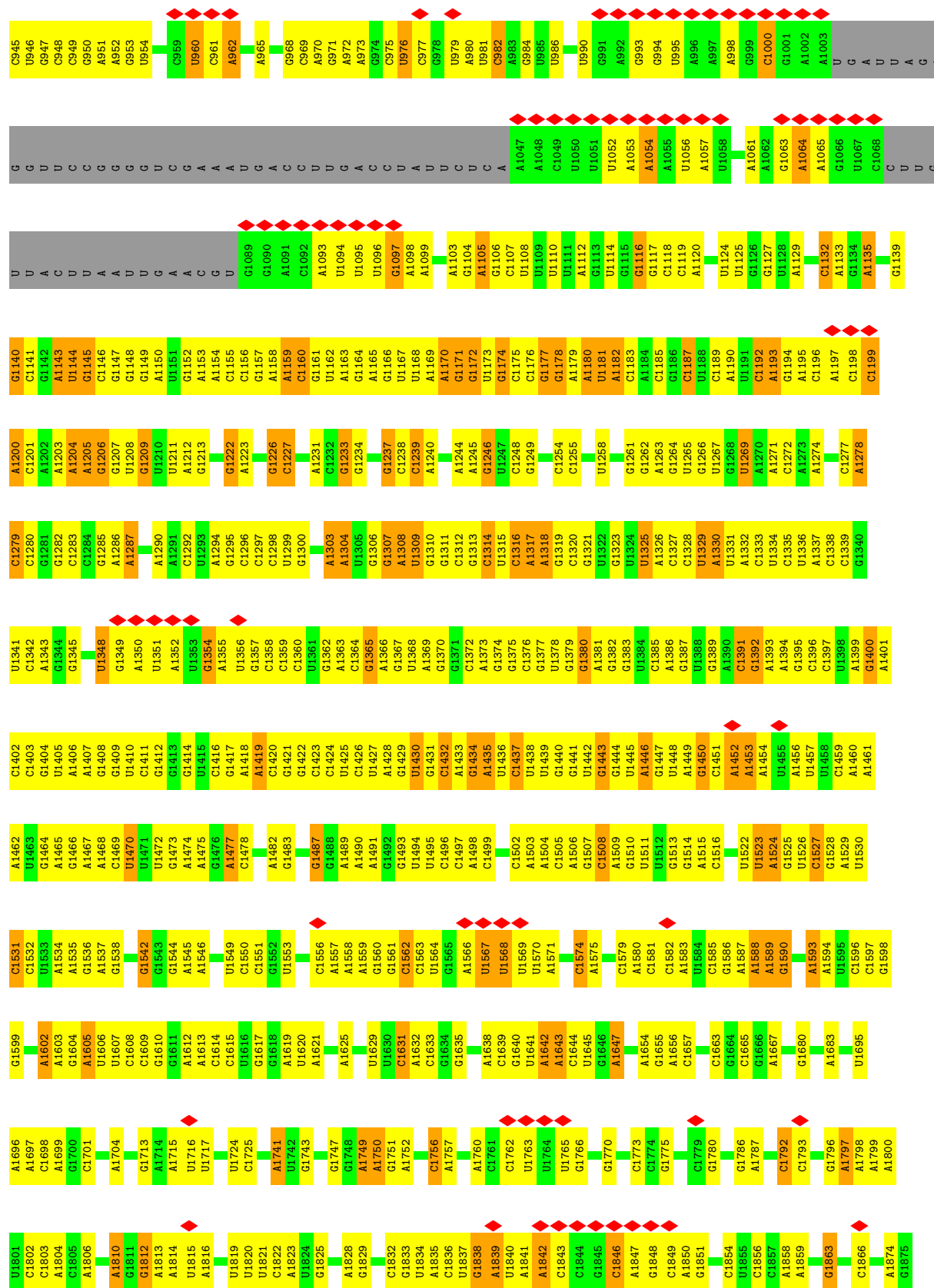
- Molecule 40: Ribosome biogenesis protein RLP7



HIS
THR
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PHE
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ARG
PHE

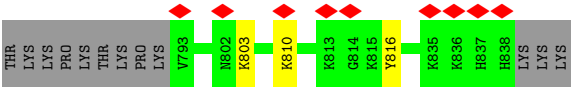
● Molecule 44: 25S rRNA











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.483	Depositor
Minimum map value	-0.257	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.055	Depositor
Map size (\AA)	416.25598, 416.25598, 416.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	1.10	6/3152 (0.2%)	1.05	15/4239 (0.4%)
2	C	1.33	14/2801 (0.5%)	1.10	22/3792 (0.6%)
3	E	0.95	0/1260	0.96	9/1694 (0.5%)
4	F	1.23	5/1821 (0.3%)	1.00	10/2451 (0.4%)
5	G	0.91	5/1542 (0.3%)	0.92	3/2083 (0.1%)
6	H	0.86	0/1539	0.95	8/2073 (0.4%)
7	K	0.47	0/2098	0.75	0/2830
8	L	1.08	2/1524 (0.1%)	1.12	13/2046 (0.6%)
9	M	1.04	3/1074 (0.3%)	0.98	6/1446 (0.4%)
10	N	1.49	12/1575 (0.8%)	1.28	29/2106 (1.4%)
11	O	1.51	13/1585 (0.8%)	1.11	13/2128 (0.6%)
12	P	1.35	12/1419 (0.8%)	1.06	9/1904 (0.5%)
13	Q	1.10	1/1050 (0.1%)	1.06	8/1419 (0.6%)
14	R	0.69	0/1275	0.91	7/1702 (0.4%)
15	S	1.01	1/1473 (0.1%)	1.01	9/1980 (0.5%)
16	T	0.44	0/440	0.93	2/594 (0.3%)
17	U	0.56	0/861	0.73	0/1167
18	V	0.68	0/1018	0.89	2/1369 (0.1%)
19	W	0.50	0/1918	0.81	0/2586
20	X	1.18	3/1116 (0.3%)	0.93	4/1503 (0.3%)
21	Y	1.17	2/1004 (0.2%)	1.06	7/1341 (0.5%)
22	Z	0.54	0/1118	0.78	2/1497 (0.1%)
23	a	0.80	0/751	0.96	3/1013 (0.3%)
24	b	0.57	1/3885 (0.0%)	0.85	6/5242 (0.1%)
25	c	0.43	0/751	0.72	0/1008
26	d	1.00	1/887 (0.1%)	0.98	4/1191 (0.3%)
27	e	1.40	7/1041 (0.7%)	1.09	10/1394 (0.7%)
28	f	1.72	7/868 (0.8%)	1.25	12/1168 (1.0%)
29	g	0.80	0/891	1.07	8/1191 (0.7%)
30	h	1.12	0/978	1.03	2/1301 (0.2%)
31	i	0.73	0/778	0.91	2/1034 (0.2%)
32	j	1.49	8/696 (1.1%)	1.34	10/923 (1.1%)
33	k	0.64	0/618	0.89	0/826
34	l	0.69	0/443	1.12	4/588 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	n	0.74	0/3101	0.91	12/4187 (0.3%)
36	o	0.55	0/1129	0.84	0/1502
37	q	0.47	0/733	0.90	4/977 (0.4%)
38	r	0.63	0/1789	0.91	3/2389 (0.1%)
39	s	0.70	0/301	1.15	3/386 (0.8%)
40	t	0.54	0/2333	0.89	3/3128 (0.1%)
41	u	0.72	0/1061	0.99	6/1410 (0.4%)
42	y	0.52	0/1872	0.79	2/2548 (0.1%)
43	z	0.58	0/445	0.89	0/585
44	1	1.93	1801/60703 (3.0%)	1.96	3153/94630 (3.3%)
45	2	2.45	221/3746 (5.9%)	2.31	330/5832 (5.7%)
46	6	0.96	1/1527 (0.1%)	1.50	26/2371 (1.1%)
47	w	0.46	0/2952	0.76	0/3965
All	All	1.55	2126/126942 (1.7%)	1.61	3781/184739 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	7
2	C	0	6
4	F	0	2
5	G	0	5
6	H	0	3
7	K	0	1
8	L	0	5
9	M	0	1
10	N	0	1
12	P	0	1
14	R	0	1
15	S	0	2
18	V	0	1
19	W	0	2
20	X	0	1
23	a	0	2
24	b	0	3
26	d	0	1
27	e	0	1
28	f	0	2
29	g	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	h	0	3
31	i	0	2
33	k	0	2
35	n	0	11
36	o	0	5
37	q	0	1
38	r	0	1
39	s	0	1
40	t	0	5
41	u	0	2
42	y	0	1
47	w	0	2
All	All	0	86

All (2126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	346	C	N1-C6	-13.06	1.29	1.37
44	1	945	C	C4-C5	-12.55	1.32	1.43
44	1	1437	C	C4-C5	-12.42	1.33	1.43
44	1	1332	A	N7-C5	-12.41	1.31	1.39
44	1	407	A	N9-C4	-12.35	1.30	1.37
44	1	1432	C	N1-C6	-12.07	1.29	1.37
45	2	105	A	N7-C5	-11.84	1.32	1.39
44	1	1381	A	N9-C4	-11.44	1.30	1.37
44	1	1419	A	N9-C4	-11.36	1.31	1.37
44	1	1426	C	C4-C5	-11.30	1.33	1.43
45	2	21	C	C4-C5	-11.06	1.34	1.43
44	1	344	A	N7-C5	-11.02	1.32	1.39
44	1	342	A	N9-C4	-10.87	1.31	1.37
44	1	630	A	C5-C6	-10.84	1.31	1.41
44	1	352	A	C6-N6	-10.64	1.25	1.33
44	1	27	C	C4-C5	-10.55	1.34	1.43
44	1	3004	C	C4-C5	-10.54	1.34	1.43
44	1	1435	A	N9-C4	-10.53	1.31	1.37
44	1	54	C	C4-C5	-10.49	1.34	1.43
44	1	1444	G	N7-C5	-10.44	1.32	1.39
44	1	1175	C	N1-C6	-10.39	1.30	1.37
44	1	1175	C	C4-C5	-10.27	1.34	1.43
44	1	634	C	C4-C5	-10.13	1.34	1.43
44	1	656	A	N7-C5	-10.13	1.33	1.39
44	1	29	C	C4-C5	-10.13	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1376	C	C4-C5	-10.05	1.34	1.43
44	1	1165	A	C6-N6	-10.03	1.25	1.33
44	1	334	A	N9-C4	-10.03	1.31	1.37
44	1	1161	G	N7-C5	-10.02	1.33	1.39
44	1	660	A	N9-C4	-9.96	1.31	1.37
45	2	44	A	C6-N6	-9.96	1.25	1.33
44	1	630	A	N7-C5	-9.89	1.33	1.39
44	1	1150	A	N7-C5	-9.88	1.33	1.39
44	1	1372	C	C4-C5	-9.86	1.35	1.43
44	1	1423	C	C4-C5	-9.85	1.35	1.43
45	2	19	C	C4-C5	-9.82	1.35	1.43
44	1	633	C	C4-C5	-9.80	1.35	1.43
44	1	944	C	N1-C6	-9.80	1.31	1.37
44	1	340	C	C4-C5	-9.75	1.35	1.43
44	1	346	C	C4-C5	-9.73	1.35	1.43
45	2	14	C	C4-C5	-9.73	1.35	1.43
44	1	3137	C	C4-C5	-9.72	1.35	1.43
44	1	345	G	N7-C5	-9.67	1.33	1.39
44	1	347	G	N7-C5	-9.66	1.33	1.39
44	1	655	C	C4-C5	-9.66	1.35	1.43
44	1	2354	C	C4-C5	-9.65	1.35	1.43
44	1	1424	C	C4-C5	-9.63	1.35	1.43
44	1	1332	A	C5-C6	-9.61	1.32	1.41
44	1	344	A	C5-C6	-9.56	1.32	1.41
44	1	1333	C	C4-C5	-9.52	1.35	1.43
44	1	1342	C	C4-C5	-9.42	1.35	1.43
44	1	1614	C	C4-C5	-9.41	1.35	1.43
44	1	65	A	N9-C4	-9.38	1.32	1.37
44	1	16	A	C5-C6	-9.36	1.32	1.41
45	2	13	A	N7-C5	-9.36	1.33	1.39
44	1	801	A	N7-C5	-9.31	1.33	1.39
44	1	409	A	C6-N6	-9.31	1.26	1.33
44	1	58	G	N7-C5	-9.30	1.33	1.39
44	1	680	G	N9-C8	-9.28	1.31	1.37
44	1	1170	A	N7-C5	-9.28	1.33	1.39
44	1	1836	C	C4-C5	-9.24	1.35	1.43
44	1	106	A	C6-N6	-9.23	1.26	1.33
44	1	1328	C	N1-C6	-9.20	1.31	1.37
44	1	408	A	N9-C4	-9.17	1.32	1.37
44	1	323	A	N7-C5	-9.13	1.33	1.39
45	2	40	A	N9-C4	-9.13	1.32	1.37
44	1	31	C	C4-C5	-9.09	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	350	C	C4-C5	-9.08	1.35	1.43
44	1	1496	C	C4-C5	-9.04	1.35	1.43
44	1	396	A	C6-N6	-9.03	1.26	1.33
44	1	332	C	C4-C5	-9.02	1.35	1.43
44	1	1420	C	C4-C5	-9.02	1.35	1.43
44	1	3008	A	C6-N6	-9.01	1.26	1.33
45	2	40	A	C6-N6	-8.98	1.26	1.33
44	1	665	A	N9-C4	-8.98	1.32	1.37
44	1	696	C	C4-C5	-8.96	1.35	1.43
45	2	12	A	N9-C4	-8.96	1.32	1.37
45	2	96	A	C6-N6	-8.96	1.26	1.33
44	1	660	A	N3-C4	-8.96	1.29	1.34
44	1	323	A	C5-C6	-8.96	1.32	1.41
44	1	1434	G	N7-C5	-8.95	1.33	1.39
44	1	51	A	N9-C4	-8.95	1.32	1.37
44	1	3046	A	N9-C4	-8.94	1.32	1.37
44	1	1426	C	N3-C4	-8.94	1.27	1.33
44	1	407	A	C6-N6	-8.90	1.26	1.33
44	1	28	C	N1-C6	-8.89	1.31	1.37
44	1	342	A	N9-C8	-8.87	1.30	1.37
44	1	1312	C	N1-C6	-8.86	1.31	1.37
45	2	40	A	C6-N1	-8.86	1.29	1.35
44	1	344	A	C6-N6	-8.86	1.26	1.33
44	1	947	G	N7-C5	-8.85	1.33	1.39
44	1	341	G	N7-C5	-8.83	1.33	1.39
44	1	504	A	N9-C4	-8.83	1.32	1.37
44	1	1338	C	C4-C5	-8.82	1.35	1.43
45	2	26	U	C4-C5	-8.79	1.35	1.43
44	1	1383	G	N7-C5	-8.79	1.33	1.39
44	1	349	A	N9-C4	-8.79	1.32	1.37
44	1	1146	C	C4-C5	-8.79	1.35	1.43
44	1	375	A	N9-C4	-8.79	1.32	1.37
44	1	1446	A	N9-C4	-8.77	1.32	1.37
44	1	1298	C	C4-C5	-8.76	1.35	1.43
44	1	1428	A	C6-N6	-8.76	1.26	1.33
44	1	1403	C	C4-C5	-8.76	1.35	1.43
44	1	16	A	N9-C4	-8.74	1.32	1.37
44	1	363	G	N7-C5	-8.74	1.34	1.39
44	1	20	A	N9-C4	-8.71	1.32	1.37
44	1	1158	A	N7-C5	-8.70	1.34	1.39
45	2	103	G	N7-C5	-8.67	1.34	1.39
44	1	1160	C	C4-C5	-8.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	16	A	N7-C5	-8.64	1.34	1.39
44	1	1338	C	N1-C6	-8.63	1.31	1.37
45	2	28	C	C4-C5	-8.63	1.36	1.43
44	1	1179	A	C6-N6	-8.60	1.27	1.33
44	1	1338	C	N3-C4	-8.59	1.27	1.33
44	1	810	A	N9-C4	-8.59	1.32	1.37
44	1	3150	A	N9-C4	-8.59	1.32	1.37
44	1	52	A	C6-N6	-8.58	1.27	1.33
44	1	1310	G	N9-C4	-8.57	1.31	1.38
44	1	349	A	C5-C6	-8.57	1.33	1.41
44	1	663	C	C4-C5	-8.56	1.36	1.43
44	1	1377	G	C2-N2	-8.55	1.26	1.34
44	1	346	C	C5-C6	-8.53	1.27	1.34
44	1	801	A	C6-N6	-8.52	1.27	1.33
44	1	972	A	N9-C4	-8.49	1.32	1.37
44	1	1437	C	N3-C4	-8.49	1.28	1.33
44	1	1615	C	C4-C5	-8.47	1.36	1.43
44	1	944	C	C4-C5	-8.46	1.36	1.43
44	1	1177	G	N9-C8	-8.46	1.31	1.37
44	1	589	A	C6-N6	-8.45	1.27	1.33
44	1	695	C	C4-C5	-8.44	1.36	1.43
44	1	2367	A	N9-C4	-8.43	1.32	1.37
44	1	77	A	N9-C4	-8.43	1.32	1.37
45	2	141	C	N3-C4	-8.43	1.28	1.33
44	1	941	G	N9-C8	-8.42	1.31	1.37
44	1	691	A	N9-C4	-8.39	1.32	1.37
44	1	1147	G	N7-C5	-8.38	1.34	1.39
44	1	350	C	C5-C6	-8.38	1.27	1.34
44	1	428	A	C6-N6	-8.37	1.27	1.33
44	1	56	G	N9-C4	-8.36	1.31	1.38
44	1	3379	C	C4-C5	-8.36	1.36	1.43
44	1	1317	A	N9-C4	-8.34	1.32	1.37
44	1	2356	A	N9-C4	-8.34	1.32	1.37
44	1	1594	A	C6-N6	-8.33	1.27	1.33
44	1	23	A	N9-C4	-8.32	1.32	1.37
45	2	137	C	C4-C5	-8.32	1.36	1.43
44	1	1613	A	N9-C4	-8.30	1.32	1.37
44	1	1363	A	C5-C6	-8.28	1.33	1.41
44	1	803	C	C4-C5	-8.27	1.36	1.43
44	1	1416	C	C4-C5	-8.26	1.36	1.43
44	1	409	A	N9-C8	-8.25	1.31	1.37
45	2	43	A	N9-C4	-8.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	120	C	C4-C5	-8.25	1.36	1.43
44	1	27	C	C5-C6	-8.23	1.27	1.34
44	1	1420	C	N1-C6	-8.23	1.32	1.37
44	1	656	A	C6-N6	-8.23	1.27	1.33
45	2	105	A	C5-C6	-8.22	1.33	1.41
44	1	82	C	C4-C5	-8.21	1.36	1.43
44	1	63	A	N7-C5	-8.21	1.34	1.39
44	1	1428	A	C5-C6	-8.21	1.33	1.41
44	1	225	C	C4-C5	-8.20	1.36	1.43
44	1	658	G	N7-C5	-8.19	1.34	1.39
45	2	42	G	N9-C4	-8.18	1.31	1.38
44	1	407	A	C5-C6	-8.17	1.33	1.41
44	1	60	A	N7-C5	-8.16	1.34	1.39
44	1	349	A	N7-C5	-8.16	1.34	1.39
44	1	928	C	C4-C5	-8.15	1.36	1.43
44	1	692	A	N9-C4	-8.15	1.32	1.37
44	1	804	C	C4-C5	-8.15	1.36	1.43
44	1	1337	A	N9-C4	-8.15	1.32	1.37
44	1	433	A	C6-N6	-8.14	1.27	1.33
44	1	65	A	N9-C8	-8.14	1.31	1.37
44	1	1422	G	N7-C5	-8.14	1.34	1.39
45	2	45	C	C4-C5	-8.12	1.36	1.43
44	1	1175	C	N3-C4	-8.12	1.28	1.33
44	1	224	C	C4-C5	-8.10	1.36	1.43
44	1	693	A	N9-C4	-8.10	1.32	1.37
45	2	105	A	N9-C8	-8.08	1.31	1.37
44	1	1836	C	N3-C4	-8.07	1.28	1.33
44	1	3273	A	C6-N6	-8.07	1.27	1.33
44	1	657	A	N9-C4	-8.07	1.33	1.37
44	1	348	A	N7-C5	-8.06	1.34	1.39
44	1	1179	A	C5-C6	-8.04	1.33	1.41
44	1	931	C	C4-C5	-8.04	1.36	1.43
44	1	1396	C	C4-C5	-8.03	1.36	1.43
44	1	28	C	N3-C4	-8.03	1.28	1.33
44	1	3173	G	C2-N2	-8.02	1.26	1.34
44	1	427	C	C4-C5	-8.02	1.36	1.43
44	1	660	A	N7-C5	-8.01	1.34	1.39
44	1	28	C	C4-C5	-8.00	1.36	1.43
44	1	1165	A	N9-C4	-8.00	1.33	1.37
44	1	1179	A	N9-C4	-8.00	1.33	1.37
44	1	1446	A	C6-N6	-7.99	1.27	1.33
44	1	34	A	N9-C4	-7.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	672	A	N9-C4	-7.97	1.33	1.37
44	1	64	G	N9-C8	-7.96	1.32	1.37
45	2	35	C	C4-C5	-7.96	1.36	1.43
44	1	2367	A	C6-N6	-7.95	1.27	1.33
44	1	2352	A	N9-C4	-7.94	1.33	1.37
44	1	1404	G	N9-C4	-7.94	1.31	1.38
44	1	111	C	N1-C6	-7.93	1.32	1.37
44	1	349	A	C6-N6	-7.92	1.27	1.33
44	1	344	A	N9-C4	-7.92	1.33	1.37
44	1	628	A	C6-N6	-7.91	1.27	1.33
44	1	1178	G	N9-C8	-7.91	1.32	1.37
44	1	1496	C	N3-C4	-7.90	1.28	1.33
44	1	1527	C	C4-C5	-7.89	1.36	1.43
44	1	1397	C	C4-C5	-7.87	1.36	1.43
44	1	322	U	C4-C5	-7.87	1.36	1.43
44	1	3139	A	N7-C5	-7.86	1.34	1.39
45	2	142	C	C4-C5	-7.86	1.36	1.43
44	1	808	A	N9-C4	-7.83	1.33	1.37
45	2	13	A	C6-N6	-7.83	1.27	1.33
45	2	104	A	N7-C5	-7.83	1.34	1.39
44	1	949	C	C4-C5	-7.83	1.36	1.43
44	1	226	C	N1-C6	-7.81	1.32	1.37
44	1	1170	A	C5-C6	-7.81	1.34	1.41
44	1	3183	A	C5-C6	-7.80	1.34	1.41
45	2	104	A	N9-C4	-7.79	1.33	1.37
44	1	368	G	N9-C4	-7.76	1.31	1.38
44	1	1159	A	N7-C5	-7.76	1.34	1.39
44	1	945	C	N3-C4	-7.74	1.28	1.33
45	2	17	A	N7-C5	-7.73	1.34	1.39
44	1	1363	A	C6-N6	-7.73	1.27	1.33
44	1	1420	C	C5-C6	-7.72	1.28	1.34
44	1	12	A	N7-C5	-7.72	1.34	1.39
28	f	102	LEU	C-N	-7.72	1.16	1.34
44	1	933	A	C5-C6	-7.71	1.34	1.41
44	1	428	A	C5-C6	-7.71	1.34	1.41
44	1	663	C	C5-C6	-7.71	1.28	1.34
44	1	500	C	C4-C5	-7.70	1.36	1.43
44	1	1496	C	C5-C6	-7.70	1.28	1.34
44	1	1602	A	N9-C4	-7.69	1.33	1.37
44	1	345	G	N9-C8	-7.69	1.32	1.37
44	1	369	A	C5-C6	-7.68	1.34	1.41
44	1	1308	A	C6-N6	-7.68	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	2910	A	C6-N6	-7.68	1.27	1.33
44	1	971	G	N9-C4	-7.68	1.31	1.38
44	1	927	C	C4-C5	-7.67	1.36	1.43
44	1	338	A	C6-N6	-7.67	1.27	1.33
12	P	119	VAL	CB-CG2	-7.66	1.36	1.52
44	1	353	G	C2-N3	-7.66	1.26	1.32
44	1	653	A	N7-C5	-7.65	1.34	1.39
44	1	340	C	N1-C6	-7.64	1.32	1.37
44	1	670	C	C4-C5	-7.62	1.36	1.43
44	1	693	A	C6-N6	-7.61	1.27	1.33
44	1	371	G	N9-C8	-7.61	1.32	1.37
44	1	1440	G	N9-C8	-7.61	1.32	1.37
44	1	3008	A	C5-C6	-7.61	1.34	1.41
44	1	3308	C	C4-C5	-7.60	1.36	1.43
44	1	654	C	C4-C5	-7.59	1.36	1.43
44	1	2355	G	N9-C4	-7.59	1.31	1.38
45	2	43	A	C5-C6	-7.59	1.34	1.41
44	1	22	G	N9-C8	-7.58	1.32	1.37
44	1	64	G	N7-C5	-7.58	1.34	1.39
44	1	353	G	N9-C4	-7.57	1.31	1.38
44	1	665	A	C5-C6	-7.56	1.34	1.41
44	1	1598	G	N7-C5	-7.56	1.34	1.39
44	1	339	C	N1-C6	-7.55	1.32	1.37
44	1	1333	C	N3-C4	-7.55	1.28	1.33
44	1	363	G	N9-C8	-7.55	1.32	1.37
45	2	97	A	N9-C4	-7.54	1.33	1.37
44	1	630	A	C6-N6	-7.54	1.27	1.33
44	1	1176	C	N1-C6	-7.54	1.32	1.37
45	2	36	G	N7-C5	-7.53	1.34	1.39
45	2	37	A	N9-C4	-7.53	1.33	1.37
12	P	119	VAL	CB-CG1	-7.53	1.37	1.52
44	1	63	A	C6-N6	-7.53	1.27	1.33
44	1	29	C	N1-C6	-7.52	1.32	1.37
45	2	10	A	N7-C5	-7.51	1.34	1.39
44	1	1420	C	C4-N4	-7.51	1.27	1.33
45	2	21	C	N3-C4	-7.50	1.28	1.33
44	1	2357	A	N9-C4	-7.50	1.33	1.37
45	2	44	A	C5-C6	-7.50	1.34	1.41
44	1	1187	C	N3-C4	-7.49	1.28	1.33
45	2	105	A	C6-N6	-7.49	1.27	1.33
45	2	40	A	N3-C4	-7.48	1.30	1.34
45	2	30	C	C4-C5	-7.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	667	C	C4-C5	-7.47	1.36	1.43
44	1	321	C	C4-C5	-7.46	1.36	1.43
44	1	356	C	N1-C6	-7.46	1.32	1.37
44	1	1339	C	C4-C5	-7.46	1.36	1.43
44	1	3008	A	N9-C4	-7.46	1.33	1.37
44	1	943	U	N3-C4	-7.44	1.31	1.38
44	1	60	A	C5-C6	-7.43	1.34	1.41
44	1	1439	U	C4-C5	-7.43	1.36	1.43
44	1	69	C	N3-C4	-7.42	1.28	1.33
44	1	86	G	C2-N3	-7.41	1.26	1.32
44	1	657	A	C6-N6	-7.39	1.28	1.33
44	1	3273	A	N9-C4	-7.39	1.33	1.37
44	1	1437	C	C5-C6	-7.39	1.28	1.34
44	1	1332	A	C8-N7	-7.38	1.26	1.31
27	e	28	VAL	CB-CG2	-7.37	1.37	1.52
44	1	1363	A	N7-C5	-7.37	1.34	1.39
44	1	3097	C	C4-C5	-7.37	1.37	1.43
45	2	22	U	N1-C6	-7.36	1.31	1.38
44	1	27	C	N1-C6	-7.35	1.32	1.37
44	1	144	A	C6-N6	-7.35	1.28	1.33
44	1	611	A	N9-C4	-7.35	1.33	1.37
45	2	104	A	N9-C8	-7.35	1.31	1.37
44	1	52	A	C5-C6	-7.35	1.34	1.41
44	1	106	A	C6-N1	-7.34	1.30	1.35
44	1	321	C	N1-C6	-7.34	1.32	1.37
44	1	31	C	N3-C4	-7.34	1.28	1.33
44	1	416	A	N9-C4	-7.34	1.33	1.37
45	2	115	C	C4-C5	-7.33	1.37	1.43
44	1	638	C	C4-C5	-7.33	1.37	1.43
44	1	1406	A	C6-N6	-7.33	1.28	1.33
44	1	1150	A	C5-C6	-7.33	1.34	1.41
44	1	1609	C	C4-C5	-7.32	1.37	1.43
44	1	792	G	N7-C5	-7.32	1.34	1.39
44	1	58	G	C5-C6	-7.32	1.35	1.42
44	1	407	A	N7-C5	-7.32	1.34	1.39
44	1	661	G	N9-C4	-7.31	1.32	1.38
44	1	81	C	C4-C5	-7.31	1.37	1.43
44	1	367	A	C6-N6	-7.31	1.28	1.33
44	1	1402	C	C4-C5	-7.30	1.37	1.43
44	1	656	A	C5-C6	-7.29	1.34	1.41
44	1	102	C	C4-C5	-7.29	1.37	1.43
44	1	586	C	C4-C5	-7.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	336	A	N7-C5	-7.29	1.34	1.39
44	1	334	A	N7-C5	-7.28	1.34	1.39
44	1	10	C	C4-C5	-7.27	1.37	1.43
44	1	369	A	N9-C8	-7.27	1.31	1.37
44	1	1179	A	N7-C5	-7.27	1.34	1.39
44	1	327	A	N9-C4	-7.27	1.33	1.37
44	1	652	G	N9-C8	-7.27	1.32	1.37
44	1	366	A	N7-C5	-7.26	1.34	1.39
44	1	933	A	N9-C4	-7.26	1.33	1.37
44	1	353	G	C2-N2	-7.26	1.27	1.34
44	1	373	A	C5-C6	-7.26	1.34	1.41
44	1	1163	A	C5-C6	-7.25	1.34	1.41
44	1	805	G	N9-C8	-7.25	1.32	1.37
44	1	1373	A	N9-C4	-7.24	1.33	1.37
44	1	1614	C	N3-C4	-7.24	1.28	1.33
44	1	341	G	N9-C8	-7.24	1.32	1.37
45	2	20	U	C4-C5	-7.24	1.37	1.43
44	1	2352	A	N7-C5	-7.24	1.34	1.39
44	1	1147	G	N9-C8	-7.23	1.32	1.37
44	1	1419	A	C6-N6	-7.23	1.28	1.33
44	1	1155	C	N3-C4	-7.23	1.28	1.33
44	1	1337	A	C5-C6	-7.23	1.34	1.41
45	2	94	C	C4-C5	-7.23	1.37	1.43
44	1	585	A	N9-C4	-7.22	1.33	1.37
44	1	3141	A	C5-C6	-7.22	1.34	1.41
45	2	32	C	C4-C5	-7.22	1.37	1.43
45	2	48	A	N9-C4	-7.22	1.33	1.37
45	2	92	A	N9-C4	-7.22	1.33	1.37
44	1	409	A	N7-C5	-7.22	1.34	1.39
44	1	345	G	N1-C2	-7.21	1.31	1.37
44	1	1426	C	C4-N4	-7.21	1.27	1.33
45	2	41	A	N9-C8	-7.21	1.31	1.37
44	1	633	C	C4-N4	-7.20	1.27	1.33
44	1	1377	G	N9-C4	-7.20	1.32	1.38
45	2	108	C	N1-C6	-7.20	1.32	1.37
44	1	27	C	N3-C4	-7.19	1.28	1.33
44	1	504	A	C5-C6	-7.18	1.34	1.41
44	1	1326	A	C6-N6	-7.18	1.28	1.33
44	1	1183	C	C4-C5	-7.18	1.37	1.43
45	2	65	A	N9-C4	-7.17	1.33	1.37
44	1	585	A	C6-N6	-7.16	1.28	1.33
44	1	802	C	C4-C5	-7.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	17	G	N9-C8	-7.16	1.32	1.37
44	1	927	C	N1-C6	-7.16	1.32	1.37
44	1	3139	A	C5-C6	-7.16	1.34	1.41
44	1	63	A	N9-C4	-7.16	1.33	1.37
44	1	1407	A	C6-N6	-7.16	1.28	1.33
44	1	2366	C	C4-C5	-7.16	1.37	1.43
45	2	41	A	N9-C4	-7.16	1.33	1.37
44	1	680	G	N9-C4	-7.16	1.32	1.38
44	1	693	A	C5-C6	-7.16	1.34	1.41
44	1	349	A	N9-C8	-7.15	1.32	1.37
44	1	1365	G	N9-C8	-7.15	1.32	1.37
44	1	585	A	N7-C5	-7.15	1.34	1.39
44	1	107	A	N9-C8	-7.15	1.32	1.37
45	2	19	C	C5-C6	-7.14	1.28	1.34
44	1	396	A	N9-C4	-7.14	1.33	1.37
44	1	341	G	C5-C6	-7.13	1.35	1.42
44	1	334	A	C6-N6	-7.13	1.28	1.33
44	1	815	G	N7-C5	-7.13	1.34	1.39
44	1	1337	A	C6-N6	-7.13	1.28	1.33
44	1	1155	C	C4-C5	-7.12	1.37	1.43
44	1	1437	C	C4-N4	-7.12	1.27	1.33
44	1	405	U	C4-C5	-7.12	1.37	1.43
44	1	266	A	N9-C4	-7.12	1.33	1.37
44	1	1163	A	N9-C4	-7.11	1.33	1.37
45	2	13	A	C5-C6	-7.11	1.34	1.41
44	1	663	C	N1-C6	-7.11	1.32	1.37
44	1	373	A	C6-N6	-7.10	1.28	1.33
44	1	352	A	C5-C4	-7.10	1.33	1.38
44	1	3211	C	C4-C5	-7.10	1.37	1.43
44	1	639	G	N9-C8	-7.10	1.32	1.37
44	1	1558	A	C6-N6	-7.10	1.28	1.33
44	1	369	A	C6-N6	-7.09	1.28	1.33
44	1	1546	A	N9-C4	-7.09	1.33	1.37
44	1	3375	A	N7-C5	-7.09	1.34	1.39
45	2	140	G	N9-C8	-7.09	1.32	1.37
44	1	1509	A	N9-C4	-7.09	1.33	1.37
44	1	289	A	N7-C5	-7.08	1.34	1.39
44	1	62	A	N7-C5	-7.08	1.35	1.39
44	1	948	C	C4-C5	-7.08	1.37	1.43
44	1	20	A	N9-C8	-7.08	1.32	1.37
44	1	633	C	N1-C6	-7.08	1.32	1.37
45	2	40	A	N7-C5	-7.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	141	C	C4-N4	-7.08	1.27	1.33
44	1	1698	C	C4-C5	-7.08	1.37	1.43
44	1	793	C	C4-C5	-7.08	1.37	1.43
44	1	3296	A	N9-C4	-7.07	1.33	1.37
44	1	3139	A	N9-C8	-7.07	1.32	1.37
27	e	17	PHE	CD1-CE1	-7.07	1.25	1.39
44	1	1419	A	C5-C6	-7.07	1.34	1.41
44	1	1435	A	N7-C5	-7.06	1.35	1.39
45	2	15	G	N9-C8	-7.06	1.32	1.37
44	1	1160	C	N1-C6	-7.05	1.32	1.37
44	1	3137	C	N3-C4	-7.05	1.29	1.33
44	1	3006	A	N7-C5	-7.05	1.35	1.39
44	1	331	G	N7-C5	-7.05	1.35	1.39
44	1	659	G	N7-C5	-7.05	1.35	1.39
44	1	396	A	C5-C6	-7.04	1.34	1.41
44	1	500	C	N3-C4	-7.04	1.29	1.33
32	j	37	CYS	CB-SG	-7.04	1.70	1.82
44	1	375	A	C6-N6	-7.04	1.28	1.33
44	1	368	G	N9-C8	-7.04	1.32	1.37
44	1	2910	A	N9-C4	-7.04	1.33	1.37
44	1	1394	A	N9-C4	-7.03	1.33	1.37
44	1	3139	A	C6-N6	-7.03	1.28	1.33
44	1	26	A	N9-C4	-7.03	1.33	1.37
44	1	377	A	N9-C4	-7.03	1.33	1.37
44	1	1314	C	N1-C6	-7.03	1.32	1.37
44	1	2354	C	C5-C6	-7.03	1.28	1.34
44	1	1435	A	C6-N6	-7.02	1.28	1.33
44	1	409	A	C5-C6	-7.02	1.34	1.41
44	1	109	A	N9-C4	-7.01	1.33	1.37
44	1	12	A	C5-C6	-7.01	1.34	1.41
44	1	3186	A	N9-C4	-7.01	1.33	1.37
44	1	3187	A	N7-C5	-7.00	1.35	1.39
44	1	344	A	C5-C4	-7.00	1.33	1.38
44	1	947	G	N9-C8	-7.00	1.32	1.37
44	1	804	C	C5-C6	-7.00	1.28	1.34
44	1	54	C	C5-C6	-6.99	1.28	1.34
44	1	804	C	N1-C6	-6.99	1.32	1.37
44	1	1194	G	C6-N1	-6.98	1.34	1.39
44	1	1443	G	N7-C5	-6.98	1.35	1.39
44	1	100	A	N7-C5	-6.98	1.35	1.39
44	1	3183	A	N9-C4	-6.97	1.33	1.37
44	1	200	C	N1-C6	-6.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1401	A	C5-C6	-6.97	1.34	1.41
44	1	1432	C	C4-C5	-6.97	1.37	1.43
45	2	40	A	N1-C2	-6.97	1.28	1.34
44	1	1296	C	C4-C5	-6.96	1.37	1.43
45	2	57	C	C4-C5	-6.96	1.37	1.43
44	1	57	A	N9-C4	-6.96	1.33	1.37
44	1	334	A	C5-C6	-6.96	1.34	1.41
44	1	107	A	C5-C6	-6.95	1.34	1.41
44	1	655	C	C5-C6	-6.95	1.28	1.34
45	2	10	A	C5-C6	-6.95	1.34	1.41
44	1	296	A	C6-N6	-6.95	1.28	1.33
44	1	649	A	N7-C5	-6.95	1.35	1.39
44	1	1181	U	C2-N3	-6.95	1.32	1.37
44	1	364	G	C2-N2	-6.95	1.27	1.34
44	1	1522	U	C2-N3	-6.95	1.32	1.37
44	1	1330	A	C5-C6	-6.94	1.34	1.41
44	1	788	C	C4-C5	-6.93	1.37	1.43
44	1	353	G	N1-C2	-6.92	1.32	1.37
44	1	60	A	N9-C8	-6.92	1.32	1.37
44	1	320	G	N9-C8	-6.92	1.33	1.37
44	1	1165	A	C5-C6	-6.92	1.34	1.41
45	2	18	U	C4-C5	-6.91	1.37	1.43
44	1	226	C	C4-C5	-6.91	1.37	1.43
44	1	803	C	N3-C4	-6.91	1.29	1.33
44	1	1332	A	C6-N6	-6.90	1.28	1.33
45	2	47	C	N1-C6	-6.90	1.33	1.37
45	2	96	A	N9-C4	-6.90	1.33	1.37
44	1	1307	G	N7-C5	-6.90	1.35	1.39
44	1	26	A	N7-C5	-6.89	1.35	1.39
44	1	628	A	C5-C6	-6.89	1.34	1.41
45	2	16	G	N9-C4	-6.89	1.32	1.38
44	1	410	U	C4-C5	-6.88	1.37	1.43
11	O	80	PHE	CB-CG	-6.87	1.39	1.51
44	1	672	A	N7-C5	-6.87	1.35	1.39
44	1	788	C	N1-C6	-6.87	1.33	1.37
44	1	701	G	N7-C5	-6.86	1.35	1.39
44	1	700	C	N1-C6	-6.86	1.33	1.37
45	2	9	A	N7-C5	-6.86	1.35	1.39
44	1	8	C	C4-C5	-6.86	1.37	1.43
44	1	102	C	N1-C6	-6.86	1.33	1.37
44	1	3004	C	C5-C6	-6.86	1.28	1.34
44	1	662	U	C2-N3	-6.85	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	23	VAL	CB-CG2	-6.85	1.38	1.52
45	2	105	A	C5-C4	-6.84	1.33	1.38
45	2	41	A	N7-C5	-6.84	1.35	1.39
44	1	65	A	C5-C4	-6.84	1.33	1.38
44	1	1173	U	C4-C5	-6.84	1.37	1.43
45	2	92	A	N7-C5	-6.84	1.35	1.39
44	1	343	U	C2-N3	-6.83	1.32	1.37
44	1	661	G	C2-N3	-6.82	1.27	1.32
44	1	1376	C	N3-C4	-6.82	1.29	1.33
44	1	1171	G	N9-C8	-6.82	1.33	1.37
44	1	3089	C	C4-C5	-6.82	1.37	1.43
44	1	945	C	C4-N4	-6.81	1.27	1.33
44	1	200	C	C4-N4	-6.81	1.27	1.33
44	1	1162	U	C4-C5	-6.81	1.37	1.43
44	1	1397	C	N3-C4	-6.81	1.29	1.33
44	1	1429	G	N1-C2	-6.80	1.32	1.37
45	2	44	A	N7-C5	-6.80	1.35	1.39
44	1	920	A	C6-N6	-6.80	1.28	1.33
44	1	1444	G	C8-N7	-6.79	1.26	1.30
44	1	115	A	N9-C4	-6.79	1.33	1.37
44	1	665	A	N7-C5	-6.79	1.35	1.39
32	j	19	CYS	CB-SG	-6.79	1.70	1.82
45	2	13	A	N9-C4	-6.79	1.33	1.37
44	1	1165	A	C5-C4	-6.79	1.33	1.38
44	1	1321	G	N9-C8	-6.79	1.33	1.37
44	1	1797	A	C6-N6	-6.78	1.28	1.33
44	1	1327	C	N3-C4	-6.78	1.29	1.33
44	1	412	G	N7-C5	-6.78	1.35	1.39
44	1	3145	C	N1-C6	-6.78	1.33	1.37
44	1	47	C	C4-C5	-6.77	1.37	1.43
44	1	585	A	C5-C6	-6.76	1.34	1.41
44	1	1799	A	N9-C4	-6.76	1.33	1.37
44	1	3173	G	N1-C2	-6.76	1.32	1.37
44	1	35	A	N9-C4	-6.76	1.33	1.37
44	1	68	C	N1-C6	-6.75	1.33	1.37
44	1	1429	G	C2-N3	-6.75	1.27	1.32
44	1	1441	G	N9-C8	-6.75	1.33	1.37
44	1	665	A	C6-N6	-6.75	1.28	1.33
44	1	1158	A	C5-C6	-6.75	1.34	1.41
44	1	2360	C	C4-C5	-6.75	1.37	1.43
44	1	396	A	C5-C4	-6.75	1.34	1.38
44	1	941	G	N9-C4	-6.75	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	355	A	N9-C4	-6.74	1.33	1.37
44	1	1527	C	N3-C4	-6.74	1.29	1.33
45	2	58	G	N7-C5	-6.74	1.35	1.39
11	O	16	VAL	CB-CG2	-6.74	1.38	1.52
44	1	2353	G	N7-C5	-6.74	1.35	1.39
44	1	1330	A	N9-C4	-6.73	1.33	1.37
44	1	364	G	N9-C4	-6.73	1.32	1.38
44	1	1335	C	C4-C5	-6.73	1.37	1.43
44	1	656	A	N9-C8	-6.73	1.32	1.37
44	1	288	C	C4-C5	-6.72	1.37	1.43
44	1	936	A	C6-N6	-6.72	1.28	1.33
44	1	938	C	C4-C5	-6.72	1.37	1.43
44	1	353	G	N3-C4	-6.71	1.30	1.35
45	2	21	C	C5-C6	-6.71	1.28	1.34
44	1	107	A	N7-C5	-6.71	1.35	1.39
44	1	929	A	N9-C4	-6.71	1.33	1.37
44	1	1358	C	C4-C5	-6.71	1.37	1.43
45	2	37	A	N9-C8	-6.71	1.32	1.37
44	1	365	A	N7-C5	-6.71	1.35	1.39
44	1	1433	A	N9-C4	-6.71	1.33	1.37
44	1	1439	U	N1-C6	-6.71	1.31	1.38
44	1	222	A	N7-C5	-6.70	1.35	1.39
44	1	367	A	N9-C4	-6.70	1.33	1.37
44	1	1881	A	C5-C6	-6.69	1.35	1.41
44	1	1401	A	N9-C4	-6.69	1.33	1.37
45	2	4	C	C4-C5	-6.69	1.37	1.43
44	1	1379	G	N7-C5	-6.69	1.35	1.39
45	2	37	A	N7-C5	-6.69	1.35	1.39
1	B	220	VAL	CB-CG1	-6.69	1.38	1.52
44	1	372	A	N9-C4	-6.68	1.33	1.37
44	1	3008	A	N7-C5	-6.68	1.35	1.39
44	1	658	G	N9-C8	-6.68	1.33	1.37
44	1	3103	A	C6-N6	-6.67	1.28	1.33
44	1	105	C	N1-C6	-6.67	1.33	1.37
45	2	141	C	C4-C5	-6.67	1.37	1.43
44	1	291	C	C4-C5	-6.67	1.37	1.43
44	1	662	U	N3-C4	-6.66	1.32	1.38
44	1	349	A	C5-C4	-6.66	1.34	1.38
45	2	44	A	N9-C4	-6.66	1.33	1.37
44	1	56	G	N9-C8	-6.66	1.33	1.37
44	1	1176	C	N3-C4	-6.65	1.29	1.33
44	1	355	A	C6-N6	-6.65	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	3187	A	N9-C8	-6.65	1.32	1.37
44	1	324	A	C6-N6	-6.65	1.28	1.33
44	1	1297	C	C4-C5	-6.64	1.37	1.43
44	1	1423	C	N3-C4	-6.64	1.29	1.33
44	1	1178	G	N7-C5	-6.64	1.35	1.39
44	1	929	A	N7-C5	-6.64	1.35	1.39
44	1	3144	G	N9-C8	-6.64	1.33	1.37
28	f	98	VAL	CB-CG1	-6.63	1.39	1.52
44	1	342	A	C5-C6	-6.63	1.35	1.41
2	C	100	PHE	CB-CG	-6.63	1.40	1.51
44	1	267	G	N1-C2	-6.63	1.32	1.37
44	1	357	A	C5-C6	-6.63	1.35	1.41
44	1	685	G	N7-C5	-6.63	1.35	1.39
44	1	1459	C	N3-C4	-6.63	1.29	1.33
44	1	2352	A	N9-C8	-6.63	1.32	1.37
44	1	1319	G	N9-C4	-6.62	1.32	1.38
44	1	1194	G	N7-C5	-6.62	1.35	1.39
44	1	1372	C	N1-C6	-6.62	1.33	1.37
44	1	802	C	N1-C6	-6.62	1.33	1.37
44	1	1508	C	C4-C5	-6.62	1.37	1.43
44	1	3094	A	N9-C4	-6.62	1.33	1.37
44	1	1147	G	C6-N1	-6.61	1.34	1.39
44	1	1330	A	N9-C8	-6.61	1.32	1.37
44	1	1447	G	N9-C4	-6.61	1.32	1.38
44	1	330	G	N7-C5	-6.61	1.35	1.39
44	1	411	U	N1-C6	-6.61	1.32	1.38
44	1	399	A	N9-C4	-6.61	1.33	1.37
44	1	951	A	N7-C5	-6.60	1.35	1.39
44	1	11	A	C6-N6	-6.60	1.28	1.33
44	1	51	A	N7-C5	-6.60	1.35	1.39
44	1	1172	G	N3-C4	-6.60	1.30	1.35
44	1	1460	A	C5-C6	-6.60	1.35	1.41
44	1	222	A	C5-C6	-6.60	1.35	1.41
44	1	1156	C	C4-C5	-6.60	1.37	1.43
44	1	3274	A	N9-C4	-6.60	1.33	1.37
44	1	2367	A	C5-C6	-6.60	1.35	1.41
44	1	113	C	C4-C5	-6.59	1.37	1.43
44	1	1498	A	N7-C5	-6.59	1.35	1.39
44	1	3173	G	C2-N3	-6.59	1.27	1.32
44	1	3305	A	C6-N6	-6.59	1.28	1.33
44	1	3005	A	C5-C6	-6.59	1.35	1.41
44	1	215	G	N9-C4	-6.58	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1175	C	C4-N4	-6.58	1.28	1.33
44	1	1368	U	C4-C5	-6.58	1.37	1.43
45	2	42	G	N7-C5	-6.58	1.35	1.39
45	2	35	C	N3-C4	-6.58	1.29	1.33
44	1	295	A	N9-C4	-6.58	1.33	1.37
44	1	1369	A	N9-C4	-6.58	1.33	1.37
44	1	1426	C	C5-C6	-6.58	1.29	1.34
44	1	801	A	C5-C6	-6.58	1.35	1.41
44	1	920	A	N9-C4	-6.58	1.33	1.37
44	1	1175	C	C5-C6	-6.58	1.29	1.34
44	1	805	G	N9-C4	-6.57	1.32	1.38
44	1	339	C	N3-C4	-6.57	1.29	1.33
44	1	389	A	C6-N6	-6.57	1.28	1.33
44	1	611	A	C6-N6	-6.57	1.28	1.33
45	2	11	C	C4-C5	-6.57	1.37	1.43
44	1	123	A	N9-C4	-6.56	1.33	1.37
44	1	17	G	N7-C5	-6.56	1.35	1.39
44	1	406	G	N7-C5	-6.56	1.35	1.39
44	1	61	A	N7-C5	-6.56	1.35	1.39
44	1	3102	G	N7-C5	-6.55	1.35	1.39
44	1	1383	G	N9-C8	-6.55	1.33	1.37
44	1	2358	A	N7-C5	-6.55	1.35	1.39
44	1	2381	G	N9-C8	-6.54	1.33	1.37
44	1	354	U	C4-C5	-6.54	1.37	1.43
44	1	1377	G	N3-C4	-6.54	1.30	1.35
44	1	111	C	N3-C4	-6.54	1.29	1.33
44	1	1534	A	C6-N6	-6.54	1.28	1.33
44	1	406	G	C2-N3	-6.54	1.27	1.32
44	1	3094	A	C6-N6	-6.54	1.28	1.33
44	1	1510	G	C6-N1	-6.53	1.34	1.39
44	1	1799	A	C6-N6	-6.53	1.28	1.33
44	1	3126	C	N1-C6	-6.53	1.33	1.37
44	1	323	A	N9-C4	-6.53	1.33	1.37
44	1	58	G	C6-N1	-6.52	1.34	1.39
44	1	663	C	N3-C4	-6.51	1.29	1.33
44	1	405	U	N1-C6	-6.51	1.32	1.38
44	1	114	A	C5-C6	-6.50	1.35	1.41
2	C	25	VAL	CB-CG2	-6.50	1.39	1.52
44	1	110	G	N9-C8	-6.50	1.33	1.37
45	2	41	A	C6-N6	-6.50	1.28	1.33
44	1	369	A	N7-C5	-6.49	1.35	1.39
44	1	1328	C	C4-C5	-6.49	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	631	U	N1-C6	-6.49	1.32	1.38
44	1	632	G	N9-C8	-6.48	1.33	1.37
44	1	3243	A	N9-C4	-6.48	1.33	1.37
44	1	637	C	C4-C5	-6.48	1.37	1.43
44	1	1146	C	N1-C6	-6.48	1.33	1.37
44	1	1376	C	N1-C6	-6.48	1.33	1.37
44	1	942	U	C2-N3	-6.47	1.33	1.37
44	1	213	A	C6-N6	-6.47	1.28	1.33
44	1	345	G	C2-N2	-6.47	1.28	1.34
44	1	1459	C	C4-C5	-6.47	1.37	1.43
11	O	104	VAL	CB-CG2	-6.47	1.39	1.52
44	1	187	A	C6-N6	-6.46	1.28	1.33
44	1	632	G	N7-C5	-6.46	1.35	1.39
44	1	940	G	N7-C5	-6.46	1.35	1.39
44	1	353	G	C5-C4	-6.46	1.33	1.38
44	1	1170	A	C6-N6	-6.45	1.28	1.33
44	1	3040	A	N7-C5	-6.45	1.35	1.39
44	1	85	A	N9-C4	-6.45	1.33	1.37
44	1	31	C	C4-N4	-6.44	1.28	1.33
44	1	649	A	C6-N6	-6.44	1.28	1.33
44	1	3141	A	C6-N6	-6.44	1.28	1.33
44	1	3002	C	C4-C5	-6.44	1.37	1.43
44	1	1608	C	C4-C5	-6.43	1.37	1.43
45	2	24	G	N1-C2	-6.43	1.32	1.37
44	1	1393	A	N7-C5	-6.43	1.35	1.39
44	1	3178	A	N9-C4	-6.43	1.33	1.37
44	1	1187	C	N1-C6	-6.43	1.33	1.37
44	1	339	C	C4-C5	-6.43	1.37	1.43
44	1	352	A	C5-C6	-6.43	1.35	1.41
45	2	145	U	C4-C5	-6.43	1.37	1.43
45	2	65	A	C5-C6	-6.42	1.35	1.41
44	1	373	A	N9-C4	-6.42	1.33	1.37
44	1	3134	A	C6-N6	-6.42	1.28	1.33
45	2	43	A	N7-C5	-6.42	1.35	1.39
44	1	1360	C	C4-C5	-6.42	1.37	1.43
44	1	624	G	N7-C5	-6.42	1.35	1.39
44	1	693	A	N7-C5	-6.42	1.35	1.39
44	1	3121	U	N1-C6	-6.42	1.32	1.38
45	2	34	U	C4-C5	-6.42	1.37	1.43
45	2	91	C	C4-C5	-6.42	1.37	1.43
44	1	1145	G	N7-C5	-6.42	1.35	1.39
44	1	2383	C	C4-C5	-6.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	573	C	C4-C5	-6.41	1.37	1.43
45	2	25	G	N1-C2	-6.41	1.32	1.37
44	1	323	A	C6-N6	-6.41	1.28	1.33
44	1	1372	C	N3-C4	-6.41	1.29	1.33
44	1	1405	U	C4-C5	-6.41	1.37	1.43
11	O	118	VAL	CB-CG1	-6.40	1.39	1.52
44	1	1440	G	N7-C5	-6.40	1.35	1.39
44	1	1797	A	N9-C4	-6.40	1.34	1.37
44	1	3183	A	N7-C5	-6.40	1.35	1.39
44	1	389	A	N7-C5	-6.39	1.35	1.39
44	1	948	C	N3-C4	-6.39	1.29	1.33
44	1	1312	C	N3-C4	-6.39	1.29	1.33
44	1	343	U	C4-C5	-6.38	1.37	1.43
44	1	1446	A	C5-C6	-6.38	1.35	1.41
44	1	934	G	N7-C5	-6.38	1.35	1.39
45	2	17	A	N9-C4	-6.38	1.34	1.37
44	1	358	G	N9-C4	-6.38	1.32	1.38
44	1	1161	G	C8-N7	-6.38	1.27	1.30
44	1	659	G	N1-C2	-6.38	1.32	1.37
44	1	1369	A	C6-N6	-6.37	1.28	1.33
44	1	1401	A	N7-C5	-6.37	1.35	1.39
44	1	1432	C	C4-N4	-6.37	1.28	1.33
44	1	54	C	N3-C4	-6.37	1.29	1.33
44	1	1364	C	N1-C6	-6.37	1.33	1.37
44	1	62	A	N9-C4	-6.36	1.34	1.37
44	1	135	C	N1-C6	-6.36	1.33	1.37
45	2	101	U	C4-C5	-6.36	1.37	1.43
44	1	317	A	N9-C4	-6.36	1.34	1.37
44	1	702	C	C4-C5	-6.36	1.37	1.43
44	1	813	G	N7-C5	-6.35	1.35	1.39
44	1	1428	A	N9-C4	-6.35	1.34	1.37
44	1	650	C	C4-C5	-6.35	1.37	1.43
44	1	3138	U	C4-C5	-6.35	1.37	1.43
44	1	3140	G	N7-C5	-6.35	1.35	1.39
45	2	71	A	N9-C4	-6.35	1.34	1.37
44	1	1317	A	N7-C5	-6.34	1.35	1.39
44	1	2890	A	C6-N6	-6.34	1.28	1.33
44	1	54	C	N1-C6	-6.34	1.33	1.37
44	1	662	U	C4-C5	-6.34	1.37	1.43
44	1	1602	A	C5-C6	-6.34	1.35	1.41
44	1	289	A	C5-C6	-6.34	1.35	1.41
44	1	1497	C	C4-C5	-6.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	103	G	N7-C5	-6.33	1.35	1.39
44	1	1163	A	N7-C5	-6.33	1.35	1.39
44	1	1177	G	N7-C5	-6.33	1.35	1.39
44	1	3085	G	N9-C4	-6.33	1.32	1.38
44	1	969	C	C4-C5	-6.33	1.37	1.43
44	1	1190	A	N7-C5	-6.33	1.35	1.39
44	1	3211	C	N3-C4	-6.33	1.29	1.33
11	O	36	VAL	CB-CG2	-6.33	1.39	1.52
45	2	103	G	C6-N1	-6.33	1.35	1.39
44	1	1195	A	N9-C4	-6.32	1.34	1.37
44	1	1375	G	N9-C8	-6.32	1.33	1.37
44	1	1304	A	N7-C5	-6.32	1.35	1.39
44	1	2936	A	C6-N6	-6.32	1.28	1.33
44	1	1446	A	C5-C4	-6.32	1.34	1.38
44	1	320	G	N9-C4	-6.32	1.32	1.38
44	1	3296	A	C5-C6	-6.32	1.35	1.41
2	C	77	VAL	CB-CG2	-6.31	1.39	1.52
44	1	1433	A	N9-C8	-6.31	1.32	1.37
44	1	668	G	N7-C5	-6.31	1.35	1.39
44	1	1596	C	N1-C6	-6.31	1.33	1.37
44	1	113	C	N3-C4	-6.31	1.29	1.33
44	1	58	G	C8-N7	-6.30	1.27	1.30
44	1	364	G	N7-C5	-6.30	1.35	1.39
44	1	661	G	C2-N2	-6.30	1.28	1.34
44	1	1438	U	C4-C5	-6.30	1.37	1.43
44	1	501	A	C6-N6	-6.29	1.28	1.33
44	1	1170	A	N9-C4	-6.29	1.34	1.37
44	1	1423	C	C4-N4	-6.29	1.28	1.33
44	1	3323	A	N7-C5	-6.29	1.35	1.39
44	1	1381	A	N7-C5	-6.29	1.35	1.39
45	2	39	G	N7-C5	-6.29	1.35	1.39
44	1	342	A	C6-N6	-6.29	1.28	1.33
44	1	53	G	N7-C5	-6.28	1.35	1.39
44	1	1320	C	C4-C5	-6.28	1.38	1.43
44	1	225	C	N3-C4	-6.28	1.29	1.33
44	1	341	G	N1-C2	-6.28	1.32	1.37
44	1	1435	A	C5-C6	-6.28	1.35	1.41
44	1	1306	G	N7-C5	-6.28	1.35	1.39
44	1	2368	A	N7-C5	-6.28	1.35	1.39
44	1	3137	C	C4-N4	-6.28	1.28	1.33
44	1	1185	C	N1-C6	-6.28	1.33	1.37
44	1	1380	G	N7-C5	-6.28	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1412	G	N7-C5	-6.27	1.35	1.39
44	1	30	G	N7-C5	-6.27	1.35	1.39
44	1	3060	C	C4-C5	-6.27	1.38	1.43
44	1	3110	C	C4-C5	-6.27	1.38	1.43
44	1	367	A	C5-C6	-6.27	1.35	1.41
44	1	3046	A	C6-N6	-6.27	1.28	1.33
45	2	108	C	C4-C5	-6.26	1.38	1.43
44	1	1179	A	N9-C8	-6.26	1.32	1.37
44	1	672	A	C5-C6	-6.26	1.35	1.41
44	1	1598	G	N9-C8	-6.26	1.33	1.37
44	1	23	A	C6-N6	-6.25	1.28	1.33
44	1	58	G	N9-C8	-6.25	1.33	1.37
44	1	409	A	C6-N1	-6.25	1.31	1.35
44	1	425	G	N7-C5	-6.25	1.35	1.39
45	2	62	C	C4-C5	-6.25	1.38	1.43
44	1	154	U	C2-N3	-6.25	1.33	1.37
45	2	39	G	C6-N1	-6.25	1.35	1.39
44	1	1161	G	C5-C6	-6.25	1.36	1.42
44	1	322	U	N1-C6	-6.25	1.32	1.38
44	1	681	U	N1-C6	-6.25	1.32	1.38
44	1	1145	G	N1-C2	-6.25	1.32	1.37
44	1	89	A	C6-N6	-6.25	1.28	1.33
44	1	142	C	C4-C5	-6.25	1.38	1.43
44	1	608	A	N9-C4	-6.24	1.34	1.37
44	1	1312	C	C4-C5	-6.24	1.38	1.43
45	2	44	A	C5-C4	-6.24	1.34	1.38
44	1	1382	G	N9-C8	-6.24	1.33	1.37
44	1	141	C	N3-C4	-6.24	1.29	1.33
44	1	1444	G	N9-C8	-6.24	1.33	1.37
44	1	1318	A	N9-C4	-6.23	1.34	1.37
44	1	944	C	C4-N4	-6.23	1.28	1.33
44	1	1160	C	C4-N4	-6.23	1.28	1.33
44	1	920	A	C5-C4	-6.23	1.34	1.38
44	1	35	A	C6-N6	-6.23	1.28	1.33
44	1	61	A	C6-N6	-6.23	1.28	1.33
45	2	120	C	N3-C4	-6.23	1.29	1.33
45	2	22	U	C2-N3	-6.22	1.33	1.37
44	1	655	C	N1-C6	-6.22	1.33	1.37
44	1	17	G	N9-C4	-6.22	1.32	1.38
44	1	20	A	C6-N6	-6.22	1.28	1.33
45	2	21	C	C4-N4	-6.21	1.28	1.33
44	1	3046	A	C5-C6	-6.21	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	788	C	C5-C6	-6.21	1.29	1.34
44	1	945	C	C5-C6	-6.21	1.29	1.34
44	1	84	U	C4-C5	-6.20	1.38	1.43
44	1	122	A	N9-C4	-6.20	1.34	1.37
44	1	700	C	C4-C5	-6.20	1.38	1.43
44	1	1441	G	N9-C4	-6.20	1.32	1.38
44	1	1460	A	C6-N6	-6.20	1.28	1.33
44	1	3134	A	N7-C5	-6.20	1.35	1.39
44	1	1172	G	N1-C2	-6.20	1.32	1.37
44	1	1532	C	C4-C5	-6.20	1.38	1.43
44	1	342	A	C5-C4	-6.20	1.34	1.38
44	1	657	A	C5-C4	-6.20	1.34	1.38
44	1	676	G	N7-C5	-6.20	1.35	1.39
44	1	1420	C	N3-C4	-6.20	1.29	1.33
44	1	348	A	N9-C8	-6.19	1.32	1.37
44	1	943	U	C2-N3	-6.19	1.33	1.37
44	1	1364	C	N3-C4	-6.19	1.29	1.33
11	O	145	VAL	CB-CG1	-6.19	1.39	1.52
44	1	1309	U	C2-N3	-6.19	1.33	1.37
44	1	355	A	N7-C5	-6.18	1.35	1.39
44	1	1313	G	N9-C8	-6.18	1.33	1.37
44	1	16	A	C6-N6	-6.18	1.29	1.33
44	1	2341	A	C6-N6	-6.18	1.29	1.33
32	j	70	VAL	CB-CG2	-6.17	1.39	1.52
44	1	503	C	C4-C5	-6.17	1.38	1.43
44	1	1370	G	N9-C4	-6.17	1.33	1.38
44	1	1400	G	N9-C8	-6.17	1.33	1.37
44	1	1534	A	N9-C4	-6.17	1.34	1.37
44	1	23	A	C5-C6	-6.17	1.35	1.41
44	1	1330	A	N7-C5	-6.17	1.35	1.39
44	1	2361	A	N9-C4	-6.16	1.34	1.37
45	2	27	U	N1-C6	-6.16	1.32	1.38
44	1	1182	A	C6-N6	-6.16	1.29	1.33
44	1	69	C	N1-C6	-6.16	1.33	1.37
44	1	1433	A	N7-C5	-6.16	1.35	1.39
45	2	28	C	N3-C4	-6.16	1.29	1.33
44	1	23	A	N7-C5	-6.16	1.35	1.39
44	1	1367	G	N9-C8	-6.16	1.33	1.37
44	1	52	A	N9-C4	-6.16	1.34	1.37
44	1	1403	C	N3-C4	-6.16	1.29	1.33
44	1	2352	A	C6-N6	-6.16	1.29	1.33
44	1	15	C	C4-C5	-6.16	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1433	A	C5-C6	-6.16	1.35	1.41
44	1	113	C	C5-C6	-6.15	1.29	1.34
44	1	344	A	N9-C8	-6.15	1.32	1.37
44	1	1832	C	C4-C5	-6.15	1.38	1.43
44	1	29	C	N3-C4	-6.15	1.29	1.33
44	1	3003	G	N9-C8	-6.15	1.33	1.37
44	1	63	A	C5-C6	-6.15	1.35	1.41
45	2	61	A	N9-C4	-6.15	1.34	1.37
44	1	2353	G	N9-C8	-6.15	1.33	1.37
44	1	3005	A	C6-N6	-6.15	1.29	1.33
44	1	88	A	C5-C6	-6.15	1.35	1.41
44	1	1395	G	C2-N2	-6.14	1.28	1.34
44	1	1562	C	N1-C6	-6.14	1.33	1.37
44	1	1798	A	C6-N6	-6.14	1.29	1.33
44	1	926	A	N7-C5	-6.14	1.35	1.39
44	1	2367	A	N7-C5	-6.13	1.35	1.39
44	1	1499	C	C4-C5	-6.13	1.38	1.43
44	1	16	A	C8-N7	-6.13	1.27	1.31
44	1	34	A	C6-N6	-6.13	1.29	1.33
44	1	3101	G	N9-C4	-6.13	1.33	1.38
44	1	2355	G	N3-C4	-6.13	1.31	1.35
44	1	3096	C	C4-C5	-6.13	1.38	1.43
44	1	282	G	N9-C8	-6.12	1.33	1.37
44	1	325	A	N7-C5	-6.12	1.35	1.39
44	1	1334	U	C4-C5	-6.12	1.38	1.43
44	1	3311	C	C4-C5	-6.12	1.38	1.43
44	1	330	G	N9-C8	-6.12	1.33	1.37
44	1	347	G	C6-N1	-6.12	1.35	1.39
44	1	3008	A	C5-C4	-6.12	1.34	1.38
44	1	651	G	N7-C5	-6.12	1.35	1.39
44	1	3001	C	C4-C5	-6.12	1.38	1.43
44	1	341	G	N9-C4	-6.12	1.33	1.38
44	1	3299	A	N7-C5	-6.12	1.35	1.39
44	1	1310	G	N3-C4	-6.11	1.31	1.35
44	1	1835	A	C6-N6	-6.11	1.29	1.33
44	1	655	C	N3-C4	-6.11	1.29	1.33
44	1	1510	G	N1-C2	-6.11	1.32	1.37
44	1	357	A	C6-N6	-6.11	1.29	1.33
45	2	33	A	C6-N6	-6.11	1.29	1.33
44	1	589	A	C5-C4	-6.11	1.34	1.38
44	1	1190	A	C5-C6	-6.11	1.35	1.41
44	1	1382	G	N7-C5	-6.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	3008	A	N9-C8	-6.11	1.32	1.37
44	1	347	G	C5-C6	-6.10	1.36	1.42
44	1	659	G	N9-C8	-6.10	1.33	1.37
44	1	946	U	C4-C5	-6.10	1.38	1.43
44	1	2911	A	N7-C5	-6.10	1.35	1.39
44	1	26	A	C6-N6	-6.10	1.29	1.33
44	1	366	A	C5-C6	-6.09	1.35	1.41
44	1	3323	A	C5-C6	-6.09	1.35	1.41
44	1	321	C	C5-C6	-6.09	1.29	1.34
44	1	1193	A	N9-C4	-6.09	1.34	1.37
44	1	3181	C	N1-C6	-6.09	1.33	1.37
44	1	1416	C	C4-N4	-6.09	1.28	1.33
45	2	43	A	C6-N6	-6.09	1.29	1.33
44	1	504	A	C6-N6	-6.09	1.29	1.33
44	1	1460	A	N7-C5	-6.09	1.35	1.39
44	1	2888	U	C4-C5	-6.08	1.38	1.43
4	F	203	TRP	CB-CG	-6.08	1.39	1.50
32	j	49	TRP	CB-CG	-6.08	1.39	1.50
44	1	634	C	C4-N4	-6.08	1.28	1.33
44	1	221	A	N9-C8	-6.08	1.32	1.37
44	1	3000	A	N9-C4	-6.08	1.34	1.37
44	1	107	A	C6-N6	-6.08	1.29	1.33
44	1	361	A	N7-C5	-6.08	1.35	1.39
44	1	346	C	N3-C4	-6.07	1.29	1.33
45	2	30	C	N3-C4	-6.07	1.29	1.33
44	1	803	C	N1-C6	-6.07	1.33	1.37
44	1	54	C	C4-N4	-6.06	1.28	1.33
44	1	1443	G	N9-C8	-6.06	1.33	1.37
44	1	583	G	N9-C8	-6.06	1.33	1.37
44	1	702	C	N1-C6	-6.06	1.33	1.37
44	1	5	G	N9-C4	-6.05	1.33	1.38
32	j	26	SER	CA-CB	-6.05	1.43	1.52
44	1	225	C	N1-C6	-6.05	1.33	1.37
44	1	791	A	N7-C5	-6.05	1.35	1.39
44	1	1506	A	N7-C5	-6.05	1.35	1.39
44	1	1749	A	N9-C4	-6.05	1.34	1.37
45	2	117	C	C4-C5	-6.05	1.38	1.43
11	O	118	VAL	CB-CG2	-6.05	1.40	1.52
44	1	1406	A	N9-C4	-6.05	1.34	1.37
44	1	1432	C	C5-C6	-6.04	1.29	1.34
44	1	296	A	N9-C4	-6.04	1.34	1.37
44	1	3305	A	N9-C4	-6.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	3007	U	C4-C5	-6.04	1.38	1.43
44	1	1437	C	N1-C6	-6.03	1.33	1.37
44	1	1445	U	N1-C6	-6.03	1.32	1.38
44	1	805	G	N7-C5	-6.03	1.35	1.39
44	1	3113	A	N7-C5	-6.03	1.35	1.39
44	1	1497	C	N3-C4	-6.03	1.29	1.33
44	1	3005	A	N7-C5	-6.03	1.35	1.39
44	1	1159	A	C5-C6	-6.02	1.35	1.41
44	1	320	G	N7-C5	-6.02	1.35	1.39
44	1	1381	A	C5-C6	-6.02	1.35	1.41
44	1	1589	A	N9-C4	-6.02	1.34	1.37
44	1	346	C	C4-N4	-6.02	1.28	1.33
44	1	404	G	N9-C8	-6.02	1.33	1.37
44	1	3210	A	C5-C6	-6.02	1.35	1.41
2	C	94	CYS	CB-SG	-6.02	1.72	1.82
2	C	199	TRP	CB-CG	-6.02	1.39	1.50
9	M	12	TRP	CB-CG	-6.02	1.39	1.50
44	1	611	A	N7-C5	-6.02	1.35	1.39
45	2	134	G	N7-C5	-6.02	1.35	1.39
44	1	347	G	C2-N2	-6.02	1.28	1.34
44	1	113	C	N1-C6	-6.01	1.33	1.37
44	1	506	U	N1-C6	-6.01	1.32	1.38
45	2	10	A	C6-N6	-6.01	1.29	1.33
44	1	3210	A	C6-N6	-6.01	1.29	1.33
2	C	193	LYS	CB-CG	-6.01	1.36	1.52
44	1	6	A	C5-C6	-6.01	1.35	1.41
45	2	98	U	N1-C6	-6.01	1.32	1.38
44	1	356	C	C4-C5	-6.01	1.38	1.43
44	1	1372	C	C5-C6	-6.01	1.29	1.34
44	1	3140	G	N9-C8	-6.01	1.33	1.37
44	1	1406	A	C6-N1	-6.00	1.31	1.35
45	2	57	C	N3-C4	-6.00	1.29	1.33
44	1	325	A	C6-N6	-6.00	1.29	1.33
44	1	801	A	N9-C4	-6.00	1.34	1.37
44	1	26	A	N9-C8	-6.00	1.32	1.37
44	1	116	A	N9-C4	-6.00	1.34	1.37
44	1	21	G	C2-N2	-6.00	1.28	1.34
44	1	697	A	N9-C4	-6.00	1.34	1.37
45	2	139	U	C4-C5	-6.00	1.38	1.43
44	1	659	G	C6-N1	-6.00	1.35	1.39
44	1	200	C	C4-C5	-5.99	1.38	1.43
44	1	1157	G	N9-C4	-5.99	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	814	U	N1-C6	-5.99	1.32	1.38
45	2	35	C	C4-N4	-5.99	1.28	1.33
44	1	942	U	N1-C6	-5.99	1.32	1.38
2	C	39	PHE	CB-CG	-5.99	1.41	1.51
44	1	928	C	N3-C4	-5.99	1.29	1.33
44	1	1474	A	C6-N6	-5.98	1.29	1.33
45	2	106	C	C4-C5	-5.98	1.38	1.43
44	1	321	C	C4-N4	-5.98	1.28	1.33
44	1	336	A	N9-C4	-5.98	1.34	1.37
44	1	2887	A	C6-N6	-5.98	1.29	1.33
44	1	1701	C	N3-C4	-5.98	1.29	1.33
44	1	52	A	N7-C5	-5.97	1.35	1.39
44	1	408	A	N9-C8	-5.97	1.32	1.37
44	1	83	U	C4-C5	-5.97	1.38	1.43
44	1	1617	G	N9-C8	-5.97	1.33	1.37
44	1	786	A	N9-C4	-5.97	1.34	1.37
44	1	1379	G	N9-C8	-5.97	1.33	1.37
10	N	132	VAL	CB-CG1	-5.97	1.40	1.52
44	1	1474	A	C5-C6	-5.97	1.35	1.41
44	1	345	G	C5-C6	-5.97	1.36	1.42
44	1	1363	A	N9-C4	-5.97	1.34	1.37
44	1	289	A	N9-C4	-5.96	1.34	1.37
44	1	3181	C	N3-C4	-5.96	1.29	1.33
44	1	363	G	C8-N7	-5.96	1.27	1.30
44	1	1614	C	C5-C6	-5.96	1.29	1.34
45	2	88	A	N7-C5	-5.96	1.35	1.39
45	2	120	C	C4-N4	-5.96	1.28	1.33
44	1	1428	A	N7-C5	-5.96	1.35	1.39
44	1	354	U	N3-C4	-5.95	1.33	1.38
44	1	1164	G	N7-C5	-5.95	1.35	1.39
44	1	1836	C	C4-N4	-5.95	1.28	1.33
44	1	1526	U	N1-C6	-5.95	1.32	1.38
8	L	69	VAL	CB-CG2	-5.95	1.40	1.52
44	1	22	G	N7-C5	-5.95	1.35	1.39
44	1	358	G	N9-C8	-5.95	1.33	1.37
44	1	951	A	N9-C8	-5.95	1.32	1.37
44	1	1174	G	N7-C5	-5.95	1.35	1.39
1	B	93	VAL	CB-CG1	-5.95	1.40	1.52
44	1	22	G	C5-C4	-5.95	1.34	1.38
44	1	369	A	C5-C4	-5.95	1.34	1.38
44	1	672	A	N9-C8	-5.95	1.32	1.37
44	1	366	A	N9-C4	-5.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	76	C	C4-C5	-5.94	1.38	1.43
44	1	628	A	N7-C5	-5.94	1.35	1.39
44	1	696	C	N3-C4	-5.94	1.29	1.33
44	1	1315	U	N1-C6	-5.94	1.32	1.38
44	1	1414	G	N7-C5	-5.94	1.35	1.39
44	1	3052	G	N9-C8	-5.94	1.33	1.37
44	1	229	G	N7-C5	-5.94	1.35	1.39
44	1	2352	A	C5-C6	-5.94	1.35	1.41
44	1	2382	G	N7-C5	-5.94	1.35	1.39
45	2	144	G	N9-C4	-5.94	1.33	1.38
44	1	18	G	N7-C5	-5.93	1.35	1.39
44	1	1596	C	C4-C5	-5.93	1.38	1.43
44	1	361	A	C6-N6	-5.93	1.29	1.33
45	2	24	G	C2-N2	-5.93	1.28	1.34
44	1	671	U	C4-C5	-5.93	1.38	1.43
44	1	1166	G	N9-C8	-5.93	1.33	1.37
44	1	2365	C	C4-C5	-5.93	1.38	1.43
44	1	1370	G	N9-C8	-5.93	1.33	1.37
44	1	696	C	C5-C6	-5.93	1.29	1.34
44	1	72	C	N1-C6	-5.93	1.33	1.37
44	1	3375	A	C5-C6	-5.92	1.35	1.41
44	1	1491	A	C6-N6	-5.92	1.29	1.33
4	F	133	TYR	CD2-CE2	-5.92	1.30	1.39
44	1	516	A	N9-C4	-5.92	1.34	1.37
44	1	1148	G	N9-C4	-5.92	1.33	1.38
44	1	1468	A	C6-N6	-5.92	1.29	1.33
44	1	101	G	N9-C8	-5.91	1.33	1.37
44	1	335	G	N7-C5	-5.91	1.35	1.39
44	1	1603	A	C6-N1	-5.91	1.31	1.35
44	1	199	A	C6-N6	-5.91	1.29	1.33
44	1	222	A	N9-C4	-5.91	1.34	1.37
44	1	589	A	N7-C5	-5.91	1.35	1.39
44	1	2934	A	C6-N6	-5.91	1.29	1.33
44	1	372	A	C5-C6	-5.90	1.35	1.41
44	1	946	U	N1-C2	-5.90	1.33	1.38
45	2	62	C	N1-C6	-5.90	1.33	1.37
28	f	16	TYR	CE2-CZ	-5.90	1.30	1.38
44	1	114	A	C6-N6	-5.90	1.29	1.33
44	1	630	A	C8-N7	-5.90	1.27	1.31
44	1	1474	A	N9-C4	-5.90	1.34	1.37
44	1	1531	C	N3-C4	-5.90	1.29	1.33
44	1	15	C	N3-C4	-5.90	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1529	A	C6-N6	-5.90	1.29	1.33
2	C	52	VAL	CB-CG2	-5.89	1.40	1.52
44	1	60	A	C5-C4	-5.89	1.34	1.38
44	1	1404	G	N1-C2	-5.89	1.33	1.37
44	1	1593	A	C6-N6	-5.89	1.29	1.33
44	1	1169	A	N9-C4	-5.89	1.34	1.37
44	1	1613	A	C6-N6	-5.89	1.29	1.33
44	1	1319	G	N7-C5	-5.89	1.35	1.39
44	1	337	G	N9-C8	-5.88	1.33	1.37
44	1	3314	A	C6-N6	-5.88	1.29	1.33
44	1	941	G	N7-C5	-5.88	1.35	1.39
44	1	815	G	C8-N7	-5.88	1.27	1.30
44	1	1414	G	N9-C8	-5.88	1.33	1.37
44	1	2350	C	C4-C5	-5.88	1.38	1.43
44	1	1854	C	C4-C5	-5.88	1.38	1.43
45	2	28	C	C4-N4	-5.88	1.28	1.33
44	1	930	U	C4-C5	-5.87	1.38	1.43
44	1	1148	G	N9-C8	-5.87	1.33	1.37
44	1	6	A	C6-N6	-5.87	1.29	1.33
44	1	17	G	C5-C6	-5.87	1.36	1.42
44	1	1146	C	C5-C6	-5.87	1.29	1.34
44	1	3004	C	N3-C4	-5.87	1.29	1.33
45	2	58	G	C5-C6	-5.87	1.36	1.42
44	1	397	A	N7-C5	-5.87	1.35	1.39
44	1	1444	G	C6-N1	-5.87	1.35	1.39
44	1	2368	A	C6-N6	-5.87	1.29	1.33
44	1	3091	A	N7-C5	-5.87	1.35	1.39
45	2	46	G	N7-C5	-5.87	1.35	1.39
44	1	685	G	N9-C8	-5.87	1.33	1.37
44	1	649	A	C5-C6	-5.87	1.35	1.41
44	1	1469	C	C2-N3	-5.86	1.31	1.35
45	2	15	G	C6-N1	-5.86	1.35	1.39
44	1	428	A	N7-C5	-5.86	1.35	1.39
44	1	1173	U	N1-C6	-5.86	1.32	1.38
44	1	2890	A	N9-C4	-5.86	1.34	1.37
44	1	353	G	C6-N1	-5.86	1.35	1.39
44	1	656	A	N9-C4	-5.86	1.34	1.37
44	1	78	U	C4-C5	-5.85	1.38	1.43
44	1	1416	C	N1-C6	-5.85	1.33	1.37
44	1	680	G	N7-C5	-5.85	1.35	1.39
44	1	1332	A	C6-N1	-5.85	1.31	1.35
44	1	1832	C	N1-C6	-5.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	194	TYR	CE1-CZ	-5.85	1.30	1.38
44	1	209	A	N9-C8	-5.85	1.33	1.37
45	2	100	U	C4-C5	-5.85	1.38	1.43
44	1	321	C	N3-C4	-5.85	1.29	1.33
44	1	368	G	N7-C5	-5.85	1.35	1.39
44	1	105	C	C4-C5	-5.84	1.38	1.43
44	1	338	A	N9-C4	-5.84	1.34	1.37
44	1	340	C	N3-C4	-5.84	1.29	1.33
44	1	352	A	C6-N1	-5.84	1.31	1.35
44	1	654	C	N1-C6	-5.84	1.33	1.37
45	2	33	A	N9-C4	-5.84	1.34	1.37
2	C	113	VAL	CB-CG2	-5.84	1.40	1.52
44	1	2357	A	N9-C8	-5.84	1.33	1.37
26	d	35	GLU	CB-CG	-5.84	1.41	1.52
44	1	359	U	N1-C6	-5.84	1.32	1.38
45	2	66	A	N9-C4	-5.84	1.34	1.37
44	1	395	A	C6-N6	-5.83	1.29	1.33
44	1	810	A	C6-N6	-5.83	1.29	1.33
44	1	1343	A	C6-N6	-5.83	1.29	1.33
44	1	1394	A	C6-N6	-5.83	1.29	1.33
44	1	347	G	N1-C2	-5.83	1.33	1.37
44	1	3375	A	C6-N6	-5.83	1.29	1.33
45	2	36	G	C6-N1	-5.83	1.35	1.39
44	1	1385	C	C4-C5	-5.83	1.38	1.43
45	2	96	A	C5-C6	-5.83	1.35	1.41
44	1	271	C	N1-C6	-5.82	1.33	1.37
44	1	1190	A	C6-N6	-5.82	1.29	1.33
44	1	1166	G	N1-C2	-5.82	1.33	1.37
44	1	64	G	C5-C6	-5.82	1.36	1.42
44	1	271	C	C4-C5	-5.82	1.38	1.43
44	1	336	A	C6-N6	-5.82	1.29	1.33
44	1	1532	C	N1-C6	-5.82	1.33	1.37
44	1	3134	A	C5-C6	-5.82	1.35	1.41
44	1	927	C	N3-C4	-5.81	1.29	1.33
44	1	1497	C	N1-C6	-5.81	1.33	1.37
45	2	143	U	C4-C5	-5.81	1.38	1.43
44	1	106	A	C5-C6	-5.81	1.35	1.41
44	1	589	A	C5-C6	-5.81	1.35	1.41
44	1	933	A	N7-C5	-5.81	1.35	1.39
44	1	1409	G	N9-C8	-5.81	1.33	1.37
44	1	1537	A	N9-C4	-5.81	1.34	1.37
44	1	26	A	C5-C6	-5.81	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	214	G	N7-C5	-5.81	1.35	1.39
44	1	3048	A	C6-N6	-5.81	1.29	1.33
44	1	52	A	C5-C4	-5.80	1.34	1.38
44	1	143	G	N9-C8	-5.80	1.33	1.37
45	2	105	A	C8-N7	-5.80	1.27	1.31
44	1	428	A	C5-C4	-5.80	1.34	1.38
44	1	214	G	N9-C8	-5.80	1.33	1.37
44	1	216	G	N7-C5	-5.80	1.35	1.39
44	1	666	A	C6-N6	-5.80	1.29	1.33
45	2	8	C	C4-C5	-5.80	1.38	1.43
44	1	1165	A	N7-C5	-5.79	1.35	1.39
44	1	1212	A	C6-N6	-5.79	1.29	1.33
44	1	504	A	N7-C5	-5.79	1.35	1.39
45	2	27	U	C4-C5	-5.79	1.38	1.43
44	1	403	C	N1-C6	-5.79	1.33	1.37
12	P	143	PRO	CB-CG	-5.79	1.21	1.50
44	1	408	A	N3-C4	-5.79	1.31	1.34
44	1	1168	U	N1-C6	-5.79	1.32	1.38
44	1	1856	C	C4-C5	-5.79	1.38	1.43
11	O	54	TYR	CD1-CE1	-5.78	1.30	1.39
44	1	665	A	N9-C8	-5.78	1.33	1.37
44	1	1183	C	C5-C6	-5.78	1.29	1.34
44	1	1195	A	N9-C8	-5.78	1.33	1.37
44	1	1462	A	C6-N6	-5.78	1.29	1.33
45	2	63	G	C2-N3	-5.78	1.28	1.32
44	1	1441	G	N7-C5	-5.78	1.35	1.39
44	1	3186	A	C6-N6	-5.78	1.29	1.33
45	2	28	C	N1-C6	-5.78	1.33	1.37
44	1	1377	G	C2-N3	-5.77	1.28	1.32
44	1	3027	A	N3-C4	-5.77	1.31	1.34
44	1	3213	A	C5-C6	-5.77	1.35	1.41
44	1	634	C	N1-C6	-5.77	1.33	1.37
44	1	800	G	N7-C5	-5.77	1.35	1.39
45	2	19	C	N1-C6	-5.77	1.33	1.37
45	2	22	U	N3-C4	-5.77	1.33	1.38
44	1	1365	G	C5-C6	-5.76	1.36	1.42
44	1	6	A	N7-C5	-5.76	1.35	1.39
44	1	371	G	N7-C5	-5.76	1.35	1.39
44	1	347	G	C8-N7	-5.76	1.27	1.30
44	1	1469	C	N3-C4	-5.76	1.29	1.33
44	1	355	A	C5-C6	-5.76	1.35	1.41
44	1	1424	C	N1-C6	-5.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1372	C	C4-N4	-5.75	1.28	1.33
44	1	1107	C	C4-C5	-5.75	1.38	1.43
45	2	33	A	N9-C8	-5.75	1.33	1.37
44	1	76	G	N7-C5	-5.75	1.35	1.39
44	1	677	A	N7-C5	-5.75	1.35	1.39
44	1	1171	G	C6-N1	-5.75	1.35	1.39
10	N	66	VAL	CB-CG1	-5.74	1.40	1.52
44	1	12	A	C6-N6	-5.74	1.29	1.33
44	1	813	G	N3-C4	-5.74	1.31	1.35
44	1	1598	G	C8-N7	-5.74	1.27	1.30
12	P	88	VAL	CB-CG1	-5.74	1.40	1.52
44	1	580	C	C4-C5	-5.74	1.38	1.43
44	1	695	C	C4-N4	-5.74	1.28	1.33
44	1	1498	A	C5-C6	-5.74	1.35	1.41
44	1	2365	C	C5-C6	-5.74	1.29	1.34
44	1	634	C	C5-C6	-5.73	1.29	1.34
44	1	657	A	C5-C6	-5.73	1.35	1.41
44	1	715	A	C6-N6	-5.73	1.29	1.33
44	1	1177	G	C6-N1	-5.73	1.35	1.39
45	2	107	G	N9-C4	-5.73	1.33	1.38
44	1	1338	C	C4-N4	-5.73	1.28	1.33
44	1	1881	A	N9-C4	-5.73	1.34	1.37
44	1	586	C	C4-N4	-5.73	1.28	1.33
44	1	790	U	C4-C5	-5.73	1.38	1.43
44	1	2892	A	C6-N6	-5.73	1.29	1.33
44	1	3040	A	C5-C6	-5.73	1.35	1.41
44	1	3226	A	N9-C4	-5.73	1.34	1.37
44	1	677	A	C6-N6	-5.73	1.29	1.33
44	1	588	G	N7-C5	-5.72	1.35	1.39
44	1	1193	A	C6-N6	-5.72	1.29	1.33
44	1	1387	G	N1-C2	-5.72	1.33	1.37
44	1	1426	C	N1-C6	-5.72	1.33	1.37
5	G	190	VAL	CB-CG1	-5.72	1.40	1.52
44	1	111	C	C4-C5	-5.72	1.38	1.43
44	1	2889	C	N1-C6	-5.72	1.33	1.37
45	2	58	G	N9-C8	-5.72	1.33	1.37
44	1	651	G	N9-C8	-5.71	1.33	1.37
44	1	942	U	N1-C2	-5.71	1.33	1.38
44	1	3310	A	N9-C4	-5.71	1.34	1.37
44	1	88	A	N9-C4	-5.71	1.34	1.37
44	1	1325	U	C4-C5	-5.71	1.38	1.43
44	1	366	A	C6-N6	-5.71	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1181	U	N3-C4	-5.71	1.33	1.38
45	2	118	C	C4-C5	-5.71	1.38	1.43
12	P	114	VAL	CB-CG2	-5.71	1.40	1.52
44	1	61	A	C5-C6	-5.70	1.35	1.41
44	1	214	G	C5-C6	-5.70	1.36	1.42
44	1	584	G	N9-C4	-5.70	1.33	1.38
44	1	686	G	N7-C5	-5.70	1.35	1.39
44	1	2368	A	C5-C6	-5.70	1.35	1.41
45	2	9	A	N9-C8	-5.70	1.33	1.37
44	1	3206	C	N1-C6	-5.70	1.33	1.37
45	2	30	C	N1-C6	-5.70	1.33	1.37
44	1	1298	C	N3-C4	-5.70	1.29	1.33
44	1	200	C	N3-C4	-5.70	1.29	1.33
44	1	1183	C	N3-C4	-5.69	1.29	1.33
44	1	931	C	C4-N4	-5.69	1.28	1.33
44	1	67	A	N9-C4	-5.69	1.34	1.37
44	1	333	G	N9-C8	-5.69	1.33	1.37
44	1	1337	A	C5-C4	-5.69	1.34	1.38
44	1	3101	G	N9-C8	-5.69	1.33	1.37
44	1	107	A	N9-C4	-5.69	1.34	1.37
44	1	668	G	N1-C2	-5.69	1.33	1.37
44	1	1381	A	N3-C4	-5.69	1.31	1.34
45	2	22	U	C4-C5	-5.69	1.38	1.43
44	1	201	A	N7-C5	-5.69	1.35	1.39
44	1	432	G	N1-C2	-5.69	1.33	1.37
44	1	926	A	C6-N6	-5.69	1.29	1.33
44	1	3086	A	C6-N6	-5.69	1.29	1.33
44	1	1160	C	C5-C6	-5.69	1.29	1.34
44	1	350	C	C4-N4	-5.68	1.28	1.33
44	1	657	A	N3-C4	-5.68	1.31	1.34
44	1	1411	C	C4-C5	-5.68	1.38	1.43
44	1	614	C	C4-C5	-5.68	1.38	1.43
44	1	1385	C	N1-C6	-5.68	1.33	1.37
44	1	1475	A	N9-C4	-5.68	1.34	1.37
44	1	701	G	C6-N1	-5.68	1.35	1.39
44	1	944	C	C5-C6	-5.68	1.29	1.34
45	2	66	A	C5-C6	-5.68	1.35	1.41
44	1	7	C	N1-C6	-5.68	1.33	1.37
44	1	1279	C	N3-C4	-5.68	1.29	1.33
45	2	42	G	N9-C8	-5.68	1.33	1.37
44	1	1159	A	C6-N6	-5.68	1.29	1.33
44	1	1404	G	N9-C8	-5.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	55	G	N9-C4	-5.67	1.33	1.38
44	1	375	A	C5-C6	-5.67	1.35	1.41
44	1	1194	G	N1-C2	-5.67	1.33	1.37
45	2	46	G	N1-C2	-5.67	1.33	1.37
12	P	83	TRP	CB-CG	-5.67	1.40	1.50
28	f	80	VAL	CB-CG1	-5.67	1.41	1.52
44	1	1396	C	N3-C4	-5.67	1.29	1.33
44	1	410	U	N1-C2	-5.66	1.33	1.38
44	1	497	C	C4-C5	-5.66	1.38	1.43
44	1	1594	A	C6-N1	-5.66	1.31	1.35
44	1	1167	U	C4-C5	-5.66	1.38	1.43
44	1	670	C	C4-N4	-5.65	1.28	1.33
44	1	806	A	C6-N6	-5.65	1.29	1.33
27	e	53	PRO	CB-CG	-5.65	1.21	1.50
44	1	34	A	N9-C8	-5.65	1.33	1.37
44	1	361	A	N9-C8	-5.65	1.33	1.37
44	1	3244	A	N7-C5	-5.65	1.35	1.39
44	1	673	U	C4-C5	-5.65	1.38	1.43
44	1	1316	C	N1-C6	-5.65	1.33	1.37
44	1	1329	U	N3-C4	-5.65	1.33	1.38
44	1	1431	G	N1-C2	-5.64	1.33	1.37
44	1	59	G	N9-C4	-5.64	1.33	1.38
44	1	224	C	C4-N4	-5.64	1.28	1.33
44	1	1465	A	N9-C4	-5.64	1.34	1.37
44	1	2912	G	C2-N2	-5.64	1.28	1.34
44	1	353	G	N9-C8	-5.64	1.33	1.37
44	1	1422	G	N9-C8	-5.64	1.33	1.37
10	N	132	VAL	CB-CG2	-5.64	1.41	1.52
44	1	700	C	C5-C6	-5.64	1.29	1.34
44	1	1449	A	N7-C5	-5.64	1.35	1.39
44	1	3128	G	N9-C4	-5.64	1.33	1.38
44	1	1176	C	C4-C5	-5.63	1.38	1.43
44	1	1303	A	C6-N6	-5.63	1.29	1.33
44	1	1466	G	N7-C5	-5.63	1.35	1.39
45	2	103	G	C2-N2	-5.63	1.28	1.34
44	1	123	A	C6-N1	-5.63	1.31	1.35
44	1	435	C	N1-C6	-5.63	1.33	1.37
44	1	694	C	C4-C5	-5.63	1.38	1.43
44	1	1370	G	N7-C5	-5.63	1.35	1.39
28	f	66	VAL	CB-CG2	-5.63	1.41	1.52
44	1	1407	A	C5-C6	-5.63	1.35	1.41
44	1	63	A	C5-C4	-5.63	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1407	A	N7-C5	-5.63	1.35	1.39
44	1	3016	A	C6-N6	-5.63	1.29	1.33
44	1	20	A	C5-C6	-5.62	1.35	1.41
44	1	943	U	N1-C6	-5.62	1.32	1.38
44	1	1409	G	N7-C5	-5.62	1.35	1.39
44	1	2936	A	N9-C4	-5.62	1.34	1.37
44	1	1158	A	N9-C8	-5.62	1.33	1.37
44	1	613	G	N7-C5	-5.62	1.35	1.39
44	1	2354	C	N3-C4	-5.62	1.30	1.33
45	2	12	A	N7-C5	-5.62	1.35	1.39
44	1	3296	A	C6-N6	-5.62	1.29	1.33
9	M	20	VAL	CB-CG1	-5.61	1.41	1.52
44	1	1112	A	C6-N6	-5.61	1.29	1.33
45	2	91	C	C5-C6	-5.61	1.29	1.34
44	1	1320	C	N3-C4	-5.61	1.30	1.33
45	2	37	A	C6-N6	-5.61	1.29	1.33
44	1	3298	C	N3-C4	-5.61	1.30	1.33
44	1	1150	A	N9-C4	-5.61	1.34	1.37
44	1	1180	A	N9-C8	-5.60	1.33	1.37
45	2	19	C	N3-C4	-5.60	1.30	1.33
45	2	150	G	N9-C8	-5.60	1.33	1.37
44	1	130	A	C5-C6	-5.60	1.36	1.41
44	1	3370	A	N9-C4	-5.60	1.34	1.37
44	1	363	G	C5-C6	-5.59	1.36	1.42
44	1	944	C	N3-C4	-5.59	1.30	1.33
44	1	325	A	N9-C8	-5.59	1.33	1.37
44	1	56	G	N3-C4	-5.59	1.31	1.35
44	1	1447	G	N9-C8	-5.59	1.33	1.37
44	1	2884	C	N3-C4	-5.59	1.30	1.33
45	2	149	A	C6-N6	-5.59	1.29	1.33
44	1	2892	A	C5-C6	-5.59	1.36	1.41
44	1	3123	A	C6-N6	-5.59	1.29	1.33
44	1	920	A	C5-C6	-5.58	1.36	1.41
44	1	1144	U	C2-N3	-5.58	1.33	1.37
44	1	2356	A	N7-C5	-5.58	1.35	1.39
45	2	77	A	C5-C6	-5.58	1.36	1.41
44	1	209	A	N7-C5	-5.58	1.35	1.39
44	1	638	C	N3-C4	-5.57	1.30	1.33
44	1	1204	A	N7-C5	-5.57	1.35	1.39
44	1	677	A	N9-C4	-5.57	1.34	1.37
8	L	28	GLN	CB-CG	-5.57	1.37	1.52
44	1	147	U	C5-C6	-5.57	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1323	G	N9-C4	-5.57	1.33	1.38
44	1	2381	G	N9-C4	-5.57	1.33	1.38
44	1	1182	A	N9-C4	-5.57	1.34	1.37
44	1	1367	G	N9-C4	-5.57	1.33	1.38
44	1	1603	A	N9-C8	-5.56	1.33	1.37
44	1	1159	A	C8-N7	-5.56	1.27	1.31
44	1	633	C	C5-C6	-5.56	1.29	1.34
44	1	583	G	N7-C5	-5.56	1.35	1.39
44	1	2355	G	N7-C5	-5.56	1.35	1.39
45	2	42	G	N3-C4	-5.56	1.31	1.35
44	1	1378	U	C4-C5	-5.55	1.38	1.43
44	1	1407	A	C6-N1	-5.55	1.31	1.35
44	1	1429	G	C5-C4	-5.55	1.34	1.38
44	1	348	A	C5-C6	-5.55	1.36	1.41
45	2	98	U	C4-C5	-5.55	1.38	1.43
44	1	95	A	N9-C4	-5.55	1.34	1.37
45	2	140	G	C2-N2	-5.55	1.28	1.34
44	1	1799	A	C5-C6	-5.55	1.36	1.41
44	1	213	A	C6-N1	-5.55	1.31	1.35
44	1	404	G	N7-C5	-5.55	1.35	1.39
44	1	75	G	N7-C5	-5.55	1.35	1.39
44	1	408	A	C6-N6	-5.55	1.29	1.33
44	1	81	C	N1-C6	-5.54	1.33	1.37
44	1	226	C	N3-C4	-5.54	1.30	1.33
44	1	104	G	N9-C8	-5.54	1.33	1.37
44	1	1183	C	N1-C6	-5.54	1.33	1.37
44	1	1394	A	N9-C8	-5.54	1.33	1.37
45	2	92	A	N3-C4	-5.54	1.31	1.34
44	1	272	G	N7-C5	-5.54	1.35	1.39
44	1	661	G	N1-C2	-5.54	1.33	1.37
44	1	345	G	C6-N1	-5.54	1.35	1.39
44	1	215	G	N7-C5	-5.54	1.35	1.39
44	1	1528	G	N7-C5	-5.54	1.35	1.39
45	2	25	G	N9-C8	-5.54	1.33	1.37
44	1	3210	A	N7-C5	-5.54	1.35	1.39
45	2	42	G	N1-C2	-5.54	1.33	1.37
44	1	22	G	N1-C2	-5.53	1.33	1.37
44	1	3147	G	N7-C5	-5.53	1.35	1.39
45	2	99	C	N1-C6	-5.53	1.33	1.37
44	1	1448	U	C4-C5	-5.53	1.38	1.43
44	1	33	G	N9-C8	-5.53	1.33	1.37
44	1	1146	C	N3-C4	-5.53	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	3033	A	N9-C4	-5.53	1.34	1.37
10	N	202	TYR	CE2-CZ	-5.53	1.31	1.38
44	1	1161	G	N9-C8	-5.53	1.33	1.37
44	1	1403	C	C5-C6	-5.53	1.29	1.34
44	1	3130	A	N9-C8	-5.53	1.33	1.37
32	j	22	CYS	CB-SG	-5.52	1.72	1.81
44	1	76	G	N1-C2	-5.52	1.33	1.37
44	1	948	C	C5-C6	-5.52	1.29	1.34
44	1	1438	U	N3-C4	-5.52	1.33	1.38
44	1	3086	A	N9-C4	-5.52	1.34	1.37
44	1	51	A	C5-C6	-5.52	1.36	1.41
44	1	372	A	N7-C5	-5.52	1.35	1.39
44	1	389	A	C5-C6	-5.51	1.36	1.41
4	F	240	VAL	CB-CG1	-5.51	1.41	1.52
27	e	28	VAL	CB-CG1	-5.51	1.41	1.52
44	1	341	G	C6-N1	-5.51	1.35	1.39
45	2	94	C	N1-C6	-5.51	1.33	1.37
44	1	56	G	N7-C5	-5.51	1.35	1.39
44	1	1419	A	N7-C5	-5.51	1.35	1.39
44	1	1558	A	N9-C4	-5.50	1.34	1.37
44	1	938	C	N3-C4	-5.50	1.30	1.33
44	1	1181	U	C4-C5	-5.50	1.38	1.43
44	1	1395	G	N1-C2	-5.50	1.33	1.37
12	P	51	VAL	CB-CG2	-5.50	1.41	1.52
44	1	22	G	N9-C4	-5.50	1.33	1.38
44	1	1380	G	N9-C4	-5.50	1.33	1.38
44	1	21	G	N1-C2	-5.50	1.33	1.37
44	1	144	A	C5-C6	-5.50	1.36	1.41
44	1	1461	A	N9-C4	-5.50	1.34	1.37
44	1	1895	A	C6-N6	-5.50	1.29	1.33
44	1	30	G	N9-C8	-5.50	1.34	1.37
44	1	412	G	N9-C8	-5.50	1.34	1.37
44	1	426	G	N9-C4	-5.50	1.33	1.38
44	1	578	A	N9-C8	-5.50	1.33	1.37
44	1	48	A	N9-C8	-5.50	1.33	1.37
44	1	1169	A	N7-C5	-5.49	1.35	1.39
44	1	3046	A	C5-C4	-5.49	1.34	1.38
44	1	3311	C	N3-C4	-5.49	1.30	1.33
44	1	618	C	N1-C6	-5.49	1.33	1.37
44	1	792	G	N9-C8	-5.49	1.34	1.37
44	1	1495	U	N3-C4	-5.49	1.33	1.38
44	1	1505	C	C4-C5	-5.49	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	3144	G	C5-C4	-5.49	1.34	1.38
44	1	27	C	C4-N4	-5.49	1.29	1.33
44	1	791	A	N9-C4	-5.49	1.34	1.37
45	2	34	U	N1-C2	-5.49	1.33	1.38
44	1	430	U	N1-C6	-5.49	1.33	1.38
44	1	695	C	N3-C4	-5.49	1.30	1.33
44	1	122	A	N9-C8	-5.48	1.33	1.37
44	1	141	C	C4-C5	-5.48	1.38	1.43
2	C	109	TRP	CB-CG	-5.48	1.40	1.50
44	1	1558	A	C5-C4	-5.48	1.34	1.38
44	1	104	G	N7-C5	-5.48	1.35	1.39
44	1	670	C	N3-C4	-5.48	1.30	1.33
45	2	65	A	C6-N6	-5.48	1.29	1.33
44	1	127	G	N9-C8	-5.48	1.34	1.37
44	1	339	C	C5-C6	-5.48	1.29	1.34
44	1	197	G	N9-C4	-5.48	1.33	1.38
44	1	102	C	C4-N4	-5.47	1.29	1.33
44	1	107	A	C5-C4	-5.47	1.34	1.38
44	1	144	A	N7-C5	-5.47	1.35	1.39
44	1	1537	A	C6-N6	-5.47	1.29	1.33
44	1	51	A	N3-C4	-5.47	1.31	1.34
44	1	1317	A	N9-C8	-5.47	1.33	1.37
45	2	39	G	N1-C2	-5.47	1.33	1.37
44	1	10	C	N1-C6	-5.47	1.33	1.37
44	1	1180	A	C6-N6	-5.47	1.29	1.33
44	1	1412	G	N9-C8	-5.47	1.34	1.37
44	1	1756	C	C4-C5	-5.47	1.38	1.43
44	1	3136	G	N7-C5	-5.47	1.35	1.39
44	1	1311	G	N7-C5	-5.47	1.35	1.39
44	1	1614	C	C4-N4	-5.47	1.29	1.33
45	2	8	C	N1-C6	-5.47	1.33	1.37
45	2	103	G	N9-C8	-5.47	1.34	1.37
44	1	368	G	C5-C4	-5.46	1.34	1.38
44	1	586	C	N3-C4	-5.46	1.30	1.33
44	1	3048	A	N7-C5	-5.46	1.35	1.39
44	1	62	A	C5-C6	-5.46	1.36	1.41
10	N	146	ALA	CA-C	-5.46	1.38	1.52
44	1	611	A	C5-C6	-5.46	1.36	1.41
44	1	1310	G	C2-N3	-5.46	1.28	1.32
44	1	425	G	C5-C6	-5.46	1.36	1.42
44	1	1428	A	C5-C4	-5.46	1.34	1.38
44	1	2358	A	N9-C4	-5.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1171	G	C8-N7	-5.46	1.27	1.30
44	1	32	U	N3-C4	-5.45	1.33	1.38
44	1	1495	U	N1-C6	-5.45	1.33	1.38
44	1	622	A	N7-C5	-5.45	1.35	1.39
44	1	3330	A	N7-C5	-5.45	1.35	1.39
44	1	373	A	C5-C4	-5.45	1.34	1.38
44	1	1456	A	N7-C5	-5.45	1.35	1.39
44	1	1833	G	N1-C2	-5.45	1.33	1.37
44	1	11	A	N9-C4	-5.45	1.34	1.37
44	1	1462	A	N7-C5	-5.45	1.35	1.39
44	1	1490	A	N9-C4	-5.45	1.34	1.37
44	1	332	C	N3-C4	-5.45	1.30	1.33
44	1	585	A	C6-N1	-5.45	1.31	1.35
44	1	1303	A	N7-C5	-5.45	1.35	1.39
45	2	32	C	N1-C6	-5.45	1.33	1.37
44	1	29	C	C4-N4	-5.45	1.29	1.33
44	1	1594	A	C5-C4	-5.45	1.34	1.38
44	1	3112	G	N9-C4	-5.45	1.33	1.38
45	2	38	U	C4-C5	-5.44	1.38	1.43
44	1	369	A	N9-C4	-5.44	1.34	1.37
44	1	1563	C	N3-C4	-5.44	1.30	1.33
44	1	1800	A	N7-C5	-5.44	1.35	1.39
44	1	3103	A	C5-C6	-5.44	1.36	1.41
44	1	1522	U	N1-C2	-5.44	1.33	1.38
44	1	3091	A	C5-C6	-5.44	1.36	1.41
44	1	590	G	N9-C4	-5.44	1.33	1.38
44	1	938	C	C5-C6	-5.44	1.29	1.34
44	1	1586	G	N9-C8	-5.44	1.34	1.37
44	1	3001	C	N1-C6	-5.44	1.33	1.37
44	1	3051	U	C4-C5	-5.44	1.38	1.43
44	1	1328	C	N3-C4	-5.44	1.30	1.33
44	1	397	A	N3-C4	-5.44	1.31	1.34
44	1	674	G	C6-N1	-5.43	1.35	1.39
44	1	687	U	C2-N3	-5.43	1.33	1.37
44	1	59	G	C2-N2	-5.43	1.29	1.34
44	1	1404	G	C2-N3	-5.43	1.28	1.32
45	2	62	C	C5-C6	-5.43	1.30	1.34
44	1	1402	C	N1-C6	-5.43	1.33	1.37
44	1	3052	G	N7-C5	-5.43	1.35	1.39
44	1	3104	U	C4-C5	-5.43	1.38	1.43
44	1	361	A	C5-C4	-5.42	1.34	1.38
44	1	639	G	N3-C4	-5.42	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	2933	A	C6-N6	-5.42	1.29	1.33
44	1	1836	C	N1-C6	-5.42	1.33	1.37
44	1	1112	A	N9-C4	-5.42	1.34	1.37
45	2	22	U	C5-C6	-5.42	1.29	1.34
44	1	375	A	C5-C4	-5.42	1.34	1.38
44	1	1165	A	N9-C8	-5.42	1.33	1.37
44	1	1491	A	C6-N1	-5.42	1.31	1.35
44	1	233	C	C4-C5	-5.42	1.38	1.43
44	1	3322	A	C6-N6	-5.42	1.29	1.33
44	1	32	U	C4-C5	-5.42	1.38	1.43
11	O	145	VAL	CB-CG2	-5.41	1.41	1.52
44	1	328	U	N3-C4	-5.41	1.33	1.38
45	2	55	U	C4-C5	-5.41	1.38	1.43
44	1	1515	A	N7-C5	-5.41	1.36	1.39
44	1	331	G	N9-C8	-5.41	1.34	1.37
44	1	364	G	N9-C8	-5.41	1.34	1.37
44	1	65	A	N7-C5	-5.40	1.36	1.39
44	1	659	G	C5-C6	-5.40	1.36	1.42
44	1	660	A	C6-N1	-5.40	1.31	1.35
44	1	1447	G	C2-N2	-5.40	1.29	1.34
44	1	427	C	C5-C6	-5.40	1.30	1.34
44	1	1537	A	C5-C6	-5.40	1.36	1.41
44	1	127	G	N9-C4	-5.40	1.33	1.38
44	1	946	U	N1-C6	-5.40	1.33	1.38
44	1	3123	A	N7-C5	-5.40	1.36	1.39
45	2	36	G	N9-C8	-5.40	1.34	1.37
44	1	683	U	N1-C2	-5.40	1.33	1.38
44	1	2359	C	C4-C5	-5.40	1.38	1.43
44	1	2368	A	N9-C8	-5.40	1.33	1.37
44	1	3012	A	C6-N6	-5.40	1.29	1.33
44	1	347	G	N9-C8	-5.39	1.34	1.37
44	1	1374	G	N7-C5	-5.39	1.36	1.39
44	1	1440	G	C6-N1	-5.39	1.35	1.39
5	G	125	ALA	C-N	-5.39	1.21	1.34
44	1	323	A	C8-N7	-5.39	1.27	1.31
44	1	1158	A	C8-N7	-5.39	1.27	1.31
44	1	1380	G	N3-C4	-5.39	1.31	1.35
45	2	47	C	C4-C5	-5.39	1.38	1.43
44	1	213	A	N9-C4	-5.39	1.34	1.37
44	1	416	A	C6-N6	-5.39	1.29	1.33
44	1	633	C	N3-C4	-5.39	1.30	1.33
44	1	1143	A	N9-C4	-5.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1311	G	N9-C4	-5.39	1.33	1.38
44	1	1407	A	C5-C4	-5.39	1.34	1.38
44	1	2910	A	C5-C4	-5.39	1.34	1.38
44	1	3276	G	N9-C8	-5.39	1.34	1.37
5	G	140	VAL	CB-CG2	-5.39	1.41	1.52
44	1	35	A	N7-C5	-5.39	1.36	1.39
44	1	14	U	C2-N3	-5.38	1.33	1.37
44	1	941	G	N3-C4	-5.38	1.31	1.35
44	1	3139	A	N9-C4	-5.38	1.34	1.37
44	1	3309	G	N1-C2	-5.38	1.33	1.37
44	1	3314	A	C5-C6	-5.38	1.36	1.41
45	2	37	A	C5-C4	-5.38	1.34	1.38
45	2	56	G	N9-C8	-5.38	1.34	1.37
44	1	430	U	C4-C5	-5.38	1.38	1.43
44	1	970	A	N9-C4	-5.38	1.34	1.37
44	1	215	G	N9-C8	-5.38	1.34	1.37
44	1	1172	G	C2-N2	-5.38	1.29	1.34
44	1	683	U	C4-C5	-5.38	1.38	1.43
9	M	94	TRP	CB-CG	-5.38	1.40	1.50
44	1	1419	A	N9-C8	-5.38	1.33	1.37
44	1	1696	A	C6-N6	-5.38	1.29	1.33
44	1	1373	A	C6-N6	-5.38	1.29	1.33
44	1	1489	A	N9-C4	-5.37	1.34	1.37
44	1	665	A	C5-C4	-5.37	1.34	1.38
44	1	683	U	C2-N3	-5.37	1.33	1.37
45	2	103	G	N1-C2	-5.37	1.33	1.37
44	1	668	G	C6-N1	-5.37	1.35	1.39
44	1	268	A	N7-C5	-5.37	1.36	1.39
44	1	1406	A	C5-C4	-5.37	1.34	1.38
44	1	1419	A	C5-C4	-5.37	1.34	1.38
44	1	1496	C	C4-N4	-5.37	1.29	1.33
44	1	28	C	C4-N4	-5.36	1.29	1.33
44	1	1363	A	N9-C8	-5.36	1.33	1.37
44	1	1389	G	N7-C5	-5.36	1.36	1.39
44	1	706	A	C6-N6	-5.36	1.29	1.33
20	X	86	VAL	CB-CG1	-5.36	1.41	1.52
44	1	1366	A	N9-C4	-5.36	1.34	1.37
44	1	1377	G	N7-C5	-5.36	1.36	1.39
44	1	1436	U	N1-C2	-5.36	1.33	1.38
44	1	1506	A	N9-C4	-5.36	1.34	1.37
44	1	696	C	C4-N4	-5.36	1.29	1.33
44	1	1590	G	N7-C5	-5.36	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	VAL	CB-CG1	-5.36	1.41	1.52
44	1	1179	A	C6-N1	-5.36	1.31	1.35
44	1	2360	C	N3-C4	-5.36	1.30	1.33
44	1	3213	A	N7-C5	-5.36	1.36	1.39
45	2	24	G	N3-C4	-5.36	1.31	1.35
44	1	1402	C	N3-C4	-5.35	1.30	1.33
44	1	3296	A	N7-C5	-5.35	1.36	1.39
1	B	92	TYR	CD1-CE1	-5.35	1.31	1.39
5	G	139	VAL	CB-CG2	-5.35	1.41	1.52
44	1	235	A	N9-C4	-5.35	1.34	1.37
44	1	312	C	C4-C5	-5.35	1.38	1.43
45	2	43	A	C5-C4	-5.35	1.35	1.38
45	2	68	G	N7-C5	-5.35	1.36	1.39
44	1	406	G	N9-C4	-5.35	1.33	1.38
44	1	637	C	N3-C4	-5.35	1.30	1.33
44	1	661	G	N3-C4	-5.35	1.31	1.35
44	1	1307	G	C8-N7	-5.35	1.27	1.30
44	1	282	G	C6-N1	-5.35	1.35	1.39
44	1	436	A	N9-C4	-5.35	1.34	1.37
44	1	396	A	N9-C8	-5.35	1.33	1.37
44	1	333	G	N7-C5	-5.34	1.36	1.39
44	1	1474	A	N7-C5	-5.34	1.36	1.39
44	1	2368	A	N9-C4	-5.34	1.34	1.37
44	1	74	G	N9-C4	-5.34	1.33	1.38
44	1	1365	G	C6-N1	-5.34	1.35	1.39
44	1	51	A	N9-C8	-5.34	1.33	1.37
44	1	729	C	C4-C5	-5.34	1.38	1.43
44	1	1603	A	C6-N6	-5.34	1.29	1.33
44	1	2910	A	C5-C6	-5.34	1.36	1.41
45	2	105	A	N9-C4	-5.34	1.34	1.37
44	1	1177	G	C8-N7	-5.34	1.27	1.30
44	1	1433	A	C6-N6	-5.34	1.29	1.33
2	C	109	TRP	CE2-CZ2	-5.34	1.30	1.39
4	F	134	VAL	CB-CG1	-5.34	1.41	1.52
44	1	1204	A	C5-C6	-5.34	1.36	1.41
44	1	2353	G	C6-N1	-5.34	1.35	1.39
44	1	3046	A	N7-C5	-5.34	1.36	1.39
45	2	35	C	C5-C6	-5.34	1.30	1.34
44	1	387	A	N7-C5	-5.33	1.36	1.39
44	1	2361	A	N7-C5	-5.33	1.36	1.39
44	1	2912	G	N7-C5	-5.33	1.36	1.39
10	N	64	VAL	CB-CG2	-5.33	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	357	A	C5-C4	-5.33	1.35	1.38
44	1	516	A	C5-C6	-5.33	1.36	1.41
10	N	150	TRP	CB-CG	-5.33	1.40	1.50
44	1	928	C	N1-C6	-5.33	1.33	1.37
44	1	1169	A	C5-C6	-5.33	1.36	1.41
44	1	689	U	C2-N3	-5.33	1.34	1.37
21	Y	80	VAL	CB-CG2	-5.33	1.41	1.52
44	1	3035	A	C5-C6	-5.33	1.36	1.41
44	1	140	C	C4-C5	-5.32	1.38	1.43
44	1	385	A	N9-C4	-5.32	1.34	1.37
44	1	1429	G	N3-C4	-5.32	1.31	1.35
44	1	508	U	C4-C5	-5.32	1.38	1.43
44	1	693	A	C5-C4	-5.32	1.35	1.38
10	N	106	VAL	CB-CG2	-5.32	1.41	1.52
44	1	3005	A	N9-C4	-5.32	1.34	1.37
44	1	1332	A	C5-C4	-5.32	1.35	1.38
44	1	2378	C	N3-C4	-5.32	1.30	1.33
44	1	1152	G	N1-C2	-5.32	1.33	1.37
44	1	29	C	C5-C6	-5.31	1.30	1.34
44	1	335	G	N9-C4	-5.31	1.33	1.38
44	1	1510	G	N9-C8	-5.31	1.34	1.37
12	P	88	VAL	CB-CG2	-5.31	1.41	1.52
44	1	409	A	N9-C4	-5.31	1.34	1.37
44	1	1297	C	N1-C6	-5.31	1.33	1.37
44	1	270	U	C4-C5	-5.31	1.38	1.43
44	1	1336	U	C4-C5	-5.31	1.38	1.43
44	1	1494	U	C4-C5	-5.31	1.38	1.43
44	1	1883	A	N7-C5	-5.31	1.36	1.39
44	1	355	A	N9-C8	-5.31	1.33	1.37
44	1	641	C	C4-C5	-5.31	1.38	1.43
44	1	1464	G	C6-N1	-5.30	1.35	1.39
44	1	1498	A	C6-N6	-5.30	1.29	1.33
44	1	3012	A	N9-C4	-5.30	1.34	1.37
44	1	622	A	C5-C6	-5.30	1.36	1.41
45	2	143	U	N1-C6	-5.30	1.33	1.38
44	1	68	C	C4-C5	-5.30	1.38	1.43
44	1	787	G	N9-C8	-5.30	1.34	1.37
44	1	1834	U	C2-N3	-5.30	1.34	1.37
45	2	133	G	N9-C8	-5.30	1.34	1.37
44	1	36	C	C4-C5	-5.30	1.38	1.43
44	1	366	A	C8-N7	-5.30	1.27	1.31
44	1	1359	C	N3-C4	-5.30	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1160	C	N3-C4	-5.30	1.30	1.33
44	1	1318	A	N3-C4	-5.30	1.31	1.34
44	1	3299	A	C5-C6	-5.30	1.36	1.41
44	1	3140	G	N9-C4	-5.30	1.33	1.38
44	1	209	A	C5-C6	-5.29	1.36	1.41
44	1	1449	A	N9-C4	-5.29	1.34	1.37
44	1	1171	G	N7-C5	-5.29	1.36	1.39
44	1	1306	G	N9-C8	-5.29	1.34	1.37
44	1	2354	C	C4-N4	-5.29	1.29	1.33
44	1	3141	A	N7-C5	-5.29	1.36	1.39
44	1	3172	A	C6-N6	-5.29	1.29	1.33
11	O	109	PRO	N-CA	-5.29	1.38	1.47
27	e	64	LYS	CB-CG	-5.29	1.38	1.52
44	1	364	G	C6-N1	-5.29	1.35	1.39
44	1	425	G	N9-C8	-5.29	1.34	1.37
44	1	428	A	N9-C4	-5.29	1.34	1.37
44	1	48	A	N9-C4	-5.28	1.34	1.37
44	1	123	A	N3-C4	-5.28	1.31	1.34
45	2	146	U	C4-C5	-5.28	1.38	1.43
46	6	42	G	C2-N3	-5.28	1.28	1.32
44	1	1427	U	C4-C5	-5.28	1.38	1.43
44	1	1444	G	C5-C6	-5.28	1.37	1.42
44	1	328	U	C4-C5	-5.28	1.38	1.43
44	1	405	U	N1-C2	-5.28	1.33	1.38
44	1	1168	U	C4-C5	-5.28	1.38	1.43
44	1	227	G	C6-N1	-5.28	1.35	1.39
44	1	1433	A	C5-C4	-5.28	1.35	1.38
44	1	1362	G	N9-C8	-5.28	1.34	1.37
44	1	1374	G	N9-C8	-5.27	1.34	1.37
44	1	1587	A	N9-C4	-5.27	1.34	1.37
44	1	637	C	C5-C6	-5.27	1.30	1.34
44	1	3273	A	C5-C6	-5.27	1.36	1.41
44	1	1378	U	N1-C6	-5.27	1.33	1.38
44	1	1536	G	N9-C4	-5.27	1.33	1.38
44	1	687	U	C4-C5	-5.27	1.38	1.43
12	P	26	PHE	CB-CG	-5.26	1.42	1.51
44	1	209	A	N9-C4	-5.26	1.34	1.37
44	1	422	A	N7-C5	-5.26	1.36	1.39
44	1	1423	C	C5-C6	-5.26	1.30	1.34
45	2	133	G	N7-C5	-5.26	1.36	1.39
44	1	676	G	C5-C6	-5.26	1.37	1.42
44	1	1105	A	N7-C5	-5.26	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1179	A	C5-C4	-5.26	1.35	1.38
44	1	1193	A	C5-C6	-5.26	1.36	1.41
44	1	1161	G	C5-C4	-5.26	1.34	1.38
44	1	3097	C	C5-C6	-5.26	1.30	1.34
44	1	376	G	N7-C5	-5.26	1.36	1.39
44	1	2380	U	C4-C5	-5.26	1.38	1.43
44	1	801	A	C5-C4	-5.26	1.35	1.38
44	1	936	A	C5-C4	-5.26	1.35	1.38
44	1	3180	A	N9-C4	-5.26	1.34	1.37
44	1	432	G	C6-N1	-5.25	1.35	1.39
44	1	2353	G	N3-C4	-5.25	1.31	1.35
45	2	131	A	N9-C4	-5.25	1.34	1.37
44	1	88	A	C6-N6	-5.25	1.29	1.33
44	1	703	G	N1-C2	-5.25	1.33	1.37
44	1	931	C	C5-C6	-5.25	1.30	1.34
44	1	1161	G	C6-N1	-5.25	1.35	1.39
44	1	3004	C	N1-C6	-5.25	1.33	1.37
44	1	1163	A	C5-C4	-5.25	1.35	1.38
44	1	1835	A	N7-C5	-5.25	1.36	1.39
45	2	65	A	N7-C5	-5.25	1.36	1.39
44	1	1407	A	N9-C8	-5.25	1.33	1.37
44	1	399	A	N9-C8	-5.25	1.33	1.37
44	1	622	A	C6-N6	-5.25	1.29	1.33
44	1	3091	A	N9-C8	-5.25	1.33	1.37
44	1	3139	A	C5-C4	-5.25	1.35	1.38
44	1	3310	A	N7-C5	-5.25	1.36	1.39
20	X	86	VAL	CB-CG2	-5.25	1.41	1.52
44	1	1411	C	N1-C6	-5.25	1.34	1.37
44	1	291	C	C4-N4	-5.24	1.29	1.33
44	1	1158	A	N9-C4	-5.24	1.34	1.37
45	2	129	C	N3-C4	-5.24	1.30	1.33
44	1	929	A	N9-C8	-5.24	1.33	1.37
44	1	1835	A	N9-C4	-5.24	1.34	1.37
45	2	66	A	C6-N6	-5.24	1.29	1.33
44	1	1174	G	N9-C8	-5.24	1.34	1.37
44	1	1298	C	N1-C6	-5.24	1.34	1.37
44	1	1410	U	N1-C2	-5.24	1.33	1.38
44	1	50	U	C4-C5	-5.24	1.38	1.43
44	1	1168	U	C2-N3	-5.24	1.34	1.37
44	1	343	U	N1-C6	-5.24	1.33	1.38
44	1	1156	C	N1-C6	-5.24	1.34	1.37
44	1	1163	A	C6-N6	-5.24	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	12	A	N3-C4	-5.24	1.31	1.34
45	2	45	C	N3-C4	-5.24	1.30	1.33
44	1	630	A	N9-C4	-5.23	1.34	1.37
44	1	1392	G	N3-C4	-5.23	1.31	1.35
44	1	99	A	N7-C5	-5.23	1.36	1.39
44	1	662	U	N1-C2	-5.23	1.33	1.38
44	1	1308	A	C6-N1	-5.23	1.31	1.35
44	1	1430	U	C4-C5	-5.23	1.38	1.43
44	1	1562	C	N3-C4	-5.23	1.30	1.33
44	1	220	G	N1-C2	-5.23	1.33	1.37
45	2	107	G	N7-C5	-5.23	1.36	1.39
44	1	62	A	N9-C8	-5.22	1.33	1.37
44	1	793	C	C5-C6	-5.22	1.30	1.34
44	1	1343	A	N9-C4	-5.22	1.34	1.37
44	1	1389	G	N9-C8	-5.22	1.34	1.37
44	1	2378	C	C4-C5	-5.22	1.38	1.43
44	1	51	A	C6-N6	-5.22	1.29	1.33
44	1	789	A	N7-C5	-5.22	1.36	1.39
44	1	1112	A	C5-C6	-5.22	1.36	1.41
44	1	1563	C	C4-C5	-5.22	1.38	1.43
44	1	1609	C	N1-C6	-5.22	1.34	1.37
45	2	47	C	N3-C4	-5.22	1.30	1.33
44	1	363	G	N9-C4	-5.22	1.33	1.38
44	1	811	U	N1-C6	-5.22	1.33	1.38
44	1	1339	C	N3-C4	-5.22	1.30	1.33
1	B	158	VAL	CB-CG1	-5.22	1.41	1.52
44	1	10	C	N3-C4	-5.22	1.30	1.33
44	1	125	C	C4-C5	-5.22	1.38	1.43
12	P	139	TYR	CD1-CE1	-5.21	1.31	1.39
44	1	696	C	N1-C6	-5.21	1.34	1.37
44	1	1333	C	C4-N4	-5.21	1.29	1.33
44	1	1410	U	N1-C6	-5.21	1.33	1.38
44	1	1421	G	N7-C5	-5.21	1.36	1.39
44	1	3273	A	N9-C8	-5.21	1.33	1.37
44	1	1375	G	N7-C5	-5.21	1.36	1.39
44	1	154	U	N1-C6	-5.21	1.33	1.38
44	1	397	A	N9-C4	-5.21	1.34	1.37
44	1	1308	A	N9-C4	-5.21	1.34	1.37
44	1	1422	G	C5-C6	-5.21	1.37	1.42
44	1	291	C	N3-C4	-5.21	1.30	1.33
44	1	415	G	N7-C5	-5.21	1.36	1.39
44	1	221	A	N7-C5	-5.21	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	1407	A	N1-C2	-5.21	1.29	1.34
44	1	1169	A	C6-N6	-5.21	1.29	1.33
44	1	1309	U	N1-C6	-5.20	1.33	1.38
44	1	432	G	N9-C8	-5.20	1.34	1.37
44	1	950	G	C6-N1	-5.20	1.35	1.39
44	1	1787	A	N9-C4	-5.20	1.34	1.37
45	2	97	A	C5-C6	-5.20	1.36	1.41
44	1	55	G	N1-C2	-5.20	1.33	1.37
44	1	1453	A	N9-C4	-5.20	1.34	1.37
45	2	26	U	N3-C4	-5.20	1.33	1.38
10	N	121	VAL	CB-CG1	-5.20	1.42	1.52
44	1	1155	C	N1-C6	-5.20	1.34	1.37
44	1	701	G	C8-N7	-5.20	1.27	1.30
44	1	2891	U	N1-C6	-5.20	1.33	1.38
44	1	2906	C	N3-C4	-5.20	1.30	1.33
45	2	16	G	C2-N3	-5.20	1.28	1.32
45	2	18	U	N1-C2	-5.19	1.33	1.38
44	1	787	G	N9-C4	-5.19	1.33	1.38
44	1	814	U	C4-C5	-5.19	1.38	1.43
44	1	1147	G	C8-N7	-5.19	1.27	1.30
44	1	1369	A	N9-C8	-5.19	1.33	1.37
44	1	1434	G	C6-N1	-5.19	1.35	1.39
44	1	33	G	C5-C6	-5.19	1.37	1.42
44	1	3136	G	N9-C8	-5.19	1.34	1.37
44	1	591	G	N9-C8	-5.19	1.34	1.37
4	F	87	VAL	CB-CG2	-5.19	1.42	1.52
44	1	14	U	N1-C6	-5.19	1.33	1.38
44	1	405	U	N3-C4	-5.19	1.33	1.38
44	1	1881	A	N7-C5	-5.19	1.36	1.39
44	1	1310	G	N1-C2	-5.18	1.33	1.37
45	2	98	U	C2-N3	-5.18	1.34	1.37
45	2	140	G	N7-C5	-5.18	1.36	1.39
44	1	411	U	N3-C4	-5.18	1.33	1.38
44	1	1593	A	N9-C4	-5.18	1.34	1.37
44	1	3210	A	N9-C4	-5.18	1.34	1.37
45	2	13	A	C5-C4	-5.18	1.35	1.38
44	1	3187	A	C6-N6	-5.18	1.29	1.33
44	1	1223	A	N7-C5	-5.18	1.36	1.39
44	1	1314	C	N3-C4	-5.18	1.30	1.33
44	1	940	G	N3-C4	-5.18	1.31	1.35
44	1	950	G	C5-C6	-5.18	1.37	1.42
44	1	370	U	C4-C5	-5.17	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	783	A	N9-C4	-5.17	1.34	1.37
44	1	1382	G	N1-C2	-5.17	1.33	1.37
44	1	1615	C	N3-C4	-5.17	1.30	1.33
44	1	20	A	N7-C5	-5.17	1.36	1.39
44	1	1408	G	N9-C4	-5.17	1.33	1.38
44	1	327	A	N9-C8	-5.17	1.33	1.37
32	j	45	ARG	CZ-NH2	-5.17	1.26	1.33
44	1	647	A	N9-C8	-5.17	1.33	1.37
45	2	102	U	C4-C5	-5.17	1.38	1.43
44	1	638	C	N1-C6	-5.17	1.34	1.37
44	1	929	A	C5-C6	-5.17	1.36	1.41
44	1	1404	G	N3-C4	-5.17	1.31	1.35
44	1	1798	A	N7-C5	-5.17	1.36	1.39
45	2	17	A	C6-N6	-5.17	1.29	1.33
44	1	1194	G	N9-C8	-5.17	1.34	1.37
44	1	3129	A	N9-C4	-5.16	1.34	1.37
28	f	81	VAL	CB-CG2	-5.16	1.42	1.52
44	1	657	A	N9-C8	-5.16	1.33	1.37
44	1	1180	A	N9-C4	-5.16	1.34	1.37
44	1	1338	C	C5-C6	-5.16	1.30	1.34
44	1	64	G	C8-N7	-5.16	1.27	1.30
45	2	11	C	N1-C6	-5.16	1.34	1.37
11	O	120	VAL	CB-CG1	-5.16	1.42	1.52
44	1	1435	A	N9-C8	-5.16	1.33	1.37
44	1	1442	U	N1-C6	-5.16	1.33	1.38
44	1	1475	A	C6-N6	-5.16	1.29	1.33
44	1	3372	A	C6-N1	-5.16	1.31	1.35
45	2	104	A	C8-N7	-5.16	1.27	1.31
45	2	106	C	N3-C4	-5.16	1.30	1.33
44	1	81	C	N3-C4	-5.15	1.30	1.33
44	1	429	U	N1-C6	-5.15	1.33	1.38
44	1	433	A	C5-C6	-5.15	1.36	1.41
44	1	639	G	N9-C4	-5.15	1.33	1.38
44	1	658	G	C8-N7	-5.15	1.27	1.30
44	1	3134	A	N9-C4	-5.15	1.34	1.37
44	1	1408	G	C5-C4	-5.15	1.34	1.38
44	1	1504	A	N7-C5	-5.15	1.36	1.39
44	1	2890	A	C5-C6	-5.15	1.36	1.41
2	C	50	TYR	CD1-CE1	-5.15	1.31	1.39
45	2	61	A	N3-C4	-5.15	1.31	1.34
44	1	18	G	C8-N7	-5.15	1.27	1.30
44	1	59	G	N1-C2	-5.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	102	C	C5-C6	-5.15	1.30	1.34
44	1	799	G	N7-C5	-5.15	1.36	1.39
44	1	1211	U	N1-C6	-5.15	1.33	1.38
44	1	1377	G	N1-C2	-5.15	1.33	1.37
44	1	22	G	C6-N1	-5.14	1.35	1.39
44	1	366	A	N9-C8	-5.14	1.33	1.37
44	1	406	G	N1-C2	-5.14	1.33	1.37
44	1	700	C	N3-C4	-5.14	1.30	1.33
44	1	1162	U	C5-C6	-5.14	1.29	1.34
44	1	1308	A	C5-C4	-5.14	1.35	1.38
44	1	2365	C	N1-C6	-5.14	1.34	1.37
45	2	14	C	C5-C6	-5.14	1.30	1.34
45	2	89	A	N7-C5	-5.14	1.36	1.39
44	1	496	C	C4-C5	-5.14	1.38	1.43
44	1	634	C	N3-C4	-5.14	1.30	1.33
44	1	1833	G	N9-C8	-5.14	1.34	1.37
45	2	34	U	N1-C6	-5.14	1.33	1.38
45	2	103	G	N3-C4	-5.14	1.31	1.35
44	1	368	G	C5-C6	-5.14	1.37	1.42
44	1	1478	C	C4-C5	-5.14	1.38	1.43
44	1	1200	A	N9-C4	-5.14	1.34	1.37
44	1	1446	A	N3-C4	-5.14	1.31	1.34
44	1	3146	G	N9-C8	-5.14	1.34	1.37
44	1	146	U	C2-N3	-5.13	1.34	1.37
44	1	198	A	C6-N6	-5.13	1.29	1.33
10	N	8	GLU	CB-CG	-5.13	1.42	1.52
44	1	3172	A	N9-C4	-5.13	1.34	1.37
45	2	72	A	N9-C4	-5.13	1.34	1.37
44	1	224	C	N3-C4	-5.13	1.30	1.33
44	1	810	A	N3-C4	-5.13	1.31	1.34
44	1	942	U	N3-C4	-5.13	1.33	1.38
44	1	1313	G	N9-C4	-5.13	1.33	1.38
44	1	416	A	C5-C6	-5.13	1.36	1.41
44	1	1333	C	N1-C6	-5.13	1.34	1.37
44	1	501	A	N7-C5	-5.13	1.36	1.39
44	1	1333	C	C5-C6	-5.13	1.30	1.34
44	1	20	A	C5-C4	-5.12	1.35	1.38
44	1	361	A	N3-C4	-5.12	1.31	1.34
44	1	1832	C	C5-C6	-5.12	1.30	1.34
44	1	1461	A	C5-C6	-5.12	1.36	1.41
12	P	29	THR	CB-CG2	-5.12	1.35	1.52
44	1	1477	A	C6-N6	-5.12	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	104	A	N3-C4	-5.12	1.31	1.34
44	1	1613	A	N3-C4	-5.12	1.31	1.34
10	N	119	TYR	CD1-CE1	-5.12	1.31	1.39
44	1	931	C	N3-C4	-5.12	1.30	1.33
44	1	1585	C	C4-C5	-5.12	1.38	1.43
44	1	1599	G	N7-C5	-5.12	1.36	1.39
44	1	1182	A	C5-C6	-5.11	1.36	1.41
44	1	3372	A	C6-N6	-5.11	1.29	1.33
45	2	29	U	C4-C5	-5.11	1.39	1.43
45	2	114	G	N9-C4	-5.11	1.33	1.38
44	1	523	A	N9-C4	-5.11	1.34	1.37
44	1	32	U	C2-N3	-5.11	1.34	1.37
44	1	335	G	C5-C6	-5.11	1.37	1.42
44	1	345	G	C8-N7	-5.11	1.27	1.30
44	1	429	U	C2-N3	-5.11	1.34	1.37
44	1	1534	A	N7-C5	-5.11	1.36	1.39
44	1	3000	A	C6-N6	-5.11	1.29	1.33
44	1	1209	G	N9-C8	-5.11	1.34	1.37
44	1	214	G	C5-C4	-5.11	1.34	1.38
44	1	503	C	C4-N4	-5.11	1.29	1.33
44	1	694	C	N1-C6	-5.11	1.34	1.37
44	1	975	C	N3-C4	-5.11	1.30	1.33
44	1	1279	C	C4-C5	-5.11	1.38	1.43
44	1	2911	A	N9-C4	-5.11	1.34	1.37
44	1	3097	C	N1-C6	-5.11	1.34	1.37
44	1	334	A	C5-C4	-5.10	1.35	1.38
44	1	3077	A	N9-C4	-5.10	1.34	1.37
44	1	1110	U	N1-C2	-5.10	1.33	1.38
44	1	1531	C	C4-C5	-5.10	1.38	1.43
44	1	80	G	N7-C5	-5.10	1.36	1.39
44	1	2345	A	C5-C6	-5.10	1.36	1.41
20	X	114	VAL	CB-CG2	-5.10	1.42	1.52
44	1	47	C	N1-C6	-5.10	1.34	1.37
44	1	583	G	C2-N2	-5.10	1.29	1.34
44	1	1279	C	N1-C6	-5.10	1.34	1.37
44	1	502	U	C4-C5	-5.10	1.39	1.43
44	1	2914	G	N1-C2	-5.10	1.33	1.37
10	N	184	LYS	CA-CB	-5.09	1.42	1.53
44	1	688	G	N9-C8	-5.09	1.34	1.37
44	1	692	A	N7-C5	-5.09	1.36	1.39
44	1	1441	G	C6-N1	-5.09	1.35	1.39
44	1	3186	A	N7-C5	-5.09	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	22	VAL	CB-CG2	-5.09	1.42	1.52
44	1	225	C	C5-C6	-5.09	1.30	1.34
5	G	55	TYR	CE2-CZ	-5.09	1.31	1.38
44	1	660	A	C5-C6	-5.09	1.36	1.41
44	1	1610	G	N9-C8	-5.09	1.34	1.37
44	1	1697	A	N9-C4	-5.09	1.34	1.37
44	1	3185	U	C2-N3	-5.09	1.34	1.37
44	1	21	G	N9-C8	-5.08	1.34	1.37
44	1	654	C	N3-C4	-5.08	1.30	1.33
44	1	685	G	N9-C4	-5.08	1.33	1.38
44	1	611	A	C5-C4	-5.08	1.35	1.38
44	1	690	A	N7-C5	-5.08	1.36	1.39
44	1	1610	G	N9-C4	-5.08	1.33	1.38
44	1	1447	G	C2-N3	-5.08	1.28	1.32
44	1	583	G	N1-C2	-5.08	1.33	1.37
44	1	3298	C	C4-C5	-5.08	1.38	1.43
27	e	32	TRP	CG-CD1	-5.08	1.29	1.36
44	1	320	G	C5-C4	-5.08	1.34	1.38
44	1	417	A	C6-N6	-5.08	1.29	1.33
44	1	660	A	C2-N3	-5.08	1.28	1.33
44	1	1319	G	C5-C4	-5.08	1.34	1.38
44	1	358	G	N3-C4	-5.08	1.31	1.35
44	1	13	A	N7-C5	-5.08	1.36	1.39
44	1	114	A	N9-C4	-5.08	1.34	1.37
44	1	3295	A	C6-N6	-5.08	1.29	1.33
12	P	139	TYR	CD2-CE2	-5.07	1.31	1.39
44	1	155	G	N1-C2	-5.07	1.33	1.37
44	1	364	G	N1-C2	-5.07	1.33	1.37
44	1	3002	C	N3-C4	-5.07	1.30	1.33
44	1	1642	A	N9-C4	-5.07	1.34	1.37
45	2	42	G	C6-N1	-5.07	1.35	1.39
15	S	156	VAL	CB-CG2	-5.07	1.42	1.52
44	1	817	A	C6-N6	-5.07	1.29	1.33
44	1	1550	C	C4-C5	-5.07	1.38	1.43
44	1	1330	A	C5-C4	-5.07	1.35	1.38
44	1	801	A	N9-C8	-5.07	1.33	1.37
44	1	354	U	C2-N3	-5.06	1.34	1.37
44	1	1283	C	C4-C5	-5.06	1.38	1.43
44	1	1378	U	N3-C4	-5.06	1.33	1.38
44	1	323	A	N9-C8	-5.06	1.33	1.37
44	1	354	U	C5-C6	-5.06	1.29	1.34
44	1	3248	C	N3-C4	-5.06	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	55	G	N7-C5	-5.06	1.36	1.39
44	1	75	G	C8-N7	-5.06	1.27	1.30
44	1	789	A	C6-N6	-5.06	1.29	1.33
44	1	929	A	N3-C4	-5.06	1.31	1.34
44	1	1317	A	N3-C4	-5.06	1.31	1.34
44	1	1430	U	C2-N3	-5.06	1.34	1.37
45	2	40	A	C5-C6	-5.06	1.36	1.41
44	1	122	A	C6-N6	-5.06	1.29	1.33
44	1	431	U	C4-C5	-5.05	1.39	1.43
44	1	1148	G	N3-C4	-5.05	1.31	1.35
44	1	3089	C	N3-C4	-5.05	1.30	1.33
44	1	3240	C	N3-C4	-5.05	1.30	1.33
44	1	365	A	N9-C8	-5.05	1.33	1.37
44	1	1099	A	N9-C4	-5.05	1.34	1.37
44	1	1181	U	N1-C2	-5.05	1.34	1.38
2	C	100	PHE	CD1-CE1	-5.05	1.29	1.39
44	1	792	G	C8-N7	-5.05	1.27	1.30
44	1	1387	G	N7-C5	-5.05	1.36	1.39
44	1	59	G	N9-C8	-5.05	1.34	1.37
44	1	2906	C	C4-C5	-5.04	1.39	1.43
44	1	360	G	N1-C2	-5.04	1.33	1.37
44	1	1387	G	C8-N7	-5.04	1.27	1.30
44	1	3045	G	N9-C8	-5.04	1.34	1.37
45	2	33	A	N7-C5	-5.04	1.36	1.39
24	b	33	ILE	C-N	-5.04	1.22	1.34
44	1	325	A	C5-C4	-5.04	1.35	1.38
44	1	338	A	C5-C4	-5.04	1.35	1.38
44	1	355	A	C5-C4	-5.04	1.35	1.38
44	1	2878	G	C2-N3	-5.04	1.28	1.32
44	1	3182	G	N9-C4	-5.04	1.33	1.38
1	B	85	VAL	CB-CG1	-5.04	1.42	1.52
44	1	650	C	N1-C6	-5.04	1.34	1.37
44	1	971	G	N7-C5	-5.04	1.36	1.39
44	1	1366	A	C6-N6	-5.04	1.29	1.33
21	Y	8	VAL	CB-CG2	-5.04	1.42	1.52
44	1	1396	C	N1-C6	-5.04	1.34	1.37
45	2	9	A	C6-N6	-5.04	1.29	1.33
44	1	1446	A	N7-C5	-5.03	1.36	1.39
44	1	2887	A	C5-C6	-5.03	1.36	1.41
44	1	875	G	C8-N7	-5.03	1.27	1.30
27	e	95	GLU	CB-CG	-5.03	1.42	1.52
44	1	200	C	C2-N3	-5.03	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	367	A	C5-C4	-5.03	1.35	1.38
44	1	674	G	N9-C8	-5.03	1.34	1.37
11	O	88	VAL	CB-CG2	-5.03	1.42	1.52
44	1	813	G	N9-C8	-5.03	1.34	1.37
44	1	1394	A	N7-C5	-5.03	1.36	1.39
44	1	1406	A	N9-C8	-5.03	1.33	1.37
44	1	334	A	N9-C8	-5.03	1.33	1.37
32	j	66	TYR	CD1-CE1	-5.03	1.31	1.39
44	1	802	C	N3-C4	-5.03	1.30	1.33
44	1	1311	G	N9-C8	-5.03	1.34	1.37
44	1	1424	C	C4-N4	-5.03	1.29	1.33
44	1	3047	U	C4-C5	-5.03	1.39	1.43
44	1	3096	C	N3-C4	-5.03	1.30	1.33
44	1	24	G	N7-C5	-5.02	1.36	1.39
44	1	82	C	N1-C6	-5.02	1.34	1.37
44	1	1837	U	C4-C5	-5.02	1.39	1.43
44	1	3161	C	C4-C5	-5.02	1.39	1.43
45	2	25	G	N3-C4	-5.02	1.31	1.35
44	1	106	A	C5-C4	-5.02	1.35	1.38
44	1	1410	U	C4-C5	-5.02	1.39	1.43
44	1	336	A	C5-C6	-5.02	1.36	1.41
44	1	658	G	C6-N1	-5.02	1.36	1.39
44	1	947	G	C5-C6	-5.02	1.37	1.42
44	1	3113	A	C5-C6	-5.02	1.36	1.41
44	1	426	G	N9-C8	-5.02	1.34	1.37
44	1	1443	G	N9-C4	-5.02	1.33	1.38
13	Q	48	VAL	CB-CG2	-5.01	1.42	1.52
44	1	269	G	N9-C4	-5.01	1.33	1.38
44	1	1339	C	N1-C6	-5.01	1.34	1.37
44	1	1180	A	C5-C6	-5.01	1.36	1.41
44	1	1335	C	C4-N4	-5.01	1.29	1.33
44	1	1806	A	C5-C6	-5.01	1.36	1.41
45	2	97	A	N7-C5	-5.01	1.36	1.39
44	1	583	G	N9-C4	-5.01	1.33	1.38
44	1	678	G	N7-C5	-5.01	1.36	1.39
44	1	1825	G	N9-C4	-5.01	1.33	1.38
44	1	361	A	N9-C4	-5.00	1.34	1.37
44	1	1147	G	C5-C6	-5.00	1.37	1.42
44	1	1326	A	N9-C8	-5.00	1.33	1.37
44	1	3043	C	C4-C5	-5.00	1.39	1.43
44	1	98	G	N9-C8	-5.00	1.34	1.37
44	1	930	U	N3-C4	-5.00	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	2351	U	C4-C5	-5.00	1.39	1.43

All (3781) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	630	A	N1-C6-N6	17.03	128.82	118.60
44	1	630	A	C5-C6-N6	-16.99	110.11	123.70
44	1	1363	A	C5-C6-N6	-16.56	110.45	123.70
44	1	630	A	C4-C5-N7	16.19	118.79	110.70
44	1	1159	A	C5-C6-N6	-15.59	111.23	123.70
45	2	14	C	C5-C4-N4	-15.43	109.40	120.20
44	1	945	C	C5-C4-N4	-15.41	109.41	120.20
44	1	1376	C	C6-N1-C2	-15.32	114.17	120.30
44	1	3308	C	C5-C4-N4	-14.73	109.89	120.20
44	1	804	C	C5-C4-N4	-14.68	109.93	120.20
44	1	1363	A	N1-C6-N6	14.49	127.29	118.60
45	2	40	A	N1-C6-N6	-14.40	109.96	118.60
44	1	1496	C	N1-C2-O2	14.23	127.44	118.90
44	1	3004	C	C5-C4-N4	-14.19	110.27	120.20
44	1	630	A	C5-N7-C8	-14.17	96.82	103.90
44	1	352	A	C5-C6-N1	14.04	124.72	117.70
44	1	1337	A	C5-C6-N6	-13.96	112.53	123.70
44	1	428	A	C5-C6-N6	-13.82	112.64	123.70
44	1	1332	A	C4-C5-N7	13.70	117.55	110.70
44	1	1594	A	C5-C6-N1	13.60	124.50	117.70
44	1	1527	C	C6-N1-C2	-13.49	114.90	120.30
44	1	106	A	C5-C6-N1	13.46	124.43	117.70
44	1	630	A	N9-C4-C5	-13.46	100.42	105.80
44	1	633	C	C5-C4-N4	-13.16	110.99	120.20
44	1	16	A	C4-C5-N7	13.11	117.26	110.70
44	1	1496	C	C6-N1-C2	-13.05	115.08	120.30
44	1	16	A	C5-C6-N6	-13.01	113.29	123.70
45	2	10	A	C5-C6-N6	-12.94	113.34	123.70
45	2	21	C	C6-N1-C2	-12.83	115.17	120.30
44	1	589	A	C5-C6-N1	12.81	124.10	117.70
44	1	16	A	N1-C6-N6	12.76	126.26	118.60
44	1	637	C	C6-N1-C2	-12.74	115.20	120.30
44	1	1426	C	C5-C4-N4	-12.64	111.35	120.20
44	1	16	A	C5-N7-C8	-12.61	97.60	103.90
44	1	2354	C	C5-C4-N4	-12.54	111.42	120.20
44	1	344	A	C5-C6-N6	-12.52	113.69	123.70
45	2	44	A	C5-C6-N1	12.40	123.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1165	A	C5-C6-N1	12.35	123.87	117.70
44	1	1496	C	C2-N1-C1'	12.32	132.35	118.80
32	j	45	ARG	NE-CZ-NH1	12.27	126.43	120.30
44	1	373	A	C5-C6-N6	-12.22	113.92	123.70
44	1	1332	A	C5-N7-C8	-12.20	97.80	103.90
44	1	357	A	C5-C6-N6	-12.19	113.95	123.70
45	2	14	C	N3-C4-N4	12.15	126.50	118.00
44	1	1437	C	C6-N1-C2	-12.13	115.45	120.30
44	1	793	C	C5-C4-N4	-12.12	111.72	120.20
44	1	975	C	N1-C2-O2	12.12	126.17	118.90
44	1	1163	A	C5-C6-N6	-12.11	114.01	123.70
44	1	630	A	C6-C5-N7	-12.10	123.83	132.30
44	1	1330	A	C5-C6-N6	-12.06	114.05	123.70
44	1	323	A	C4-C5-N7	12.03	116.72	110.70
44	1	213	A	N1-C6-N6	-12.01	111.39	118.60
44	1	1146	C	C6-N1-C2	-11.98	115.51	120.30
44	1	428	A	C5-C6-N1	11.97	123.69	117.70
45	2	94	C	C5-C4-N4	-11.88	111.88	120.20
45	2	44	A	C5-C6-N6	-11.84	114.23	123.70
44	1	1159	A	C5-C6-N1	11.82	123.61	117.70
44	1	3217	C	N1-C2-O2	11.80	125.98	118.90
44	1	634	C	C5-C4-N4	-11.79	111.95	120.20
44	1	1332	A	C6-C5-N7	-11.78	124.06	132.30
44	1	323	A	C5-N7-C8	-11.77	98.02	103.90
45	2	40	A	C5-C6-N1	11.76	123.58	117.70
45	2	19	C	C5-C4-N4	-11.76	111.97	120.20
44	1	325	A	C5-C6-N1	11.76	123.58	117.70
44	1	350	C	C5-C4-N4	-11.74	111.98	120.20
44	1	29	C	C5-C4-N4	-11.71	112.00	120.20
44	1	357	A	C5-C6-N1	11.65	123.53	117.70
44	1	349	A	C5-C6-N6	-11.63	114.40	123.70
44	1	945	C	N1-C2-O2	11.63	125.88	118.90
45	2	21	C	N1-C2-O2	11.61	125.86	118.90
44	1	346	C	C5-C4-N4	-11.60	112.08	120.20
44	1	54	C	C5-C4-N4	-11.47	112.17	120.20
44	1	945	C	N3-C4-N4	11.43	126.00	118.00
44	1	344	A	C4-C5-N7	11.41	116.41	110.70
44	1	1437	C	C5-C4-N4	-11.41	112.21	120.20
44	1	12	A	C5-C6-N6	-11.36	114.61	123.70
44	1	1615	C	C6-N1-C2	-11.34	115.76	120.30
44	1	200	C	N3-C4-C5	11.29	126.42	121.90
44	1	1363	A	C4-C5-N7	11.28	116.34	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1424	C	C5-C4-N4	-11.28	112.31	120.20
44	1	3308	C	N3-C4-N4	11.26	125.88	118.00
8	L	35	ARG	NE-CZ-NH1	11.25	125.92	120.30
44	1	1342	C	C5-C4-N4	-11.24	112.33	120.20
44	1	1407	A	C5-C6-N1	11.19	123.30	117.70
44	1	344	A	C5-C6-N1	11.19	123.29	117.70
44	1	1333	C	C5-C4-N4	-11.15	112.39	120.20
44	1	659	G	C4-C5-N7	11.14	115.26	110.80
44	1	628	A	C5-C6-N6	-11.13	114.79	123.70
44	1	1406	A	C5-C6-N1	11.12	123.26	117.70
44	1	78	U	C6-N1-C2	-11.09	114.34	121.00
44	1	1423	C	C5-C4-N4	-11.08	112.44	120.20
44	1	1330	A	N1-C6-N6	11.07	125.24	118.60
45	2	21	C	C5-C6-N1	11.06	126.53	121.00
44	1	345	G	C5-N7-C8	-11.04	98.78	104.30
44	1	947	G	N7-C8-N9	11.01	118.61	113.10
44	1	1614	C	C5-C4-N4	-11.01	112.50	120.20
44	1	3004	C	N3-C4-N4	10.99	125.69	118.00
44	1	58	G	C4-C5-N7	10.97	115.19	110.80
44	1	933	A	C4-C5-N7	10.94	116.17	110.70
44	1	931	C	N3-C4-C5	10.91	126.26	121.90
44	1	367	A	C5-C6-N6	-10.87	115.01	123.70
44	1	1525	G	C4-C5-N7	10.86	115.15	110.80
45	2	43	A	C5-C6-N6	-10.86	115.01	123.70
44	1	668	G	N3-C2-N2	10.85	127.49	119.90
45	2	40	A	C4-C5-C6	-10.84	111.58	117.00
44	1	1159	A	N1-C6-N6	10.81	125.09	118.60
44	1	349	A	C5-N7-C8	-10.79	98.50	103.90
44	1	1508	C	C5-C4-N4	-10.79	112.64	120.20
44	1	345	G	N7-C8-N9	10.79	118.49	113.10
44	1	1307	G	C8-N9-C4	-10.79	102.09	106.40
44	1	102	C	C5-C4-N4	-10.77	112.66	120.20
44	1	3181	C	N1-C2-O2	10.77	125.36	118.90
45	2	104	A	C5-N7-C8	-10.77	98.52	103.90
44	1	1363	A	C5-N7-C8	-10.75	98.53	103.90
45	2	19	C	C6-N1-C2	-10.74	116.00	120.30
44	1	1332	A	N7-C8-N9	10.70	119.15	113.80
45	2	19	C	N1-C2-O2	10.70	125.32	118.90
44	1	1179	A	C5-C6-N1	10.68	123.04	117.70
45	2	94	C	N3-C4-N4	10.65	125.46	118.00
44	1	657	A	C5-C6-N1	10.65	123.03	117.70
44	1	693	A	C5-C6-N6	-10.64	115.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	628	A	C5-C6-N1	10.61	123.00	117.70
44	1	1170	A	C5-C6-N6	-10.59	115.23	123.70
44	1	696	C	C5-C4-N4	-10.57	112.80	120.20
44	1	1603	A	N1-C6-N6	-10.57	112.26	118.60
44	1	142	C	C5-C4-N4	-10.54	112.82	120.20
32	j	21	ARG	NE-CZ-NH1	10.53	125.56	120.30
44	1	345	G	C4-C5-N7	10.53	115.01	110.80
44	1	659	G	N3-C2-N2	10.51	127.26	119.90
44	1	341	G	C4-C5-N7	10.50	115.00	110.80
44	1	1496	C	N3-C2-O2	-10.49	114.55	121.90
44	1	637	C	C5-C6-N1	10.49	126.25	121.00
44	1	1159	A	N3-C4-N9	10.49	135.79	127.40
45	2	96	A	C5-C6-N1	10.49	122.94	117.70
44	1	1372	C	C5-C4-N4	-10.48	112.86	120.20
44	1	1435	A	C5-N7-C8	-10.47	98.67	103.90
44	1	1159	A	C4-C5-N7	10.46	115.93	110.70
44	1	2383	C	C6-N1-C2	-10.45	116.12	120.30
45	2	10	A	N1-C6-N6	10.44	124.86	118.60
44	1	933	A	N9-C4-C5	-10.43	101.63	105.80
44	1	1179	A	C5-N7-C8	-10.43	98.68	103.90
44	1	63	A	C5-C6-N1	10.40	122.90	117.70
44	1	1420	C	N3-C4-C5	10.39	126.06	121.90
44	1	16	A	N9-C4-C5	-10.37	101.65	105.80
44	1	665	A	C5-N7-C8	-10.35	98.72	103.90
44	1	3217	C	N3-C2-O2	-10.34	114.67	121.90
44	1	267	G	N1-C6-O6	-10.32	113.71	119.90
44	1	3019	U	N3-C2-O2	-10.32	114.98	122.20
44	1	2892	A	C5-C6-N6	-10.29	115.47	123.70
44	1	1332	A	C5-C6-N6	-10.28	115.47	123.70
44	1	665	A	C5-C6-N6	-10.28	115.48	123.70
45	2	137	C	C5-C4-N4	-10.28	113.01	120.20
44	1	224	C	C5-C4-N4	-10.27	113.01	120.20
44	1	659	G	N1-C2-N2	-10.26	106.97	116.20
44	1	975	C	N3-C2-O2	-10.20	114.76	121.90
44	1	1337	A	N9-C4-C5	-10.19	101.72	105.80
44	1	1163	A	C5-N7-C8	-10.19	98.81	103.90
44	1	12	A	C4-C5-N7	10.18	115.79	110.70
45	2	28	C	C5-C4-N4	-10.18	113.07	120.20
44	1	1158	A	C5-N7-C8	-10.17	98.82	103.90
44	1	349	A	C4-C5-N7	10.16	115.78	110.70
44	1	60	A	C5-C6-N6	-10.14	115.59	123.70
44	1	804	C	N3-C4-N4	10.13	125.09	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	407	A	C5-N7-C8	-10.13	98.84	103.90
44	1	1337	A	C5-C6-N1	10.12	122.76	117.70
44	1	213	A	C5-C6-N1	10.11	122.76	117.70
44	1	1376	C	C5-C4-N4	-10.11	113.12	120.20
44	1	3004	C	N1-C2-O2	10.11	124.96	118.90
44	1	144	A	C5-C6-N1	10.10	122.75	117.70
45	2	9	A	N7-C8-N9	10.10	118.85	113.80
44	1	3139	A	C5-C6-N6	-10.08	115.64	123.70
45	2	105	A	C5-C6-N6	-10.08	115.64	123.70
44	1	945	C	C6-N1-C2	-10.07	116.27	120.30
44	1	1342	C	N3-C4-N4	10.07	125.05	118.00
44	1	344	A	C5-N7-C8	-10.05	98.87	103.90
44	1	1527	C	N1-C2-O2	10.04	124.93	118.90
44	1	338	A	C5-C6-N1	10.04	122.72	117.70
44	1	659	G	C5-N7-C8	-10.04	99.28	104.30
44	1	1337	A	N1-C6-N6	10.04	124.62	118.60
45	2	103	G	N7-C8-N9	10.04	118.12	113.10
44	1	933	A	C5-C6-N6	-10.02	115.69	123.70
44	1	1420	C	N1-C2-O2	10.01	124.91	118.90
44	1	936	A	C5-C6-N1	10.01	122.70	117.70
44	1	3008	A	C5-C6-N1	10.01	122.70	117.70
44	1	1330	A	C5-N7-C8	-10.01	98.90	103.90
45	2	77	A	C5-C6-N6	-10.01	115.70	123.70
44	1	1296	C	C6-N1-C2	-9.99	116.30	120.30
37	q	250	ASP	CB-CG-OD1	9.99	127.29	118.30
44	1	1337	A	C4-C5-N7	9.98	115.69	110.70
44	1	3137	C	C5-C4-N4	-9.97	113.22	120.20
44	1	428	A	C4-C5-N7	9.97	115.68	110.70
44	1	655	C	N1-C2-O2	9.96	124.88	118.90
45	2	17	A	C8-N9-C4	-9.96	101.81	105.80
44	1	3183	A	C4-C5-N7	9.96	115.68	110.70
44	1	929	A	C5-N7-C8	-9.96	98.92	103.90
44	1	303	G	N3-C2-N2	9.95	126.86	119.90
44	1	433	A	C5-C6-N1	9.95	122.67	117.70
44	1	3103	A	C5-C6-N1	9.95	122.67	117.70
44	1	1381	A	C5-N7-C8	-9.94	98.93	103.90
44	1	504	A	C5-N7-C8	-9.94	98.93	103.90
44	1	815	G	N3-C2-N2	9.93	126.85	119.90
44	1	1308	A	C5-C6-N1	9.93	122.67	117.70
44	1	933	A	C5-N7-C8	-9.93	98.94	103.90
44	1	1460	A	C4-C5-N7	9.93	115.66	110.70
44	1	2836	C	N3-C2-O2	-9.92	114.95	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	504	A	C5-C6-N6	-9.91	115.77	123.70
44	1	321	C	N1-C2-O2	9.90	124.84	118.90
44	1	265	A	N1-C6-N6	-9.90	112.66	118.60
32	j	45	ARG	NE-CZ-NH2	-9.89	115.35	120.30
44	1	82	C	C5-C4-N4	-9.88	113.28	120.20
44	1	1579	C	N3-C2-O2	-9.88	114.98	121.90
44	1	1432	C	N3-C4-C5	9.88	125.85	121.90
44	1	3183	A	C5-N7-C8	-9.88	98.96	103.90
44	1	323	A	N9-C4-C5	-9.87	101.85	105.80
44	1	585	A	C5-N7-C8	-9.87	98.97	103.90
44	1	3299	A	C5-C6-N6	-9.87	115.80	123.70
44	1	1363	A	N9-C4-C5	-9.86	101.86	105.80
44	1	334	A	C5-N7-C8	-9.85	98.97	103.90
45	2	32	C	C5-C4-N4	-9.85	113.31	120.20
45	2	10	A	C4-C5-N7	9.84	115.62	110.70
44	1	3091	A	C5-C6-N6	-9.84	115.83	123.70
44	1	1460	A	C5-C6-N6	-9.83	115.83	123.70
44	1	1328	C	N1-C2-O2	9.83	124.80	118.90
45	2	104	A	N7-C8-N9	9.82	118.71	113.80
44	1	1307	G	N7-C8-N9	9.80	118.00	113.10
44	1	933	A	N1-C6-N6	9.79	124.47	118.60
44	1	373	A	C4-C5-N7	9.77	115.58	110.70
44	1	3035	A	C5-C6-N6	-9.76	115.89	123.70
44	1	1158	A	C5-C6-N6	-9.76	115.89	123.70
44	1	396	A	C5-C6-N1	9.76	122.58	117.70
44	1	665	A	C4-C5-N7	9.73	115.57	110.70
44	1	1283	C	N1-C2-O2	9.73	124.74	118.90
44	1	205	C	N1-C2-O2	9.72	124.73	118.90
44	1	1836	C	N1-C2-O2	9.72	124.73	118.90
44	1	407	A	C4-C5-N7	9.71	115.55	110.70
44	1	60	A	N1-C6-N6	9.70	124.42	118.60
44	1	1416	C	C5-C4-N4	-9.70	113.41	120.20
44	1	1190	A	C5-C6-N6	-9.68	115.95	123.70
44	1	1598	G	N7-C8-N9	9.68	117.94	113.10
44	1	373	A	N9-C4-C5	-9.67	101.93	105.80
44	1	693	A	C5-N7-C8	-9.67	99.06	103.90
44	1	1510	G	N3-C2-N2	9.65	126.65	119.90
44	1	665	A	C5-C6-N1	9.64	122.52	117.70
44	1	1376	C	N3-C2-O2	-9.64	115.15	121.90
44	1	1403	C	C5-C4-N4	-9.63	113.46	120.20
44	1	618	C	N3-C2-O2	-9.62	115.16	121.90
44	1	3103	A	C5-C6-N6	-9.60	116.02	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3379	C	C5-C4-N4	-9.59	113.49	120.20
44	1	1432	C	N1-C2-O2	9.59	124.65	118.90
8	L	39	ARG	NE-CZ-NH1	9.57	125.08	120.30
44	1	323	A	C5-C6-N6	-9.56	116.05	123.70
44	1	656	A	C5-C6-N1	9.56	122.48	117.70
44	1	1158	A	N7-C8-N9	9.56	118.58	113.80
44	1	928	C	C6-N1-C2	-9.55	116.48	120.30
45	2	58	G	C4-C5-N7	9.55	114.62	110.80
44	1	1179	A	C4-C5-N7	9.55	115.47	110.70
45	2	26	U	C6-N1-C2	-9.55	115.27	121.00
44	1	2994	A	C5-C6-N6	-9.55	116.06	123.70
44	1	1306	G	N7-C8-N9	9.54	117.87	113.10
44	1	1881	A	C4-C5-N7	9.52	115.46	110.70
45	2	13	A	C5-C6-N1	9.51	122.45	117.70
44	1	3174	A	C5-C6-N6	-9.50	116.10	123.70
44	1	630	A	N7-C8-N9	9.49	118.55	113.80
44	1	589	A	C5-C6-N6	-9.49	116.11	123.70
44	1	660	A	C5-N7-C8	-9.48	99.16	103.90
44	1	1376	C	N3-C4-N4	9.48	124.64	118.00
44	1	1159	A	O4'-C1'-N9	9.47	115.78	108.20
2	C	95	ARG	NE-CZ-NH2	-9.47	115.56	120.30
45	2	43	A	C5-N7-C8	-9.46	99.17	103.90
45	2	157	U	N1-C2-O2	9.46	129.42	122.80
44	1	693	A	C4-C5-N7	9.45	115.42	110.70
44	1	1422	G	C4-C5-N7	9.43	114.57	110.80
44	1	1190	A	C5-C6-N1	9.43	122.41	117.70
44	1	373	A	C5-C6-N1	9.42	122.41	117.70
44	1	586	C	N1-C2-O2	9.42	124.55	118.90
44	1	369	A	C5-C6-N6	-9.41	116.17	123.70
44	1	1204	A	C5-C6-N6	-9.40	116.18	123.70
44	1	1558	A	C5-C6-N1	9.40	122.40	117.70
11	O	117	ARG	NE-CZ-NH2	-9.39	115.61	120.30
45	2	19	C	N3-C4-N4	9.39	124.57	118.00
44	1	1615	C	N3-C4-N4	9.38	124.57	118.00
44	1	670	C	C5-C4-N4	-9.38	113.63	120.20
44	1	1179	A	C5-C6-N6	-9.38	116.19	123.70
44	1	1701	C	N1-C2-O2	9.38	124.53	118.90
44	1	947	G	C8-N9-C4	-9.37	102.65	106.40
44	1	1527	C	N3-C2-O2	-9.37	115.34	121.90
44	1	342	A	C8-N9-C4	9.36	109.54	105.80
44	1	366	A	C5-C6-N6	-9.35	116.22	123.70
44	1	2367	A	C5-C6-N1	9.35	122.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	949	C	C5-C4-N4	-9.35	113.66	120.20
44	1	341	G	C5-N7-C8	-9.33	99.63	104.30
45	2	41	A	N1-C6-N6	-9.33	113.00	118.60
44	1	1190	A	C4-C5-N7	9.33	115.36	110.70
44	1	1561	G	O4'-C1'-N9	9.33	115.66	108.20
44	1	1327	C	C6-N1-C2	-9.31	116.57	120.30
44	1	1326	A	C5-C6-N1	9.31	122.36	117.70
44	1	702	C	C5-C4-N4	-9.31	113.68	120.20
44	1	409	A	C5-N7-C8	-9.30	99.25	103.90
44	1	695	C	C5-C4-N4	-9.30	113.69	120.20
44	1	332	C	C5-C4-N4	-9.29	113.70	120.20
44	1	1496	C	C5-C6-N1	9.29	125.64	121.00
44	1	2983	C	N1-C2-O2	9.28	124.47	118.90
44	1	1159	A	C6-C5-N7	-9.28	125.81	132.30
44	1	1446	A	C5-C6-N1	9.27	122.34	117.70
44	1	11	A	C5-C6-N1	9.27	122.33	117.70
44	1	3354	U	C2-N1-C1'	9.27	128.82	117.70
44	1	1428	A	C4-C5-N7	9.27	115.33	110.70
44	1	1170	A	C5-N7-C8	-9.26	99.27	103.90
44	1	3181	C	N3-C2-O2	-9.25	115.42	121.90
45	2	74	U	C5-C6-N1	9.25	127.32	122.70
44	1	3089	C	C5-C4-N4	-9.24	113.73	120.20
44	1	346	C	O5'-P-OP1	-9.24	97.39	105.70
44	1	1418	A	N9-C4-C5	-9.21	102.11	105.80
44	1	1469	C	N1-C2-O2	9.21	124.42	118.90
44	1	12	A	C5-N7-C8	-9.20	99.30	103.90
44	1	114	A	C5-C6-N6	-9.19	116.35	123.70
44	1	1204	A	N1-C6-N6	9.19	124.11	118.60
45	2	19	C	N3-C2-O2	-9.19	115.47	121.90
44	1	1444	G	N7-C8-N9	9.18	117.69	113.10
44	1	3046	A	C5-C6-N6	-9.18	116.36	123.70
44	1	2892	A	C5-C6-N1	9.18	122.29	117.70
45	2	43	A	C4-C5-N7	9.16	115.28	110.70
28	f	18	ARG	NE-CZ-NH2	-9.16	115.72	120.30
44	1	3323	A	C5-C6-N6	-9.15	116.38	123.70
44	1	3323	A	C4-C5-N7	9.15	115.28	110.70
8	L	39	ARG	NE-CZ-NH2	-9.15	115.73	120.30
44	1	628	A	C4-C5-N7	9.15	115.27	110.70
44	1	1163	A	C4-C5-N7	9.14	115.27	110.70
44	1	58	G	C6-C5-N7	-9.14	124.92	130.40
44	1	222	A	C4-C5-N7	9.13	115.27	110.70
44	1	1608	C	C5-C4-N4	-9.12	113.82	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	633	C	N1-C2-O2	9.12	124.37	118.90
44	1	1161	G	C4-C5-N7	9.11	114.44	110.80
44	1	29	C	N3-C4-N4	9.11	124.38	118.00
44	1	52	A	C5-C6-N6	-9.10	116.42	123.70
44	1	1363	A	C5-C6-N1	9.09	122.25	117.70
44	1	659	G	C6-C5-N7	-9.09	124.95	130.40
44	1	1146	C	C5-C6-N1	9.09	125.54	121.00
44	1	3153	U	N1-C2-O2	9.09	129.16	122.80
44	1	1874	A	C5-C6-N6	-9.07	116.44	123.70
44	1	1175	C	C5-C4-N4	-9.07	113.85	120.20
44	1	920	A	C5-C6-N1	9.06	122.23	117.70
44	1	1163	A	C5-C6-N1	9.06	122.23	117.70
44	1	815	G	N1-C2-N2	-9.06	108.05	116.20
44	1	1419	A	C5-N7-C8	-9.06	99.37	103.90
44	1	1330	A	C4-C5-N7	9.05	115.22	110.70
44	1	2836	C	N1-C2-O2	9.04	124.33	118.90
44	1	504	A	C4-C5-N7	9.04	115.22	110.70
44	1	102	C	N3-C4-C5	9.03	125.51	121.90
44	1	2899	C	N1-C2-O2	9.02	124.31	118.90
44	1	1376	C	C5-C6-N1	9.01	125.51	121.00
45	2	77	A	C4-C5-N7	9.01	115.20	110.70
44	1	107	A	C5-N7-C8	-9.00	99.40	103.90
44	1	1614	C	N1-C2-O2	9.00	124.30	118.90
44	1	289	A	C5-N7-C8	-8.99	99.40	103.90
44	1	3164	C	N1-C2-O2	8.99	124.29	118.90
45	2	17	A	N1-C6-N6	-8.99	113.21	118.60
44	1	703	G	N1-C2-N2	-8.98	108.12	116.20
44	1	806	A	C5-C6-N1	8.98	122.19	117.70
44	1	222	A	C5-N7-C8	-8.98	99.41	103.90
44	1	366	A	C5-N7-C8	-8.97	99.42	103.90
44	1	655	C	C5-C4-N4	-8.95	113.94	120.20
44	1	51	A	C5-N7-C8	-8.95	99.42	103.90
44	1	633	C	N3-C4-C5	8.94	125.48	121.90
44	1	2367	A	C5-C6-N6	-8.93	116.56	123.70
44	1	1333	C	C6-N1-C2	-8.92	116.73	120.30
44	1	2367	A	C5-N7-C8	-8.92	99.44	103.90
44	1	10	C	C6-N1-C2	-8.92	116.73	120.30
44	1	346	C	N3-C4-C5	8.92	125.47	121.90
44	1	1307	G	N3-C4-C5	-8.92	124.14	128.60
44	1	1329	U	C6-N1-C2	-8.91	115.65	121.00
44	1	3005	A	C5-N7-C8	-8.91	99.45	103.90
44	1	375	A	C4-C5-C6	-8.90	112.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	18	ARG	NE-CZ-NH2	-8.89	115.85	120.30
44	1	928	C	C5-C4-N4	-8.89	113.98	120.20
44	1	342	A	N9-C4-C5	-8.89	102.25	105.80
44	1	638	C	C6-N1-C2	-8.87	116.75	120.30
44	1	113	C	N1-C2-O2	8.87	124.22	118.90
44	1	655	C	C6-N1-C2	-8.87	116.75	120.30
44	1	1328	C	N3-C2-O2	-8.87	115.69	121.90
44	1	1332	A	N9-C4-C5	-8.86	102.26	105.80
44	1	1843	C	C6-N1-C2	-8.86	116.75	120.30
44	1	618	C	N1-C2-O2	8.85	124.21	118.90
44	1	409	A	C5-C6-N1	8.85	122.12	117.70
44	1	1314	C	N1-C2-O2	8.85	124.21	118.90
44	1	3213	A	C5-C6-N6	-8.84	116.62	123.70
44	1	656	A	C5-N7-C8	-8.83	99.48	103.90
44	1	428	A	C5-N7-C8	-8.82	99.49	103.90
44	1	1170	A	C4-C5-N7	8.82	115.11	110.70
44	1	3006	A	C5-C6-N1	8.82	122.11	117.70
44	1	3139	A	C5-N7-C8	-8.82	99.49	103.90
44	1	1187	C	N3-C2-O2	-8.81	115.73	121.90
44	1	815	G	C4-C5-N7	8.81	114.33	110.80
44	1	12	A	N1-C6-N6	8.81	123.88	118.60
44	1	668	G	N1-C2-N2	-8.80	108.28	116.20
44	1	1657	C	C6-N1-C2	-8.80	116.78	120.30
44	1	3273	A	C5-C6-N1	8.80	122.10	117.70
45	2	21	C	C2-N1-C1'	8.79	128.47	118.80
44	1	693	A	C5-C6-N1	8.79	122.09	117.70
44	1	52	A	C5-C6-N1	8.79	122.09	117.70
44	1	1333	C	N3-C4-N4	8.78	124.15	118.00
44	1	367	A	C5-C6-N1	8.78	122.09	117.70
10	N	203	ARG	NE-CZ-NH2	-8.77	115.92	120.30
44	1	1365	G	C4-C5-N7	8.76	114.30	110.80
44	1	789	A	C5-C6-N1	8.76	122.08	117.70
44	1	701	G	C4-C5-N7	8.75	114.30	110.80
44	1	1337	A	C5-N7-C8	-8.74	99.53	103.90
44	1	389	A	C5-C6-N1	8.73	122.07	117.70
45	2	10	A	C5-N7-C8	-8.73	99.53	103.90
45	2	141	C	N3-C4-C5	8.73	125.39	121.90
45	2	44	A	C4-C5-N7	8.73	115.06	110.70
44	1	1159	A	N9-C4-C5	-8.73	102.31	105.80
44	1	1105	A	C5-C6-N6	-8.72	116.72	123.70
44	1	324	A	C5-C6-N1	8.71	122.06	117.70
44	1	1432	C	C5-C4-N4	-8.71	114.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	2354	C	N3-C4-N4	8.70	124.09	118.00
44	1	342	A	C5-N7-C8	-8.69	99.55	103.90
44	1	628	A	N9-C4-C5	-8.69	102.32	105.80
44	1	1401	A	C4-C5-N7	8.68	115.04	110.70
44	1	3034	C	N3-C4-C5	8.68	125.37	121.90
44	1	945	C	N3-C2-O2	-8.67	115.83	121.90
44	1	1298	C	C5-C4-N4	-8.67	114.13	120.20
44	1	1643	A	N1-C6-N6	-8.67	113.40	118.60
44	1	1383	G	N7-C8-N9	8.67	117.43	113.10
44	1	1493	G	N3-C2-N2	8.67	125.97	119.90
44	1	660	A	N7-C8-N9	8.66	118.13	113.80
44	1	1462	A	C5-C6-N1	8.66	122.03	117.70
44	1	1428	A	C5-C6-N6	-8.66	116.78	123.70
44	1	1423	C	N1-C2-O2	8.65	124.09	118.90
44	1	30	G	N7-C8-N9	8.65	117.42	113.10
44	1	363	G	C5-N7-C8	-8.65	99.98	104.30
44	1	1158	A	C4-C5-N7	8.64	115.02	110.70
44	1	1327	C	N3-C2-O2	-8.64	115.85	121.90
44	1	1150	A	C4-C5-N7	8.64	115.02	110.70
44	1	1498	A	C5-N7-C8	-8.63	99.58	103.90
44	1	349	A	C5-C6-N1	8.63	122.02	117.70
44	1	3097	C	N1-C2-O2	8.63	124.08	118.90
44	1	289	A	C4-C5-N7	8.62	115.01	110.70
44	1	929	A	N7-C8-N9	8.62	118.11	113.80
44	1	667	C	C5-C4-N4	-8.62	114.17	120.20
44	1	3008	A	C5-N7-C8	-8.62	99.59	103.90
44	1	1614	C	N3-C4-N4	8.60	124.02	118.00
45	2	22	U	N1-C2-O2	8.60	128.82	122.80
44	1	585	A	C4-C5-N7	8.59	115.00	110.70
44	1	3211	C	N1-C2-O2	8.59	124.05	118.90
44	1	48	A	N1-C6-N6	-8.58	113.45	118.60
44	1	801	A	C5-C6-N1	8.58	121.99	117.70
44	1	3008	A	C4-C5-N7	8.58	114.99	110.70
44	1	1183	C	C5-C4-N4	-8.57	114.20	120.20
44	1	659	G	N7-C8-N9	8.56	117.38	113.10
44	1	1613	A	C5-C6-N1	8.56	121.98	117.70
44	1	334	A	C4-C5-N7	8.56	114.98	110.70
44	1	357	A	C4-C5-N7	8.55	114.97	110.70
44	1	2934	A	C5-C6-N1	8.54	121.97	117.70
44	1	1163	A	N1-C6-N6	8.54	123.72	118.60
44	1	1460	A	N9-C4-C5	-8.53	102.39	105.80
44	1	3097	C	C6-N1-C2	-8.53	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	43	A	N1-C6-N6	8.53	123.72	118.60
44	1	663	C	C5-C4-N4	-8.52	114.24	120.20
44	1	352	A	C5-C6-N6	-8.52	116.89	123.70
44	1	1428	A	C5-C6-N1	8.51	121.96	117.70
44	1	3186	A	C5-C6-N1	8.51	121.96	117.70
44	1	1858	A	O4'-C1'-N9	8.51	115.01	108.20
44	1	369	A	N9-C4-C5	-8.51	102.40	105.80
44	1	1376	C	N1-C2-O2	8.51	124.00	118.90
2	C	197	ARG	NE-CZ-NH2	-8.50	116.05	120.30
44	1	366	A	C4-C5-N7	8.50	114.95	110.70
44	1	1698	C	C5-C4-N4	-8.50	114.25	120.20
44	1	1107	C	C5-C4-N4	-8.49	114.25	120.20
44	1	1158	A	N1-C6-N6	8.49	123.70	118.60
44	1	498	A	N1-C6-N6	-8.49	113.51	118.60
44	1	3248	C	N1-C2-O2	8.48	123.99	118.90
11	O	101	ARG	NE-CZ-NH1	8.48	124.54	120.30
44	1	30	G	C8-N9-C4	-8.48	103.01	106.40
44	1	3060	C	C5-C4-N4	-8.47	114.27	120.20
45	2	76	C	C5-C4-N4	-8.47	114.27	120.20
44	1	3141	A	C5-C6-N6	-8.47	116.93	123.70
44	1	1150	A	C5-N7-C8	-8.46	99.67	103.90
44	1	1401	A	C5-C6-N6	-8.46	116.93	123.70
44	1	1460	A	C5-N7-C8	-8.46	99.67	103.90
44	1	3138	U	C6-N1-C2	-8.46	115.92	121.00
44	1	114	A	C4-C5-N7	8.46	114.93	110.70
44	1	2910	A	C5-C6-N1	8.46	121.93	117.70
44	1	27	C	C6-N1-C2	-8.45	116.92	120.30
44	1	339	C	C6-N1-C2	-8.45	116.92	120.30
44	1	130	A	C4-C5-N7	8.45	114.92	110.70
44	1	1279	C	C6-N1-C2	-8.44	116.92	120.30
44	1	2354	C	N1-C2-O2	8.44	123.97	118.90
44	1	428	A	N1-C6-N6	8.44	123.66	118.60
44	1	107	A	C5-C6-N1	8.44	121.92	117.70
45	2	157	U	N3-C2-O2	-8.44	116.30	122.20
44	1	409	A	N7-C8-N9	8.43	118.02	113.80
1	B	232	ARG	NE-CZ-NH1	8.43	124.52	120.30
44	1	926	A	C5-C6-N1	8.43	121.91	117.70
44	1	345	G	C6-C5-N7	-8.43	125.34	130.40
44	1	347	G	C4-C5-N7	8.43	114.17	110.80
44	1	1881	A	C5-N7-C8	-8.43	99.69	103.90
44	1	364	G	C2-N3-C4	-8.42	107.69	111.90
44	1	1546	A	N9-C4-C5	-8.42	102.43	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	45	C	C5-C4-N4	-8.42	114.31	120.20
28	f	48	ARG	NE-CZ-NH1	-8.42	116.09	120.30
44	1	1365	G	N9-C4-C5	-8.41	102.03	105.40
44	1	321	C	N3-C4-C5	8.41	125.26	121.90
45	2	42	G	C5-N7-C8	-8.41	100.10	104.30
44	1	672	A	N1-C6-N6	8.40	123.64	118.60
45	2	103	G	C8-N9-C4	-8.40	103.04	106.40
44	1	672	A	C5-C6-N6	-8.40	116.98	123.70
44	1	701	G	C6-C5-N7	-8.40	125.36	130.40
44	1	1335	C	C5-C4-N4	-8.40	114.32	120.20
44	1	36	C	C5-C4-N4	-8.39	114.32	120.20
44	1	3008	A	C5-C6-N6	-8.39	116.99	123.70
44	1	423	A	N1-C6-N6	8.39	123.63	118.60
44	1	323	A	N7-C8-N9	8.38	117.99	113.80
44	1	1420	C	C5-C4-N4	-8.38	114.34	120.20
44	1	1401	A	C5-N7-C8	-8.38	99.71	103.90
44	1	228	U	C5-C6-N1	8.37	126.89	122.70
44	1	3021	A	N1-C6-N6	8.37	123.62	118.60
44	1	1593	A	C5-C6-N1	8.36	121.88	117.70
44	1	931	C	C5-C4-N4	-8.36	114.35	120.20
44	1	1196	C	C2-N1-C1'	8.36	127.99	118.80
44	1	1428	A	C5-N7-C8	-8.35	99.72	103.90
2	C	138	ARG	NE-CZ-NH1	8.34	124.47	120.30
44	1	373	A	N1-C6-N6	8.34	123.60	118.60
44	1	1310	G	C5-N7-C8	-8.34	100.13	104.30
44	1	703	G	N3-C2-N2	8.33	125.73	119.90
44	1	1510	G	N1-C2-N2	-8.33	108.70	116.20
44	1	2365	C	N3-C4-C5	8.32	125.23	121.90
44	1	3005	A	C5-C6-N6	-8.32	117.04	123.70
44	1	291	C	C5-C4-N4	-8.32	114.37	120.20
44	1	1881	A	C5-C6-N6	-8.32	117.04	123.70
44	1	60	A	C4-C5-N7	8.32	114.86	110.70
44	1	3323	A	C5-N7-C8	-8.32	99.74	103.90
44	1	344	A	N9-C4-C5	-8.31	102.47	105.80
44	1	349	A	N1-C6-N6	8.31	123.59	118.60
44	1	1343	A	C5-C6-N1	8.31	121.86	117.70
44	1	363	G	N7-C8-N9	8.31	117.25	113.10
45	2	17	A	N7-C8-N9	8.30	117.95	113.80
45	2	129	C	N1-C2-O2	8.30	123.88	118.90
44	1	130	A	C5-C6-N1	8.30	121.85	117.70
44	1	1187	C	N1-C2-O2	8.30	123.88	118.90
45	2	26	U	C5-C6-N1	8.30	126.85	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	340	C	N1-C2-O2	8.29	123.88	118.90
44	1	144	A	C5-C6-N6	-8.29	117.07	123.70
44	1	407	A	C4-C5-C6	-8.29	112.86	117.00
44	1	944	C	N3-C4-C5	8.29	125.21	121.90
44	1	213	A	C4-C5-C6	-8.28	112.86	117.00
44	1	875	G	N3-C4-N9	8.28	130.97	126.00
44	1	1332	A	N1-C2-N3	-8.28	125.16	129.30
44	1	1283	C	N3-C2-O2	-8.28	116.11	121.90
44	1	407	A	N3-C4-C5	8.27	132.59	126.80
44	1	22	G	N1-C6-O6	-8.27	114.94	119.90
44	1	1508	C	N3-C4-C5	8.27	125.21	121.90
44	1	114	A	N9-C4-C5	-8.25	102.50	105.80
44	1	1836	C	N3-C2-O2	-8.25	116.13	121.90
44	1	3323	A	N1-C6-N6	8.25	123.55	118.60
44	1	3023	U	N3-C2-O2	-8.25	116.43	122.20
44	1	6	A	C4-C5-N7	8.24	114.82	110.70
44	1	18	G	C4-C5-N7	8.24	114.10	110.80
44	1	78	U	C5-C6-N1	8.24	126.82	122.70
44	1	375	A	C5-C6-N1	8.24	121.82	117.70
44	1	16	A	C6-C5-N7	-8.24	126.53	132.30
44	1	1397	C	C6-N1-C2	-8.24	117.00	120.30
44	1	658	G	N7-C8-N9	8.23	117.22	113.10
44	1	1615	C	C5-C4-N4	-8.23	114.44	120.20
44	1	1835	A	C5-C6-N1	8.22	121.81	117.70
44	1	680	G	C5-N7-C8	-8.22	100.19	104.30
44	1	1339	C	N1-C2-O2	8.22	123.83	118.90
44	1	8	C	C6-N1-C2	-8.21	117.02	120.30
44	1	361	A	C5-C6-N1	8.21	121.81	117.70
45	2	57	C	N1-C2-O2	8.20	123.82	118.90
44	1	1525	G	C4-N9-C1'	8.20	137.16	126.50
44	1	1333	C	N3-C2-O2	-8.20	116.16	121.90
44	1	695	C	N3-C4-C5	8.20	125.18	121.90
44	1	1160	C	N3-C4-C5	8.20	125.18	121.90
44	1	1426	C	N3-C4-N4	8.19	123.73	118.00
2	C	220	ARG	NE-CZ-NH2	-8.19	116.21	120.30
44	1	586	C	C5-C4-N4	-8.19	114.47	120.20
44	1	659	G	N9-C4-C5	-8.19	102.12	105.40
44	1	187	A	C5-C6-N1	8.18	121.79	117.70
44	1	2887	A	C5-C6-N1	8.18	121.79	117.70
44	1	28	C	C6-N1-C2	-8.17	117.03	120.30
44	1	1609	C	C5-C4-N4	-8.17	114.48	120.20
44	1	3005	A	C4-C5-N7	8.16	114.78	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3019	U	N1-C2-O2	8.16	128.51	122.80
44	1	350	C	N3-C4-N4	8.16	123.71	118.00
44	1	367	A	C4-C5-N7	8.16	114.78	110.70
44	1	3123	A	C5-C6-N1	8.15	121.77	117.70
44	1	1433	A	C5-C6-N6	-8.14	117.18	123.70
45	2	11	C	C5-C4-N4	-8.14	114.50	120.20
44	1	345	G	N1-C2-N2	-8.14	108.88	116.20
39	s	10	ARG	NE-CZ-NH1	8.13	124.37	120.30
44	1	1842	A	N1-C6-N6	-8.13	113.72	118.60
44	1	389	A	C5-C6-N6	-8.12	117.20	123.70
44	1	1546	A	N1-C6-N6	8.12	123.47	118.60
44	1	363	G	C4-C5-N7	8.12	114.05	110.80
44	1	3172	A	C5-C6-N1	8.11	121.76	117.70
44	1	1579	C	N1-C2-O2	8.11	123.77	118.90
44	1	2383	C	C5-C6-N1	8.11	125.05	121.00
45	2	44	A	C5-N7-C8	-8.10	99.85	103.90
44	1	803	C	C6-N1-C2	-8.09	117.06	120.30
44	1	1598	G	C5-N7-C8	-8.09	100.25	104.30
44	1	656	A	N7-C8-N9	8.09	117.85	113.80
44	1	107	A	C5-C6-N6	-8.09	117.23	123.70
44	1	357	A	N9-C4-C5	-8.09	102.56	105.80
44	1	432	G	N1-C2-N2	-8.09	108.92	116.20
44	1	3040	A	C4-C5-N7	8.09	114.74	110.70
44	1	3048	A	C5-C6-N1	8.09	121.74	117.70
44	1	432	G	N3-C2-N2	8.08	125.56	119.90
44	1	1424	C	C6-N1-C2	-8.08	117.07	120.30
44	1	1891	A	C5-C6-N1	8.08	121.74	117.70
10	N	63	ARG	NE-CZ-NH1	8.08	124.34	120.30
44	1	2362	C	N1-C2-O2	8.08	123.75	118.90
44	1	76	G	N7-C8-N9	8.07	117.14	113.10
44	1	340	C	C5-C4-N4	-8.07	114.55	120.20
44	1	2348	A	N1-C6-N6	8.07	123.44	118.60
45	2	105	A	O4'-C1'-N9	8.07	114.66	108.20
44	1	3299	A	N1-C6-N6	8.07	123.44	118.60
44	1	649	A	C5-C6-N6	-8.06	117.25	123.70
30	h	90	ARG	NE-CZ-NH1	8.06	124.33	120.30
44	1	402	A	N1-C6-N6	8.06	123.44	118.60
44	1	2356	A	C5-N7-C8	-8.06	99.87	103.90
44	1	1161	G	C6-C5-N7	-8.05	125.57	130.40
44	1	323	A	C6-C5-N7	-8.05	126.67	132.30
44	1	2876	C	O4'-C1'-N1	8.05	114.64	108.20
44	1	219	A	N1-C6-N6	-8.03	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1203	A	N1-C6-N6	8.03	123.42	118.60
44	1	3320	A	C5-C6-N1	8.03	121.71	117.70
44	1	89	A	C5-C6-N1	8.03	121.71	117.70
6	H	124	ARG	NE-CZ-NH1	8.03	124.31	120.30
44	1	428	A	N9-C4-C5	-8.02	102.59	105.80
44	1	3183	A	N9-C4-C5	-8.02	102.59	105.80
44	1	1169	A	C5-N7-C8	-8.01	99.89	103.90
44	1	1330	A	N9-C4-C5	-8.01	102.59	105.80
44	1	1406	A	C4-C5-C6	-8.01	113.00	117.00
45	2	142	C	C5-C4-N4	-8.01	114.60	120.20
44	1	1444	G	C6-C5-N7	-8.00	125.60	130.40
44	1	226	C	N1-C2-O2	8.00	123.70	118.90
45	2	10	A	C5-C6-N1	8.00	121.70	117.70
44	1	969	C	N3-C2-O2	-8.00	116.30	121.90
44	1	501	A	C5-C6-N1	7.99	121.70	117.70
44	1	3213	A	C4-C5-N7	7.99	114.69	110.70
44	1	384	A	N9-C4-C5	-7.99	102.61	105.80
44	1	3174	A	C4-C5-N7	7.99	114.69	110.70
45	2	19	C	C2-N1-C1'	7.99	127.58	118.80
44	1	1422	G	C5-N7-C8	-7.98	100.31	104.30
44	1	815	G	C5-N7-C8	-7.98	100.31	104.30
44	1	1382	G	N7-C8-N9	7.98	117.09	113.10
44	1	788	C	C5-C4-N4	-7.98	114.62	120.20
45	2	45	C	N3-C4-N4	7.98	123.58	118.00
44	1	715	A	C5-C6-N1	7.97	121.69	117.70
44	1	632	G	N7-C8-N9	7.97	117.08	113.10
44	1	1374	G	C4-C5-N7	7.97	113.99	110.80
45	2	74	U	C5-C4-O4	-7.97	121.12	125.90
44	1	1279	C	N1-C2-O2	7.96	123.68	118.90
45	2	9	A	C5-N7-C8	-7.96	99.92	103.90
44	1	1416	C	N3-C4-C5	7.96	125.08	121.90
44	1	1169	A	C4-C5-N7	7.95	114.68	110.70
44	1	1474	A	C4-C5-N7	7.95	114.67	110.70
44	1	1474	A	C5-N7-C8	-7.95	99.93	103.90
44	1	1525	G	C8-N9-C1'	-7.94	116.68	127.00
44	1	815	G	N7-C8-N9	7.94	117.07	113.10
44	1	3035	A	N1-C6-N6	7.94	123.36	118.60
45	2	66	A	C4-C5-N7	7.93	114.67	110.70
44	1	347	G	N7-C8-N9	7.93	117.07	113.10
44	1	3100	U	N1-C2-O2	7.93	128.35	122.80
45	2	65	A	C5-C6-N6	-7.93	117.35	123.70
44	1	2348	A	C5-C6-N6	-7.93	117.36	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	655	C	N3-C2-O2	-7.92	116.36	121.90
44	1	672	A	C5-N7-C8	-7.92	99.94	103.90
44	1	634	C	N3-C4-C5	7.91	125.06	121.90
44	1	1447	G	O4'-C1'-N9	7.91	114.53	108.20
44	1	573	C	C5-C4-N4	-7.91	114.66	120.20
44	1	3322	A	C5-C6-N1	7.91	121.65	117.70
44	1	369	A	C5-C6-N1	7.91	121.65	117.70
44	1	793	C	N3-C4-N4	7.91	123.53	118.00
44	1	3211	C	C5-C4-N4	-7.91	114.67	120.20
44	1	633	C	N3-C4-N4	7.90	123.53	118.00
44	1	951	A	N7-C8-N9	7.90	117.75	113.80
44	1	288	C	C5-C4-N4	-7.90	114.67	120.20
44	1	1459	C	C6-N1-C2	-7.90	117.14	120.30
44	1	3210	A	C4-C5-N7	7.90	114.65	110.70
45	2	77	A	N9-C4-C5	-7.90	102.64	105.80
44	1	1460	A	C5-C6-N1	7.89	121.65	117.70
44	1	1106	G	N7-C8-N9	7.89	117.04	113.10
44	1	1377	G	N3-C4-N9	-7.87	121.28	126.00
44	1	3138	U	C5-C6-N1	7.87	126.64	122.70
44	1	58	G	C5-N7-C8	-7.87	100.37	104.30
44	1	516	A	C5-C6-N6	-7.87	117.41	123.70
44	1	1165	A	C5-C6-N6	-7.87	117.41	123.70
44	1	1283	C	C6-N1-C2	-7.87	117.15	120.30
44	1	1514	G	N3-C2-N2	-7.87	114.39	119.90
28	f	86	ARG	NE-CZ-NH2	-7.85	116.38	120.30
44	1	1326	A	C5-C6-N6	-7.85	117.42	123.70
44	1	1327	C	N1-C2-O2	7.84	123.61	118.90
44	1	1107	C	N3-C4-N4	7.84	123.48	118.00
44	1	1749	A	N1-C6-N6	-7.84	113.90	118.60
45	2	58	G	C5-N7-C8	-7.83	100.38	104.30
44	1	990	U	N3-C2-O2	-7.83	116.72	122.20
44	1	1419	A	C4-C5-N7	7.83	114.61	110.70
44	1	1434	G	C8-N9-C4	-7.83	103.27	106.40
44	1	1613	A	C4-C5-C6	-7.83	113.09	117.00
44	1	1182	A	C5-C6-N6	-7.83	117.44	123.70
44	1	1836	C	C5-C4-N4	-7.82	114.73	120.20
45	2	97	A	C5-N7-C8	-7.82	99.99	103.90
44	1	106	A	N1-C6-N6	-7.82	113.91	118.60
44	1	3100	U	O4'-C1'-N1	7.82	114.45	108.20
44	1	1383	G	C5-N7-C8	-7.81	100.39	104.30
44	1	367	A	C5-N7-C8	-7.81	99.99	103.90
44	1	665	A	N9-C4-C5	-7.81	102.68	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	13	A	C5-N7-C8	-7.81	100.00	103.90
44	1	3046	A	C4-C5-N7	7.80	114.60	110.70
44	1	1380	G	N7-C8-N9	7.80	117.00	113.10
44	1	3139	A	C5-C6-N1	7.80	121.60	117.70
44	1	3043	C	N3-C4-C5	7.79	125.02	121.90
44	1	349	A	N9-C4-C5	-7.79	102.68	105.80
10	N	96	ARG	NE-CZ-NH2	-7.79	116.41	120.30
44	1	410	U	N3-C4-O4	7.79	124.85	119.40
44	1	1298	C	C6-N1-C2	-7.78	117.19	120.30
44	1	1298	C	N3-C4-N4	7.78	123.45	118.00
44	1	646	A	C5-C6-N6	-7.78	117.48	123.70
44	1	1335	C	N3-C4-C5	7.78	125.01	121.90
44	1	3110	C	C5-C4-N4	-7.78	114.76	120.20
44	1	1435	A	N7-C8-N9	7.77	117.69	113.80
45	2	13	A	C4-C5-N7	7.77	114.58	110.70
44	1	60	A	C5-N7-C8	-7.76	100.02	103.90
44	1	1170	A	N1-C6-N6	7.76	123.26	118.60
44	1	2887	A	C5-C6-N6	-7.76	117.49	123.70
45	2	92	A	C5-N7-C8	-7.76	100.02	103.90
44	1	427	C	C5-C4-N4	-7.75	114.77	120.20
44	1	2948	C	C6-N1-C2	-7.75	117.20	120.30
44	1	3100	U	N3-C2-O2	-7.75	116.77	122.20
44	1	1459	C	N3-C2-O2	-7.75	116.47	121.90
44	1	1461	A	C5-C6-N6	-7.75	117.50	123.70
44	1	1160	C	C5-C4-N4	-7.75	114.78	120.20
44	1	1893	A	C5-C6-N6	-7.75	117.50	123.70
44	1	3043	C	N1-C2-O2	7.75	123.55	118.90
44	1	130	A	C5-N7-C8	-7.74	100.03	103.90
44	1	1312	C	N1-C2-O2	7.74	123.54	118.90
44	1	2886	U	C5-C6-N1	7.73	126.57	122.70
44	1	54	C	N3-C4-N4	7.73	123.41	118.00
44	1	204	A	C5-C6-N1	7.73	121.56	117.70
44	1	2836	C	C6-N1-C2	-7.72	117.21	120.30
44	1	656	A	C4-C5-N7	7.71	114.56	110.70
44	1	2913	C	N3-C4-C5	7.71	124.98	121.90
44	1	1403	C	N1-C2-O2	7.71	123.52	118.90
44	1	130	A	C5-C6-N6	-7.70	117.54	123.70
44	1	1307	G	N3-C4-N9	7.70	130.62	126.00
44	1	2892	A	C4-C5-N7	7.70	114.55	110.70
44	1	3046	A	C5-N7-C8	-7.69	100.05	103.90
44	1	806	A	C5-C6-N6	-7.69	117.55	123.70
44	1	3006	A	C5-N7-C8	-7.69	100.05	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3134	A	C4-C5-N7	7.69	114.55	110.70
44	1	1422	G	C6-C5-N7	-7.69	125.79	130.40
44	1	114	A	C5-C6-N1	7.68	121.54	117.70
45	2	40	A	C5-N7-C8	-7.67	100.06	103.90
44	1	2358	A	C5-N7-C8	-7.67	100.06	103.90
44	1	2994	A	N1-C6-N6	7.67	123.20	118.60
44	1	663	C	N3-C4-N4	7.67	123.37	118.00
44	1	27	C	C5-C6-N1	7.67	124.83	121.00
44	1	1498	A	C4-C5-N7	7.67	114.53	110.70
44	1	3145	C	N1-C2-O2	7.67	123.50	118.90
44	1	3019	U	C6-N1-C2	-7.66	116.40	121.00
45	2	45	C	N1-C2-O2	7.66	123.50	118.90
11	O	18	ARG	NE-CZ-NH1	7.66	124.13	120.30
44	1	1226	G	C4-C5-N7	7.66	113.86	110.80
44	1	1525	G	C5-N7-C8	-7.66	100.47	104.30
44	1	2925	C	C2-N1-C1'	7.65	127.22	118.80
44	1	3021	A	C5-C6-N6	-7.65	117.58	123.70
44	1	3139	A	C4-C5-N7	7.65	114.53	110.70
44	1	2376	G	N3-C2-N2	7.65	125.25	119.90
44	1	2910	A	C4-C5-C6	-7.65	113.18	117.00
44	1	2136	C	C6-N1-C2	-7.64	117.24	120.30
44	1	389	A	C4-C5-N7	7.64	114.52	110.70
45	2	66	A	C5-C6-N6	-7.64	117.59	123.70
2	C	182	LEU	CA-CB-CG	7.64	132.87	115.30
44	1	1187	C	N3-C4-N4	-7.64	112.65	118.00
44	1	801	A	C5-C6-N6	-7.63	117.59	123.70
44	1	1333	C	N1-C2-O2	7.63	123.48	118.90
44	1	64	G	C4-C5-N7	7.63	113.85	110.80
44	1	666	A	C5-C6-N1	7.63	121.52	117.70
44	1	1498	A	N7-C8-N9	7.63	117.61	113.80
44	1	613	G	N7-C8-N9	7.63	116.91	113.10
44	1	3141	A	N9-C4-C5	-7.63	102.75	105.80
45	2	120	C	C5-C4-N4	-7.63	114.86	120.20
44	1	701	G	N3-C2-N2	7.62	125.24	119.90
44	1	926	A	C5-C6-N6	-7.62	117.60	123.70
44	1	3089	C	N1-C2-O2	7.62	123.47	118.90
45	2	9	A	C5-C6-N1	7.62	121.51	117.70
44	1	804	C	N3-C4-C5	7.62	124.95	121.90
44	1	1420	C	C5-C6-N1	7.62	124.81	121.00
45	2	137	C	N3-C4-N4	7.62	123.33	118.00
44	1	1423	C	N3-C4-C5	7.62	124.95	121.90
44	1	16	A	N7-C8-N9	7.61	117.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	19	C	C5-C6-N1	7.61	124.81	121.00
44	1	3273	A	C4-C5-C6	-7.61	113.20	117.00
44	1	3295	A	C5-C6-N1	7.61	121.50	117.70
44	1	3091	A	C5-C6-N1	7.61	121.50	117.70
44	1	1474	A	C5-C6-N6	-7.60	117.62	123.70
44	1	1443	G	C5-N7-C8	-7.60	100.50	104.30
44	1	1895	A	C5-C6-N1	7.60	121.50	117.70
44	1	1382	G	C5-N7-C8	-7.60	100.50	104.30
45	2	36	G	N7-C8-N9	7.59	116.90	113.10
10	N	38	ARG	NE-CZ-NH1	7.59	124.09	120.30
44	1	58	G	N9-C4-C5	-7.58	102.37	105.40
44	1	347	G	C5-N7-C8	-7.58	100.51	104.30
44	1	323	A	N1-C6-N6	7.58	123.14	118.60
44	1	113	C	N3-C2-O2	-7.57	116.60	121.90
44	1	369	A	C4-C5-N7	7.57	114.48	110.70
44	1	2367	A	C4-C5-N7	7.57	114.48	110.70
44	1	345	G	N3-C2-N2	7.57	125.20	119.90
44	1	2352	A	C5-N7-C8	-7.56	100.12	103.90
44	1	12	A	C5-C6-N1	7.56	121.48	117.70
44	1	815	G	C6-C5-N7	-7.56	125.86	130.40
44	1	503	C	C5-C4-N4	-7.55	114.91	120.20
44	1	882	A	C8-N9-C4	-7.55	102.78	105.80
45	2	113	U	C5-C6-N1	7.55	126.48	122.70
44	1	56	G	C5-N7-C8	-7.55	100.53	104.30
44	1	1190	A	N9-C4-C5	-7.55	102.78	105.80
44	1	1437	C	N3-C4-N4	7.54	123.28	118.00
44	1	3016	A	C5-C6-N1	7.54	121.47	117.70
44	1	928	C	N3-C4-N4	7.54	123.28	118.00
45	2	12	A	C5-N7-C8	-7.54	100.13	103.90
44	1	1456	A	C5-N7-C8	-7.54	100.13	103.90
45	2	21	C	N3-C2-O2	-7.54	116.63	121.90
44	1	1394	A	C5-C6-N1	7.53	121.47	117.70
44	1	107	A	C4-C5-N7	7.53	114.47	110.70
44	1	947	G	C5-N7-C8	-7.53	100.53	104.30
44	1	3097	C	C5-C4-N4	-7.53	114.93	120.20
44	1	2936	A	C5-C6-N1	7.53	121.47	117.70
44	1	3210	A	C5-N7-C8	-7.53	100.14	103.90
44	1	1161	G	C5-N7-C8	-7.53	100.54	104.30
44	1	123	A	N1-C6-N6	-7.53	114.08	118.60
44	1	1418	A	C8-N9-C4	7.53	108.81	105.80
44	1	1426	C	N1-C2-O2	7.53	123.42	118.90
44	1	1881	A	N9-C4-C5	-7.53	102.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	2933	A	C5-C6-N1	7.53	121.46	117.70
44	1	1162	U	C5-C4-O4	-7.52	121.39	125.90
44	1	3086	A	C5-C6-N1	7.52	121.46	117.70
44	1	3043	C	C5-C4-N4	-7.52	114.94	120.20
44	1	990	U	C5-C6-N1	7.52	126.46	122.70
44	1	3164	C	N3-C2-O2	-7.51	116.64	121.90
44	1	1290	A	N7-C8-N9	7.50	117.55	113.80
44	1	1161	G	N7-C8-N9	7.50	116.85	113.10
44	1	875	G	C6-C5-N7	-7.50	125.90	130.40
45	2	57	C	N3-C2-O2	-7.50	116.65	121.90
44	1	114	A	C5-N7-C8	-7.49	100.15	103.90
44	1	1112	A	C5-C6-N1	7.49	121.45	117.70
44	1	292	U	C2-N1-C1'	7.49	126.69	117.70
45	2	8	C	N1-C2-O2	7.49	123.39	118.90
44	1	3012	A	C5-C6-N1	7.49	121.44	117.70
46	6	23	U	C2-N1-C1'	7.49	126.68	117.70
44	1	803	C	N3-C4-N4	7.48	123.24	118.00
44	1	1179	A	N9-C4-C5	-7.48	102.81	105.80
44	1	1299	U	C2-N1-C1'	7.48	126.68	117.70
44	1	1615	C	N3-C2-O2	-7.48	116.66	121.90
44	1	228	U	C6-N1-C2	-7.48	116.52	121.00
44	1	365	A	C5-N7-C8	-7.47	100.16	103.90
24	b	370	ASP	CB-CG-OD2	7.47	125.02	118.30
44	1	1527	C	C5-C6-N1	7.47	124.74	121.00
44	1	2366	C	C6-N1-C2	-7.47	117.31	120.30
44	1	3040	A	C5-N7-C8	-7.47	100.17	103.90
44	1	637	C	N1-C2-O2	7.47	123.38	118.90
45	2	105	A	C5-C6-N1	7.47	121.43	117.70
44	1	373	A	C5-N7-C8	-7.46	100.17	103.90
44	1	1194	G	N3-C2-N2	7.46	125.12	119.90
44	1	1426	C	N3-C4-C5	7.46	124.89	121.90
44	1	303	G	N1-C2-N2	-7.46	109.48	116.20
44	1	423	A	C5-C6-N6	-7.46	117.73	123.70
44	1	1446	A	C4-C5-C6	-7.46	113.27	117.00
44	1	3083	G	C4-C5-N7	7.46	113.78	110.80
44	1	340	C	C2-N1-C1'	7.46	127.01	118.80
44	1	952	A	C5-C6-N1	7.46	121.43	117.70
44	1	3299	A	C4-C5-N7	7.46	114.43	110.70
46	6	231	A	N1-C6-N6	-7.46	114.12	118.60
44	1	355	A	C5-N7-C8	-7.45	100.17	103.90
44	1	1332	A	N1-C6-N6	7.44	123.07	118.60
44	1	3248	C	N3-C2-O2	-7.44	116.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	f	82	ARG	NE-CZ-NH1	7.44	124.02	120.30
44	1	1194	G	C4-C5-N7	7.43	113.77	110.80
44	1	622	A	C5-C6-N6	-7.43	117.76	123.70
44	1	29	C	N1-C2-O2	7.43	123.36	118.90
44	1	715	A	C5-C6-N6	-7.42	117.76	123.70
44	1	3296	A	C4-C5-N7	7.42	114.41	110.70
44	1	1132	C	C6-N1-C2	-7.42	117.33	120.30
44	1	3134	A	C5-N7-C8	-7.42	100.19	103.90
44	1	1381	A	N3-C4-C5	7.42	131.99	126.80
44	1	226	C	C5-C4-N4	-7.42	115.01	120.20
44	1	1105	A	C4-C5-N7	7.42	114.41	110.70
44	1	2355	G	C5-N7-C8	-7.42	100.59	104.30
14	R	42	ARG	NE-CZ-NH2	-7.41	116.59	120.30
44	1	1382	G	C4-C5-N7	7.41	113.77	110.80
44	1	1444	G	C4-C5-N7	7.41	113.77	110.80
44	1	1427	U	C5-C6-N1	7.41	126.41	122.70
44	1	3103	A	C4-C5-N7	7.41	114.40	110.70
44	1	663	C	N1-C2-O2	7.40	123.34	118.90
44	1	1752	A	C5-C6-N1	7.40	121.40	117.70
44	1	216	G	C4-C5-N7	7.40	113.76	110.80
44	1	1303	A	C5-C6-N1	7.40	121.40	117.70
44	1	215	G	C4-C5-N7	7.39	113.76	110.80
44	1	1493	G	N1-C2-N2	-7.39	109.55	116.20
44	1	1377	G	C2-N3-C4	-7.39	108.20	111.90
44	1	1514	G	N1-C2-N2	7.39	122.85	116.20
44	1	1332	A	C5-C6-N1	7.38	121.39	117.70
44	1	1342	C	N1-C2-O2	7.38	123.33	118.90
44	1	61	A	C4-C5-N7	7.38	114.39	110.70
44	1	1459	C	N1-C2-O2	7.38	123.33	118.90
8	L	101	ARG	NE-CZ-NH1	7.38	123.99	120.30
10	N	159	ARG	NE-CZ-NH1	7.38	123.99	120.30
41	u	32	CYS	CA-CB-SG	7.37	127.26	114.00
44	1	427	C	N1-C2-O2	7.37	123.32	118.90
44	1	1426	C	C6-N1-C2	-7.37	117.35	120.30
44	1	3320	A	C5-C6-N6	-7.37	117.81	123.70
44	1	342	A	C4-C5-C6	-7.36	113.32	117.00
44	1	352	A	C4-C5-C6	-7.36	113.32	117.00
44	1	705	A	N1-C6-N6	7.36	123.02	118.60
44	1	60	A	N9-C4-C5	-7.36	102.86	105.80
44	1	2114	C	C6-N1-C2	-7.36	117.36	120.30
44	1	3323	A	N9-C4-C5	-7.36	102.86	105.80
44	1	342	A	C5-C6-N1	7.35	121.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3097	C	N3-C2-O2	-7.35	116.75	121.90
44	1	344	A	N1-C6-N6	7.35	123.01	118.60
44	1	660	A	C8-N9-C4	-7.35	102.86	105.80
44	1	27	C	N1-C2-O2	7.35	123.31	118.90
45	2	37	A	C5-C6-N1	7.35	121.37	117.70
44	1	321	C	C5-C4-N4	-7.34	115.06	120.20
44	1	803	C	C5-C4-N4	-7.34	115.06	120.20
44	1	1159	A	C2-N3-C4	7.34	114.27	110.60
44	1	1420	C	C4-C5-C6	-7.34	113.73	117.40
44	1	1526	U	C2-N1-C1'	7.34	126.51	117.70
44	1	2940	A	C5-C6-N1	7.34	121.37	117.70
44	1	3046	A	C5-C6-N1	7.34	121.37	117.70
44	1	948	C	C5-C4-N4	-7.34	115.06	120.20
45	2	62	C	C5-C4-N4	-7.34	115.06	120.20
44	1	1635	G	N3-C2-N2	7.33	125.03	119.90
44	1	790	U	N3-C4-O4	7.33	124.53	119.40
44	1	3006	A	N7-C8-N9	7.33	117.47	113.80
44	1	3185	U	C5-C6-N1	7.33	126.37	122.70
44	1	347	G	N1-C2-N2	-7.33	109.60	116.20
44	1	1304	A	N7-C8-N9	7.33	117.46	113.80
44	1	800	G	N7-C8-N9	7.33	116.76	113.10
44	1	655	C	N3-C4-N4	7.32	123.13	118.00
44	1	667	C	N3-C4-N4	7.32	123.13	118.00
44	1	225	C	C5-C4-N4	-7.32	115.07	120.20
44	1	1437	C	C5-C6-N1	7.32	124.66	121.00
44	1	1395	G	N1-C2-N2	-7.32	109.61	116.20
44	1	3314	A	C4-C5-N7	7.32	114.36	110.70
44	1	1307	G	N3-C2-N2	7.32	125.02	119.90
44	1	367	A	N9-C4-C5	-7.32	102.87	105.80
44	1	586	C	N3-C2-O2	-7.32	116.78	121.90
44	1	1165	A	C4-C5-N7	7.31	114.36	110.70
44	1	1435	A	C4-C5-C6	-7.31	113.34	117.00
44	1	342	A	C4-C5-N7	7.31	114.35	110.70
44	1	2360	C	C5-C4-N4	-7.31	115.08	120.20
45	2	103	G	C5-N7-C8	-7.31	100.65	104.30
44	1	969	C	N1-C2-O2	7.31	123.28	118.90
44	1	123	A	C4-C5-C6	-7.30	113.35	117.00
45	2	10	A	N7-C8-N9	7.30	117.45	113.80
44	1	12	A	N9-C4-C5	-7.30	102.88	105.80
44	1	1380	G	C5-N7-C8	-7.30	100.65	104.30
44	1	1546	A	C5-C6-N6	-7.30	117.86	123.70
44	1	397	A	C8-N9-C4	-7.30	102.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1170	A	N7-C8-N9	7.30	117.45	113.80
44	1	1204	A	C4-C5-N7	7.29	114.35	110.70
44	1	585	A	N7-C8-N9	7.29	117.45	113.80
44	1	1588	A	N1-C6-N6	-7.29	114.22	118.60
44	1	2983	C	N3-C2-O2	-7.29	116.80	121.90
44	1	2986	U	C5-C6-N1	7.29	126.35	122.70
1	B	116	ARG	NE-CZ-NH1	7.29	123.95	120.30
44	1	651	G	C4-C5-N7	7.29	113.72	110.80
15	S	152	LEU	CB-CG-CD1	7.29	123.39	111.00
44	1	2114	C	N3-C2-O2	-7.29	116.80	121.90
44	1	2390	A	C5-C6-N1	7.29	121.34	117.70
44	1	1150	A	C5-C6-N6	-7.29	117.87	123.70
44	1	1475	A	C5-C6-N1	7.28	121.34	117.70
44	1	2985	C	O5'-P-OP2	-7.28	99.14	105.70
44	1	1806	A	C5-C6-N6	-7.28	117.88	123.70
45	2	157	U	C2-N1-C1'	7.28	126.44	117.70
2	C	95	ARG	NE-CZ-NH1	7.28	123.94	120.30
44	1	334	A	C5-C6-N6	-7.28	117.88	123.70
44	1	649	A	C5-C6-N1	7.28	121.34	117.70
44	1	23	A	C5-N7-C8	-7.27	100.26	103.90
44	1	920	A	C4-C5-N7	7.27	114.34	110.70
44	1	1304	A	C5-C6-N1	7.27	121.34	117.70
44	1	376	G	O4'-C1'-N9	7.27	114.02	108.20
44	1	1843	C	N3-C4-N4	7.27	123.09	118.00
44	1	516	A	N9-C4-C5	-7.26	102.89	105.80
44	1	1422	G	N7-C8-N9	7.26	116.73	113.10
45	2	77	A	C5-N7-C8	-7.26	100.27	103.90
44	1	209	A	N9-C4-C5	-7.26	102.90	105.80
44	1	2341	A	C5-C6-N1	7.26	121.33	117.70
44	1	357	A	C6-N1-C2	-7.26	114.25	118.60
44	1	2366	C	C5-C4-N4	-7.25	115.12	120.20
44	1	338	A	C4-C5-C6	-7.25	113.38	117.00
44	1	1279	C	N3-C2-O2	-7.25	116.83	121.90
44	1	1306	G	C5-N7-C8	-7.25	100.68	104.30
44	1	3127	A	N9-C4-C5	-7.25	102.90	105.80
44	1	3286	G	N3-C2-N2	7.25	124.97	119.90
44	1	1477	A	C5-C6-N1	7.25	121.32	117.70
44	1	649	A	C4-C5-N7	7.25	114.32	110.70
44	1	347	G	N3-C2-N2	7.24	124.97	119.90
44	1	1667	A	N7-C8-N9	7.24	117.42	113.80
44	1	1152	G	C8-N9-C1'	-7.24	117.59	127.00
44	1	1428	A	N9-C4-C5	-7.24	102.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	969	C	C6-N1-C2	-7.24	117.41	120.30
44	1	1433	A	C5-N7-C8	-7.24	100.28	103.90
44	1	1491	A	C5-C6-N1	7.24	121.32	117.70
44	1	3375	A	C5-C6-N1	7.24	121.32	117.70
44	1	588	G	N7-C8-N9	7.23	116.72	113.10
45	2	36	G	C5-N7-C8	-7.23	100.68	104.30
45	2	66	A	N1-C6-N6	7.23	122.94	118.60
44	1	3008	A	N9-C4-C5	-7.22	102.91	105.80
45	2	66	A	C5-N7-C8	-7.22	100.29	103.90
44	1	341	G	C6-C5-N7	-7.22	126.07	130.40
44	1	366	A	C5-C6-N1	7.22	121.31	117.70
44	1	1290	A	C5-N7-C8	-7.22	100.29	103.90
44	1	1329	U	C5-C6-N1	7.22	126.31	122.70
44	1	64	G	C5-N7-C8	-7.22	100.69	104.30
45	2	104	A	C4-C5-N7	7.22	114.31	110.70
44	1	1440	G	C5-N7-C8	-7.22	100.69	104.30
44	1	1695	U	O4'-C1'-N1	7.22	113.97	108.20
44	1	130	A	N9-C4-C5	-7.22	102.91	105.80
44	1	1603	A	C5-C6-N1	7.22	121.31	117.70
44	1	3127	A	C5-C6-N6	-7.21	117.93	123.70
44	1	1105	A	C5-C6-N1	7.21	121.31	117.70
44	1	792	G	C6-C5-N7	-7.21	126.08	130.40
44	1	1420	C	N3-C2-O2	-7.21	116.85	121.90
44	1	1835	A	C5-N7-C8	-7.21	100.30	103.90
44	1	1169	A	C5-C6-N6	-7.21	117.94	123.70
44	1	326	U	C5-C6-N1	7.20	126.30	122.70
44	1	1146	C	N3-C4-N4	7.20	123.04	118.00
44	1	1307	G	C6-C5-N7	-7.20	126.08	130.40
44	1	66	A	N1-C6-N6	-7.20	114.28	118.60
44	1	1546	A	C4-C5-N7	7.20	114.30	110.70
44	1	3021	A	C4-C5-N7	7.20	114.30	110.70
44	1	3097	C	C5-C6-N1	7.20	124.60	121.00
44	1	1461	A	C4-C5-N7	7.20	114.30	110.70
44	1	1203	A	C5-C6-N6	-7.19	117.95	123.70
44	1	1105	A	C5-N7-C8	-7.19	100.31	103.90
32	j	63	ARG	NE-CZ-NH1	-7.19	116.71	120.30
44	1	384	A	C5-C6-N6	-7.19	117.95	123.70
44	1	613	G	C5-N7-C8	-7.19	100.71	104.30
44	1	1337	A	C8-N9-C4	7.19	108.67	105.80
44	1	1799	A	C5-C6-N1	7.18	121.29	117.70
44	1	2884	C	N1-C2-O2	7.18	123.21	118.90
44	1	23	A	C5-C6-N1	7.18	121.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3382	U	C5-C6-N1	7.18	126.29	122.70
4	F	156	ILE	C-N-CA	7.17	139.63	121.70
44	1	55	G	C4-C5-N7	7.17	113.67	110.80
44	1	655	C	C5-C6-N1	7.17	124.59	121.00
1	B	19	ARG	NE-CZ-NH2	-7.17	116.71	120.30
27	e	24	ARG	NE-CZ-NH2	-7.17	116.71	120.30
44	1	205	C	N3-C2-O2	-7.17	116.88	121.90
44	1	1401	A	N1-C6-N6	7.17	122.90	118.60
44	1	3091	A	N9-C4-C5	-7.17	102.93	105.80
44	1	1874	A	N1-C6-N6	7.17	122.90	118.60
44	1	3181	C	C2-N1-C1'	7.17	126.69	118.80
8	L	35	ARG	NE-CZ-NH2	-7.17	116.72	120.30
44	1	1621	A	N7-C8-N9	7.17	117.38	113.80
44	1	519	A	C5-C6-N6	-7.17	117.97	123.70
44	1	1194	G	N7-C8-N9	7.17	116.68	113.10
45	2	46	G	C8-N9-C4	-7.17	103.53	106.40
44	1	1381	A	C4-C5-N7	7.16	114.28	110.70
44	1	6	A	N9-C4-C5	-7.16	102.94	105.80
44	1	1443	G	C4-C5-N7	7.16	113.66	110.80
44	1	3006	A	C4-C5-N7	7.16	114.28	110.70
44	1	1406	A	N1-C6-N6	-7.16	114.31	118.60
44	1	1615	C	N1-C2-O2	7.16	123.20	118.90
44	1	799	G	N3-C2-N2	7.16	124.91	119.90
44	1	1332	A	N3-C4-N9	7.16	133.12	127.40
44	1	504	A	N1-C6-N6	7.15	122.89	118.60
44	1	1404	G	N3-C4-C5	7.15	132.18	128.60
44	1	3295	A	C5-C6-N6	-7.15	117.98	123.70
44	1	497	C	N3-C4-C5	7.15	124.76	121.90
44	1	1190	A	C5-N7-C8	-7.15	100.32	103.90
44	1	1696	A	C5-C6-N1	7.15	121.28	117.70
44	1	3085	G	N3-C4-C5	7.15	132.18	128.60
44	1	355	A	C5-C6-N1	7.15	121.28	117.70
45	2	105	A	N1-C6-N6	7.15	122.89	118.60
44	1	1342	C	C6-N1-C2	-7.15	117.44	120.30
44	1	1800	A	C5-C6-N6	-7.15	117.98	123.70
44	1	76	G	N3-C2-N2	7.14	124.90	119.90
44	1	1469	C	C2-N3-C4	7.14	123.47	119.90
45	2	43	A	C5-C6-N1	7.14	121.27	117.70
44	1	3375	A	C5-C6-N6	-7.14	117.99	123.70
44	1	3196	U	C2-N1-C1'	7.13	126.26	117.70
44	1	348	A	N1-C6-N6	7.13	122.88	118.60
44	1	1314	C	N3-C2-O2	-7.13	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	6	A	C5-C6-N6	-7.13	118.00	123.70
44	1	1525	G	N9-C4-C5	-7.13	102.55	105.40
44	1	944	C	C5-C4-N4	-7.13	115.21	120.20
44	1	348	A	C5-C6-N6	-7.13	118.00	123.70
44	1	35	A	C5-C6-N1	7.12	121.26	117.70
44	1	641	C	C5-C4-N4	-7.12	115.21	120.20
39	s	27	ARG	NE-CZ-NH1	7.12	123.86	120.30
44	1	1895	A	C5-C6-N6	-7.12	118.00	123.70
44	1	793	C	N3-C4-C5	7.12	124.75	121.90
44	1	3085	G	N3-C4-N9	-7.12	121.73	126.00
44	1	81	C	C5-C4-N4	-7.11	115.22	120.20
44	1	142	C	N3-C4-N4	7.11	122.98	118.00
44	1	636	C	C5-C4-N4	-7.11	115.22	120.20
44	1	1598	G	C6-C5-N7	-7.11	126.13	130.40
44	1	2341	A	C4-C5-N7	7.11	114.25	110.70
44	1	1159	A	N3-C4-C5	-7.11	121.82	126.80
44	1	1896	A	C5-C6-N6	-7.11	118.01	123.70
44	1	1394	A	C5-N7-C8	-7.11	100.35	103.90
44	1	64	G	C4-N9-C1'	7.10	135.74	126.50
45	2	115	C	C5-C4-N4	-7.10	115.23	120.20
44	1	397	A	N7-C8-N9	7.10	117.35	113.80
44	1	2828	G	N3-C2-N2	7.10	124.87	119.90
44	1	3210	A	C5-C6-N1	7.10	121.25	117.70
44	1	1609	C	C5-C6-N1	7.10	124.55	121.00
2	C	195	ARG	NE-CZ-NH1	7.09	123.85	120.30
44	1	5	G	N3-C4-N9	-7.09	121.74	126.00
44	1	1312	C	N3-C2-O2	-7.09	116.93	121.90
44	1	2896	A	C5-C6-N1	7.09	121.25	117.70
44	1	1444	G	C8-N9-C4	-7.09	103.56	106.40
44	1	51	A	C4-C5-N7	7.09	114.24	110.70
44	1	20	A	C5-C6-N1	7.08	121.24	117.70
44	1	634	C	N3-C4-N4	7.08	122.96	118.00
44	1	705	A	C5-C6-N6	-7.08	118.03	123.70
44	1	929	A	C5-C6-N1	7.08	121.24	117.70
44	1	1493	G	C4-N9-C1'	7.08	135.71	126.50
44	1	319	A	C5-C6-N1	7.08	121.24	117.70
44	1	1535	A	C5-C6-N1	7.08	121.24	117.70
44	1	1203	A	N9-C4-C5	-7.08	102.97	105.80
44	1	53	G	C5-N7-C8	-7.08	100.76	104.30
44	1	1435	A	C5-C6-N1	7.07	121.24	117.70
23	a	87	ARG	NE-CZ-NH1	7.07	123.84	120.30
44	1	199	A	C5-C6-N1	7.07	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	296	A	C5-C6-N1	7.07	121.23	117.70
44	1	1904	C	C6-N1-C2	-7.07	117.47	120.30
44	1	1496	C	C6-N1-C1'	-7.07	112.32	120.80
45	2	9	A	C5-C6-N6	-7.07	118.05	123.70
44	1	47	C	C5-C4-N4	-7.07	115.25	120.20
44	1	1171	G	N3-C2-N2	7.07	124.85	119.90
44	1	1176	C	C6-N1-C2	-7.07	117.47	120.30
44	1	2345	A	C4-C5-N7	7.06	114.23	110.70
44	1	1786	G	C4-C5-N7	7.06	113.62	110.80
44	1	1178	G	O5'-P-OP1	-7.06	99.35	105.70
44	1	3183	A	C5-C6-N6	-7.06	118.05	123.70
44	1	1558	A	C4-C5-C6	-7.06	113.47	117.00
44	1	2993	G	N3-C2-N2	7.06	124.84	119.90
44	1	1165	A	C5-N7-C8	-7.05	100.37	103.90
44	1	2355	G	C5-C6-O6	-7.05	124.37	128.60
44	1	670	C	N3-C4-C5	7.05	124.72	121.90
45	2	74	U	N3-C2-O2	-7.05	117.26	122.20
44	1	2994	A	N9-C4-C5	-7.05	102.98	105.80
44	1	672	A	C4-C5-N7	7.04	114.22	110.70
44	1	729	C	C6-N1-C2	-7.04	117.48	120.30
44	1	1418	A	C4-C5-N7	7.04	114.22	110.70
45	2	33	A	C5-C6-N1	7.04	121.22	117.70
45	2	45	C	C6-N1-C2	-7.04	117.48	120.30
44	1	947	G	C4-N9-C1'	7.04	135.65	126.50
44	1	3104	U	C6-N1-C2	-7.04	116.78	121.00
44	1	1116	G	C4-N9-C1'	7.04	135.65	126.50
44	1	2878	G	C5-C6-O6	7.04	132.82	128.60
44	1	1797	A	C4-C5-C6	-7.04	113.48	117.00
44	1	215	G	C5-N7-C8	-7.03	100.78	104.30
44	1	990	U	C6-N1-C2	-7.03	116.78	121.00
44	1	3163	A	N9-C4-C5	-7.03	102.99	105.80
45	2	110	C	C5-C4-N4	-7.03	115.28	120.20
44	1	573	C	N1-C2-O2	7.03	123.12	118.90
44	1	637	C	N3-C2-O2	-7.03	116.98	121.90
44	1	70	A	C5-C6-N1	7.03	121.21	117.70
44	1	920	A	C5-C6-N6	-7.02	118.08	123.70
44	1	3094	A	C5-C6-N1	7.02	121.21	117.70
44	1	106	A	C4-C5-N7	7.02	114.21	110.70
44	1	1462	A	C4-C5-N7	7.02	114.21	110.70
44	1	2355	G	N3-C2-N2	-7.02	114.99	119.90
46	6	2	C	C6-N1-C2	-7.02	117.49	120.30
44	1	384	A	C4-C5-N7	7.02	114.21	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	365	A	N7-C8-N9	7.01	117.31	113.80
44	1	1496	C	C5-C4-N4	-7.01	115.29	120.20
44	1	1527	C	C2-N1-C1'	7.01	126.52	118.80
6	H	124	ARG	NE-CZ-NH2	-7.01	116.79	120.30
44	1	2892	A	N9-C4-C5	-7.01	103.00	105.80
44	1	64	G	C8-N9-C1'	-7.01	117.89	127.00
44	1	628	A	C5-N7-C8	-7.01	100.39	103.90
44	1	3174	A	C5-C6-N1	7.01	121.20	117.70
44	1	1424	C	N3-C4-N4	7.01	122.91	118.00
10	N	143	ARG	NE-CZ-NH1	7.00	123.80	120.30
27	e	45	ARG	NE-CZ-NH2	-7.00	116.80	120.30
44	1	1456	A	N7-C8-N9	7.00	117.30	113.80
44	1	3174	A	N9-C4-C5	-7.00	103.00	105.80
45	2	46	G	N7-C8-N9	7.00	116.60	113.10
44	1	667	C	C6-N1-C2	-7.00	117.50	120.30
44	1	932	U	N1-C2-O2	7.00	127.70	122.80
44	1	960	U	C2-N1-C1'	7.00	126.09	117.70
44	1	2925	C	N1-C2-O2	7.00	123.10	118.90
44	1	1462	A	C5-C6-N6	-7.00	118.10	123.70
45	2	133	G	C4-C5-N7	7.00	113.60	110.80
44	1	399	A	C5-C6-N1	6.99	121.20	117.70
44	1	435	C	N1-C2-O2	6.99	123.10	118.90
44	1	659	G	C2-N3-C4	-6.99	108.40	111.90
44	1	1339	C	N3-C2-O2	-6.99	117.00	121.90
44	1	794	U	C5-C6-N1	6.99	126.19	122.70
44	1	3057	U	N3-C2-O2	-6.99	117.31	122.20
44	1	1376	C	C2-N1-C1'	6.99	126.49	118.80
44	1	1402	C	C5-C4-N4	-6.99	115.31	120.20
44	1	3214	U	N3-C2-O2	-6.99	117.31	122.20
45	2	40	A	O5'-P-OP1	-6.99	99.41	105.70
45	2	105	A	C4-C5-N7	6.99	114.19	110.70
44	1	367	A	N1-C6-N6	6.99	122.79	118.60
44	1	1836	C	C6-N1-C2	-6.98	117.51	120.30
44	1	1446	A	C5-N7-C8	-6.98	100.41	103.90
44	1	500	C	N1-C2-O2	6.98	123.08	118.90
44	1	1360	C	C5-C4-N4	-6.98	115.32	120.20
44	1	282	G	C4-N9-C1'	6.97	135.57	126.50
44	1	652	G	C8-N9-C1'	-6.97	117.93	127.00
45	2	10	A	N9-C4-C5	-6.97	103.01	105.80
45	2	30	C	N1-C2-O2	6.97	123.08	118.90
44	1	1509	A	C5-N7-C8	-6.96	100.42	103.90
11	O	117	ARG	NE-CZ-NH1	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	932	U	N3-C2-O2	-6.96	117.33	122.20
44	1	1175	C	N3-C4-C5	6.96	124.68	121.90
44	1	1358	C	C5-C4-N4	-6.96	115.33	120.20
44	1	289	A	N1-C6-N6	6.96	122.78	118.60
44	1	1799	A	C5-N7-C8	-6.96	100.42	103.90
45	2	149	A	C5-C6-N1	6.96	121.18	117.70
45	2	26	U	N3-C2-O2	-6.95	117.33	122.20
44	1	75	G	C4-C5-N7	6.95	113.58	110.80
45	2	96	A	C4-C5-C6	-6.95	113.52	117.00
44	1	422	A	C8-N9-C4	-6.95	103.02	105.80
44	1	3035	A	C4-C5-N7	6.95	114.17	110.70
44	1	800	G	C8-N9-C4	-6.95	103.62	106.40
44	1	1430	U	C5-C6-N1	6.95	126.17	122.70
44	1	61	A	C5-C6-N1	6.94	121.17	117.70
44	1	1303	A	C4-C5-N7	6.94	114.17	110.70
44	1	632	G	C4-N9-C1'	6.93	135.51	126.50
44	1	1893	A	C4-C5-N7	6.93	114.17	110.70
44	1	3103	A	N9-C4-C5	-6.93	103.03	105.80
44	1	1456	A	C5-C6-N6	-6.93	118.16	123.70
44	1	3182	G	C4-C5-N7	6.93	113.57	110.80
44	1	1329	U	N3-C2-O2	-6.92	117.35	122.20
44	1	159	A	C5-C6-N1	6.92	121.16	117.70
44	1	683	U	C5-C6-N1	6.92	126.16	122.70
44	1	1699	A	N1-C6-N6	-6.92	114.45	118.60
44	1	3314	A	C5-C6-N6	-6.92	118.16	123.70
45	2	132	G	N7-C8-N9	6.92	116.56	113.10
44	1	3213	A	N9-C4-C5	-6.92	103.03	105.80
44	1	3145	C	N3-C2-O2	-6.92	117.06	121.90
45	2	4	C	N1-C2-O2	6.92	123.05	118.90
4	F	232	ARG	NE-CZ-NH1	6.92	123.76	120.30
44	1	2376	G	C4-C5-N7	6.92	113.57	110.80
44	1	315	C	N1-C2-O2	6.92	123.05	118.90
32	j	25	ARG	NE-CZ-NH1	6.91	123.76	120.30
44	1	63	A	C5-N7-C8	-6.91	100.44	103.90
44	1	1396	C	C5-C4-N4	-6.91	115.36	120.20
4	F	88	ARG	NE-CZ-NH1	6.91	123.75	120.30
44	1	500	C	C6-N1-C2	-6.91	117.54	120.30
44	1	701	G	N3-C4-N9	6.91	130.14	126.00
44	1	88	A	C5-C6-N6	-6.90	118.18	123.70
45	2	30	C	C5-C4-N4	-6.90	115.37	120.20
44	1	1108	U	N3-C2-O2	-6.90	117.37	122.20
44	1	1338	C	C5-C4-N4	-6.90	115.37	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1146	C	C5-C4-N4	-6.90	115.37	120.20
44	1	588	G	C5-N7-C8	-6.90	100.85	104.30
44	1	614	C	C5-C4-N4	-6.89	115.38	120.20
44	1	1613	A	C6-N1-C2	-6.89	114.47	118.60
44	1	55	G	C5-N7-C8	-6.89	100.86	104.30
44	1	212	G	C4-N9-C1'	6.89	135.46	126.50
44	1	1280	C	N3-C2-O2	-6.89	117.08	121.90
45	2	65	A	C5-N7-C8	-6.89	100.46	103.90
44	1	52	A	C4-C5-N7	6.89	114.14	110.70
44	1	1336	U	C5-C6-N1	6.89	126.14	122.70
44	1	1837	U	C5-C6-N1	6.89	126.14	122.70
44	1	3085	G	N3-C2-N2	-6.89	115.08	119.90
44	1	3139	A	N1-C6-N6	6.89	122.73	118.60
44	1	585	A	C5-C6-N1	6.88	121.14	117.70
44	1	2348	A	N9-C4-C5	-6.88	103.05	105.80
44	1	497	C	N1-C2-O2	6.88	123.03	118.90
44	1	1135	A	C4-C5-N7	6.88	114.14	110.70
44	1	1364	C	N1-C2-O2	6.88	123.03	118.90
44	1	2899	C	N3-C2-O2	-6.88	117.09	121.90
10	N	31	ARG	NE-CZ-NH1	6.87	123.74	120.30
44	1	28	C	C5-C6-N1	6.87	124.44	121.00
44	1	100	A	N7-C8-N9	6.87	117.23	113.80
44	1	928	C	C2-N1-C1'	6.86	126.35	118.80
45	2	10	A	C6-C5-N7	-6.86	127.50	132.30
44	1	1418	A	N1-C6-N6	6.86	122.72	118.60
44	1	1444	G	C5-N7-C8	-6.86	100.87	104.30
44	1	20	A	C5-N7-C8	-6.86	100.47	103.90
44	1	1152	G	N3-C2-N2	6.86	124.70	119.90
44	1	1419	A	C5-C6-N1	6.85	121.12	117.70
44	1	1529	A	C5-C6-N1	6.85	121.13	117.70
44	1	658	G	C5-N7-C8	-6.85	100.88	104.30
44	1	693	A	N1-C6-N6	6.85	122.71	118.60
44	1	1306	G	C8-N9-C4	-6.85	103.66	106.40
44	1	1608	C	N3-C4-C5	6.85	124.64	121.90
44	1	3048	A	C5-C6-N6	-6.85	118.22	123.70
44	1	282	G	N1-C2-N2	-6.85	110.04	116.20
44	1	242	C	N3-C4-N4	-6.84	113.21	118.00
44	1	1424	C	N3-C4-C5	6.84	124.64	121.90
44	1	3161	C	C6-N1-C2	-6.84	117.56	120.30
44	1	3257	C	N3-C4-C5	6.84	124.64	121.90
45	2	13	A	C5-C6-N6	-6.84	118.22	123.70
44	1	1342	C	C5-C6-N1	6.84	124.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	39	G	N3-C2-N2	6.84	124.69	119.90
44	1	3083	G	N9-C4-C5	-6.84	102.67	105.40
44	1	2345	A	C5-N7-C8	-6.84	100.48	103.90
44	1	805	G	C5-N7-C8	-6.83	100.88	104.30
44	1	3048	A	C4-C5-N7	6.83	114.12	110.70
44	1	653	A	N7-C8-N9	6.83	117.22	113.80
44	1	3012	A	C4-C5-C6	-6.83	113.58	117.00
44	1	8	C	C5-C6-N1	6.83	124.42	121.00
44	1	519	A	N9-C4-C5	-6.83	103.07	105.80
44	1	630	A	N1-C2-N3	-6.83	125.89	129.30
44	1	945	C	C2-N1-C1'	6.83	126.31	118.80
44	1	1800	A	C4-C5-N7	6.83	114.11	110.70
45	2	37	A	C4-C5-C6	-6.83	113.59	117.00
44	1	882	A	N7-C8-N9	6.82	117.21	113.80
44	1	516	A	C4-C5-N7	6.82	114.11	110.70
44	1	1106	G	C8-N9-C4	-6.82	103.67	106.40
44	1	2348	A	C4-C5-N7	6.82	114.11	110.70
44	1	3052	G	N7-C8-N9	6.82	116.51	113.10
44	1	3174	A	N1-C6-N6	6.82	122.69	118.60
45	2	89	A	C5-C6-N1	6.82	121.11	117.70
44	1	57	A	C5-N7-C8	-6.82	100.49	103.90
44	1	1603	A	C4-C5-C6	-6.82	113.59	117.00
45	2	148	G	C8-N9-C4	-6.82	103.67	106.40
44	1	430	U	C5-C6-N1	6.81	126.11	122.70
44	1	1657	C	N3-C4-N4	6.81	122.77	118.00
44	1	2360	C	N1-C2-O2	6.81	122.98	118.90
44	1	3296	A	C5-C6-N6	-6.80	118.26	123.70
44	1	3307	A	C5-C6-N1	6.80	121.10	117.70
44	1	224	C	N3-C4-N4	6.80	122.76	118.00
44	1	342	A	C5-C6-N6	-6.80	118.26	123.70
44	1	1411	C	C5-C4-N4	-6.80	115.44	120.20
44	1	1823	A	C5-C6-N1	6.80	121.10	117.70
44	1	3097	C	C2-N1-C1'	6.80	126.28	118.80
45	2	28	C	N3-C4-N4	6.80	122.76	118.00
44	1	58	G	N7-C8-N9	6.80	116.50	113.10
44	1	242	C	N1-C2-O2	6.80	122.98	118.90
44	1	676	G	C4-C5-N7	6.80	113.52	110.80
44	1	1404	G	C2-N3-C4	-6.80	108.50	111.90
44	1	1546	A	C8-N9-C4	6.80	108.52	105.80
44	1	402	A	C5-C6-N6	-6.79	118.27	123.70
44	1	1193	A	C5-C6-N6	-6.79	118.27	123.70
44	1	2370	G	N3-C2-N2	6.79	124.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	100	U	C6-N1-C2	-6.79	116.93	121.00
44	1	200	C	N1-C2-O2	6.79	122.97	118.90
44	1	676	G	C5-N7-C8	-6.79	100.91	104.30
44	1	3314	A	N9-C4-C5	-6.79	103.09	105.80
44	1	282	G	N3-C2-N2	6.78	124.65	119.90
44	1	1594	A	N1-C6-N6	-6.78	114.53	118.60
44	1	2378	C	C6-N1-C2	-6.78	117.59	120.30
45	2	4	C	C6-N1-C2	-6.78	117.59	120.30
44	1	226	C	N3-C2-O2	-6.78	117.16	121.90
45	2	89	A	C5-N7-C8	-6.78	100.51	103.90
44	1	3305	A	C5-C6-N1	6.78	121.09	117.70
44	1	216	G	C5-N7-C8	-6.77	100.91	104.30
44	1	3091	A	N1-C6-N6	6.77	122.67	118.60
44	1	1419	A	C4-C5-C6	-6.77	113.61	117.00
45	2	17	A	C5-C6-N1	6.77	121.09	117.70
3	E	31	ARG	NE-CZ-NH1	6.77	123.69	120.30
44	1	696	C	N3-C4-N4	6.77	122.74	118.00
44	1	656	A	C5-C6-N6	-6.77	118.29	123.70
45	2	66	A	N9-C4-C5	-6.76	103.09	105.80
44	1	1510	G	N1-C6-O6	-6.76	115.84	119.90
44	1	2098	C	N3-C2-O2	-6.76	117.17	121.90
44	1	430	U	C6-N1-C2	-6.76	116.94	121.00
44	1	1108	U	N1-C2-O2	6.76	127.53	122.80
44	1	1177	G	C8-N9-C1'	-6.75	118.22	127.00
44	1	1363	A	C6-C5-N7	-6.75	127.57	132.30
44	1	328	U	C5-C6-N1	6.75	126.08	122.70
44	1	630	A	C5-C6-N1	6.75	121.08	117.70
44	1	1444	G	C4-N9-C1'	6.75	135.28	126.50
44	1	1461	A	C5-N7-C8	-6.75	100.52	103.90
44	1	1883	A	C5-C6-N1	6.75	121.08	117.70
44	1	3235	C	C6-N1-C2	-6.75	117.60	120.30
44	1	418	A	C4-C5-N7	6.75	114.07	110.70
44	1	76	G	N1-C2-N2	-6.74	110.13	116.20
44	1	1440	G	N7-C8-N9	6.74	116.47	113.10
44	1	3004	C	C6-N1-C2	-6.74	117.60	120.30
44	1	2899	C	C2-N1-C1'	6.74	126.22	118.80
44	1	928	C	N3-C2-O2	-6.74	117.18	121.90
44	1	1741	A	N1-C6-N6	-6.74	114.56	118.60
44	1	2101	C	C6-N1-C2	-6.74	117.61	120.30
44	1	3296	A	C5-N7-C8	-6.74	100.53	103.90
10	N	105	ARG	NE-CZ-NH1	6.74	123.67	120.30
44	1	630	A	N3-C4-N9	6.74	132.79	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	94	ARG	NE-CZ-NH1	6.74	123.67	120.30
44	1	53	G	N7-C8-N9	6.74	116.47	113.10
44	1	1150	A	N7-C8-N9	6.73	117.17	113.80
44	1	1802	C	C5-C4-N4	-6.73	115.49	120.20
44	1	651	G	C5-N7-C8	-6.73	100.93	104.30
45	2	16	G	N3-C4-N9	-6.73	121.96	126.00
44	1	116	A	C4-C5-C6	-6.73	113.64	117.00
44	1	332	C	N1-C2-O2	6.73	122.94	118.90
44	1	1527	C	N3-C4-N4	6.73	122.71	118.00
44	1	396	A	N9-C4-C5	-6.73	103.11	105.80
44	1	336	A	C5-C6-N1	6.72	121.06	117.70
44	1	3091	A	C4-C5-N7	6.72	114.06	110.70
44	1	293	C	N3-C4-C5	6.72	124.59	121.90
44	1	50	U	C6-N1-C2	-6.71	116.97	121.00
44	1	366	A	N9-C4-C5	-6.71	103.11	105.80
45	2	47	C	N1-C2-O2	6.71	122.93	118.90
44	1	3137	C	N3-C4-N4	6.71	122.70	118.00
1	B	21	ARG	NE-CZ-NH1	6.71	123.65	120.30
44	1	63	A	C4-C5-N7	6.71	114.06	110.70
44	1	1171	G	C4-C5-N7	6.71	113.48	110.80
44	1	586	C	C6-N1-C2	-6.71	117.62	120.30
44	1	3004	C	C5-C6-N1	6.71	124.35	121.00
45	2	115	C	N3-C4-N4	6.71	122.69	118.00
45	2	74	U	C6-N1-C2	-6.70	116.98	121.00
45	2	61	A	N1-C6-N6	-6.70	114.58	118.60
44	1	106	A	C4-C5-C6	-6.70	113.65	117.00
45	2	65	A	C4-C5-N7	6.70	114.05	110.70
44	1	951	A	C5-N7-C8	-6.70	100.55	103.90
44	1	1680	G	N3-C2-N2	6.70	124.59	119.90
44	1	1609	C	N3-C4-N4	6.70	122.69	118.00
44	1	1680	G	N1-C2-N2	-6.70	110.17	116.20
44	1	929	A	C4-C5-N7	6.69	114.05	110.70
44	1	794	U	C6-N1-C2	-6.69	116.98	121.00
44	1	1493	G	C8-N9-C1'	-6.69	118.30	127.00
44	1	1525	G	C6-C5-N7	-6.69	126.38	130.40
44	1	396	A	C4-C5-N7	6.69	114.05	110.70
44	1	410	U	C5-C6-N1	6.69	126.04	122.70
44	1	1474	A	C5-C6-N1	6.69	121.04	117.70
44	1	3211	C	N3-C4-N4	6.69	122.68	118.00
44	1	328	U	C6-N1-C2	-6.69	116.99	121.00
44	1	990	U	N1-C2-O2	6.69	127.48	122.80
44	1	920	A	N9-C4-C5	-6.69	103.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	181	ARG	NE-CZ-NH2	6.68	123.64	120.30
44	1	945	C	N3-C4-C5	6.68	124.57	121.90
44	1	34	A	C5-N7-C8	-6.68	100.56	103.90
44	1	641	C	N3-C4-C5	6.68	124.57	121.90
44	1	657	A	C4-C5-C6	-6.68	113.66	117.00
44	1	657	A	C5-C6-N6	-6.68	118.36	123.70
44	1	721	G	O5'-P-OP2	-6.68	99.69	105.70
44	1	3307	A	C5-N7-C8	-6.68	100.56	103.90
45	2	65	A	N1-C6-N6	6.68	122.61	118.60
44	1	20	A	C5-C6-N6	-6.67	118.36	123.70
44	1	117	U	C2-N1-C1'	6.67	125.71	117.70
44	1	1462	A	C5-N7-C8	-6.67	100.56	103.90
44	1	1189	C	C6-N1-C2	-6.67	117.63	120.30
44	1	1381	A	C2-N3-C4	-6.67	107.27	110.60
44	1	1654	A	C5-C6-N1	6.67	121.03	117.70
44	1	2828	G	C4-C5-N7	6.67	113.47	110.80
46	6	232	A	C5-C6-N1	6.66	121.03	117.70
44	1	3163	A	C4-C5-N7	6.66	114.03	110.70
44	1	3186	A	C5-N7-C8	-6.66	100.57	103.90
44	1	1856	C	N1-C2-O2	6.66	122.89	118.90
44	1	3005	A	C5-C6-N1	6.66	121.03	117.70
45	2	149	A	C5-C6-N6	-6.66	118.38	123.70
44	1	150	A	C5-C6-N1	6.65	121.03	117.70
44	1	397	A	N1-C6-N6	-6.65	114.61	118.60
44	1	1383	G	C8-N9-C4	-6.65	103.74	106.40
45	2	96	A	C4-C5-N7	6.65	114.03	110.70
44	1	1297	C	C5-C4-N4	-6.65	115.55	120.20
44	1	1404	G	C5-N7-C8	-6.65	100.98	104.30
44	1	1800	A	N1-C6-N6	6.65	122.59	118.60
44	1	3139	A	N7-C8-N9	6.65	117.12	113.80
44	1	3213	A	N1-C6-N6	6.65	122.59	118.60
2	C	197	ARG	NE-CZ-NH1	6.64	123.62	120.30
44	1	61	A	C5-N7-C8	-6.64	100.58	103.90
44	1	289	A	C5-C6-N6	-6.64	118.39	123.70
44	1	1255	C	C2-N1-C1'	6.64	126.11	118.80
44	1	923	C	N1-C2-O2	6.64	122.88	118.90
44	1	15	C	C6-N1-C2	-6.64	117.64	120.30
44	1	504	A	C5-C6-N1	6.64	121.02	117.70
44	1	1307	G	C4-N9-C1'	6.63	135.12	126.50
44	1	1602	A	N9-C4-C5	-6.63	103.15	105.80
44	1	407	A	C5-C6-N6	-6.63	118.40	123.70
44	1	1365	G	C8-N9-C1'	-6.63	118.38	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	938	C	N3-C4-C5	6.63	124.55	121.90
44	1	6	A	C5-N7-C8	-6.62	100.59	103.90
38	r	16	LYS	CB-CA-C	-6.62	97.15	110.40
44	1	1182	A	C5-C6-N1	6.62	121.01	117.70
44	1	1495	U	C5-C4-O4	6.62	129.87	125.90
44	1	3126	C	N1-C2-O2	6.62	122.87	118.90
44	1	1194	G	C5-N7-C8	-6.62	100.99	104.30
44	1	1372	C	N3-C4-N4	6.62	122.63	118.00
44	1	2343	C	N3-C2-O2	-6.62	117.27	121.90
44	1	347	G	C6-C5-N7	-6.61	126.43	130.40
44	1	402	A	C5-N7-C8	-6.61	100.59	103.90
44	1	3298	C	N1-C2-O2	6.61	122.87	118.90
44	1	366	A	N7-C8-N9	6.61	117.10	113.80
44	1	715	A	C4-C5-N7	6.61	114.00	110.70
44	1	1185	C	N1-C2-O2	6.61	122.86	118.90
44	1	23	A	C4-C5-N7	6.60	114.00	110.70
2	C	47	ARG	NE-CZ-NH1	6.60	123.60	120.30
44	1	802	C	C6-N1-C2	-6.60	117.66	120.30
44	1	1822	C	C6-N1-C2	-6.60	117.66	120.30
44	1	1863	G	N3-C4-N9	-6.60	122.04	126.00
44	1	3001	C	C5-C4-N4	-6.60	115.58	120.20
44	1	3083	G	C5-C6-O6	-6.60	124.64	128.60
44	1	2368	A	C5-C6-N6	-6.60	118.42	123.70
45	2	58	G	C6-C5-N7	-6.60	126.44	130.40
44	1	1859	A	C5-C6-N6	-6.59	118.42	123.70
44	1	1304	A	C5-N7-C8	-6.59	100.60	103.90
44	1	691	A	C4-C5-C6	-6.59	113.70	117.00
44	1	1749	A	C4-C5-C6	-6.59	113.70	117.00
45	2	16	G	N3-C4-C5	6.59	131.90	128.60
44	1	233	C	C5-C4-N4	-6.59	115.59	120.20
44	1	1203	A	C4-C5-N7	6.59	113.99	110.70
44	1	651	G	N7-C8-N9	6.59	116.39	113.10
44	1	3187	A	C5-C6-N1	6.59	120.99	117.70
44	1	395	A	C5-C6-N1	6.58	120.99	117.70
44	1	289	A	N9-C4-C5	-6.58	103.17	105.80
44	1	1449	A	N9-C4-C5	-6.58	103.17	105.80
44	1	1834	U	C5-C6-N1	6.58	125.99	122.70
44	1	3141	A	N1-C6-N6	6.58	122.55	118.60
30	h	89	ARG	NE-CZ-NH2	-6.58	117.01	120.30
44	1	1456	A	N1-C6-N6	6.58	122.55	118.60
44	1	151	A	C5-C6-N6	-6.58	118.44	123.70
44	1	1846	C	N1-C2-O2	6.57	122.84	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	142	C	N3-C4-N4	6.57	122.60	118.00
40	t	167	ARG	NE-CZ-NH1	6.57	123.58	120.30
44	1	18	G	C5-N7-C8	-6.57	101.02	104.30
44	1	1426	C	N3-C2-O2	-6.57	117.30	121.90
44	1	1437	C	N3-C2-O2	-6.57	117.30	121.90
44	1	1786	G	C6-C5-N7	-6.57	126.46	130.40
45	2	16	G	C5-N7-C8	-6.57	101.02	104.30
44	1	775	A	C4-C5-N7	6.56	113.98	110.70
44	1	1437	C	C2-N1-C1'	6.56	126.02	118.80
44	1	3131	U	N3-C4-O4	6.56	124.00	119.40
44	1	416	A	C4-C5-C6	-6.56	113.72	117.00
44	1	1403	C	N3-C4-N4	6.56	122.59	118.00
44	1	1424	C	C5-C6-N1	6.56	124.28	121.00
45	2	15	G	C2-N3-C4	-6.56	108.62	111.90
44	1	693	A	N9-C4-C5	-6.56	103.18	105.80
44	1	1335	C	N1-C2-O2	6.56	122.83	118.90
44	1	1435	A	C4-C5-N7	6.56	113.98	110.70
44	1	2844	C	C6-N1-C2	-6.56	117.68	120.30
45	2	18	U	C5-C6-N1	6.56	125.98	122.70
45	2	97	A	C4-C5-N7	6.56	113.98	110.70
44	1	418	A	C5-N7-C8	-6.55	100.62	103.90
44	1	1296	C	C5-C6-N1	6.55	124.28	121.00
44	1	1432	C	C6-N1-C2	6.55	122.92	120.30
44	1	2352	A	C5-C6-N1	6.54	120.97	117.70
12	P	82	ARG	NE-CZ-NH1	6.54	123.57	120.30
44	1	589	A	C6-N1-C2	-6.54	114.68	118.60
44	1	648	C	C6-N1-C2	-6.54	117.68	120.30
44	1	76	G	C5-N7-C8	-6.54	101.03	104.30
44	1	518	G	C4-N9-C1'	6.54	135.00	126.50
44	1	198	A	C5-C6-N1	6.53	120.97	117.70
44	1	205	C	N3-C4-C5	6.53	124.51	121.90
44	1	1380	G	C8-N9-C4	-6.53	103.79	106.40
44	1	3161	C	N3-C4-N4	6.53	122.57	118.00
44	1	1145	G	N3-C2-N2	6.53	124.47	119.90
44	1	1226	G	C6-C5-N7	-6.53	126.48	130.40
44	1	1504	A	C5-N7-C8	-6.53	100.63	103.90
44	1	12	A	N7-C8-N9	6.53	117.06	113.80
44	1	701	G	N9-C4-C5	-6.53	102.79	105.40
45	2	61	A	C4-C5-C6	-6.53	113.74	117.00
44	1	17	G	C4-C5-N7	6.53	113.41	110.80
44	1	1460	A	N1-C6-N6	6.53	122.52	118.60
45	2	129	C	N3-C2-O2	-6.52	117.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	19	ARG	NE-CZ-NH2	-6.52	117.04	120.30
44	1	680	G	C4-C5-N7	6.52	113.41	110.80
44	1	775	A	N9-C4-C5	-6.51	103.19	105.80
44	1	1468	A	C5-C6-N6	-6.51	118.49	123.70
44	1	1372	C	N3-C4-C5	6.51	124.50	121.90
45	2	140	G	N1-C2-N2	-6.51	110.34	116.20
44	1	225	C	N1-C2-O2	6.51	122.81	118.90
44	1	369	A	C5-N7-C8	-6.51	100.65	103.90
44	1	1423	C	N3-C4-N4	6.51	122.56	118.00
44	1	1874	A	C4-C5-N7	6.51	113.95	110.70
45	2	96	A	C5-N7-C8	-6.51	100.65	103.90
44	1	922	U	C2-N1-C1'	6.51	125.51	117.70
44	1	1112	A	C5-C6-N6	-6.51	118.50	123.70
44	1	2358	A	C5-C6-N6	-6.51	118.50	123.70
44	1	3163	A	C5-N7-C8	-6.51	100.65	103.90
44	1	3196	U	N1-C2-O2	6.50	127.35	122.80
44	1	412	G	C4-C5-N7	6.50	113.40	110.80
44	1	1497	C	N3-C2-O2	-6.50	117.35	121.90
44	1	58	G	C4-N9-C1'	6.50	134.95	126.50
44	1	220	G	N1-C2-N2	-6.50	110.35	116.20
44	1	1365	G	C5-N7-C8	-6.50	101.05	104.30
44	1	1504	A	C4-C5-N7	6.50	113.95	110.70
44	1	357	A	N1-C6-N6	6.50	122.50	118.60
44	1	715	A	C5-N7-C8	-6.50	100.65	103.90
44	1	1183	C	N1-C2-O2	6.50	122.80	118.90
44	1	335	G	C4-C5-N7	6.50	113.40	110.80
44	1	1437	C	N3-C4-C5	6.50	124.50	121.90
44	1	1303	A	C5-N7-C8	-6.49	100.65	103.90
44	1	928	C	N1-C2-O2	6.49	122.80	118.90
44	1	1443	G	N7-C8-N9	6.49	116.35	113.10
44	1	498	A	C5-C6-N1	6.49	120.94	117.70
44	1	1423	C	N3-C2-O2	-6.49	117.36	121.90
44	1	1843	C	N3-C4-C5	-6.49	119.30	121.90
44	1	82	C	N3-C4-N4	6.49	122.54	118.00
44	1	971	G	N3-C4-C5	6.49	131.84	128.60
44	1	1159	A	C6-N1-C2	-6.49	114.71	118.60
44	1	1701	C	N3-C2-O2	-6.49	117.36	121.90
44	1	1308	A	C4-C5-C6	-6.48	113.76	117.00
44	1	3121	U	P-O3'-C3'	6.48	127.48	119.70
44	1	2345	A	N9-C4-C5	-6.48	103.21	105.80
44	1	1598	G	C4-C5-N7	6.48	113.39	110.80
45	2	51	G	C8-N9-C1'	-6.48	118.58	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	2114	C	N1-C2-O2	6.48	122.79	118.90
1	B	26	ARG	NE-CZ-NH2	-6.47	117.06	120.30
45	2	91	C	N1-C2-O2	6.47	122.78	118.90
44	1	947	G	C6-C5-N7	-6.47	126.52	130.40
44	1	1422	G	N3-C2-N2	6.47	124.43	119.90
44	1	3362	A	N1-C6-N6	-6.47	114.72	118.60
44	1	426	G	C5-N7-C8	-6.46	101.07	104.30
44	1	1382	G	N3-C2-N2	6.46	124.42	119.90
44	1	1377	G	N3-C4-C5	6.46	131.83	128.60
44	1	1505	C	C6-N1-C2	-6.46	117.72	120.30
44	1	312	C	C5-C4-N4	-6.46	115.68	120.20
44	1	1609	C	N1-C2-O2	6.46	122.78	118.90
27	e	19	ARG	NE-CZ-NH1	6.46	123.53	120.30
44	1	56	G	C4-C5-N7	6.46	113.38	110.80
44	1	1835	A	C4-C5-N7	6.46	113.93	110.70
45	2	57	C	C6-N1-C2	-6.46	117.72	120.30
44	1	792	G	C4-C5-N7	6.46	113.38	110.80
44	1	1590	G	C4-C5-N7	6.46	113.38	110.80
44	1	2362	C	N3-C2-O2	-6.46	117.38	121.90
1	B	58	ARG	NE-CZ-NH1	6.45	123.53	120.30
6	H	91	ARG	NE-CZ-NH2	6.45	123.53	120.30
44	1	303	G	N3-C4-N9	6.45	129.87	126.00
44	1	1363	A	N7-C8-N9	6.45	117.03	113.80
44	1	22	G	C5-C6-N1	6.45	114.73	111.50
44	1	29	C	N3-C2-O2	-6.45	117.38	121.90
44	1	1332	A	C8-N9-C4	-6.45	103.22	105.80
44	1	1602	A	C5-C6-N6	-6.45	118.54	123.70
44	1	1307	G	N1-C2-N2	-6.45	110.40	116.20
44	1	3329	U	C6-N1-C2	-6.45	117.13	121.00
44	1	366	A	N1-C6-N6	6.44	122.47	118.60
44	1	519	A	C4-C5-N7	6.44	113.92	110.70
44	1	1496	C	N3-C4-N4	6.44	122.51	118.00
44	1	1550	C	C6-N1-C2	-6.44	117.72	120.30
44	1	1665	C	C5-C4-N4	-6.44	115.69	120.20
45	2	132	G	C5-N7-C8	-6.44	101.08	104.30
44	1	1537	A	C4-C5-N7	6.43	113.92	110.70
44	1	2361	A	C5-N7-C8	-6.43	100.68	103.90
44	1	3299	A	C5-N7-C8	-6.43	100.68	103.90
44	1	3021	A	N9-C4-C5	-6.43	103.23	105.80
44	1	408	A	C5-N7-C8	-6.43	100.69	103.90
44	1	1667	A	C5-N7-C8	-6.43	100.69	103.90
44	1	340	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	387	A	C5-C6-N6	-6.43	118.56	123.70
44	1	508	U	C5-C6-N1	6.43	125.91	122.70
10	N	159	ARG	NE-CZ-NH2	-6.42	117.09	120.30
44	1	3092	C	N1-C2-O2	6.42	122.75	118.90
44	1	810	A	C4-C5-C6	-6.42	113.79	117.00
44	1	2354	C	N3-C4-C5	6.42	124.47	121.90
29	g	60	ARG	NE-CZ-NH1	6.42	123.51	120.30
44	1	355	A	C4-C5-N7	6.42	113.91	110.70
44	1	937	G	C4-N9-C1'	6.42	134.84	126.50
44	1	212	G	C8-N9-C1'	-6.42	118.66	127.00
44	1	1640	G	C4-C5-N7	6.42	113.37	110.80
44	1	1800	A	C5-N7-C8	-6.42	100.69	103.90
44	1	2343	C	N1-C2-O2	6.42	122.75	118.90
44	1	791	A	C5-N7-C8	-6.41	100.69	103.90
44	1	3354	U	N1-C2-O2	6.41	127.29	122.80
45	2	30	C	N3-C2-O2	-6.41	117.41	121.90
44	1	1406	A	C5-N7-C8	-6.41	100.70	103.90
44	1	1491	A	N9-C4-C5	-6.41	103.24	105.80
44	1	652	G	C4-N9-C1'	6.41	134.83	126.50
44	1	1304	A	C5-C6-N6	-6.41	118.58	123.70
44	1	3249	C	C6-N1-C2	-6.41	117.74	120.30
10	N	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
44	1	792	G	N7-C8-N9	6.40	116.30	113.10
41	u	44	ARG	NE-CZ-NH1	-6.40	117.10	120.30
44	1	345	G	C4-N9-C1'	6.40	134.82	126.50
44	1	3053	G	C6-C5-N7	-6.40	126.56	130.40
45	2	39	G	C4-C5-N7	6.40	113.36	110.80
44	1	75	G	C6-C5-N7	-6.40	126.56	130.40
44	1	283	G	C8-N9-C1'	-6.40	118.68	127.00
44	1	1397	C	C5-C4-N4	-6.40	115.72	120.20
44	1	936	A	C4-C5-N7	6.40	113.90	110.70
44	1	945	C	C5-C6-N1	6.40	124.20	121.00
44	1	935	U	C5-C6-N1	6.39	125.90	122.70
45	2	119	C	N3-C4-C5	6.39	124.46	121.90
44	1	1799	A	C4-C5-N7	6.39	113.90	110.70
45	2	77	A	N1-C6-N6	6.39	122.44	118.60
44	1	3375	A	C4-C5-N7	6.39	113.89	110.70
44	1	2353	G	C5-N7-C8	-6.39	101.11	104.30
45	2	117	C	C5-C4-N4	-6.39	115.73	120.20
44	1	1135	A	N9-C4-C5	-6.39	103.25	105.80
28	f	103	TYR	CA-CB-CG	6.39	125.53	113.40
44	1	123	A	C5-C6-N1	6.39	120.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	696	C	N3-C4-C5	6.39	124.45	121.90
44	1	48	A	C5-C6-N1	6.38	120.89	117.70
44	1	622	A	C4-C5-N7	6.38	113.89	110.70
44	1	1563	C	N3-C4-C5	6.38	124.45	121.90
35	n	47	ARG	NE-CZ-NH1	6.38	123.49	120.30
44	1	1602	A	C8-N9-C4	6.38	108.35	105.80
45	2	118	C	C5-C4-N4	-6.38	115.73	120.20
44	1	54	C	N1-C2-O2	6.38	122.73	118.90
44	1	595	G	N3-C4-N9	-6.38	122.17	126.00
44	1	1330	A	N7-C8-N9	6.38	116.99	113.80
44	1	3379	C	N3-C4-C5	6.38	124.45	121.90
44	1	289	A	N7-C8-N9	6.38	116.99	113.80
44	1	3140	G	C2-N3-C4	-6.38	108.71	111.90
44	1	52	A	C5-N7-C8	-6.37	100.71	103.90
44	1	1304	A	C4-C5-N7	6.37	113.89	110.70
44	1	1594	A	C6-N1-C2	-6.37	114.78	118.60
27	e	27	ARG	NE-CZ-NH2	-6.37	117.11	120.30
44	1	936	A	C4-C5-C6	-6.37	113.81	117.00
44	1	3011	A	C5-C6-N1	6.37	120.89	117.70
44	1	109	A	C4-C5-C6	-6.37	113.82	117.00
44	1	1158	A	C6-C5-N7	-6.37	127.84	132.30
44	1	962	A	C8-N9-C4	-6.37	103.25	105.80
44	1	611	A	C5-C6-N1	6.37	120.88	117.70
44	1	1468	A	C5-C6-N1	6.37	120.88	117.70
44	1	1625	A	N9-C4-C5	-6.37	103.25	105.80
44	1	335	G	C5-N7-C8	-6.36	101.12	104.30
44	1	666	A	C5-C6-N6	-6.36	118.61	123.70
44	1	936	A	C5-C6-N6	-6.36	118.61	123.70
44	1	1599	G	C4-C5-N7	6.36	113.34	110.80
44	1	3137	C	C6-N1-C2	-6.36	117.76	120.30
44	1	668	G	N7-C8-N9	6.36	116.28	113.10
32	j	73	ARG	NE-CZ-NH1	6.36	123.48	120.30
44	1	950	G	C4-C5-N7	6.36	113.34	110.80
44	1	972	A	C4-C5-C6	-6.36	113.82	117.00
44	1	3002	C	C5-C4-N4	-6.36	115.75	120.20
44	1	341	G	N7-C8-N9	6.36	116.28	113.10
44	1	2836	C	C2-N1-C1'	6.36	125.79	118.80
44	1	527	A	C5-C6-N1	6.35	120.88	117.70
44	1	282	G	N7-C8-N9	6.35	116.28	113.10
44	1	1437	C	N1-C2-O2	6.35	122.71	118.90
44	1	1837	U	C5-C4-O4	-6.35	122.09	125.90
44	1	1896	A	N1-C6-N6	6.35	122.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3244	A	C5-N7-C8	-6.35	100.72	103.90
45	2	35	C	N1-C2-O2	6.35	122.71	118.90
44	1	1802	C	N3-C4-C5	6.35	124.44	121.90
44	1	77	A	C5-N7-C8	-6.34	100.73	103.90
44	1	931	C	N1-C2-O2	6.34	122.71	118.90
44	1	1295	G	N3-C2-N2	6.34	124.34	119.90
44	1	497	C	C5-C4-N4	-6.34	115.76	120.20
45	2	105	A	N9-C4-C5	-6.34	103.26	105.80
44	1	387	A	C5-N7-C8	-6.34	100.73	103.90
44	1	701	G	N7-C8-N9	6.34	116.27	113.10
44	1	1909	A	C4-C5-N7	6.34	113.87	110.70
44	1	1643	A	C5-C6-N1	6.34	120.87	117.70
8	L	49	ARG	NE-CZ-NH2	6.33	123.47	120.30
44	1	279	U	C5-C6-N1	6.33	125.87	122.70
44	1	3131	U	C5-C4-O4	-6.33	122.10	125.90
14	R	42	ARG	NE-CZ-NH1	6.33	123.47	120.30
44	1	673	U	N3-C4-O4	6.33	123.83	119.40
44	1	2358	A	N7-C8-N9	6.33	116.97	113.80
45	2	156	U	C2-N1-C1'	6.33	125.30	117.70
44	1	3354	U	N3-C2-O2	-6.33	117.77	122.20
44	1	1163	A	N7-C8-N9	6.33	116.97	113.80
44	1	820	A	C5-C6-N6	-6.33	118.64	123.70
29	g	31	ARG	NE-CZ-NH1	6.33	123.46	120.30
44	1	3296	A	N9-C4-C5	-6.33	103.27	105.80
44	1	159	A	C5-C6-N6	-6.32	118.64	123.70
44	1	3023	U	N1-C2-O2	6.32	127.23	122.80
44	1	3314	A	C5-C6-N1	6.32	120.86	117.70
44	1	3213	A	C5-N7-C8	-6.32	100.74	103.90
44	1	1295	G	N1-C2-N2	-6.32	110.51	116.20
44	1	12	A	C6-C5-N7	-6.32	127.88	132.30
44	1	315	C	C5-C4-N4	-6.32	115.78	120.20
44	1	820	A	C5-C6-N1	6.32	120.86	117.70
44	1	965	A	C8-N9-C4	6.32	108.33	105.80
10	N	68	ARG	NE-CZ-NH2	-6.31	117.14	120.30
44	1	3214	U	N1-C2-O2	6.31	127.22	122.80
44	1	3372	A	C5-C6-N1	6.31	120.86	117.70
2	C	73	ARG	NE-CZ-NH1	6.31	123.45	120.30
44	1	282	G	C8-N9-C1'	-6.31	118.80	127.00
44	1	292	U	C6-N1-C1'	-6.31	112.37	121.20
44	1	1222	G	O4'-C1'-N9	6.31	113.25	108.20
44	1	1593	A	N1-C6-N6	-6.31	114.82	118.60
44	1	204	A	C5-C6-N6	-6.30	118.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	932	U	C5-C6-N1	6.30	125.85	122.70
44	1	3375	A	C5-N7-C8	-6.30	100.75	103.90
45	2	58	G	N9-C4-C5	-6.30	102.88	105.40
44	1	1881	A	N1-C6-N6	6.30	122.38	118.60
44	1	3086	A	C4-C5-C6	-6.30	113.85	117.00
45	2	77	A	C5-C6-N1	6.30	120.85	117.70
44	1	1404	G	N3-C4-N9	-6.30	122.22	126.00
44	1	1594	A	N9-C4-C5	-6.30	103.28	105.80
44	1	907	G	O4'-C1'-N9	6.30	113.24	108.20
44	1	653	A	C5-N7-C8	-6.30	100.75	103.90
44	1	1145	G	C4-C5-N7	6.30	113.32	110.80
44	1	10	C	N3-C4-N4	6.29	122.41	118.00
44	1	88	A	C4-C5-N7	6.29	113.85	110.70
44	1	407	A	C5-C6-N1	6.29	120.85	117.70
44	1	729	C	N1-C2-O2	6.29	122.68	118.90
44	1	1514	G	C2-N3-C4	6.29	115.05	111.90
10	N	172	ARG	NE-CZ-NH1	6.29	123.44	120.30
44	1	361	A	C5-N7-C8	-6.29	100.75	103.90
44	1	572	A	N1-C6-N6	-6.29	114.83	118.60
44	1	1177	G	C4-N9-C1'	6.29	134.68	126.50
44	1	1431	G	C5-N7-C8	-6.29	101.15	104.30
44	1	2914	G	N1-C6-O6	-6.29	116.12	119.90
44	1	3186	A	C4-C5-C6	-6.29	113.85	117.00
44	1	3214	U	C2-N1-C1'	6.29	125.25	117.70
44	1	1171	G	N3-C4-N9	6.29	129.77	126.00
44	1	3127	A	C4-C5-N7	6.29	113.84	110.70
44	1	3335	A	C5-C6-N1	6.29	120.84	117.70
11	O	37	ARG	NE-CZ-NH1	6.29	123.44	120.30
9	M	55	ARG	NE-CZ-NH1	6.29	123.44	120.30
44	1	54	C	N3-C4-C5	6.29	124.41	121.90
44	1	1156	C	C5-C4-N4	-6.29	115.80	120.20
44	1	1194	G	C4-N9-C1'	6.29	134.67	126.50
44	1	1411	C	N3-C4-C5	6.29	124.41	121.90
44	1	1657	C	C5-C4-N4	-6.29	115.80	120.20
44	1	2943	G	N3-C2-N2	6.29	124.30	119.90
44	1	353	G	C5-N7-C8	-6.28	101.16	104.30
44	1	3164	C	N3-C4-N4	-6.28	113.60	118.00
44	1	1854	C	C5-C4-N4	-6.28	115.80	120.20
44	1	2366	C	N1-C2-O2	6.28	122.67	118.90
44	1	1432	C	C6-N1-C1'	-6.28	113.27	120.80
44	1	1695	U	N3-C2-O2	-6.28	117.81	122.20
44	1	805	G	C4-C5-N7	6.28	113.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1169	A	C5-C6-N1	6.27	120.84	117.70
44	1	3132	C	N3-C4-N4	6.27	122.39	118.00
44	1	6	A	C5-C6-N1	6.27	120.84	117.70
44	1	283	G	C4-N9-C1'	6.27	134.65	126.50
44	1	331	G	N7-C8-N9	6.27	116.23	113.10
44	1	499	G	C5-N7-C8	-6.27	101.17	104.30
44	1	971	G	C5-N7-C8	-6.27	101.17	104.30
44	1	192	C	N3-C4-C5	6.27	124.41	121.90
44	1	920	A	C4-C5-C6	-6.27	113.87	117.00
44	1	1806	A	N9-C4-C5	-6.27	103.29	105.80
44	1	3244	A	N7-C8-N9	6.27	116.93	113.80
27	e	45	ARG	NE-CZ-NH1	6.27	123.43	120.30
44	1	2341	A	C5-N7-C8	-6.27	100.77	103.90
44	1	1162	U	N3-C4-O4	6.26	123.79	119.40
44	1	33	G	C4-C5-N7	6.26	113.31	110.80
44	1	841	A	C5-N7-C8	-6.26	100.77	103.90
44	1	1294	A	C4-C5-C6	-6.26	113.87	117.00
44	1	1341	U	C5-C4-O4	-6.26	122.14	125.90
2	C	69	ARG	NE-CZ-NH2	6.26	123.43	120.30
44	1	271	C	C5-C4-N4	-6.26	115.82	120.20
44	1	346	C	C6-N1-C1'	-6.26	113.29	120.80
44	1	3004	C	N3-C2-O2	-6.26	117.52	121.90
2	C	69	ARG	NE-CZ-NH1	-6.26	117.17	120.30
44	1	1278	A	N7-C8-N9	6.26	116.93	113.80
44	1	1526	U	C5-C6-N1	6.26	125.83	122.70
45	2	22	U	N3-C2-O2	-6.26	117.82	122.20
45	2	42	G	N7-C8-N9	6.26	116.23	113.10
44	1	932	U	C6-N1-C2	-6.25	117.25	121.00
44	1	1195	A	C4-C5-C6	-6.25	113.87	117.00
44	1	3148	U	C5-C6-N1	6.25	125.83	122.70
44	1	339	C	N3-C4-N4	6.25	122.38	118.00
45	2	9	A	C4-C5-N7	6.25	113.83	110.70
45	2	88	A	C5-N7-C8	-6.25	100.77	103.90
44	1	1524	A	C5-C6-N1	6.25	120.83	117.70
15	S	152	LEU	CA-CB-CG	6.25	129.68	115.30
44	1	30	G	C5-N7-C8	-6.25	101.17	104.30
44	1	677	A	C5-C6-N1	6.25	120.82	117.70
44	1	3354	U	C6-N1-C1'	-6.25	112.46	121.20
44	1	325	A	C2-N3-C4	6.25	113.72	110.60
44	1	1599	G	C6-C5-N7	-6.24	126.65	130.40
45	2	39	G	C5-N7-C8	-6.24	101.18	104.30
45	2	100	U	C5-C6-N1	6.24	125.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3165	A	N7-C8-N9	6.24	116.92	113.80
44	1	3320	A	C4-C5-N7	6.24	113.82	110.70
44	1	402	A	C4-C5-N7	6.24	113.82	110.70
44	1	1374	G	N9-C4-C5	-6.24	102.90	105.40
10	N	164	LEU	CA-CB-CG	6.24	129.65	115.30
44	1	973	A	C5-C6-N1	6.24	120.82	117.70
44	1	10	C	C5-C4-N4	-6.23	115.84	120.20
44	1	622	A	N1-C6-N6	6.23	122.34	118.60
44	1	1328	C	C5-C4-N4	-6.23	115.84	120.20
45	2	103	G	C4-N9-C1'	6.23	134.60	126.50
44	1	1414	G	C4-C5-N7	6.23	113.29	110.80
44	1	2353	G	N7-C8-N9	6.22	116.21	113.10
44	1	3000	A	C5-N7-C8	-6.22	100.79	103.90
23	a	117	ARG	NE-CZ-NH2	-6.22	117.19	120.30
44	1	1537	A	N9-C4-C5	-6.22	103.31	105.80
44	1	3181	C	C6-N1-C1'	-6.22	113.33	120.80
44	1	1364	C	N3-C2-O2	-6.22	117.55	121.90
44	1	3001	C	N1-C2-O2	6.22	122.63	118.90
2	C	188	ARG	NE-CZ-NH1	6.22	123.41	120.30
44	1	580	C	C5-C4-N4	-6.22	115.85	120.20
44	1	934	G	C5-N7-C8	-6.22	101.19	104.30
44	1	63	A	C5-C6-N6	-6.22	118.73	123.70
44	1	1196	C	N1-C2-O2	6.22	122.63	118.90
44	1	2366	C	N3-C4-N4	6.21	122.35	118.00
44	1	375	A	OP1-P-O3'	6.21	118.86	105.20
44	1	2341	A	C5-C6-N6	-6.21	118.73	123.70
44	1	658	G	C4-N9-C1'	6.21	134.57	126.50
44	1	3087	A	C5-C6-N6	-6.21	118.73	123.70
12	P	131	ARG	NE-CZ-NH1	6.21	123.40	120.30
44	1	678	G	C4-C5-N7	6.21	113.28	110.80
44	1	1204	A	N9-C4-C5	-6.21	103.32	105.80
4	F	107	ARG	NE-CZ-NH2	-6.21	117.20	120.30
44	1	325	A	N7-C8-N9	6.21	116.90	113.80
44	1	407	A	N9-C4-C5	-6.21	103.32	105.80
44	1	65	A	C4-C5-C6	-6.20	113.90	117.00
44	1	64	G	C6-C5-N7	-6.20	126.68	130.40
44	1	323	A	C5-C6-N1	6.20	120.80	117.70
44	1	2994	A	C4-C5-N7	6.20	113.80	110.70
21	Y	27	ARG	NE-CZ-NH2	-6.20	117.20	120.30
44	1	1846	C	N3-C2-O2	-6.20	117.56	121.90
44	1	658	G	C4-C5-N7	6.20	113.28	110.80
44	1	3049	A	C5-N7-C8	-6.20	100.80	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	48	ARG	NE-CZ-NH2	-6.19	117.20	120.30
44	1	841	A	C4-C5-N7	6.19	113.80	110.70
44	1	702	C	N3-C4-N4	6.19	122.33	118.00
44	1	1170	A	C5-C6-N1	6.19	120.80	117.70
45	2	133	G	C5-N7-C8	-6.19	101.20	104.30
1	B	232	ARG	NE-CZ-NH2	-6.19	117.21	120.30
34	l	8	ARG	NE-CZ-NH1	6.19	123.39	120.30
44	1	624	G	C6-C5-N7	-6.19	126.69	130.40
44	1	1612	A	C5-N7-C8	-6.19	100.81	103.90
44	1	3097	C	N3-C4-N4	6.19	122.33	118.00
44	1	26	A	C5-N7-C8	-6.18	100.81	103.90
44	1	686	G	N7-C8-N9	6.18	116.19	113.10
44	1	611	A	C5-N7-C8	-6.18	100.81	103.90
44	1	3153	U	C2-N1-C1'	6.18	125.12	117.70
44	1	904	A	N9-C4-C5	-6.18	103.33	105.80
44	1	58	G	N3-C2-N2	6.18	124.22	119.90
44	1	667	C	N1-C2-O2	6.18	122.61	118.90
44	1	1797	A	N1-C6-N6	-6.18	114.89	118.60
44	1	2390	A	C5-C6-N6	-6.18	118.76	123.70
45	2	141	C	N1-C2-O2	6.18	122.61	118.90
29	g	4	ARG	NE-CZ-NH2	-6.18	117.21	120.30
44	1	1105	A	N7-C8-N9	6.18	116.89	113.80
44	1	1299	U	N3-C2-O2	-6.18	117.88	122.20
44	1	1749	A	C5-C6-N1	6.18	120.79	117.70
44	1	3144	G	C4-C5-N7	6.18	113.27	110.80
44	1	1311	G	C5-N7-C8	-6.17	101.21	104.30
14	R	38	ARG	NE-CZ-NH1	6.17	123.39	120.30
14	R	62	ARG	NE-CZ-NH2	6.17	123.39	120.30
44	1	1152	G	C4-N9-C1'	6.17	134.52	126.50
44	1	3141	A	C4-C5-N7	6.17	113.79	110.70
44	1	107	A	N7-C8-N9	6.17	116.89	113.80
14	R	71	ARG	NE-CZ-NH1	6.17	123.38	120.30
44	1	1419	A	N9-C4-C5	-6.17	103.33	105.80
44	1	3112	G	C2-N3-C4	-6.17	108.82	111.90
44	1	1612	A	C4-C5-N7	6.17	113.78	110.70
45	2	51	G	C4-N9-C1'	6.17	134.51	126.50
44	1	3150	A	C5-C6-N1	6.16	120.78	117.70
44	1	1163	A	C6-N1-C2	-6.16	114.90	118.60
44	1	1392	G	C5-N7-C8	-6.16	101.22	104.30
44	1	3310	A	C5-N7-C8	-6.16	100.82	103.90
44	1	2881	C	N3-C2-O2	-6.16	117.59	121.90
41	u	44	ARG	NE-CZ-NH2	6.15	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1381	A	C4-C5-C6	-6.15	113.92	117.00
44	1	1655	G	C2-N3-C4	-6.15	108.82	111.90
1	B	339	ARG	NE-CZ-NH2	-6.15	117.22	120.30
16	T	139	ARG	NE-CZ-NH2	6.15	123.38	120.30
44	1	45	A	C5-C6-N1	6.15	120.78	117.70
44	1	417	A	C5-C6-N1	6.15	120.78	117.70
44	1	969	C	C5-C4-N4	-6.15	115.89	120.20
44	1	3057	U	N1-C2-O2	6.15	127.11	122.80
44	1	34	A	C4-C5-C6	-6.15	113.92	117.00
44	1	589	A	O4'-C1'-N9	-6.15	103.28	108.20
44	1	1798	A	C5-C6-N1	6.15	120.77	117.70
42	y	237	ARG	NE-CZ-NH1	6.15	123.37	120.30
44	1	1226	G	C4-N9-C1'	6.15	134.49	126.50
44	1	1602	A	C4-C5-N7	6.15	113.77	110.70
44	1	1524	A	C4-C5-C6	-6.14	113.93	117.00
44	1	3309	G	N3-C2-N2	6.14	124.20	119.90
46	6	47	A	C5-C6-N1	6.14	120.77	117.70
44	1	1116	G	O4'-C1'-N9	-6.14	103.29	108.20
45	2	130	C	N1-C2-O2	6.14	122.59	118.90
44	1	1176	C	N3-C2-O2	-6.14	117.60	121.90
44	1	2358	A	C4-C5-N7	6.14	113.77	110.70
45	2	74	U	N1-C2-O2	6.14	127.09	122.80
44	1	3172	A	N9-C4-C5	-6.13	103.35	105.80
44	1	2881	C	C6-N1-C2	-6.13	117.85	120.30
44	1	2890	A	C5-C6-N1	6.13	120.76	117.70
44	1	3029	A	N1-C6-N6	6.13	122.28	118.60
45	2	76	C	N3-C4-N4	6.13	122.29	118.00
44	1	496	C	C5-C4-N4	-6.13	115.91	120.20
44	1	75	G	N9-C4-C5	-6.12	102.95	105.40
44	1	516	A	C8-N9-C4	6.12	108.25	105.80
44	1	3031	G	N9-C4-C5	-6.12	102.95	105.40
44	1	3060	C	N3-C4-C5	6.12	124.35	121.90
44	1	2943	G	N1-C2-N2	-6.12	110.69	116.20
44	1	649	A	N9-C4-C5	-6.12	103.35	105.80
44	1	3046	A	N1-C6-N6	6.12	122.27	118.60
44	1	3147	G	C4-C5-N7	6.12	113.25	110.80
44	1	3314	A	C5-N7-C8	-6.12	100.84	103.90
44	1	2946	A	C5-C6-N6	-6.12	118.81	123.70
44	1	3213	A	C5-C6-N1	6.12	120.76	117.70
44	1	786	A	N9-C4-C5	-6.12	103.35	105.80
44	1	33	G	C2-N3-C4	-6.11	108.84	111.90
44	1	1833	G	N3-C2-N2	6.11	124.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	701	G	C5-N7-C8	-6.11	101.24	104.30
44	1	346	C	N3-C4-N4	6.11	122.28	118.00
44	1	658	G	C6-C5-N7	-6.11	126.73	130.40
44	1	324	A	N1-C6-N6	-6.11	114.94	118.60
44	1	972	A	N3-C4-N9	-6.11	122.51	127.40
44	1	1212	A	C5-C6-N1	6.11	120.75	117.70
44	1	1587	A	C5-N7-C8	-6.11	100.85	103.90
44	1	3040	A	N9-C4-C5	-6.10	103.36	105.80
44	1	332	C	N3-C4-N4	6.10	122.27	118.00
44	1	3311	C	C6-N1-C2	-6.10	117.86	120.30
44	1	64	G	N7-C8-N9	6.10	116.15	113.10
44	1	1804	A	C5-C6-N1	6.10	120.75	117.70
44	1	2340	U	C5-C6-N1	6.10	125.75	122.70
44	1	62	A	OP2-P-O3'	6.10	118.61	105.20
44	1	1412	G	C5-N7-C8	-6.10	101.25	104.30
44	1	88	A	N9-C4-C5	-6.09	103.36	105.80
9	M	128	ARG	NE-CZ-NH1	6.09	123.34	120.30
44	1	1643	A	C4-C5-C6	-6.09	113.96	117.00
27	e	44	ARG	NE-CZ-NH1	6.09	123.34	120.30
44	1	58	G	C8-N9-C1'	-6.09	119.09	127.00
44	1	106	A	N9-C4-C5	-6.09	103.36	105.80
44	1	663	C	N3-C2-O2	-6.09	117.64	121.90
44	1	1182	A	C4-C5-N7	6.08	113.74	110.70
44	1	291	C	N3-C4-C5	6.08	124.33	121.90
44	1	1280	C	N1-C2-O2	6.08	122.55	118.90
44	1	1451	C	N3-C4-C5	6.08	124.33	121.90
44	1	504	A	N9-C4-C5	-6.08	103.37	105.80
44	1	657	A	C6-N1-C2	-6.08	114.95	118.60
44	1	661	G	O4'-C1'-N9	6.08	113.06	108.20
44	1	1806	A	C4-C5-N7	6.08	113.74	110.70
44	1	2831	G	N7-C8-N9	6.08	116.14	113.10
44	1	3223	A	C4-C5-C6	-6.08	113.96	117.00
44	1	2886	U	O4'-C1'-N1	6.08	113.06	108.20
44	1	3131	U	C6-N1-C2	-6.08	117.35	121.00
44	1	341	G	N9-C4-C5	-6.07	102.97	105.40
44	1	646	A	C5-C6-N1	6.07	120.74	117.70
44	1	671	U	C5-C6-N1	6.07	125.74	122.70
44	1	961	C	N1-C2-O2	6.07	122.54	118.90
44	1	1145	G	N1-C2-N2	-6.07	110.73	116.20
44	1	3181	C	N3-C4-C5	6.07	124.33	121.90
44	1	3269	U	P-O3'-C3'	6.07	126.99	119.70
10	N	68	ARG	NE-CZ-NH1	6.07	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	e	24	ARG	NE-CZ-NH1	6.07	123.34	120.30
44	1	1165	A	C4-C5-C6	-6.07	113.96	117.00
44	1	1379	G	C5-N7-C8	-6.07	101.26	104.30
44	1	3112	G	N3-C4-C5	6.07	131.63	128.60
44	1	125	C	C6-N1-C2	-6.07	117.87	120.30
44	1	303	G	C4-C5-N7	6.07	113.23	110.80
44	1	409	A	C4-C5-N7	6.07	113.73	110.70
44	1	400	G	O4'-C1'-N9	6.07	113.05	108.20
44	1	505	G	C4-C5-N7	6.06	113.23	110.80
44	1	3101	G	C5-N7-C8	-6.06	101.27	104.30
44	1	1169	A	N9-C4-C5	-6.06	103.38	105.80
44	1	1172	G	N1-C6-O6	-6.06	116.26	119.90
44	1	1317	A	C5-N7-C8	-6.06	100.87	103.90
45	2	39	G	N1-C2-N2	-6.06	110.74	116.20
44	1	320	G	C5-N7-C8	-6.06	101.27	104.30
44	1	1152	G	N1-C2-N2	-6.06	110.75	116.20
44	1	1615	C	C5-C6-N1	6.06	124.03	121.00
44	1	3040	A	N7-C8-N9	6.06	116.83	113.80
46	6	31	G	N3-C4-N9	-6.06	122.36	126.00
11	O	128	ARG	NE-CZ-NH1	6.06	123.33	120.30
44	1	341	G	C5-C6-O6	-6.06	124.97	128.60
44	1	1373	A	C5-C6-N1	6.06	120.73	117.70
44	1	1527	C	C5-C4-N4	-6.06	115.96	120.20
45	2	41	A	C5-C6-N1	6.06	120.73	117.70
44	1	128	G	C6-C5-N7	-6.05	126.77	130.40
44	1	334	A	C5-C6-N1	6.05	120.73	117.70
44	1	813	G	C8-N9-C4	-6.05	103.98	106.40
44	1	497	C	N3-C2-O2	-6.05	117.66	121.90
44	1	368	G	C5-N7-C8	-6.05	101.28	104.30
44	1	1409	G	C4-C5-N7	6.05	113.22	110.80
44	1	3186	A	C4-C5-N7	6.05	113.73	110.70
12	P	30	ARG	NE-CZ-NH1	6.05	123.32	120.30
44	1	319	A	C4-C5-C6	-6.05	113.98	117.00
44	1	3089	C	N3-C4-N4	6.04	122.23	118.00
44	1	9	U	C5-C4-O4	-6.04	122.27	125.90
44	1	1524	A	C5-N7-C8	-6.04	100.88	103.90
44	1	1446	A	C4-C5-N7	6.04	113.72	110.70
44	1	2366	C	N3-C2-O2	-6.04	117.67	121.90
45	2	31	G	N3-C4-N9	-6.04	122.38	126.00
44	1	435	C	C5-C4-N4	-6.04	115.97	120.20
44	1	800	G	C4-N9-C1'	6.04	134.35	126.50
13	Q	59	ARG	NE-CZ-NH1	6.04	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	66	ARG	NE-CZ-NH1	6.04	123.32	120.30
44	1	1239	C	C6-N1-C2	-6.04	117.89	120.30
44	1	1374	G	C6-C5-N7	-6.04	126.78	130.40
44	1	1515	A	C5-C6-N1	6.04	120.72	117.70
45	2	20	U	C5-C4-O4	-6.04	122.28	125.90
44	1	103	G	N7-C8-N9	6.03	116.12	113.10
44	1	341	G	C4-N9-C1'	6.03	134.34	126.50
44	1	391	A	C5-C6-N1	6.03	120.72	117.70
44	1	817	A	C5-C6-N1	6.03	120.72	117.70
44	1	1339	C	C6-N1-C2	-6.03	117.89	120.30
44	1	2831	G	C8-N9-C4	-6.03	103.99	106.40
44	1	145	G	N7-C8-N9	6.03	116.11	113.10
44	1	209	A	C4-C5-N7	6.03	113.72	110.70
44	1	406	G	O4'-C1'-N9	6.03	113.02	108.20
44	1	689	U	N1-C2-O2	6.03	127.02	122.80
44	1	376	G	N7-C8-N9	6.03	116.11	113.10
44	1	1612	A	N1-C6-N6	6.03	122.22	118.60
44	1	144	A	C6-N1-C2	-6.03	114.98	118.60
44	1	408	A	N1-C6-N6	-6.03	114.98	118.60
44	1	621	A	C4-C5-N7	6.03	113.71	110.70
44	1	1621	A	C5-N7-C8	-6.03	100.89	103.90
44	1	1625	A	C4-C5-N7	6.03	113.71	110.70
44	1	267	G	C5-C6-N1	6.03	114.51	111.50
44	1	1394	A	C4-C5-C6	-6.03	113.99	117.00
44	1	3005	A	N7-C8-N9	6.03	116.81	113.80
44	1	3035	A	C5-C6-N1	6.03	120.71	117.70
44	1	3330	A	C4-C5-N7	6.03	113.71	110.70
44	1	66	A	N7-C8-N9	6.02	116.81	113.80
44	1	2378	C	N3-C2-O2	-6.02	117.68	121.90
44	1	3006	A	C5-C6-N6	-6.02	118.88	123.70
44	1	1901	A	C5-C6-N1	6.02	120.71	117.70
44	1	422	A	N7-C8-N9	6.02	116.81	113.80
44	1	1393	A	C5-N7-C8	-6.02	100.89	103.90
44	1	1279	C	O4'-C1'-N1	6.02	113.01	108.20
44	1	2892	A	N1-C6-N6	6.02	122.21	118.60
44	1	3053	G	C4-C5-N7	6.02	113.21	110.80
44	1	1196	C	C6-N1-C2	-6.02	117.89	120.30
44	1	347	G	C4-N9-C1'	6.01	134.32	126.50
44	1	659	G	C4-N9-C1'	6.01	134.32	126.50
45	2	102	U	C5-C6-N1	6.01	125.71	122.70
45	2	149	A	N9-C4-C5	-6.01	103.39	105.80
44	1	387	A	C5-C6-N1	6.01	120.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3219	G	N3-C2-N2	6.01	124.11	119.90
44	1	621	A	C5-N7-C8	-6.01	100.89	103.90
44	1	907	G	C4-C5-N7	6.01	113.20	110.80
44	1	3395	G	C6-C5-N7	-6.01	126.79	130.40
23	a	139	ARG	NE-CZ-NH1	6.01	123.30	120.30
44	1	5	G	N3-C4-C5	6.01	131.60	128.60
44	1	224	C	C6-N1-C2	-6.01	117.90	120.30
44	1	573	C	C6-N1-C2	-6.01	117.90	120.30
44	1	2912	G	N1-C2-N2	-6.01	110.79	116.20
45	2	91	C	C5-C4-N4	-6.01	115.99	120.20
44	1	372	A	C5-N7-C8	-6.01	100.90	103.90
44	1	387	A	C4-C5-N7	6.01	113.70	110.70
44	1	614	C	N1-C2-O2	6.01	122.50	118.90
44	1	1614	C	N3-C2-O2	-6.01	117.69	121.90
44	1	1893	A	N1-C6-N6	6.01	122.20	118.60
13	Q	16	ARG	NE-CZ-NH1	6.01	123.30	120.30
44	1	222	A	C5-C6-N6	-6.01	118.89	123.70
44	1	3153	U	N3-C2-O2	-6.01	118.00	122.20
45	2	88	A	C4-C5-N7	6.01	113.70	110.70
44	1	53	G	C4-C5-N7	6.00	113.20	110.80
44	1	371	G	C5-N7-C8	-6.00	101.30	104.30
44	1	1838	G	N9-C4-C5	-6.00	103.00	105.40
45	2	42	G	C2-N3-C4	-6.00	108.90	111.90
44	1	736	A	C5-C6-N6	-6.00	118.90	123.70
44	1	1878	G	C4-N9-C1'	6.00	134.30	126.50
11	O	85	ARG	NE-CZ-NH1	6.00	123.30	120.30
44	1	375	A	C5-N7-C8	-6.00	100.90	103.90
44	1	1949	G	C5-C6-O6	6.00	132.20	128.60
44	1	3288	G	N3-C2-N2	6.00	124.10	119.90
44	1	100	A	C5-N7-C8	-6.00	100.90	103.90
44	1	1551	C	N1-C2-O2	6.00	122.50	118.90
45	2	41	A	N7-C8-N9	6.00	116.80	113.80
44	1	653	A	C5-C6-N6	-6.00	118.90	123.70
20	X	115	ARG	NE-CZ-NH1	6.00	123.30	120.30
44	1	303	G	N9-C4-C5	-6.00	103.00	105.40
44	1	1542	G	C4-C5-N7	5.99	113.20	110.80
44	1	336	A	C5-N7-C8	-5.99	100.90	103.90
44	1	253	A	N1-C2-N3	-5.99	126.31	129.30
44	1	1308	A	C5-N7-C8	-5.99	100.91	103.90
44	1	1379	G	C4-C5-N7	5.99	113.20	110.80
44	1	1450	G	C5-N7-C8	-5.99	101.31	104.30
44	1	3299	A	C5-C6-N1	5.99	120.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1170	A	C6-C5-N7	-5.99	128.11	132.30
35	n	34	ARG	NE-CZ-NH2	5.99	123.29	120.30
44	1	101	G	C4-N9-C1'	5.99	134.28	126.50
44	1	333	G	C4-C5-N7	5.99	113.19	110.80
44	1	1195	A	C8-N9-C4	5.99	108.19	105.80
44	1	3293	U	C5-C6-N1	5.99	125.69	122.70
44	1	949	C	N3-C4-N4	5.98	122.19	118.00
44	1	1909	A	C5-C6-N6	-5.98	118.92	123.70
44	1	227	G	C4-N9-C1'	5.98	134.27	126.50
44	1	2341	A	N9-C4-C5	-5.98	103.41	105.80
44	1	31	C	N3-C4-C5	5.98	124.29	121.90
44	1	344	A	C6-C5-N7	-5.98	128.12	132.30
44	1	1385	C	N1-C2-O2	5.98	122.49	118.90
44	1	1499	C	C5-C4-N4	-5.98	116.02	120.20
44	1	3034	C	C5-C4-N4	-5.98	116.02	120.20
45	2	32	C	N3-C4-N4	5.98	122.18	118.00
44	1	1446	A	C5-C6-N6	-5.98	118.92	123.70
44	1	276	U	N3-C4-O4	5.97	123.58	119.40
10	N	50	ARG	NE-CZ-NH1	5.97	123.29	120.30
44	1	1596	C	C5-C4-N4	-5.97	116.02	120.20
44	1	671	U	C6-N1-C2	-5.97	117.42	121.00
44	1	1332	A	C4-N9-C1'	5.97	137.05	126.30
44	1	371	G	C4-C5-N7	5.97	113.19	110.80
44	1	933	A	N1-C2-N3	-5.96	126.32	129.30
44	1	1185	C	N3-C2-O2	-5.96	117.72	121.90
44	1	350	C	N3-C4-C5	5.96	124.28	121.90
44	1	1116	G	C8-N9-C1'	-5.96	119.25	127.00
44	1	3104	U	C5-C6-N1	5.96	125.68	122.70
45	2	44	A	C6-N1-C2	-5.96	115.02	118.60
1	B	58	ARG	NE-CZ-NH2	-5.96	117.32	120.30
44	1	1362	G	C4-C5-N7	5.96	113.18	110.80
44	1	23	A	C4-C5-C6	-5.96	114.02	117.00
44	1	1428	A	C4-C5-C6	-5.96	114.02	117.00
44	1	1655	G	O5'-P-OP1	-5.96	100.34	105.70
44	1	3395	G	N3-C2-N2	5.96	124.07	119.90
44	1	346	C	C2-N1-C1'	5.96	125.35	118.80
44	1	729	C	C5-C4-N4	-5.96	116.03	120.20
44	1	1120	A	C5-N7-C8	-5.95	100.92	103.90
44	1	1593	A	C4-C5-C6	-5.95	114.02	117.00
44	1	3096	C	C5-C4-N4	-5.95	116.03	120.20
44	1	3150	A	C4-C5-C6	-5.95	114.02	117.00
44	1	659	G	C8-N9-C1'	-5.95	119.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1193	A	C4-C5-N7	5.95	113.68	110.70
44	1	3163	A	N1-C2-N3	-5.95	126.32	129.30
44	1	3177	G	C4-C5-N7	5.95	113.18	110.80
44	1	3241	G	N1-C2-N2	-5.95	110.84	116.20
46	6	31	G	N3-C4-C5	5.95	131.58	128.60
13	Q	16	ARG	NE-CZ-NH2	-5.95	117.32	120.30
44	1	369	A	N1-C6-N6	5.95	122.17	118.60
44	1	969	C	N3-C4-N4	5.95	122.17	118.00
44	1	1574	C	N1-C2-O2	5.95	122.47	118.90
44	1	1836	C	N3-C4-N4	5.95	122.17	118.00
44	1	1389	G	C4-C5-N7	5.95	113.18	110.80
44	1	1460	A	C6-C5-N7	-5.95	128.13	132.30
44	1	1833	G	N3-C4-N9	5.95	129.57	126.00
44	1	3164	C	C6-N1-C2	-5.95	117.92	120.30
21	Y	27	ARG	NE-CZ-NH1	5.95	123.27	120.30
44	1	972	A	C5-N7-C8	-5.95	100.93	103.90
9	M	124	ARG	NE-CZ-NH2	-5.95	117.33	120.30
44	1	58	G	N3-C4-N9	5.95	129.57	126.00
44	1	944	C	N1-C2-O2	5.95	122.47	118.90
44	1	1193	A	C5-C6-N1	5.95	120.67	117.70
44	1	1461	A	N1-C6-N6	5.95	122.17	118.60
27	e	43	ARG	NE-CZ-NH1	5.94	123.27	120.30
44	1	145	G	C5-N7-C8	-5.94	101.33	104.30
44	1	501	A	C5-C6-N6	-5.94	118.94	123.70
44	1	926	A	C4-C5-N7	5.94	113.67	110.70
44	1	3087	A	C4-C5-N7	5.94	113.67	110.70
2	C	198	ARG	NE-CZ-NH2	-5.94	117.33	120.30
34	l	8	ARG	NE-CZ-NH2	-5.94	117.33	120.30
44	1	609	G	N3-C2-N2	5.94	124.06	119.90
44	1	1383	G	C4-C5-N7	5.94	113.17	110.80
45	2	17	A	C5-N7-C8	-5.94	100.93	103.90
35	n	23	ARG	NE-CZ-NH1	5.93	123.27	120.30
44	1	1477	A	C4-C5-N7	5.93	113.67	110.70
44	1	3052	G	C5-N7-C8	-5.93	101.33	104.30
45	2	45	C	N3-C2-O2	-5.93	117.75	121.90
44	1	1504	A	C5-C6-N6	-5.93	118.96	123.70
44	1	1587	A	C4-C5-N7	5.93	113.67	110.70
44	1	2910	A	C5-N7-C8	-5.93	100.94	103.90
44	1	13	A	C5-N7-C8	-5.93	100.94	103.90
44	1	1433	A	C5-C6-N1	5.93	120.66	117.70
44	1	694	C	C5-C4-N4	-5.93	116.05	120.20
44	1	976	U	C5-C4-O4	5.93	129.46	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1299	U	C5-C6-N1	5.93	125.66	122.70
44	1	1441	G	C5-N7-C8	-5.93	101.34	104.30
44	1	3182	G	C5-N7-C8	-5.93	101.34	104.30
44	1	1502	C	N3-C4-C5	5.92	124.27	121.90
44	1	8	C	N1-C2-O2	5.92	122.45	118.90
44	1	934	G	N7-C8-N9	5.92	116.06	113.10
44	1	3077	A	N9-C4-C5	-5.92	103.43	105.80
44	1	118	U	C6-N1-C2	-5.92	117.45	121.00
44	1	3134	A	C5-C6-N6	-5.92	118.96	123.70
44	1	1407	A	C4-C5-C6	-5.92	114.04	117.00
44	1	2934	A	N1-C6-N6	-5.92	115.05	118.60
45	2	42	G	N1-C2-N2	-5.92	110.87	116.20
8	L	67	ARG	NE-CZ-NH1	5.92	123.26	120.30
44	1	1382	G	O5'-P-OP2	-5.92	100.37	105.70
44	1	1508	C	N3-C4-N4	5.92	122.14	118.00
44	1	1909	A	C5-N7-C8	-5.92	100.94	103.90
44	1	3150	A	C5-N7-C8	-5.92	100.94	103.90
44	1	76	G	C8-N9-C4	-5.92	104.03	106.40
44	1	221	A	O4'-C1'-N9	5.92	112.93	108.20
44	1	658	G	C8-N9-C4	-5.92	104.03	106.40
44	1	1428	A	N1-C2-N3	-5.92	126.34	129.30
44	1	1336	U	N3-C4-O4	5.92	123.54	119.40
44	1	3391	A	C4-C5-N7	5.92	113.66	110.70
44	1	1433	A	N1-C6-N6	5.91	122.15	118.60
44	1	585	A	N1-C2-N3	-5.91	126.34	129.30
44	1	1366	A	C5-C6-N6	-5.91	118.97	123.70
45	2	11	C	N3-C4-C5	5.91	124.27	121.90
44	1	498	A	C8-N9-C4	-5.91	103.44	105.80
44	1	666	A	N9-C4-C5	-5.91	103.44	105.80
44	1	831	G	N7-C8-N9	5.91	116.06	113.10
44	1	1205	A	C4-C5-N7	5.91	113.66	110.70
44	1	1656	A	C5-C6-N1	5.91	120.66	117.70
44	1	1874	A	C5-C6-N1	5.91	120.66	117.70
44	1	3372	A	C4-C5-N7	5.91	113.66	110.70
45	2	18	U	C6-N1-C2	-5.91	117.45	121.00
44	1	412	G	C5-N7-C8	-5.91	101.35	104.30
44	1	1159	A	C5-N7-C8	-5.91	100.95	103.90
44	1	1369	A	C5-C6-N1	5.91	120.66	117.70
45	2	141	C	C5-C4-N4	-5.91	116.06	120.20
44	1	810	A	C5-N7-C8	-5.91	100.95	103.90
44	1	1615	C	C2-N1-C1'	5.91	125.30	118.80
45	2	145	U	N3-C4-O4	5.91	123.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	u	111	ARG	NE-CZ-NH2	5.91	123.25	120.30
44	1	428	A	C6-N1-C2	-5.91	115.06	118.60
44	1	1304	A	C8-N9-C4	-5.91	103.44	105.80
44	1	1450	G	C4-C5-N7	5.91	113.16	110.80
44	1	1559	A	N1-C6-N6	-5.91	115.06	118.60
44	1	499	G	C4-C5-N7	5.90	113.16	110.80
44	1	915	A	C2-N3-C4	5.90	113.55	110.60
44	1	1330	A	C5-C6-N1	5.90	120.65	117.70
44	1	3077	A	C4-C5-N7	5.90	113.65	110.70
44	1	3095	U	N3-C4-O4	5.90	123.53	119.40
44	1	663	C	C6-N1-C2	-5.90	117.94	120.30
15	S	12	ARG	NE-CZ-NH1	5.90	123.25	120.30
29	g	74	ARG	NE-CZ-NH2	-5.90	117.35	120.30
44	1	816	A	N7-C8-N9	5.90	116.75	113.80
44	1	2892	A	C5-N7-C8	-5.90	100.95	103.90
45	2	150	G	N9-C4-C5	-5.90	103.04	105.40
44	1	29	C	C6-N1-C2	-5.90	117.94	120.30
44	1	1333	C	C2-N1-C1'	5.90	125.29	118.80
44	1	2101	C	O4'-C1'-N1	5.90	112.92	108.20
44	1	3087	A	N9-C4-C5	-5.90	103.44	105.80
44	1	931	C	C4-C5-C6	-5.90	114.45	117.40
44	1	1810	A	C5-C6-N1	5.90	120.65	117.70
44	1	80	G	C5-N7-C8	-5.89	101.35	104.30
44	1	628	A	N1-C6-N6	5.89	122.14	118.60
44	1	3381	U	N1-C2-O2	5.89	126.93	122.80
45	2	42	G	N3-C4-C5	5.89	131.55	128.60
24	b	43	ARG	NE-CZ-NH2	5.89	123.25	120.30
44	1	3021	A	C5-N7-C8	-5.89	100.95	103.90
44	1	1374	G	C5-N7-C8	-5.89	101.36	104.30
44	1	3033	A	C5-C6-N1	5.89	120.64	117.70
44	1	226	C	C2-N1-C1'	5.89	125.28	118.80
44	1	3103	A	C5-N7-C8	-5.89	100.96	103.90
44	1	311	C	C6-N1-C2	-5.89	117.94	120.30
44	1	622	A	N9-C4-C5	-5.89	103.44	105.80
44	1	952	A	C5-C6-N6	-5.89	118.99	123.70
44	1	932	U	C2-N3-C4	5.88	130.53	127.00
44	1	934	G	C4-C5-N7	5.88	113.15	110.80
2	C	202	ARG	NE-CZ-NH2	-5.88	117.36	120.30
44	1	2946	A	N9-C4-C5	-5.88	103.45	105.80
45	2	105	A	C6-C5-N7	-5.88	128.18	132.30
44	1	373	A	C8-N9-C4	5.88	108.15	105.80
44	1	634	C	N1-C2-O2	5.88	122.42	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	2361	A	C4-C5-N7	5.88	113.64	110.70
44	1	3053	G	N3-C4-N9	5.88	129.53	126.00
44	1	1108	U	C2-N1-C1'	5.88	124.75	117.70
44	1	3296	A	C5-C6-N1	5.88	120.64	117.70
45	2	44	A	C4-C5-C6	-5.88	114.06	117.00
44	1	1223	A	C5-C6-N6	-5.87	119.00	123.70
44	1	150	A	C4-C5-C6	-5.87	114.06	117.00
44	1	238	A	N9-C4-C5	-5.87	103.45	105.80
44	1	1190	A	C2-N3-C4	5.87	113.54	110.60
44	1	1294	A	C5-C6-N1	5.87	120.64	117.70
44	1	588	G	C4-C5-N7	5.87	113.15	110.80
44	1	1537	A	C5-C6-N6	-5.87	119.00	123.70
44	1	348	A	C5-N7-C8	-5.87	100.97	103.90
45	2	148	G	N7-C8-N9	5.87	116.03	113.10
46	6	53	A	C5-N7-C8	-5.87	100.97	103.90
11	O	128	ARG	NE-CZ-NH2	-5.87	117.37	120.30
44	1	1298	C	N1-C2-O2	5.87	122.42	118.90
44	1	349	A	C4-C5-C6	-5.86	114.07	117.00
44	1	690	A	N7-C8-N9	5.86	116.73	113.80
44	1	396	A	C8-N9-C4	5.86	108.14	105.80
44	1	1365	G	N3-C2-N2	5.86	124.00	119.90
44	1	1581	C	N1-C2-O2	5.86	122.42	118.90
44	1	3286	G	N1-C2-N2	-5.86	110.92	116.20
44	1	266	A	C8-N9-C4	5.86	108.14	105.80
44	1	312	C	N1-C2-O2	5.86	122.42	118.90
44	1	3211	C	N3-C2-O2	-5.86	117.80	121.90
44	1	201	A	C5-C6-N6	-5.85	119.02	123.70
44	1	1227	C	C6-N1-C2	-5.85	117.96	120.30
44	1	327	A	C5-N7-C8	-5.85	100.97	103.90
44	1	389	A	C5-N7-C8	-5.85	100.97	103.90
44	1	802	C	C5-C6-N1	5.85	123.92	121.00
44	1	875	G	C4-N9-C1'	5.85	134.10	126.50
44	1	1310	G	C4-C5-N7	5.85	113.14	110.80
44	1	1422	G	N9-C4-C5	-5.85	103.06	105.40
44	1	3367	C	N1-C2-O2	5.85	122.41	118.90
45	2	114	G	N3-C4-C5	5.85	131.52	128.60
44	1	1362	G	N9-C4-C5	-5.85	103.06	105.40
44	1	78	U	C2-N1-C1'	5.84	124.71	117.70
44	1	1528	G	C5-N7-C8	-5.84	101.38	104.30
44	1	672	A	N9-C4-C5	-5.84	103.46	105.80
44	1	2348	A	C5-N7-C8	-5.84	100.98	103.90
44	1	88	A	C5-N7-C8	-5.84	100.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	114	A	N1-C6-N6	5.84	122.11	118.60
44	1	350	C	C6-N1-C2	-5.84	117.96	120.30
44	1	2833	A	N9-C4-C5	-5.84	103.46	105.80
45	2	113	U	C6-N1-C2	-5.84	117.50	121.00
44	1	415	G	N7-C8-N9	5.84	116.02	113.10
44	1	101	G	C8-N9-C1'	-5.84	119.41	127.00
44	1	613	G	C4-C5-N7	5.84	113.14	110.80
44	1	3089	C	N3-C2-O2	-5.84	117.81	121.90
44	1	106	A	C5-N7-C8	-5.84	100.98	103.90
44	1	347	G	C8-N9-C4	-5.84	104.07	106.40
44	1	396	A	C5-C6-N6	-5.84	119.03	123.70
44	1	1182	A	N9-C4-C5	-5.84	103.47	105.80
45	2	102	U	C6-N1-C2	-5.84	117.50	121.00
45	2	106	C	C5-C4-N4	-5.84	116.11	120.20
44	1	1876	U	C5-C4-O4	-5.83	122.40	125.90
44	1	324	A	C4-C5-C6	-5.83	114.08	117.00
44	1	377	A	C4-C5-C6	-5.83	114.08	117.00
44	1	1385	C	C5-C4-N4	-5.83	116.12	120.20
45	2	92	A	N7-C8-N9	5.83	116.72	113.80
44	1	928	C	C5-C6-N1	5.83	123.92	121.00
44	1	345	G	N9-C4-C5	-5.83	103.07	105.40
44	1	1310	G	N3-C4-C5	5.83	131.51	128.60
44	1	1166	G	C4-C5-N7	5.83	113.13	110.80
44	1	247	C	N1-C2-O2	5.82	122.39	118.90
44	1	1162	U	C5-C6-N1	5.82	125.61	122.70
45	2	17	A	N9-C4-C5	5.82	108.13	105.80
45	2	36	G	C4-C5-N7	5.82	113.13	110.80
44	1	224	C	N3-C4-C5	5.82	124.23	121.90
44	1	341	G	C8-N9-C1'	-5.82	119.44	127.00
44	1	705	A	N9-C4-C5	-5.82	103.47	105.80
44	1	1564	U	C5-C4-O4	-5.82	122.41	125.90
44	1	3039	C	C6-N1-C2	-5.82	117.97	120.30
44	1	3210	A	N9-C4-C5	-5.82	103.47	105.80
44	1	611	A	C4-C5-C6	-5.82	114.09	117.00
44	1	3103	A	C6-N1-C2	-5.82	115.11	118.60
45	2	9	A	C8-N9-C4	-5.82	103.47	105.80
44	1	209	A	C5-N7-C8	-5.81	100.99	103.90
44	1	850	U	C5-C6-N1	5.81	125.61	122.70
44	1	1499	C	N1-C2-O2	5.81	122.39	118.90
44	1	267	G	O4'-C1'-N9	-5.81	103.55	108.20
44	1	950	G	C5-N7-C8	-5.81	101.39	104.30
44	1	1882	G	C4-C5-N7	5.81	113.12	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3308	C	N3-C4-C5	5.81	124.22	121.90
3	E	26	ARG	NE-CZ-NH1	5.81	123.20	120.30
44	1	1832	C	C5-C4-N4	-5.81	116.13	120.20
35	n	92	ARG	NE-CZ-NH2	5.81	123.20	120.30
38	r	163	ARG	NE-CZ-NH1	5.81	123.20	120.30
44	1	2130	G	C8-N9-C1'	5.81	134.55	127.00
44	1	651	G	C4-N9-C1'	5.81	134.05	126.50
44	1	2130	G	C4-N9-C1'	-5.81	118.95	126.50
44	1	157	A	N1-C6-N6	-5.80	115.12	118.60
45	2	58	G	N3-C2-N2	5.80	123.96	119.90
45	2	101	U	N3-C4-O4	5.80	123.46	119.40
21	Y	115	ARG	NE-CZ-NH1	5.80	123.20	120.30
44	1	418	A	C5-C6-N1	5.80	120.60	117.70
44	1	1158	A	N9-C4-C5	-5.80	103.48	105.80
44	1	2994	A	C5-C6-N1	5.80	120.60	117.70
44	1	3379	C	N3-C4-N4	5.80	122.06	118.00
45	2	132	G	C8-N9-C4	-5.80	104.08	106.40
46	6	50	U	C5-C6-N1	5.80	125.60	122.70
44	1	516	A	C5-C6-N1	5.80	120.60	117.70
44	1	1397	C	N3-C2-O2	-5.80	117.84	121.90
44	1	1506	A	C5-N7-C8	-5.80	101.00	103.90
44	1	1516	C	N1-C2-O2	5.80	122.38	118.90
44	1	1833	G	N9-C4-C5	-5.80	103.08	105.40
44	1	214	G	C4-C5-N7	5.80	113.12	110.80
44	1	357	A	C5-N7-C8	-5.80	101.00	103.90
44	1	1187	C	C2-N1-C1'	5.80	125.18	118.80
44	1	3167	A	C5-N7-C8	-5.80	101.00	103.90
44	1	500	C	C5-C4-N4	-5.79	116.14	120.20
44	1	736	A	N9-C4-C5	-5.79	103.48	105.80
44	1	1204	A	C5-N7-C8	-5.79	101.00	103.90
44	1	1418	A	C5-N7-C8	-5.79	101.00	103.90
45	2	26	U	N1-C2-O2	5.79	126.85	122.80
44	1	2911	A	N1-C6-N6	-5.79	115.13	118.60
44	1	3273	A	C8-N9-C4	5.79	108.11	105.80
45	2	62	C	N3-C4-N4	5.79	122.05	118.00
44	1	1796	G	N1-C6-O6	-5.79	116.43	119.90
44	1	3016	A	N9-C4-C5	-5.79	103.48	105.80
44	1	586	C	N3-C4-C5	5.78	124.21	121.90
44	1	3165	A	C5-N7-C8	-5.78	101.01	103.90
44	1	961	C	N3-C2-O2	-5.78	117.85	121.90
44	1	1155	C	C6-N1-C2	-5.78	117.99	120.30
44	1	3016	A	C4-C5-N7	5.78	113.59	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	74	U	N3-C4-O4	5.78	123.44	119.40
12	P	90	PHE	CB-CG-CD1	5.78	124.84	120.80
15	S	28	ARG	NE-CZ-NH2	5.78	123.19	120.30
44	1	929	A	C5-C6-N6	-5.78	119.08	123.70
44	1	201	A	C5-C6-N1	5.77	120.59	117.70
44	1	736	A	N1-C6-N6	5.77	122.06	118.60
45	2	9	A	C4-N9-C1'	5.77	136.69	126.30
44	1	345	G	C2-N3-C4	-5.77	109.01	111.90
44	1	588	G	C8-N9-C4	-5.77	104.09	106.40
44	1	1633	C	N1-C2-O2	5.77	122.36	118.90
44	1	60	A	C6-C5-N7	-5.77	128.26	132.30
21	Y	20	PHE	CB-CG-CD2	5.77	124.84	120.80
34	l	46	ARG	NE-CZ-NH1	5.77	123.18	120.30
44	1	510	G	N1-C2-N2	-5.77	111.01	116.20
44	1	1410	U	C5-C6-N1	5.77	125.58	122.70
44	1	701	G	C4-N9-C1'	5.77	134.00	126.50
44	1	1159	A	N7-C8-N9	5.77	116.68	113.80
44	1	3131	U	C5-C6-N1	5.77	125.58	122.70
44	1	364	G	N1-C2-N3	5.76	127.36	123.90
44	1	389	A	N9-C4-C5	-5.76	103.49	105.80
44	1	20	A	C4-C5-C6	-5.76	114.12	117.00
44	1	920	A	C5-N7-C8	-5.76	101.02	103.90
45	2	103	G	N1-C2-N2	-5.76	111.02	116.20
44	1	1638	A	C5-C6-N1	5.76	120.58	117.70
44	1	1587	A	C5-C6-N1	5.76	120.58	117.70
44	1	3321	C	N3-C4-C5	5.76	124.20	121.90
44	1	792	G	C4-N9-C1'	5.75	133.98	126.50
44	1	1172	G	C5-C6-O6	5.75	132.05	128.60
44	1	220	G	N3-C2-N2	5.75	123.93	119.90
44	1	1354	G	N3-C2-N2	-5.75	115.87	119.90
45	2	42	G	C4-C5-N7	5.75	113.10	110.80
45	2	149	A	C4-C5-N7	5.75	113.58	110.70
44	1	926	A	C4-N9-C1'	5.75	136.65	126.30
44	1	1190	A	N3-C4-N9	5.75	132.00	127.40
44	1	1392	G	N7-C8-N9	5.75	115.98	113.10
44	1	3218	A	C4-C5-N7	5.75	113.58	110.70
44	1	803	C	N3-C2-O2	-5.75	117.88	121.90
1	B	100	ARG	NE-CZ-NH1	5.75	123.17	120.30
44	1	288	C	N3-C4-N4	5.75	122.02	118.00
44	1	1290	A	C4-C5-N7	5.75	113.57	110.70
44	1	2827	U	C5-C6-N1	5.75	125.58	122.70
45	2	126	A	C5-C6-N1	5.75	120.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1329	U	P-O3'-C3'	5.75	126.59	119.70
44	1	3060	C	N1-C2-O2	5.75	122.35	118.90
45	2	11	C	N1-C2-O2	5.75	122.35	118.90
44	1	1385	C	N3-C2-O2	-5.75	117.88	121.90
44	1	1829	G	C8-N9-C4	5.74	108.70	106.40
46	6	5	C	N3-C2-O2	-5.74	117.88	121.90
44	1	1294	A	N1-C6-N6	-5.74	115.16	118.60
44	1	1472	U	C5-C4-O4	-5.74	122.46	125.90
44	1	1173	U	C5-C6-N1	5.74	125.57	122.70
44	1	1320	C	N1-C2-O2	5.74	122.34	118.90
44	1	1393	A	N7-C8-N9	5.74	116.67	113.80
44	1	1607	U	C6-N1-C2	-5.74	117.56	121.00
44	1	368	G	N3-C4-C5	5.73	131.47	128.60
44	1	415	G	C5-N7-C8	-5.73	101.43	104.30
44	1	1309	U	OP1-P-O3'	5.73	117.81	105.20
44	1	3007	U	C5-C6-N1	5.73	125.57	122.70
44	1	1506	A	N9-C4-C5	-5.73	103.51	105.80
44	1	1589	A	C5-N7-C8	-5.73	101.03	103.90
44	1	1833	G	C8-N9-C1'	-5.73	119.55	127.00
44	1	2382	G	C5-N7-C8	-5.73	101.43	104.30
44	1	2890	A	C5-N7-C8	-5.73	101.03	103.90
44	1	17	G	C5-N7-C8	-5.73	101.44	104.30
44	1	585	A	C4-C5-C6	-5.73	114.14	117.00
44	1	659	G	OP2-P-O3'	5.73	117.81	105.20
44	1	2876	C	C6-N1-C2	-5.73	118.01	120.30
44	1	1391	C	N3-C4-C5	5.73	124.19	121.90
45	2	35	C	C5-C6-N1	5.73	123.86	121.00
45	2	106	C	N1-C2-O2	5.73	122.34	118.90
44	1	495	G	N3-C2-N2	5.72	123.91	119.90
44	1	803	C	N1-C2-O2	5.72	122.33	118.90
44	1	1561	G	N1-C2-N2	-5.72	111.05	116.20
45	2	47	C	N3-C2-O2	-5.72	117.89	121.90
44	1	24	G	C2-N3-C4	-5.72	109.04	111.90
44	1	1377	G	N1-C2-N3	5.72	127.33	123.90
44	1	1607	U	C5-C6-N1	5.72	125.56	122.70
45	2	20	U	N3-C4-O4	5.72	123.41	119.40
44	1	56	G	N3-C4-C5	5.72	131.46	128.60
44	1	3330	A	C5-N7-C8	-5.72	101.04	103.90
45	2	59	A	N9-C4-C5	-5.72	103.51	105.80
44	1	78	U	N1-C2-N3	5.72	118.33	114.90
44	1	1179	A	N7-C8-N9	5.72	116.66	113.80
44	1	1278	A	C8-N9-C4	-5.72	103.51	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	89	A	N7-C8-N9	5.72	116.66	113.80
4	F	47	ARG	NE-CZ-NH2	-5.72	117.44	120.30
44	1	33	G	C5-N7-C8	-5.71	101.44	104.30
44	1	1161	G	C4-N9-C1'	5.71	133.93	126.50
44	1	1528	G	N7-C8-N9	5.71	115.96	113.10
44	1	1886	A	N1-C6-N6	-5.71	115.17	118.60
44	1	753	C	C6-N1-C2	-5.71	118.02	120.30
44	1	2948	C	N3-C2-O2	-5.71	117.90	121.90
45	2	1	A	N1-C6-N6	-5.71	115.17	118.60
44	1	729	C	C5-C6-N1	5.71	123.85	121.00
44	1	340	C	N3-C4-C5	5.71	124.18	121.90
44	1	2356	A	C4-C5-N7	5.71	113.55	110.70
44	1	3330	A	N7-C8-N9	5.71	116.65	113.80
44	1	433	A	C4-C5-N7	5.71	113.55	110.70
44	1	638	C	N3-C4-N4	5.70	121.99	118.00
44	1	1589	A	C4-C5-C6	-5.70	114.15	117.00
44	1	2352	A	C5-C6-N6	-5.70	119.14	123.70
1	B	100	ARG	NE-CZ-NH2	-5.70	117.45	120.30
29	g	16	ARG	NE-CZ-NH1	5.70	123.15	120.30
44	1	1537	A	C5-C6-N1	5.70	120.55	117.70
44	1	3033	A	C8-N9-C4	5.70	108.08	105.80
44	1	125	C	C5-C4-N4	-5.70	116.21	120.20
44	1	1395	G	N1-C2-N3	5.70	127.32	123.90
44	1	1837	U	N3-C4-O4	5.70	123.39	119.40
44	1	935	U	N1-C2-O2	5.70	126.79	122.80
44	1	1180	A	C5-N7-C8	-5.70	101.05	103.90
44	1	1473	G	N7-C8-N9	5.70	115.95	113.10
44	1	1553	U	N1-C2-O2	5.70	126.79	122.80
44	1	3187	A	N7-C8-N9	5.69	116.65	113.80
20	X	33	ARG	NE-CZ-NH1	5.69	123.15	120.30
44	1	384	A	C5-C6-N1	5.69	120.55	117.70
44	1	1593	A	N9-C4-C5	-5.69	103.52	105.80
44	1	3108	G	N7-C8-N9	5.69	115.95	113.10
44	1	3004	C	C2-N1-C1'	5.69	125.06	118.80
44	1	222	A	C5-C6-N1	5.69	120.55	117.70
38	r	16	LYS	CA-CB-CG	5.69	125.91	113.40
44	1	349	A	O5'-P-OP2	-5.69	100.58	105.70
44	1	1154	A	C5-C6-N1	5.69	120.54	117.70
44	1	638	C	C5-C6-N1	5.68	123.84	121.00
44	1	812	G	N7-C8-N9	5.68	115.94	113.10
44	1	1757	A	C4-C5-C6	-5.68	114.16	117.00
44	1	3139	A	N9-C4-C5	-5.68	103.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	120	C	N3-C4-C5	5.68	124.17	121.90
28	f	65	ARG	NE-CZ-NH2	-5.68	117.46	120.30
44	1	113	C	C6-N1-C2	-5.68	118.03	120.30
44	1	1319	G	C5-N7-C8	-5.68	101.46	104.30
44	1	365	A	C4-C5-N7	5.68	113.54	110.70
44	1	374	A	C5-C6-N1	5.68	120.54	117.70
44	1	792	G	C5-N7-C8	-5.68	101.46	104.30
44	1	1381	A	N7-C8-N9	5.68	116.64	113.80
44	1	1498	A	N9-C4-C5	-5.68	103.53	105.80
44	1	682	U	C5-C6-N1	5.68	125.54	122.70
44	1	1787	A	C5-N7-C8	-5.68	101.06	103.90
45	2	28	C	C6-N1-C2	-5.68	118.03	120.30
45	2	142	C	C5-C6-N1	5.68	123.84	121.00
44	1	644	G	C8-N9-C1'	-5.67	119.62	127.00
44	1	671	U	N3-C4-O4	5.67	123.37	119.40
44	1	1149	G	O4'-C1'-N9	5.67	112.74	108.20
44	1	1165	A	N9-C4-C5	-5.67	103.53	105.80
44	1	1419	A	C5-C6-N6	-5.67	119.16	123.70
44	1	1699	A	C5-C6-N1	5.67	120.54	117.70
6	H	62	ARG	NE-CZ-NH1	5.67	123.14	120.30
44	1	363	G	C6-C5-N7	-5.67	127.00	130.40
32	j	49	TRP	CA-CB-CG	5.67	124.47	113.70
44	1	364	G	N3-C4-C5	5.67	131.43	128.60
44	1	561	C	N1-C2-O2	5.67	122.30	118.90
44	1	621	A	C5-C6-N6	-5.67	119.17	123.70
44	1	1360	C	N1-C2-O2	5.67	122.30	118.90
44	1	1839	A	C8-N9-C4	-5.67	103.53	105.80
44	1	3062	G	N3-C4-C5	5.67	131.43	128.60
44	1	3327	G	C4-C5-N7	5.67	113.07	110.80
45	2	70	G	C4-C5-N7	5.67	113.07	110.80
44	1	2849	C	C6-N1-C2	-5.67	118.03	120.30
44	1	3026	G	N3-C4-N9	-5.67	122.60	126.00
44	1	3094	A	C4-C5-C6	-5.67	114.17	117.00
45	2	35	C	N3-C4-C5	5.67	124.17	121.90
45	2	37	A	C5-N7-C8	-5.67	101.07	103.90
44	1	151	A	N1-C6-N6	5.66	122.00	118.60
44	1	325	A	C5-N7-C8	-5.66	101.07	103.90
44	1	1141	C	C5-C4-N4	-5.66	116.24	120.20
44	1	1881	A	C5-C6-N1	5.66	120.53	117.70
45	2	39	G	N7-C8-N9	5.66	115.93	113.10
44	1	233	C	N3-C4-C5	5.66	124.17	121.90
44	1	3243	A	C4-C5-C6	-5.66	114.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3295	A	C5-N7-C8	-5.66	101.07	103.90
46	6	23	U	N1-C2-O2	5.66	126.76	122.80
44	1	355	A	C4-C5-C6	-5.66	114.17	117.00
44	1	1833	G	C5-C6-N1	5.66	114.33	111.50
44	1	3095	U	C5-C4-O4	-5.66	122.50	125.90
44	1	107	A	N9-C4-C5	-5.66	103.54	105.80
44	1	1534	A	C5-N7-C8	-5.65	101.07	103.90
44	1	631	U	C5-C6-N1	5.65	125.53	122.70
44	1	2881	C	N1-C2-O2	5.65	122.29	118.90
44	1	3113	A	C5-N7-C8	-5.65	101.07	103.90
44	1	11	A	C5-C6-N6	-5.65	119.18	123.70
44	1	1800	A	N9-C4-C5	-5.65	103.54	105.80
44	1	3187	A	C5-N7-C8	-5.65	101.08	103.90
3	E	48	ARG	NE-CZ-NH1	5.65	123.12	120.30
44	1	3307	A	C4-C5-N7	5.65	113.52	110.70
45	2	130	C	N3-C2-O2	-5.65	117.95	121.90
44	1	1431	G	C4-C5-N7	5.65	113.06	110.80
44	1	2393	G	C5-C6-O6	-5.65	125.21	128.60
44	1	693	A	C4-C5-C6	-5.64	114.18	117.00
26	d	88	PRO	N-CA-C	5.64	126.77	112.10
44	1	1299	U	N1-C2-O2	5.64	126.75	122.80
44	1	1786	G	N7-C8-N9	5.64	115.92	113.10
44	1	1747	G	C4-C5-N7	5.64	113.06	110.80
44	1	3273	A	C5-C6-N6	-5.64	119.19	123.70
44	1	36	C	N3-C4-N4	5.64	121.95	118.00
44	1	1828	A	C5-C6-N1	5.64	120.52	117.70
45	2	87	G	N7-C8-N9	5.63	115.92	113.10
44	1	775	A	N1-C6-N6	5.63	121.98	118.60
44	1	990	U	C2-N1-C1'	5.63	124.46	117.70
44	1	385	A	C4-C5-N7	5.63	113.52	110.70
44	1	352	A	C6-N1-C2	-5.63	115.22	118.60
44	1	356	C	N3-C2-O2	-5.63	117.96	121.90
44	1	1619	A	C4-C5-C6	-5.63	114.19	117.00
44	1	495	G	N1-C2-N2	-5.63	111.14	116.20
44	1	622	A	C5-N7-C8	-5.63	101.09	103.90
44	1	665	A	N1-C6-N6	5.63	121.98	118.60
44	1	1863	G	N3-C4-C5	5.63	131.41	128.60
44	1	1896	A	C4-C5-N7	5.63	113.51	110.70
44	1	2884	C	N3-C2-O2	-5.63	117.96	121.90
44	1	1374	G	N3-C2-N2	5.62	123.84	119.90
45	2	142	C	C6-N1-C2	-5.62	118.05	120.30
12	P	18	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	632	G	C5-N7-C8	-5.62	101.49	104.30
44	1	3034	C	C2-N3-C4	-5.62	117.09	119.90
44	1	77	A	C4-C5-N7	5.62	113.51	110.70
44	1	397	A	C5-N7-C8	-5.62	101.09	103.90
44	1	1329	U	C5-C4-O4	5.62	129.27	125.90
44	1	1506	A	C4-C5-N7	5.62	113.51	110.70
44	1	1663	C	N3-C4-C5	5.62	124.15	121.90
44	1	3335	A	C5-C6-N6	-5.62	119.20	123.70
8	L	15	ARG	NE-CZ-NH1	5.62	123.11	120.30
44	1	1502	C	C5-C4-N4	-5.62	116.27	120.20
44	1	3053	G	N9-C4-C5	-5.62	103.15	105.40
44	1	3138	U	N3-C4-O4	5.62	123.33	119.40
45	2	32	C	N3-C4-C5	5.62	124.15	121.90
44	1	810	A	C5-C6-N1	5.62	120.51	117.70
44	1	333	G	C5-N7-C8	-5.62	101.49	104.30
44	1	1196	C	C6-N1-C1'	-5.62	114.06	120.80
44	1	1460	A	N7-C8-N9	5.62	116.61	113.80
44	1	65	A	C5-C6-N1	5.61	120.51	117.70
44	1	638	C	N1-C2-O2	5.61	122.27	118.90
44	1	668	G	C4-N9-C1'	5.61	133.80	126.50
44	1	1823	A	N9-C4-C5	-5.61	103.56	105.80
45	2	138	A	C5-C6-N1	5.61	120.51	117.70
44	1	522	A	C5-C6-N6	-5.61	119.21	123.70
44	1	1663	C	C5-C4-N4	-5.61	116.27	120.20
8	L	21	ARG	NE-CZ-NH2	-5.61	117.50	120.30
44	1	1525	G	N3-C4-N9	5.61	129.37	126.00
44	1	62	A	C5-N7-C8	-5.61	101.10	103.90
44	1	1119	C	C5-C4-N4	-5.61	116.27	120.20
44	1	3012	A	C8-N9-C4	5.61	108.04	105.80
44	1	1193	A	C5-N7-C8	-5.61	101.10	103.90
44	1	3140	G	C5-N7-C8	-5.61	101.50	104.30
44	1	1147	G	N7-C8-N9	5.60	115.90	113.10
44	1	3379	C	C6-N1-C2	-5.60	118.06	120.30
21	Y	12	ARG	NE-CZ-NH2	-5.60	117.50	120.30
44	1	632	G	C8-N9-C4	-5.60	104.16	106.40
44	1	3172	A	C5-C6-N6	-5.60	119.22	123.70
44	1	806	A	C4-C5-N7	5.60	113.50	110.70
44	1	1372	C	N1-C2-O2	5.60	122.26	118.90
44	1	1575	A	C5-C6-N1	5.60	120.50	117.70
45	2	76	C	N1-C2-O2	5.60	122.26	118.90
45	2	131	A	C5-N7-C8	-5.60	101.10	103.90
44	1	209	A	C5-C6-N6	-5.59	119.22	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1303	A	C5-C6-N6	-5.59	119.22	123.70
10	N	99	ARG	NE-CZ-NH2	-5.59	117.50	120.30
44	1	1498	A	C5-C6-N6	-5.59	119.22	123.70
46	6	13	U	N1-C2-O2	5.59	126.72	122.80
8	L	100	ARG	NE-CZ-NH1	5.59	123.09	120.30
44	1	815	G	N9-C4-C5	-5.59	103.16	105.40
44	1	1318	A	N1-C6-N6	-5.59	115.25	118.60
44	1	1585	C	C5-C4-N4	-5.59	116.29	120.20
44	1	142	C	N3-C4-C5	5.59	124.14	121.90
44	1	198	A	N1-C6-N6	-5.59	115.25	118.60
44	1	947	G	C4-C5-N7	5.59	113.04	110.80
10	N	12	ARG	NE-CZ-NH2	-5.59	117.51	120.30
42	y	100	ARG	NE-CZ-NH2	5.59	123.09	120.30
44	1	26	A	C5-C6-N1	5.59	120.49	117.70
44	1	1208	U	N1-C2-O2	5.59	126.71	122.80
44	1	1231	A	C8-N9-C4	5.59	108.03	105.80
44	1	1589	A	C5-C6-N1	5.59	120.49	117.70
44	1	3279	A	C4-C5-N7	5.59	113.49	110.70
44	1	396	A	C5-N7-C8	-5.58	101.11	103.90
44	1	1135	A	C5-C6-N6	-5.58	119.23	123.70
44	1	1337	A	C6-N1-C2	-5.58	115.25	118.60
44	1	2946	A	C5-C6-N1	5.58	120.49	117.70
44	1	282	G	P-O3'-C3'	5.58	126.40	119.70
44	1	1300	G	N1-C2-N2	-5.58	111.17	116.20
45	2	105	A	C5-N7-C8	-5.58	101.11	103.90
32	j	55	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	E	77	ARG	NE-CZ-NH2	-5.58	117.51	120.30
35	n	18	ARG	NE-CZ-NH2	5.58	123.09	120.30
44	1	77	A	C5-C6-N6	-5.58	119.24	123.70
44	1	412	G	C6-C5-N7	-5.58	127.05	130.40
44	1	2380	U	C5-C4-O4	-5.58	122.55	125.90
44	1	3294	A	C5-C6-N1	5.58	120.49	117.70
44	1	3196	U	N3-C2-O2	-5.58	118.30	122.20
44	1	2890	A	C5-C6-N6	-5.57	119.24	123.70
45	2	13	A	N7-C8-N9	5.57	116.59	113.80
44	1	232	G	N3-C4-N9	-5.57	122.66	126.00
44	1	529	A	C4-C5-N7	5.57	113.49	110.70
44	1	1382	G	N1-C2-N2	-5.57	111.19	116.20
24	b	159	ARG	NE-CZ-NH1	5.57	123.08	120.30
44	1	729	C	N3-C4-N4	5.57	121.90	118.00
44	1	1537	A	C5-N7-C8	-5.57	101.11	103.90
44	1	1895	A	C4-C5-N7	5.57	113.49	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3172	A	C4-C5-C6	-5.57	114.22	117.00
44	1	360	G	N1-C2-N2	-5.57	111.19	116.20
44	1	1546	A	C5-N7-C8	-5.57	101.11	103.90
44	1	289	A	C6-C5-N7	-5.57	128.40	132.30
45	2	81	U	N3-C2-O2	-5.57	118.30	122.20
44	1	276	U	C5-C4-O4	-5.57	122.56	125.90
44	1	348	A	N7-C8-N9	5.57	116.58	113.80
44	1	657	A	C5-N7-C8	-5.57	101.12	103.90
44	1	3113	A	C5-C6-N1	5.57	120.48	117.70
44	1	3190	C	C5-C4-N4	-5.57	116.31	120.20
44	1	347	G	C5-C6-O6	-5.56	125.26	128.60
44	1	1440	G	C4-C5-N7	5.56	113.03	110.80
44	1	1874	A	C5-N7-C8	-5.56	101.12	103.90
44	1	3141	A	C5-C6-N1	5.56	120.48	117.70
10	N	65	ARG	NE-CZ-NH1	5.56	123.08	120.30
44	1	875	G	N9-C4-C5	-5.56	103.18	105.40
44	1	1194	G	C6-C5-N7	-5.56	127.06	130.40
45	2	8	C	C5-C4-N4	-5.56	116.31	120.20
15	S	113	ARG	NE-CZ-NH1	5.56	123.08	120.30
44	1	690	A	C4-C5-N7	5.56	113.48	110.70
44	1	803	C	C5-C6-N1	5.56	123.78	121.00
44	1	1169	A	OP2-P-O3'	5.56	117.43	105.20
46	6	5	C	C6-N1-C1'	5.56	127.47	120.80
44	1	1798	A	C4-C5-N7	5.56	113.48	110.70
26	d	87	ASN	C-N-CD	-5.55	108.38	120.60
44	1	690	A	C5-N7-C8	-5.55	101.12	103.90
44	1	789	A	C5-N7-C8	-5.55	101.12	103.90
44	1	818	C	N3-C4-C5	5.55	124.12	121.90
44	1	976	U	C6-N1-C2	-5.55	117.67	121.00
44	1	3166	C	C6-N1-C2	-5.55	118.08	120.30
45	2	139	U	N3-C4-O4	5.55	123.29	119.40
44	1	85	A	C4-C5-C6	-5.55	114.22	117.00
44	1	614	C	N3-C4-C5	5.55	124.12	121.90
44	1	2926	A	N1-C6-N6	-5.55	115.27	118.60
44	1	3193	C	C6-N1-C2	-5.55	118.08	120.30
2	C	119	ARG	NE-CZ-NH1	5.55	123.08	120.30
13	Q	39	ARG	NE-CZ-NH1	5.55	123.07	120.30
44	1	1594	A	C4-C5-C6	-5.55	114.23	117.00
44	1	3157	U	N3-C2-O2	-5.55	118.31	122.20
44	1	398	A	O4'-C1'-N9	5.55	112.64	108.20
44	1	784	A	C5-C6-N1	5.55	120.47	117.70
44	1	2358	A	C5-C6-N1	5.55	120.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	110	C	N3-C4-N4	5.55	121.88	118.00
45	2	146	U	C5-C4-O4	-5.55	122.57	125.90
12	P	23	ARG	NE-CZ-NH2	-5.54	117.53	120.30
44	1	17	G	N9-C4-C5	-5.54	103.18	105.40
44	1	267	G	C5-N7-C8	-5.54	101.53	104.30
37	q	421	ARG	NE-CZ-NH2	5.54	123.07	120.30
44	1	106	A	C6-N1-C2	-5.54	115.27	118.60
44	1	315	C	N3-C2-O2	-5.54	118.02	121.90
44	1	2350	C	N3-C4-C5	5.54	124.12	121.90
44	1	3033	A	C4-C5-C6	-5.54	114.23	117.00
44	1	3073	A	C5-C6-N1	5.54	120.47	117.70
44	1	3183	A	N7-C8-N9	5.54	116.57	113.80
44	1	50	U	C5-C6-N1	5.54	125.47	122.70
44	1	790	U	C5-C4-O4	-5.54	122.58	125.90
44	1	1246	G	N3-C2-N2	-5.54	116.02	119.90
44	1	1842	A	C4-C5-C6	-5.54	114.23	117.00
45	2	88	A	N7-C8-N9	5.54	116.57	113.80
9	M	55	ARG	NE-CZ-NH2	-5.54	117.53	120.30
13	Q	39	ARG	NE-CZ-NH2	-5.54	117.53	120.30
44	1	1110	U	N1-C2-O2	-5.54	118.93	122.80
44	1	1377	G	C5-N7-C8	-5.54	101.53	104.30
44	1	1477	A	C5-N7-C8	-5.54	101.13	103.90
44	1	1698	C	N3-C4-N4	5.54	121.88	118.00
44	1	3242	G	N3-C2-N2	5.54	123.78	119.90
45	2	28	C	N1-C2-O2	5.54	122.22	118.90
44	1	624	G	C4-N9-C1'	5.53	133.69	126.50
44	1	1532	C	C5-C4-N4	-5.53	116.33	120.20
44	1	3129	A	C5-N7-C8	-5.53	101.13	103.90
44	1	2378	C	N1-C2-O2	5.53	122.22	118.90
8	L	42	ARG	NE-CZ-NH1	-5.53	117.53	120.30
44	1	431	U	C5-C4-O4	-5.53	122.58	125.90
44	1	705	A	O4'-C1'-N9	-5.53	103.78	108.20
44	1	1185	C	C2-N1-C1'	5.53	124.88	118.80
44	1	3147	G	C4-N9-C1'	5.53	133.69	126.50
46	6	45	U	C6-N1-C2	-5.53	117.68	121.00
29	g	74	ARG	NE-CZ-NH1	5.53	123.06	120.30
44	1	325	A	C6-N1-C2	-5.53	115.28	118.60
44	1	944	C	C2-N3-C4	-5.53	117.14	119.90
44	1	1409	G	C5-N7-C8	-5.53	101.54	104.30
44	1	2930	A	C5-C6-N1	5.53	120.46	117.70
44	1	3008	A	N1-C2-N3	-5.53	126.54	129.30
44	1	650	C	N3-C4-N4	5.52	121.87	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1269	U	C2-N1-C1'	5.52	124.33	117.70
44	1	3079	U	C5-C4-O4	-5.52	122.59	125.90
44	1	598	A	C5-N7-C8	-5.52	101.14	103.90
44	1	1255	C	N3-C2-O2	-5.52	118.03	121.90
44	1	1171	G	N9-C4-C5	-5.52	103.19	105.40
44	1	2991	A	C8-N9-C4	-5.52	103.59	105.80
45	2	50	C	N3-C4-C5	5.52	124.11	121.90
16	T	136	ARG	NE-CZ-NH1	5.52	123.06	120.30
44	1	1157	G	C5-N7-C8	-5.52	101.54	104.30
44	1	375	A	N3-C4-C5	5.52	130.66	126.80
3	E	51	ARG	NE-CZ-NH1	5.51	123.06	120.30
44	1	1194	G	N3-C4-N9	5.51	129.31	126.00
44	1	3305	A	C4-C5-C6	-5.51	114.24	117.00
45	2	8	C	N3-C2-O2	-5.51	118.04	121.90
44	1	1282	G	N7-C8-N9	5.51	115.86	113.10
44	1	1315	U	C5-C6-N1	5.51	125.45	122.70
44	1	1389	G	C5-N7-C8	-5.51	101.55	104.30
44	1	1699	A	C4-C5-C6	-5.51	114.25	117.00
44	1	2370	G	N1-C2-N2	-5.51	111.24	116.20
44	1	3298	C	C6-N1-C2	-5.51	118.10	120.30
9	M	124	ARG	NE-CZ-NH1	5.51	123.06	120.30
44	1	1750	A	C4-C5-C6	-5.51	114.25	117.00
44	1	2910	A	C4-C5-N7	5.51	113.45	110.70
44	1	3295	A	C4-C5-N7	5.51	113.45	110.70
44	1	407	A	C2-N3-C4	-5.51	107.85	110.60
44	1	410	U	C5-C4-O4	-5.51	122.59	125.90
45	2	92	A	C4-C5-N7	5.51	113.45	110.70
44	1	88	A	C4-C5-C6	-5.51	114.25	117.00
44	1	233	C	N1-C2-O2	5.51	122.20	118.90
44	1	813	G	N7-C8-N9	5.51	115.85	113.10
44	1	1203	A	C5-N7-C8	-5.51	101.15	103.90
14	R	9	ARG	NE-CZ-NH2	-5.50	117.55	120.30
15	S	13	ARG	NE-CZ-NH1	5.50	123.05	120.30
44	1	26	A	C4-C5-N7	5.50	113.45	110.70
44	1	812	G	C5-N7-C8	-5.50	101.55	104.30
44	1	1179	A	C4-C5-C6	-5.50	114.25	117.00
44	1	1190	A	N1-C2-N3	-5.50	126.55	129.30
44	1	64	G	N1-C6-O6	5.50	123.20	119.90
44	1	1000	C	N1-C2-O2	5.50	122.20	118.90
44	1	1165	A	C6-N1-C2	-5.50	115.30	118.60
44	1	1474	A	N9-C4-C5	-5.50	103.60	105.80
44	1	1493	G	C6-C5-N7	-5.50	127.10	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	909	G	N1-C6-O6	-5.50	116.60	119.90
44	1	3040	A	C5-C6-N6	-5.50	119.30	123.70
45	2	104	A	C5-C6-N1	5.50	120.45	117.70
4	F	100	ARG	NE-CZ-NH2	5.50	123.05	120.30
44	1	48	A	C4-C5-C6	-5.50	114.25	117.00
44	1	638	C	C5-C4-N4	-5.50	116.35	120.20
44	1	875	G	N3-C4-C5	-5.50	125.85	128.60
44	1	1326	A	N9-C4-C5	-5.50	103.60	105.80
44	1	1667	A	C8-N9-C4	-5.50	103.60	105.80
26	d	28	ARG	NE-CZ-NH1	5.50	123.05	120.30
44	1	1443	G	C6-C5-N7	-5.49	127.10	130.40
44	1	3124	G	N3-C2-N2	5.49	123.75	119.90
44	1	633	C	N3-C2-O2	-5.49	118.06	121.90
44	1	652	G	N9-C4-C5	-5.49	103.20	105.40
40	t	297	ARG	NE-CZ-NH1	5.49	123.05	120.30
44	1	1466	G	C6-C5-N7	-5.49	127.11	130.40
45	2	12	A	C4-C5-C6	-5.49	114.25	117.00
13	Q	69	ARG	NE-CZ-NH2	-5.49	117.56	120.30
18	V	128	ARG	NE-CZ-NH1	5.49	123.04	120.30
45	2	105	A	N3-C4-N9	5.49	131.79	127.40
44	1	1105	A	N1-C6-N6	5.49	121.89	118.60
44	1	596	C	C5-C4-N4	-5.48	116.36	120.20
44	1	820	A	N9-C4-C5	-5.48	103.61	105.80
44	1	1459	C	C5-C4-N4	-5.48	116.36	120.20
11	O	172	ARG	NE-CZ-NH2	-5.48	117.56	120.30
20	X	125	ARG	NE-CZ-NH2	5.48	123.04	120.30
44	1	88	A	C5-C6-N1	5.48	120.44	117.70
44	1	638	C	N3-C2-O2	-5.48	118.06	121.90
44	1	946	U	N3-C4-O4	5.48	123.24	119.40
44	1	3005	A	N1-C6-N6	5.48	121.89	118.60
44	1	3019	U	C5-C4-O4	5.48	129.19	125.90
44	1	3113	A	C5-C6-N6	-5.48	119.32	123.70
45	2	37	A	N9-C4-C5	-5.48	103.61	105.80
44	1	80	G	C4-C5-N7	5.48	112.99	110.80
11	O	160	ARG	NE-CZ-NH1	5.47	123.04	120.30
27	e	125	ARG	NE-CZ-NH2	-5.47	117.56	120.30
44	1	225	C	N3-C4-N4	5.47	121.83	118.00
44	1	3092	C	N3-C2-O2	-5.47	118.07	121.90
44	1	1803	C	C5-C4-N4	-5.47	116.37	120.20
44	1	2993	G	N3-C4-N9	5.47	129.28	126.00
44	1	3242	G	N7-C8-N9	5.47	115.84	113.10
46	6	231	A	C5-C6-N1	5.47	120.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1192	C	C5-C4-N4	-5.47	116.37	120.20
44	1	1654	A	OP1-P-O3'	5.47	117.24	105.20
3	E	46	ARG	NE-CZ-NH1	5.47	123.03	120.30
44	1	361	A	N7-C8-N9	5.47	116.53	113.80
44	1	1280	C	C6-N1-C2	-5.47	118.11	120.30
44	1	3149	G	C4-C5-N7	5.47	112.99	110.80
46	6	49	C	N1-C2-O2	5.47	122.18	118.90
44	1	13	A	C4-C5-N7	5.47	113.43	110.70
44	1	102	C	N3-C4-N4	5.47	121.83	118.00
44	1	1635	G	N1-C2-N2	-5.47	111.28	116.20
44	1	2887	A	N9-C4-C5	-5.46	103.61	105.80
44	1	661	G	C5-N7-C8	-5.46	101.57	104.30
44	1	661	G	N3-C4-C5	5.46	131.33	128.60
44	1	3113	A	C4-C5-N7	5.46	113.43	110.70
44	1	3218	A	C5-N7-C8	-5.46	101.17	103.90
44	1	503	C	N3-C4-C5	5.46	124.08	121.90
44	1	1544	G	N3-C4-N9	-5.46	122.72	126.00
44	1	1594	A	C4-C5-N7	5.46	113.43	110.70
44	1	29	C	C2-N1-C1'	5.46	124.80	118.80
44	1	1466	G	C4-N9-C1'	5.46	133.59	126.50
44	1	1612	A	C5-C6-N6	-5.46	119.33	123.70
44	1	1833	G	C4-C5-N7	5.46	112.98	110.80
45	2	33	A	C5-N7-C8	-5.46	101.17	103.90
45	2	44	A	N9-C4-C5	-5.46	103.62	105.80
27	e	27	ARG	NE-CZ-NH1	5.46	123.03	120.30
44	1	657	A	OP2-P-O3'	5.46	117.20	105.20
44	1	790	U	C5-C6-N1	5.46	125.43	122.70
44	1	1417	G	C4-C5-N7	5.46	112.98	110.80
44	1	327	A	N1-C6-N6	-5.45	115.33	118.60
44	1	1434	G	N7-C8-N9	5.45	115.83	113.10
44	1	1787	A	C4-C5-N7	5.45	113.43	110.70
44	1	3039	C	C5-C4-N4	-5.45	116.38	120.20
44	1	187	A	C4-C5-C6	-5.45	114.27	117.00
44	1	1373	A	C4-C5-C6	-5.45	114.27	117.00
44	1	318	A	C5-N7-C8	-5.45	101.17	103.90
44	1	651	G	C6-C5-N7	-5.45	127.13	130.40
44	1	1449	A	C4-C5-N7	5.45	113.42	110.70
44	1	688	G	N3-C2-N2	-5.45	116.09	119.90
44	1	1311	G	C4-C5-N7	5.45	112.98	110.80
44	1	1797	A	C5-C6-N1	5.45	120.42	117.70
44	1	66	A	C8-N9-C4	-5.44	103.62	105.80
44	1	3323	A	C6-C5-N7	-5.44	128.49	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	6	2	C	N3-C2-O2	-5.44	118.09	121.90
44	1	415	G	C4-C5-N7	5.44	112.98	110.80
44	1	965	A	N9-C4-C5	-5.44	103.62	105.80
44	1	3019	U	C5-C6-N1	5.44	125.42	122.70
45	2	46	G	C4-N9-C1'	5.44	133.57	126.50
44	1	1199	C	C6-N1-C2	-5.44	118.12	120.30
44	1	1419	A	N3-C4-C5	5.44	130.61	126.80
44	1	226	C	N3-C4-C5	5.44	124.08	121.90
44	1	1209	G	C8-N9-C4	5.44	108.58	106.40
44	1	1590	G	C6-C5-N7	-5.44	127.14	130.40
44	1	3123	A	C5-C6-N6	-5.44	119.35	123.70
44	1	686	G	C5-N7-C8	-5.44	101.58	104.30
44	1	3137	C	N3-C4-C5	5.44	124.07	121.90
45	2	145	U	C5-C4-O4	-5.44	122.64	125.90
44	1	1320	C	C6-N1-C2	-5.43	118.13	120.30
44	1	3184	A	N7-C8-N9	5.43	116.52	113.80
44	1	529	A	C5-N7-C8	-5.43	101.18	103.90
44	1	680	G	N7-C8-N9	5.43	115.82	113.10
44	1	831	G	C8-N9-C4	-5.43	104.23	106.40
44	1	938	C	C5-C4-N4	-5.43	116.40	120.20
44	1	1829	G	N9-C4-C5	-5.43	103.23	105.40
45	2	45	C	C5-C6-N1	5.43	123.72	121.00
24	b	130	ARG	NE-CZ-NH1	5.43	123.02	120.30
35	n	424	ARG	NE-CZ-NH1	5.43	123.02	120.30
44	1	108	A	C5-N7-C8	-5.43	101.19	103.90
44	1	1528	G	C4-C5-N7	5.43	112.97	110.80
3	E	26	ARG	NE-CZ-NH2	-5.43	117.58	120.30
44	1	720	A	C5-C6-N6	-5.43	119.36	123.70
44	1	1433	A	C4-C5-N7	5.43	113.42	110.70
44	1	3279	A	N9-C4-C5	-5.43	103.63	105.80
44	1	1343	A	C5-N7-C8	-5.43	101.19	103.90
44	1	1786	G	C5-N7-C8	-5.43	101.59	104.30
44	1	1133	A	C4-C5-N7	5.42	113.41	110.70
44	1	1193	A	N9-C4-C5	-5.42	103.63	105.80
44	1	1195	A	N9-C4-C5	-5.42	103.63	105.80
44	1	2376	G	N1-C2-N2	-5.42	111.32	116.20
44	1	3046	A	C4-C5-C6	-5.42	114.29	117.00
44	1	3303	G	C5-N7-C8	-5.42	101.59	104.30
44	1	1145	G	C4-N9-C1'	5.42	133.55	126.50
44	1	3279	A	C5-C6-N6	-5.42	119.36	123.70
11	O	172	ARG	NE-CZ-NH1	5.42	123.01	120.30
6	H	173	ARG	NE-CZ-NH2	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	80	ARG	NE-CZ-NH1	5.42	123.01	120.30
44	1	1532	C	N1-C2-O2	5.42	122.15	118.90
44	1	2900	A	C4-C5-N7	5.42	113.41	110.70
44	1	3240	C	N1-C2-O2	5.42	122.15	118.90
46	6	53	A	C4-C5-N7	5.42	113.41	110.70
4	F	41	ARG	NE-CZ-NH1	5.41	123.01	120.30
44	1	2322	C	C6-N1-C2	-5.41	118.14	120.30
44	1	216	G	N7-C8-N9	5.41	115.81	113.10
20	X	42	ARG	NE-CZ-NH1	5.41	123.00	120.30
44	1	589	A	C4-C5-N7	5.41	113.41	110.70
44	1	1158	A	C5-C6-N1	5.41	120.41	117.70
44	1	3126	C	N3-C2-O2	-5.41	118.11	121.90
44	1	3136	G	N1-C2-N2	-5.41	111.33	116.20
44	1	841	A	N9-C4-C5	-5.41	103.64	105.80
1	B	117	ARG	NE-CZ-NH1	5.41	123.00	120.30
44	1	1143	A	C5-C6-N1	5.41	120.40	117.70
44	1	1161	G	C8-N9-C4	-5.41	104.24	106.40
44	1	268	A	C5-N7-C8	-5.40	101.20	103.90
44	1	501	A	C4-C5-N7	5.40	113.40	110.70
44	1	1395	G	C2-N3-C4	-5.40	109.20	111.90
44	1	2356	A	N7-C8-N9	5.40	116.50	113.80
44	1	2925	C	C6-N1-C1'	-5.40	114.32	120.80
44	1	3091	A	C5-N7-C8	-5.40	101.20	103.90
24	b	27	ARG	NE-CZ-NH2	5.40	123.00	120.30
44	1	1190	A	C6-C5-N7	-5.40	128.52	132.30
44	1	1473	G	C5-N7-C8	-5.40	101.60	104.30
45	2	4	C	N3-C2-O2	-5.40	118.12	121.90
45	2	9	A	C6-C5-N7	-5.40	128.52	132.30
44	1	3125	U	N3-C2-O2	-5.40	118.42	122.20
44	1	495	G	C4-N9-C1'	5.40	133.52	126.50
44	1	1379	G	N7-C8-N9	5.40	115.80	113.10
44	1	1412	G	N7-C8-N9	5.40	115.80	113.10
44	1	2368	A	C5-N7-C8	-5.40	101.20	103.90
44	1	2900	A	N9-C4-C5	-5.40	103.64	105.80
44	1	3273	A	C5-N7-C8	-5.40	101.20	103.90
44	1	3310	A	N7-C8-N9	5.40	116.50	113.80
44	1	152	U	C6-N1-C2	-5.40	117.76	121.00
44	1	344	A	N7-C8-N9	5.40	116.50	113.80
44	1	1328	C	N3-C4-C5	5.40	124.06	121.90
44	1	433	A	N9-C4-C5	-5.39	103.64	105.80
44	1	666	A	C4-C5-N7	5.39	113.40	110.70
44	1	677	A	C5-N7-C8	-5.39	101.20	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1417	G	C5-N7-C8	-5.39	101.60	104.30
44	1	2381	G	C5-N7-C8	-5.39	101.60	104.30
44	1	3019	U	C2-N1-C1'	5.39	124.17	117.70
44	1	3323	A	N7-C8-N9	5.39	116.50	113.80
45	2	41	A	C5-N7-C8	-5.39	101.20	103.90
44	1	214	G	C5-C6-O6	-5.39	125.36	128.60
44	1	3035	A	N9-C4-C5	-5.39	103.64	105.80
45	2	72	A	C4-C5-C6	-5.39	114.30	117.00
10	N	108	ARG	NE-CZ-NH1	5.39	123.00	120.30
44	1	8	C	N3-C4-N4	5.39	121.77	118.00
44	1	1370	G	C5-N7-C8	-5.39	101.61	104.30
44	1	1883	A	N7-C8-N9	5.39	116.49	113.80
44	1	3096	C	N1-C2-O2	5.39	122.13	118.90
44	1	346	C	C2-N3-C4	-5.39	117.21	119.90
44	1	573	C	N3-C2-O2	-5.39	118.13	121.90
1	B	244	ARG	NE-CZ-NH1	5.39	122.99	120.30
44	1	1306	G	C4-C5-N7	5.39	112.95	110.80
44	1	1428	A	O4'-C1'-N9	5.39	112.51	108.20
44	1	3159	C	N3-C2-O2	-5.39	118.13	121.90
44	1	3273	A	N9-C4-C5	-5.39	103.65	105.80
46	6	13	U	N3-C2-O2	-5.39	118.43	122.20
44	1	144	A	C4-C5-N7	5.38	113.39	110.70
44	1	1125	U	C5-C6-N1	5.38	125.39	122.70
44	1	1475	A	C4-C5-N7	5.38	113.39	110.70
44	1	1099	A	C4-C5-C6	-5.38	114.31	117.00
44	1	334	A	N9-C4-C5	-5.38	103.65	105.80
44	1	706	A	C5-C6-N1	5.38	120.39	117.70
44	1	1183	C	N3-C4-C5	5.38	124.05	121.90
44	1	2317	A	P-O3'-C3'	5.38	126.16	119.70
44	1	3033	A	N9-C4-C5	-5.38	103.65	105.80
44	1	499	G	N7-C8-N9	5.38	115.79	113.10
44	1	1054	A	C2-N3-C4	5.38	113.29	110.60
44	1	1466	G	N7-C8-N9	5.38	115.79	113.10
44	1	2352	A	C4-C5-N7	5.38	113.39	110.70
45	2	91	C	N3-C4-C5	5.38	124.05	121.90
44	1	598	A	N9-C4-C5	-5.38	103.65	105.80
44	1	1182	A	C5-N7-C8	-5.38	101.21	103.90
44	1	1316	C	N1-C2-O2	5.38	122.13	118.90
44	1	1632	A	N1-C6-N6	-5.38	115.37	118.60
44	1	3293	U	C6-N1-C2	-5.38	117.78	121.00
44	1	1798	A	C5-N7-C8	-5.37	101.21	103.90
44	1	2350	C	C5-C4-N4	-5.37	116.44	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	2946	A	C4-C5-N7	5.37	113.39	110.70
15	S	12	ARG	NE-CZ-NH2	-5.37	117.61	120.30
44	1	373	A	C4-C5-C6	-5.37	114.31	117.00
44	1	590	G	N3-C4-C5	5.37	131.28	128.60
44	1	1640	G	C5-N7-C8	-5.37	101.61	104.30
44	1	1803	C	N1-C2-O2	5.37	122.12	118.90
44	1	3059	G	C5-N7-C8	-5.37	101.61	104.30
44	1	3391	A	N9-C4-C5	-5.37	103.65	105.80
2	C	98	ARG	NE-CZ-NH1	5.37	122.98	120.30
44	1	331	G	C5-N7-C8	-5.37	101.61	104.30
44	1	1414	G	C5-N7-C8	-5.37	101.61	104.30
44	1	2828	G	N9-C4-C5	-5.37	103.25	105.40
44	1	403	C	N3-C2-O2	-5.37	118.14	121.90
44	1	1604	G	C4-N9-C1'	5.37	133.48	126.50
44	1	2878	G	N1-C6-O6	-5.37	116.68	119.90
44	1	3153	U	C6-N1-C1'	-5.37	113.69	121.20
44	1	3110	C	N3-C4-N4	5.37	121.76	118.00
44	1	3372	A	C5-N7-C8	-5.37	101.22	103.90
44	1	344	A	C6-N1-C2	-5.37	115.38	118.60
44	1	1336	U	C5-C4-O4	-5.37	122.68	125.90
44	1	1631	C	N1-C2-O2	5.37	122.12	118.90
44	1	1800	A	N7-C8-N9	5.37	116.48	113.80
44	1	1882	G	C5-N7-C8	-5.37	101.62	104.30
8	L	115	ARG	NE-CZ-NH1	5.36	122.98	120.30
44	1	421	G	C4-N9-C1'	5.36	133.47	126.50
44	1	736	A	C4-C5-N7	5.36	113.38	110.70
44	1	1585	C	C6-N1-C2	-5.36	118.16	120.30
45	2	14	C	N3-C4-C5	5.36	124.05	121.90
45	2	71	A	C8-N9-C4	5.36	107.94	105.80
45	2	107	G	C5-N7-C8	-5.36	101.62	104.30
44	1	372	A	C4-C5-N7	5.36	113.38	110.70
44	1	3371	G	N7-C8-N9	5.36	115.78	113.10
45	2	37	A	C4-C5-N7	5.36	113.38	110.70
31	i	41	ARG	NE-CZ-NH2	-5.36	117.62	120.30
44	1	63	A	C6-N1-C2	-5.36	115.39	118.60
44	1	1472	U	N3-C4-O4	5.36	123.15	119.40
44	1	1574	C	N3-C2-O2	-5.36	118.15	121.90
44	1	3017	A	C5-C6-N1	5.36	120.38	117.70
10	N	109	ARG	NE-CZ-NH1	5.35	122.98	120.30
44	1	690	A	C5-C6-N6	-5.35	119.42	123.70
44	1	2898	G	N3-C2-N2	5.35	123.65	119.90
44	1	3112	G	C5-N7-C8	-5.35	101.62	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	15	ARG	NE-CZ-NH1	5.35	122.97	120.30
44	1	1237	G	N3-C4-N9	-5.35	122.79	126.00
44	1	1550	C	N1-C2-O2	5.35	122.11	118.90
44	1	3077	A	C5-N7-C8	-5.35	101.22	103.90
45	2	68	G	C5-N7-C8	-5.35	101.63	104.30
44	1	515	C	C6-N1-C2	-5.35	118.16	120.30
44	1	656	A	C6-N1-C2	-5.35	115.39	118.60
44	1	680	G	N9-C4-C5	-5.35	103.26	105.40
45	2	50	C	N1-C2-O2	5.35	122.11	118.90
44	1	2345	A	C5-C6-N6	-5.34	119.42	123.70
44	1	402	A	N7-C8-N9	5.34	116.47	113.80
44	1	570	A	C4-C5-C6	-5.34	114.33	117.00
44	1	775	A	C5-N7-C8	-5.34	101.23	103.90
37	q	261	ARG	NE-CZ-NH1	5.34	122.97	120.30
44	1	887	G	N7-C8-N9	5.34	115.77	113.10
44	1	1475	A	C5-C6-N6	-5.34	119.43	123.70
44	1	2898	G	C4-C5-N7	5.34	112.94	110.80
44	1	332	C	N3-C2-O2	-5.34	118.16	121.90
44	1	1097	G	OP2-P-O3'	5.34	116.94	105.20
44	1	1171	G	C5-N7-C8	-5.34	101.63	104.30
44	1	2325	G	N3-C4-N9	-5.34	122.80	126.00
44	1	2394	G	N3-C2-N2	5.34	123.64	119.90
44	1	3035	A	C5-N7-C8	-5.34	101.23	103.90
2	C	195	ARG	NE-CZ-NH2	-5.34	117.63	120.30
44	1	1310	G	N3-C4-N9	-5.34	122.80	126.00
44	1	1373	A	C5-N7-C8	-5.33	101.23	103.90
44	1	3130	A	C8-N9-C1'	-5.33	118.10	127.70
35	n	18	ARG	NE-CZ-NH1	-5.33	117.63	120.30
44	1	34	A	N1-C6-N6	-5.33	115.40	118.60
44	1	799	G	N1-C2-N2	-5.33	111.40	116.20
44	1	2993	G	C4-N9-C1'	5.33	133.43	126.50
44	1	363	G	N3-C2-N2	5.33	123.63	119.90
44	1	1183	C	N3-C4-N4	5.33	121.73	118.00
44	1	2376	G	C6-C5-N7	-5.33	127.20	130.40
44	1	1269	U	N3-C2-O2	-5.33	118.47	122.20
44	1	1363	A	C6-N1-C2	-5.33	115.40	118.60
44	1	3127	A	C5-C6-N1	5.33	120.36	117.70
44	1	1874	A	N9-C4-C5	-5.33	103.67	105.80
44	1	227	G	C8-N9-C1'	-5.33	120.08	127.00
44	1	1452	A	O4'-C1'-N9	5.33	112.46	108.20
45	2	134	G	C4-N9-C1'	5.33	133.42	126.50
46	6	231	A	C2-N3-C4	5.32	113.26	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	15	C	N1-C2-O2	5.32	122.09	118.90
44	1	332	C	C6-N1-C2	-5.32	118.17	120.30
44	1	349	A	N7-C8-N9	5.32	116.46	113.80
44	1	1317	A	C5-C6-N1	5.32	120.36	117.70
44	1	3031	G	N3-C2-N2	5.32	123.62	119.90
44	1	1145	G	C5-N7-C8	-5.32	101.64	104.30
44	1	1310	G	N7-C8-N9	5.32	115.76	113.10
44	1	1447	G	C2-N3-C4	-5.32	109.24	111.90
44	1	1806	A	C5-C6-N1	5.32	120.36	117.70
44	1	527	A	C4-C5-N7	5.32	113.36	110.70
44	1	1233	G	N3-C2-N2	5.32	123.62	119.90
10	N	201	ARG	NE-CZ-NH1	5.32	122.96	120.30
44	1	346	C	N1-C2-O2	5.32	122.09	118.90
44	1	982	C	C6-N1-C2	-5.32	118.17	120.30
44	1	1277	C	O4'-C1'-N1	5.32	112.45	108.20
44	1	1418	A	C5-C6-N6	-5.32	119.45	123.70
44	1	1453	A	N3-C4-C5	5.32	130.52	126.80
44	1	2146	C	N1-C2-O2	5.32	122.09	118.90
44	1	1475	A	C5-N7-C8	-5.31	101.24	103.90
44	1	944	C	O4'-C1'-N1	5.31	112.45	108.20
44	1	1097	G	P-O3'-C3'	5.31	126.07	119.70
44	1	3391	A	C5-C6-N1	5.31	120.36	117.70
44	1	1274	A	C5-C6-N1	5.31	120.36	117.70
44	1	2844	C	N1-C2-O2	5.31	122.09	118.90
1	B	300	ARG	NE-CZ-NH2	-5.31	117.64	120.30
44	1	865	U	C6-N1-C2	-5.31	117.81	121.00
44	1	3026	G	N3-C4-C5	5.31	131.25	128.60
44	1	519	A	C5-C6-N1	5.31	120.35	117.70
44	1	646	A	N1-C6-N6	5.31	121.78	118.60
44	1	656	A	C6-C5-N7	-5.31	128.58	132.30
44	1	789	A	C6-N1-C2	-5.31	115.42	118.60
44	1	1883	A	C8-N9-C4	-5.31	103.68	105.80
44	1	268	A	C4-C5-N7	5.31	113.35	110.70
44	1	1598	G	C8-N9-C4	-5.30	104.28	106.40
45	2	131	A	C4-C5-N7	5.30	113.35	110.70
44	1	2367	A	C4-C5-C6	-5.30	114.35	117.00
45	2	5	U	C5-C6-N1	5.30	125.35	122.70
44	1	143	G	N3-C4-N9	-5.30	122.82	126.00
44	1	1106	G	C5-N7-C8	-5.30	101.65	104.30
44	1	1597	C	C6-N1-C2	-5.30	118.18	120.30
44	1	3049	A	C4-C5-N7	5.30	113.35	110.70
10	N	147	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	34	A	C5-C6-N1	5.30	120.35	117.70
44	1	103	G	C5-N7-C8	-5.30	101.65	104.30
44	1	1120	A	C4-C5-N7	5.30	113.35	110.70
45	2	41	A	C4-C5-C6	-5.30	114.35	117.00
44	1	720	A	C4-C5-N7	5.30	113.35	110.70
44	1	650	C	C6-N1-C2	-5.30	118.18	120.30
44	1	806	A	C4-C5-C6	-5.30	114.35	117.00
44	1	1150	A	N1-C6-N6	5.30	121.78	118.60
44	1	3382	U	C6-N1-C2	-5.30	117.82	121.00
45	2	62	C	N1-C2-O2	5.30	122.08	118.90
44	1	1139	G	C4-C5-N7	5.29	112.92	110.80
44	1	1064	A	P-O3'-C3'	5.29	126.05	119.70
45	2	157	U	C6-N1-C1'	-5.29	113.79	121.20
9	M	13	ARG	NE-CZ-NH1	5.29	122.94	120.30
44	1	1374	G	C5-C6-O6	-5.29	125.43	128.60
44	1	578	A	C5-C6-N1	5.29	120.34	117.70
44	1	650	C	C5-C4-N4	-5.29	116.50	120.20
44	1	1261	G	C4-N9-C1'	5.29	133.38	126.50
44	1	1285	G	N3-C2-N2	5.29	123.60	119.90
10	N	150	TRP	CA-CB-CG	5.29	123.75	113.70
44	1	660	A	C4-C5-N7	5.29	113.34	110.70
44	1	806	A	N1-C2-N3	-5.29	126.66	129.30
44	1	1282	G	C5-N7-C8	-5.29	101.66	104.30
44	1	3002	C	N3-C4-C5	5.29	124.01	121.90
44	1	187	A	C5-N7-C8	-5.28	101.26	103.90
44	1	1655	G	C5-N7-C8	-5.28	101.66	104.30
44	1	2902	A	N9-C4-C5	-5.28	103.69	105.80
44	1	3134	A	C5-C6-N1	5.28	120.34	117.70
45	2	28	C	N3-C4-C5	5.28	124.01	121.90
45	2	9	A	N3-C4-N9	5.28	131.62	127.40
45	2	17	A	C4-C5-C6	-5.28	114.36	117.00
21	Y	12	ARG	NE-CZ-NH1	5.28	122.94	120.30
44	1	936	A	C5-N7-C8	-5.28	101.26	103.90
44	1	1135	A	C5-N7-C8	-5.28	101.26	103.90
44	1	3031	G	C8-N9-C4	5.28	108.51	106.40
44	1	3138	U	N3-C2-O2	-5.28	118.50	122.20
44	1	3144	G	C5-N7-C8	-5.28	101.66	104.30
44	1	3366	G	C4-C5-N7	5.28	112.91	110.80
45	2	40	A	N7-C8-N9	5.28	116.44	113.80
44	1	1452	A	N1-C6-N6	-5.28	115.44	118.60
44	1	1863	G	N3-C2-N2	-5.28	116.21	119.90
45	2	73	U	P-O3'-C3'	5.28	126.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	136	G	C5-N7-C8	-5.28	101.66	104.30
44	1	1466	G	C4-C5-N7	5.27	112.91	110.80
41	u	33	ARG	NE-CZ-NH2	5.27	122.94	120.30
44	1	1194	G	C8-N9-C1'	-5.27	120.14	127.00
45	2	58	G	C5-C6-O6	-5.27	125.44	128.60
44	1	267	G	C5-C6-O6	5.27	131.76	128.60
44	1	3070	A	C5-C6-N6	-5.27	119.48	123.70
44	1	338	A	N1-C6-N6	-5.27	115.44	118.60
44	1	1523	U	C5-C6-N1	5.27	125.33	122.70
44	1	3024	A	N1-C6-N6	-5.27	115.44	118.60
44	1	3032	A	N9-C4-C5	-5.27	103.69	105.80
45	2	144	G	N3-C4-C5	5.27	131.24	128.60
44	1	288	C	C6-N1-C2	-5.27	118.19	120.30
44	1	661	G	C2-N3-C4	-5.27	109.27	111.90
44	1	703	G	C5-N7-C8	-5.27	101.67	104.30
44	1	1667	A	C4-C5-N7	5.27	113.33	110.70
44	1	1843	C	C4-C5-C6	5.27	120.03	117.40
44	1	1878	G	C2-N3-C4	5.27	114.53	111.90
35	n	96	ARG	NE-CZ-NH1	-5.27	117.67	120.30
44	1	598	A	C4-C5-N7	5.27	113.33	110.70
44	1	283	G	N3-C4-N9	5.26	129.16	126.00
44	1	937	G	C8-N9-C1'	-5.26	120.16	127.00
44	1	1605	A	C5-N7-C8	-5.26	101.27	103.90
44	1	3009	G	N7-C8-N9	5.26	115.73	113.10
44	1	3226	A	C4-C5-C6	-5.26	114.37	117.00
35	n	9	ARG	NE-CZ-NH1	5.26	122.93	120.30
44	1	1401	A	N9-C4-C5	-5.26	103.69	105.80
44	1	1493	G	C4-C5-N7	5.26	112.91	110.80
45	2	75	G	C4-C5-N7	5.26	112.91	110.80
44	1	99	A	N7-C8-N9	5.26	116.43	113.80
44	1	367	A	C4-C5-C6	-5.26	114.37	117.00
44	1	812	G	C8-N9-C4	-5.26	104.30	106.40
44	1	1140	G	C4-N9-C1'	5.26	133.34	126.50
44	1	1439	U	C5-C4-O4	-5.26	122.74	125.90
44	1	2368	A	C5-C6-N1	5.26	120.33	117.70
44	1	3016	A	C5-C6-N6	-5.26	119.49	123.70
45	2	89	A	C4-C5-N7	5.26	113.33	110.70
45	2	104	A	C5-C6-N6	-5.26	119.49	123.70
44	1	89	A	C5-C6-N6	-5.26	119.49	123.70
44	1	321	C	N3-C2-O2	-5.26	118.22	121.90
45	2	28	C	N3-C2-O2	-5.26	118.22	121.90
45	2	126	A	C4-C5-C6	-5.26	114.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	135	ARG	NE-CZ-NH2	-5.25	117.67	120.30
44	1	52	A	C4-C5-C6	-5.25	114.37	117.00
44	1	1321	G	C8-N9-C1'	-5.25	120.17	127.00
44	1	1369	A	C4-C5-C6	-5.25	114.37	117.00
44	1	701	G	C8-N9-C1'	-5.25	120.17	127.00
44	1	3183	A	N1-C6-N6	5.25	121.75	118.60
2	C	246	ARG	NE-CZ-NH1	5.25	122.93	120.30
44	1	786	A	C4-C5-N7	5.25	113.33	110.70
45	2	95	G	C5-N7-C8	-5.25	101.67	104.30
44	1	117	U	N3-C2-O2	-5.25	118.53	122.20
44	1	578	A	C4-C5-C6	-5.25	114.38	117.00
44	1	408	A	C4-C5-C6	-5.25	114.38	117.00
44	1	2828	G	N1-C6-O6	-5.25	116.75	119.90
13	Q	92	ARG	NE-CZ-NH1	-5.25	117.68	120.30
44	1	904	A	C4-C5-N7	5.25	113.32	110.70
44	1	1374	G	N3-C4-N9	5.25	129.15	126.00
44	1	3055	U	C5-C6-N1	5.25	125.32	122.70
44	1	1456	A	C4-C5-N7	5.25	113.32	110.70
2	C	138	ARG	NE-CZ-NH2	-5.24	117.68	120.30
44	1	325	A	N1-C6-N6	-5.24	115.45	118.60
44	1	342	A	N3-C4-C5	5.24	130.47	126.80
44	1	632	G	C8-N9-C1'	-5.24	120.18	127.00
44	1	2983	C	C2-N1-C1'	5.24	124.57	118.80
44	1	3031	G	N1-C2-N2	-5.24	111.48	116.20
24	b	396	ARG	NE-CZ-NH1	5.24	122.92	120.30
44	1	3009	G	C5-N7-C8	-5.24	101.68	104.30
44	1	282	G	N3-C4-N9	5.24	129.15	126.00
12	P	69	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	Y	20	PHE	CB-CG-CD1	-5.24	117.13	120.80
44	1	609	G	N1-C2-N2	-5.24	111.48	116.20
44	1	1893	A	C5-N7-C8	-5.24	101.28	103.90
44	1	3302	U	C5-C4-O4	-5.24	122.76	125.90
45	2	97	A	C5-C6-N1	5.24	120.32	117.70
44	1	775	A	C5-C6-N6	-5.24	119.51	123.70
45	2	44	A	N1-C6-N6	5.24	121.74	118.60
44	1	345	G	C8-N9-C1'	-5.24	120.19	127.00
44	1	802	C	C5-C4-N4	-5.24	116.54	120.20
44	1	1461	A	C5-C6-N1	5.24	120.32	117.70
44	1	1383	G	C6-C5-N7	-5.23	127.26	130.40
44	1	1799	A	C4-C5-C6	-5.23	114.38	117.00
29	g	60	ARG	NE-CZ-NH2	-5.23	117.68	120.30
32	j	72	ARG	NE-CZ-NH1	5.23	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	288	C	N1-C2-O2	5.23	122.04	118.90
44	1	875	G	C4-C5-N7	5.23	112.89	110.80
44	1	1124	U	C2-N1-C1'	5.23	123.98	117.70
44	1	14	U	N1-C2-O2	5.23	126.46	122.80
44	1	660	A	C4-C5-C6	-5.23	114.39	117.00
44	1	1140	G	C8-N9-C4	-5.23	104.31	106.40
44	1	1317	A	O4'-C1'-N9	5.23	112.38	108.20
44	1	2909	U	C5-C4-O4	-5.23	122.76	125.90
46	6	22	G	N3-C4-C5	5.23	131.21	128.60
44	1	27	C	N3-C2-O2	-5.22	118.24	121.90
44	1	369	A	N1-C2-N3	-5.22	126.69	129.30
44	1	3184	A	C5-N7-C8	-5.22	101.29	103.90
4	F	33	ARG	NE-CZ-NH1	5.22	122.91	120.30
44	1	128	G	N3-C4-N9	5.22	129.13	126.00
44	1	583	G	N7-C8-N9	5.22	115.71	113.10
44	1	1326	A	C4-C5-N7	5.22	113.31	110.70
44	1	57	A	N7-C8-N9	5.22	116.41	113.80
44	1	706	A	C4-C5-N7	5.22	113.31	110.70
44	1	3241	G	C4-C5-N7	5.22	112.89	110.80
44	1	3291	G	N3-C2-N2	5.22	123.55	119.90
35	n	109	ARG	NE-CZ-NH2	5.22	122.91	120.30
44	1	720	A	N9-C4-C5	-5.22	103.71	105.80
44	1	941	G	C5-N7-C8	-5.22	101.69	104.30
44	1	1171	G	C4-N9-C1'	5.22	133.28	126.50
44	1	1180	A	C5-C6-N1	5.22	120.31	117.70
44	1	1299	U	C6-N1-C2	-5.22	117.87	121.00
44	1	273	A	C5-N7-C8	-5.21	101.29	103.90
44	1	427	C	N3-C4-N4	5.21	121.65	118.00
44	1	1172	G	N3-C4-N9	-5.21	122.87	126.00
44	1	1337	A	C4-C5-C6	-5.21	114.39	117.00
44	1	1387	G	C4-N9-C1'	5.21	133.28	126.50
44	1	1402	C	N3-C4-C5	5.21	123.99	121.90
44	1	3219	G	N1-C2-N2	-5.21	111.51	116.20
44	1	1606	U	N3-C2-O2	-5.21	118.55	122.20
44	1	1833	G	C4-N9-C1'	5.21	133.28	126.50
45	2	155	A	C5-N7-C8	-5.21	101.29	103.90
44	1	33	G	N9-C4-C5	-5.21	103.31	105.40
44	1	332	C	N3-C4-C5	5.21	123.98	121.90
44	1	816	A	C8-N9-C4	-5.21	103.72	105.80
44	1	1327	C	C5-C6-N1	5.21	123.61	121.00
44	1	1000	C	N3-C2-O2	-5.21	118.25	121.90
44	1	1444	G	C8-N9-C1'	-5.21	120.23	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3148	U	C6-N1-C2	-5.21	117.87	121.00
44	1	200	C	C5-C4-N4	-5.21	116.55	120.20
44	1	522	A	C4-C5-N7	5.21	113.30	110.70
44	1	1323	G	N3-C4-C5	5.21	131.20	128.60
44	1	662	U	C6-N1-C2	-5.21	117.88	121.00
44	1	806	A	N9-C4-C5	-5.21	103.72	105.80
44	1	1287	A	C4-C5-C6	-5.21	114.40	117.00
44	1	3150	A	C4-C5-N7	5.21	113.30	110.70
34	l	41	ARG	NE-CZ-NH1	5.21	122.90	120.30
41	u	56	ARG	NE-CZ-NH2	5.21	122.90	120.30
44	1	76	G	C4-C5-N7	5.21	112.88	110.80
44	1	529	A	N9-C4-C5	-5.21	103.72	105.80
44	1	1382	G	C4-N9-C1'	5.21	133.27	126.50
35	n	130	ARG	NE-CZ-NH1	5.20	122.90	120.30
44	1	1896	A	C5-N7-C8	-5.20	101.30	103.90
44	1	2380	U	N3-C4-O4	5.20	123.04	119.40
44	1	3166	C	C5-C6-N1	5.20	123.60	121.00
8	L	55	ARG	NE-CZ-NH1	5.20	122.90	120.30
15	S	115	ARG	NE-CZ-NH1	5.20	122.90	120.30
44	1	3101	G	N3-C4-C5	5.20	131.20	128.60
44	1	20	A	C4-C5-N7	5.20	113.30	110.70
44	1	159	A	C4-C5-N7	5.20	113.30	110.70
44	1	1366	A	C5-C6-N1	5.20	120.30	117.70
44	1	1536	G	N3-C4-N9	-5.20	122.88	126.00
44	1	1567	U	P-O3'-C3'	5.20	125.94	119.70
44	1	2925	C	N3-C2-O2	-5.20	118.26	121.90
44	1	138	U	C5-C4-O4	-5.20	122.78	125.90
44	1	1493	G	N3-C4-N9	5.20	129.12	126.00
44	1	1493	G	N9-C4-C5	-5.20	103.32	105.40
44	1	1454	A	C4-C5-C6	-5.20	114.40	117.00
44	1	3141	A	C8-N9-C4	5.20	107.88	105.80
44	1	3213	A	C6-C5-N7	-5.20	128.66	132.30
5	G	204	ARG	NE-CZ-NH1	5.19	122.90	120.30
44	1	595	G	N3-C4-C5	5.19	131.20	128.60
44	1	64	G	C5-C6-O6	-5.19	125.48	128.60
44	1	788	C	N3-C4-N4	5.19	121.63	118.00
44	1	1133	A	C5-N7-C8	-5.19	101.30	103.90
44	1	1196	C	N3-C4-N4	5.19	121.63	118.00
44	1	1389	G	N1-C2-N2	-5.19	111.53	116.20
44	1	1319	G	N3-C4-C5	5.19	131.19	128.60
44	1	3059	G	C4-C5-N7	5.19	112.88	110.80
44	1	199	A	C4-C5-C6	-5.19	114.41	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1099	A	C4-C5-N7	5.19	113.30	110.70
45	2	43	A	C4-C5-C6	-5.19	114.41	117.00
28	f	43	PHE	CB-CG-CD2	-5.19	117.17	120.80
44	1	64	G	N9-C4-C5	-5.19	103.33	105.40
44	1	1525	G	N7-C8-N9	5.19	115.69	113.10
44	1	18	G	N7-C8-N9	5.19	115.69	113.10
44	1	416	A	N3-C4-C5	5.19	130.43	126.80
44	1	562	C	C5-C4-N4	-5.19	116.57	120.20
44	1	8	C	C5-C4-N4	-5.18	116.57	120.20
44	1	798	G	C5-N7-C8	-5.18	101.71	104.30
44	1	1348	U	N3-C2-O2	-5.18	118.57	122.20
44	1	1497	C	N1-C2-O2	5.18	122.01	118.90
44	1	3048	A	C5-N7-C8	-5.18	101.31	103.90
45	2	4	C	C5-C4-N4	-5.18	116.57	120.20
45	2	114	G	N3-C4-N9	-5.18	122.89	126.00
44	1	1602	A	C4-C5-C6	-5.18	114.41	117.00
44	1	151	A	N9-C4-C5	-5.18	103.73	105.80
44	1	1825	G	N3-C4-C5	5.18	131.19	128.60
44	1	151	A	C4-C5-N7	5.18	113.29	110.70
44	1	670	C	N3-C4-N4	5.18	121.62	118.00
44	1	851	C	C6-N1-C2	-5.18	118.23	120.30
44	1	3372	A	N9-C4-C5	-5.18	103.73	105.80
45	2	16	G	C2-N3-C4	-5.18	109.31	111.90
44	1	1298	C	N3-C2-O2	-5.18	118.28	121.90
44	1	2390	A	C4-C5-N7	5.18	113.29	110.70
28	f	60	ARG	NE-CZ-NH2	5.18	122.89	120.30
44	1	636	C	N3-C4-N4	5.18	121.62	118.00
44	1	935	U	N3-C2-O2	-5.18	118.58	122.20
44	1	3121	U	N3-C4-O4	5.18	123.02	119.40
44	1	3172	A	C4-C5-N7	5.18	113.29	110.70
1	B	118	PHE	CB-CG-CD2	-5.17	117.18	120.80
32	j	11	ARG	NE-CZ-NH1	5.17	122.89	120.30
44	1	127	G	C5-N7-C8	-5.17	101.71	104.30
44	1	1212	A	N9-C4-C5	-5.17	103.73	105.80
44	1	3182	G	C5-C6-O6	-5.17	125.50	128.60
44	1	720	A	P-O3'-C3'	5.17	125.91	119.70
44	1	1173	U	C5-C4-O4	-5.17	122.80	125.90
10	N	31	ARG	NE-CZ-NH2	-5.17	117.71	120.30
44	1	148	G	C4-N9-C1'	5.17	133.22	126.50
44	1	2936	A	C4-C5-C6	-5.17	114.42	117.00
44	1	655	C	C2-N1-C1'	5.17	124.49	118.80
44	1	1303	A	N7-C8-N9	5.17	116.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1561	G	N7-C8-N9	5.17	115.69	113.10
44	1	1470	U	N3-C4-O4	5.17	123.02	119.40
44	1	1373	A	C5-C6-N6	-5.17	119.57	123.70
44	1	2993	G	N1-C2-N2	-5.17	111.55	116.20
44	1	583	G	C5-N7-C8	-5.17	101.72	104.30
44	1	1545	A	C5-N7-C8	-5.17	101.32	103.90
2	C	98	ARG	NE-CZ-NH2	-5.16	117.72	120.30
44	1	290	G	N1-C2-N2	-5.16	111.55	116.20
44	1	3378	C	N3-C2-O2	-5.16	118.29	121.90
44	1	222	A	N7-C8-N9	5.16	116.38	113.80
44	1	815	G	C2-N3-C4	-5.16	109.32	111.90
44	1	2984	C	OP2-P-O3'	5.16	116.56	105.20
44	1	3304	U	N3-C2-O2	-5.16	118.59	122.20
44	1	3307	A	N7-C8-N9	5.16	116.38	113.80
44	1	64	G	N3-C2-N2	5.16	123.51	119.90
44	1	108	A	C4-C5-N7	5.16	113.28	110.70
44	1	360	G	N3-C2-N2	5.16	123.51	119.90
44	1	148	G	C8-N9-C1'	-5.16	120.29	127.00
44	1	3322	A	C4-C5-N7	5.16	113.28	110.70
44	1	1407	A	C5-C6-N6	-5.16	119.57	123.70
44	1	668	G	C8-N9-C4	-5.16	104.34	106.40
44	1	1838	G	C4-C5-N7	5.15	112.86	110.80
44	1	1832	C	N1-C2-O2	5.15	121.99	118.90
44	1	3147	G	C6-C5-N7	-5.15	127.31	130.40
45	2	42	G	N3-C2-N2	5.15	123.51	119.90
45	2	140	G	C2-N3-C4	-5.15	109.32	111.90
22	Z	48	ARG	NE-CZ-NH1	5.15	122.88	120.30
44	1	75	G	N1-C6-O6	5.15	122.99	119.90
44	1	422	A	C4-C5-N7	5.15	113.28	110.70
44	1	551	A	O4'-C1'-N9	5.15	112.32	108.20
44	1	1806	A	C5-N7-C8	-5.15	101.33	103.90
44	1	1893	A	N9-C4-C5	-5.15	103.74	105.80
44	1	3391	A	C5-N7-C8	-5.15	101.33	103.90
46	6	39	U	N3-C2-O2	-5.15	118.59	122.20
44	1	703	G	C4-C5-N7	5.15	112.86	110.80
44	1	1207	G	C8-N9-C4	-5.15	104.34	106.40
44	1	1407	A	C5-N7-C8	-5.15	101.33	103.90
44	1	3123	A	C5-N7-C8	-5.15	101.33	103.90
44	1	85	A	C5-N7-C8	-5.15	101.33	103.90
44	1	1343	A	C4-C5-C6	-5.15	114.43	117.00
44	1	1883	A	C5-N7-C8	-5.15	101.33	103.90
44	1	3005	A	C4-C5-C6	-5.15	114.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	57	ARG	NE-CZ-NH1	5.14	122.87	120.30
44	1	665	A	C6-N1-C2	-5.14	115.51	118.60
44	1	1834	U	C6-N1-C2	-5.14	117.91	121.00
44	1	2382	G	C4-C5-N7	5.14	112.86	110.80
44	1	51	A	N7-C8-N9	5.14	116.37	113.80
44	1	214	G	C5-N7-C8	-5.14	101.73	104.30
45	2	150	G	C8-N9-C4	5.14	108.46	106.40
44	1	1558	A	C5-C6-N6	-5.14	119.59	123.70
6	H	168	ARG	NE-CZ-NH2	5.14	122.87	120.30
44	1	1538	G	N9-C4-C5	-5.14	103.34	105.40
44	1	667	C	C5-C6-N1	5.14	123.57	121.00
44	1	1326	A	C5-N7-C8	-5.14	101.33	103.90
44	1	3006	A	C6-N1-C2	-5.14	115.52	118.60
44	1	3161	C	C5-C4-N4	-5.14	116.61	120.20
18	V	87	ARG	NE-CZ-NH1	5.13	122.87	120.30
28	f	67	MET	CG-SD-CE	-5.13	91.98	100.20
44	1	31	C	C5-C4-N4	-5.13	116.61	120.20
44	1	500	C	N3-C4-N4	5.13	121.59	118.00
44	1	1756	C	C5-C4-N4	-5.13	116.61	120.20
44	1	3204	C	N3-C2-O2	-5.13	118.31	121.90
44	1	705	A	C4-C5-N7	5.13	113.27	110.70
44	1	296	A	C4-C5-C6	-5.13	114.43	117.00
44	1	972	A	C8-N9-C4	-5.13	103.75	105.80
44	1	3004	C	N3-C4-C5	5.13	123.95	121.90
44	1	438	A	C8-N9-C4	-5.13	103.75	105.80
44	1	953	G	N3-C2-N2	-5.13	116.31	119.90
44	1	21	G	N1-C6-O6	-5.13	116.82	119.90
44	1	691	A	C5-N7-C8	-5.13	101.34	103.90
44	1	3293	U	N3-C2-O2	-5.13	118.61	122.20
44	1	412	G	N7-C8-N9	5.13	115.66	113.10
44	1	3150	A	C5-C6-N6	-5.13	119.60	123.70
44	1	3212	C	N3-C4-C5	5.13	123.95	121.90
45	2	58	G	N7-C8-N9	5.13	115.66	113.10
44	1	1112	A	C4-C5-C6	-5.12	114.44	117.00
44	1	1145	G	N7-C8-N9	5.12	115.66	113.10
44	1	1478	C	C5-C4-N4	-5.12	116.61	120.20
44	1	1792	C	N3-C2-O2	-5.12	118.31	121.90
44	1	522	A	N9-C4-C5	-5.12	103.75	105.80
44	1	1587	A	C4-C5-C6	-5.12	114.44	117.00
44	1	3087	A	C5-C6-N1	5.12	120.26	117.70
44	1	352	A	C5-N7-C8	-5.12	101.34	103.90
44	1	1403	C	N3-C4-C5	5.12	123.95	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	110	ARG	NE-CZ-NH2	5.12	122.86	120.30
35	n	121	ARG	NE-CZ-NH1	5.12	122.86	120.30
44	1	500	C	N3-C2-O2	-5.12	118.32	121.90
44	1	1366	A	N9-C4-C5	-5.12	103.75	105.80
44	1	1382	G	C6-C5-N7	-5.12	127.33	130.40
28	f	65	ARG	NE-CZ-NH1	5.12	122.86	120.30
44	1	1397	C	N3-C4-C5	5.12	123.95	121.90
44	1	519	A	N1-C6-N6	5.12	121.67	118.60
6	H	31	ARG	NE-CZ-NH1	5.11	122.86	120.30
44	1	75	G	C5-C6-O6	-5.11	125.53	128.60
44	1	253	A	N9-C4-C5	-5.11	103.75	105.80
44	1	399	A	C4-C5-C6	-5.11	114.44	117.00
44	1	1196	C	C5-C6-N1	5.11	123.56	121.00
44	1	1279	C	C5-C6-N1	5.11	123.56	121.00
44	1	1292	C	N3-C4-C5	5.11	123.95	121.90
44	1	1489	A	C5-C6-N1	5.11	120.26	117.70
44	1	3006	A	N3-C4-N9	5.11	131.49	127.40
44	1	3212	C	C5-C4-N4	-5.11	116.62	120.20
44	1	6	A	N1-C2-N3	-5.11	126.74	129.30
44	1	656	A	N9-C4-C5	-5.11	103.75	105.80
44	1	1154	A	C4-C5-C6	-5.11	114.44	117.00
44	1	1756	C	C6-N1-C2	-5.11	118.25	120.30
44	1	3369	G	C2-N3-C4	5.11	114.46	111.90
45	2	118	C	N3-C4-N4	5.11	121.58	118.00
44	1	361	A	C4-C5-C6	-5.11	114.44	117.00
44	1	810	A	C4-C5-N7	5.11	113.25	110.70
45	2	156	U	C5-C6-N1	5.11	125.26	122.70
44	1	3177	G	N9-C4-C5	-5.11	103.36	105.40
44	1	24	G	N7-C8-N9	5.11	115.65	113.10
44	1	651	G	C8-N9-C1'	-5.11	120.36	127.00
44	1	1396	C	C6-N1-C2	-5.11	118.26	120.30
44	1	3075	G	C8-N9-C4	-5.11	104.36	106.40
44	1	3172	A	C8-N9-C4	5.11	107.84	105.80
44	1	314	U	C6-N1-C2	-5.11	117.94	121.00
44	1	423	A	C4-C5-N7	5.11	113.25	110.70
44	1	430	U	N3-C4-C5	-5.11	111.54	114.60
44	1	504	A	C4-C5-C6	-5.11	114.45	117.00
44	1	675	C	N3-C4-C5	5.11	123.94	121.90
44	1	1223	A	N1-C6-N6	5.11	121.66	118.60
44	1	1893	A	C5-C6-N1	5.11	120.25	117.70
44	1	215	G	N3-C4-C5	5.10	131.15	128.60
44	1	1171	G	C8-N9-C1'	-5.10	120.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	3300	U	C6-N1-C2	-5.10	117.94	121.00
44	1	3307	A	C5-C6-N6	-5.10	119.62	123.70
45	2	131	A	C5-C6-N1	5.10	120.25	117.70
44	1	339	C	N3-C2-O2	-5.10	118.33	121.90
44	1	2844	C	N3-C2-O2	-5.10	118.33	121.90
44	1	3243	A	O4'-C1'-N9	-5.10	104.12	108.20
44	1	3291	G	N1-C2-N2	-5.10	111.61	116.20
44	1	1397	C	N1-C2-O2	5.10	121.96	118.90
44	1	1532	C	N3-C4-N4	5.10	121.57	118.00
44	1	1704	A	C5-C6-N6	-5.10	119.62	123.70
44	1	3051	U	N3-C4-O4	5.10	122.97	119.40
45	2	26	U	C2-N1-C1'	5.10	123.82	117.70
6	H	166	ARG	NE-CZ-NH2	5.10	122.85	120.30
44	1	86	G	C8-N9-C1'	5.10	133.63	127.00
44	1	886	C	C6-N1-C2	-5.10	118.26	120.30
44	1	1394	A	N7-C8-N9	5.10	116.35	113.80
44	1	1582	C	N3-C4-N4	-5.10	114.43	118.00
44	1	683	U	O5'-P-OP2	-5.10	101.11	105.70
44	1	3196	U	C6-N1-C1'	-5.10	114.06	121.20
44	1	518	G	C8-N9-C1'	-5.09	120.38	127.00
44	1	648	C	N3-C2-O2	-5.09	118.33	121.90
44	1	1147	G	C4-N9-C1'	5.09	133.12	126.50
44	1	3241	G	C5-N7-C8	-5.09	101.75	104.30
14	R	98	ARG	NE-CZ-NH1	5.09	122.85	120.30
15	S	167	ARG	NE-CZ-NH1	5.09	122.85	120.30
44	1	235	A	C5-C6-N1	5.09	120.25	117.70
44	1	949	C	N3-C4-C5	5.09	123.94	121.90
44	1	1170	A	P-O3'-C3'	5.09	125.81	119.70
44	1	3276	G	N1-C2-N2	-5.09	111.62	116.20
44	1	1513	G	N7-C8-N9	5.09	115.64	113.10
44	1	3164	C	C5-C4-N4	5.09	123.76	120.20
44	1	3298	C	N3-C2-O2	-5.09	118.34	121.90
10	N	162	ARG	NE-CZ-NH1	5.09	122.84	120.30
44	1	350	C	O4'-C1'-N1	-5.09	104.13	108.20
44	1	385	A	C5-N7-C8	-5.09	101.36	103.90
44	1	644	G	C4-N9-C1'	5.09	133.11	126.50
44	1	875	G	N3-C2-N2	5.09	123.46	119.90
44	1	1274	A	N1-C6-N6	-5.09	115.55	118.60
44	1	1469	C	N3-C4-N4	-5.09	114.44	118.00
44	1	1680	G	N1-C6-O6	-5.09	116.85	119.90
44	1	1326	A	C6-N1-C2	-5.08	115.55	118.60
44	1	340	C	C6-N1-C1'	-5.08	114.70	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	678	G	C5-N7-C8	-5.08	101.76	104.30
44	1	3240	C	N3-C2-O2	-5.08	118.34	121.90
44	1	352	A	C4-C5-N7	5.08	113.24	110.70
44	1	396	A	O4'-C1'-N9	-5.08	104.14	108.20
44	1	3134	A	N9-C4-C5	-5.08	103.77	105.80
4	F	157	ASN	C-N-CA	5.08	134.40	121.70
44	1	212	G	O4'-C1'-N9	5.08	112.26	108.20
44	1	970	A	N1-C6-N6	-5.08	115.55	118.60
44	1	972	A	N7-C8-N9	5.08	116.34	113.80
44	1	3259	U	C6-N1-C2	-5.08	117.95	121.00
45	2	37	A	O5'-P-OP2	-5.08	101.13	105.70
44	1	115	A	P-O3'-C3'	5.08	125.79	119.70
44	1	1155	C	C5-C4-N4	-5.08	116.65	120.20
44	1	3049	A	C5-C6-N6	-5.08	119.64	123.70
44	1	3128	G	C5-N7-C8	-5.08	101.76	104.30
10	N	203	ARG	NE-CZ-NH1	5.08	122.84	120.30
44	1	1451	C	OP1-P-O3'	5.08	116.37	105.20
2	C	3	ARG	NE-CZ-NH1	-5.07	117.76	120.30
44	1	42	C	N3-C4-C5	5.07	123.93	121.90
44	1	521	A	C5-N7-C8	-5.07	101.36	103.90
44	1	2914	G	N3-C2-N2	5.07	123.45	119.90
44	1	3218	A	C5-C6-N6	-5.07	119.64	123.70
44	1	3330	A	C5-C6-N6	-5.07	119.64	123.70
44	1	3391	A	C5-C6-N6	-5.07	119.64	123.70
45	2	94	C	C6-N1-C2	-5.07	118.27	120.30
44	1	3167	A	C4-C5-N7	5.07	113.24	110.70
28	f	43	PHE	CB-CG-CD1	5.07	124.35	120.80
44	1	1206	G	C4-C5-N7	5.07	112.83	110.80
44	1	1542	G	C5-N7-C8	-5.07	101.77	104.30
44	1	1799	A	N9-C4-C5	-5.07	103.77	105.80
28	f	90	PRO	CA-N-CD	-5.07	104.40	111.50
44	1	3127	A	N1-C6-N6	5.07	121.64	118.60
45	2	134	G	C6-C5-N7	-5.07	127.36	130.40
44	1	334	A	N7-C8-N9	5.07	116.33	113.80
44	1	1226	G	C8-N9-C1'	-5.07	120.41	127.00
44	1	1406	A	C4-C5-N7	5.07	113.23	110.70
10	N	12	ARG	NE-CZ-NH1	5.07	122.83	120.30
44	1	1306	G	N3-C2-N2	5.07	123.45	119.90
44	1	1487	G	N3-C4-N9	-5.07	122.96	126.00
44	1	1647	A	C5-N7-C8	-5.07	101.37	103.90
45	2	140	G	N3-C2-N2	5.07	123.45	119.90
5	G	185	ARG	NE-CZ-NH1	5.06	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1608	C	N3-C4-N4	5.06	121.55	118.00
44	1	754	G	N3-C2-N2	5.06	123.44	119.90
44	1	2367	A	N7-C8-N9	5.06	116.33	113.80
46	6	17	G	C5-C6-O6	5.06	131.64	128.60
46	6	53	A	N1-C6-N6	5.06	121.64	118.60
44	1	10	C	C2-N1-C1'	5.06	124.36	118.80
44	1	330	G	N7-C8-N9	5.06	115.63	113.10
44	1	1152	G	N9-C4-C5	-5.06	103.38	105.40
44	1	1594	A	N3-C4-N9	5.06	131.45	127.40
44	1	1148	G	N3-C4-C5	5.06	131.13	128.60
44	1	1598	G	N1-C6-O6	5.06	122.94	119.90
44	1	2342	U	N3-C4-O4	5.06	122.94	119.40
45	2	136	G	N7-C8-N9	5.06	115.63	113.10
44	1	3273	A	C4-C5-N7	5.06	113.23	110.70
40	t	148	ARG	NE-CZ-NH2	5.05	122.83	120.30
44	1	422	A	C5-N7-C8	-5.05	101.37	103.90
44	1	1285	G	N7-C8-N9	5.05	115.63	113.10
44	1	1822	C	C5-C4-N4	-5.05	116.66	120.20
44	1	3126	C	C2-N1-C1'	5.05	124.36	118.80
44	1	3366	G	C5-N7-C8	-5.05	101.77	104.30
45	2	85	G	N3-C2-N2	-5.05	116.36	119.90
39	s	6	ARG	NE-CZ-NH1	-5.05	117.77	120.30
44	1	1354	G	C8-N9-C4	-5.05	104.38	106.40
3	E	31	ARG	NE-CZ-NH2	-5.05	117.77	120.30
44	1	313	A	C5-C6-N1	5.05	120.23	117.70
44	1	338	A	C5-N7-C8	-5.05	101.37	103.90
44	1	900	G	C8-N9-C4	-5.05	104.38	106.40
44	1	1365	G	C4-N9-C1'	5.05	133.07	126.50
44	1	1936	A	N7-C8-N9	5.05	116.33	113.80
44	1	267	G	C4-C5-C6	-5.05	115.77	118.80
44	1	1396	C	N3-C4-N4	5.05	121.53	118.00
44	1	1812	G	N1-C2-N2	-5.05	111.66	116.20
44	1	3308	C	C2-N3-C4	-5.05	117.38	119.90
44	1	1190	A	C4-N9-C1'	5.05	135.39	126.30
44	1	1901	A	C4-N9-C1'	5.05	135.39	126.30
45	2	21	C	C2-N3-C4	5.05	122.42	119.90
44	1	1114	U	N1-C2-O2	5.05	126.33	122.80
44	1	1704	A	N1-C6-N6	5.04	121.63	118.60
10	N	162	ARG	NE-CZ-NH2	-5.04	117.78	120.30
44	1	253	A	C4-C5-N7	5.04	113.22	110.70
44	1	909	G	C6-C5-N7	5.04	133.43	130.40
44	1	926	A	C6-N1-C2	-5.04	115.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1365	G	N3-C4-N9	5.04	129.03	126.00
44	1	1447	G	N3-C4-C5	5.04	131.12	128.60
45	2	96	A	C5-C6-N6	-5.04	119.67	123.70
45	2	134	G	N7-C8-N9	5.04	115.62	113.10
44	1	890	C	C6-N1-C2	-5.04	118.28	120.30
44	1	1330	A	O5'-P-OP1	-5.04	101.16	105.70
44	1	1568	U	P-O3'-C3'	5.04	125.75	119.70
44	1	1604	G	C8-N9-C1'	-5.04	120.44	127.00
44	1	2903	A	C4-C5-N7	5.04	113.22	110.70
45	2	32	C	N1-C2-O2	5.04	121.92	118.90
44	1	112	U	C3'-C2'-C1'	5.04	105.53	101.50
44	1	1464	G	C2-N3-C4	-5.04	109.38	111.90
10	N	197	LEU	CA-CB-CG	5.04	126.89	115.30
44	1	384	A	C8-N9-C4	5.04	107.81	105.80
44	1	836	A	C4-C5-N7	5.04	113.22	110.70
44	1	1608	C	N1-C2-O2	5.04	121.92	118.90
44	1	2337	C	N1-C2-O2	5.04	121.92	118.90
44	1	265	A	C5-C6-N1	5.04	120.22	117.70
45	2	63	G	N3-C4-N9	-5.04	122.98	126.00
45	2	76	C	C6-N1-C2	-5.04	118.28	120.30
44	1	348	A	C4-C5-N7	5.04	113.22	110.70
44	1	35	A	C5-N7-C8	-5.03	101.38	103.90
44	1	1812	G	N3-C2-N2	5.03	123.42	119.90
44	1	3101	G	N7-C8-N9	5.03	115.62	113.10
44	1	3147	G	C8-N9-C1'	-5.03	120.46	127.00
44	1	65	A	C5-N7-C8	-5.03	101.38	103.90
44	1	86	G	C4-C5-C6	-5.03	115.78	118.80
44	1	135	C	C5-C4-N4	5.03	123.72	120.20
44	1	1389	G	N3-C2-N2	5.03	123.42	119.90
44	1	1619	A	N1-C2-N3	-5.03	126.78	129.30
44	1	3166	C	N1-C2-O2	5.03	121.92	118.90
44	1	340	C	C6-N1-C2	-5.03	118.29	120.30
44	1	396	A	C4-C5-C6	-5.03	114.48	117.00
44	1	968	G	N7-C8-N9	5.03	115.61	113.10
44	1	1468	A	C4-C5-N7	5.03	113.22	110.70
46	6	53	A	C5-C6-N6	-5.03	119.68	123.70
44	1	801	A	C5-N7-C8	-5.03	101.39	103.90
44	1	376	G	C5-N7-C8	-5.03	101.79	104.30
44	1	608	A	C5-N7-C8	-5.03	101.39	103.90
45	2	31	G	N3-C4-C5	5.03	131.11	128.60
45	2	36	G	C8-N9-C4	-5.03	104.39	106.40
44	1	678	G	C6-C5-N7	-5.03	127.38	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1190	A	N1-C6-N6	5.03	121.61	118.60
44	1	2906	C	N1-C2-O2	5.02	121.91	118.90
44	1	59	G	N1-C2-N2	-5.02	111.68	116.20
44	1	651	G	N9-C4-C5	-5.02	103.39	105.40
44	1	1829	G	C4-C5-N7	5.02	112.81	110.80
44	1	3091	A	C6-N1-C2	-5.02	115.59	118.60
44	1	3395	G	N3-C4-N9	5.02	129.01	126.00
44	1	24	G	C5-N7-C8	-5.02	101.79	104.30
44	1	18	G	C6-C5-N7	-5.02	127.39	130.40
44	1	505	G	C6-C5-N7	-5.02	127.39	130.40
44	1	1397	C	C2-N1-C1'	5.02	124.32	118.80
44	1	1856	C	C5-C4-N4	-5.02	116.69	120.20
44	1	2377	G	N3-C2-N2	-5.02	116.39	119.90
44	1	2876	C	N3-C2-O2	-5.02	118.39	121.90
44	1	1124	U	N1-C2-O2	5.02	126.31	122.80
44	1	2887	A	C4-C5-N7	5.02	113.21	110.70
44	1	3044	G	C5-N7-C8	-5.02	101.79	104.30
45	2	97	A	C4-C5-C6	-5.02	114.49	117.00
44	1	950	G	C2-N3-C4	-5.02	109.39	111.90
45	2	71	A	C4-C5-C6	-5.02	114.49	117.00
44	1	3136	G	N3-C2-N2	5.01	123.41	119.90
44	1	926	A	C5-N7-C8	-5.01	101.39	103.90
44	1	953	G	C5-N7-C8	-5.01	101.79	104.30
44	1	103	G	C8-N9-C4	-5.01	104.40	106.40
44	1	2821	C	N1-C2-O2	5.01	121.91	118.90
44	1	3243	A	C5-N7-C8	-5.01	101.39	103.90
45	2	149	A	C5-N7-C8	-5.01	101.39	103.90
46	6	23	U	N3-C2-O2	-5.01	118.69	122.20
31	i	68	ARG	NE-CZ-NH1	5.01	122.81	120.30
44	1	85	A	C5-C6-N1	5.01	120.20	117.70
44	1	803	C	C2-N1-C1'	5.01	124.31	118.80
44	1	1226	G	N7-C8-N9	5.01	115.60	113.10
44	1	3320	A	N9-C4-C5	-5.01	103.80	105.80
45	2	36	G	C4-N9-C1'	5.01	133.01	126.50
44	1	140	C	C5-C4-N4	-5.01	116.69	120.20
44	1	573	C	N3-C4-N4	5.01	121.50	118.00
44	1	1550	C	N3-C2-O2	-5.00	118.40	121.90
37	q	252	ARG	NE-CZ-NH2	5.00	122.80	120.30
44	1	1806	A	N1-C6-N6	5.00	121.60	118.60
44	1	2367	A	C6-N1-C2	-5.00	115.60	118.60
44	1	3122	A	N1-C6-N6	-5.00	115.60	118.60
44	1	3140	G	C4-C5-N7	5.00	112.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	111	C	O4'-C1'-N1	5.00	112.20	108.20
44	1	841	A	N7-C8-N9	5.00	116.30	113.80
44	1	926	A	C8-N9-C1'	-5.00	118.70	127.70
44	1	1285	G	N1-C2-N2	-5.00	111.70	116.20
44	1	1510	G	C5-C6-O6	5.00	131.60	128.60
44	1	2917	G	C4-C5-N7	5.00	112.80	110.80

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	PRO	Peptide
1	B	221	THR	Peptide
1	B	241	LYS	Peptide
1	B	340	LYS	Peptide
1	B	35	ASP	Peptide
1	B	353	GLU	Peptide
1	B	37	ARG	Peptide
2	C	182	LEU	Peptide
2	C	269	SER	Peptide
2	C	3	ARG	Peptide
2	C	318	LEU	Peptide
2	C	338	LYS	Peptide
2	C	4	PRO	Peptide
4	F	158	LYS	Peptide
4	F	215	GLY	Peptide
5	G	120	LYS	Peptide
5	G	226	TYR	Peptide
5	G	76	ALA	Peptide
5	G	79	GLN	Peptide
5	G	83	ASP	Peptide
6	H	20	ILE	Peptide
6	H	21	LYS	Peptide
6	H	49	ASN	Peptide
7	K	164	TYR	Peptide
8	L	12	ASN	Peptide
8	L	130	GLY	Peptide
8	L	166	ALA	Mainchain
8	L	27	ASP	Peptide
8	L	46	ILE	Peptide
9	M	12	TRP	Peptide
10	N	93	LYS	Peptide

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Mol	Chain	Res	Type	Group
12	P	144	SER	Peptide
14	R	54	ALA	Peptide
15	S	13	ARG	Peptide
15	S	22	PRO	Peptide
18	V	89	ASP	Peptide
19	W	127	PRO	Peptide
19	W	177	ALA	Peptide
20	X	65	GLN	Peptide
23	a	77	LYS	Peptide
23	a	97	GLU	Peptide
24	b	227	ARG	Peptide
24	b	368	ALA	Peptide
24	b	399	ALA	Peptide
26	d	87	ASN	Peptide
27	e	121	ASN	Peptide
28	f	66	VAL	Peptide
28	f	89	LEU	Peptide
29	g	6	THR	Peptide
29	g	82	ALA	Mainchain
30	h	119	LYS	Peptide
30	h	83	LYS	Peptide
30	h	91	ALA	Peptide
31	i	49	GLY	Peptide
31	i	78	GLY	Peptide
33	k	32	ASN	Peptide
33	k	33	LYS	Peptide
35	n	1	MET	Peptide
35	n	123	PRO	Peptide
35	n	240	SER	Peptide
35	n	3	ILE	Peptide
35	n	374	ASP	Peptide
35	n	375	ILE	Peptide
35	n	455	PRO	Peptide
35	n	53	ASN	Peptide
35	n	54	LYS	Peptide
35	n	55	GLY	Peptide
35	n	73	HIS	Peptide
36	o	139	PHE	Peptide
36	o	140	VAL	Peptide
36	o	158	MET	Peptide
36	o	171	ALA	Peptide
36	o	176	LEU	Peptide

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Mol	Chain	Res	Type	Group
37	q	225	LYS	Peptide
38	r	45	TRP	Mainchain
39	s	2	ARG	Peptide
40	t	150	PRO	Peptide
40	t	170	GLU	Peptide
40	t	220	ASN	Peptide
40	t	260	SER	Peptide
40	t	280	PHE	Peptide
41	u	61	LYS	Peptide
41	u	79	VAL	Peptide
47	w	126	LEU	Peptide
47	w	56	ALA	Peptide
42	y	7	PHE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	B	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
2	C	359/362 (99%)	338 (94%)	20 (6%)	1 (0%)	37	70
3	E	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
4	F	220/244 (90%)	206 (94%)	14 (6%)	0	100	100
5	G	190/256 (74%)	183 (96%)	7 (4%)	0	100	100
6	H	189/191 (99%)	182 (96%)	6 (3%)	1 (0%)	25	60
7	K	252/376 (67%)	242 (96%)	10 (4%)	0	100	100
8	L	185/199 (93%)	176 (95%)	8 (4%)	1 (0%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	M	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
10	N	176/204 (86%)	167 (95%)	9 (5%)	0	100	100
11	O	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
12	P	172/184 (94%)	167 (97%)	5 (3%)	0	100	100
13	Q	132/186 (71%)	132 (100%)	0	0	100	100
14	R	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
15	S	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
16	T	54/160 (34%)	53 (98%)	1 (2%)	0	100	100
17	U	104/121 (86%)	103 (99%)	1 (1%)	0	100	100
18	V	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
19	W	232/236 (98%)	229 (99%)	3 (1%)	0	100	100
20	X	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
21	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
22	Z	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
23	a	91/149 (61%)	87 (96%)	4 (4%)	0	100	100
24	b	468/647 (72%)	451 (96%)	17 (4%)	0	100	100
25	c	95/105 (90%)	95 (100%)	0	0	100	100
26	d	105/113 (93%)	103 (98%)	2 (2%)	0	100	100
27	e	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
28	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
29	g	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
30	h	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
31	i	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
32	j	85/88 (97%)	82 (96%)	3 (4%)	0	100	100
33	k	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
34	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
35	n	365/605 (60%)	339 (93%)	26 (7%)	0	100	100
36	o	131/220 (60%)	123 (94%)	8 (6%)	0	100	100
37	q	83/455 (18%)	80 (96%)	3 (4%)	0	100	100
38	r	211/261 (81%)	200 (95%)	11 (5%)	0	100	100
39	s	34/520 (6%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	t	283/322 (88%)	267 (94%)	16 (6%)	0	100	100
41	u	121/199 (61%)	115 (95%)	6 (5%)	0	100	100
42	y	242/245 (99%)	240 (99%)	2 (1%)	0	100	100
43	z	53/106 (50%)	52 (98%)	1 (2%)	0	100	100
47	w	350/841 (42%)	347 (99%)	3 (1%)	0	100	100
All	All	7377/10105 (73%)	7124 (97%)	250 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	339	LEU
8	L	63	VAL
6	H	50	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	322/323 (100%)	316 (98%)	6 (2%)	52	70
2	C	288/289 (100%)	286 (99%)	2 (1%)	81	86
3	E	134/153 (88%)	133 (99%)	1 (1%)	81	86
4	F	186/205 (91%)	186 (100%)	0	100	100
5	G	159/208 (76%)	156 (98%)	3 (2%)	52	70
6	H	171/171 (100%)	171 (100%)	0	100	100
7	K	236/346 (68%)	235 (100%)	1 (0%)	89	91
8	L	149/159 (94%)	148 (99%)	1 (1%)	81	86
9	M	108/109 (99%)	107 (99%)	1 (1%)	75	83
10	N	156/176 (89%)	151 (97%)	5 (3%)	34	56
11	O	160/162 (99%)	159 (99%)	1 (1%)	84	88
12	P	142/146 (97%)	141 (99%)	1 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Q	110/151 (73%)	110 (100%)	0	100	100
14	R	129/154 (84%)	128 (99%)	1 (1%)	79	84
15	S	155/156 (99%)	155 (100%)	0	100	100
16	T	45/137 (33%)	45 (100%)	0	100	100
17	U	93/107 (87%)	93 (100%)	0	100	100
18	V	104/105 (99%)	103 (99%)	1 (1%)	73	81
19	W	211/213 (99%)	211 (100%)	0	100	100
20	X	117/118 (99%)	117 (100%)	0	100	100
21	Y	109/110 (99%)	108 (99%)	1 (1%)	75	83
22	Z	115/116 (99%)	114 (99%)	1 (1%)	75	83
23	a	76/119 (64%)	75 (99%)	1 (1%)	65	76
24	b	424/573 (74%)	423 (100%)	1 (0%)	92	94
25	c	81/88 (92%)	81 (100%)	0	100	100
26	d	94/97 (97%)	92 (98%)	2 (2%)	48	67
27	e	109/111 (98%)	107 (98%)	2 (2%)	54	71
28	f	90/91 (99%)	89 (99%)	1 (1%)	70	79
29	g	95/103 (92%)	94 (99%)	1 (1%)	70	79
30	h	104/105 (99%)	104 (100%)	0	100	100
31	i	81/82 (99%)	81 (100%)	0	100	100
32	j	70/71 (99%)	69 (99%)	1 (1%)	62	75
33	k	68/69 (99%)	68 (100%)	0	100	100
34	l	45/46 (98%)	44 (98%)	1 (2%)	47	65
35	n	334/548 (61%)	333 (100%)	1 (0%)	91	92
36	o	118/199 (59%)	116 (98%)	2 (2%)	56	72
37	q	80/420 (19%)	80 (100%)	0	100	100
38	r	191/229 (83%)	191 (100%)	0	100	100
39	s	32/445 (7%)	32 (100%)	0	100	100
40	t	256/287 (89%)	253 (99%)	3 (1%)	67	78
41	u	108/180 (60%)	107 (99%)	1 (1%)	75	83
42	y	210/211 (100%)	210 (100%)	0	100	100
43	z	48/95 (50%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	w	319/745 (43%)	311 (98%)	8 (2%)	42 62
All	All	6432/8728 (74%)	6381 (99%)	51 (1%)	77 84

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	PHE
1	B	63	PRO
1	B	236	LYS
1	B	255	TRP
1	B	332	ARG
1	B	385	LYS
2	C	145	ILE
2	C	283	THR
3	E	79	VAL
5	G	120	LYS
5	G	158	ASP
5	G	180	VAL
7	K	39	LYS
8	L	104	ARG
9	M	102	LYS
10	N	43	THR
10	N	49	ARG
10	N	132	VAL
10	N	164	LEU
10	N	183	THR
11	O	143	THR
12	P	120	ASN
14	R	71	ARG
18	V	23	MET
21	Y	125	LYS
22	Z	14	VAL
23	a	130	VAL
24	b	367	GLN
26	d	16	LEU
26	d	23	VAL
27	e	14	THR
27	e	63	THR
28	f	72	THR
29	g	99	LYS
32	j	75	LYS
34	l	41	ARG

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Mol	Chain	Res	Type
35	n	17	THR
36	o	213	LYS
36	o	219	LYS
40	t	22	LYS
40	t	141	LEU
40	t	198	LYS
41	u	9	CYS
47	w	28	ARG
47	w	48	LYS
47	w	207	ARG
47	w	294	LYS
47	w	690	ARG
47	w	803	LYS
47	w	810	LYS
47	w	816	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	59	GLN
5	G	123	GLN
6	H	5	GLN
7	K	84	ASN
8	L	37	ASN
10	N	57	GLN
11	O	50	ASN
13	Q	73	GLN
15	S	157	GLN
17	U	87	ASN
18	V	24	ASN
19	W	74	GLN
24	b	70	ASN
24	b	217	GLN
24	b	454	GLN
27	e	104	ASN
27	e	121	ASN
30	h	59	ASN
33	k	40	GLN
35	n	160	GLN
35	n	437	ASN
36	o	163	GLN
38	r	13	GLN

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Mol	Chain	Res	Type
38	r	183	ASN
41	u	110	ASN
42	y	9	ASN
42	y	75	GLN
42	y	82	GLN
47	w	276	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	1	2523/3396 (74%)	688 (27%)	34 (1%)
45	2	157/158 (99%)	46 (29%)	3 (1%)
46	6	63/232 (27%)	29 (46%)	0
All	All	2743/3786 (72%)	763 (27%)	37 (1%)

All (763) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	1	2	U
44	1	3	U
44	1	7	C
44	1	13	A
44	1	14	U
44	1	15	C
44	1	18	G
44	1	22	G
44	1	26	A
44	1	40	A
44	1	43	A
44	1	44	U
44	1	49	A
44	1	57	A
44	1	59	G
44	1	60	A
44	1	65	A
44	1	66	A
44	1	73	C
44	1	74	G
44	1	77	A
44	1	85	A
44	1	92	G

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Mol	Chain	Res	Type
44	1	96	G
44	1	108	A
44	1	110	G
44	1	111	C
44	1	116	A
44	1	117	U
44	1	121	A
44	1	122	A
44	1	124	U
44	1	133	U
44	1	136	G
44	1	142	C
44	1	145	G
44	1	149	U
44	1	156	G
44	1	157	A
44	1	161	G
44	1	165	A
44	1	166	C
44	1	169	U
44	1	170	G
44	1	172	G
44	1	173	G
44	1	187	A
44	1	189	G
44	1	190	U
44	1	191	U
44	1	200	C
44	1	201	A
44	1	206	G
44	1	210	U
44	1	211	A
44	1	213	A
44	1	218	G
44	1	219	A
44	1	220	G
44	1	221	A
44	1	224	C
44	1	234	G
44	1	237	G
44	1	240	U
44	1	241	G

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Mol	Chain	Res	Type
44	1	243	G
44	1	248	U
44	1	250	U
44	1	251	G
44	1	252	U
44	1	253	A
44	1	268	A
44	1	269	G
44	1	270	U
44	1	283	G
44	1	284	A
44	1	285	A
44	1	286	U
44	1	295	A
44	1	304	G
44	1	307	A
44	1	311	C
44	1	317	A
44	1	323	A
44	1	329	U
44	1	334	A
44	1	337	G
44	1	338	A
44	1	339	C
44	1	341	G
44	1	343	U
44	1	346	C
44	1	347	G
44	1	349	A
44	1	350	C
44	1	351	A
44	1	359	U
44	1	370	U
44	1	373	A
44	1	375	A
44	1	376	G
44	1	390	G
44	1	397	A
44	1	399	A
44	1	401	U
44	1	402	A
44	1	403	C

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Mol	Chain	Res	Type
44	1	404	G
44	1	420	G
44	1	421	G
44	1	422	A
44	1	439	C
44	1	440	A
44	1	495	G
44	1	498	A
44	1	503	C
44	1	515	C
44	1	520	U
44	1	521	A
44	1	523	A
44	1	525	C
44	1	535	G
44	1	542	G
44	1	544	C
44	1	545	U
44	1	546	C
44	1	547	G
44	1	552	G
44	1	555	U
44	1	557	A
44	1	559	A
44	1	560	G
44	1	578	A
44	1	579	G
44	1	591	G
44	1	592	A
44	1	597	G
44	1	604	G
44	1	609	G
44	1	610	G
44	1	611	A
44	1	619	A
44	1	620	U
44	1	636	C
44	1	637	C
44	1	638	C
44	1	641	C
44	1	642	U
44	1	643	U

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Mol	Chain	Res	Type
44	1	644	G
44	1	645	A
44	1	646	A
44	1	647	A
44	1	650	C
44	1	660	A
44	1	661	G
44	1	677	A
44	1	678	G
44	1	681	U
44	1	683	U
44	1	689	U
44	1	691	A
44	1	692	A
44	1	701	G
44	1	705	A
44	1	706	A
44	1	708	G
44	1	709	A
44	1	712	G
44	1	716	A
44	1	719	U
44	1	721	G
44	1	735	A
44	1	742	G
44	1	750	G
44	1	762	U
44	1	765	C
44	1	767	U
44	1	774	G
44	1	776	U
44	1	780	A
44	1	781	G
44	1	784	A
44	1	785	G
44	1	786	A
44	1	794	U
44	1	801	A
44	1	817	A
44	1	818	C
44	1	830	A
44	1	832	G

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Mol	Chain	Res	Type
44	1	837	A
44	1	849	C
44	1	861	C
44	1	865	U
44	1	866	A
44	1	870	G
44	1	873	C
44	1	874	U
44	1	875	G
44	1	879	U
44	1	880	G
44	1	887	G
44	1	888	A
44	1	892	U
44	1	894	G
44	1	907	G
44	1	908	G
44	1	914	A
44	1	916	G
44	1	917	A
44	1	922	U
44	1	924	G
44	1	925	A
44	1	926	A
44	1	932	U
44	1	933	A
44	1	934	G
44	1	938	C
44	1	944	C
44	1	954	U
44	1	960	U
44	1	962	A
44	1	976	U
44	1	977	C
44	1	979	U
44	1	980	A
44	1	981	U
44	1	982	C
44	1	984	G
44	1	986	U
44	1	993	G
44	1	994	G

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Mol	Chain	Res	Type
44	1	995	U
44	1	998	A
44	1	1000	C
44	1	1052	U
44	1	1053	A
44	1	1054	A
44	1	1056	U
44	1	1057	A
44	1	1061	A
44	1	1063	G
44	1	1064	A
44	1	1065	A
44	1	1093	A
44	1	1094	U
44	1	1095	U
44	1	1096	U
44	1	1097	G
44	1	1098	A
44	1	1103	A
44	1	1104	G
44	1	1105	A
44	1	1116	G
44	1	1117	G
44	1	1118	C
44	1	1127	G
44	1	1129	A
44	1	1132	C
44	1	1135	A
44	1	1140	G
44	1	1143	A
44	1	1144	U
44	1	1145	G
44	1	1153	A
44	1	1159	A
44	1	1160	C
44	1	1170	A
44	1	1171	G
44	1	1172	G
44	1	1174	G
44	1	1177	G
44	1	1178	G
44	1	1180	A

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Mol	Chain	Res	Type
44	1	1181	U
44	1	1182	A
44	1	1187	C
44	1	1192	C
44	1	1193	A
44	1	1197	A
44	1	1198	C
44	1	1199	C
44	1	1200	A
44	1	1201	C
44	1	1204	A
44	1	1206	G
44	1	1209	G
44	1	1213	G
44	1	1222	G
44	1	1226	G
44	1	1227	C
44	1	1233	G
44	1	1234	G
44	1	1237	G
44	1	1238	C
44	1	1239	C
44	1	1240	A
44	1	1244	A
44	1	1245	A
44	1	1246	G
44	1	1248	C
44	1	1249	G
44	1	1254	C
44	1	1258	U
44	1	1262	G
44	1	1263	A
44	1	1264	G
44	1	1265	U
44	1	1266	G
44	1	1267	U
44	1	1269	U
44	1	1271	A
44	1	1272	C
44	1	1278	A
44	1	1279	C
44	1	1286	A

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Mol	Chain	Res	Type
44	1	1287	A
44	1	1303	A
44	1	1304	A
44	1	1307	G
44	1	1308	A
44	1	1309	U
44	1	1314	C
44	1	1316	C
44	1	1317	A
44	1	1318	A
44	1	1325	U
44	1	1330	A
44	1	1331	U
44	1	1345	G
44	1	1348	U
44	1	1349	G
44	1	1350	A
44	1	1351	U
44	1	1352	A
44	1	1354	G
44	1	1356	U
44	1	1357	G
44	1	1365	G
44	1	1380	G
44	1	1386	A
44	1	1391	C
44	1	1392	G
44	1	1399	A
44	1	1400	G
44	1	1419	A
44	1	1425	U
44	1	1430	U
44	1	1432	C
44	1	1434	G
44	1	1435	A
44	1	1437	C
44	1	1443	G
44	1	1446	A
44	1	1450	G
44	1	1452	A
44	1	1453	A
44	1	1457	U

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Mol	Chain	Res	Type
44	1	1467	A
44	1	1470	U
44	1	1477	A
44	1	1482	A
44	1	1483	G
44	1	1487	G
44	1	1503	A
44	1	1507	G
44	1	1508	C
44	1	1511	U
44	1	1523	U
44	1	1524	A
44	1	1527	C
44	1	1530	U
44	1	1531	C
44	1	1542	G
44	1	1549	U
44	1	1556	C
44	1	1557	A
44	1	1560	G
44	1	1562	C
44	1	1566	A
44	1	1567	U
44	1	1568	U
44	1	1569	U
44	1	1570	U
44	1	1571	A
44	1	1574	C
44	1	1580	A
44	1	1583	A
44	1	1588	A
44	1	1589	A
44	1	1590	G
44	1	1593	A
44	1	1602	A
44	1	1605	A
44	1	1620	U
44	1	1629	U
44	1	1631	C
44	1	1639	C
44	1	1642	A
44	1	1643	A

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Mol	Chain	Res	Type
44	1	1644	C
44	1	1645	U
44	1	1647	A
44	1	1683	A
44	1	1713	G
44	1	1715	A
44	1	1716	U
44	1	1717	U
44	1	1724	U
44	1	1725	C
44	1	1741	A
44	1	1743	G
44	1	1749	A
44	1	1750	A
44	1	1751	G
44	1	1756	C
44	1	1760	A
44	1	1762	C
44	1	1763	U
44	1	1765	U
44	1	1766	G
44	1	1770	G
44	1	1773	C
44	1	1775	G
44	1	1780	G
44	1	1792	C
44	1	1793	C
44	1	1797	A
44	1	1810	A
44	1	1812	G
44	1	1813	A
44	1	1814	A
44	1	1815	U
44	1	1816	A
44	1	1819	U
44	1	1820	U
44	1	1821	U
44	1	1839	A
44	1	1840	U
44	1	1841	A
44	1	1842	A
44	1	1846	C

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Mol	Chain	Res	Type
44	1	1847	A
44	1	1848	G
44	1	1849	C
44	1	1850	A
44	1	1851	G
44	1	1863	G
44	1	1866	C
44	1	1878	G
44	1	1879	A
44	1	1886	A
44	1	1892	G
44	1	1893	A
44	1	1906	G
44	1	1913	A
44	1	1921	A
44	1	1922	A
44	1	1924	U
44	1	1926	C
44	1	1928	G
44	1	1929	G
44	1	1935	G
44	1	1948	G
44	1	1953	G
44	1	2094	C
44	1	2101	C
44	1	2111	G
44	1	2112	U
44	1	2113	A
44	1	2114	C
44	1	2116	G
44	1	2117	A
44	1	2118	C
44	1	2119	A
44	1	2121	G
44	1	2122	G
44	1	2126	A
44	1	2130	G
44	1	2131	A
44	1	2132	C
44	1	2145	A
44	1	2149	A
44	1	2188	A

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Mol	Chain	Res	Type
44	1	2315	G
44	1	2316	G
44	1	2317	A
44	1	2318	U
44	1	2319	U
44	1	2335	G
44	1	2336	U
44	1	2339	C
44	1	2340	U
44	1	2347	U
44	1	2352	A
44	1	2363	A
44	1	2364	G
44	1	2365	C
44	1	2371	G
44	1	2378	C
44	1	2388	U
44	1	2393	G
44	1	2394	G
44	1	2397	A
44	1	2821	C
44	1	2822	U
44	1	2824	G
44	1	2826	U
44	1	2830	G
44	1	2834	G
44	1	2838	A
44	1	2839	G
44	1	2842	U
44	1	2843	U
44	1	2845	A
44	1	2846	U
44	1	2847	A
44	1	2848	G
44	1	2850	G
44	1	2857	C
44	1	2858	U
44	1	2859	U
44	1	2861	U
44	1	2863	G
44	1	2864	A
44	1	2866	U

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Mol	Chain	Res	Type
44	1	2867	C
44	1	2868	U
44	1	2870	C
44	1	2872	A
44	1	2873	U
44	1	2876	C
44	1	2877	G
44	1	2878	G
44	1	2879	C
44	1	2881	C
44	1	2887	A
44	1	2889	C
44	1	2894	C
44	1	2897	A
44	1	2898	G
44	1	2899	C
44	1	2901	G
44	1	2911	A
44	1	2918	G
44	1	2920	U
44	1	2921	U
44	1	2922	G
44	1	2923	U
44	1	2924	U
44	1	2926	A
44	1	2927	C
44	1	2928	C
44	1	2930	A
44	1	2935	U
44	1	2936	A
44	1	2944	U
44	1	2946	A
44	1	2947	G
44	1	2950	G
44	1	2952	G
44	1	2953	U
44	1	2982	A
44	1	2983	C
44	1	2996	U
44	1	2997	G
44	1	3011	A
44	1	3012	A

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Mol	Chain	Res	Type
44	1	3017	A
44	1	3019	U
44	1	3021	A
44	1	3022	G
44	1	3023	U
44	1	3027	A
44	1	3032	A
44	1	3034	C
44	1	3049	A
44	1	3058	U
44	1	3059	G
44	1	3061	G
44	1	3078	U
44	1	3080	G
44	1	3086	A
44	1	3092	C
44	1	3093	C
44	1	3099	C
44	1	3104	U
44	1	3115	C
44	1	3116	G
44	1	3117	C
44	1	3118	C
44	1	3121	U
44	1	3122	A
44	1	3129	A
44	1	3130	A
44	1	3131	U
44	1	3142	A
44	1	3143	C
44	1	3150	A
44	1	3152	U
44	1	3153	U
44	1	3154	C
44	1	3155	U
44	1	3156	U
44	1	3164	C
44	1	3165	A
44	1	3168	A
44	1	3170	A
44	1	3172	A
44	1	3173	G

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Mol	Chain	Res	Type
44	1	3174	A
44	1	3175	U
44	1	3176	G
44	1	3179	U
44	1	3180	A
44	1	3181	C
44	1	3187	A
44	1	3188	G
44	1	3196	U
44	1	3198	U
44	1	3207	U
44	1	3208	G
44	1	3209	A
44	1	3212	C
44	1	3216	G
44	1	3217	C
44	1	3218	A
44	1	3219	G
44	1	3222	U
44	1	3235	C
44	1	3243	A
44	1	3245	A
44	1	3246	G
44	1	3247	G
44	1	3253	G
44	1	3259	U
44	1	3260	G
44	1	3263	G
44	1	3269	U
44	1	3270	U
44	1	3272	C
44	1	3273	A
44	1	3274	A
44	1	3276	G
44	1	3278	C
44	1	3281	U
44	1	3286	G
44	1	3289	G
44	1	3293	U
44	1	3294	A
44	1	3295	A
44	1	3304	U

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Mol	Chain	Res	Type
44	1	3305	A
44	1	3306	U
44	1	3308	C
44	1	3309	G
44	1	3313	U
44	1	3316	A
44	1	3319	U
44	1	3320	A
44	1	3324	C
44	1	3329	U
44	1	3330	A
44	1	3334	U
44	1	3341	U
44	1	3342	A
44	1	3345	G
44	1	3347	A
44	1	3348	G
44	1	3349	C
44	1	3350	C
44	1	3351	U
44	1	3352	U
44	1	3353	G
44	1	3354	U
44	1	3355	U
44	1	3356	G
44	1	3357	U
44	1	3359	A
44	1	3369	G
44	1	3375	A
44	1	3378	C
44	1	3382	U
44	1	3386	G
44	1	3389	U
44	1	3390	G
44	1	3396	U
45	2	2	A
45	2	23	U
45	2	34	U
45	2	35	C
45	2	37	A
45	2	38	U
45	2	39	G

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Mol	Chain	Res	Type
45	2	40	A
45	2	46	G
45	2	48	A
45	2	49	G
45	2	51	G
45	2	59	A
45	2	61	A
45	2	62	C
45	2	63	G
45	2	70	G
45	2	73	U
45	2	74	U
45	2	78	G
45	2	79	A
45	2	80	A
45	2	81	U
45	2	82	U
45	2	83	C
45	2	84	C
45	2	86	U
45	2	87	G
45	2	90	U
45	2	91	C
45	2	94	C
45	2	95	G
45	2	97	A
45	2	100	U
45	2	104	A
45	2	105	A
45	2	106	C
45	2	111	A
45	2	113	U
45	2	116	G
45	2	125	U
45	2	126	A
45	2	127	U
45	2	136	G
45	2	138	A
45	2	151	C
46	6	4	U
46	6	5	C
46	6	7	C

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Mol	Chain	Res	Type
46	6	9	A
46	6	15	C
46	6	16	U
46	6	23	U
46	6	24	A
46	6	25	G
46	6	26	U
46	6	29	G
46	6	34	A
46	6	40	U
46	6	41	G
46	6	42	G
46	6	43	A
46	6	47	A
46	6	49	C
46	6	52	G
46	6	53	A
46	6	54	A
46	6	56	U
46	6	57	U
46	6	58	G
46	6	59	C
46	6	66	U
46	6	230	A
46	6	231	A
46	6	232	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	1	13	A
44	1	42	C
44	1	121	A
44	1	148	G
44	1	160	G
44	1	282	G
44	1	338	A
44	1	637	C
44	1	645	A
44	1	649	A
44	1	705	A
44	1	720	A

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Mol	Chain	Res	Type
44	1	761	A
44	1	916	G
44	1	1064	A
44	1	1097	G
44	1	1200	A
44	1	1205	A
44	1	1307	G
44	1	1329	U
44	1	1355	A
44	1	1567	U
44	1	1568	U
44	1	1605	A
44	1	1641	U
44	1	1838	G
44	1	2110	G
44	1	2187	G
44	1	2317	A
44	1	2920	U
44	1	3269	U
44	1	3341	U
44	1	3350	C
44	1	3375	A
45	2	39	G
45	2	73	U
45	2	79	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
28	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	102:LEU	C	103:TYR	N	1.16

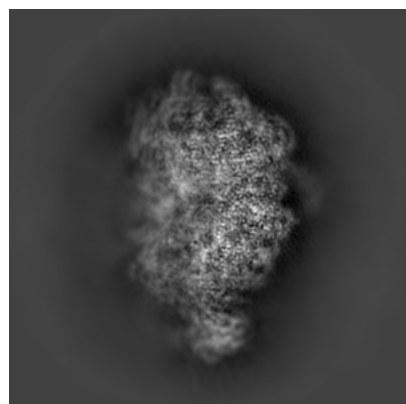
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10841. These allow visual inspection of the internal detail of the map and identification of artifacts.

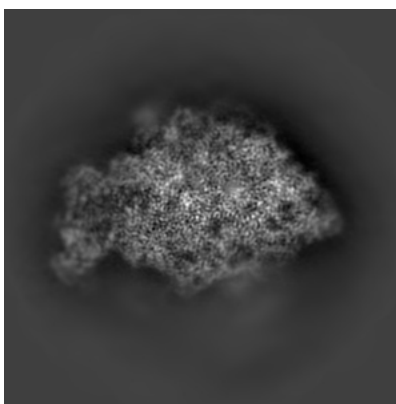
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

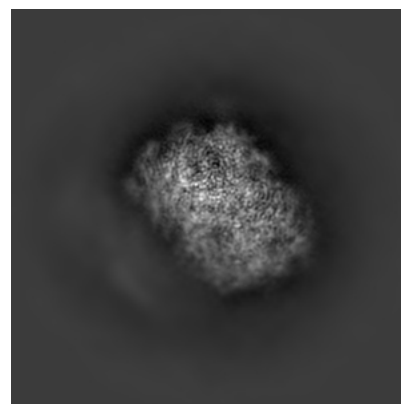
6.1.1 Primary map



X

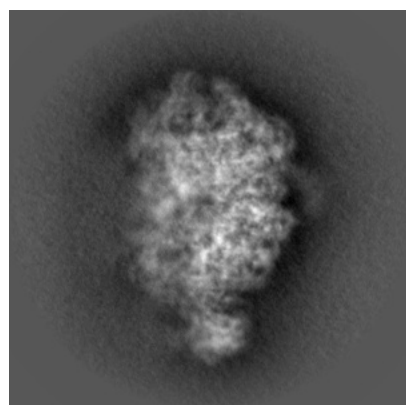


Y

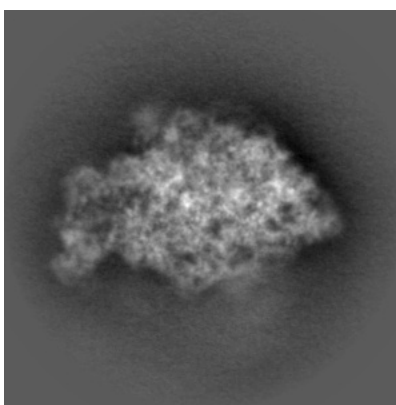


Z

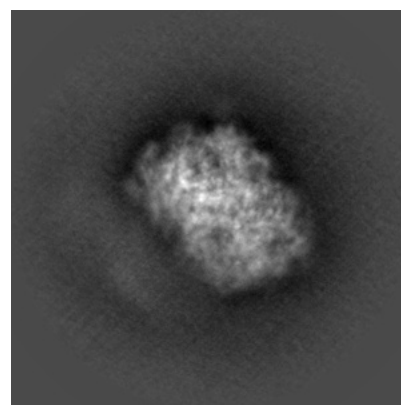
6.1.2 Raw map



X



Y

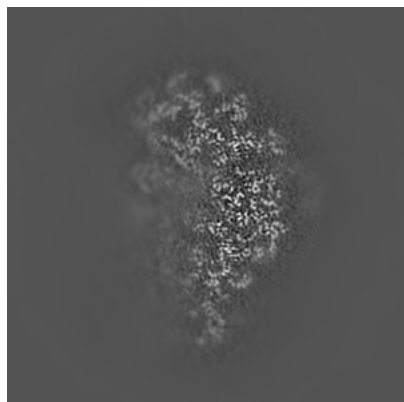


Z

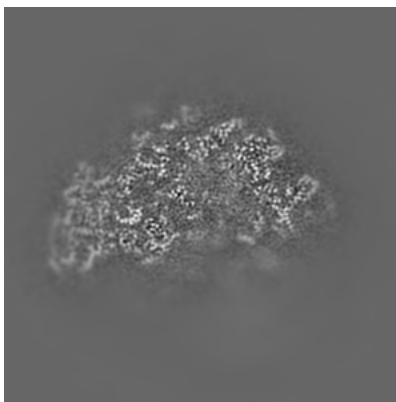
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

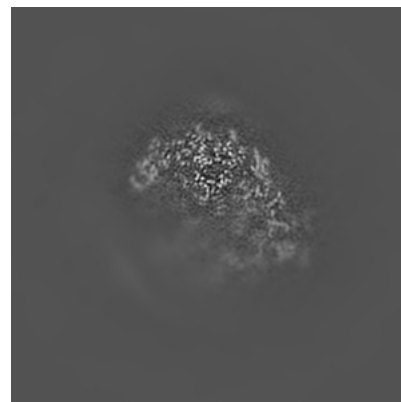
6.2.1 Primary map



X Index: 192

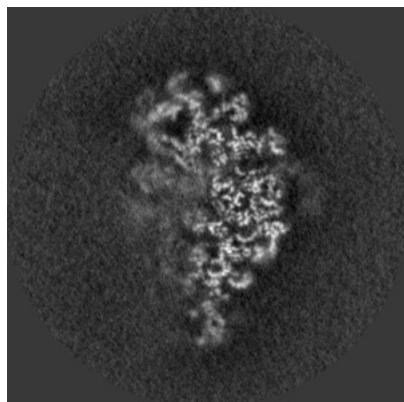


Y Index: 192

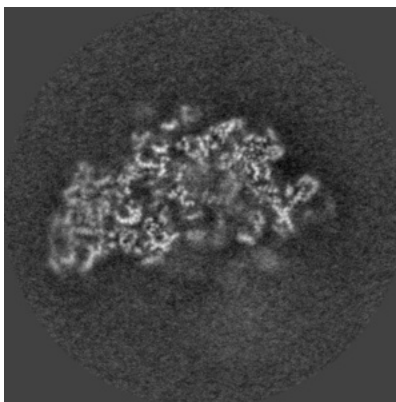


Z Index: 192

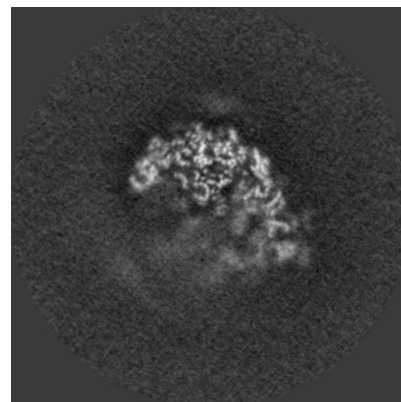
6.2.2 Raw map



X Index: 192



Y Index: 192

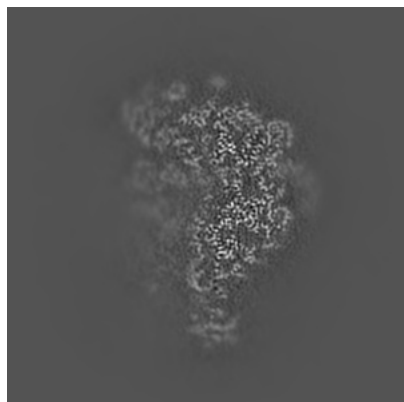


Z Index: 192

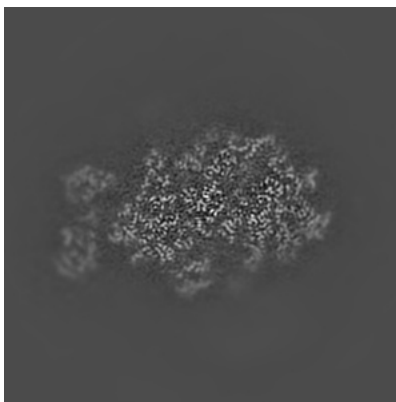
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

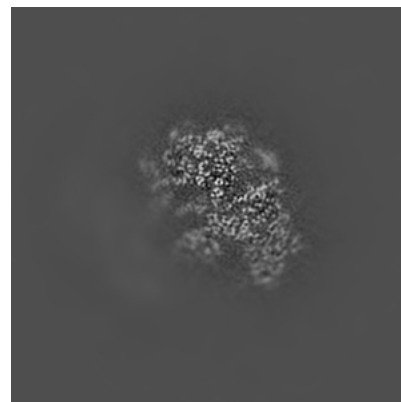
6.3.1 Primary map



X Index: 201

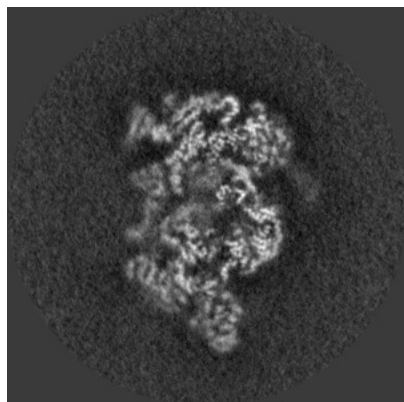


Y Index: 216

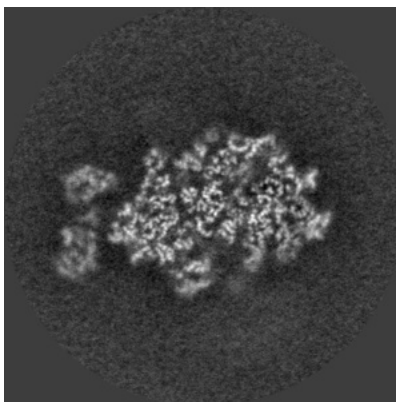


Z Index: 245

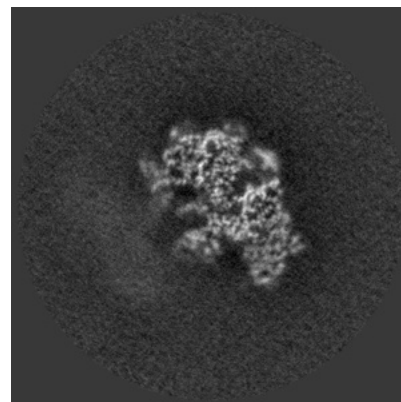
6.3.2 Raw map



X Index: 217



Y Index: 216

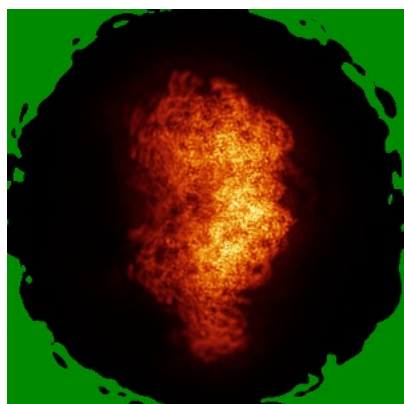


Z Index: 244

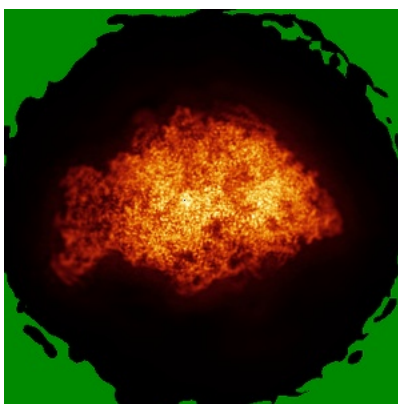
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

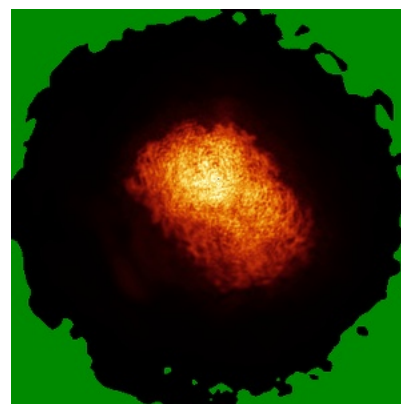
6.4.1 Primary map



X

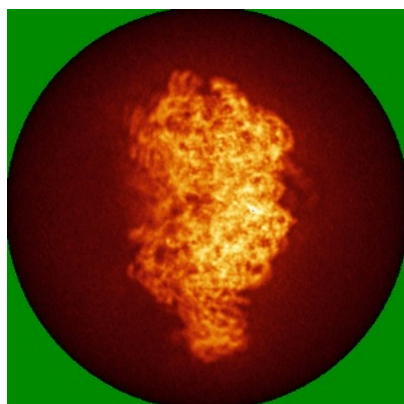


Y

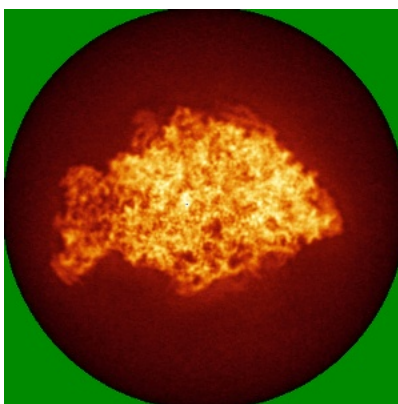


Z

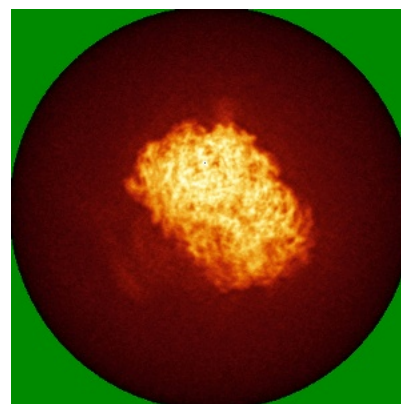
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

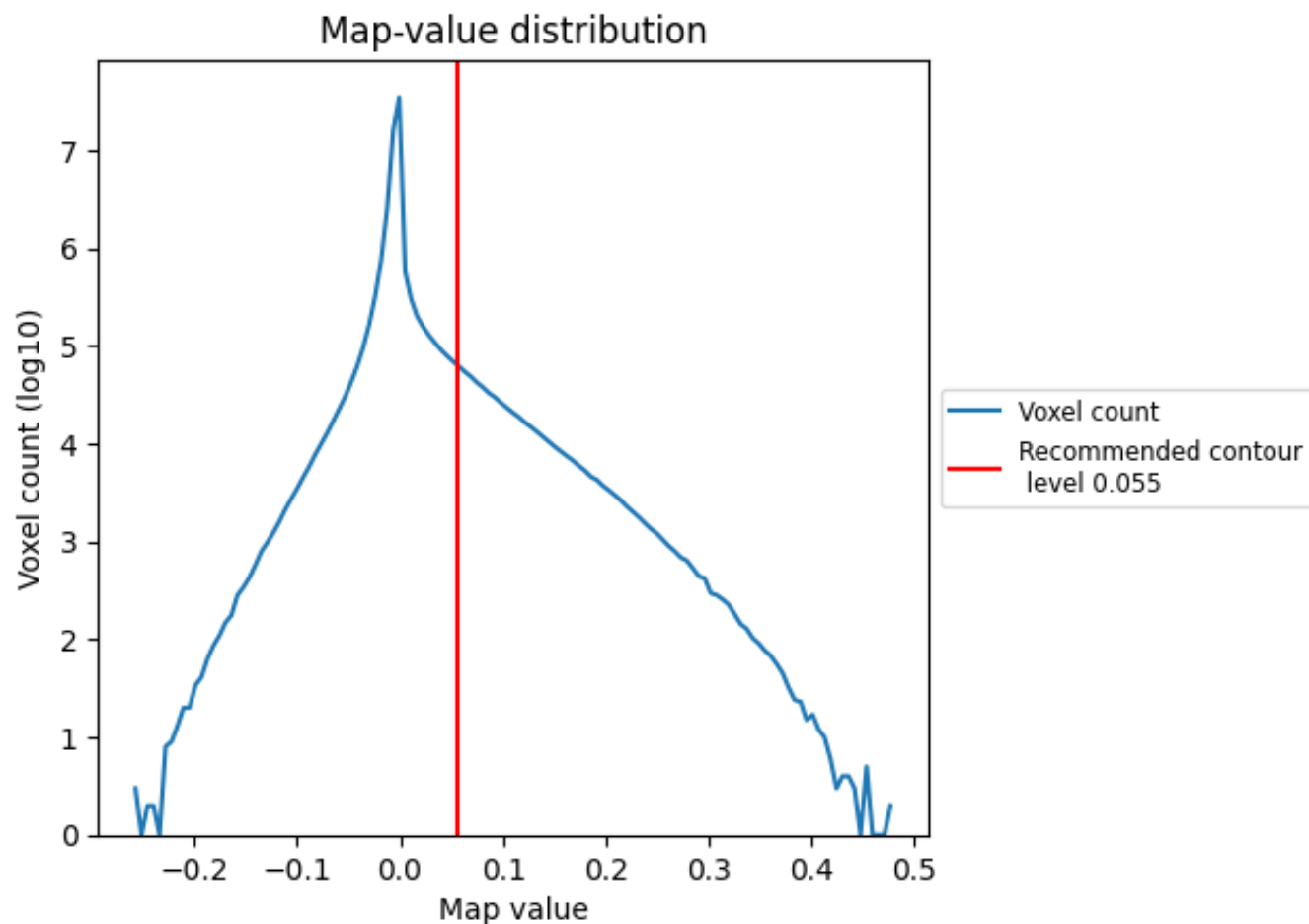
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

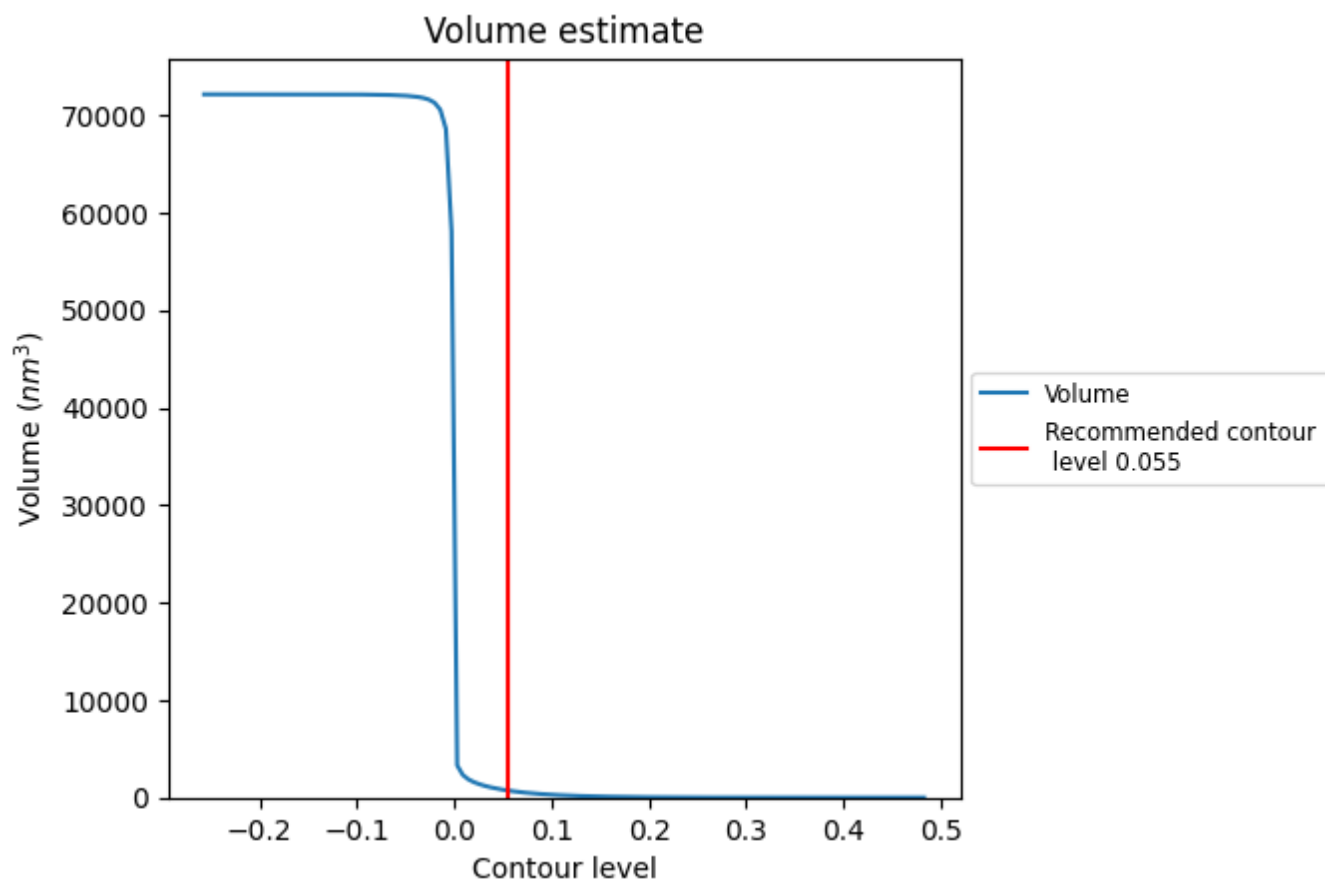
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

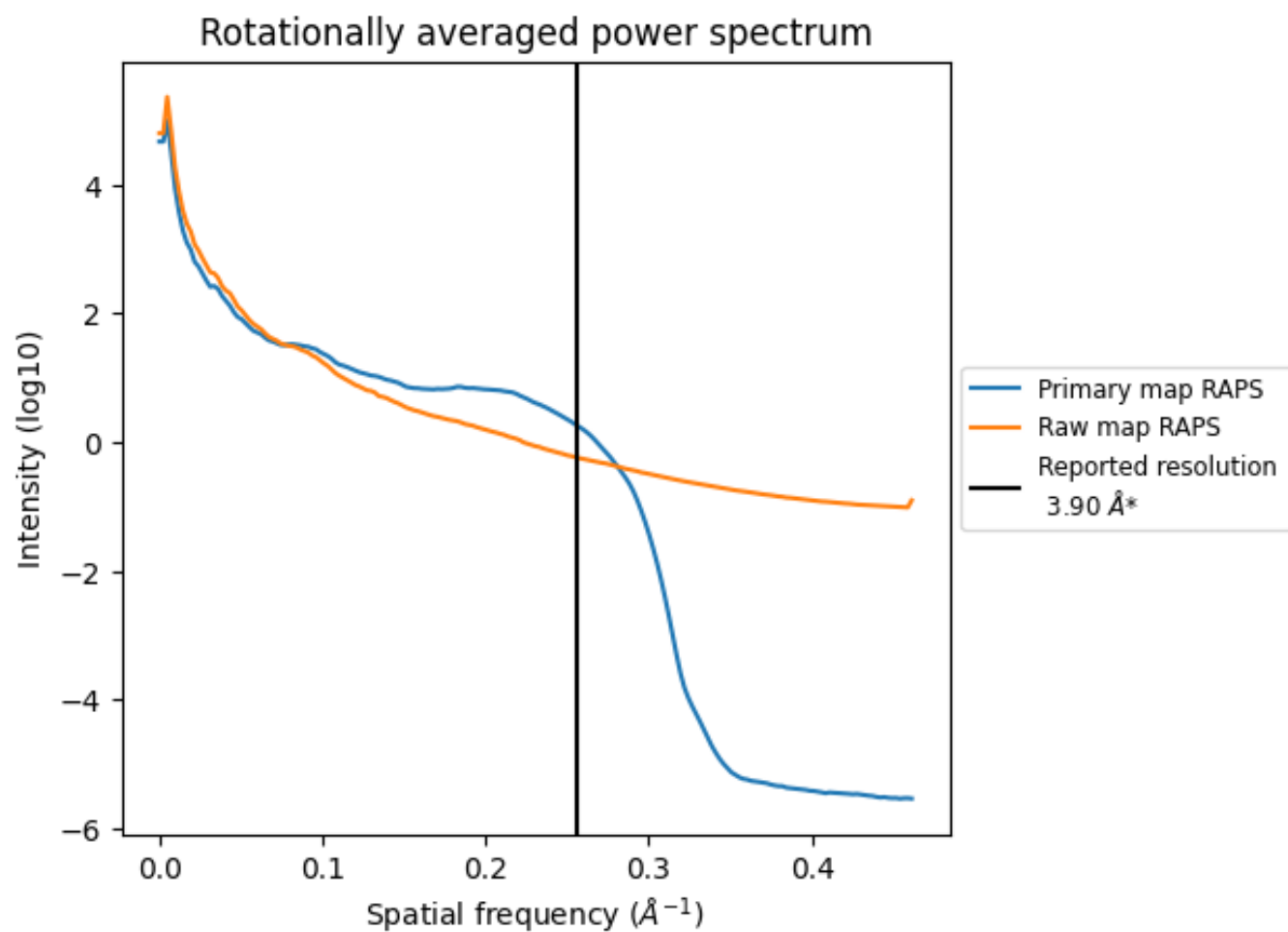
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 656 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 ⓘ

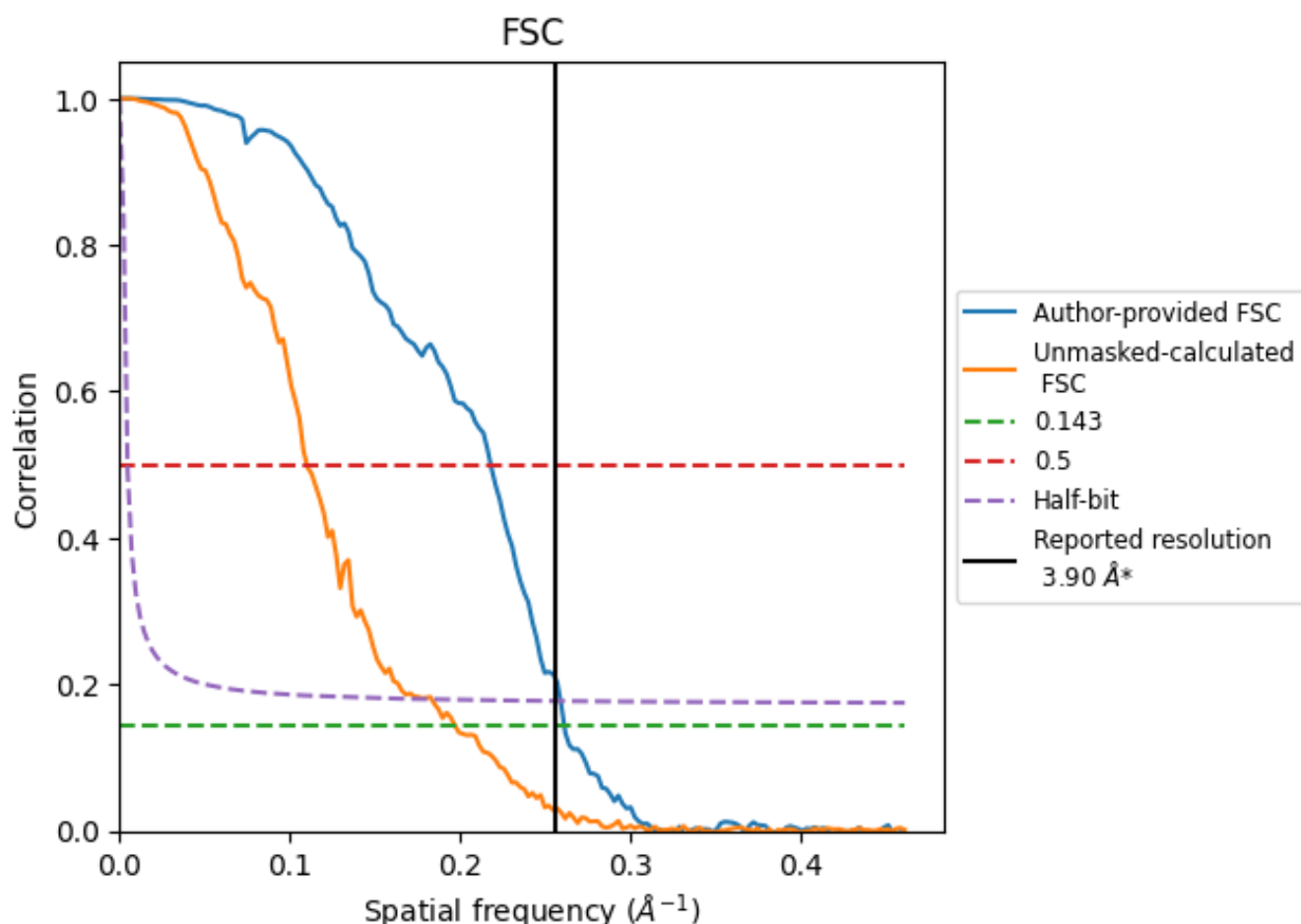


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

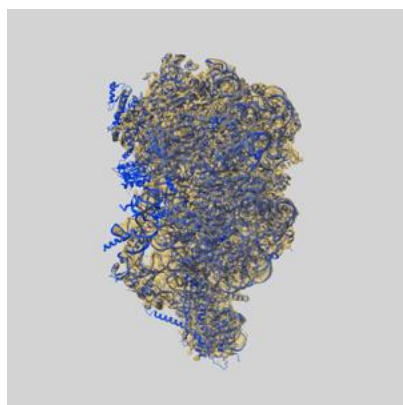
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	4.59	3.86
Unmasked-calculated*	5.07	9.08	5.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.07 differs from the reported value 3.9 by more than 10 %

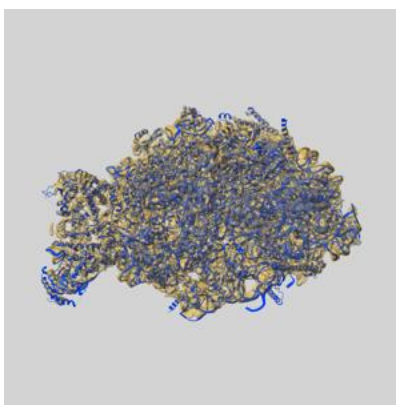
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10841 and PDB model 6YLX. Per-residue inclusion information can be found in section 3 on page 12.

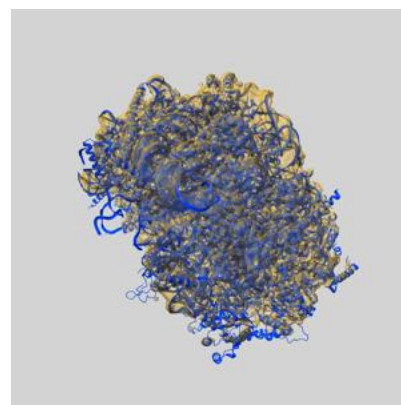
9.1 Map-model overlay [i](#)



X



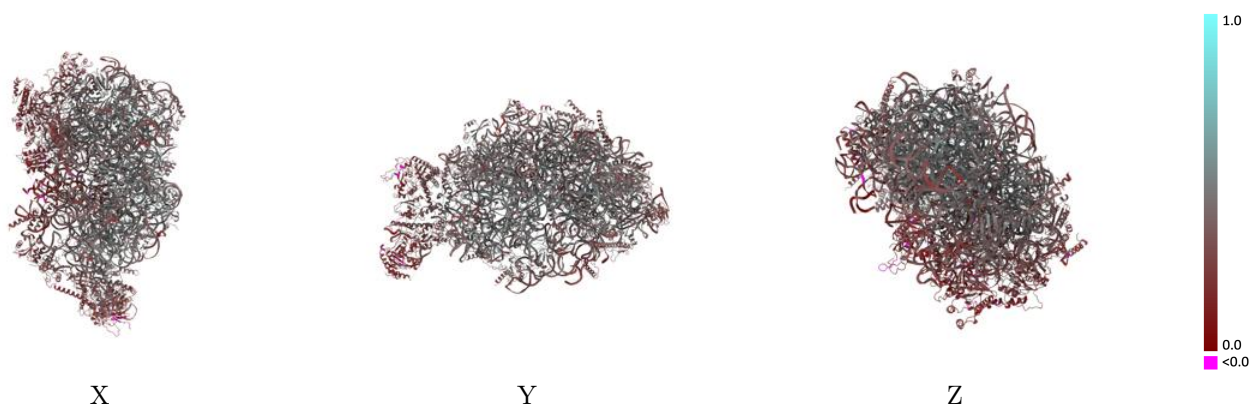
Y



Z

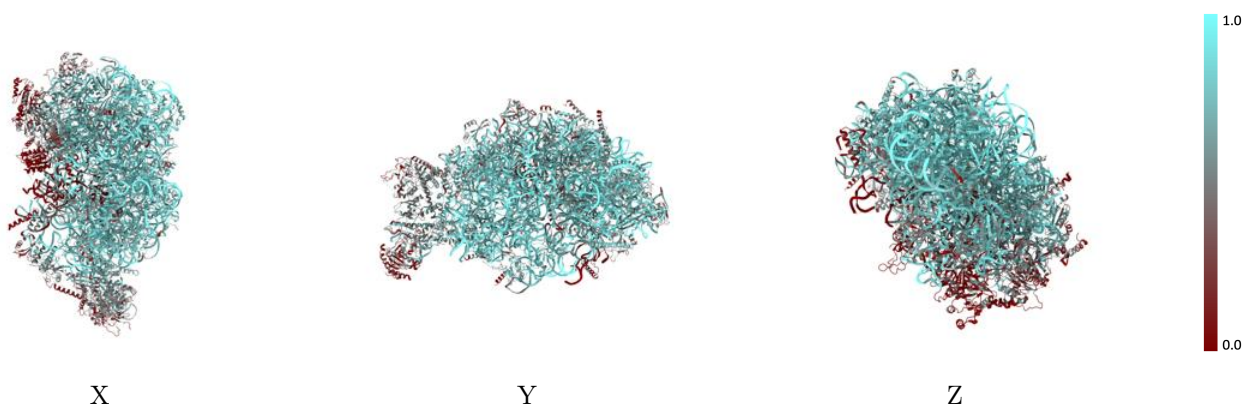
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



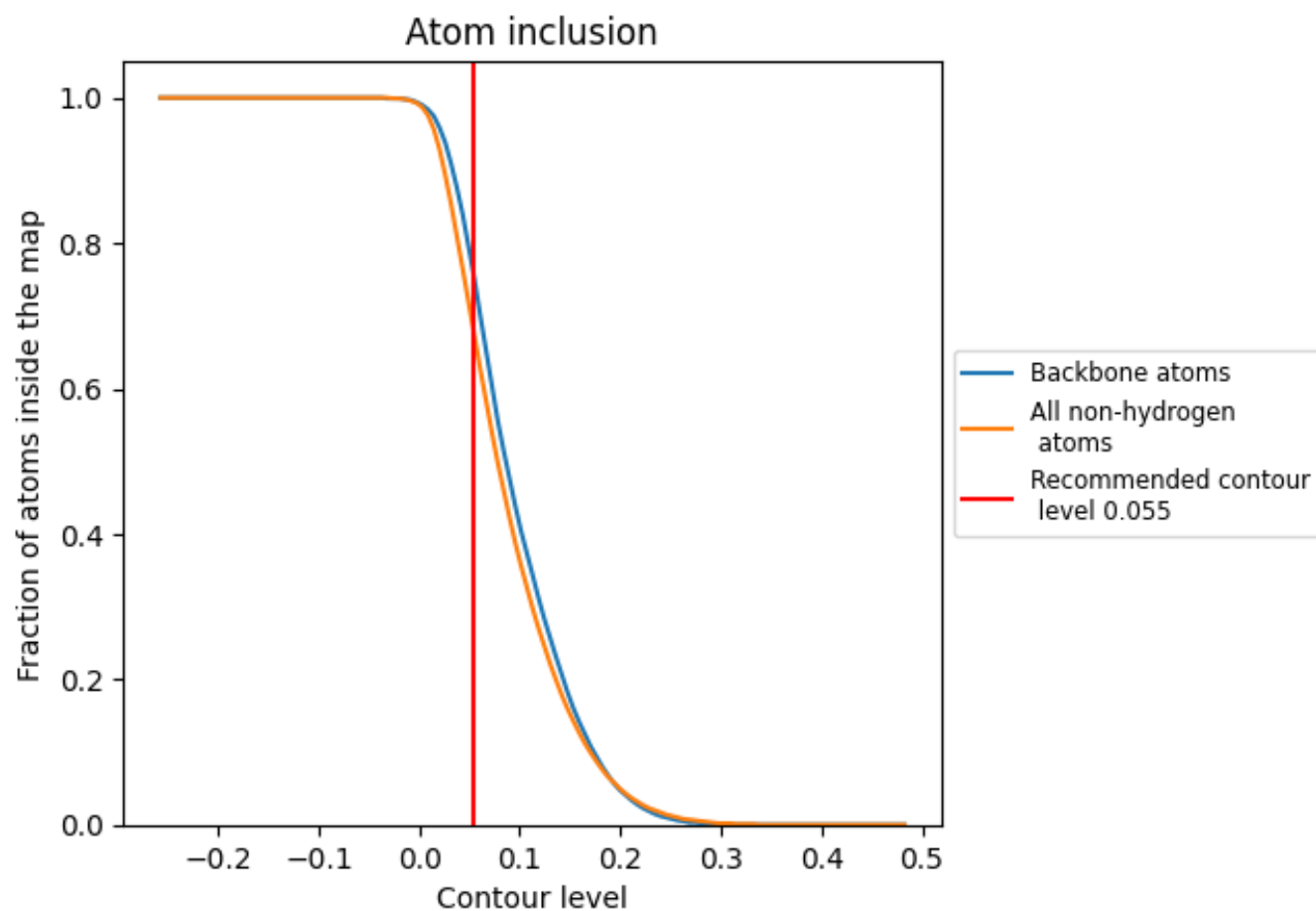
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.055).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6730	 0.3840
1	 0.7890	 0.3960
2	 0.8920	 0.4560
6	 0.6830	 0.3070
B	 0.6810	 0.4290
C	 0.7750	 0.4690
E	 0.7250	 0.4280
F	 0.7770	 0.4300
G	 0.6420	 0.3890
H	 0.6870	 0.4150
K	 0.2690	 0.2150
L	 0.6910	 0.4310
M	 0.7610	 0.4410
N	 0.8020	 0.4900
O	 0.8060	 0.4790
P	 0.7620	 0.4590
Q	 0.7510	 0.4440
R	 0.4550	 0.3430
S	 0.7070	 0.4280
T	 0.1880	 0.3110
U	 0.4610	 0.3320
V	 0.5390	 0.3800
W	 0.4070	 0.2770
X	 0.7080	 0.4430
Y	 0.7800	 0.4720
Z	 0.5030	 0.3200
a	 0.6190	 0.3960
b	 0.3230	 0.2730
c	 0.3410	 0.2580
d	 0.7040	 0.4430
e	 0.8010	 0.4980
f	 0.8390	 0.5110
g	 0.5810	 0.3980
h	 0.7410	 0.4570
i	 0.5930	 0.3700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.7500	 0.4660
k	 0.5410	 0.3910
l	 0.2800	 0.3650
n	 0.5320	 0.3380
o	 0.3760	 0.2480
q	 0.1930	 0.2420
r	 0.2480	 0.2720
s	 0.4770	 0.4100
t	 0.4620	 0.3010
u	 0.5330	 0.3480
w	 0.1110	 0.2630
y	 0.4430	 0.2890
z	 0.4560	 0.3770