



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 04:18 pm GMT

PDB ID : 6S13
EMDB ID : EMD-10079
Title : Erythromycin Resistant Staphylococcus aureus 70S ribosome (delta R88 A89 uL22).
Authors : Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on : 2019-06-18
Resolution : 3.58 Å(reported)

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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

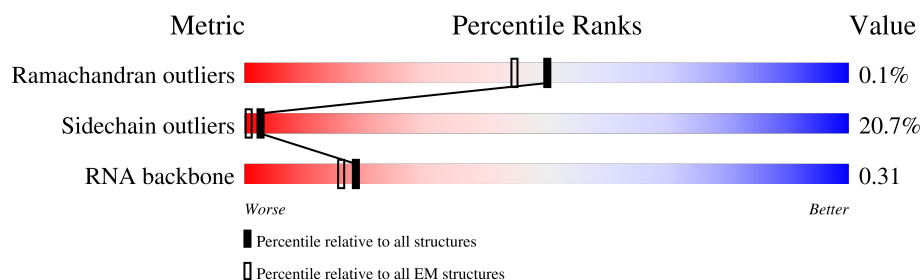
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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.














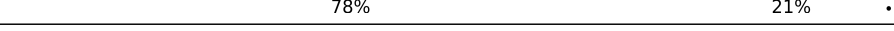



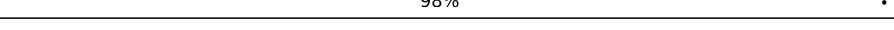



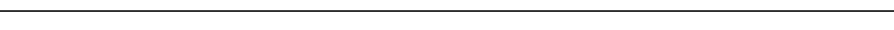

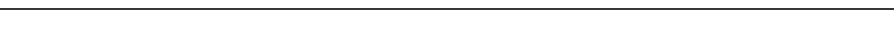
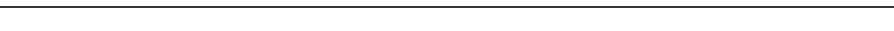


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2905	
2	B	115	
3	C	274	
4	D	215	
5	E	206	
6	F	175	
7	G	175	
8	H	145	
9	I	122	










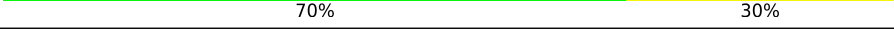



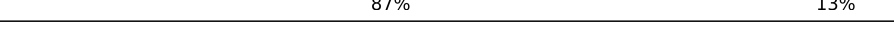




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Mol	Chain	Length	Quality of chain
10	J	146	 91% 9%
11	K	137	 86% 14%
12	L	120	 88% 12%
13	M	119	 79% 20% .
14	N	114	 88% 12%
15	O	116	 89% 11%
16	P	102	 78% 22%
17	Q	110	 73% 27%
18	R	89	 82% 18%
19	S	103	 79% 20% .
20	T	94	 81% 19%
21	U	82	 78% 21% .
22	V	58	 81% 19%
23	W	67	 88% 12%
24	X	58	 86% 14%
25	Y	59	 98% .
26	Z	48	 75% 23% .
27	1	47	 74% 26%
28	2	43	 91% 9%
29	3	64	 88% 12%
30	4	37	 76% 19% 5%
31	a	1539	 35% 54% 10%
32	b	226	 84% 15% .
33	c	202	 86% 13%
34	d	198	 81% 17% .

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Mol	Chain	Length	Quality of chain
35	e	156	 87% 13%
36	f	95	 81% 19%
37	g	152	 76% 22% ..
38	h	131	 82% 18% .
39	i	127	 85% 15%
40	j	97	 82% 14% .
41	k	114	 77% 21% .
42	l	135	 75% 22% .
43	m	104	 87% 12% .
44	n	60	 70% 30%
45	o	88	 76% 22% .
46	p	89	 81% 19%
47	q	80	 78% 18% 5%
48	r	54	 87% 13%
49	s	80	 74% 24% .
50	t	81	 84% 16%
51	u	52	 75% 23% .
52	v	162	 78% 21% .

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 233957 atoms, of which 93218 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2905	Total	C	H	N	O	P	0	0
			93564	27803	31287	11387	20182	2905		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	115	Total	C	H	N	O	P	0	0
			3685	1094	1240	436	801	114		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	274	Total	C	H	N	O	S	0	0
			4291	1301	2201	415	369	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	215	Total	C	H	N	O	S	0	0
			3294	1018	1667	299	305	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	206	Total	C	H	N	O	S	0	0
			3192	986	1620	288	296	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	175	Total	C	H	N	O	S	0	0
			2667	837	1342	227	255	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	175	Total	C	H	N	O	S	0	0
			2488	790	1225	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	145	Total	C	H	N	O	S	0	0
			2277	714	1134	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	122	Total	C	H	N	O	S	0	0
			1899	572	981	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	146	Total	C	H	N	O	S	0	0
			2211	674	1125	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	137	Total	C	H	N	O	S	0	0
			2194	689	1123	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	120	Total	C	H	N	O	S	0	0
			1915	576	983	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1816	557	925	174	159	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	H	N	O	0	0
			1826	563	937	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	116	Total	C	H	N	O	S	0	0
			1956	593	1014	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	102	Total	C	H	N	O	S	0	0
			1620	503	830	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	110	Total	C	H	N	O	S	0	0
			1724	523	887	158	153	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	89	Total	C	H	N	O	S	0	0
			1463	453	748	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
19	S	103	Total	C	H	N	O	S	0	0
			1579	486	809	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	H	N	O	0	0
			1488	463	766	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	H	N	O	0	0
			1265	385	643	122	115		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	58	Total	C	H	N	O	0	0
			911	277	466	96	72		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	67	Total	C	H	N	O	0	0
			1104	333	563	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	58	Total	C	H	N	O	0	0
			940	280	491	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	Y	59	Total	C	H	N	O	S	0	0
			613	225	243	68	76	1		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	Z	48	Total	C	H	N	O	S	0	0
			718	222	358	77	59	2		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	47	Total	C	H	N	O	S	0	0
			784	238	394	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	43	Total	C	H	N	O	S	0	0
			782	225	415	89	52	1		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	64	Total	C	H	N	O	S	0	0
			1107	324	586	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	37	Total	C	H	N	O	S	0	0
			635	186	340	60	44	5		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	a	1539	Total	C	H	N	O	P	0	0
			49563	14719	16594	6017	10694	1539		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	b	226	Total	C	H	N	O	S	0	0
			3705	1159	1886	317	335	8		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	c	202	Total	C	H	N	O	S	0	0
			2965	945	1464	284	271	1		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	d	198	Total	C	H	N	O	S	0	0
			2946	952	1449	275	268	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	e	156	Total	C	H	N	O	S	0	0
			2347	723	1202	211	209	2		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	f	95	Total	C	H	N	O	S	0	0
			1553	493	775	138	145	2		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	g	152	Total	C	H	N	O	S	0	0
			2326	722	1165	218	217	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	h	131	Total	C	H	N	O	S	0	0
			2103	650	1077	183	189	4		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	i	127	Total	C	H	N	O	S	0	0
			1812	576	890	179	166	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	j	97	Total	C	H	N	O	S	0	0
			1527	475	775	140	136	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	k	114	Total	C	H	N	O	S	0	0
			1594	498	784	151	159	2		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	l	135	Total	C	H	N	O	S	0	0
			2128	646	1091	211	178	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	m	104	Total	C	H	N	O	S	0	0
			1401	453	674	139	135			

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	n	60	Total	C	H	N	O	S	0	0
			979	307	492	98	77	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	o	88	Total	C	H	N	O	S	0	0
			1475	448	752	150	124	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	p	89	Total	C	H	N	O	S	0	0
			1403	436	709	128	129	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	q	80	Total	C	H	N	O	S	0	0
			1237	392	616	112	117			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	r	54	Total	C	H	N	O	S	0	0
			927	284	482	86	73	2		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	s	80	Total	C	H	N	O	S	0	0
			1262	410	626	113	111	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	t	81	Total	C	H	N	O	S	0	0
			1207	358	616	117	115	1		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	52	Total	C	H	N	O		
			807	249	407	79	72	0	0

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	162	Total	C	H	N	O	S	0	0
			2682	835	1349	242	254	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	PHE	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	LEU	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	MET	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

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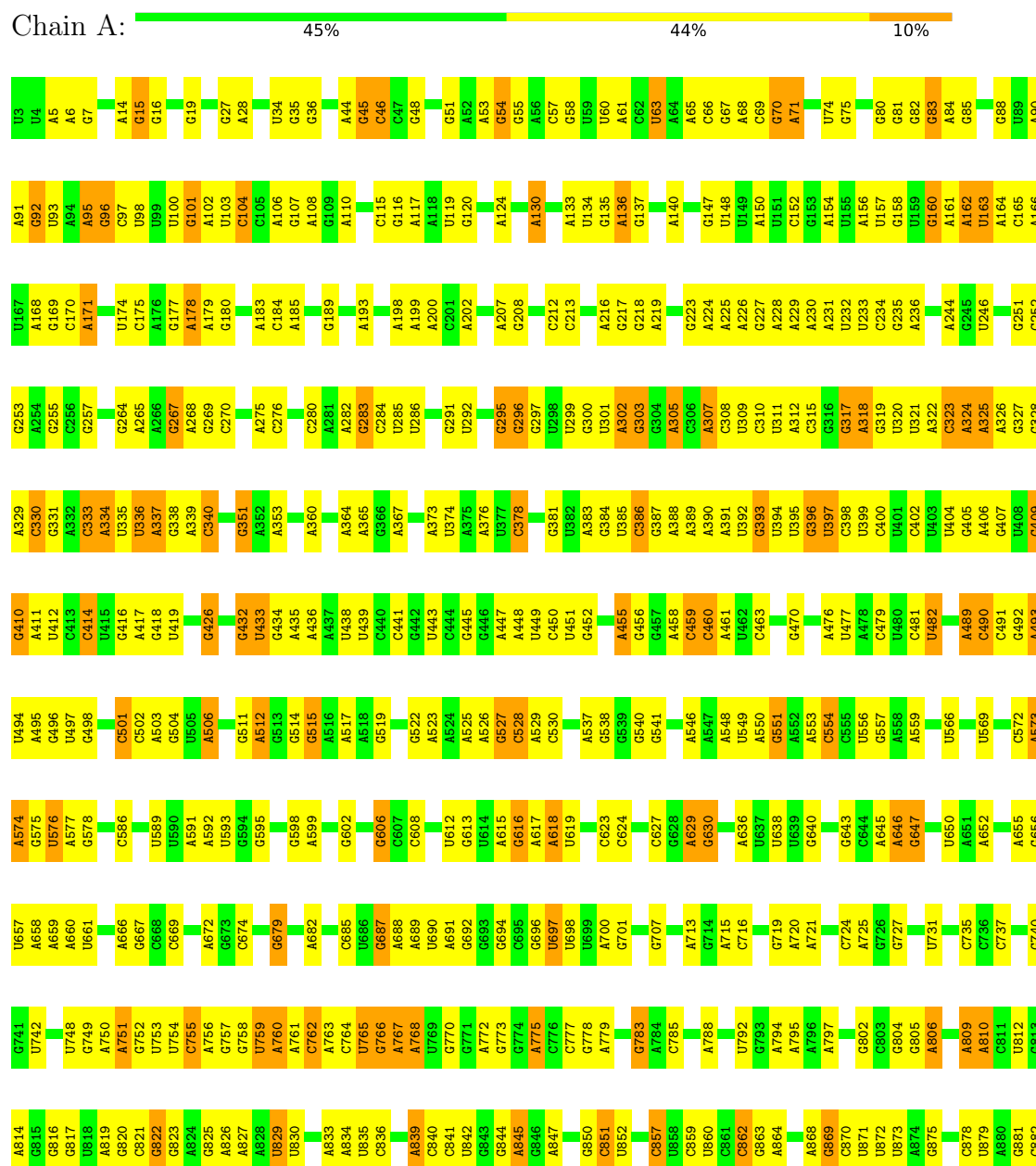
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Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	THR	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	TYR	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

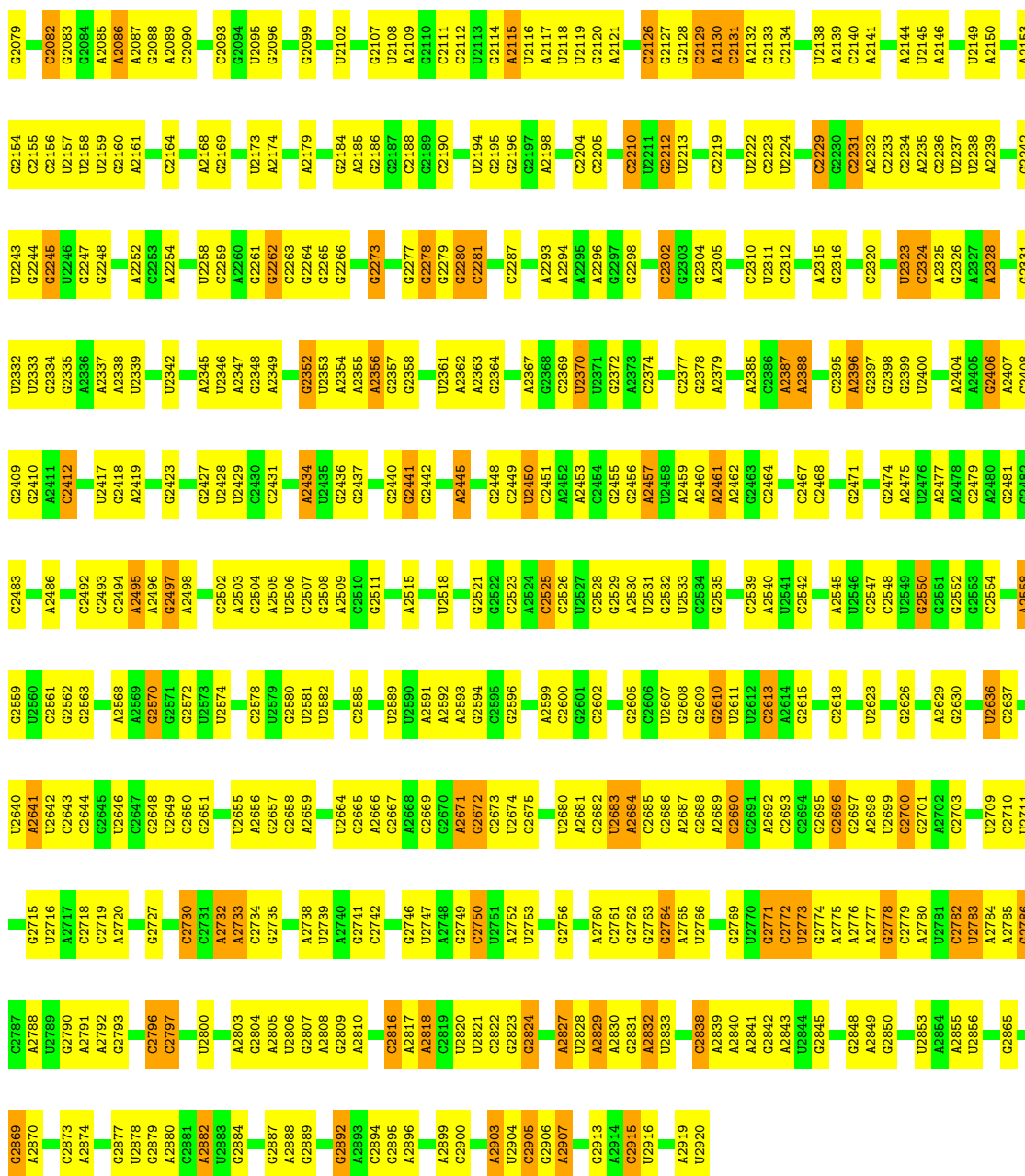
3 Residue-property plots

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

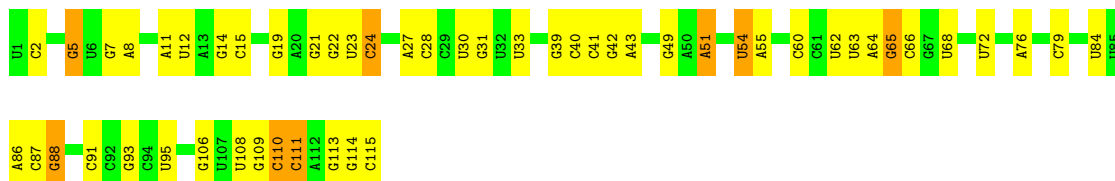
• Molecule 1: 23S ribosomal RNA



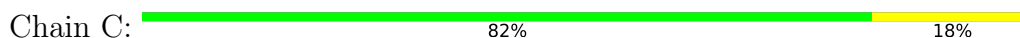


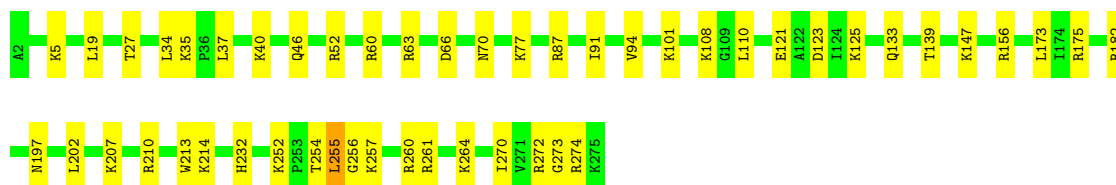


• Molecule 2: 5S ribosomal RNA



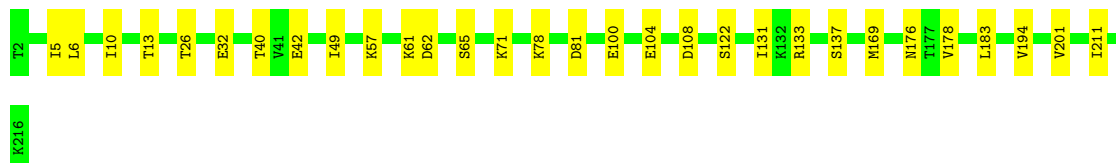
• Molecule 3: 50S ribosomal protein L2





- Molecule 4: 50S ribosomal protein L3

Chain D: 86% 14%



- Molecule 5: 50S ribosomal protein L4

Chain E: 79% 20%



- Molecule 6: 50S ribosomal protein L5

Chain F: 85% 15%



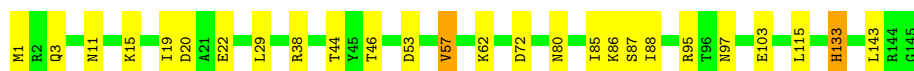
- Molecule 7: 50S ribosomal protein L6

Chain G: 87% 13%




- Molecule 8: 50S ribosomal protein L13

Chain H: 82% 17%



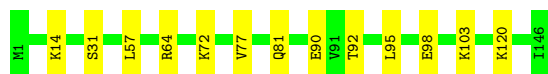
- Molecule 9: 50S ribosomal protein L14

Chain I:  83% 17%



- Molecule 10: 50S ribosomal protein L15

Chain J:  91% 9%




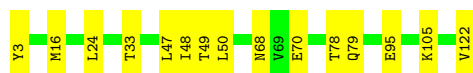
- Molecule 11: 50S ribosomal protein L16

Chain K:  86% 14%




- Molecule 12: 50S ribosomal protein L17

Chain L:  88% 12%




- Molecule 13: 50S ribosomal protein L18

Chain M:  79% 20%



- Molecule 14: 50S ribosomal protein L19

Chain N:  88% 12%




- Molecule 15: 50S ribosomal protein L20

Chain O:  89% 11%



- Molecule 16: 50S ribosomal protein L21

Chain P:  78% 22%




- Molecule 17: 50S ribosomal protein L22

Chain Q:  73% 27%




- Molecule 18: 50S ribosomal protein L23

Chain R:  82% 18%




- Molecule 19: 50S ribosomal protein L24

Chain S:  79% 20%




- Molecule 20: 50S ribosomal protein L25

Chain T:  81% 19%




- Molecule 21: 50S ribosomal protein L27

Chain U:  78% 21%




- Molecule 22: 50S ribosomal protein L28

Chain V:  81% 19%




- Molecule 23: 50S ribosomal protein L29

Chain W:  88% 12%



- Molecule 24: 50S ribosomal protein L30

Chain X:  86% 14%



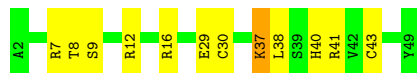
- Molecule 25: 50S ribosomal protein L31 type B

Chain Y:  98% .



- Molecule 26: 50S ribosomal protein L32

Chain Z:  75% 23% .




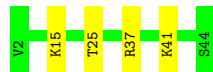
- Molecule 27: 50S ribosomal protein L33

Chain 1:  74% 26%




- Molecule 28: 50S ribosomal protein L34

Chain 2:  91% 9%




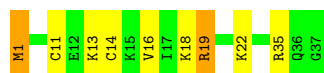
- Molecule 29: 50S ribosomal protein L35

Chain 3:  88% 12%



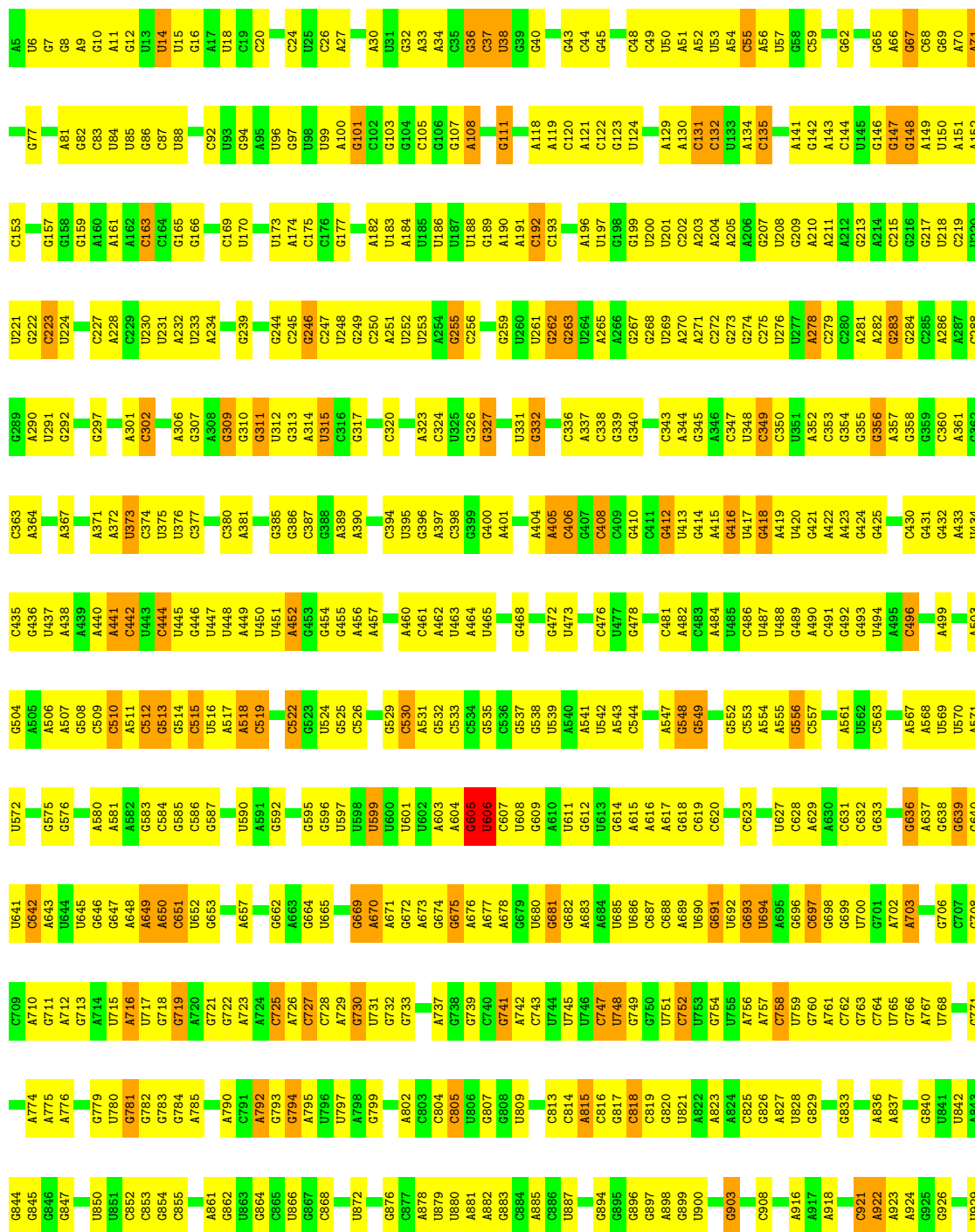
- Molecule 30: 50S ribosomal protein L36

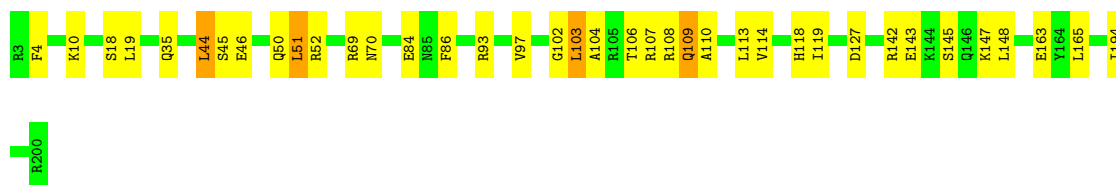
Chain 4:  76% 19% 5%



● Molecule 31: 16S ribosomal RNA

Chain a:  35% 54% 10%





- Molecule 35: 30S ribosomal protein S5

Chain e: 87% 13%



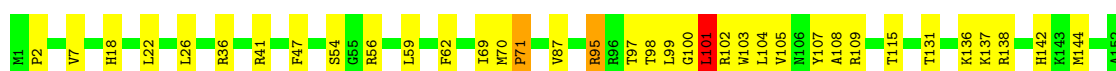
- Molecule 36: 30S ribosomal protein S6

Chain f: 81% 19%



- Molecule 37: 30S ribosomal protein S7

Chain g: 76% 22% ..



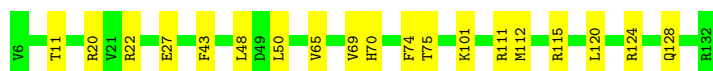
- Molecule 38: 30S ribosomal protein S8

Chain h: 82% 18%



- Molecule 39: 30S ribosomal protein S9

Chain i: 85% 15%




- Molecule 40: 30S ribosomal protein S10

Chain j: 82% 14%



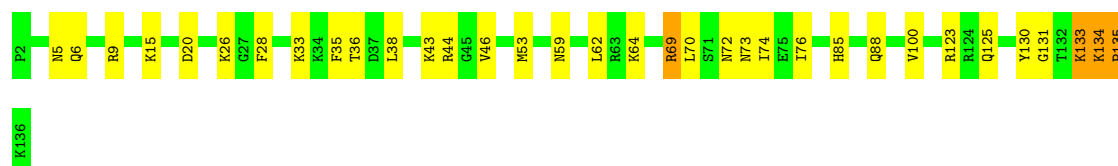
- Molecule 41: 30S ribosomal protein S11

Chain k:  77% 21% .



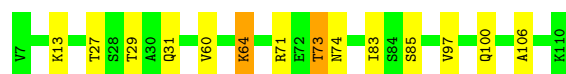
- Molecule 42: 30S ribosomal protein S12

Chain l:  75% 22% .



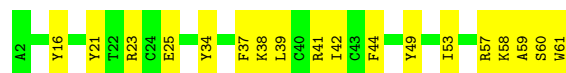
- Molecule 43: 30S ribosomal protein S13

Chain m:  87% 12% .




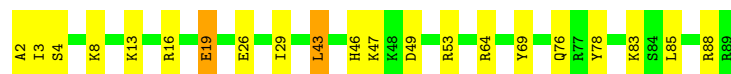
- Molecule 44: 30S ribosomal protein S14 type Z

Chain n:  70% 30% .




- Molecule 45: 30S ribosomal protein S15

Chain o:  76% 22% .




- Molecule 46: 30S ribosomal protein S16

Chain p:  81% 19% .




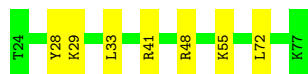
- Molecule 47: 30S ribosomal protein S17

Chain q:  78% 18% 5% .



- Molecule 48: 30S ribosomal protein S18

Chain r:  87% 13%




- Molecule 49: 30S ribosomal protein S19

Chain s:  74% 24% .



- Molecule 50: 30S ribosomal protein S20

Chain t:  84% 16%




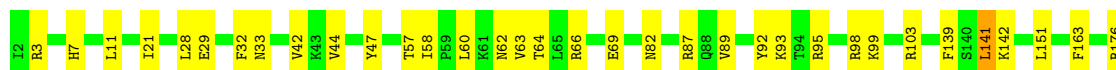
- Molecule 51: 30S ribosomal protein S21

Chain u:  75% 23% .



- Molecule 52: Ribosome hibernation promoting factor

Chain v:  78% 21% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145897	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 ($e^-/\text{\AA}^2$)	1.076	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.69	183/69739 (0.3%)	1.60	1291/108751 (1.2%)
2	B	1.04	0/2733	1.42	26/4257 (0.6%)
3	C	0.61	0/2125	0.82	2/2853 (0.1%)
4	D	0.70	0/1651	0.70	1/2215 (0.0%)
5	E	0.69	1/1595 (0.1%)	0.74	0/2154
6	F	0.37	0/1339	0.66	0/1805
7	G	0.38	0/1281	0.66	0/1736
8	H	0.66	0/1165	0.71	0/1570
9	I	0.65	0/925	0.80	0/1242
10	J	0.62	0/1100	0.71	0/1467
11	K	2.44	1/1095 (0.1%)	0.78	1/1472 (0.1%)
12	L	0.59	0/936	0.79	0/1253
13	M	0.45	0/900	0.70	0/1205
14	N	0.65	0/901	0.74	0/1209
15	O	0.71	0/954	0.76	0/1264
16	P	0.72	0/800	0.76	0/1070
17	Q	0.65	0/845	0.80	0/1140
18	R	0.60	0/723	0.68	0/966
19	S	0.49	0/779	0.69	0/1043
20	T	0.39	0/730	0.64	0/981
21	U	0.66	0/628	0.81	1/833 (0.1%)
22	V	0.49	0/451	0.76	0/603
23	W	0.45	0/542	0.73	0/722
24	X	0.64	0/451	0.71	0/606
25	Y	0.31	0/378	0.57	0/521
26	Z	0.63	0/366	0.85	0/489
27	1	0.44	0/395	0.77	0/530
28	2	0.78	0/371	0.81	0/484
29	3	0.60	0/526	0.83	1/690 (0.1%)
30	4	0.50	0/298	0.88	1/392 (0.3%)
31	a	2.36	45/36913 (0.1%)	1.54	698/57564 (1.2%)
32	b	1.12	1/1846 (0.1%)	0.63	1/2477 (0.0%)
33	c	0.29	0/1523	0.65	0/2062
34	d	0.31	0/1526	0.69	1/2063 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	e	0.32	0/1159	0.63	0/1566
36	f	0.36	0/789	0.66	0/1060
37	g	0.39	0/1175	0.87	2/1584 (0.1%)
38	h	1.16	4/1037 (0.4%)	0.96	7/1392 (0.5%)
39	i	0.34	0/937	0.71	0/1269
40	j	0.33	0/764	0.76	0/1034
41	k	0.34	0/824	0.75	1/1119 (0.1%)
42	l	6.63	7/1054 (0.7%)	0.87	4/1415 (0.3%)
43	m	0.32	0/732	0.71	0/991
44	n	6.34	3/497 (0.6%)	1.03	4/662 (0.6%)
45	o	0.33	0/732	0.72	1/979 (0.1%)
46	p	0.33	0/705	0.65	0/952
47	q	0.35	0/629	0.81	1/849 (0.1%)
48	r	0.35	0/452	0.72	0/604
49	s	6.45	8/654 (1.2%)	1.28	11/879 (1.3%)
50	t	0.37	0/591	0.73	0/793
51	u	0.45	0/403	0.83	1/535 (0.2%)
52	v	0.33	0/1350	0.72	1/1812 (0.1%)
All	All	1.85	253/153014 (0.2%)	1.41	2057/229184 (0.9%)

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
3	C	0	5
5	E	0	1
6	F	0	2
7	G	0	1
8	H	0	4
11	K	0	3
12	L	0	1
13	M	0	1
16	P	0	2
19	S	0	1
26	Z	0	2
30	4	0	2
31	a	0	2
32	b	0	4
33	c	0	1
34	d	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	g	0	10
39	i	0	1
40	j	0	4
41	k	0	5
42	l	0	2
43	m	0	5
44	n	0	4
45	o	0	4
47	q	0	5
49	s	0	3
50	t	0	1
51	u	0	3
52	v	0	3
All	All	0	89

All (253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	n	16	TYR	CB-CG	140.63	3.62	1.51
1	A	333	C	N1-C6	139.55	2.20	1.37
31	a	606	U	C2-N3	135.46	2.32	1.37
31	a	605	G	N3-C4	131.79	2.27	1.35
31	a	605	G	C2-N3	128.80	2.35	1.32
31	a	606	U	N1-C2	124.77	2.50	1.38
42	l	134	LYS	CD-CE	120.00	4.51	1.51
1	A	333	C	N3-C4	117.33	2.16	1.33
31	a	605	G	C6-N1	113.71	2.19	1.39
31	a	606	U	N1-C6	106.92	2.34	1.38
1	A	333	C	C2-N3	106.04	2.20	1.35
31	a	605	G	N1-C2	103.25	2.20	1.37
31	a	606	U	C4-C5	99.71	2.33	1.43
42	l	130	TYR	CD1-CE1	99.09	2.88	1.39
31	a	989	C	N1-C6	97.12	1.95	1.37
31	a	606	U	N3-C4	95.63	2.24	1.38
42	l	130	TYR	CD2-CE2	95.02	2.81	1.39
1	A	333	C	C4-C5	94.11	2.18	1.43
1	A	333	C	C5-C6	91.01	2.07	1.34
49	s	74	PHE	CD2-CE2	90.66	3.20	1.39
31	a	605	G	C5-C4	87.78	1.99	1.38
31	a	606	U	C5-C6	85.91	2.11	1.34
31	a	989	C	N3-C4	82.25	1.91	1.33
1	A	333	C	N1-C2	80.64	2.20	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	2	LEU	CG-CD1	78.91	4.43	1.51
31	a	989	C	C2-N3	74.72	1.95	1.35
49	s	74	PHE	CD1-CE1	73.03	2.85	1.39
31	a	605	G	C5-C6	70.56	2.12	1.42
49	s	74	PHE	CE1-CZ	70.36	2.71	1.37
49	s	74	PHE	CE2-CZ	67.60	2.65	1.37
1	A	393	G	C1'-N9	66.91	2.49	1.48
42	l	130	TYR	CE2-CZ	63.48	2.21	1.38
42	l	130	TYR	CE1-CZ	62.35	2.19	1.38
31	a	989	C	C4-C5	61.37	1.92	1.43
31	a	989	C	C5-C6	60.26	1.82	1.34
31	a	989	C	N1-C2	58.49	1.98	1.40
42	l	130	TYR	CG-CD1	50.42	2.04	1.39
42	l	130	TYR	CG-CD2	49.24	2.03	1.39
31	a	405	A	N9-C4	47.29	1.66	1.37
32	b	107	ILE	CG1-CD1	46.30	4.70	1.50
31	a	405	A	N7-C5	45.82	1.66	1.39
49	s	74	PHE	CG-CD1	42.95	2.03	1.38
49	s	74	PHE	CG-CD2	41.51	2.01	1.38
31	a	405	A	C8-N7	40.18	1.59	1.31
31	a	405	A	N9-C8	39.41	1.69	1.37
1	A	917	U	C2-N3	35.89	1.62	1.37
1	A	393	G	N9-C4	35.24	1.66	1.38
1	A	393	G	N9-C8	34.87	1.62	1.37
31	a	36	G	O3'-P	33.12	2.00	1.61
38	h	90	LYS	CA-C	29.85	2.30	1.52
1	A	917	U	N3-C4	28.67	1.64	1.38
31	a	1112	A	N3-C4	28.57	1.51	1.34
1	A	917	U	N1-C6	28.22	1.63	1.38
1	A	917	U	N1-C2	28.18	1.64	1.38
31	a	1112	A	C6-N1	27.92	1.55	1.35
1	A	917	U	C4-C5	26.44	1.67	1.43
31	a	405	A	C5-C4	25.48	1.56	1.38
1	A	917	U	C5-C6	25.29	1.56	1.34
31	a	36	G	C3'-O3'	22.72	1.74	1.42
1	A	393	G	N7-C5	-22.27	1.25	1.39
31	a	1112	A	N1-C2	20.36	1.52	1.34
49	s	36	ARG	CA-C	20.30	2.05	1.52
31	a	1112	A	C5-C4	18.29	1.51	1.38
31	a	1112	A	C2-N3	18.25	1.50	1.33
31	a	1112	A	C5-C6	17.78	1.57	1.41
38	h	90	LYS	N-CA	16.46	1.79	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2497	G	C8-N7	-8.76	1.25	1.30
1	A	1465	G	N7-C5	-7.94	1.34	1.39
1	A	393	G	C8-N7	-7.81	1.26	1.30
44	n	16	TYR	CG-CD1	7.76	1.49	1.39
1	A	2497	G	N7-C5	-7.13	1.34	1.39
5	E	132	GLU	C-N	-7.12	1.17	1.34
1	A	461	A	C5-C6	-7.12	1.34	1.41
31	a	263	G	N9-C8	-7.11	1.32	1.37
1	A	393	G	C2'-C1'	6.78	1.60	1.53
38	h	90	LYS	CB-CG	6.77	1.70	1.52
1	A	629	A	N9-C4	-6.77	1.33	1.37
1	A	766	G	C8-N7	-6.70	1.26	1.30
1	A	1059	A	N9-C4	-6.68	1.33	1.37
1	A	1633	A	N7-C5	-6.57	1.35	1.39
1	A	1468	G	N7-C5	-6.53	1.35	1.39
1	A	2044	C	N1-C6	-6.47	1.33	1.37
1	A	554	C	N1-C6	-6.40	1.33	1.37
1	A	1634	A	C5-C6	-6.40	1.35	1.41
1	A	1823	U	C4-C5	-6.38	1.37	1.43
38	h	90	LYS	CA-CB	6.38	1.68	1.53
1	A	1850	G	C6-N1	-6.37	1.35	1.39
1	A	1850	G	N9-C4	-6.35	1.32	1.38
1	A	2045	A	N9-C4	-6.33	1.34	1.37
1	A	396	G	C8-N7	-6.33	1.27	1.30
1	A	2242	G	C8-N7	-6.31	1.27	1.30
1	A	2849	A	N9-C4	-6.26	1.34	1.37
1	A	985	A	N9-C4	-6.24	1.34	1.37
1	A	1521	A	N3-C4	-6.21	1.31	1.34
1	A	303	G	N9-C8	-6.20	1.33	1.37
1	A	490	C	N1-C6	-6.16	1.33	1.37
1	A	1159	A	N9-C4	-6.15	1.34	1.37
1	A	756	A	N7-C5	-6.14	1.35	1.39
1	A	1468	G	C8-N7	-6.13	1.27	1.30
44	n	16	TYR	CG-CD2	6.11	1.47	1.39
31	a	1205	C	C4-C5	-6.09	1.38	1.43
1	A	1410	A	N9-C4	-6.09	1.34	1.37
1	A	1492	G	N9-C4	-6.06	1.33	1.38
1	A	1500	G	N7-C5	-6.05	1.35	1.39
1	A	2388	A	N9-C4	-6.04	1.34	1.37
1	A	2477	A	N9-C4	-6.01	1.34	1.37
1	A	2771	G	N7-C5	-6.00	1.35	1.39
1	A	200	A	N9-C4	-5.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	C	N3-C4	-5.96	1.29	1.33
1	A	845	A	N9-C4	-5.96	1.34	1.37
1	A	1500	G	C8-N7	-5.95	1.27	1.30
1	A	825	G	N9-C4	-5.94	1.33	1.38
1	A	1694	A	N9-C4	-5.93	1.34	1.37
1	A	624	C	N1-C6	-5.93	1.33	1.37
1	A	2818	A	N7-C5	-5.91	1.35	1.39
1	A	2028	A	N9-C4	-5.90	1.34	1.37
1	A	755	C	C4-C5	-5.88	1.38	1.43
1	A	1480	G	C2-N2	-5.87	1.28	1.34
1	A	737	C	C4-C5	-5.87	1.38	1.43
31	a	605	G	C8-N7	5.84	1.34	1.30
1	A	1850	G	N1-C2	-5.84	1.33	1.37
1	A	461	A	C8-N7	-5.83	1.27	1.31
1	A	1852	G	N3-C4	-5.82	1.31	1.35
31	a	1489	A	N9-C4	-5.81	1.34	1.37
1	A	2915	C	C2-N3	-5.80	1.31	1.35
1	A	2848	G	N9-C4	-5.79	1.33	1.38
1	A	336	U	C4-C5	-5.78	1.38	1.43
1	A	845	A	C5-C6	-5.76	1.35	1.41
1	A	2651	G	N9-C4	-5.73	1.33	1.38
1	A	2248	G	N9-C4	-5.72	1.33	1.38
1	A	870	C	N1-C6	-5.72	1.33	1.37
1	A	864	A	N9-C4	-5.71	1.34	1.37
1	A	1841	G	N9-C4	-5.71	1.33	1.38
31	a	1478	G	C8-N7	-5.67	1.27	1.30
1	A	493	A	N9-C4	-5.67	1.34	1.37
1	A	2850	G	N9-C4	-5.67	1.33	1.38
1	A	721	A	N7-C5	-5.65	1.35	1.39
1	A	476	A	N9-C4	-5.63	1.34	1.37
1	A	727	G	N9-C4	-5.63	1.33	1.38
1	A	1759	G	N9-C8	-5.60	1.33	1.37
1	A	548	A	N9-C4	-5.60	1.34	1.37
1	A	461	A	C6-N1	-5.60	1.31	1.35
1	A	919	G	C6-N1	-5.60	1.35	1.39
1	A	2400	U	C4-C5	-5.58	1.38	1.43
1	A	154	A	N9-C4	-5.57	1.34	1.37
1	A	334	A	N7-C5	-5.56	1.35	1.39
1	A	1037	A	C6-N6	-5.56	1.29	1.33
1	A	1622	C	C4-C5	-5.54	1.38	1.43
1	A	2698	A	N9-C4	-5.54	1.34	1.37
1	A	2671	A	N9-C4	-5.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	A	N9-C4	-5.52	1.34	1.37
1	A	512	A	N9-C4	-5.51	1.34	1.37
1	A	2076	A	C6-N1	-5.48	1.31	1.35
49	s	36	ARG	CA-CB	5.46	1.66	1.53
1	A	2437	G	N3-C4	-5.46	1.31	1.35
1	A	2281	C	N1-C6	-5.44	1.33	1.37
1	A	1494	G	C2-N3	-5.42	1.28	1.32
1	A	1881	A	N9-C4	-5.41	1.34	1.37
1	A	557	G	N9-C4	-5.41	1.33	1.38
1	A	1467	G	C8-N7	-5.40	1.27	1.30
1	A	1400	C	C4-C5	-5.39	1.38	1.43
31	a	263	G	N7-C5	-5.37	1.36	1.39
1	A	461	A	N7-C5	-5.36	1.36	1.39
1	A	2542	C	N1-C6	-5.34	1.33	1.37
1	A	2907	A	C6-N1	-5.34	1.31	1.35
1	A	402	C	N1-C6	-5.34	1.33	1.37
31	a	263	G	C8-N7	-5.33	1.27	1.30
1	A	44	A	N9-C4	-5.32	1.34	1.37
1	A	1017	A	N9-C4	-5.31	1.34	1.37
1	A	862	C	N3-C4	-5.31	1.30	1.33
1	A	2029	G	N9-C4	-5.30	1.33	1.38
1	A	2387	A	N9-C4	-5.30	1.34	1.37
1	A	713	A	N9-C4	-5.30	1.34	1.37
31	a	1173	G	N7-C5	-5.29	1.36	1.39
1	A	2732	A	C8-N7	-5.29	1.27	1.31
1	A	2919	A	N9-C4	-5.29	1.34	1.37
1	A	1471	A	N9-C4	-5.29	1.34	1.37
1	A	1622	C	C5-C6	-5.28	1.30	1.34
1	A	2810	A	N9-C4	-5.25	1.34	1.37
1	A	2877	G	N9-C4	-5.25	1.33	1.38
31	a	301	A	N7-C5	-5.25	1.36	1.39
1	A	1823	U	C5'-C4'	5.25	1.57	1.51
1	A	721	A	C5-C6	-5.25	1.36	1.41
1	A	2907	A	C5-C6	-5.25	1.36	1.41
1	A	897	A	C5-C6	-5.25	1.36	1.41
31	a	263	G	P-O5'	5.25	1.65	1.59
1	A	1445	C	C4-C5	-5.24	1.38	1.43
1	A	951	G	C2-N3	-5.24	1.28	1.32
1	A	1015	C	C4-C5	-5.24	1.38	1.43
1	A	1466	G	N1-C2	-5.24	1.33	1.37
1	A	2907	A	C6-N6	-5.23	1.29	1.33
1	A	1561	G	C6-N1	-5.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	A	N9-C4	-5.22	1.34	1.37
1	A	1634	A	N7-C5	-5.22	1.36	1.39
1	A	1851	G	C2-N2	-5.22	1.29	1.34
1	A	2497	G	C6-N1	-5.21	1.35	1.39
1	A	1772	G	C8-N7	-5.21	1.27	1.30
1	A	882	C	N1-C6	-5.21	1.34	1.37
1	A	2071	C	C4-C5	-5.20	1.38	1.43
1	A	208	G	C2-N3	-5.19	1.28	1.32
1	A	2408	C	C4-C5	-5.19	1.38	1.43
31	a	1381	G	N1-C2	-5.18	1.33	1.37
1	A	503	A	N9-C4	-5.18	1.34	1.37
1	A	517	A	N9-C4	-5.17	1.34	1.37
1	A	1207	G	N9-C4	-5.17	1.33	1.38
1	A	198	A	N9-C4	-5.17	1.34	1.37
1	A	1044	A	N9-C4	-5.17	1.34	1.37
1	A	1817	C	N1-C6	-5.17	1.34	1.37
1	A	2666	A	N9-C4	-5.16	1.34	1.37
1	A	881	G	N9-C4	-5.16	1.33	1.38
1	A	2838	C	N3-C4	-5.15	1.30	1.33
1	A	495	A	N9-C4	-5.14	1.34	1.37
1	A	1198	G	N9-C8	-5.14	1.34	1.37
1	A	2082	C	N1-C6	-5.14	1.34	1.37
31	a	1478	G	N7-C5	-5.14	1.36	1.39
1	A	559	A	N9-C4	-5.14	1.34	1.37
1	A	1359	A	N9-C4	-5.13	1.34	1.37
1	A	2248	G	C2-N3	-5.13	1.28	1.32
1	A	1987	A	N3-C4	-5.12	1.31	1.34
1	A	501	C	N1-C6	-5.12	1.34	1.37
1	A	777	C	N1-C6	-5.12	1.34	1.37
1	A	1853	C	N1-C6	-5.11	1.34	1.37
1	A	1954	A	N9-C8	-5.11	1.33	1.37
1	A	96	G	N9-C4	-5.10	1.33	1.38
1	A	2036	G	N9-C4	-5.09	1.33	1.38
1	A	15	G	N9-C4	-5.09	1.33	1.38
1	A	823	G	N9-C4	-5.09	1.33	1.38
1	A	2752	A	C5-C6	-5.09	1.36	1.41
1	A	2483	C	N1-C6	-5.08	1.34	1.37
31	a	263	G	N9-C4	5.07	1.42	1.38
1	A	859	C	C4-C5	-5.07	1.38	1.43
1	A	2896	A	N9-C4	-5.07	1.34	1.37
1	A	983	G	N9-C4	-5.07	1.33	1.38
1	A	613	G	N9-C8	-5.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1851	G	C2-N3	-5.06	1.28	1.32
1	A	1693	G	N9-C4	-5.06	1.33	1.38
1	A	178	A	N9-C4	-5.06	1.34	1.37
1	A	1222	A	C5-C6	-5.06	1.36	1.41
1	A	1480	G	C2-N3	-5.06	1.28	1.32
1	A	2738	A	C6-N6	-5.05	1.29	1.33
1	A	624	C	N3-C4	-5.05	1.30	1.33
1	A	1031	C	N1-C6	-5.05	1.34	1.37
1	A	627	C	C4-C5	-5.04	1.39	1.43
1	A	2771	G	C5-C6	-5.04	1.37	1.42
31	a	1395	G	N7-C5	-5.04	1.36	1.39
1	A	2738	A	C5-C6	-5.04	1.36	1.41
1	A	2497	G	C5-C6	-5.04	1.37	1.42
1	A	1991	G	N9-C4	-5.03	1.33	1.38
1	A	996	G	N9-C4	-5.03	1.33	1.38
1	A	1538	A	N9-C8	-5.03	1.33	1.37
1	A	1042	C	N1-C6	-5.02	1.34	1.37
1	A	1415	A	N9-C4	-5.02	1.34	1.37
1	A	491	C	N1-C6	-5.00	1.34	1.37

All (2057) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	G	C8-N9-C4	-101.80	65.68	106.40
1	A	393	G	N7-C8-N9	65.13	145.66	113.10
1	A	393	G	N9-C4-C5	52.43	126.37	105.40
1	A	393	G	N3-C4-C5	-40.30	108.45	128.60
31	a	605	G	C2-N3-C4	36.17	129.98	111.90
31	a	36	G	P-O3'-C3'	34.97	161.66	119.70
31	a	605	G	N1-C2-N3	-34.92	102.95	123.90
31	a	605	G	C4-C5-N7	-33.51	97.40	110.80
31	a	405	A	N7-C8-N9	-32.87	97.37	113.80
31	a	605	G	N3-C2-N2	32.23	142.46	119.90
31	a	605	G	N3-C4-N9	30.80	144.48	126.00
31	a	605	G	N3-C4-C5	-29.37	113.92	128.60
31	a	1112	A	N1-C2-N3	-27.78	115.41	129.30
31	a	605	G	N7-C8-N9	26.27	126.23	113.10
1	A	1823	U	C5-C6-N1	25.11	135.26	122.70
1	A	393	G	C2-N3-C4	24.61	124.20	111.90
31	a	405	A	C5-N7-C8	24.42	116.11	103.90
31	a	405	A	C8-N9-C4	22.87	114.95	105.80
31	a	1112	A	C2-N3-C4	22.70	121.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	G	C4-C5-C6	20.16	130.90	118.80
1	A	1822	C	C6-N1-C2	-19.14	112.64	120.30
1	A	393	G	C5-N7-C8	-18.72	94.94	104.30
31	a	37	C	N1-C2-O2	17.49	129.40	118.90
1	A	1823	U	C6-N1-C2	-17.32	110.61	121.00
31	a	605	G	C5-C6-N1	16.80	119.90	111.50
1	A	393	G	C4-N9-C1'	16.79	148.32	126.50
31	a	697	C	OP1-P-OP2	16.58	144.47	119.60
1	A	1634	A	N1-C6-N6	15.72	128.03	118.60
1	A	393	G	O4'-C1'-N9	15.65	120.72	108.20
38	h	90	LYS	O-C-N	-15.30	98.22	122.70
31	a	696	G	OP2-P-O3'	-14.82	72.60	105.20
31	a	696	G	OP1-P-O3'	-14.70	72.87	105.20
1	A	393	G	C8-N9-C1'	14.60	145.97	127.00
31	a	989	C	C2-N3-C4	14.55	127.17	119.90
1	A	393	G	C6-C5-N7	-14.48	121.71	130.40
31	a	989	C	N1-C2-N3	-14.44	109.09	119.20
49	s	36	ARG	N-CA-CB	-14.44	84.61	110.60
31	a	1381	G	N1-C6-O6	-14.09	111.45	119.90
31	a	697	C	N1-C2-O2	13.70	127.12	118.90
31	a	263	G	N3-C4-N9	13.51	134.11	126.00
1	A	1906	C	N1-C2-O2	13.37	126.92	118.90
1	A	919	G	C5-C6-O6	13.20	136.52	128.60
1	A	393	G	N9-C1'-C2'	13.19	131.14	114.00
1	A	2262	G	O5'-P-OP1	-13.15	93.87	105.70
31	a	263	G	C4-N9-C1'	12.88	143.25	126.50
1	A	1228	A	OP1-P-O3'	-12.74	77.17	105.20
1	A	461	A	N9-C4-C5	-12.74	100.70	105.80
31	a	989	C	C6-N1-C2	12.64	125.36	120.30
31	a	1125	C	N1-C2-O2	12.61	126.47	118.90
31	a	263	G	C6-C5-N7	-12.54	122.88	130.40
31	a	605	G	N1-C6-O6	-12.47	112.42	119.90
31	a	556	G	N9-C4-C5	-12.34	100.46	105.40
1	A	1461	C	N1-C2-O2	12.24	126.24	118.90
31	a	1381	G	C8-N9-C4	-12.20	101.52	106.40
1	A	461	A	C4-C5-N7	12.17	116.78	110.70
1	A	919	G	N1-C6-O6	-12.15	112.61	119.90
31	a	556	G	N3-C2-N2	12.11	128.38	119.90
1	A	333	C	C6-N1-C2	12.02	125.11	120.30
49	s	36	ARG	CB-CA-C	11.95	134.29	110.40
1	A	2497	G	C6-C5-N7	-11.77	123.34	130.40
49	s	36	ARG	O-C-N	-11.64	104.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	556	G	C4-C5-N7	11.54	115.42	110.80
31	a	263	G	N7-C8-N9	11.51	118.86	113.10
31	a	1381	G	C2-N3-C4	11.46	117.63	111.90
1	A	878	C	N3-C2-O2	-11.46	113.88	121.90
31	a	649	A	C8-N9-C4	-11.26	101.30	105.80
1	A	1633	A	N1-C6-N6	11.23	125.34	118.60
1	A	1634	A	C5-C6-N6	-11.22	114.73	123.70
31	a	1381	G	N3-C4-C5	-11.16	123.02	128.60
31	a	38	U	N3-C2-O2	-11.15	114.39	122.20
1	A	333	C	N1-C2-N3	-11.07	111.45	119.20
1	A	1468	G	C6-C5-N7	-11.06	123.77	130.40
31	a	1381	G	C5-C6-O6	11.03	135.22	128.60
31	a	1112	A	C6-N1-C2	10.97	125.18	118.60
31	a	1196	G	N3-C2-N2	10.96	127.57	119.90
1	A	336	U	C5-C6-N1	10.94	128.17	122.70
31	a	1381	G	N9-C4-C5	10.91	109.76	105.40
1	A	1467	G	C4-C5-N7	10.87	115.15	110.80
1	A	1822	C	C2-N1-C1'	10.87	130.75	118.80
49	s	74	PHE	CB-CG-CD1	-10.76	113.27	120.80
31	a	263	G	C8-N9-C1'	-10.75	113.03	127.00
1	A	333	C	C2-N3-C4	10.72	125.26	119.90
1	A	1906	C	N3-C2-O2	-10.72	114.40	121.90
38	h	90	LYS	N-CA-CB	-10.67	91.39	110.60
1	A	2915	C	N3-C2-O2	-10.66	114.43	121.90
1	A	756	A	C6-C5-N7	-10.62	124.86	132.30
31	a	37	C	N3-C2-O2	-10.60	114.48	121.90
1	A	751	A	N1-C6-N6	10.56	124.94	118.60
31	a	263	G	N3-C4-C5	-10.51	123.35	128.60
31	a	606	U	C6-N1-C1'	-10.50	106.50	121.20
31	a	687	C	C6-N1-C2	-10.49	116.10	120.30
31	a	1405	C	N1-C2-O2	10.49	125.19	118.90
1	A	333	C	N3-C4-C5	-10.48	117.71	121.90
31	a	606	U	C2-N1-C1'	10.43	130.21	117.70
31	a	1205	C	N1-C2-O2	10.41	125.15	118.90
1	A	396	G	C4-N9-C1'	10.41	140.03	126.50
1	A	1823	U	O4'-C1'-N1	10.40	116.52	108.20
31	a	989	C	N3-C4-C5	-10.29	117.78	121.90
31	a	725	C	C6-N1-C2	-10.24	116.20	120.30
31	a	1155	C	N1-C2-O2	10.23	125.04	118.90
31	a	605	G	C6-C5-N7	10.19	136.52	130.40
1	A	1822	C	C5-C6-N1	10.18	126.09	121.00
1	A	1228	A	OP2-P-O3'	-10.18	82.81	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1125	C	N3-C2-O2	-10.16	114.78	121.90
1	A	1480	G	N3-C2-N2	-10.14	112.80	119.90
1	A	806	A	N1-C6-N6	10.04	124.62	118.60
1	A	1906	C	C2-N1-C1'	10.04	129.84	118.80
31	a	1440	C	N3-C2-O2	-10.03	114.88	121.90
31	a	1405	C	C2-N1-C1'	10.01	129.81	118.80
1	A	1634	A	N9-C4-C5	-9.99	101.80	105.80
1	A	461	A	C6-C5-N7	-9.94	125.34	132.30
31	a	1173	G	C6-C5-N7	-9.94	124.44	130.40
1	A	396	G	N3-C4-N9	9.91	131.94	126.00
1	A	461	A	C5-N7-C8	-9.85	98.97	103.90
31	a	150	U	C5-C4-O4	-9.81	120.01	125.90
1	A	751	A	C5-C6-N6	-9.80	115.86	123.70
1	A	2525	C	N3-C2-O2	-9.78	115.05	121.90
31	a	1196	G	C4-C5-N7	9.77	114.71	110.80
1	A	2497	G	N9-C4-C5	-9.73	101.51	105.40
31	a	706	G	N9-C4-C5	-9.72	101.51	105.40
1	A	396	G	C8-N9-C1'	-9.69	114.41	127.00
31	a	1155	C	N3-C2-O2	-9.69	115.12	121.90
1	A	2782	C	C2-N1-C1'	9.68	129.45	118.80
1	A	1825	U	C5-C6-N1	9.66	127.53	122.70
1	A	2210	C	N3-C2-O2	-9.64	115.16	121.90
1	A	766	G	N9-C4-C5	-9.62	101.55	105.40
1	A	1467	G	N9-C4-C5	-9.62	101.55	105.40
31	a	605	G	N9-C4-C5	-9.61	101.56	105.40
31	a	1315	G	O4'-C1'-N9	9.61	115.89	108.20
1	A	2525	C	N1-C2-O2	9.59	124.65	118.90
1	A	333	C	C5-C4-N4	9.55	126.89	120.20
1	A	2734	C	N1-C2-O2	9.55	124.63	118.90
1	A	2797	C	N3-C2-O2	-9.55	115.22	121.90
49	s	74	PHE	CD1-CG-CD2	9.54	130.71	118.30
31	a	349	C	N1-C2-O2	9.54	124.62	118.90
31	a	758	C	N3-C2-O2	-9.51	115.24	121.90
1	A	1822	C	N3-C2-O2	-9.49	115.26	121.90
1	A	2361	U	C2-N1-C1'	9.48	129.08	117.70
1	A	2774	G	N1-C6-O6	-9.46	114.22	119.90
31	a	1019	C	N1-C2-O2	9.46	124.58	118.90
1	A	1823	U	C2-N3-C4	9.44	132.66	127.00
1	A	1461	C	N3-C2-O2	-9.44	115.29	121.90
1	A	2850	G	N3-C4-N9	-9.37	120.38	126.00
1	A	1467	G	C6-C5-N7	-9.37	124.78	130.40
1	A	1465	G	C8-N9-C4	-9.37	102.65	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	U	C5-C4-O4	-9.35	120.29	125.90
1	A	1850	G	N3-C4-C5	9.32	133.26	128.60
31	a	1382	U	C5-C6-N1	9.32	127.36	122.70
31	a	556	G	N3-C4-N9	9.32	131.59	126.00
1	A	284	C	C6-N1-C2	-9.27	116.59	120.30
31	a	989	C	N1-C2-O2	9.25	124.45	118.90
1	A	1500	G	C6-C5-N7	-9.23	124.86	130.40
31	a	697	C	N3-C2-O2	-9.22	115.44	121.90
1	A	1468	G	N7-C8-N9	9.19	117.69	113.10
1	A	1468	G	C4-C5-N7	9.18	114.47	110.80
1	A	2782	C	N1-C2-O2	9.16	124.40	118.90
1	A	756	A	N1-C6-N6	9.14	124.08	118.60
1	A	2210	C	N1-C2-O2	9.14	124.38	118.90
1	A	2907	A	N9-C4-C5	-9.13	102.15	105.80
42	l	130	TYR	CB-CG-CD2	-9.12	115.53	121.00
1	A	2497	G	C4-C5-N7	9.11	114.44	110.80
1	A	1500	G	C4-C5-N7	9.06	114.42	110.80
31	a	1395	G	C6-C5-N7	-9.06	124.97	130.40
1	A	917	U	C2-N1-C1'	-9.05	106.84	117.70
1	A	951	G	N3-C2-N2	-9.05	113.56	119.90
1	A	2150	A	C5-N7-C8	9.02	108.41	103.90
1	A	393	G	C4-C5-N7	-9.01	107.20	110.80
1	A	1822	C	P-O3'-C3'	8.98	130.48	119.70
1	A	897	A	N9-C4-C5	-8.97	102.21	105.80
1	A	1759	G	N7-C8-N9	8.97	117.59	113.10
1	A	2686	G	C8-N9-C4	-8.97	102.81	106.40
1	A	1824	C	C6-N1-C2	-8.97	116.71	120.30
31	a	1083	G	C6-C5-N7	-8.96	125.02	130.40
38	h	90	LYS	N-CA-C	8.97	135.21	111.00
31	a	706	G	C4-C5-N7	8.95	114.38	110.80
1	A	333	C	C4-C5-C6	8.93	121.87	117.40
1	A	2497	G	N3-C4-N9	8.92	131.35	126.00
31	a	1205	C	N3-C2-O2	-8.91	115.66	121.90
31	a	1196	G	N3-C4-N9	8.87	131.32	126.00
1	A	917	U	O4'-C1'-N1	8.86	115.28	108.20
31	a	1155	C	C2-N1-C1'	8.85	128.54	118.80
1	A	902	A	N1-C6-N6	8.85	123.91	118.60
31	a	781	G	C4-C5-N7	8.84	114.34	110.80
31	a	970	U	N3-C2-O2	-8.84	116.01	122.20
1	A	1467	G	N3-C2-N2	8.83	126.08	119.90
1	A	1823	U	N1-C2-O2	8.82	128.98	122.80
11	K	2	LEU	CB-CG-CD1	8.81	125.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	A	N1-C6-N6	8.81	123.88	118.60
31	a	1196	G	N9-C4-C5	-8.80	101.88	105.40
1	A	482	U	C5-C4-O4	-8.79	120.63	125.90
31	a	1382	U	C6-N1-C2	-8.74	115.75	121.00
1	A	160	G	N3-C4-C5	-8.73	124.23	128.60
1	A	623	C	N1-C2-O2	8.70	124.12	118.90
31	a	1028	G	N3-C4-N9	8.70	131.22	126.00
1	A	755	C	N1-C2-O2	8.66	124.09	118.90
1	A	414	C	N1-C2-O2	8.65	124.09	118.90
1	A	679	G	C6-C5-N7	-8.65	125.21	130.40
1	A	652	A	N1-C6-N6	8.63	123.78	118.60
31	a	1395	G	N3-C4-N9	8.62	131.17	126.00
31	a	135	C	C6-N1-C2	-8.62	116.85	120.30
1	A	1093	C	C6-N1-C2	-8.62	116.85	120.30
1	A	1492	G	N3-C4-N9	-8.61	120.83	126.00
31	a	605	G	C4-C5-C6	8.60	123.96	118.80
31	a	605	G	C5-N7-C8	8.60	108.60	104.30
31	a	606	U	C5-C6-N1	-8.58	118.41	122.70
31	a	122	C	C6-N1-C2	-8.58	116.87	120.30
31	a	1083	G	C4-C5-N7	8.57	114.23	110.80
1	A	1622	C	N1-C2-O2	8.56	124.04	118.90
31	a	967	A	N1-C6-N6	-8.52	113.49	118.60
1	A	393	G	C6-N1-C2	-8.52	119.99	125.10
31	a	405	A	C6-C5-N7	8.51	138.25	132.30
31	a	606	U	N3-C4-C5	8.50	119.70	114.60
1	A	1409	U	C5-C4-O4	-8.50	120.80	125.90
1	A	1222	A	N9-C4-C5	-8.48	102.41	105.80
44	n	16	TYR	CD1-CG-CD2	-8.48	108.57	117.90
1	A	917	U	C6-N1-C2	8.48	126.09	121.00
31	a	1421	C	C6-N1-C2	-8.46	116.92	120.30
31	a	549	G	C6-C5-N7	-8.46	125.32	130.40
31	a	1294	C	C6-N1-C2	-8.46	116.92	120.30
1	A	756	A	N9-C4-C5	-8.45	102.42	105.80
31	a	1293	C	N3-C2-O2	-8.44	115.99	121.90
31	a	150	U	N3-C4-O4	8.44	125.31	119.40
31	a	583	G	N3-C4-N9	-8.44	120.94	126.00
1	A	878	C	N1-C2-O2	8.41	123.95	118.90
1	A	988	C	N1-C2-O2	8.40	123.94	118.90
1	A	917	U	N1-C2-N3	-8.40	109.86	114.90
1	A	95	A	N1-C6-N6	8.40	123.64	118.60
1	A	433	U	C5-C4-O4	-8.38	120.87	125.90
1	A	917	U	N1-C2-O2	8.38	128.66	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1633	A	C5-C6-N6	-8.37	117.00	123.70
31	a	135	C	C2-N1-C1'	8.37	128.01	118.80
2	B	21	G	N3-C4-C5	8.36	132.78	128.60
31	a	344	A	N9-C4-C5	-8.36	102.46	105.80
3	C	256	GLY	N-CA-C	8.35	133.98	113.10
1	A	1851	G	N1-C6-O6	-8.34	114.89	119.90
1	A	2248	G	N3-C4-N9	-8.34	121.00	126.00
31	a	263	G	C4-C5-C6	8.33	123.80	118.80
1	A	2461	A	C5-C6-N6	-8.33	117.04	123.70
31	a	697	C	O5'-P-OP2	-8.33	98.21	105.70
31	a	1421	C	C5-C6-N1	8.33	125.16	121.00
1	A	1467	G	N3-C4-N9	8.32	130.99	126.00
1	A	2797	C	N1-C2-O2	8.31	123.89	118.90
1	A	942	C	N3-C2-O2	-8.30	116.09	121.90
1	A	752	G	N1-C6-O6	8.30	124.88	119.90
1	A	2915	C	N3-C4-N4	-8.30	112.19	118.00
1	A	2782	C	N3-C2-O2	-8.29	116.10	121.90
1	A	1759	G	C5-N7-C8	-8.29	100.16	104.30
1	A	1759	G	C6-C5-N7	-8.28	125.43	130.40
1	A	988	C	C2-N1-C1'	8.27	127.90	118.80
1	A	851	C	N1-C2-O2	8.27	123.86	118.90
31	a	1381	G	C4-N9-C1'	8.24	137.22	126.50
31	a	301	A	N7-C8-N9	8.22	117.91	113.80
31	a	332	G	C6-C5-N7	-8.22	125.47	130.40
31	a	350	C	N3-C2-O2	-8.22	116.15	121.90
1	A	1830	A	N1-C6-N6	8.21	123.53	118.60
31	a	1494	A	C5-C6-N6	-8.20	117.14	123.70
31	a	687	C	N3-C2-O2	-8.18	116.17	121.90
1	A	1823	U	C4-C5-C6	-8.18	114.79	119.70
31	a	599	U	N1-C2-O2	8.18	128.53	122.80
31	a	1348	G	C4-N9-C1'	8.18	137.13	126.50
1	A	766	G	N3-C4-N9	8.17	130.90	126.00
1	A	1607	A	C8-N9-C4	8.16	109.06	105.80
31	a	1382	U	O4'-C1'-N1	8.15	114.72	108.20
1	A	450	C	N3-C4-C5	8.13	125.15	121.90
49	s	74	PHE	CZ-CE2-CD2	-8.12	110.36	120.10
1	A	340	C	C6-N1-C2	-8.09	117.06	120.30
31	a	940	C	C6-N1-C2	-8.07	117.07	120.30
1	A	7	G	N3-C4-N9	-8.07	121.16	126.00
2	B	21	G	N3-C4-N9	-8.07	121.16	126.00
31	a	1381	G	C4-C5-N7	-8.06	107.57	110.80
1	A	942	C	N1-C2-O2	8.06	123.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	38	U	N1-C2-N3	8.06	119.74	114.90
1	A	2437	G	C2-N3-C4	8.05	115.93	111.90
1	A	2280	G	N7-C8-N9	8.05	117.12	113.10
1	A	265	A	N1-C6-N6	8.04	123.42	118.60
1	A	1823	U	N3-C2-O2	-8.04	116.57	122.20
31	a	1294	C	C6-N1-C1'	8.03	130.44	120.80
1	A	2130	A	O5'-P-OP2	-8.02	98.48	105.70
1	A	2907	A	C4-C5-N7	8.02	114.71	110.70
31	a	488	U	C2-N1-C1'	8.01	127.31	117.70
1	A	1850	G	C2-N3-C4	-8.00	107.90	111.90
1	A	1500	G	N7-C8-N9	8.00	117.10	113.10
1	A	751	A	C4-C5-N7	7.99	114.69	110.70
1	A	756	A	C4-C5-N7	7.99	114.69	110.70
1	A	2686	G	N7-C8-N9	7.98	117.09	113.10
1	A	1079	U	C5-C4-O4	7.98	130.69	125.90
31	a	1109	C	N1-C2-O2	7.97	123.68	118.90
1	A	1438	G	N3-C4-N9	-7.97	121.22	126.00
44	n	16	TYR	CB-CG-CD1	7.97	125.78	121.00
1	A	721	A	C5-N7-C8	-7.96	99.92	103.90
31	a	1395	G	N9-C4-C5	-7.96	102.22	105.40
1	A	1492	G	N3-C4-C5	7.94	132.57	128.60
31	a	135	C	N1-C2-O2	7.93	123.66	118.90
31	a	349	C	N3-C2-O2	-7.93	116.35	121.90
31	a	533	C	N1-C2-O2	7.92	123.65	118.90
31	a	651	C	C2-N3-C4	7.90	123.85	119.90
1	A	2461	A	N1-C6-N6	7.89	123.34	118.60
31	a	818	C	N3-C2-O2	-7.89	116.38	121.90
1	A	1441	C	C5-C6-N1	7.89	124.94	121.00
31	a	1028	G	N3-C2-N2	7.88	125.42	119.90
1	A	2248	G	N3-C4-C5	7.87	132.54	128.60
1	A	397	U	O5'-P-OP1	-7.87	98.62	105.70
31	a	1184	G	C4-C5-N7	7.87	113.95	110.80
1	A	2818	A	N1-C6-N6	7.87	123.32	118.60
1	A	460	C	O5'-P-OP2	-7.87	98.62	105.70
31	a	643	A	N9-C4-C5	-7.86	102.66	105.80
1	A	751	A	C5-N7-C8	-7.85	99.97	103.90
1	A	1851	G	N9-C4-C5	7.85	108.54	105.40
31	a	989	C	C4-C5-C6	7.85	121.32	117.40
44	n	16	TYR	CA-CB-CG	7.82	128.26	113.40
31	a	111	G	N3-C4-N9	-7.82	121.31	126.00
1	A	2730	C	N1-C2-O2	7.82	123.59	118.90
1	A	1468	G	N1-C6-O6	7.79	124.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	706	G	N3-C2-N2	7.79	125.35	119.90
1	A	2523	C	N3-C2-O2	-7.79	116.45	121.90
31	a	967	A	C5-C6-N6	7.78	129.93	123.70
1	A	95	A	C5-C6-N6	-7.78	117.48	123.70
31	a	122	C	C5-C6-N1	7.78	124.89	121.00
1	A	2563	G	N3-C4-N9	-7.77	121.34	126.00
31	a	344	A	C4-C5-N7	7.76	114.58	110.70
31	a	815	A	N1-C6-N6	7.76	123.26	118.60
1	A	1468	G	C5-N7-C8	-7.75	100.42	104.30
1	A	19	G	N1-C2-N2	-7.74	109.23	116.20
1	A	2696	G	N3-C4-N9	-7.74	121.36	126.00
1	A	2495	A	N1-C6-N6	-7.74	113.96	118.60
1	A	721	A	C4-C5-N7	7.74	114.57	110.70
1	A	924	G	C5-C6-O6	-7.73	123.96	128.60
1	A	284	C	C2-N1-C1'	7.72	127.30	118.80
31	a	148	G	C6-C5-N7	-7.72	125.77	130.40
31	a	1002	G	C6-C5-N7	-7.72	125.77	130.40
1	A	1391	A	N1-C6-N6	7.71	123.22	118.60
31	a	1098	G	N9-C4-C5	-7.71	102.32	105.40
1	A	897	A	C4-C5-N7	7.70	114.55	110.70
31	a	135	C	N3-C2-O2	-7.70	116.51	121.90
1	A	825	G	N3-C4-C5	7.70	132.45	128.60
1	A	1158	G	C5-C6-O6	-7.70	123.98	128.60
31	a	1332	C	C6-N1-C2	-7.69	117.22	120.30
1	A	2672	G	O4'-C1'-N9	7.69	114.35	108.20
1	A	104	C	N1-C2-O2	7.68	123.51	118.90
31	a	1152	G	N3-C4-N9	7.68	130.61	126.00
31	a	548	G	C6-C5-N7	-7.67	125.80	130.40
1	A	1441	C	C6-N1-C2	-7.67	117.23	120.30
1	A	1991	G	N3-C4-N9	-7.66	121.40	126.00
1	A	2131	C	C6-N1-C1'	7.66	129.99	120.80
31	a	1131	C	C2-N1-C1'	7.65	127.22	118.80
1	A	2778	G	N1-C6-O6	-7.65	115.31	119.90
1	A	2732	A	N9-C4-C5	-7.65	102.74	105.80
1	A	1607	A	N9-C4-C5	-7.64	102.74	105.80
1	A	767	A	N9-C4-C5	-7.63	102.75	105.80
1	A	951	G	N9-C4-C5	7.63	108.45	105.40
31	a	71	A	C5-C6-N6	-7.62	117.60	123.70
1	A	721	A	N7-C8-N9	7.61	117.61	113.80
1	A	1824	C	C5-C6-N1	7.61	124.81	121.00
1	A	208	G	N3-C2-N2	-7.61	114.58	119.90
31	a	781	G	C6-C5-N7	-7.61	125.83	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1083	G	N9-C4-C5	-7.60	102.36	105.40
1	A	806	A	C5-C6-N6	-7.60	117.62	123.70
31	a	649	A	C2-N3-C4	7.59	114.40	110.60
31	a	606	U	N1-C2-N3	-7.58	110.35	114.90
1	A	924	G	C6-C5-N7	-7.58	125.85	130.40
44	n	16	TYR	CB-CG-CD2	7.57	125.54	121.00
1	A	1759	G	C4-C5-N7	7.57	113.83	110.80
31	a	807	G	N9-C4-C5	-7.56	102.38	105.40
1	A	2850	G	N3-C4-C5	7.56	132.38	128.60
1	A	1841	G	N3-C4-C5	7.55	132.37	128.60
2	B	76	A	C5-C6-N6	-7.55	117.66	123.70
31	a	583	G	C8-N9-C1'	7.55	136.81	127.00
31	a	1405	C	C6-N1-C1'	-7.53	111.76	120.80
1	A	1622	C	C5-C4-N4	-7.53	114.93	120.20
1	A	766	G	N3-C2-N2	7.53	125.17	119.90
1	A	1004	A	N1-C6-N6	7.52	123.11	118.60
1	A	165	C	C6-N1-C2	-7.52	117.29	120.30
1	A	721	A	C6-C5-N7	-7.52	127.03	132.30
1	A	1823	U	N3-C4-O4	7.52	124.66	119.40
31	a	332	G	C4-C5-N7	7.51	113.81	110.80
31	a	1155	C	C6-N1-C2	-7.51	117.29	120.30
51	u	33	ARG	NE-CZ-NH1	7.51	124.06	120.30
31	a	1098	G	C4-C5-N7	7.50	113.80	110.80
31	a	514	G	N3-C2-N2	7.50	125.15	119.90
1	A	2641	A	N1-C6-N6	-7.49	114.10	118.60
31	a	279	C	N1-C2-O2	7.47	123.39	118.90
1	A	988	C	C6-N1-C1'	-7.47	111.83	120.80
31	a	807	G	C4-C5-N7	7.46	113.78	110.80
31	a	921	C	N3-C2-O2	-7.45	116.68	121.90
31	a	1173	G	N3-C4-N9	7.45	130.47	126.00
1	A	1468	G	C4-N9-C1'	7.45	136.19	126.50
31	a	556	G	N1-C2-N2	-7.44	109.50	116.20
1	A	1634	A	C8-N9-C4	7.43	108.77	105.80
2	B	111	C	C6-N1-C2	-7.43	117.33	120.30
31	a	1112	A	C4-C5-N7	-7.43	106.98	110.70
1	A	1229	G	OP1-P-OP2	7.42	130.74	119.60
1	A	1851	G	C8-N9-C4	-7.42	103.43	106.40
2	B	111	C	N3-C2-O2	-7.42	116.71	121.90
31	a	556	G	C6-C5-N7	-7.41	125.95	130.40
1	A	1719	C	C5-C4-N4	-7.41	115.02	120.20
31	a	246	G	N9-C4-C5	-7.40	102.44	105.40
31	a	302	C	C5-C6-N1	7.40	124.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	37	C	OP1-P-OP2	-7.40	108.50	119.60
1	A	2696	G	N3-C4-C5	7.39	132.30	128.60
31	a	675	G	N1-C6-O6	-7.39	115.47	119.90
31	a	405	A	C4-C5-N7	-7.37	107.01	110.70
31	a	670	A	N9-C4-C5	-7.37	102.85	105.80
1	A	576	U	N1-C2-O2	7.37	127.96	122.80
1	A	679	G	N9-C4-C5	-7.37	102.45	105.40
31	a	1470	U	C5-C4-O4	-7.36	121.48	125.90
31	a	549	G	N3-C4-N9	7.36	130.41	126.00
31	a	643	A	C4-C5-N7	7.35	114.38	110.70
1	A	2734	C	N3-C2-O2	-7.34	116.76	121.90
1	A	2771	G	C5-C6-O6	-7.34	124.20	128.60
1	A	133	A	N9-C4-C5	-7.33	102.87	105.80
31	a	1395	G	C8-N9-C1'	-7.33	117.47	127.00
1	A	762	C	N1-C2-O2	7.33	123.30	118.90
1	A	459	C	C6-N1-C2	-7.32	117.37	120.30
1	A	735	C	N3-C2-O2	-7.32	116.77	121.90
1	A	817	G	N1-C6-O6	-7.32	115.51	119.90
1	A	340	C	N3-C2-O2	-7.32	116.78	121.90
31	a	719	G	N1-C6-O6	-7.32	115.51	119.90
1	A	655	A	N9-C4-C5	-7.32	102.87	105.80
31	a	1173	G	C4-C5-N7	7.32	113.73	110.80
1	A	1494	G	N3-C4-N9	-7.31	121.61	126.00
31	a	918	A	C5-C6-N6	-7.31	117.86	123.70
1	A	2259	C	N1-C2-O2	7.30	123.28	118.90
31	a	1405	C	N3-C2-O2	-7.30	116.79	121.90
1	A	685	C	N1-C2-O2	7.29	123.28	118.90
1	A	752	G	C5-C6-O6	-7.29	124.22	128.60
31	a	315	U	N3-C2-O2	-7.29	117.10	122.20
1	A	396	G	N3-C4-C5	-7.27	124.96	128.60
31	a	1125	C	C6-N1-C2	-7.27	117.39	120.30
31	a	1383	G	C4-N9-C1'	7.26	135.94	126.50
1	A	1906	C	C6-N1-C2	-7.26	117.40	120.30
31	a	1395	G	C4-N9-C1'	7.25	135.93	126.50
1	A	2877	G	N3-C4-N9	-7.25	121.65	126.00
31	a	599	U	N3-C2-O2	-7.25	117.13	122.20
31	a	1173	G	C4-N9-C1'	7.24	135.91	126.50
1	A	396	G	C5-C6-O6	-7.24	124.26	128.60
1	A	924	G	C4-C5-N7	7.23	113.69	110.80
31	a	1263	G	N1-C6-O6	-7.22	115.56	119.90
31	a	583	G	C4-N9-C1'	-7.22	117.11	126.50
31	a	1494	A	N1-C6-N6	7.22	122.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	344	A	C6-C5-N7	-7.22	127.25	132.30
1	A	1759	G	C4-N9-C1'	7.21	135.88	126.50
1	A	961	G	C4-C5-N7	7.20	113.68	110.80
31	a	1236	C	N3-C2-O2	-7.19	116.87	121.90
31	a	675	G	C5-C6-O6	7.19	132.91	128.60
1	A	902	A	C5-C6-N6	-7.18	117.95	123.70
1	A	2342	U	C5-C4-O4	-7.18	121.59	125.90
31	a	696	G	C8-N9-C1'	7.18	136.34	127.00
1	A	1608	C	C5-C6-N1	7.18	124.59	121.00
31	a	263	G	N9-C4-C5	-7.17	102.53	105.40
1	A	450	C	N3-C4-N4	-7.17	112.98	118.00
1	A	766	G	C4-C5-N7	7.17	113.67	110.80
38	h	90	LYS	CA-C-N	7.17	132.97	117.20
31	a	1083	G	N3-C4-N9	7.16	130.30	126.00
1	A	303	G	N7-C8-N9	7.16	116.68	113.10
1	A	1466	G	C2-N3-C4	-7.16	108.32	111.90
1	A	608	C	C5-C4-N4	-7.16	115.19	120.20
31	a	670	A	C4-C5-N7	7.16	114.28	110.70
31	a	670	A	C6-C5-N7	-7.16	127.29	132.30
31	a	794	G	N1-C6-O6	-7.15	115.61	119.90
31	a	1428	A	N1-C6-N6	-7.15	114.31	118.60
31	a	1440	C	C6-N1-C2	-7.15	117.44	120.30
1	A	1881	A	N3-C4-N9	-7.14	121.69	127.40
1	A	1069	G	N3-C2-N2	-7.13	114.91	119.90
31	a	344	A	C5-N7-C8	-7.13	100.34	103.90
31	a	344	A	N1-C6-N6	7.13	122.88	118.60
1	A	2436	G	N1-C6-O6	7.12	124.17	119.90
1	A	1021	G	N3-C4-C5	7.12	132.16	128.60
1	A	2131	C	C2-N1-C1'	-7.12	110.97	118.80
31	a	792	A	C6-N1-C2	-7.12	114.33	118.60
1	A	334	A	N1-C6-N6	7.11	122.87	118.60
1	A	724	C	C6-N1-C2	-7.11	117.45	120.30
1	A	623	C	N3-C2-O2	-7.10	116.93	121.90
1	A	1467	G	N1-C2-N2	-7.09	109.81	116.20
1	A	133	A	C4-C5-N7	7.09	114.25	110.70
1	A	1534	G	N3-C4-N9	-7.09	121.75	126.00
1	A	1823	U	C4'-C3'-O3'	7.09	127.18	113.00
31	a	71	A	N1-C6-N6	7.09	122.85	118.60
31	a	416	G	N3-C4-N9	-7.09	121.75	126.00
1	A	924	G	N1-C6-O6	7.08	124.15	119.90
31	a	514	G	N9-C4-C5	-7.08	102.57	105.40
31	a	1383	G	N1-C6-O6	-7.08	115.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2436	G	C4-C5-N7	7.07	113.63	110.80
1	A	919	G	N3-C4-N9	-7.07	121.76	126.00
31	a	1184	G	N9-C4-C5	-7.07	102.57	105.40
31	a	1196	G	C6-C5-N7	-7.06	126.16	130.40
31	a	706	G	N3-C4-N9	7.06	130.24	126.00
1	A	386	C	N3-C4-C5	7.05	124.72	121.90
1	A	414	C	N3-C2-O2	-7.05	116.97	121.90
31	a	994	C	N3-C2-O2	-7.05	116.97	121.90
31	a	1002	G	C4-N9-C1'	7.05	135.66	126.50
1	A	2703	C	N3-C2-O2	-7.04	116.97	121.90
31	a	1125	C	C2-N1-C1'	7.04	126.54	118.80
31	a	1395	G	C4-C5-N7	7.04	113.62	110.80
31	a	123	G	C4-C5-N7	7.04	113.61	110.80
31	a	1294	C	N3-C2-O2	-7.04	116.97	121.90
31	a	1421	C	C2-N3-C4	7.04	123.42	119.90
31	a	1131	C	C6-N1-C2	-7.03	117.49	120.30
31	a	36	G	C8-N9-C4	-7.02	103.59	106.40
1	A	2848	G	N3-C4-C5	7.02	132.11	128.60
1	A	2437	G	N9-C4-C5	7.02	108.21	105.40
1	A	2797	C	C6-N1-C2	-7.02	117.49	120.30
1	A	1881	A	C2-N3-C4	-7.01	107.10	110.60
1	A	1850	G	C6-N1-C2	7.00	129.30	125.10
1	A	2047	A	C5-C6-N6	-7.00	118.10	123.70
31	a	418	G	C4-N9-C1'	6.99	135.59	126.50
31	a	956	G	C4-N9-C1'	6.99	135.58	126.50
1	A	396	G	C6-C5-N7	-6.99	126.21	130.40
1	A	2361	U	N3-C2-O2	-6.99	117.31	122.20
1	A	1757	U	C2-N3-C4	6.98	131.19	127.00
1	A	1850	G	C5-C6-O6	6.98	132.79	128.60
31	a	518	A	N1-C6-N6	6.98	122.79	118.60
1	A	919	G	C6-N1-C2	6.98	129.29	125.10
1	A	1494	G	C5-C6-O6	6.97	132.78	128.60
1	A	1158	G	C4-C5-N7	6.97	113.59	110.80
1	A	489	A	N1-C6-N6	6.96	122.78	118.60
1	A	2782	C	C6-N1-C1'	-6.96	112.44	120.80
31	a	606	U	N3-C4-O4	-6.96	114.53	119.40
1	A	2610	G	O4'-C1'-N9	6.96	113.76	108.20
31	a	1098	G	C8-N9-C1'	-6.95	117.96	127.00
1	A	1148	C	N3-C2-O2	-6.95	117.03	121.90
31	a	696	G	C4-N9-C1'	-6.95	117.47	126.50
49	s	74	PHE	CB-CG-CD2	-6.95	115.94	120.80
31	a	781	G	N9-C4-C5	-6.94	102.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	G	N3-C2-N2	6.93	124.75	119.90
1	A	160	G	C4-N9-C1'	6.93	135.51	126.50
31	a	549	G	C4-N9-C1'	6.93	135.50	126.50
31	a	1123	C	C2-N1-C1'	6.92	126.42	118.80
31	a	1453	A	N1-C6-N6	6.92	122.75	118.60
1	A	751	A	C6-C5-N7	-6.91	127.46	132.30
1	A	1905	G	C4-N9-C1'	6.91	135.48	126.50
1	A	2786	G	N3-C2-N2	-6.91	115.06	119.90
31	a	1441	C	C6-N1-C2	-6.91	117.54	120.30
1	A	1179	C	N1-C2-O2	6.90	123.04	118.90
2	B	76	A	N1-C6-N6	6.89	122.73	118.60
31	a	1233	C	C6-N1-C2	-6.89	117.54	120.30
1	A	2525	C	C6-N1-C2	-6.88	117.55	120.30
31	a	122	C	N1-C2-O2	6.88	123.03	118.90
1	A	924	G	N9-C4-C5	-6.88	102.65	105.40
31	a	510	C	C6-N1-C2	-6.88	117.55	120.30
31	a	649	A	N7-C8-N9	6.88	117.24	113.80
31	a	1324	C	N1-C2-O2	6.88	123.03	118.90
31	a	1072	G	N9-C4-C5	-6.87	102.65	105.40
31	a	1348	G	C8-N9-C1'	-6.87	118.07	127.00
1	A	756	A	C4-C5-C6	6.87	120.43	117.00
31	a	1383	G	O4'-C1'-N9	6.86	113.69	108.20
1	A	1634	A	C4-C5-N7	6.86	114.13	110.70
1	A	721	A	N1-C6-N6	6.86	122.71	118.60
1	A	1500	G	C5-N7-C8	-6.85	100.87	104.30
31	a	535	G	N9-C4-C5	-6.85	102.66	105.40
1	A	1603	U	C5-C4-O4	-6.85	121.79	125.90
31	a	1123	C	C6-N1-C2	-6.85	117.56	120.30
1	A	1015	C	C6-N1-C2	-6.85	117.56	120.30
31	a	792	A	C5-C6-N6	-6.84	118.22	123.70
1	A	1207	G	N3-C4-C5	6.84	132.02	128.60
1	A	629	A	N1-C6-N6	-6.84	114.50	118.60
1	A	1438	G	N3-C4-C5	6.84	132.02	128.60
31	a	719	G	C5-C6-O6	6.83	132.70	128.60
1	A	1158	G	N1-C6-O6	6.83	124.00	119.90
1	A	1385	G	N3-C4-C5	6.83	132.01	128.60
2	B	51	A	N1-C6-N6	6.83	122.70	118.60
1	A	652	A	C5-C6-N6	-6.82	118.24	123.70
1	A	1222	A	C4-C5-N7	6.82	114.11	110.70
1	A	1986	G	N3-C4-N9	-6.82	121.91	126.00
1	A	95	A	C4-C5-N7	6.82	114.11	110.70
31	a	604	A	N9-C4-C5	-6.82	103.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	148	G	C4-N9-C1'	6.81	135.36	126.50
31	a	1098	G	N3-C4-N9	6.81	130.09	126.00
31	a	1173	G	N9-C4-C5	-6.81	102.68	105.40
31	a	510	C	C5-C6-N1	6.81	124.40	121.00
42	l	130	TYR	CD1-CG-CD2	6.81	125.39	117.90
1	A	2651	G	N3-C4-C5	6.81	132.00	128.60
1	A	1469	G	N7-C8-N9	6.80	116.50	113.10
1	A	721	A	C5-C6-N6	-6.80	118.26	123.70
1	A	1367	C	N1-C2-O2	6.80	122.98	118.90
1	A	1906	C	C6-N1-C1'	-6.80	112.64	120.80
31	a	1494	A	C4-C5-N7	6.80	114.10	110.70
31	a	727	C	O5'-P-OP2	-6.79	99.58	105.70
1	A	1268	C	N1-C2-O2	6.79	122.98	118.90
1	A	2915	C	C5-C4-N4	6.79	124.95	120.20
1	A	575	G	N1-C2-N2	-6.79	110.09	116.20
1	A	2877	G	N3-C4-C5	6.78	131.99	128.60
31	a	1453	A	N9-C4-C5	-6.78	103.09	105.80
1	A	2905	C	N1-C2-O2	6.77	122.96	118.90
1	A	92	G	C5-C6-O6	6.77	132.66	128.60
1	A	2397	G	N3-C4-N9	-6.77	121.94	126.00
31	a	246	G	C4-C5-N7	6.77	113.51	110.80
1	A	1518	G	O4'-C1'-N9	6.76	113.61	108.20
1	A	2280	G	C8-N9-C4	-6.75	103.70	106.40
1	A	857	C	N3-C4-C5	6.75	124.60	121.90
1	A	1627	G	C6-C5-N7	-6.75	126.35	130.40
31	a	643	A	N1-C6-N6	6.75	122.65	118.60
1	A	1838	G	N3-C4-N9	-6.75	121.95	126.00
31	a	519	C	C6-N1-C2	-6.74	117.60	120.30
1	A	944	G	C6-C5-N7	-6.74	126.36	130.40
31	a	1218	C	N3-C2-O2	-6.74	117.18	121.90
31	a	1294	C	O4'-C1'-N1	6.74	113.59	108.20
1	A	95	A	N9-C4-C5	-6.74	103.11	105.80
31	a	263	G	C8-N9-C4	-6.74	103.71	106.40
1	A	1075	G	C8-N9-C1'	6.73	135.75	127.00
1	A	756	A	N3-C4-N9	6.73	132.79	127.40
1	A	333	C	C2-N1-C1'	-6.73	111.40	118.80
1	A	919	G	N3-C4-C5	6.72	131.96	128.60
1	A	412	U	C5-C4-O4	-6.72	121.87	125.90
1	A	2690	G	C4-C5-N7	6.72	113.49	110.80
49	s	36	ARG	N-CA-C	6.71	129.12	111.00
1	A	751	A	N7-C8-N9	6.71	117.16	113.80
2	B	76	A	C4-C5-N7	6.71	114.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1196	G	N1-C2-N2	-6.71	110.16	116.20
1	A	1283	G	N3-C4-N9	-6.70	121.98	126.00
31	a	1098	G	C6-C5-N7	-6.70	126.38	130.40
1	A	1075	G	C4-N9-C1'	-6.70	117.80	126.50
1	A	1480	G	N1-C2-N3	6.69	127.91	123.90
1	A	1851	G	C5-C6-O6	6.69	132.61	128.60
1	A	2764	G	C4-C5-N7	6.69	113.47	110.80
31	a	37	C	C2-N1-C1'	6.69	126.16	118.80
1	A	265	A	C5-C6-N6	-6.68	118.35	123.70
31	a	747	C	N3-C2-O2	-6.68	117.22	121.90
31	a	24	C	N3-C4-N4	-6.68	113.32	118.00
2	B	5	G	N3-C4-N9	-6.67	122.00	126.00
1	A	1603	U	N3-C4-O4	6.67	124.07	119.40
1	A	1024	A	C5-C6-N6	-6.67	118.36	123.70
1	A	755	C	C6-N1-C2	-6.67	117.63	120.30
1	A	7	G	N9-C4-C5	6.66	108.06	105.40
31	a	950	G	N9-C4-C5	6.65	108.06	105.40
31	a	111	G	N3-C2-N2	-6.65	115.25	119.90
31	a	514	G	N3-C4-N9	6.65	129.99	126.00
37	g	100	GLY	N-CA-C	6.63	129.68	113.10
1	A	96	G	N3-C4-N9	-6.63	122.02	126.00
1	A	2264	G	N3-C4-N9	-6.63	122.02	126.00
31	a	752	C	C6-N1-C2	-6.63	117.65	120.30
1	A	1410	A	N1-C6-N6	6.63	122.58	118.60
31	a	1072	G	C4-C5-N7	6.63	113.45	110.80
1	A	752	G	C4-C5-N7	6.63	113.45	110.80
31	a	416	G	C8-N9-C1'	6.63	135.61	127.00
1	A	1468	G	N9-C4-C5	-6.62	102.75	105.40
31	a	535	G	C4-C5-N7	6.62	113.45	110.80
31	a	725	C	N3-C2-O2	-6.62	117.26	121.90
31	a	903	G	N3-C4-C5	6.62	131.91	128.60
1	A	679	G	N3-C4-N9	6.62	129.97	126.00
38	h	90	LYS	CB-CA-C	6.62	123.64	110.40
31	a	1263	G	O4'-C1'-N9	6.62	113.49	108.20
1	A	1465	G	C4-N9-C1'	6.61	135.10	126.50
1	A	817	G	C5-C6-O6	6.61	132.57	128.60
1	A	2613	C	N3-C4-N4	-6.61	113.37	118.00
1	A	160	G	C8-N9-C4	-6.61	103.76	106.40
1	A	2408	C	N1-C2-O2	6.60	122.86	118.90
1	A	1986	G	C5-C6-O6	6.59	132.55	128.60
1	A	1822	C	N3-C4-C5	-6.58	119.27	121.90
1	A	1033	G	N1-C2-N2	-6.58	110.28	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1472	C	C6-N1-C2	-6.58	117.67	120.30
31	a	208	U	C5-C6-N1	6.57	125.99	122.70
1	A	16	G	N3-C4-C5	6.57	131.88	128.60
31	a	934	G	N7-C8-N9	6.57	116.38	113.10
1	A	878	C	N3-C4-N4	-6.56	113.41	118.00
31	a	1446	C	N3-C4-N4	6.55	122.59	118.00
31	a	37	C	C5-C6-N1	6.54	124.27	121.00
31	a	669	G	C4-N9-C1'	-6.54	117.99	126.50
1	A	2244	G	N9-C4-C5	6.54	108.02	105.40
1	A	2361	U	N1-C2-O2	6.54	127.38	122.80
31	a	794	G	N3-C4-C5	-6.54	125.33	128.60
31	a	549	G	C4-C5-N7	6.54	113.42	110.80
1	A	756	A	N7-C8-N9	6.54	117.07	113.80
1	A	2772	C	N3-C4-C5	6.54	124.51	121.90
1	A	2884	G	C4-C5-N7	6.53	113.41	110.80
31	a	213	G	C6-C5-N7	-6.53	126.48	130.40
31	a	1028	G	N9-C4-C5	-6.52	102.79	105.40
1	A	1213	C	C5-C4-N4	-6.52	115.64	120.20
1	A	1534	G	N3-C2-N2	-6.51	115.34	119.90
1	A	1608	C	N1-C2-O2	6.51	122.81	118.90
1	A	2326	G	C4-C5-N7	6.51	113.41	110.80
1	A	2727	G	C4-C5-N7	6.51	113.40	110.80
31	a	833	G	C5-C6-O6	6.51	132.50	128.60
31	a	833	G	N1-C6-O6	-6.51	116.00	119.90
1	A	1207	G	N3-C4-N9	-6.50	122.10	126.00
31	a	512	C	N1-C2-O2	6.50	122.80	118.90
1	A	2280	G	C4-N9-C1'	6.50	134.95	126.50
1	A	1495	C	C6-N1-C1'	6.49	128.59	120.80
1	A	1759	G	C8-N9-C1'	-6.49	118.56	127.00
1	A	2126	C	C6-N1-C2	-6.49	117.70	120.30
31	a	37	C	O5'-P-OP1	-6.49	99.86	105.70
1	A	2013	G	N3-C2-N2	6.48	124.44	119.90
31	a	416	G	C5-C6-O6	6.48	132.49	128.60
1	A	2013	G	C8-N9-C4	6.48	108.99	106.40
31	a	514	G	C4-C5-N7	6.48	113.39	110.80
31	a	807	G	N3-C4-N9	6.48	129.89	126.00
1	A	767	A	C4-C5-N7	6.48	113.94	110.70
1	A	918	G	N1-C6-O6	-6.47	116.02	119.90
1	A	2000	G	N3-C4-C5	6.47	131.84	128.60
31	a	301	A	C5-N7-C8	-6.47	100.66	103.90
1	A	208	G	O4'-C1'-N9	6.47	113.38	108.20
1	A	2398	G	N3-C4-C5	6.47	131.84	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	488	U	N3-C2-O2	-6.47	117.67	122.20
1	A	2651	G	C2-N3-C4	-6.47	108.67	111.90
31	a	1152	G	N3-C4-C5	-6.47	125.37	128.60
1	A	1701	U	N3-C4-O4	6.47	123.93	119.40
31	a	283	G	C5-C6-O6	-6.47	124.72	128.60
31	a	1453	A	C5-C6-N6	-6.46	118.53	123.70
1	A	1466	G	N1-C2-N2	-6.46	110.38	116.20
1	A	1828	U	N1-C2-O2	6.46	127.32	122.80
1	A	2436	G	N9-C4-C5	-6.46	102.82	105.40
31	a	989	C	N3-C2-O2	6.46	126.42	121.90
31	a	1098	G	C4-N9-C1'	6.46	134.90	126.50
31	a	548	G	C4-N9-C1'	6.46	134.89	126.50
1	A	528	C	N3-C4-N4	-6.45	113.48	118.00
1	A	2242	G	N9-C4-C5	-6.45	102.82	105.40
31	a	406	C	N1-C2-O2	6.45	122.77	118.90
1	A	410	G	C4-C5-N7	6.45	113.38	110.80
1	A	1635	A	O4'-C1'-N9	6.45	113.36	108.20
31	a	262	G	O4'-C1'-N9	6.45	113.36	108.20
31	a	956	G	C6-C5-N7	-6.45	126.53	130.40
1	A	882	C	C6-N1-C1'	-6.45	113.06	120.80
31	a	918	A	N1-C6-N6	6.45	122.47	118.60
1	A	1994	C	C2-N1-C1'	6.45	125.89	118.80
31	a	283	G	N1-C6-O6	6.45	123.77	119.90
31	a	1263	G	C5-C6-O6	6.45	132.47	128.60
31	a	263	G	N3-C2-N2	6.45	124.41	119.90
31	a	1441	C	N1-C2-N3	6.44	123.71	119.20
1	A	1954	A	N7-C8-N9	6.44	117.02	113.80
1	A	2818	A	C6-C5-N7	-6.44	127.79	132.30
1	A	2212	G	C5-C6-O6	6.44	132.46	128.60
31	a	669	G	C8-N9-C1'	6.44	135.37	127.00
31	a	1173	G	C8-N9-C1'	-6.44	118.63	127.00
1	A	96	G	N3-C4-C5	6.43	131.82	128.60
1	A	576	U	N3-C2-O2	-6.43	117.70	122.20
1	A	766	G	C6-C5-N7	-6.43	126.54	130.40
1	A	1467	G	C5-N7-C8	-6.43	101.08	104.30
2	B	51	A	C5-C6-N6	-6.43	118.55	123.70
31	a	649	A	C4-N9-C1'	6.43	137.88	126.30
31	a	1441	C	N3-C2-O2	-6.43	117.40	121.90
1	A	482	U	N3-C4-O4	6.43	123.90	119.40
31	a	1108	C	C6-N1-C2	-6.43	117.73	120.30
1	A	432	G	N3-C4-C5	-6.43	125.39	128.60
1	A	1496	G	O4'-C1'-N9	6.43	113.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	510	C	N1-C2-O2	6.43	122.76	118.90
31	a	747	C	C6-N1-C2	-6.42	117.73	120.30
1	A	2280	G	N3-C2-N2	-6.41	115.41	119.90
1	A	1654	A	N1-C6-N6	6.41	122.45	118.60
1	A	2064	A	C5-C6-N6	-6.41	118.57	123.70
31	a	1202	C	C6-N1-C2	-6.41	117.74	120.30
31	a	350	C	C6-N1-C2	-6.41	117.74	120.30
1	A	589	U	C5-C4-O4	-6.41	122.06	125.90
1	A	1410	A	C5-C6-N6	-6.41	118.58	123.70
1	A	1495	C	N1-C2-N3	6.41	123.68	119.20
1	A	1269	A	C4-C5-N7	6.40	113.90	110.70
31	a	571	A	N9-C4-C5	-6.40	103.24	105.80
31	a	758	C	C6-N1-C2	-6.40	117.74	120.30
32	b	97	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	7	G	C5-C6-O6	6.40	132.44	128.60
1	A	788	A	N9-C4-C5	-6.39	103.24	105.80
1	A	1024	A	N1-C6-N6	6.39	122.44	118.60
1	A	1633	A	N9-C4-C5	-6.39	103.24	105.80
1	A	2036	G	N3-C4-C5	6.39	131.79	128.60
1	A	647	G	C4-C5-N7	6.38	113.35	110.80
1	A	426	G	C6-C5-N7	-6.38	126.57	130.40
1	A	2212	G	N1-C6-O6	-6.38	116.07	119.90
31	a	1510	A	N9-C4-C5	-6.38	103.25	105.80
1	A	1634	A	C6-C5-N7	-6.38	127.84	132.30
31	a	548	G	N1-C6-O6	6.37	123.72	119.90
52	v	141	LEU	CA-CB-CG	6.37	129.96	115.30
31	a	781	G	C5-N7-C8	-6.37	101.11	104.30
1	A	685	C	N3-C2-O2	-6.37	117.44	121.90
1	A	2771	G	C6-C5-N7	-6.36	126.58	130.40
31	a	696	G	O4'-C1'-N9	6.36	113.29	108.20
31	a	344	A	N7-C8-N9	6.36	116.98	113.80
1	A	765	U	N3-C4-O4	6.36	123.85	119.40
31	a	14	U	C5-C4-O4	-6.36	122.09	125.90
1	A	1890	G	C2-N3-C4	-6.36	108.72	111.90
1	A	2523	C	N1-C2-O2	6.35	122.71	118.90
31	a	513	G	N3-C4-N9	-6.35	122.19	126.00
31	a	716	A	O5'-P-OP1	-6.35	99.98	105.70
1	A	432	G	C8-N9-C4	-6.35	103.86	106.40
31	a	1000	U	N3-C2-O2	-6.34	117.76	122.20
1	A	640	G	C2-N3-C4	-6.34	108.73	111.90
1	A	2099	G	N1-C2-N2	-6.34	110.50	116.20
1	A	2247	G	N3-C4-C5	6.33	131.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	647	G	N9-C4-C5	-6.33	102.87	105.40
1	A	1463	A	C4-C5-N7	6.33	113.86	110.70
1	A	2715	G	N3-C4-C5	6.33	131.76	128.60
1	A	2773	U	C5-C6-N1	6.33	125.86	122.70
31	a	416	G	C4-N9-C1'	-6.33	118.28	126.50
49	s	36	ARG	CA-C-N	6.32	131.11	117.20
1	A	1823	U	C5'-C4'-C3'	6.32	126.11	116.00
1	A	162	A	C4-N9-C1'	6.32	137.67	126.30
1	A	759	U	O4'-C1'-N1	6.31	113.25	108.20
1	A	1908	A	O4'-C1'-N9	6.31	113.25	108.20
47	q	77	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	53	A	N1-C6-N6	6.31	122.39	118.60
1	A	2036	G	C2-N3-C4	-6.30	108.75	111.90
1	A	1691	G	O5'-P-OP2	-6.30	100.03	105.70
1	A	882	C	C2-N1-C1'	6.30	125.73	118.80
1	A	629	A	C4-C5-C6	-6.29	113.85	117.00
31	a	263	G	C4-C5-N7	6.29	113.32	110.80
1	A	82	G	N3-C4-N9	-6.29	122.23	126.00
31	a	681	G	N1-C6-O6	-6.29	116.13	119.90
31	a	1072	G	N3-C4-N9	6.29	129.77	126.00
1	A	1075	G	N3-C4-N9	-6.28	122.23	126.00
31	a	1510	A	C5-C6-N6	-6.28	118.68	123.70
1	A	324	A	N1-C6-N6	6.27	122.36	118.60
1	A	333	C	N3-C2-O2	6.27	126.29	121.90
31	a	807	G	C5-C6-O6	-6.27	124.84	128.60
31	a	970	U	C2-N1-C1'	6.27	125.22	117.70
1	A	2610	G	C4-N9-C1'	-6.26	118.36	126.50
2	B	21	G	C2-N3-C4	-6.26	108.77	111.90
31	a	1002	G	C8-N9-C1'	-6.26	118.86	127.00
21	U	22	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	823	G	N3-C4-C5	6.26	131.73	128.60
1	A	1470	G	C2-N3-C4	-6.25	108.77	111.90
1	A	997	G	N1-C2-N2	-6.25	110.57	116.20
1	A	1053	A	C4-C5-N7	6.25	113.83	110.70
1	A	2102	U	C5-C4-O4	-6.25	122.15	125.90
1	A	2442	G	N7-C8-N9	6.25	116.23	113.10
31	a	1333	G	N3-C4-N9	6.25	129.75	126.00
31	a	1494	A	N9-C4-C5	-6.24	103.30	105.80
1	A	2774	G	N3-C2-N2	6.24	124.27	119.90
1	A	1509	G	C8-N9-C4	-6.24	103.90	106.40
31	a	604	A	C4-C5-N7	6.24	113.82	110.70
1	A	2379	A	N9-C4-C5	-6.24	103.31	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	956	G	N3-C4-N9	6.24	129.74	126.00
1	A	1468	G	C8-N9-C1'	-6.24	118.89	127.00
1	A	1754	C	N1-C2-O2	6.24	122.64	118.90
1	A	95	A	C5-N7-C8	-6.23	100.78	103.90
1	A	1622	C	N3-C4-N4	6.23	122.36	118.00
1	A	15	G	C2-N3-C4	-6.23	108.78	111.90
1	A	1409	U	N3-C4-O4	6.23	123.76	119.40
31	a	970	U	C6-N1-C2	-6.23	117.26	121.00
1	A	1496	G	C5-C6-N1	6.23	114.61	111.50
1	A	1336	G	N3-C4-C5	6.23	131.71	128.60
31	a	123	G	N9-C4-C5	-6.22	102.91	105.40
31	a	833	G	N3-C4-N9	-6.22	122.27	126.00
31	a	1395	G	N3-C2-N2	6.22	124.25	119.90
1	A	2610	G	C8-N9-C1'	6.21	135.08	127.00
31	a	1382	U	O5'-P-OP2	-6.21	100.11	105.70
1	A	2441	G	N7-C8-N9	6.21	116.20	113.10
1	A	1440	A	C8-N9-C4	6.21	108.28	105.80
1	A	1825	U	C2-N1-C1'	6.21	125.15	117.70
31	a	213	G	N7-C8-N9	6.21	116.20	113.10
31	a	1019	C	N3-C2-O2	-6.21	117.55	121.90
31	a	1028	G	C6-C5-N7	-6.21	126.67	130.40
31	a	693	G	N3-C2-N2	-6.21	115.56	119.90
1	A	7	G	C8-N9-C4	-6.21	103.92	106.40
1	A	1311	A	N7-C8-N9	6.20	116.90	113.80
1	A	1169	G	N7-C8-N9	6.20	116.20	113.10
31	a	1294	C	C5-C4-N4	6.19	124.53	120.20
1	A	1164	G	N1-C6-O6	6.19	123.61	119.90
31	a	681	G	C8-N9-C1'	6.19	135.05	127.00
31	a	1434	U	C5-C6-N1	6.19	125.80	122.70
1	A	1654	A	C5-C6-N6	-6.19	118.75	123.70
31	a	122	C	C2-N3-C4	6.19	122.99	119.90
1	A	1261	G	N1-C2-N2	-6.18	110.64	116.20
2	B	76	A	C5-N7-C8	-6.18	100.81	103.90
1	A	317	G	C2-N3-C4	-6.18	108.81	111.90
31	a	1083	G	C4-N9-C1'	6.18	134.53	126.50
31	a	444	C	C6-N1-C2	-6.18	117.83	120.30
38	h	90	LYS	CA-CB-CG	6.18	126.99	113.40
1	A	917	U	C5-C6-N1	-6.18	119.61	122.70
1	A	1541	C	C6-N1-C2	-6.18	117.83	120.30
1	A	1822	C	N1-C2-O2	6.18	122.61	118.90
31	a	478	G	C4-N9-C1'	6.18	134.53	126.50
31	a	1028	G	C4-C5-N7	6.17	113.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2231	C	C6-N1-C2	-6.17	117.83	120.30
31	a	697	C	C5-C6-N1	6.17	124.08	121.00
31	a	1002	G	N3-C4-N9	6.17	129.70	126.00
1	A	2397	G	N1-C6-O6	-6.16	116.20	119.90
31	a	1173	G	N1-C6-O6	6.16	123.60	119.90
1	A	2408	C	C6-N1-C2	-6.16	117.84	120.30
31	a	1451	G	C4-C5-N7	6.16	113.26	110.80
1	A	1093	C	C5-C6-N1	6.16	124.08	121.00
31	a	192	C	C6-N1-C2	-6.16	117.84	120.30
31	a	1453	A	C4-C5-N7	6.16	113.78	110.70
31	a	1028	G	C4-N9-C1'	6.15	134.49	126.50
31	a	1077	C	C6-N1-C2	-6.15	117.84	120.30
1	A	284	C	C5-C6-N1	6.15	124.07	121.00
1	A	751	A	N9-C4-C5	-6.15	103.34	105.80
31	a	122	C	N3-C4-N4	6.15	122.30	118.00
1	A	1991	G	N3-C4-C5	6.14	131.67	128.60
1	A	2750	C	N3-C2-O2	-6.14	117.60	121.90
49	s	72	GLY	N-CA-C	6.14	128.46	113.10
1	A	2771	G	C4-C5-N7	6.14	113.26	110.80
31	a	163	C	N3-C2-O2	-6.14	117.60	121.90
31	a	332	G	N9-C4-C5	-6.14	102.94	105.40
1	A	1406	G	N3-C4-C5	6.14	131.67	128.60
1	A	814	A	C5-C6-N6	-6.14	118.79	123.70
1	A	1463	A	N9-C4-C5	-6.14	103.34	105.80
31	a	488	U	N1-C2-O2	6.13	127.09	122.80
1	A	162	A	N7-C8-N9	6.13	116.86	113.80
1	A	324	A	N7-C8-N9	6.13	116.86	113.80
1	A	160	G	C2-N3-C4	6.13	114.96	111.90
31	a	442	C	N3-C2-O2	-6.13	117.61	121.90
1	A	735	C	N1-C2-O2	6.12	122.58	118.90
1	A	825	G	C2-N3-C4	-6.12	108.84	111.90
31	a	1466	G	C4-N9-C1'	6.12	134.46	126.50
1	A	862	C	N1-C2-O2	6.12	122.58	118.90
1	A	2247	G	N3-C4-N9	-6.12	122.33	126.00
31	a	387	C	C2-N1-C1'	6.12	125.54	118.80
31	a	1107	C	N1-C2-O2	6.12	122.57	118.90
31	a	794	G	C4-C5-N7	-6.12	108.35	110.80
1	A	2816	C	N1-C2-O2	6.12	122.57	118.90
1	A	2021	C	C5-C4-N4	-6.12	115.92	120.20
31	a	148	G	N3-C4-N9	6.12	129.67	126.00
31	a	807	G	C6-C5-N7	-6.11	126.73	130.40
1	A	1380	G	C8-N9-C1'	-6.11	119.06	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1463	A	C6-C5-N7	-6.11	128.03	132.30
31	a	36	G	OP2-P-O3'	6.11	118.64	105.20
31	a	612	G	N3-C4-N9	6.10	129.66	126.00
31	a	815	A	N9-C4-C5	-6.10	103.36	105.80
1	A	2892	G	N3-C2-N2	-6.10	115.63	119.90
1	A	1286	G	N1-C2-N2	-6.09	110.72	116.20
31	a	36	G	C4'-C3'-O3'	6.09	125.18	113.00
1	A	2361	U	C6-N1-C1'	-6.09	112.68	121.20
31	a	781	G	N1-C6-O6	6.09	123.55	119.90
1	A	2783	U	OP1-P-O3'	6.08	118.58	105.20
31	a	553	C	N3-C2-O2	-6.08	117.64	121.90
1	A	307	A	N9-C4-C5	-6.08	103.37	105.80
1	A	589	U	N3-C4-O4	6.08	123.66	119.40
1	A	2733	A	N9-C4-C5	-6.08	103.37	105.80
1	A	1269	A	N9-C4-C5	-6.08	103.37	105.80
1	A	2816	C	C6-N1-C2	-6.08	117.87	120.30
31	a	1383	G	N3-C4-C5	-6.07	125.56	128.60
1	A	2764	G	N9-C4-C5	-6.07	102.97	105.40
1	A	2400	U	N3-C4-O4	6.07	123.65	119.40
1	A	2408	C	C2-N1-C1'	6.07	125.48	118.80
29	3	42	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	983	G	C2-N3-C4	-6.07	108.87	111.90
1	A	1465	G	N7-C8-N9	6.07	116.13	113.10
1	A	1513	A	N7-C8-N9	6.06	116.83	113.80
1	A	2397	G	C6-C5-N7	6.06	134.04	130.40
1	A	679	G	C4-C5-N7	6.05	113.22	110.80
1	A	740	G	C2-N3-C4	-6.05	108.87	111.90
1	A	1380	G	C4-N9-C1'	6.05	134.37	126.50
31	a	1421	C	N1-C2-O2	6.05	122.53	118.90
1	A	107	G	N3-C4-C5	6.05	131.63	128.60
1	A	1834	G	N3-C4-N9	-6.05	122.37	126.00
1	A	1841	G	N3-C4-N9	-6.05	122.37	126.00
1	A	2644	C	C5-C4-N4	-6.05	115.97	120.20
1	A	1186	A	C5-C6-N6	-6.04	118.86	123.70
1	A	1825	U	C6-N1-C2	-6.04	117.38	121.00
1	A	2029	G	N3-C4-C5	6.04	131.62	128.60
1	A	1815	C	N3-C4-C5	6.04	124.31	121.90
1	A	1627	G	C4-C5-N7	6.03	113.21	110.80
1	A	624	C	C2-N1-C1'	6.03	125.43	118.80
1	A	546	A	N1-C6-N6	6.03	122.22	118.60
1	A	2277	G	N3-C2-N2	-6.03	115.68	119.90
31	a	1072	G	C6-C5-N7	-6.03	126.78	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1742	A	N1-C6-N6	6.03	122.22	118.60
31	a	315	U	C6-N1-C2	-6.03	117.39	121.00
31	a	1293	C	N1-C2-O2	6.03	122.52	118.90
31	a	642	C	C5-C4-N4	-6.02	115.98	120.20
31	a	263	G	C5-N7-C8	-6.02	101.29	104.30
31	a	643	A	C6-C5-N7	-6.02	128.09	132.30
31	a	815	A	C5-C6-N6	-6.01	118.89	123.70
1	A	1539	A	N1-C6-N6	-6.01	114.99	118.60
31	a	1028	G	C8-N9-C1'	-6.01	119.19	127.00
1	A	522	G	C2-N3-C4	-6.00	108.90	111.90
1	A	2497	G	N1-C6-O6	6.00	123.50	119.90
31	a	553	C	N1-C2-O2	6.00	122.50	118.90
1	A	1452	C	N3-C4-N4	-6.00	113.80	118.00
1	A	2675	G	N3-C2-N2	6.00	124.10	119.90
1	A	1004	A	C5-C6-N6	-6.00	118.90	123.70
1	A	2437	G	N1-C6-O6	-6.00	116.30	119.90
31	a	1451	G	N3-C4-N9	6.00	129.60	126.00
1	A	1719	C	N3-C4-N4	6.00	122.20	118.00
31	a	249	G	C4-C5-N7	5.99	113.20	110.80
31	a	583	G	C6-C5-N7	5.99	133.99	130.40
1	A	452	G	N3-C4-N9	-5.99	122.41	126.00
31	a	548	G	N3-C4-N9	5.99	129.59	126.00
31	a	1143	C	N3-C2-O2	-5.99	117.71	121.90
1	A	897	A	N1-C6-N6	5.99	122.19	118.60
1	A	303	G	C5-N7-C8	-5.98	101.31	104.30
31	a	496	C	N1-C2-O2	5.98	122.49	118.90
31	a	37	C	C2-N3-C4	5.98	122.89	119.90
1	A	756	A	C4-N9-C1'	5.98	137.06	126.30
1	A	1283	G	N3-C4-C5	5.97	131.59	128.60
31	a	955	A	O4'-C1'-N9	5.97	112.98	108.20
1	A	755	C	N3-C2-O2	-5.97	117.72	121.90
3	C	156	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	1015	C	C5-C6-N1	5.97	123.98	121.00
1	A	1521	A	N1-C2-N3	-5.97	126.31	129.30
31	a	1197	G	P-O3'-C3'	5.97	126.86	119.70
31	a	918	A	C4-C5-N7	5.97	113.68	110.70
1	A	2448	G	N9-C4-C5	-5.97	103.01	105.40
1	A	1709	A	N7-C8-N9	5.97	116.78	113.80
1	A	1837	A	N1-C6-N6	5.96	122.18	118.60
1	A	2578	C	C6-N1-C2	5.96	122.69	120.30
1	A	1245	G	N3-C4-C5	5.96	131.58	128.60
1	A	636	A	C5-N7-C8	-5.96	100.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2115	A	C5-N7-C8	-5.96	100.92	103.90
1	A	2596	G	N3-C4-C5	5.96	131.58	128.60
1	A	92	G	N3-C4-N9	-5.96	122.42	126.00
1	A	851	C	N3-C2-O2	-5.96	117.73	121.90
1	A	1932	C	C2-N1-C1'	5.96	125.36	118.80
31	a	758	C	C5-C4-N4	5.96	124.37	120.20
1	A	546	A	C5-C6-N6	-5.96	118.94	123.70
1	A	918	G	C5-C6-O6	5.96	132.17	128.60
1	A	1480	G	C5-C6-O6	5.96	132.17	128.60
1	A	2842	G	N1-C2-N2	-5.96	110.84	116.20
31	a	794	G	N9-C4-C5	5.96	107.78	105.40
31	a	956	G	C8-N9-C1'	-5.96	119.26	127.00
1	A	506	A	N1-C6-N6	5.95	122.17	118.60
31	a	1478	G	C6-C5-N7	-5.95	126.83	130.40
1	A	768	A	N9-C4-C5	-5.95	103.42	105.80
1	A	1196	C	N1-C2-O2	5.95	122.47	118.90
31	a	549	G	C8-N9-C1'	-5.95	119.27	127.00
1	A	14	A	C5-C6-N6	-5.94	118.94	123.70
1	A	1021	G	C4-C5-N7	5.94	113.18	110.80
1	A	1838	G	N3-C4-C5	5.94	131.57	128.60
1	A	1079	U	N3-C4-O4	-5.94	115.24	119.40
1	A	27	G	N3-C4-C5	5.94	131.57	128.60
1	A	1709	A	N1-C6-N6	5.94	122.16	118.60
31	a	418	G	C8-N9-C1'	-5.94	119.28	127.00
1	A	45	G	C4-N9-C1'	-5.93	118.79	126.50
1	A	752	G	C5-N7-C8	-5.93	101.33	104.30
1	A	333	C	C5-C6-N1	-5.93	118.03	121.00
1	A	2778	G	C5-C6-O6	5.93	132.16	128.60
31	a	706	G	C6-C5-N7	-5.92	126.84	130.40
1	A	1030	C	C5-C4-N4	-5.92	116.06	120.20
1	A	2056	G	N3-C4-C5	5.92	131.56	128.60
1	A	2408	C	C5-C6-N1	5.92	123.96	121.00
31	a	159	G	N3-C4-N9	-5.92	122.45	126.00
1	A	2115	A	C4-C5-N7	5.92	113.66	110.70
1	A	461	A	N7-C8-N9	5.92	116.76	113.80
1	A	1908	A	N9-C4-C5	5.92	108.17	105.80
2	B	108	U	C2-N1-C1'	5.92	124.80	117.70
1	A	439	U	N1-C2-O2	5.92	126.94	122.80
1	A	1158	G	C6-C5-N7	-5.91	126.85	130.40
1	A	1511	C	C6-N1-C2	-5.91	117.93	120.30
1	A	768	A	C4-C5-N7	5.91	113.66	110.70
1	A	1008	C	N3-C4-N4	-5.91	113.86	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2441	G	C8-N9-C4	-5.91	104.04	106.40
31	a	1383	G	C8-N9-C1'	-5.91	119.32	127.00
31	a	1394	C	N1-C2-O2	5.91	122.44	118.90
31	a	101	G	N3-C4-N9	-5.91	122.46	126.00
1	A	1400	C	C5-C4-N4	-5.90	116.07	120.20
1	A	2763	G	N3-C2-N2	5.90	124.03	119.90
1	A	396	G	N9-C4-C5	-5.90	103.04	105.40
1	A	439	U	N3-C2-O2	-5.90	118.07	122.20
31	a	681	G	N9-C4-C5	5.90	107.76	105.40
31	a	1507	C	C6-N1-C1'	5.90	127.88	120.80
1	A	881	G	N3-C4-N9	-5.89	122.46	126.00
31	a	583	G	N3-C2-N2	-5.89	115.77	119.90
31	a	650	A	N1-C6-N6	-5.89	115.06	118.60
1	A	1850	G	N3-C4-N9	-5.89	122.47	126.00
1	A	1500	G	C8-N9-C4	-5.89	104.05	106.40
1	A	2845	G	N3-C4-C5	5.89	131.54	128.60
1	A	1222	A	C8-N9-C4	5.89	108.15	105.80
1	A	46	C	C6-N1-C2	-5.88	117.95	120.30
1	A	951	G	C8-N9-C4	-5.88	104.05	106.40
1	A	160	G	N3-C4-N9	5.88	129.53	126.00
1	A	1400	C	N1-C2-O2	5.88	122.43	118.90
1	A	1687	G	N3-C4-C5	5.88	131.54	128.60
1	A	1637	A	C4-C5-N7	5.88	113.64	110.70
1	A	2727	G	N3-C2-N2	5.87	124.01	119.90
31	a	515	C	C6-N1-C2	-5.87	117.95	120.30
1	A	988	C	N3-C2-O2	-5.87	117.79	121.90
1	A	1286	G	N3-C2-N2	5.87	124.01	119.90
1	A	1268	C	N3-C2-O2	-5.87	117.79	121.90
1	A	2261	G	O3'-P-O5'	5.87	115.15	104.00
1	A	2323	U	O4'-C1'-N1	5.87	112.89	108.20
31	a	1184	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1905	G	C8-N9-C1'	-5.86	119.38	127.00
31	a	175	C	C6-N1-C2	-5.86	117.95	120.30
31	a	263	G	N1-C2-N2	-5.86	110.92	116.20
1	A	280	C	C6-N1-C2	-5.86	117.95	120.30
1	A	2102	U	N3-C4-O4	5.86	123.50	119.40
1	A	1038	C	N3-C4-C5	5.86	124.24	121.90
1	A	2019	G	N1-C2-N2	-5.86	110.93	116.20
1	A	1823	U	N3-C4-C5	-5.86	111.09	114.60
31	a	1489	A	N3-C4-N9	-5.86	122.71	127.40
31	a	696	G	C6-C5-N7	5.86	133.91	130.40
1	A	470	G	N3-C4-N9	-5.85	122.49	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1226	G	C2-N3-C4	-5.85	108.97	111.90
1	A	897	A	C6-C5-N7	-5.85	128.20	132.30
1	A	2771	G	N9-C4-C5	-5.85	103.06	105.40
31	a	681	G	C6-C5-N7	5.85	133.91	130.40
2	B	79	C	N3-C4-C5	5.85	124.24	121.90
1	A	1495	C	C6-N1-C2	-5.85	117.96	120.30
31	a	1510	A	C4-C5-N7	5.85	113.62	110.70
1	A	1475	A	C4-C5-N7	5.84	113.62	110.70
31	a	818	C	C6-N1-C2	-5.84	117.96	120.30
1	A	961	G	C5-N7-C8	-5.84	101.38	104.30
1	A	1296	C	N1-C2-O2	5.84	122.41	118.90
1	A	2061	U	C5-C4-O4	-5.84	122.39	125.90
31	a	442	C	C5-C4-N4	5.84	124.29	120.20
1	A	450	C	C6-N1-C2	5.84	122.64	120.30
1	A	655	A	C4-C5-N7	5.83	113.62	110.70
1	A	1361	G	O4'-C1'-N9	5.83	112.87	108.20
1	A	2796	C	C6-N1-C2	-5.83	117.97	120.30
31	a	1002	G	C4-C5-N7	5.83	113.13	110.80
1	A	252	C	C5-C4-N4	-5.83	116.12	120.20
1	A	636	A	C4-C5-N7	5.83	113.62	110.70
1	A	1759	G	N9-C4-C5	-5.83	103.07	105.40
1	A	2442	G	C5-N7-C8	-5.83	101.38	104.30
31	a	1446	C	C5-C4-N4	-5.83	116.12	120.20
1	A	2223	C	C2-N3-C4	5.83	122.81	119.90
31	a	530	C	N1-C2-O2	5.83	122.40	118.90
31	a	1109	C	N3-C2-O2	-5.83	117.82	121.90
1	A	687	G	N3-C4-C5	5.83	131.51	128.60
31	a	478	G	C8-N9-C1'	-5.83	119.43	127.00
31	a	994	C	N1-C2-O2	5.83	122.39	118.90
1	A	80	G	C5-N7-C8	-5.82	101.39	104.30
1	A	325	A	C5-C6-N1	5.82	120.61	117.70
31	a	246	G	C5-C6-O6	-5.82	125.11	128.60
1	A	2436	G	C5-C6-O6	-5.82	125.11	128.60
1	A	1468	G	N3-C4-N9	5.81	129.49	126.00
1	A	2596	G	N3-C4-N9	-5.81	122.51	126.00
31	a	1382	U	C5'-C4'-O4'	5.81	116.08	109.10
1	A	396	G	N1-C6-O6	5.81	123.39	119.90
1	A	770	G	N3-C2-N2	-5.81	115.83	119.90
1	A	2750	C	N1-C2-O2	5.81	122.39	118.90
1	A	2874	A	C4-C5-C6	-5.81	114.09	117.00
31	a	643	A	C5-C6-N6	-5.81	119.05	123.70
1	A	2548	C	N1-C2-O2	5.81	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2865	G	C2-N3-C4	-5.81	108.99	111.90
31	a	752	C	N3-C2-O2	-5.81	117.83	121.90
31	a	1294	C	N1-C2-N3	5.81	123.27	119.20
31	a	583	G	N3-C4-C5	5.81	131.50	128.60
1	A	135	G	N3-C2-N2	5.80	123.96	119.90
31	a	725	C	N1-C2-O2	5.80	122.38	118.90
31	a	111	G	N3-C4-C5	5.80	131.50	128.60
31	a	697	C	O5'-P-OP1	-5.80	100.48	105.70
1	A	2352	G	N3-C4-C5	5.80	131.50	128.60
1	A	1336	G	N3-C4-N9	-5.79	122.52	126.00
31	a	1394	C	N3-C2-O2	-5.79	117.84	121.90
1	A	162	A	N1-C6-N6	5.79	122.08	118.60
1	A	2052	C	N1-C2-O2	5.79	122.38	118.90
31	a	669	G	O4'-C1'-N9	5.79	112.83	108.20
31	a	1419	C	C6-N1-C2	-5.79	117.98	120.30
31	a	670	A	N7-C8-N9	5.79	116.69	113.80
1	A	470	G	N3-C4-C5	5.79	131.50	128.60
1	A	1410	A	C5-N7-C8	-5.79	101.01	103.90
1	A	737	C	C5-C4-N4	-5.79	116.15	120.20
1	A	1518	G	N1-C6-O6	-5.79	116.43	119.90
1	A	2719	C	N1-C2-O2	5.78	122.37	118.90
1	A	574	A	C5-C6-N6	-5.78	119.07	123.70
1	A	2746	G	N3-C4-N9	-5.78	122.53	126.00
31	a	604	A	C5-C6-N6	-5.78	119.08	123.70
31	a	1287	C	C6-N1-C2	-5.78	117.99	120.30
31	a	1445	G	O4'-C1'-N9	5.78	112.83	108.20
1	A	2648	G	C4-C5-N7	5.78	113.11	110.80
31	a	148	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	2131	C	O4'-C1'-N1	-5.77	103.58	108.20
1	A	2684	A	C5-C6-N6	-5.77	119.08	123.70
1	A	455	A	C4-C5-N7	5.77	113.58	110.70
1	A	1767	G	C4-N9-C1'	5.77	134.00	126.50
1	A	1908	A	N1-C6-N6	-5.77	115.14	118.60
31	a	693	G	N3-C4-N9	-5.77	122.54	126.00
1	A	2423	G	N3-C4-C5	5.76	131.48	128.60
1	A	1391	A	C5-C6-N6	-5.76	119.09	123.70
31	a	1505	G	C8-N9-C1'	-5.76	119.51	127.00
1	A	452	G	N3-C4-C5	5.76	131.48	128.60
1	A	1638	G	N3-C2-N2	5.76	123.93	119.90
1	A	2397	G	N9-C4-C5	5.76	107.70	105.40
2	B	24	C	C6-N1-C2	-5.76	118.00	120.30
1	A	2763	G	C2-N3-C4	-5.76	109.02	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2326	G	C5-N7-C8	-5.76	101.42	104.30
1	A	863	G	N3-C4-C5	5.75	131.48	128.60
1	A	2400	U	C5-C6-N1	5.75	125.58	122.70
1	A	1016	G	C8-N9-C4	-5.75	104.10	106.40
1	A	2839	A	N9-C4-C5	-5.75	103.50	105.80
1	A	2882	A	N9-C4-C5	-5.75	103.50	105.80
31	a	1152	G	C4-N9-C1'	5.75	133.98	126.50
1	A	162	A	C8-N9-C1'	-5.75	117.35	127.70
1	A	1560	A	C2-N3-C4	5.75	113.47	110.60
31	a	926	G	N3-C4-N9	-5.75	122.55	126.00
31	a	1440	C	N1-C2-N3	5.75	123.22	119.20
1	A	2326	G	C6-C5-N7	-5.74	126.95	130.40
31	a	1083	G	C8-N9-C1'	-5.74	119.54	127.00
31	a	604	A	N3-C4-N9	5.74	131.99	127.40
1	A	694	G	N1-C6-O6	5.73	123.34	119.90
1	A	1520	A	P-O3'-C3'	5.73	126.58	119.70
1	A	2258	U	C5-C4-O4	-5.73	122.46	125.90
31	a	670	A	C5-N7-C8	-5.73	101.03	103.90
1	A	461	A	C6-N1-C2	5.73	122.04	118.60
1	A	924	G	N3-C4-N9	5.73	129.44	126.00
31	a	1420	A	N9-C4-C5	5.73	108.09	105.80
1	A	755	C	C2-N1-C1'	5.72	125.10	118.80
1	A	2845	G	C2-N3-C4	-5.72	109.04	111.90
1	A	809	A	O4'-C1'-N9	5.72	112.78	108.20
1	A	1480	G	N3-C4-N9	-5.72	122.57	126.00
1	A	2450	U	P-O3'-C3'	5.72	126.56	119.70
31	a	36	G	O3'-P-O5'	5.72	114.87	104.00
31	a	725	C	C5-C6-N1	5.72	123.86	121.00
1	A	1440	A	N9-C4-C5	-5.72	103.51	105.80
31	a	311	G	C4-C5-N7	5.72	113.09	110.80
1	A	2278	G	N3-C4-N9	5.72	129.43	126.00
1	A	2298	G	C2-N3-C4	-5.71	109.04	111.90
1	A	305	A	N1-C6-N6	5.71	122.03	118.60
1	A	1424	A	N9-C4-C5	-5.71	103.52	105.80
1	A	1623	U	C5-C6-N1	5.71	125.55	122.70
1	A	2229	C	O4'-C1'-N1	5.71	112.77	108.20
31	a	131	C	N3-C2-O2	-5.71	117.91	121.90
1	A	2655	U	N3-C2-O2	-5.70	118.21	122.20
31	a	968	A	N1-C6-N6	-5.70	115.18	118.60
31	a	675	G	N9-C4-C5	5.70	107.68	105.40
1	A	2497	G	N3-C2-N2	5.70	123.89	119.90
31	a	442	C	N3-C4-N4	-5.70	114.01	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	454	G	N9-C4-C5	-5.70	103.12	105.40
1	A	162	A	C6-C5-N7	-5.70	128.31	132.30
1	A	2550	G	N3-C4-N9	-5.70	122.58	126.00
31	a	669	G	N3-C4-N9	-5.70	122.58	126.00
31	a	612	G	N9-C4-C5	-5.70	103.12	105.40
1	A	296	G	C8-N9-C1'	5.69	134.40	127.00
1	A	727	G	N3-C4-C5	5.69	131.45	128.60
31	a	1466	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	806	A	C5-N7-C8	-5.69	101.06	103.90
1	A	919	G	C6-C5-N7	5.69	133.81	130.40
1	A	1615	G	N3-C4-N9	-5.69	122.59	126.00
31	a	122	C	C2-N1-C1'	5.69	125.06	118.80
31	a	1112	A	C6-C5-N7	5.69	136.28	132.30
1	A	1627	G	C4-N9-C1'	5.69	133.90	126.50
31	a	147	G	N9-C4-C5	5.69	107.67	105.40
1	A	515	G	C2-N3-C4	-5.69	109.06	111.90
31	a	1505	G	C4-C5-N7	5.68	113.07	110.80
31	a	549	G	N3-C2-N2	5.68	123.88	119.90
1	A	2273	G	C2-N3-C4	-5.68	109.06	111.90
1	A	1069	G	N1-C2-N2	5.68	121.31	116.20
1	A	1881	A	N3-C4-C5	5.68	130.77	126.80
1	A	452	G	C2-N3-C4	-5.67	109.06	111.90
1	A	902	A	C5-N7-C8	-5.67	101.06	103.90
1	A	2738	A	C4-C5-N7	5.67	113.53	110.70
1	A	223	G	N3-C4-C5	5.67	131.44	128.60
1	A	496	G	C2-N3-C4	-5.67	109.06	111.90
1	A	1424	A	C4-C5-N7	5.67	113.53	110.70
1	A	2915	C	N1-C2-O2	5.67	122.30	118.90
1	A	655	A	C8-N9-C4	5.66	108.07	105.80
31	a	1173	G	N7-C8-N9	5.66	115.93	113.10
38	h	89	ALA	CA-C-O	-5.66	108.21	120.10
1	A	1466	G	N3-C2-N2	5.66	123.86	119.90
1	A	1622	C	C2-N1-C1'	5.66	125.03	118.80
1	A	608	C	N3-C4-C5	5.66	124.16	121.90
1	A	2434	A	N9-C4-C5	-5.66	103.54	105.80
31	a	861	A	N9-C4-C5	-5.66	103.54	105.80
1	A	1469	G	C5-N7-C8	-5.66	101.47	104.30
1	A	1975	G	C4-C5-N7	5.66	113.06	110.80
1	A	15	G	N3-C4-C5	5.66	131.43	128.60
1	A	575	G	O4'-C1'-N9	5.66	112.73	108.20
31	a	548	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	133	A	C5-N7-C8	-5.66	101.07	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	301	A	C6-C5-N7	-5.65	128.34	132.30
1	A	337	A	O4'-C1'-N9	5.65	112.72	108.20
1	A	762	C	N3-C2-O2	-5.65	117.94	121.90
1	A	2486	A	N9-C4-C5	-5.65	103.54	105.80
1	A	1742	A	N9-C4-C5	-5.65	103.54	105.80
1	A	1812	A	C5-C6-N6	-5.65	119.18	123.70
1	A	2326	G	N1-C6-O6	5.65	123.29	119.90
1	A	2436	G	N3-C4-C5	5.65	131.43	128.60
31	a	278	A	N1-C6-N6	5.65	121.99	118.60
31	a	1114	C	N3-C4-C5	5.65	124.16	121.90
31	a	1416	U	O4'-C1'-N1	5.65	112.72	108.20
31	a	165	G	N3-C4-N9	-5.65	122.61	126.00
31	a	815	A	C4-C5-N7	5.65	113.52	110.70
1	A	165	C	C2-N1-C1'	5.64	125.01	118.80
1	A	721	A	N1-C2-N3	5.64	132.12	129.30
1	A	340	C	N1-C2-O2	5.64	122.28	118.90
31	a	1468	G	O4'-C1'-N9	5.64	112.71	108.20
37	g	101	LEU	N-CA-C	5.64	126.22	111.00
31	a	132	C	N3-C2-O2	-5.64	117.95	121.90
1	A	1494	G	N3-C4-C5	5.63	131.42	128.60
31	a	263	G	N1-C6-O6	5.63	123.28	119.90
1	A	624	C	C5-C6-N1	5.63	123.82	121.00
1	A	1747	G	N3-C4-C5	5.63	131.42	128.60
1	A	2370	U	C6-N1-C1'	5.63	129.09	121.20
1	A	1307	G	N3-C4-N9	-5.63	122.62	126.00
31	a	522	C	C6-N1-C2	-5.63	118.05	120.30
1	A	1534	G	C8-N9-C1'	5.63	134.32	127.00
1	A	1701	U	C2-N1-C1'	5.63	124.45	117.70
1	A	2497	G	C4-C5-C6	5.63	122.18	118.80
1	A	2262	G	C4-C5-N7	5.63	113.05	110.80
31	a	54	A	N9-C4-C5	-5.63	103.55	105.80
31	a	249	G	N9-C4-C5	-5.63	103.15	105.40
31	a	1419	C	O4'-C1'-N1	5.63	112.70	108.20
31	a	441	A	N7-C8-N9	5.62	116.61	113.80
31	a	1294	C	C2-N1-C1'	-5.62	112.61	118.80
1	A	881	G	N3-C4-C5	5.62	131.41	128.60
1	A	1521	A	C5-C6-N6	5.62	128.20	123.70
1	A	1647	A	N1-C6-N6	-5.62	115.23	118.60
1	A	432	G	N1-C2-N2	-5.62	111.14	116.20
1	A	2396	A	C4-C5-N7	5.62	113.51	110.70
1	A	2302	C	C6-N1-C2	-5.62	118.05	120.30
1	A	527	G	O4'-C1'-N9	5.62	112.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	249	G	C6-C5-N7	-5.62	127.03	130.40
1	A	602	G	C2-N3-C4	-5.61	109.09	111.90
1	A	1987	A	N9-C4-C5	5.61	108.05	105.80
31	a	533	C	N3-C2-O2	-5.61	117.97	121.90
1	A	636	A	C5-C6-N6	-5.61	119.21	123.70
1	A	759	U	C2-N1-C1'	5.61	124.43	117.70
1	A	1092	A	C4-N9-C1'	5.61	136.40	126.30
1	A	1636	U	C5-C6-N1	5.61	125.50	122.70
1	A	1438	G	C2-N3-C4	-5.60	109.10	111.90
31	a	921	C	N1-C2-O2	5.60	122.26	118.90
1	A	1227	U	C2-N1-C1'	5.60	124.42	117.70
31	a	696	G	N3-C4-N9	-5.60	122.64	126.00
1	A	1087	C	N3-C2-O2	-5.60	117.98	121.90
1	A	1365	G	C2-N3-C4	-5.60	109.10	111.90
1	A	2636	U	N1-C2-O2	5.60	126.72	122.80
1	A	1004	A	N9-C4-C5	-5.60	103.56	105.80
1	A	2690	G	C5-N7-C8	-5.60	101.50	104.30
31	a	703	A	N1-C2-N3	5.60	132.10	129.30
31	a	950	G	N3-C4-N9	-5.60	122.64	126.00
1	A	1033	G	N7-C8-N9	5.60	115.90	113.10
1	A	902	A	C4-C5-N7	5.59	113.50	110.70
1	A	2494	C	N3-C2-O2	-5.59	117.98	121.90
31	a	970	U	N1-C2-N3	5.59	118.26	114.90
1	A	1081	G	C2-N3-C4	-5.59	109.10	111.90
1	A	1087	C	O4'-C1'-N1	5.59	112.67	108.20
1	A	1701	U	C5-C6-N1	5.59	125.50	122.70
1	A	1723	A	C4-C5-N7	5.59	113.50	110.70
31	a	1505	G	C4-N9-C1'	5.59	133.77	126.50
1	A	330	C	N1-C2-O2	5.59	122.25	118.90
1	A	2865	G	N1-C2-N2	-5.59	111.17	116.20
1	A	1709	A	C5-N7-C8	-5.59	101.11	103.90
30	4	19	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	595	G	N3-C4-N9	-5.59	122.65	126.00
31	a	556	G	C8-N9-C1'	-5.59	119.74	127.00
1	A	962	A	N1-C6-N6	5.58	121.95	118.60
1	A	2481	G	N1-C6-O6	-5.58	116.55	119.90
31	a	1326	G	C4-N9-C1'	5.58	133.76	126.50
31	a	1416	U	N3-C2-O2	-5.58	118.29	122.20
31	a	344	A	C5-C6-N6	-5.58	119.23	123.70
1	A	844	G	C8-N9-C4	-5.58	104.17	106.40
1	A	19	G	C4-N9-C1'	5.58	133.75	126.50
1	A	1501	G	C5-N7-C8	-5.58	101.51	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2771	G	N1-C6-O6	5.58	123.25	119.90
1	A	1183	G	N3-C4-C5	5.57	131.39	128.60
1	A	2013	G	N1-C2-N2	-5.57	111.18	116.20
31	a	818	C	N1-C2-O2	5.57	122.24	118.90
1	A	2818	A	C4-C5-C6	5.57	119.79	117.00
1	A	575	G	C4-N9-C1'	5.57	133.74	126.50
1	A	961	G	C6-C5-N7	-5.57	127.06	130.40
1	A	1991	G	C8-N9-C1'	5.57	134.24	127.00
31	a	1198	A	C8-N9-C4	-5.57	103.57	105.80
1	A	396	G	N7-C8-N9	5.57	115.88	113.10
1	A	636	A	N1-C6-N6	5.57	121.94	118.60
31	a	452	A	N1-C6-N6	5.57	121.94	118.60
1	A	2014	G	N3-C4-C5	5.56	131.38	128.60
31	a	1007	C	C2-N1-C1'	5.56	124.92	118.80
31	a	1155	C	C6-N1-C1'	-5.56	114.13	120.80
1	A	768	A	N1-C6-N6	5.56	121.94	118.60
31	a	279	C	N3-C2-O2	-5.56	118.01	121.90
31	a	1336	U	P-O3'-C3'	5.56	126.37	119.70
1	A	806	A	C6-C5-N7	-5.56	128.41	132.30
1	A	351	G	N3-C4-N9	-5.56	122.67	126.00
1	A	1496	G	C8-N9-C4	5.56	108.62	106.40
31	a	548	G	C5-C6-O6	-5.56	125.27	128.60
1	A	2747	U	C6-N1-C2	-5.55	117.67	121.00
31	a	649	A	N3-C4-C5	-5.55	122.91	126.80
1	A	630	G	O4'-C1'-N9	5.55	112.64	108.20
1	A	280	C	C5-C6-N1	5.55	123.78	121.00
1	A	2763	G	N1-C2-N2	-5.55	111.20	116.20
34	d	51	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	2150	A	N7-C8-N9	5.55	116.58	113.80
1	A	323	C	C2-N3-C4	5.55	122.67	119.90
31	a	412	G	C4-N9-C1'	5.55	133.71	126.50
1	A	1691	G	OP1-P-OP2	5.55	127.92	119.60
1	A	2099	G	N3-C2-N2	5.55	123.78	119.90
1	A	2326	G	N9-C4-C5	-5.55	103.18	105.40
31	a	549	G	N7-C8-N9	5.55	115.87	113.10
31	a	1007	C	C6-N1-C2	-5.55	118.08	120.30
1	A	887	A	C5-N7-C8	-5.54	101.13	103.90
1	A	1465	G	C6-C5-N7	-5.54	127.08	130.40
1	A	814	A	N1-C6-N6	5.54	121.92	118.60
1	A	897	A	C5-N7-C8	-5.54	101.13	103.90
1	A	410	G	N9-C4-C5	-5.54	103.19	105.40
1	A	2342	U	N3-C4-O4	5.54	123.28	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	G	OP1-P-O3'	5.54	117.38	105.20
1	A	756	A	C5-N7-C8	-5.54	101.13	103.90
1	A	1633	A	C6-C5-N7	-5.54	128.43	132.30
1	A	1742	A	C5-C6-N6	-5.54	119.27	123.70
31	a	278	A	N9-C4-C5	-5.53	103.59	105.80
31	a	1125	C	C5-C6-N1	5.53	123.77	121.00
1	A	557	G	N3-C2-N2	-5.53	116.03	119.90
1	A	819	A	C5-C6-N6	-5.53	119.28	123.70
1	A	1307	G	N3-C4-C5	5.53	131.37	128.60
31	a	1420	A	N1-C6-N6	-5.53	115.28	118.60
31	a	1415	G	N3-C2-N2	-5.53	116.03	119.90
1	A	1627	G	N3-C4-N9	5.53	129.32	126.00
1	A	2464	C	N1-C2-O2	5.53	122.22	118.90
1	A	1633	A	C4-C5-C6	5.52	119.76	117.00
1	A	857	C	C2-N3-C4	-5.52	117.14	119.90
1	A	1723	A	C5-C6-N6	-5.52	119.28	123.70
2	B	65	G	N3-C2-N2	5.52	123.77	119.90
31	a	548	G	N7-C8-N9	5.52	115.86	113.10
1	A	1091	G	O4'-C1'-N9	5.52	112.62	108.20
1	A	2774	G	C5-C6-N1	5.52	114.26	111.50
2	B	88	G	N3-C4-C5	5.52	131.36	128.60
1	A	1378	U	N1-C2-O2	5.52	126.66	122.80
1	A	1441	C	C2-N1-C1'	5.52	124.87	118.80
1	A	2262	G	C5-N7-C8	-5.52	101.54	104.30
1	A	1480	G	N9-C4-C5	5.52	107.61	105.40
1	A	1520	A	C5-C6-N6	5.52	128.11	123.70
1	A	212	C	N1-C2-O2	5.51	122.21	118.90
1	A	1815	C	C6-N1-C2	5.51	122.51	120.30
31	a	983	A	C8-N9-C4	-5.51	103.59	105.80
31	a	1233	C	C5-C6-N1	5.51	123.76	121.00
1	A	66	C	N1-C2-O2	5.51	122.21	118.90
1	A	101	G	N3-C2-N2	5.51	123.76	119.90
1	A	1016	G	N7-C8-N9	5.51	115.86	113.10
1	A	2832	A	N9-C4-C5	-5.51	103.59	105.80
31	a	123	G	N3-C4-N9	5.51	129.31	126.00
31	a	956	G	N7-C8-N9	5.51	115.86	113.10
31	a	518	A	C5-C6-N6	-5.51	119.29	123.70
1	A	2129	C	P-O3'-C3'	5.51	126.31	119.70
1	A	806	A	C4-C5-N7	5.50	113.45	110.70
1	A	130	A	N9-C4-C5	-5.50	103.60	105.80
1	A	503	A	C5-N7-C8	-5.50	101.15	103.90
1	A	1376	G	C8-N9-C4	5.50	108.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1186	A	N1-C6-N6	5.50	121.90	118.60
1	A	2445	A	C8-N9-C4	5.50	108.00	105.80
1	A	2849	A	C8-N9-C4	5.50	108.00	105.80
1	A	554	C	N1-C2-O2	5.50	122.20	118.90
1	A	1465	G	N3-C4-C5	-5.50	125.85	128.60
1	A	1655	C	C6-N1-C2	-5.50	118.10	120.30
1	A	2782	C	C6-N1-C2	-5.50	118.10	120.30
1	A	459	C	C2-N1-C1'	5.49	124.84	118.80
1	A	919	G	C4-C5-C6	-5.49	115.50	118.80
1	A	1776	A	C4-C5-N7	5.49	113.45	110.70
1	A	2434	A	C4-C5-N7	5.49	113.45	110.70
1	A	2056	G	C2-N3-C4	-5.49	109.16	111.90
1	A	2328	A	N1-C6-N6	5.49	121.89	118.60
31	a	1108	C	OP1-P-O3'	5.49	117.28	105.20
1	A	378	C	C5-C4-N4	-5.49	116.36	120.20
31	a	941	C	N1-C2-O2	5.49	122.19	118.90
1	A	426	G	C4-C5-N7	5.49	112.99	110.80
1	A	2764	G	C5-C6-O6	-5.49	125.31	128.60
31	a	922	A	P-O3'-C3'	5.49	126.28	119.70
1	A	694	G	C6-C5-N7	-5.48	127.11	130.40
1	A	1391	A	C6-C5-N7	-5.48	128.46	132.30
1	A	2827	A	C5-C6-N1	5.48	120.44	117.70
1	A	2710	C	N3-C2-O2	-5.48	118.06	121.90
31	a	36	G	C5'-C4'-O4'	-5.48	102.52	109.10
1	A	1410	A	C4-C5-N7	5.48	113.44	110.70
1	A	1520	A	C2-N3-C4	-5.48	107.86	110.60
1	A	2711	U	C5-C4-O4	-5.48	122.61	125.90
31	a	315	U	N1-C2-O2	5.48	126.63	122.80
31	a	326	G	N1-C6-O6	5.48	123.19	119.90
31	a	681	G	C4-N9-C1'	-5.48	119.38	126.50
1	A	816	G	N3-C4-N9	-5.48	122.71	126.00
1	A	2061	U	N3-C4-O4	5.48	123.23	119.40
1	A	624	C	C6-N1-C2	-5.47	118.11	120.30
1	A	1053	A	C5-N7-C8	-5.47	101.16	103.90
1	A	137	G	N7-C8-N9	5.47	115.84	113.10
1	A	2047	A	C5-C6-N1	5.47	120.44	117.70
1	A	2869	G	N3-C4-C5	5.47	131.34	128.60
31	a	263	G	OP1-P-OP2	-5.47	111.39	119.60
1	A	2715	G	C2-N3-C4	-5.47	109.17	111.90
1	A	788	A	C5-N7-C8	-5.47	101.17	103.90
1	A	2273	G	N3-C4-C5	5.47	131.33	128.60
1	A	2818	A	N9-C4-C5	-5.46	103.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	643	A	C5-N7-C8	-5.46	101.17	103.90
31	a	651	C	N1-C2-N3	-5.46	115.38	119.20
1	A	862	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2618	C	N3-C4-N4	-5.46	114.18	118.00
1	A	1232	G	N1-C2-N2	-5.46	111.28	116.20
1	A	1841	G	C4-N9-C1'	-5.46	119.40	126.50
1	A	2442	G	C2-N3-C4	-5.46	109.17	111.90
31	a	1494	A	C5-N7-C8	-5.46	101.17	103.90
1	A	2764	G	N1-C6-O6	5.46	123.18	119.90
1	A	2884	G	N9-C4-C5	-5.46	103.22	105.40
1	A	426	G	N9-C4-C5	-5.46	103.22	105.40
1	A	223	G	N3-C4-N9	-5.46	122.73	126.00
1	A	395	U	C6-N1-C1'	5.46	128.84	121.20
1	A	2727	G	N9-C4-C5	-5.46	103.22	105.40
31	a	861	A	N1-C6-N6	5.46	121.87	118.60
1	A	432	G	N7-C8-N9	5.46	115.83	113.10
1	A	2572	G	N3-C4-N9	-5.46	122.73	126.00
1	A	1158	G	N9-C4-C5	-5.45	103.22	105.40
1	A	2457	A	C4-C5-N7	5.45	113.42	110.70
31	a	1116	A	N9-C4-C5	-5.45	103.62	105.80
1	A	679	G	N1-C6-O6	5.45	123.17	119.90
1	A	860	U	C5-C4-O4	-5.45	122.63	125.90
1	A	918	G	C5-N7-C8	5.45	107.02	104.30
31	a	302	C	C6-N1-C2	-5.45	118.12	120.30
1	A	16	G	C2-N3-C4	-5.44	109.18	111.90
1	A	163	U	N3-C4-O4	-5.44	115.59	119.40
1	A	1476	G	C4-C5-N7	5.44	112.98	110.80
1	A	2210	C	C6-N1-C2	-5.44	118.12	120.30
1	A	863	G	C2-N3-C4	-5.44	109.18	111.90
1	A	1081	G	N3-C4-C5	5.44	131.32	128.60
1	A	1506	C	C5-C4-N4	5.44	124.01	120.20
31	a	670	A	N3-C4-N9	5.44	131.75	127.40
1	A	80	G	C4-C5-N7	5.44	112.97	110.80
1	A	1161	A	N1-C6-N6	5.44	121.86	118.60
1	A	2720	A	C4-C5-N7	5.44	113.42	110.70
1	A	1627	G	N9-C4-C5	-5.43	103.23	105.40
1	A	1823	U	O4'-C4'-C3'	-5.43	98.57	104.00
1	A	2431	C	N3-C2-O2	-5.43	118.10	121.90
2	B	8	A	C8-N9-C4	5.43	107.97	105.80
1	A	1834	G	N3-C4-C5	5.43	131.31	128.60
1	A	63	U	N3-C2-O2	-5.43	118.40	122.20
1	A	2752	A	C4-C5-N7	5.43	113.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2746	G	N3-C4-C5	5.43	131.31	128.60
31	a	951	G	N3-C4-N9	5.43	129.26	126.00
2	B	111	C	N1-C2-O2	5.42	122.16	118.90
1	A	45	G	C8-N9-C1'	5.42	134.05	127.00
1	A	822	G	N3-C4-N9	-5.42	122.75	126.00
1	A	2842	G	N3-C2-N2	5.42	123.69	119.90
31	a	758	C	N1-C2-O2	5.42	122.15	118.90
1	A	1898	C	C6-N1-C2	-5.42	118.13	120.30
1	A	2231	C	O4'-C1'-N1	5.42	112.53	108.20
31	a	255	G	N3-C2-N2	-5.42	116.11	119.90
31	a	1510	A	O4'-C1'-N9	-5.42	103.86	108.20
1	A	2896	A	C4-C5-N7	5.42	113.41	110.70
31	a	55	C	C2-N1-C1'	5.42	124.76	118.80
31	a	636	G	N7-C8-N9	5.42	115.81	113.10
1	A	996	G	N3-C4-C5	5.41	131.31	128.60
1	A	1008	C	N3-C4-C5	5.41	124.07	121.90
1	A	1733	A	C5-C6-N6	-5.41	119.37	123.70
1	A	2832	A	C4-C5-N7	5.41	113.41	110.70
1	A	2563	G	N3-C4-C5	5.41	131.31	128.60
1	A	2738	A	C5-C6-N1	5.41	120.41	117.70
1	A	496	G	N3-C4-C5	5.41	131.31	128.60
1	A	2497	G	C4-N9-C1'	5.41	133.53	126.50
1	A	756	A	C8-N9-C1'	-5.41	117.97	127.70
1	A	1081	G	N3-C4-N9	-5.41	122.76	126.00
1	A	1828	U	N3-C2-O2	-5.40	118.42	122.20
1	A	2848	G	N3-C4-N9	-5.40	122.76	126.00
1	A	397	U	C5-C6-N1	5.40	125.40	122.70
1	A	955	A	N9-C4-C5	5.40	107.96	105.80
31	a	239	G	N3-C4-N9	-5.40	122.76	126.00
1	A	768	A	C5-C6-N6	-5.40	119.38	123.70
1	A	961	G	N9-C4-C5	-5.40	103.24	105.40
1	A	1051	C	C5-C4-N4	-5.40	116.42	120.20
1	A	1534	G	C4-N9-C1'	-5.40	119.48	126.50
1	A	1723	A	C5-N7-C8	-5.40	101.20	103.90
31	a	583	G	N9-C4-C5	5.40	107.56	105.40
31	a	148	G	C4-C5-C6	5.40	122.04	118.80
31	a	549	G	N9-C4-C5	-5.40	103.24	105.40
1	A	2259	C	C5-C4-N4	-5.39	116.42	120.20
1	A	2073	G	N3-C2-N2	-5.39	116.12	119.90
1	A	2824	G	C2-N3-C4	-5.39	109.20	111.90
31	a	741	G	N3-C2-N2	-5.39	116.13	119.90
1	A	395	U	C2-N1-C1'	-5.39	111.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	887	A	C4-C5-N7	5.39	113.39	110.70
1	A	2328	A	C4-C5-N7	5.39	113.39	110.70
1	A	2397	G	C8-N9-C1'	5.39	134.01	127.00
1	A	2558	A	C2-N3-C4	5.39	113.30	110.60
1	A	351	G	C8-N9-C1'	5.39	134.00	127.00
1	A	997	G	C2-N3-C4	-5.39	109.21	111.90
1	A	2326	G	N7-C8-N9	5.39	115.79	113.10
31	a	842	U	C5-C4-O4	-5.38	122.67	125.90
1	A	1509	G	O4'-C1'-N9	5.38	112.51	108.20
1	A	624	C	N1-C2-O2	5.38	122.13	118.90
1	A	2783	U	P-O3'-C3'	5.38	126.16	119.70
31	a	669	G	C6-C5-N7	5.38	133.63	130.40
1	A	2735	G	C5-N7-C8	-5.38	101.61	104.30
1	A	766	G	C8-N9-C1'	-5.38	120.01	127.00
1	A	1691	G	C4-N9-C1'	5.38	133.49	126.50
1	A	295	G	C4-N9-C1'	5.38	133.49	126.50
31	a	166	G	N3-C4-C5	5.38	131.29	128.60
31	a	1364	U	C5-C6-N1	5.38	125.39	122.70
1	A	810	A	C4-C5-N7	5.38	113.39	110.70
1	A	2437	G	C8-N9-C4	-5.38	104.25	106.40
1	A	2328	A	C5-C6-N6	-5.37	119.40	123.70
1	A	2747	U	C5-C6-N1	5.37	125.39	122.70
31	a	36	G	N1-C6-O6	-5.37	116.67	119.90
1	A	656	G	N3-C4-C5	5.37	131.29	128.60
1	A	2684	A	C5-C6-N1	5.37	120.39	117.70
31	a	604	A	C5-C6-N1	5.37	120.39	117.70
1	A	1776	A	N9-C4-C5	-5.37	103.65	105.80
1	A	758	G	C8-N9-C4	-5.37	104.25	106.40
31	a	301	A	C2-N3-C4	-5.37	107.92	110.60
31	a	415	A	O4'-C1'-N9	5.37	112.49	108.20
31	a	1481	G	N3-C4-N9	-5.37	122.78	126.00
1	A	576	U	P-O3'-C3'	5.36	126.14	119.70
31	a	694	U	O4'-C1'-N1	5.36	112.49	108.20
1	A	1385	G	N3-C4-N9	-5.36	122.78	126.00
1	A	2658	G	N3-C4-C5	5.36	131.28	128.60
1	A	1469	G	C2-N3-C4	-5.36	109.22	111.90
1	A	2052	C	C2-N1-C1'	5.36	124.70	118.80
31	a	1090	G	O4'-C1'-N9	-5.36	103.91	108.20
1	A	1775	G	C4-C5-N7	5.36	112.94	110.80
1	A	669	C	C5-C4-N4	-5.36	116.45	120.20
1	A	2833	U	N3-C2-O2	-5.36	118.45	122.20
31	a	639	G	O4'-C1'-N9	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1205	C	C5-C4-N4	-5.36	116.45	120.20
31	a	1324	C	N3-C2-O2	-5.36	118.15	121.90
31	a	246	G	C6-C5-N7	-5.35	127.19	130.40
1	A	336	U	C4-C5-C6	-5.35	116.49	119.70
1	A	2756	G	C2-N3-C4	-5.35	109.22	111.90
31	a	1152	G	C8-N9-C1'	-5.35	120.05	127.00
31	a	1414	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2641	A	C5-C6-N1	5.35	120.37	117.70
1	A	2896	A	N9-C4-C5	-5.35	103.66	105.80
31	a	940	C	C5-C6-N1	5.35	123.67	121.00
31	a	1059	G	N1-C6-O6	5.35	123.11	119.90
1	A	83	G	C8-N9-C4	-5.34	104.26	106.40
31	a	571	A	C8-N9-C1'	-5.34	118.08	127.70
31	a	693	G	C8-N9-C1'	5.34	133.95	127.00
1	A	1479	G	O4'-C1'-N9	5.34	112.47	108.20
1	A	1557	C	N3-C2-O2	-5.34	118.16	121.90
31	a	108	A	C8-N9-C4	-5.34	103.66	105.80
1	A	616	G	C2-N3-C4	-5.34	109.23	111.90
1	A	627	C	C5-C4-N4	-5.34	116.47	120.20
1	A	1750	U	C5-C4-O4	-5.34	122.70	125.90
1	A	2304	G	N3-C4-C5	5.34	131.27	128.60
1	A	2873	C	N1-C2-O2	5.34	122.10	118.90
31	a	1131	C	N1-C2-O2	5.34	122.10	118.90
1	A	1627	G	C8-N9-C1'	-5.33	120.07	127.00
31	a	24	C	C5-C4-N4	5.33	123.93	120.20
31	a	1505	G	N9-C4-C5	-5.33	103.27	105.40
1	A	1492	G	C8-N9-C1'	5.33	133.93	127.00
31	a	549	G	N1-C6-O6	5.33	123.10	119.90
1	A	207	A	C8-N9-C4	5.33	107.93	105.80
1	A	1615	G	C8-N9-C1'	5.33	133.93	127.00
1	A	2245	G	C4-C5-N7	5.33	112.93	110.80
1	A	2720	A	N9-C4-C5	-5.33	103.67	105.80
31	a	1409	C	O4'-C1'-N1	5.33	112.46	108.20
1	A	810	A	N9-C4-C5	-5.33	103.67	105.80
1	A	1905	G	N3-C4-C5	-5.33	125.94	128.60
1	A	15	G	C8-N9-C4	5.33	108.53	106.40
1	A	1406	G	N3-C4-N9	-5.33	122.81	126.00
1	A	1826	G	C4-C5-N7	5.33	112.93	110.80
1	A	2508	G	C8-N9-C4	5.33	108.53	106.40
31	a	743	C	N1-C2-O2	5.33	122.09	118.90
1	A	2440	G	N1-C2-N2	-5.32	111.41	116.20
31	a	165	G	N3-C4-C5	5.32	131.26	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	918	A	N9-C4-C5	-5.32	103.67	105.80
1	A	2498	A	N1-C6-N6	5.32	121.79	118.60
1	A	2548	C	N3-C2-O2	-5.32	118.18	121.90
2	B	54	U	C5-C6-N1	5.32	125.36	122.70
1	A	1378	U	C2-N1-C1'	5.32	124.08	117.70
31	a	255	G	N9-C4-C5	5.32	107.53	105.40
1	A	2829	A	C4-C5-N7	5.31	113.36	110.70
1	A	955	A	N1-C6-N6	-5.31	115.41	118.60
31	a	1000	U	N1-C2-O2	5.31	126.52	122.80
1	A	302	A	C8-N9-C4	5.31	107.92	105.80
1	A	814	A	C4-C5-N7	5.31	113.35	110.70
31	a	1390	U	N3-C2-O2	-5.31	118.48	122.20
1	A	829	U	O4'-C1'-N1	-5.30	103.96	108.20
31	a	612	G	C5-C6-O6	-5.30	125.42	128.60
31	a	687	C	N1-C2-O2	5.30	122.08	118.90
1	A	461	A	C5-C6-N6	-5.30	119.46	123.70
1	A	1701	U	C5-C4-O4	-5.30	122.72	125.90
31	a	373	U	C2-N1-C1'	5.30	124.06	117.70
1	A	2248	G	C2-N3-C4	-5.30	109.25	111.90
1	A	257	G	C8-N9-C4	5.30	108.52	106.40
1	A	839	A	C5-C6-N1	5.30	120.35	117.70
1	A	1571	G	N3-C4-C5	-5.30	125.95	128.60
1	A	1637	A	N9-C4-C5	-5.30	103.68	105.80
31	a	1319	G	N3-C4-N9	5.30	129.18	126.00
1	A	2021	C	N3-C4-N4	5.29	121.71	118.00
1	A	541	G	N3-C4-C5	5.29	131.25	128.60
1	A	1435	C	N1-C2-O2	5.29	122.08	118.90
1	A	2494	C	N1-C2-O2	5.29	122.08	118.90
1	A	2643	C	C5-C4-N4	-5.29	116.50	120.20
1	A	19	G	C8-N9-C1'	-5.29	120.12	127.00
41	k	120	GLY	N-CA-C	5.29	126.33	113.10
1	A	851	C	N3-C4-C5	5.29	124.02	121.90
1	A	1465	G	C4-C5-C6	5.29	121.97	118.80
1	A	2715	G	N3-C4-N9	-5.29	122.83	126.00
2	B	110	C	N3-C4-N4	-5.29	114.30	118.00
31	a	861	A	C6-C5-N7	-5.29	128.60	132.30
31	a	1083	G	N7-C8-N9	5.29	115.74	113.10
1	A	70	G	N3-C4-C5	5.29	131.24	128.60
1	A	432	G	N3-C4-N9	5.29	129.17	126.00
1	A	788	A	C4-C5-N7	5.29	113.34	110.70
31	a	950	G	N3-C2-N2	-5.29	116.20	119.90
1	A	1232	G	N3-C2-N2	5.28	123.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1608	C	C6-N1-C2	-5.28	118.19	120.30
31	a	997	A	N1-C6-N6	-5.28	115.43	118.60
1	A	575	G	N3-C2-N2	5.28	123.60	119.90
1	A	869	G	N3-C4-N9	-5.28	122.83	126.00
31	a	758	C	N3-C4-N4	-5.28	114.30	118.00
1	A	2352	G	N3-C4-N9	-5.28	122.83	126.00
1	A	2827	A	C4-C5-C6	-5.28	114.36	117.00
1	A	1501	G	N3-C4-N9	-5.28	122.83	126.00
1	A	2089	A	N1-C6-N6	5.28	121.77	118.60
1	A	685	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1180	G	N3-C4-N9	-5.27	122.84	126.00
1	A	1284	A	C5-C6-N6	-5.27	119.48	123.70
1	A	2877	G	N3-C2-N2	-5.27	116.21	119.90
31	a	1313	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1772	G	C8-N9-C1'	-5.27	120.15	127.00
1	A	915	U	C5-C6-N1	5.27	125.33	122.70
1	A	1425	G	C4-C5-N7	5.27	112.91	110.80
1	A	296	G	O4'-C1'-N9	5.27	112.42	108.20
1	A	707	G	C2-N3-C4	-5.27	109.27	111.90
1	A	1383	G	N3-C4-N9	-5.27	122.84	126.00
1	A	1479	G	C4-N9-C1'	-5.27	119.65	126.50
1	A	2849	A	C4-C5-C6	-5.27	114.37	117.00
1	A	1261	G	C2-N3-C4	-5.26	109.27	111.90
1	A	2497	G	C8-N9-C1'	-5.26	120.16	127.00
31	a	1467	A	C5-C6-N6	-5.26	119.49	123.70
1	A	707	G	N3-C4-C5	5.26	131.23	128.60
31	a	730	G	C4-N9-C1'	5.26	133.34	126.50
1	A	130	A	C4-C5-N7	5.26	113.33	110.70
1	A	551	G	O4'-C1'-N9	5.26	112.41	108.20
31	a	311	G	N9-C4-C5	-5.26	103.30	105.40
31	a	1421	C	C2-N1-C1'	5.26	124.58	118.80
1	A	742	U	C5-C4-O4	-5.25	122.75	125.90
1	A	2643	C	N1-C2-O2	5.25	122.05	118.90
1	A	606	G	C2-N3-C4	-5.25	109.27	111.90
1	A	1179	C	C2-N1-C1'	5.25	124.58	118.80
1	A	1218	G	N1-C6-O6	-5.25	116.75	119.90
1	A	1850	G	C4-C5-C6	-5.25	115.65	118.80
1	A	2115	A	C6-C5-N7	-5.25	128.62	132.30
1	A	2355	A	C6-N1-C2	-5.25	115.45	118.60
1	A	1492	G	N3-C2-N2	-5.25	116.22	119.90
1	A	2231	C	C5-C6-N1	5.25	123.63	121.00
31	a	1433	G	N3-C4-N9	-5.25	122.85	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	A	N9-C4-C5	-5.25	103.70	105.80
1	A	2816	C	N3-C2-O2	-5.25	118.22	121.90
31	a	122	C	N3-C4-C5	-5.25	119.80	121.90
31	a	1131	C	C5-C6-N1	5.25	123.62	121.00
1	A	1148	C	N1-C2-O2	5.25	122.05	118.90
31	a	691	G	N9-C4-C5	5.25	107.50	105.40
31	a	1028	G	N3-C4-C5	-5.25	125.98	128.60
1	A	351	G	C4-N9-C1'	-5.25	119.68	126.50
1	A	2013	G	N3-C4-C5	5.25	131.22	128.60
31	a	283	G	C4-C5-N7	5.25	112.90	110.80
31	a	950	G	N1-C6-O6	-5.25	116.75	119.90
1	A	101	G	N1-C2-N2	-5.24	111.48	116.20
1	A	479	C	N3-C2-O2	-5.24	118.23	121.90
31	a	292	G	N3-C4-C5	5.24	131.22	128.60
1	A	2786	G	C8-N9-C4	-5.24	104.31	106.40
1	A	455	A	N9-C4-C5	-5.24	103.71	105.80
1	A	1622	C	N3-C2-O2	-5.24	118.24	121.90
1	A	2686	G	C6-C5-N7	-5.24	127.26	130.40
45	o	43	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	2115	A	N7-C8-N9	5.23	116.42	113.80
1	A	383	A	N1-C6-N6	5.23	121.74	118.60
1	A	1045	A	N1-C6-N6	5.23	121.74	118.60
1	A	1994	C	C6-N1-C1'	-5.23	114.52	120.80
1	A	2412	C	N3-C2-O2	-5.23	118.24	121.90
31	a	416	G	N9-C4-C5	5.23	107.49	105.40
1	A	116	G	N3-C4-C5	5.23	131.22	128.60
1	A	432	G	N3-C2-N2	5.23	123.56	119.90
1	A	1183	G	N3-C4-N9	-5.23	122.86	126.00
31	a	1451	G	C5-C6-O6	-5.23	125.46	128.60
1	A	65	A	N9-C4-C5	-5.23	103.71	105.80
1	A	778	G	C2-N3-C4	-5.23	109.29	111.90
1	A	1759	G	C5-C6-N1	-5.23	108.89	111.50
1	A	160	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1162	C	N3-C2-O2	-5.23	118.24	121.90
1	A	1767	G	N3-C4-N9	5.23	129.14	126.00
1	A	2356	A	C5-N7-C8	-5.23	101.29	103.90
31	a	1348	G	N3-C4-C5	-5.23	125.99	128.60
1	A	2064	A	N1-C6-N6	5.23	121.74	118.60
31	a	309	G	N3-C4-N9	-5.23	122.86	126.00
1	A	1686	G	C2-N3-C4	-5.22	109.29	111.90
31	a	223	C	C6-N1-C2	-5.22	118.21	120.30
1	A	441	C	N1-C2-O2	5.22	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	C	C2-N3-C4	-5.22	117.29	119.90
1	A	944	G	C4-N9-C1'	5.22	133.29	126.50
1	A	1268	C	N3-C4-C5	5.22	123.99	121.90
1	A	1490	G	O4'-C1'-N9	5.22	112.38	108.20
1	A	2689	A	N1-C6-N6	5.22	121.73	118.60
1	A	646	A	N1-C6-N6	5.22	121.73	118.60
31	a	36	G	N9-C4-C5	5.22	107.49	105.40
31	a	671	A	N1-C6-N6	5.22	121.73	118.60
31	a	1405	C	C2-N3-C4	5.22	122.51	119.90
31	a	792	A	N1-C6-N6	5.22	121.73	118.60
1	A	2747	U	N3-C2-O2	-5.22	118.55	122.20
31	a	54	A	C4-C5-N7	5.22	113.31	110.70
1	A	212	C	C2-N1-C1'	5.21	124.54	118.80
31	a	934	G	C8-N9-C4	-5.21	104.31	106.40
1	A	1776	A	C5-C6-N6	-5.21	119.53	123.70
1	A	2845	G	N3-C4-N9	-5.21	122.87	126.00
1	A	503	A	N1-C6-N6	5.21	121.73	118.60
31	a	548	G	C4-C5-N7	5.21	112.89	110.80
31	a	748	U	N3-C2-O2	-5.21	118.55	122.20
1	A	1494	G	C4-N9-C1'	-5.21	119.73	126.50
1	A	1799	G	N3-C4-C5	5.21	131.21	128.60
1	A	1163	U	N3-C2-O2	-5.21	118.55	122.20
1	A	2431	C	N1-C2-O2	5.21	122.03	118.90
1	A	2526	C	C5-C4-N4	-5.21	116.55	120.20
1	A	160	G	N7-C8-N9	5.21	115.70	113.10
1	A	1390	A	C5-C6-N1	5.21	120.30	117.70
1	A	2397	G	C5-C6-O6	5.21	131.72	128.60
2	B	60	C	N1-C2-O2	5.21	122.02	118.90
31	a	794	G	C2-N3-C4	5.21	114.50	111.90
1	A	1762	U	N3-C2-O2	5.20	125.84	122.20
1	A	2406	G	N9-C4-C5	-5.20	103.32	105.40
1	A	2771	G	N3-C4-N9	5.20	129.12	126.00
1	A	2869	G	C4-N9-C1'	-5.20	119.74	126.50
31	a	255	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	334	A	C5-C6-N1	-5.20	115.10	117.70
1	A	822	G	N3-C4-C5	5.20	131.20	128.60
1	A	1687	G	N3-C4-N9	-5.20	122.88	126.00
1	A	1986	G	N1-C6-O6	-5.20	116.78	119.90
1	A	1762	U	N1-C2-O2	-5.20	119.16	122.80
1	A	2261	G	P-O3'-C3'	-5.20	113.46	119.70
31	a	794	G	C8-N9-C4	-5.20	104.32	106.40
31	a	1002	G	N9-C4-C5	-5.20	103.32	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	512	C	N3-C2-O2	-5.20	118.26	121.90
1	A	506	A	C5-C6-N6	-5.20	119.54	123.70
1	A	1989	C	C6-N1-C2	-5.20	118.22	120.30
1	A	27	G	C2-N3-C4	-5.19	109.30	111.90
1	A	1812	A	N1-C6-N6	5.19	121.72	118.60
1	A	2047	A	C4-C5-N7	5.19	113.30	110.70
31	a	1002	G	N1-C6-O6	5.19	123.02	119.90
31	a	1348	G	N3-C4-N9	5.19	129.12	126.00
31	a	408	C	N1-C2-O2	5.19	122.01	118.90
1	A	2400	U	C5-C4-O4	-5.19	122.79	125.90
1	A	305	A	N9-C4-C5	-5.19	103.73	105.80
31	a	693	G	C4-N9-C1'	-5.19	119.76	126.50
1	A	922	G	N3-C4-N9	-5.18	122.89	126.00
1	A	1316	G	C4-C5-N7	5.18	112.87	110.80
1	A	1991	G	N3-C2-N2	-5.18	116.27	119.90
1	A	162	A	C4-C5-C6	5.18	119.59	117.00
1	A	573	A	C5-C6-N1	5.18	120.29	117.70
1	A	806	A	N9-C4-C5	-5.18	103.73	105.80
1	A	2636	U	C2-N1-C1'	5.18	123.92	117.70
1	A	955	A	N3-C4-N9	-5.18	123.26	127.40
1	A	1253	G	C4-N9-C1'	5.18	133.23	126.50
31	a	356	G	N1-C2-N2	-5.18	111.54	116.20
1	A	284	C	N3-C2-O2	-5.17	118.28	121.90
1	A	1015	C	N1-C2-O2	5.17	122.00	118.90
1	A	1467	G	C8-N9-C1'	-5.17	120.27	127.00
1	A	1991	G	C4-N9-C1'	-5.17	119.77	126.50
31	a	488	U	C6-N1-C1'	-5.17	113.96	121.20
31	a	1482	G	N3-C4-N9	-5.17	122.90	126.00
1	A	267	G	N3-C4-C5	5.17	131.19	128.60
1	A	1740	G	N3-C4-C5	5.17	131.19	128.60
1	A	2735	G	C4-C5-N7	5.17	112.87	110.80
31	a	514	G	C6-C5-N7	-5.17	127.30	130.40
31	a	649	A	O4'-C1'-N9	5.17	112.34	108.20
1	A	1694	A	C8-N9-C4	5.17	107.87	105.80
31	a	67	G	C6-C5-N7	-5.17	127.30	130.40
31	a	457	A	C4-N9-C1'	5.17	135.60	126.30
1	A	1283	G	N3-C2-N2	-5.17	116.28	119.90
1	A	1481	A	C4-C5-C6	-5.17	114.42	117.00
1	A	2895	G	C2-N3-C4	-5.17	109.32	111.90
31	a	159	G	N3-C4-C5	5.17	131.18	128.60
1	A	1987	A	N1-C6-N6	-5.16	115.50	118.60
1	A	2703	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	725	C	C2-N1-C1'	5.16	124.48	118.80
1	A	1198	G	C2-N3-C4	-5.16	109.32	111.90
1	A	2086	A	O4'-C1'-N9	5.16	112.33	108.20
31	a	1498	G	N3-C4-C5	5.16	131.18	128.60
31	a	213	G	N1-C6-O6	5.16	122.99	119.90
42	l	134	LYS	CA-CB-CG	5.16	124.74	113.40
1	A	1986	G	C2-N3-C4	-5.15	109.32	111.90
1	A	2764	G	C6-C5-N7	-5.15	127.31	130.40
1	A	775	A	N9-C4-C5	-5.15	103.74	105.80
1	A	1407	C	N3-C4-C5	5.15	123.96	121.90
1	A	908	A	C5-N7-C8	-5.15	101.32	103.90
31	a	326	G	N3-C4-C5	5.15	131.18	128.60
31	a	1329	A	P-O3'-C3'	5.15	125.88	119.70
42	l	69	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	384	G	N1-C2-N2	-5.15	111.57	116.20
1	A	1793	C	N3-C4-N4	-5.15	114.40	118.00
1	A	95	A	C6-C5-N7	-5.14	128.70	132.30
1	A	575	G	C8-N9-C1'	-5.14	120.31	127.00
1	A	778	G	N3-C4-C5	5.14	131.17	128.60
1	A	1039	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1905	G	N3-C4-N9	5.14	129.09	126.00
1	A	1503	U	P-O3'-C3'	5.14	125.87	119.70
1	A	1534	G	N9-C4-C5	5.14	107.46	105.40
1	A	165	C	N3-C2-O2	-5.14	118.30	121.90
1	A	759	U	C5'-C4'-O4'	5.14	115.27	109.10
31	a	522	C	C5-C6-N1	5.14	123.57	121.00
49	s	36	ARG	CA-CB-CG	5.14	124.71	113.40
31	a	1333	G	N9-C4-C5	-5.14	103.34	105.40
31	a	556	G	C8-N9-C4	5.14	108.45	106.40
1	A	1053	A	N9-C4-C5	-5.13	103.75	105.80
1	A	2907	A	C5-N7-C8	-5.13	101.33	103.90
1	A	1198	G	N3-C4-C5	5.13	131.17	128.60
31	a	452	A	C5-C6-N6	-5.13	119.59	123.70
1	A	15	G	C4-C5-N7	5.13	112.85	110.80
1	A	618	A	C5-C6-N6	-5.13	119.60	123.70
1	A	756	A	C5-C6-N6	-5.13	119.60	123.70
1	A	2907	A	C6-C5-N7	-5.13	128.71	132.30
31	a	213	G	C4-N9-C1'	5.13	133.17	126.50
1	A	2774	G	C8-N9-C4	5.12	108.45	106.40
2	B	5	G	N3-C4-C5	5.12	131.16	128.60
31	a	670	A	N1-C6-N6	5.12	121.67	118.60
1	A	878	C	C5-C4-N4	5.12	123.79	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	513	G	C8-N9-C1'	5.12	133.66	127.00
1	A	253	G	C2-N3-C4	-5.12	109.34	111.90
1	A	2112	C	N1-C2-O2	5.12	121.97	118.90
1	A	136	A	N7-C8-N9	5.12	116.36	113.80
1	A	2742	C	C2-N1-C1'	5.12	124.43	118.80
31	a	693	G	N1-C2-N2	5.12	120.81	116.20
31	a	1028	G	N1-C2-N2	-5.12	111.59	116.20
1	A	450	C	N1-C2-O2	5.12	121.97	118.90
1	A	2324	C	C2-N3-C4	5.12	122.46	119.90
1	A	804	G	N3-C4-N9	-5.11	122.93	126.00
31	a	940	C	C2-N1-C1'	5.11	124.42	118.80
1	A	71	A	N1-C6-N6	5.11	121.67	118.60
1	A	1080	G	C6-C5-N7	-5.11	127.33	130.40
1	A	2248	G	C8-N9-C1'	5.11	133.65	127.00
2	B	114	G	N7-C8-N9	5.11	115.66	113.10
31	a	1156	A	N1-C6-N6	-5.11	115.53	118.60
1	A	640	G	N3-C4-C5	5.11	131.16	128.60
1	A	1378	U	N3-C2-O2	-5.11	118.62	122.20
31	a	805	C	N3-C2-O2	-5.11	118.32	121.90
31	a	1510	A	N3-C4-N9	5.11	131.49	127.40
1	A	1733	A	N1-C6-N6	5.11	121.67	118.60
1	A	2747	U	C2-N1-C1'	5.11	123.83	117.70
1	A	951	G	N3-C4-N9	-5.11	122.94	126.00
31	a	123	G	C6-C5-N7	-5.11	127.33	130.40
1	A	2903	A	C5-C6-N1	5.10	120.25	117.70
1	A	1411	G	N3-C2-N2	5.10	123.47	119.90
2	B	108	U	C5-C6-N1	5.10	125.25	122.70
1	A	2905	C	N3-C2-O2	-5.10	118.33	121.90
1	A	983	G	N3-C4-C5	5.10	131.15	128.60
1	A	1383	G	N3-C4-C5	5.10	131.15	128.60
1	A	104	C	C2-N3-C4	5.10	122.45	119.90
1	A	1538	A	N7-C8-N9	5.10	116.35	113.80
1	A	845	A	C5-C6-N6	-5.10	119.62	123.70
31	a	387	C	N3-C2-O2	-5.09	118.33	121.90
1	A	2602	C	N3-C4-C5	5.09	123.94	121.90
1	A	760	A	O4'-C1'-N9	5.09	112.27	108.20
1	A	1632	A	C3'-C2'-C1'	5.09	105.57	101.50
31	a	681	G	C4-C5-N7	-5.09	108.76	110.80
1	A	1493	U	N1-C2-O2	5.09	126.36	122.80
1	A	1571	G	C4-N9-C1'	5.09	133.12	126.50
1	A	2895	G	N3-C4-C5	5.09	131.15	128.60
31	a	478	G	N3-C4-N9	5.09	129.05	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1143	C	N1-C2-O2	5.09	121.95	118.90
1	A	1021	G	N1-C6-O6	5.09	122.95	119.90
1	A	1320	G	N3-C4-C5	5.09	131.14	128.60
1	A	2441	G	C5-N7-C8	-5.09	101.76	104.30
1	A	697	U	P-O3'-C3'	5.08	125.80	119.70
1	A	860	U	N3-C4-O4	5.08	122.96	119.40
1	A	1423	C	N3-C2-O2	-5.08	118.34	121.90
1	A	1466	G	N3-C4-C5	5.08	131.14	128.60
1	A	727	G	C2-N3-C4	-5.08	109.36	111.90
1	A	1445	C	C2-N3-C4	5.08	122.44	119.90
31	a	649	A	N9-C4-C5	5.08	107.83	105.80
1	A	1741	G	N3-C4-N9	-5.08	122.95	126.00
1	A	1906	C	C5-C6-N1	5.08	123.54	121.00
1	A	783	G	N3-C4-C5	5.08	131.14	128.60
1	A	1037	A	C5-C6-N6	-5.08	119.64	123.70
1	A	1794	C	N3-C4-N4	-5.08	114.45	118.00
1	A	2829	A	N9-C4-C5	-5.08	103.77	105.80
1	A	887	A	N9-C4-C5	-5.08	103.77	105.80
1	A	1041	G	N3-C4-C5	5.08	131.14	128.60
1	A	1637	A	C5-N7-C8	-5.08	101.36	103.90
1	A	1638	G	C4-C5-N7	5.08	112.83	110.80
1	A	2064	A	C4-C5-N7	5.08	113.24	110.70
1	A	2570	G	C2-N3-C4	-5.08	109.36	111.90
1	A	2671	A	C4-C5-C6	-5.08	114.46	117.00
31	a	1002	G	N7-C8-N9	5.08	115.64	113.10
1	A	515	G	N9-C4-C5	-5.07	103.37	105.40
1	A	1830	A	N7-C8-N9	5.07	116.34	113.80
1	A	1501	G	N3-C4-C5	5.07	131.14	128.60
31	a	1441	C	C6-N1-C1'	5.07	126.89	120.80
1	A	1759	G	C2-N3-C4	-5.07	109.36	111.90
31	a	444	C	C5-C6-N1	5.07	123.53	121.00
31	a	681	G	N9-C1'-C2'	5.07	120.59	114.00
31	a	722	G	C4-N9-C1'	5.07	133.09	126.50
31	a	1445	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	1976	G	N3-C4-C5	5.07	131.13	128.60
1	A	115	C	N3-C4-C5	5.07	123.93	121.90
1	A	886	A	C4-C5-N7	5.07	113.23	110.70
1	A	1822	C	O3'-P-O5'	5.07	113.62	104.00
31	a	246	G	N3-C4-N9	5.07	129.04	126.00
1	A	1534	G	C6-C5-N7	5.06	133.44	130.40
31	a	1083	G	C5-N7-C8	-5.06	101.77	104.30
1	A	1492	G	C2-N3-C4	-5.06	109.37	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	213	G	C5-N7-C8	-5.06	101.77	104.30
31	a	612	G	C6-C5-N7	-5.06	127.36	130.40
1	A	410	G	C5-N7-C8	-5.06	101.77	104.30
31	a	332	G	N7-C8-N9	5.06	115.63	113.10
1	A	171	A	N9-C4-C5	-5.06	103.78	105.80
1	A	1087	C	C6-N1-C1'	5.06	126.87	120.80
31	a	327	G	O4'-C1'-N9	5.06	112.25	108.20
31	a	765	U	C5-C6-N1	5.06	125.23	122.70
31	a	1205	C	N3-C4-N4	5.06	121.54	118.00
31	a	1398	U	O4'-C1'-N1	5.06	112.25	108.20
1	A	725	A	C5-C6-N6	-5.06	119.66	123.70
1	A	1380	G	C4-C5-N7	5.06	112.82	110.80
1	A	1723	A	N1-C6-N6	5.06	121.63	118.60
1	A	1320	G	C2-N3-C4	-5.05	109.37	111.90
1	A	2818	A	C5-C6-N6	-5.05	119.66	123.70
31	a	571	A	C4-N9-C1'	5.05	135.40	126.30
31	a	606	U	N3-C2-O2	5.05	125.74	122.20
31	a	1173	G	C4-C5-C6	5.05	121.83	118.80
1	A	917	U	C5-C4-O4	5.05	128.93	125.90
1	A	1500	G	N1-C6-O6	5.05	122.93	119.90
1	A	283	G	C4-C5-N7	5.05	112.82	110.80
1	A	660	A	N1-C6-N6	-5.05	115.57	118.60
1	A	674	C	C6-N1-C2	5.05	122.32	120.30
1	A	1494	G	C8-N9-C1'	5.05	133.57	127.00
1	A	1848	A	C4-C5-N7	5.05	113.23	110.70
31	a	1319	G	C4-C5-N7	5.05	112.82	110.80
31	a	1510	A	C5-C6-N1	5.05	120.23	117.70
1	A	1819	G	C2-N3-C4	-5.05	109.38	111.90
1	A	2261	G	OP1-P-O3'	-5.05	94.09	105.20
1	A	2669	G	N3-C4-C5	5.05	131.12	128.60
31	a	515	C	N3-C2-O2	-5.05	118.37	121.90
31	a	1453	A	C6-C5-N7	-5.05	128.77	132.30
1	A	7	G	C8-N9-C1'	5.05	133.56	127.00
1	A	1213	C	N3-C4-N4	5.05	121.53	118.00
1	A	1228	A	C5-N7-C8	-5.05	101.38	103.90
1	A	54	G	N3-C2-N2	5.05	123.43	119.90
31	a	1381	G	C6-C5-N7	5.05	133.43	130.40
31	a	1390	U	C5-C4-O4	5.05	128.93	125.90
1	A	384	G	N3-C2-N2	5.04	123.43	119.90
1	A	135	G	C4-C5-N7	5.04	112.82	110.80
31	a	283	G	C6-C5-N7	-5.04	127.37	130.40
1	A	257	G	C2-N3-C4	-5.04	109.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1053	A	C6-C5-N7	-5.04	128.77	132.30
1	A	1231	A	N9-C4-C5	-5.04	103.78	105.80
31	a	1454	G	N3-C4-N9	5.04	129.03	126.00
31	a	1505	G	N3-C4-N9	5.04	129.03	126.00
1	A	318	A	O4'-C1'-N9	5.04	112.23	108.20
31	a	1020	U	C5-C4-O4	-5.04	122.88	125.90
31	a	1333	G	N3-C2-N2	5.04	123.43	119.90
1	A	1423	C	N1-C2-O2	5.04	121.92	118.90
31	a	548	G	N9-C4-C5	-5.04	103.38	105.40
31	a	1072	G	N3-C2-N2	5.04	123.43	119.90
1	A	752	G	C6-C5-N7	-5.04	127.38	130.40
1	A	1513	A	C4-N9-C1'	5.04	135.37	126.30
31	a	262	G	P-O3'-C3'	5.04	125.74	119.70
31	a	781	G	N7-C8-N9	5.04	115.62	113.10
1	A	2896	A	C5-N7-C8	-5.03	101.38	103.90
31	a	36	G	C5-C6-O6	5.03	131.62	128.60
1	A	554	C	C6-N1-C2	5.03	122.31	120.30
1	A	888	G	N3-C4-C5	5.03	131.11	128.60
1	A	1196	C	C6-N1-C2	-5.03	118.29	120.30
1	A	2882	A	C4-C5-N7	5.03	113.21	110.70
31	a	1218	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1195	A	C5-N7-C8	-5.03	101.39	103.90
1	A	2064	A	C5-N7-C8	-5.03	101.39	103.90
31	a	24	C	N3-C2-O2	-5.03	118.38	121.90
31	a	350	C	N1-C2-O2	5.03	121.92	118.90
31	a	513	G	C6-C5-N7	5.03	133.42	130.40
31	a	1069	G	O4'-C1'-N9	5.03	112.22	108.20
1	A	330	C	N3-C2-O2	-5.03	118.38	121.90
1	A	522	G	C8-N9-C4	5.03	108.41	106.40
1	A	719	G	N1-C2-N2	-5.03	111.68	116.20
31	a	394	C	C6-N1-C2	-5.03	118.29	120.30
31	a	101	G	N3-C4-C5	5.02	131.11	128.60
4	D	133	ARG	NE-CZ-NH1	5.02	122.81	120.30
31	a	111	G	N1-C2-N2	5.02	120.72	116.20
1	A	193	A	C5-C6-N1	5.02	120.21	117.70
1	A	193	A	C5-C6-N6	-5.02	119.69	123.70
1	A	1287	U	C2-N1-C1'	5.02	123.72	117.70
1	A	1852	G	N9-C4-C5	5.02	107.41	105.40
1	A	2690	G	N9-C4-C5	-5.02	103.39	105.40
31	a	967	A	C6-N1-C2	5.02	121.61	118.60
31	a	1326	G	N3-C4-N9	5.02	129.01	126.00
1	A	1857	C	N1-C2-O2	5.02	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1428	A	C5-C6-N6	5.02	127.71	123.70
1	A	1021	G	N9-C4-C5	-5.01	103.39	105.40
1	A	1481	A	O4'-C1'-N9	5.01	112.21	108.20
1	A	1562	C	N3-C2-O2	-5.01	118.39	121.90
1	A	1987	A	C6-C5-N7	5.01	135.81	132.30
1	A	1123	C	N1-C2-O2	5.01	121.91	118.90
1	A	1522	G	N3-C4-C5	5.01	131.11	128.60
1	A	2683	U	N3-C2-O2	-5.01	118.69	122.20
2	B	19	G	C2-N3-C4	-5.01	109.39	111.90
1	A	2457	A	C5-C6-N6	-5.01	119.69	123.70
1	A	2671	A	N3-C4-C5	5.01	130.31	126.80
1	A	252	C	N3-C4-C5	5.01	123.90	121.90
1	A	409	G	N3-C2-N2	5.01	123.41	119.90
1	A	1740	G	N3-C4-N9	-5.01	123.00	126.00
1	A	997	G	N3-C2-N2	5.00	123.40	119.90
1	A	2700	G	N3-C4-C5	5.00	131.10	128.60
1	A	265	A	N9-C4-C5	-5.00	103.80	105.80
1	A	661	U	C5-C4-O4	-5.00	122.90	125.90
1	A	1179	C	N3-C2-O2	-5.00	118.40	121.90
1	A	1279	C	N1-C2-O2	5.00	121.90	118.90
1	A	2002	G	N9-C4-C5	-5.00	103.40	105.40
31	a	385	G	N3-C4-N9	-5.00	123.00	126.00

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	4	1	MET	Peptide
30	4	13	LYS	Peptide
3	C	173	LEU	Peptide
3	C	255	LEU	Peptide
3	C	257	LYS	Peptide
3	C	273	GLY	Peptide
3	C	40	LYS	Peptide
5	E	132	GLU	Peptide
6	F	16	LEU	Peptide
6	F	170	LEU	Peptide
7	G	106	ASN	Peptide
8	H	11	ASN	Peptide
8	H	133	HIS	Peptide
8	H	57	VAL	Peptide
8	H	80	ASN	Peptide

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Mol	Chain	Res	Type	Group
11	K	1	MET	Peptide
11	K	3	LEU	Peptide
11	K	68	ILE	Peptide
12	L	95	GLU	Peptide
13	M	68	THR	Peptide
16	P	50	ALA	Peptide
16	P	77	LYS	Peptide
19	S	4	LYS	Peptide
26	Z	37	LYS	Peptide
26	Z	43	CYS	Peptide
31	a	605	G	Sidechain
31	a	606	U	Sidechain
32	b	103	ASN	Peptide
32	b	104	TYR	Peptide
32	b	107	ILE	Peptide
32	b	21	ARG	Peptide
33	c	169	GLU	Peptide
34	d	102	GLY	Peptide
34	d	103	LEU	Peptide
34	d	104	ALA	Peptide
34	d	109	GLN	Peptide
34	d	44	LEU	Peptide
34	d	45	SER	Peptide
34	d	97	VAL	Peptide
37	g	101	LEU	Peptide
37	g	102	ARG	Peptide
37	g	105	VAL	Peptide
37	g	108	ALA	Peptide
37	g	138	ARG	Peptide
37	g	144	MET	Peptide
37	g	2	PRO	Peptide
37	g	70	MET	Peptide
37	g	71	PRO	Peptide
37	g	95	ARG	Peptide
39	i	128	GLN	Peptide
40	j	15	HIS	Peptide
40	j	65	PHE	Peptide
40	j	87	LEU	Peptide
40	j	9	ARG	Peptide
41	k	116	VAL	Peptide
41	k	118	HIS	Peptide
41	k	122	ARG	Peptide

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Mol	Chain	Res	Type	Group
41	k	123	PRO	Peptide
41	k	126	ARG	Peptide
42	l	133	LYS	Peptide
42	l	135	PRO	Peptide
43	m	106	ALA	Peptide
43	m	27	THR	Peptide
43	m	64	LYS	Peptide
43	m	73	THR	Peptide
43	m	74	ASN	Peptide
44	n	25	GLU	Peptide
44	n	34	TYR	Peptide
44	n	58	LYS	Peptide
44	n	59	ALA	Peptide
45	o	19	GLU	Peptide
45	o	2	ALA	Peptide
45	o	46	HIS	Peptide
45	o	47	LYS	Peptide
47	q	22	THR	Peptide
47	q	24	THR	Peptide
47	q	63	ILE	Peptide
47	q	65	GLU	Peptide
47	q	75	PHE	Peptide
49	s	71	LEU	Peptide
49	s	79	THR	Peptide
49	s	80	PHE	Peptide
50	t	69	ASN	Peptide
51	u	32	VAL	Peptide
51	u	33	ARG	Peptide
51	u	49	SER	Peptide
52	v	33	ASN	Peptide
52	v	92	TYR	Peptide
52	v	93	LYS	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	272/274 (99%)	215 (79%)	57 (21%)	0	100	100
4	D	213/215 (99%)	166 (78%)	47 (22%)	0	100	100
5	E	204/206 (99%)	175 (86%)	29 (14%)	0	100	100
6	F	173/175 (99%)	141 (82%)	32 (18%)	0	100	100
7	G	173/175 (99%)	140 (81%)	33 (19%)	0	100	100
8	H	143/145 (99%)	118 (82%)	25 (18%)	0	100	100
9	I	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
10	J	144/146 (99%)	124 (86%)	20 (14%)	0	100	100
11	K	135/137 (98%)	113 (84%)	22 (16%)	0	100	100
12	L	118/120 (98%)	101 (86%)	17 (14%)	0	100	100
13	M	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
14	N	112/114 (98%)	94 (84%)	18 (16%)	0	100	100
15	O	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
16	P	100/102 (98%)	85 (85%)	15 (15%)	0	100	100
17	Q	108/110 (98%)	90 (83%)	17 (16%)	1 (1%)	14	48
18	R	87/89 (98%)	70 (80%)	17 (20%)	0	100	100
19	S	101/103 (98%)	82 (81%)	19 (19%)	0	100	100
20	T	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
21	U	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
22	V	56/58 (97%)	46 (82%)	10 (18%)	0	100	100
23	W	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
24	X	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
25	Y	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
26	Z	46/48 (96%)	29 (63%)	17 (37%)	0	100	100
27	1	45/47 (96%)	37 (82%)	8 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	50 (81%)	12 (19%)	0	100	100
30	4	35/37 (95%)	21 (60%)	14 (40%)	0	100	100
32	b	224/226 (99%)	193 (86%)	31 (14%)	0	100	100
33	c	200/202 (99%)	161 (80%)	39 (20%)	0	100	100
34	d	196/198 (99%)	136 (69%)	59 (30%)	1 (0%)	25	59
35	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
36	f	93/95 (98%)	75 (81%)	18 (19%)	0	100	100
37	g	149/152 (98%)	99 (66%)	50 (34%)	0	100	100
38	h	127/131 (97%)	98 (77%)	29 (23%)	0	100	100
39	i	125/127 (98%)	86 (69%)	39 (31%)	0	100	100
40	j	95/97 (98%)	59 (62%)	35 (37%)	1 (1%)	12	45
41	k	112/114 (98%)	81 (72%)	31 (28%)	0	100	100
42	l	133/135 (98%)	102 (77%)	29 (22%)	2 (2%)	8	39
43	m	100/104 (96%)	62 (62%)	38 (38%)	0	100	100
44	n	58/60 (97%)	36 (62%)	22 (38%)	0	100	100
45	o	86/88 (98%)	71 (83%)	15 (17%)	0	100	100
46	p	87/89 (98%)	68 (78%)	19 (22%)	0	100	100
47	q	78/80 (98%)	51 (65%)	27 (35%)	0	100	100
48	r	52/54 (96%)	43 (83%)	9 (17%)	0	100	100
49	s	78/80 (98%)	58 (74%)	20 (26%)	0	100	100
50	t	79/81 (98%)	59 (75%)	20 (25%)	0	100	100
51	u	50/52 (96%)	32 (64%)	18 (36%)	0	100	100
52	v	158/162 (98%)	117 (74%)	41 (26%)	0	100	100
All	All	5503/5608 (98%)	4369 (79%)	1129 (20%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	l	131	GLY
34	d	110	ALA
40	j	7	ARG
17	Q	87	PRO
42	l	135	PRO

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	
3	C	220/221 (100%)	177 (80%)	43 (20%)	1	7
4	D	173/173 (100%)	144 (83%)	29 (17%)	1	11
5	E	168/168 (100%)	126 (75%)	42 (25%)	0	3
6	F	141/154 (92%)	116 (82%)	25 (18%)	1	9
7	G	124/153 (81%)	101 (82%)	23 (18%)	1	8
8	H	122/123 (99%)	98 (80%)	24 (20%)	1	7
9	I	100/100 (100%)	79 (79%)	21 (21%)	1	6
10	J	109/112 (97%)	96 (88%)	13 (12%)	4	22
11	K	108/114 (95%)	93 (86%)	15 (14%)	3	17
12	L	96/101 (95%)	82 (85%)	14 (15%)	2	16
13	M	86/95 (90%)	61 (71%)	25 (29%)	0	2
14	N	93/100 (93%)	79 (85%)	14 (15%)	2	15
15	O	96/96 (100%)	83 (86%)	13 (14%)	3	18
16	P	84/86 (98%)	64 (76%)	20 (24%)	0	4
17	Q	88/90 (98%)	59 (67%)	29 (33%)	0	1
18	R	78/80 (98%)	62 (80%)	16 (20%)	1	6
19	S	81/88 (92%)	59 (73%)	22 (27%)	0	3
20	T	78/82 (95%)	60 (77%)	18 (23%)	0	4
21	U	63/64 (98%)	45 (71%)	18 (29%)	0	2
22	V	44/49 (90%)	33 (75%)	11 (25%)	0	3
23	W	58/60 (97%)	50 (86%)	8 (14%)	3	17
24	X	52/52 (100%)	44 (85%)	8 (15%)	2	14
25	Y	23/56 (41%)	22 (96%)	1 (4%)	25	54
26	Z	35/44 (80%)	24 (69%)	11 (31%)	0	2
27	1	44/45 (98%)	32 (73%)	12 (27%)	0	2
28	2	39/39 (100%)	35 (90%)	4 (10%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	55/55 (100%)	48 (87%)	7 (13%)	3	19
30	4	35/35 (100%)	27 (77%)	8 (23%)	0	4
32	b	196/196 (100%)	160 (82%)	36 (18%)	1	8
33	c	138/164 (84%)	110 (80%)	28 (20%)	1	6
34	d	147/174 (84%)	114 (78%)	33 (22%)	1	5
35	e	118/122 (97%)	97 (82%)	21 (18%)	1	9
36	f	80/83 (96%)	62 (78%)	18 (22%)	1	5
37	g	118/128 (92%)	90 (76%)	28 (24%)	0	4
38	h	111/112 (99%)	88 (79%)	23 (21%)	1	6
39	i	86/105 (82%)	68 (79%)	18 (21%)	1	6
40	j	81/87 (93%)	66 (82%)	15 (18%)	1	8
41	k	82/90 (91%)	60 (73%)	22 (27%)	0	3
42	l	111/117 (95%)	80 (72%)	31 (28%)	0	2
43	m	62/92 (67%)	51 (82%)	11 (18%)	1	9
44	n	48/52 (92%)	35 (73%)	13 (27%)	0	3
45	o	77/80 (96%)	59 (77%)	18 (23%)	0	4
46	p	73/75 (97%)	56 (77%)	17 (23%)	0	4
47	q	65/75 (87%)	49 (75%)	16 (25%)	0	4
48	r	48/49 (98%)	41 (85%)	7 (15%)	2	16
49	s	67/70 (96%)	50 (75%)	17 (25%)	0	3
50	t	61/67 (91%)	49 (80%)	12 (20%)	1	7
51	u	40/48 (83%)	29 (72%)	11 (28%)	0	2
52	v	147/147 (100%)	115 (78%)	32 (22%)	1	5
All	All	4449/4768 (93%)	3528 (79%)	921 (21%)	3	6

All (921) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5	LYS
3	C	19	LEU
3	C	27	THR
3	C	34	LEU
3	C	35	LYS
3	C	37	LEU

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Mol	Chain	Res	Type
3	C	46	GLN
3	C	52	ARG
3	C	60	ARG
3	C	63	ARG
3	C	66	ASP
3	C	70	ASN
3	C	77	LYS
3	C	87	ARG
3	C	91	ILE
3	C	94	VAL
3	C	101	LYS
3	C	108	LYS
3	C	110	LEU
3	C	121	GLU
3	C	123	ASP
3	C	125	LYS
3	C	133	GLN
3	C	139	THR
3	C	147	LYS
3	C	175	ARG
3	C	182	ARG
3	C	197	ASN
3	C	202	LEU
3	C	207	LYS
3	C	210	ARG
3	C	213	TRP
3	C	214	LYS
3	C	232	HIS
3	C	252	LYS
3	C	254	THR
3	C	255	LEU
3	C	260	ARG
3	C	261	ARG
3	C	264	LYS
3	C	270	ILE
3	C	272	ARG
3	C	274	ARG
4	D	5	ILE
4	D	6	LEU
4	D	10	ILE
4	D	13	THR
4	D	26	THR

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Mol	Chain	Res	Type
4	D	32	GLU
4	D	40	THR
4	D	42	GLU
4	D	49	ILE
4	D	57	LYS
4	D	61	LYS
4	D	62	ASP
4	D	65	SER
4	D	71	LYS
4	D	78	LYS
4	D	81	ASP
4	D	100	GLU
4	D	104	GLU
4	D	108	ASP
4	D	122	SER
4	D	131	ILE
4	D	137	SER
4	D	169	MET
4	D	176	ASN
4	D	178	VAL
4	D	183	LEU
4	D	194	VAL
4	D	201	VAL
4	D	211	ILE
5	E	5	ASP
5	E	8	LYS
5	E	13	LYS
5	E	14	SER
5	E	27	GLU
5	E	30	ASN
5	E	33	LEU
5	E	35	GLU
5	E	43	SER
5	E	44	LEU
5	E	49	HIS
5	E	51	VAL
5	E	55	SER
5	E	72	ARG
5	E	82	GLN
5	E	99	TYR
5	E	100	LYS
5	E	101	MET

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Mol	Chain	Res	Type
5	E	105	MET
5	E	108	LEU
5	E	111	ARG
5	E	112	SER
5	E	114	LEU
5	E	116	PHE
5	E	117	LYS
5	E	119	GLN
5	E	121	ASN
5	E	125	VAL
5	E	130	ASN
5	E	135	LYS
5	E	137	LYS
5	E	139	PHE
5	E	146	LEU
5	E	150	LYS
5	E	154	VAL
5	E	159	GLU
5	E	169	ASN
5	E	173	VAL
5	E	187	THR
5	E	193	VAL
5	E	201	LYS
5	E	204	GLU
6	F	15	ASN
6	F	30	LYS
6	F	32	ASP
6	F	36	VAL
6	F	48	LYS
6	F	59	LEU
6	F	64	LYS
6	F	66	LEU
6	F	71	LYS
6	F	78	ARG
6	F	79	LEU
6	F	80	ARG
6	F	98	GLU
6	F	99	PHE
6	F	100	LEU
6	F	119	LYS
6	F	120	LYS
6	F	125	ARG

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Mol	Chain	Res	Type
6	F	127	ASN
6	F	143	TYR
6	F	152	MET
6	F	155	VAL
6	F	162	THR
6	F	168	GLU
6	F	175	MET
7	G	4	VAL
7	G	16	THR
7	G	30	LYS
7	G	44	LYS
7	G	65	HIS
7	G	69	ARG
7	G	75	MET
7	G	83	TYR
7	G	87	LEU
7	G	89	LEU
7	G	90	VAL
7	G	94	TYR
7	G	97	GLN
7	G	105	LEU
7	G	106	ASN
7	G	112	PRO
7	G	115	ILE
7	G	136	ILE
7	G	149	ARG
7	G	155	GLU
7	G	170	ARG
7	G	172	LYS
7	G	175	LYS
8	H	1	MET
8	H	3	GLN
8	H	15	LYS
8	H	19	ILE
8	H	20	ASP
8	H	22	GLU
8	H	29	LEU
8	H	38	ARG
8	H	44	THR
8	H	46	THR
8	H	53	ASP
8	H	57	VAL

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Mol	Chain	Res	Type
8	H	62	LYS
8	H	72	ASP
8	H	85	ILE
8	H	86	LYS
8	H	87	SER
8	H	88	ILE
8	H	95	ARG
8	H	97	ASN
8	H	103	GLU
8	H	115	LEU
8	H	133	HIS
8	H	143	LEU
9	I	2	ILE
9	I	4	GLN
9	I	8	LEU
9	I	10	VAL
9	I	19	VAL
9	I	21	THR
9	I	39	ILE
9	I	40	VAL
9	I	47	THR
9	I	61	VAL
9	I	64	ARG
9	I	70	ARG
9	I	75	SER
9	I	77	ILE
9	I	82	ASN
9	I	84	CYS
9	I	99	PHE
9	I	106	LEU
9	I	112	MET
9	I	117	LEU
9	I	120	GLU
10	J	14	LYS
10	J	31	SER
10	J	57	LEU
10	J	64	ARG
10	J	72	LYS
10	J	77	VAL
10	J	81	GLN
10	J	90	GLU
10	J	92	THR

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Mol	Chain	Res	Type
10	J	95	LEU
10	J	98	GLU
10	J	103	LYS
10	J	120	LYS
11	K	5	LYS
11	K	13	HIS
11	K	18	THR
11	K	20	ARG
11	K	38	THR
11	K	45	ARG
11	K	51	ARG
11	K	64	VAL
11	K	75	THR
11	K	82	ARG
11	K	91	GLU
11	K	123	HIS
11	K	130	LYS
11	K	132	VAL
11	K	133	LYS
12	L	3	TYR
12	L	16	MET
12	L	24	LEU
12	L	33	THR
12	L	47	LEU
12	L	48	ILE
12	L	49	THR
12	L	50	LEU
12	L	68	ASN
12	L	70	GLU
12	L	78	THR
12	L	79	GLN
12	L	105	LYS
12	L	122	VAL
13	M	2	ILE
13	M	6	ASP
13	M	13	LYS
13	M	14	ARG
13	M	19	ARG
13	M	21	ASN
13	M	28	LYS
13	M	31	LEU
13	M	32	ASN

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Mol	Chain	Res	Type
13	M	34	TYR
13	M	35	ARG
13	M	39	HIS
13	M	41	TYR
13	M	44	ILE
13	M	45	ILE
13	M	46	ASP
13	M	55	GLN
13	M	57	SER
13	M	58	SER
13	M	68	THR
13	M	72	LEU
13	M	87	LYS
13	M	90	LYS
13	M	95	ASP
13	M	96	ARG
14	N	17	THR
14	N	29	ARG
14	N	42	ILE
14	N	46	GLU
14	N	52	ARG
14	N	53	ARG
14	N	58	SER
14	N	67	SER
14	N	74	ARG
14	N	78	LEU
14	N	85	LYS
14	N	98	LYS
14	N	102	LEU
14	N	113	GLN
15	O	4	VAL
15	O	11	ARG
15	O	34	VAL
15	O	51	ARG
15	O	55	ARG
15	O	72	HIS
15	O	81	ASN
15	O	89	ASP
15	O	92	ARG
15	O	95	LEU
15	O	102	ASP
15	O	103	GLU

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Mol	Chain	Res	Type
15	O	104	LYS
16	P	7	THR
16	P	10	LYS
16	P	13	LYS
16	P	14	VAL
16	P	21	PHE
16	P	23	GLU
16	P	24	LYS
16	P	25	LEU
16	P	31	ASP
16	P	34	THR
16	P	37	LYS
16	P	59	THR
16	P	63	ASN
16	P	67	ARG
16	P	76	TYR
16	P	80	LYS
16	P	82	SER
16	P	96	THR
16	P	98	ASP
16	P	99	LYS
17	Q	1	MET
17	Q	4	LYS
17	Q	6	VAL
17	Q	8	ARG
17	Q	15	ARG
17	Q	17	VAL
17	Q	22	ASP
17	Q	24	ILE
17	Q	25	ARG
17	Q	36	LEU
17	Q	37	LYS
17	Q	38	LEU
17	Q	48	GLU
17	Q	49	LYS
17	Q	50	VAL
17	Q	52	MET
17	Q	62	TYR
17	Q	71	VAL
17	Q	72	LYS
17	Q	73	GLU
17	Q	75	TYR

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Mol	Chain	Res	Type
17	Q	82	LEU
17	Q	86	ARG
17	Q	88	GLN
17	Q	90	ARG
17	Q	92	SER
17	Q	101	ILE
17	Q	102	THR
17	Q	109	LYS
18	R	2	GLU
18	R	9	ARG
18	R	11	VAL
18	R	14	GLU
18	R	23	ASP
18	R	31	THR
18	R	35	LYS
18	R	36	THR
18	R	49	LYS
18	R	53	VAL
18	R	56	MET
18	R	72	THR
18	R	80	VAL
18	R	83	LYS
18	R	84	GLU
18	R	90	PHE
19	S	4	LYS
19	S	7	ASP
19	S	17	LYS
19	S	24	ILE
19	S	26	THR
19	S	27	LEU
19	S	30	LYS
19	S	33	VAL
19	S	38	VAL
19	S	41	MET
19	S	43	LYS
19	S	57	LEU
19	S	59	THR
19	S	63	ILE
19	S	70	LEU
19	S	74	LYS
19	S	76	ASN
19	S	79	THR

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Mol	Chain	Res	Type
19	S	81	VAL
19	S	87	ASP
19	S	97	SER
19	S	99	GLU
20	T	7	ILE
20	T	9	ARG
20	T	10	GLN
20	T	16	SER
20	T	18	LEU
20	T	20	GLN
20	T	30	VAL
20	T	31	VAL
20	T	32	TYR
20	T	34	TYR
20	T	36	THR
20	T	37	LYS
20	T	41	VAL
20	T	42	LYS
20	T	52	ILE
20	T	83	LYS
20	T	89	ILE
20	T	92	LEU
21	U	13	LYS
21	U	20	ASN
21	U	22	ARG
21	U	28	ARG
21	U	29	LEU
21	U	40	THR
21	U	45	LEU
21	U	47	ARG
21	U	52	LYS
21	U	53	ILE
21	U	61	ARG
21	U	67	LEU
21	U	68	PHE
21	U	72	ASP
21	U	79	ARG
21	U	82	ARG
21	U	83	ASP
21	U	84	LYS
22	V	6	PHE
22	V	11	LYS

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Mol	Chain	Res	Type
22	V	14	THR
22	V	19	SER
22	V	29	TRP
22	V	30	ASN
22	V	32	ASN
22	V	33	LEU
22	V	45	LYS
22	V	52	ARG
22	V	56	SER
23	W	2	LYS
23	W	4	LYS
23	W	11	THR
23	W	13	GLU
23	W	16	GLU
23	W	30	PHE
23	W	32	LEU
23	W	61	GLU
24	X	18	THR
24	X	24	GLU
24	X	29	LYS
24	X	40	ASN
24	X	51	LYS
24	X	56	VAL
24	X	57	GLU
24	X	59	LYS
25	Y	1	MET
26	Z	7	ARG
26	Z	8	THR
26	Z	9	SER
26	Z	12	ARG
26	Z	16	ARG
26	Z	29	GLU
26	Z	30	CYS
26	Z	37	LYS
26	Z	38	LEU
26	Z	40	HIS
26	Z	41	ARG
27	1	5	VAL
27	1	9	CYS
27	1	15	ARG
27	1	19	THR
27	1	20	THR

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Mol	Chain	Res	Type
27	1	21	LYS
27	1	22	ASN
27	1	24	ARG
27	1	26	ASN
27	1	33	LYS
27	1	34	LYS
27	1	36	CYS
28	2	15	LYS
28	2	25	THR
28	2	37	ARG
28	2	41	LYS
29	3	6	THR
29	3	32	LEU
29	3	44	LEU
29	3	52	LYS
29	3	53	SER
29	3	55	MET
29	3	65	LYS
30	4	1	MET
30	4	11	CYS
30	4	14	CYS
30	4	16	VAL
30	4	18	LYS
30	4	19	ARG
30	4	22	LYS
30	4	35	ARG
32	b	4	ILE
32	b	10	LEU
32	b	16	PHE
32	b	21	ARG
32	b	28	LYS
32	b	29	LYS
32	b	34	GLU
32	b	50	VAL
32	b	59	GLN
32	b	60	VAL
32	b	61	SER
32	b	63	ASP
32	b	73	LYS
32	b	79	SER
32	b	85	GLU
32	b	96	TRP

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Mol	Chain	Res	Type
32	b	97	LEU
32	b	103	ASN
32	b	105	LYS
32	b	106	THR
32	b	107	ILE
32	b	112	LYS
32	b	119	LYS
32	b	131	LYS
32	b	141	TYR
32	b	144	LEU
32	b	147	PHE
32	b	152	ARG
32	b	157	MET
32	b	164	VAL
32	b	168	LYS
32	b	188	ASP
32	b	211	LYS
32	b	216	LYS
32	b	217	MET
32	b	223	GLU
33	c	4	LYS
33	c	10	LEU
33	c	11	ARG
33	c	16	ARG
33	c	23	TYR
33	c	44	ASN
33	c	53	HIS
33	c	58	ARG
33	c	67	ILE
33	c	75	VAL
33	c	99	HIS
33	c	119	ILE
33	c	126	ARG
33	c	137	ILE
33	c	138	THR
33	c	142	LYS
33	c	156	LEU
33	c	160	ASP
33	c	169	GLU
33	c	172	VAL
33	c	174	LEU
33	c	180	ASP

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Mol	Chain	Res	Type
33	c	181	ILE
33	c	190	THR
33	c	192	TYR
33	c	198	LYS
33	c	199	VAL
33	c	203	ARG
34	d	4	PHE
34	d	10	LYS
34	d	18	SER
34	d	19	LEU
34	d	35	GLN
34	d	44	LEU
34	d	46	GLU
34	d	50	GLN
34	d	51	LEU
34	d	52	ARG
34	d	69	ARG
34	d	70	ASN
34	d	84	GLU
34	d	86	PHE
34	d	93	ARG
34	d	103	LEU
34	d	106	THR
34	d	107	ARG
34	d	108	ARG
34	d	109	GLN
34	d	113	LEU
34	d	114	VAL
34	d	118	HIS
34	d	119	ILE
34	d	127	ASP
34	d	142	ARG
34	d	143	GLU
34	d	145	SER
34	d	147	LYS
34	d	148	LEU
34	d	163	GLU
34	d	165	LEU
34	d	194	ILE
35	e	19	ASN
35	e	30	ARG
35	e	36	LEU

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Mol	Chain	Res	Type
35	e	37	VAL
35	e	39	VAL
35	e	43	ASN
35	e	48	PHE
35	e	61	LYS
35	e	64	VAL
35	e	78	GLU
35	e	85	ILE
35	e	112	ARG
35	e	115	LEU
35	e	116	GLU
35	e	121	THR
35	e	124	LEU
35	e	126	LYS
35	e	136	MET
35	e	144	LEU
35	e	151	GLU
35	e	155	LYS
36	f	2	ARG
36	f	6	VAL
36	f	8	TYR
36	f	9	ILE
36	f	15	GLU
36	f	19	LYS
36	f	24	GLU
36	f	39	GLU
36	f	46	ARG
36	f	50	TYR
36	f	52	ILE
36	f	57	ASP
36	f	64	ARG
36	f	66	LYS
36	f	71	LYS
36	f	78	ARG
36	f	85	ASP
36	f	92	ILE
37	g	7	VAL
37	g	18	HIS
37	g	22	LEU
37	g	26	LEU
37	g	36	ARG
37	g	41	ARG

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Mol	Chain	Res	Type
37	g	47	PHE
37	g	54	SER
37	g	56	ARG
37	g	59	LEU
37	g	62	PHE
37	g	69	ILE
37	g	71	PRO
37	g	87	VAL
37	g	95	ARG
37	g	97	THR
37	g	98	THR
37	g	99	LEU
37	g	101	LEU
37	g	103	TRP
37	g	104	LEU
37	g	107	TYR
37	g	109	ARG
37	g	115	THR
37	g	131	THR
37	g	136	LYS
37	g	137	LYS
37	g	142	HIS
38	h	10	MET
38	h	15	ARG
38	h	31	ASN
38	h	34	LYS
38	h	38	GLU
38	h	41	LYS
38	h	51	TYR
38	h	53	GLU
38	h	54	ASP
38	h	64	LEU
38	h	65	LYS
38	h	70	ASP
38	h	72	ARG
38	h	82	LYS
38	h	87	VAL
38	h	90	LYS
38	h	106	VAL
38	h	110	GLU
38	h	113	ILE
38	h	114	THR

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Mol	Chain	Res	Type
38	h	115	ASP
38	h	120	LYS
38	h	132	TRP
39	i	11	THR
39	i	20	ARG
39	i	22	ARG
39	i	27	GLU
39	i	43	PHE
39	i	48	LEU
39	i	50	LEU
39	i	65	VAL
39	i	69	VAL
39	i	70	HIS
39	i	74	PHE
39	i	75	THR
39	i	101	LYS
39	i	111	ARG
39	i	112	MET
39	i	115	ARG
39	i	120	LEU
39	i	124	ARG
40	j	9	ARG
40	j	13	TYR
40	j	21	SER
40	j	31	ARG
40	j	42	LEU
40	j	45	GLU
40	j	52	ILE
40	j	55	VAL
40	j	63	GLU
40	j	65	PHE
40	j	68	ARG
40	j	69	THR
40	j	72	ARG
40	j	75	ASP
40	j	87	LEU
41	k	18	ASN
41	k	24	ARG
41	k	27	PHE
41	k	31	ILE
41	k	50	LEU
41	k	52	PHE

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Mol	Chain	Res	Type
41	k	53	LYS
41	k	55	SER
41	k	67	SER
41	k	72	LYS
41	k	85	THR
41	k	86	VAL
41	k	97	ILE
41	k	98	ARG
41	k	111	ARG
41	k	116	VAL
41	k	118	HIS
41	k	119	ASN
41	k	121	CYS
41	k	125	LYS
41	k	127	ARG
41	k	128	ARG
42	l	5	ASN
42	l	6	GLN
42	l	9	ARG
42	l	15	LYS
42	l	20	ASP
42	l	26	LYS
42	l	28	PHE
42	l	33	LYS
42	l	35	PHE
42	l	36	THR
42	l	38	LEU
42	l	43	LYS
42	l	44	ARG
42	l	46	VAL
42	l	53	MET
42	l	59	ASN
42	l	62	LEU
42	l	64	LYS
42	l	69	ARG
42	l	70	LEU
42	l	72	ASN
42	l	73	ASN
42	l	74	ILE
42	l	76	ILE
42	l	85	HIS
42	l	88	GLN

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Mol	Chain	Res	Type
42	l	100	VAL
42	l	123	ARG
42	l	125	GLN
42	l	133	LYS
42	l	134	LYS
43	m	13	LYS
43	m	29	THR
43	m	31	GLN
43	m	60	VAL
43	m	64	LYS
43	m	71	ARG
43	m	73	THR
43	m	83	ILE
43	m	85	SER
43	m	97	VAL
43	m	100	GLN
44	n	21	TYR
44	n	23	ARG
44	n	37	PHE
44	n	38	LYS
44	n	39	LEU
44	n	41	ARG
44	n	42	ILE
44	n	44	PHE
44	n	49	TYR
44	n	53	ILE
44	n	57	ARG
44	n	60	SER
44	n	61	TRP
45	o	3	ILE
45	o	4	SER
45	o	8	LYS
45	o	13	LYS
45	o	16	ARG
45	o	19	GLU
45	o	26	GLU
45	o	29	ILE
45	o	43	LEU
45	o	49	ASP
45	o	53	ARG
45	o	64	ARG
45	o	69	TYR

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Mol	Chain	Res	Type
45	o	76	GLN
45	o	78	TYR
45	o	83	LYS
45	o	85	LEU
45	o	88	ARG
46	p	3	VAL
46	p	4	LYS
46	p	5	ILE
46	p	6	ARG
46	p	10	LEU
46	p	13	LYS
46	p	20	ILE
46	p	21	VAL
46	p	32	ARG
46	p	37	ILE
46	p	59	LYS
46	p	68	THR
46	p	70	THR
46	p	72	HIS
46	p	78	GLU
46	p	83	LYS
46	p	85	ASP
47	q	13	LYS
47	q	22	THR
47	q	23	ILE
47	q	24	THR
47	q	25	VAL
47	q	29	THR
47	q	48	THR
47	q	49	HIS
47	q	52	ASN
47	q	56	LYS
47	q	70	SER
47	q	73	LYS
47	q	75	PHE
47	q	76	ARG
47	q	77	LEU
47	q	78	VAL
48	r	28	TYR
48	r	29	LYS
48	r	33	LEU
48	r	41	ARG

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Mol	Chain	Res	Type
48	r	48	ARG
48	r	55	LYS
48	r	72	LEU
49	s	6	LYS
49	s	7	LYS
49	s	12	ASP
49	s	15	LEU
49	s	16	MET
49	s	19	VAL
49	s	27	LYS
49	s	30	VAL
49	s	36	ARG
49	s	44	PHE
49	s	48	THR
49	s	49	PHE
49	s	55	ARG
49	s	56	LYS
49	s	60	VAL
49	s	67	VAL
49	s	74	PHE
50	t	13	THR
50	t	14	THR
50	t	15	GLU
50	t	39	VAL
50	t	54	VAL
50	t	55	LYS
50	t	59	LYS
50	t	68	SER
50	t	70	LYS
50	t	75	LYS
50	t	77	GLN
50	t	79	MET
51	u	18	ARG
51	u	19	PHE
51	u	25	LYS
51	u	28	THR
51	u	29	ILE
51	u	31	GLU
51	u	33	ARG
51	u	37	PHE
51	u	38	TYR
51	u	45	ARG

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Mol	Chain	Res	Type
51	u	50	GLU
52	v	3	ARG
52	v	7	HIS
52	v	11	LEU
52	v	21	ILE
52	v	28	LEU
52	v	29	GLU
52	v	32	PHE
52	v	42	VAL
52	v	44	VAL
52	v	47	TYR
52	v	57	THR
52	v	58	ILE
52	v	60	LEU
52	v	62	ASN
52	v	63	VAL
52	v	64	THR
52	v	66	ARG
52	v	69	GLU
52	v	82	ASN
52	v	87	ARG
52	v	89	VAL
52	v	95	ARG
52	v	98	ARG
52	v	99	LYS
52	v	103	ARG
52	v	139	PHE
52	v	141	LEU
52	v	142	LYS
52	v	151	LEU
52	v	163	PHE
52	v	176	ARG
52	v	178	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	54	HIS
3	C	70	ASN
4	D	47	ASN
4	D	66	ASN
4	D	176	ASN

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Mol	Chain	Res	Type
5	E	30	ASN
5	E	119	GLN
7	G	23	HIS
7	G	97	GLN
8	H	136	GLN
9	I	4	GLN
10	J	68	ASN
10	J	81	GLN
10	J	143	HIS
12	L	79	GLN
12	L	106	GLN
21	U	20	ASN
22	V	23	ASN
22	V	34	GLN
23	W	31	GLN
29	3	43	GLN
30	4	34	GLN
32	b	203	ASN
34	d	109	GLN
34	d	149	ASN
35	e	145	GLN
38	h	22	HIS
41	k	40	ASN
41	k	119	ASN
43	m	31	GLN
45	o	68	ASN
46	p	46	ASN
46	p	62	ASN
49	s	83	HIS
50	t	69	ASN
52	v	49	ASN
52	v	152	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2896/2905 (99%)	1223 (42%)	55 (1%)
2	B	114/115 (99%)	44 (38%)	0
31	a	1537/1539 (99%)	918 (59%)	0
All	All	4547/4559 (99%)	2185 (48%)	55 (1%)

All (2185) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	6	A
1	A	15	G
1	A	28	A
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	C
1	A	48	G
1	A	51	G
1	A	54	G
1	A	55	G
1	A	57	C
1	A	58	G
1	A	60	U
1	A	61	A
1	A	63	U
1	A	67	G
1	A	68	A
1	A	70	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	81	G
1	A	83	G
1	A	84	A
1	A	85	G
1	A	88	G
1	A	90	A
1	A	91	A
1	A	92	G
1	A	93	U
1	A	95	A
1	A	96	G
1	A	97	C
1	A	98	U
1	A	100	U
1	A	101	G
1	A	102	A
1	A	103	U
1	A	104	C
1	A	106	A

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Mol	Chain	Res	Type
1	A	117	A
1	A	119	U
1	A	120	G
1	A	124	A
1	A	130	A
1	A	134	U
1	A	136	A
1	A	140	A
1	A	147	G
1	A	148	U
1	A	150	A
1	A	152	C
1	A	156	A
1	A	157	U
1	A	158	G
1	A	160	G
1	A	161	A
1	A	162	A
1	A	163	U
1	A	164	A
1	A	166	A
1	A	168	A
1	A	169	G
1	A	170	C
1	A	171	A
1	A	174	U
1	A	175	C
1	A	177	G
1	A	178	A
1	A	179	A
1	A	180	G
1	A	183	A
1	A	184	C
1	A	185	A
1	A	189	G
1	A	199	A
1	A	202	A
1	A	213	C
1	A	216	A
1	A	217	G
1	A	218	G
1	A	219	A

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Mol	Chain	Res	Type
1	A	224	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	228	A
1	A	229	A
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	U
1	A	234	C
1	A	235	G
1	A	236	A
1	A	244	A
1	A	246	U
1	A	251	G
1	A	255	G
1	A	264	G
1	A	268	A
1	A	269	G
1	A	270	C
1	A	275	A
1	A	276	C
1	A	283	G
1	A	285	U
1	A	286	U
1	A	292	U
1	A	295	G
1	A	296	G
1	A	297	G
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	305	A
1	A	307	A
1	A	308	C
1	A	309	U
1	A	310	C
1	A	311	U
1	A	312	A

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Mol	Chain	Res	Type
1	A	315	C
1	A	317	G
1	A	318	A
1	A	319	G
1	A	320	U
1	A	321	U
1	A	322	A
1	A	323	C
1	A	324	A
1	A	325	A
1	A	326	A
1	A	327	G
1	A	328	G
1	A	329	A
1	A	330	C
1	A	331	G
1	A	333	C
1	A	334	A
1	A	335	U
1	A	336	U
1	A	337	A
1	A	338	G
1	A	339	A
1	A	340	C
1	A	351	G
1	A	353	A
1	A	360	A
1	A	364	A
1	A	365	A
1	A	367	A
1	A	373	A
1	A	374	U
1	A	376	A
1	A	378	C
1	A	381	G
1	A	386	C
1	A	387	G
1	A	388	A
1	A	389	A
1	A	390	A
1	A	391	A
1	A	392	U

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Mol	Chain	Res	Type
1	A	393	G
1	A	394	U
1	A	396	G
1	A	397	U
1	A	398	C
1	A	399	U
1	A	400	C
1	A	404	U
1	A	405	G
1	A	406	A
1	A	407	G
1	A	409	G
1	A	410	G
1	A	411	A
1	A	414	C
1	A	416	G
1	A	417	A
1	A	418	G
1	A	419	U
1	A	426	G
1	A	432	G
1	A	433	U
1	A	434	G
1	A	435	A
1	A	436	A
1	A	438	U
1	A	443	U
1	A	445	G
1	A	447	A
1	A	448	A
1	A	449	U
1	A	451	U
1	A	455	A
1	A	456	G
1	A	458	A
1	A	459	C
1	A	460	C
1	A	463	C
1	A	477	U
1	A	481	C
1	A	482	U
1	A	489	A

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Mol	Chain	Res	Type
1	A	490	C
1	A	492	G
1	A	493	A
1	A	494	U
1	A	497	U
1	A	498	G
1	A	501	C
1	A	502	C
1	A	504	G
1	A	506	A
1	A	511	G
1	A	512	A
1	A	514	G
1	A	515	G
1	A	519	G
1	A	523	A
1	A	525	A
1	A	526	A
1	A	527	G
1	A	528	C
1	A	529	A
1	A	530	C
1	A	537	A
1	A	538	G
1	A	540	G
1	A	549	U
1	A	550	A
1	A	551	G
1	A	553	A
1	A	554	C
1	A	556	U
1	A	566	U
1	A	569	U
1	A	572	C
1	A	573	A
1	A	574	A
1	A	576	U
1	A	577	A
1	A	578	G
1	A	586	C
1	A	591	A
1	A	592	A

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Mol	Chain	Res	Type
1	A	593	U
1	A	598	G
1	A	599	A
1	A	606	G
1	A	612	U
1	A	615	A
1	A	616	G
1	A	617	A
1	A	618	A
1	A	619	U
1	A	629	A
1	A	630	G
1	A	638	U
1	A	643	G
1	A	645	A
1	A	646	A
1	A	647	G
1	A	650	U
1	A	657	U
1	A	658	A
1	A	659	A
1	A	666	A
1	A	667	G
1	A	672	A
1	A	679	G
1	A	682	A
1	A	687	G
1	A	689	A
1	A	690	U
1	A	691	A
1	A	692	G
1	A	696	G
1	A	698	U
1	A	700	A
1	A	701	G
1	A	715	A
1	A	716	C
1	A	720	A
1	A	731	U
1	A	748	U
1	A	749	G
1	A	750	A

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Mol	Chain	Res	Type
1	A	751	A
1	A	753	U
1	A	754	U
1	A	755	C
1	A	757	G
1	A	759	U
1	A	760	A
1	A	761	A
1	A	762	C
1	A	763	A
1	A	764	C
1	A	765	U
1	A	766	G
1	A	767	A
1	A	768	A
1	A	772	A
1	A	773	G
1	A	775	A
1	A	779	A
1	A	783	G
1	A	785	C
1	A	792	U
1	A	794	A
1	A	795	A
1	A	797	A
1	A	802	G
1	A	805	G
1	A	806	A
1	A	809	A
1	A	810	A
1	A	820	G
1	A	821	C
1	A	822	G
1	A	826	A
1	A	827	A
1	A	829	U
1	A	830	U
1	A	833	A
1	A	834	A
1	A	835	U
1	A	836	C
1	A	839	A

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Mol	Chain	Res	Type
1	A	841	C
1	A	842	U
1	A	845	A
1	A	847	A
1	A	850	G
1	A	851	C
1	A	852	U
1	A	857	C
1	A	862	C
1	A	868	A
1	A	869	G
1	A	871	U
1	A	872	U
1	A	873	U
1	A	875	G
1	A	879	U
1	A	887	A
1	A	891	A
1	A	896	U
1	A	897	A
1	A	899	U
1	A	900	G
1	A	904	G
1	A	908	A
1	A	911	A
1	A	912	C
1	A	914	G
1	A	915	U
1	A	916	U
1	A	917	U
1	A	918	G
1	A	920	A
1	A	923	A
1	A	924	G
1	A	925	G
1	A	926	G
1	A	927	G
1	A	928	C
1	A	940	U
1	A	943	C
1	A	944	G
1	A	946	A

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Mol	Chain	Res	Type
1	A	948	U
1	A	949	C
1	A	951	G
1	A	952	A
1	A	955	A
1	A	957	C
1	A	959	C
1	A	960	C
1	A	965	G
1	A	970	U
1	A	971	U
1	A	972	A
1	A	974	U
1	A	977	A
1	A	985	A
1	A	986	G
1	A	989	A
1	A	990	G
1	A	997	G
1	A	1001	A
1	A	1003	A
1	A	1005	G
1	A	1006	G
1	A	1017	A
1	A	1018	A
1	A	1019	A
1	A	1024	A
1	A	1025	A
1	A	1027	A
1	A	1029	C
1	A	1034	A
1	A	1035	C
1	A	1037	A
1	A	1038	C
1	A	1039	C
1	A	1040	A
1	A	1043	U
1	A	1046	G
1	A	1053	A
1	A	1055	A
1	A	1056	U
1	A	1057	A

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Mol	Chain	Res	Type
1	A	1058	U
1	A	1059	A
1	A	1061	G
1	A	1070	A
1	A	1074	G
1	A	1077	U
1	A	1078	G
1	A	1080	G
1	A	1083	G
1	A	1086	G
1	A	1088	C
1	A	1089	C
1	A	1090	A
1	A	1091	G
1	A	1092	A
1	A	1093	C
1	A	1095	A
1	A	1099	G
1	A	1100	G
1	A	1101	A
1	A	1105	U
1	A	1106	G
1	A	1109	U
1	A	1111	A
1	A	1114	A
1	A	1115	G
1	A	1116	C
1	A	1117	A
1	A	1118	G
1	A	1119	C
1	A	1120	C
1	A	1122	U
1	A	1125	U
1	A	1126	U
1	A	1127	U
1	A	1128	A
1	A	1129	A
1	A	1131	G
1	A	1132	A
1	A	1133	G
1	A	1134	U
1	A	1135	G

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Mol	Chain	Res	Type
1	A	1138	U
1	A	1140	A
1	A	1141	U
1	A	1142	A
1	A	1143	G
1	A	1146	C
1	A	1147	A
1	A	1148	C
1	A	1149	U
1	A	1150	A
1	A	1151	G
1	A	1153	C
1	A	1155	A
1	A	1156	G
1	A	1158	G
1	A	1160	C
1	A	1161	A
1	A	1162	C
1	A	1163	U
1	A	1164	G
1	A	1168	C
1	A	1170	A
1	A	1171	A
1	A	1173	A
1	A	1174	U
1	A	1175	G
1	A	1178	C
1	A	1179	C
1	A	1180	G
1	A	1185	U
1	A	1186	A
1	A	1192	A
1	A	1199	A
1	A	1200	A
1	A	1201	G
1	A	1208	A
1	A	1210	U
1	A	1212	U
1	A	1214	C
1	A	1216	U
1	A	1217	U
1	A	1222	A

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Mol	Chain	Res	Type
1	A	1225	G
1	A	1234	G
1	A	1245	G
1	A	1248	U
1	A	1249	U
1	A	1253	G
1	A	1258	A
1	A	1262	U
1	A	1265	G
1	A	1267	A
1	A	1271	G
1	A	1275	A
1	A	1276	G
1	A	1284	A
1	A	1289	A
1	A	1290	G
1	A	1291	A
1	A	1293	U
1	A	1294	G
1	A	1298	G
1	A	1304	G
1	A	1309	G
1	A	1310	A
1	A	1311	A
1	A	1312	A
1	A	1320	G
1	A	1326	C
1	A	1330	U
1	A	1337	A
1	A	1338	U
1	A	1339	U
1	A	1340	G
1	A	1341	A
1	A	1342	C
1	A	1345	A
1	A	1348	U
1	A	1349	U
1	A	1355	A
1	A	1359	A
1	A	1361	G
1	A	1366	U
1	A	1370	C

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Mol	Chain	Res	Type
1	A	1379	A
1	A	1382	C
1	A	1384	G
1	A	1386	U
1	A	1389	U
1	A	1392	G
1	A	1401	G
1	A	1402	A
1	A	1403	C
1	A	1405	G
1	A	1412	G
1	A	1416	U
1	A	1422	A
1	A	1423	C
1	A	1424	A
1	A	1425	G
1	A	1430	A
1	A	1431	U
1	A	1432	A
1	A	1433	U
1	A	1435	C
1	A	1440	A
1	A	1445	C
1	A	1447	A
1	A	1448	U
1	A	1450	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1454	U
1	A	1455	U
1	A	1457	U
1	A	1459	A
1	A	1460	U
1	A	1461	C
1	A	1462	G
1	A	1463	A
1	A	1464	U
1	A	1465	G
1	A	1466	G
1	A	1467	G
1	A	1469	G

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Mol	Chain	Res	Type
1	A	1471	A
1	A	1472	C
1	A	1478	A
1	A	1480	G
1	A	1483	A
1	A	1487	G
1	A	1491	C
1	A	1492	G
1	A	1493	U
1	A	1495	C
1	A	1496	G
1	A	1497	A
1	A	1498	U
1	A	1499	U
1	A	1500	G
1	A	1503	U
1	A	1504	U
1	A	1505	G
1	A	1506	C
1	A	1507	A
1	A	1508	C
1	A	1509	G
1	A	1510	U
1	A	1511	C
1	A	1512	U
1	A	1513	A
1	A	1514	A
1	A	1515	G
1	A	1516	C
1	A	1518	G
1	A	1519	U
1	A	1520	A
1	A	1521	A
1	A	1522	G
1	A	1526	G
1	A	1527	A
1	A	1529	U
1	A	1533	A
1	A	1534	G
1	A	1535	G
1	A	1536	C
1	A	1537	A

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Mol	Chain	Res	Type
1	A	1538	A
1	A	1540	U
1	A	1541	C
1	A	1542	C
1	A	1546	A
1	A	1547	C
1	A	1550	G
1	A	1551	U
1	A	1552	U
1	A	1553	A
1	A	1555	G
1	A	1559	G
1	A	1561	G
1	A	1562	C
1	A	1563	U
1	A	1564	G
1	A	1565	U
1	A	1568	U
1	A	1569	G
1	A	1570	G
1	A	1571	G
1	A	1572	G
1	A	1573	A
1	A	1575	A
1	A	1576	A
1	A	1577	G
1	A	1578	A
1	A	1579	C
1	A	1580	A
1	A	1581	U
1	A	1582	U
1	A	1583	G
1	A	1584	U
1	A	1585	G
1	A	1586	U
1	A	1593	G
1	A	1594	U
1	A	1595	C
1	A	1596	G
1	A	1599	G
1	A	1600	A
1	A	1601	U

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Mol	Chain	Res	Type
1	A	1603	U
1	A	1604	C
1	A	1605	A
1	A	1606	C
1	A	1613	G
1	A	1616	A
1	A	1623	U
1	A	1625	U
1	A	1626	A
1	A	1627	G
1	A	1629	U
1	A	1630	A
1	A	1631	G
1	A	1632	A
1	A	1633	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1638	G
1	A	1639	G
1	A	1640	U
1	A	1651	C
1	A	1653	A
1	A	1654	A
1	A	1658	A
1	A	1659	C
1	A	1660	A
1	A	1661	C
1	A	1662	A
1	A	1666	A
1	A	1675	G
1	A	1678	A
1	A	1679	A
1	A	1682	C
1	A	1690	A
1	A	1691	G
1	A	1692	C
1	A	1693	G
1	A	1698	A
1	A	1701	U
1	A	1707	U
1	A	1708	A

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Mol	Chain	Res	Type
1	A	1716	C
1	A	1718	G
1	A	1719	C
1	A	1732	U
1	A	1737	U
1	A	1738	C
1	A	1739	G
1	A	1740	G
1	A	1741	G
1	A	1742	A
1	A	1747	G
1	A	1748	G
1	A	1757	U
1	A	1758	A
1	A	1759	G
1	A	1760	G
1	A	1761	G
1	A	1762	U
1	A	1763	U
1	A	1764	A
1	A	1765	A
1	A	1768	C
1	A	1771	A
1	A	1772	G
1	A	1773	A
1	A	1775	G
1	A	1780	G
1	A	1781	C
1	A	1782	A
1	A	1783	G
1	A	1785	G
1	A	1790	G
1	A	1791	G
1	A	1796	A
1	A	1797	G
1	A	1800	A
1	A	1803	G
1	A	1806	U
1	A	1808	U
1	A	1811	A
1	A	1812	A
1	A	1814	A

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Mol	Chain	Res	Type
1	A	1822	C
1	A	1823	U
1	A	1824	C
1	A	1825	U
1	A	1827	C
1	A	1828	U
1	A	1829	A
1	A	1830	A
1	A	1838	G
1	A	1839	G
1	A	1843	U
1	A	1846	A
1	A	1847	U
1	A	1852	G
1	A	1855	G
1	A	1856	A
1	A	1858	G
1	A	1862	G
1	A	1866	G
1	A	1871	U
1	A	1875	A
1	A	1876	G
1	A	1877	G
1	A	1878	U
1	A	1879	U
1	A	1880	A
1	A	1882	G
1	A	1884	G
1	A	1885	G
1	A	1887	G
1	A	1889	G
1	A	1890	G
1	A	1892	U
1	A	1894	G
1	A	1896	U
1	A	1897	U
1	A	1899	U
1	A	1900	G
1	A	1902	G
1	A	1903	A
1	A	1904	A
1	A	1905	G

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Mol	Chain	Res	Type
1	A	1906	C
1	A	1907	U
1	A	1908	A
1	A	1911	A
1	A	1912	A
1	A	1914	C
1	A	1916	A
1	A	1919	C
1	A	1926	A
1	A	1927	A
1	A	1929	C
1	A	1933	G
1	A	1938	U
1	A	1945	A
1	A	1946	A
1	A	1950	U
1	A	1954	A
1	A	1956	G
1	A	1957	G
1	A	1958	U
1	A	1961	C
1	A	1963	A
1	A	1964	A
1	A	1965	A
1	A	1966	U
1	A	1967	U
1	A	1968	C
1	A	1970	U
1	A	1971	U
1	A	1972	G
1	A	1974	C
1	A	1976	G
1	A	1979	A
1	A	1982	U
1	A	1983	U
1	A	1984	C
1	A	1990	C
1	A	1996	A
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2008	A

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Mol	Chain	Res	Type
1	A	2009	U
1	A	2012	G
1	A	2018	U
1	A	2019	G
1	A	2020	U
1	A	2023	C
1	A	2024	A
1	A	2027	G
1	A	2029	G
1	A	2045	A
1	A	2047	A
1	A	2048	G
1	A	2049	U
1	A	2050	A
1	A	2057	A
1	A	2059	G
1	A	2060	A
1	A	2061	U
1	A	2062	G
1	A	2064	A
1	A	2070	C
1	A	2075	G
1	A	2076	A
1	A	2079	G
1	A	2082	C
1	A	2083	G
1	A	2085	A
1	A	2086	A
1	A	2087	A
1	A	2088	G
1	A	2090	C
1	A	2093	C
1	A	2095	U
1	A	2096	G
1	A	2107	G
1	A	2108	U
1	A	2109	A
1	A	2111	C
1	A	2114	G
1	A	2115	A
1	A	2116	U
1	A	2117	A

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Mol	Chain	Res	Type
1	A	2118	U
1	A	2119	U
1	A	2120	G
1	A	2121	A
1	A	2126	C
1	A	2128	G
1	A	2129	C
1	A	2130	A
1	A	2131	C
1	A	2132	A
1	A	2133	G
1	A	2134	C
1	A	2138	U
1	A	2139	A
1	A	2140	C
1	A	2141	A
1	A	2144	A
1	A	2145	U
1	A	2146	A
1	A	2149	U
1	A	2153	A
1	A	2154	G
1	A	2155	C
1	A	2156	C
1	A	2157	U
1	A	2158	U
1	A	2159	U
1	A	2160	G
1	A	2161	A
1	A	2164	C
1	A	2168	A
1	A	2169	G
1	A	2173	U
1	A	2174	A
1	A	2179	A
1	A	2184	G
1	A	2185	A
1	A	2186	G
1	A	2188	C
1	A	2190	C
1	A	2194	U
1	A	2195	G

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Mol	Chain	Res	Type
1	A	2196	G
1	A	2198	A
1	A	2204	C
1	A	2205	C
1	A	2210	C
1	A	2212	G
1	A	2213	U
1	A	2219	C
1	A	2222	U
1	A	2224	U
1	A	2229	C
1	A	2231	C
1	A	2232	A
1	A	2233	C
1	A	2234	C
1	A	2235	A
1	A	2236	C
1	A	2237	U
1	A	2238	U
1	A	2239	A
1	A	2243	U
1	A	2245	G
1	A	2252	A
1	A	2254	A
1	A	2262	G
1	A	2263	C
1	A	2265	G
1	A	2266	G
1	A	2273	G
1	A	2278	G
1	A	2279	G
1	A	2280	G
1	A	2281	C
1	A	2287	C
1	A	2293	A
1	A	2294	A
1	A	2296	A
1	A	2305	A
1	A	2310	C
1	A	2311	U
1	A	2312	C
1	A	2315	A

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Mol	Chain	Res	Type
1	A	2316	G
1	A	2320	C
1	A	2323	U
1	A	2324	C
1	A	2325	A
1	A	2328	A
1	A	2331	G
1	A	2332	U
1	A	2333	U
1	A	2334	G
1	A	2335	G
1	A	2337	A
1	A	2338	A
1	A	2339	U
1	A	2345	A
1	A	2346	U
1	A	2347	A
1	A	2348	G
1	A	2349	A
1	A	2352	G
1	A	2353	U
1	A	2354	A
1	A	2356	A
1	A	2357	G
1	A	2358	G
1	A	2362	A
1	A	2363	A
1	A	2364	G
1	A	2367	A
1	A	2369	C
1	A	2370	U
1	A	2372	G
1	A	2374	C
1	A	2377	C
1	A	2378	G
1	A	2385	A
1	A	2387	A
1	A	2388	A
1	A	2395	C
1	A	2396	A
1	A	2399	G
1	A	2404	A

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Mol	Chain	Res	Type
1	A	2406	G
1	A	2407	A
1	A	2409	G
1	A	2410	G
1	A	2412	C
1	A	2417	U
1	A	2418	G
1	A	2419	A
1	A	2427	G
1	A	2429	U
1	A	2434	A
1	A	2441	G
1	A	2445	A
1	A	2449	C
1	A	2450	U
1	A	2451	C
1	A	2453	A
1	A	2455	G
1	A	2456	G
1	A	2457	A
1	A	2459	A
1	A	2460	A
1	A	2461	A
1	A	2462	A
1	A	2467	C
1	A	2468	C
1	A	2471	G
1	A	2474	G
1	A	2475	A
1	A	2479	C
1	A	2492	C
1	A	2493	C
1	A	2495	A
1	A	2496	A
1	A	2497	G
1	A	2502	C
1	A	2503	A
1	A	2504	C
1	A	2505	A
1	A	2506	U
1	A	2507	C
1	A	2509	A

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Mol	Chain	Res	Type
1	A	2511	G
1	A	2515	A
1	A	2518	U
1	A	2521	G
1	A	2525	C
1	A	2528	C
1	A	2529	G
1	A	2530	A
1	A	2531	U
1	A	2532	G
1	A	2533	U
1	A	2535	G
1	A	2539	C
1	A	2540	A
1	A	2545	A
1	A	2547	C
1	A	2550	G
1	A	2552	G
1	A	2554	C
1	A	2558	A
1	A	2559	G
1	A	2561	C
1	A	2562	G
1	A	2568	A
1	A	2570	G
1	A	2574	U
1	A	2580	G
1	A	2581	U
1	A	2582	U
1	A	2585	C
1	A	2589	U
1	A	2591	A
1	A	2592	A
1	A	2593	A
1	A	2594	G
1	A	2599	A
1	A	2600	C
1	A	2605	G
1	A	2607	U
1	A	2609	G
1	A	2610	G
1	A	2611	U

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Mol	Chain	Res	Type
1	A	2613	C
1	A	2615	G
1	A	2623	U
1	A	2626	G
1	A	2629	A
1	A	2630	G
1	A	2636	U
1	A	2637	C
1	A	2640	U
1	A	2641	A
1	A	2642	U
1	A	2646	U
1	A	2649	U
1	A	2650	G
1	A	2656	A
1	A	2657	G
1	A	2659	A
1	A	2664	U
1	A	2665	G
1	A	2667	G
1	A	2671	A
1	A	2672	G
1	A	2673	C
1	A	2674	U
1	A	2680	U
1	A	2681	A
1	A	2682	G
1	A	2683	U
1	A	2684	A
1	A	2685	C
1	A	2687	A
1	A	2688	G
1	A	2690	G
1	A	2692	A
1	A	2693	C
1	A	2695	G
1	A	2696	G
1	A	2697	G
1	A	2699	U
1	A	2700	G
1	A	2701	G
1	A	2709	U

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Mol	Chain	Res	Type
1	A	2716	U
1	A	2718	C
1	A	2730	C
1	A	2732	A
1	A	2733	A
1	A	2739	U
1	A	2741	G
1	A	2750	C
1	A	2753	U
1	A	2760	A
1	A	2761	C
1	A	2762	G
1	A	2764	G
1	A	2765	A
1	A	2766	U
1	A	2769	G
1	A	2771	G
1	A	2772	C
1	A	2773	U
1	A	2775	A
1	A	2776	A
1	A	2777	A
1	A	2778	G
1	A	2779	C
1	A	2780	A
1	A	2782	C
1	A	2783	U
1	A	2784	A
1	A	2785	A
1	A	2786	G
1	A	2788	A
1	A	2790	G
1	A	2791	A
1	A	2792	A
1	A	2793	G
1	A	2796	C
1	A	2797	C
1	A	2800	U
1	A	2803	A
1	A	2804	G
1	A	2805	A
1	A	2806	U

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Mol	Chain	Res	Type
1	A	2807	G
1	A	2808	A
1	A	2809	G
1	A	2816	C
1	A	2817	A
1	A	2818	A
1	A	2820	U
1	A	2821	U
1	A	2822	C
1	A	2823	G
1	A	2824	G
1	A	2827	A
1	A	2828	U
1	A	2829	A
1	A	2830	A
1	A	2831	G
1	A	2832	A
1	A	2838	C
1	A	2840	A
1	A	2841	A
1	A	2843	A
1	A	2853	U
1	A	2855	A
1	A	2856	U
1	A	2869	G
1	A	2870	A
1	A	2878	U
1	A	2879	G
1	A	2880	A
1	A	2882	A
1	A	2887	G
1	A	2888	A
1	A	2889	G
1	A	2892	G
1	A	2894	C
1	A	2899	A
1	A	2900	C
1	A	2903	A
1	A	2904	U
1	A	2905	C
1	A	2906	G
1	A	2907	A

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Mol	Chain	Res	Type
1	A	2913	G
1	A	2915	C
1	A	2916	U
1	A	2920	U
2	B	2	C
2	B	5	G
2	B	7	G
2	B	11	A
2	B	12	U
2	B	14	G
2	B	15	C
2	B	22	G
2	B	23	U
2	B	24	C
2	B	27	A
2	B	28	C
2	B	30	U
2	B	31	G
2	B	33	U
2	B	39	G
2	B	40	C
2	B	41	C
2	B	42	G
2	B	43	A
2	B	49	G
2	B	51	A
2	B	54	U
2	B	55	A
2	B	62	U
2	B	63	U
2	B	64	A
2	B	65	G
2	B	66	C
2	B	68	U
2	B	72	U
2	B	84	U
2	B	86	A
2	B	87	C
2	B	88	G
2	B	91	C
2	B	93	G
2	B	95	U

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Mol	Chain	Res	Type
2	B	106	G
2	B	109	G
2	B	110	C
2	B	111	C
2	B	113	G
2	B	115	C
31	a	6	U
31	a	7	G
31	a	8	G
31	a	9	A
31	a	10	G
31	a	11	A
31	a	12	G
31	a	14	U
31	a	15	U
31	a	16	G
31	a	18	U
31	a	20	C
31	a	26	C
31	a	27	A
31	a	30	A
31	a	32	G
31	a	33	A
31	a	34	A
31	a	36	G
31	a	37	C
31	a	38	U
31	a	40	G
31	a	43	G
31	a	44	C
31	a	45	G
31	a	48	C
31	a	49	C
31	a	50	U
31	a	51	A
31	a	52	A
31	a	53	U
31	a	55	C
31	a	56	A
31	a	57	U
31	a	59	C
31	a	62	G

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Mol	Chain	Res	Type
31	a	65	G
31	a	66	A
31	a	67	G
31	a	68	C
31	a	69	G
31	a	70	A
31	a	71	A
31	a	77	G
31	a	81	A
31	a	82	G
31	a	83	C
31	a	84	U
31	a	85	U
31	a	86	G
31	a	87	C
31	a	88	U
31	a	92	C
31	a	94	G
31	a	96	U
31	a	97	G
31	a	99	U
31	a	100	A
31	a	101	G
31	a	103	G
31	a	105	C
31	a	107	G
31	a	108	A
31	a	111	G
31	a	118	A
31	a	119	A
31	a	120	C
31	a	121	A
31	a	124	U
31	a	129	A
31	a	130	A
31	a	131	C
31	a	132	C
31	a	134	A
31	a	135	C
31	a	141	A
31	a	142	G
31	a	143	A

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Mol	Chain	Res	Type
31	a	144	C
31	a	146	G
31	a	147	G
31	a	148	G
31	a	149	A
31	a	151	A
31	a	152	A
31	a	153	C
31	a	157	G
31	a	161	A
31	a	163	C
31	a	169	C
31	a	170	U
31	a	173	U
31	a	174	A
31	a	177	G
31	a	182	A
31	a	183	U
31	a	184	A
31	a	186	U
31	a	188	U
31	a	189	G
31	a	190	A
31	a	191	A
31	a	192	C
31	a	193	C
31	a	196	A
31	a	197	U
31	a	199	G
31	a	200	U
31	a	201	U
31	a	202	C
31	a	203	A
31	a	204	A
31	a	205	A
31	a	207	G
31	a	209	G
31	a	210	A
31	a	211	A
31	a	215	C
31	a	217	G
31	a	218	U

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Mol	Chain	Res	Type
31	a	219	C
31	a	221	U
31	a	222	G
31	a	223	C
31	a	224	U
31	a	227	C
31	a	228	A
31	a	230	U
31	a	231	U
31	a	232	A
31	a	233	U
31	a	234	A
31	a	244	G
31	a	245	C
31	a	246	G
31	a	247	C
31	a	248	U
31	a	250	C
31	a	251	A
31	a	252	U
31	a	253	U
31	a	255	G
31	a	256	C
31	a	259	G
31	a	261	U
31	a	262	G
31	a	263	G
31	a	265	A
31	a	267	G
31	a	268	G
31	a	269	U
31	a	270	A
31	a	271	A
31	a	272	C
31	a	273	G
31	a	274	G
31	a	275	C
31	a	276	U
31	a	278	A
31	a	281	A
31	a	282	A
31	a	283	G

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Mol	Chain	Res	Type
31	a	284	G
31	a	286	A
31	a	288	C
31	a	290	A
31	a	291	U
31	a	297	G
31	a	302	C
31	a	306	A
31	a	307	G
31	a	309	G
31	a	310	G
31	a	311	G
31	a	312	U
31	a	313	G
31	a	314	A
31	a	315	U
31	a	317	G
31	a	320	C
31	a	323	A
31	a	324	C
31	a	327	G
31	a	331	U
31	a	332	G
31	a	336	C
31	a	337	A
31	a	338	C
31	a	339	G
31	a	340	G
31	a	343	C
31	a	345	G
31	a	347	C
31	a	348	U
31	a	349	C
31	a	352	A
31	a	353	C
31	a	354	G
31	a	355	G
31	a	356	G
31	a	357	A
31	a	358	G
31	a	360	C
31	a	361	A

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Mol	Chain	Res	Type
31	a	363	C
31	a	364	A
31	a	367	A
31	a	371	A
31	a	372	A
31	a	373	U
31	a	374	C
31	a	375	U
31	a	376	U
31	a	377	C
31	a	380	C
31	a	381	A
31	a	386	G
31	a	389	A
31	a	390	A
31	a	395	U
31	a	396	G
31	a	397	A
31	a	398	C
31	a	400	G
31	a	401	A
31	a	404	A
31	a	405	A
31	a	406	C
31	a	408	C
31	a	410	G
31	a	412	G
31	a	413	U
31	a	414	G
31	a	416	G
31	a	417	U
31	a	418	G
31	a	419	A
31	a	420	U
31	a	421	G
31	a	422	A
31	a	423	A
31	a	424	G
31	a	425	G
31	a	430	C
31	a	431	G
31	a	432	G

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Mol	Chain	Res	Type
31	a	433	A
31	a	434	U
31	a	435	C
31	a	436	G
31	a	437	U
31	a	438	A
31	a	440	A
31	a	441	A
31	a	442	C
31	a	444	C
31	a	445	U
31	a	446	G
31	a	447	U
31	a	448	U
31	a	449	A
31	a	450	U
31	a	451	U
31	a	452	A
31	a	455	G
31	a	456	A
31	a	460	A
31	a	461	C
31	a	462	A
31	a	463	U
31	a	464	A
31	a	465	U
31	a	468	G
31	a	472	G
31	a	473	U
31	a	476	C
31	a	481	C
31	a	482	A
31	a	484	A
31	a	486	C
31	a	487	U
31	a	489	G
31	a	490	A
31	a	491	C
31	a	492	G
31	a	493	G
31	a	494	U
31	a	496	C

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Mol	Chain	Res	Type
31	a	499	A
31	a	503	A
31	a	504	G
31	a	506	A
31	a	507	A
31	a	508	G
31	a	509	C
31	a	510	C
31	a	511	A
31	a	512	C
31	a	513	G
31	a	515	C
31	a	516	U
31	a	517	A
31	a	518	A
31	a	519	C
31	a	522	C
31	a	524	U
31	a	525	G
31	a	526	C
31	a	529	G
31	a	530	C
31	a	531	A
31	a	532	G
31	a	537	G
31	a	538	G
31	a	539	U
31	a	541	A
31	a	542	U
31	a	543	A
31	a	544	C
31	a	547	A
31	a	548	G
31	a	549	G
31	a	552	G
31	a	554	A
31	a	555	A
31	a	556	G
31	a	557	C
31	a	561	A
31	a	563	C
31	a	567	A

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Mol	Chain	Res	Type
31	a	568	A
31	a	569	U
31	a	570	U
31	a	572	U
31	a	575	G
31	a	576	G
31	a	580	A
31	a	581	A
31	a	584	C
31	a	585	G
31	a	586	C
31	a	587	G
31	a	590	U
31	a	592	G
31	a	595	G
31	a	596	G
31	a	597	U
31	a	599	U
31	a	601	U
31	a	603	A
31	a	605	G
31	a	606	U
31	a	607	C
31	a	608	U
31	a	609	G
31	a	611	U
31	a	614	G
31	a	615	A
31	a	616	A
31	a	617	A
31	a	618	G
31	a	619	C
31	a	620	C
31	a	623	C
31	a	627	U
31	a	628	C
31	a	629	A
31	a	631	C
31	a	632	C
31	a	633	G
31	a	636	G
31	a	637	A

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Mol	Chain	Res	Type
31	a	638	G
31	a	639	G
31	a	640	G
31	a	641	U
31	a	642	C
31	a	645	U
31	a	646	G
31	a	647	G
31	a	648	A
31	a	649	A
31	a	650	A
31	a	651	C
31	a	652	U
31	a	653	G
31	a	657	A
31	a	662	G
31	a	664	G
31	a	665	U
31	a	669	G
31	a	670	A
31	a	672	G
31	a	673	A
31	a	674	G
31	a	675	G
31	a	676	A
31	a	677	A
31	a	678	A
31	a	680	U
31	a	681	G
31	a	682	G
31	a	683	A
31	a	685	U
31	a	686	U
31	a	688	C
31	a	689	A
31	a	690	U
31	a	691	G
31	a	692	U
31	a	693	G
31	a	694	U
31	a	697	C
31	a	698	G

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Mol	Chain	Res	Type
31	a	699	G
31	a	700	U
31	a	702	A
31	a	703	A
31	a	708	G
31	a	710	A
31	a	711	G
31	a	712	A
31	a	713	G
31	a	715	U
31	a	716	A
31	a	717	U
31	a	718	G
31	a	719	G
31	a	721	G
31	a	723	A
31	a	725	C
31	a	726	A
31	a	727	C
31	a	728	C
31	a	729	A
31	a	730	G
31	a	731	U
31	a	732	G
31	a	733	G
31	a	737	A
31	a	739	G
31	a	741	G
31	a	742	A
31	a	745	U
31	a	747	C
31	a	748	U
31	a	749	G
31	a	751	U
31	a	752	C
31	a	754	G
31	a	756	A
31	a	757	A
31	a	758	C
31	a	759	U
31	a	760	G
31	a	761	A

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Mol	Chain	Res	Type
31	a	762	C
31	a	763	G
31	a	764	C
31	a	766	G
31	a	767	A
31	a	768	U
31	a	771	G
31	a	774	A
31	a	775	A
31	a	776	A
31	a	779	G
31	a	780	U
31	a	781	G
31	a	782	G
31	a	783	G
31	a	784	G
31	a	785	A
31	a	790	A
31	a	792	A
31	a	793	G
31	a	794	G
31	a	795	A
31	a	797	U
31	a	799	G
31	a	802	A
31	a	804	C
31	a	805	C
31	a	809	U
31	a	813	C
31	a	814	C
31	a	815	A
31	a	816	C
31	a	817	G
31	a	818	C
31	a	819	C
31	a	820	G
31	a	821	U
31	a	823	A
31	a	825	C
31	a	826	G
31	a	827	A
31	a	828	U

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Mol	Chain	Res	Type
31	a	829	G
31	a	836	A
31	a	837	A
31	a	840	G
31	a	844	G
31	a	845	G
31	a	847	G
31	a	850	U
31	a	852	C
31	a	853	C
31	a	854	G
31	a	855	C
31	a	862	G
31	a	864	G
31	a	866	U
31	a	868	C
31	a	872	U
31	a	876	G
31	a	878	A
31	a	879	U
31	a	880	U
31	a	881	A
31	a	882	A
31	a	883	G
31	a	885	A
31	a	887	U
31	a	894	G
31	a	896	G
31	a	897	G
31	a	898	A
31	a	899	G
31	a	900	U
31	a	903	G
31	a	908	C
31	a	916	A
31	a	921	C
31	a	922	A
31	a	923	A
31	a	924	A
31	a	929	U
31	a	931	G
31	a	932	A

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Mol	Chain	Res	Type
31	a	934	G
31	a	935	G
31	a	943	C
31	a	945	C
31	a	946	A
31	a	949	C
31	a	950	G
31	a	952	U
31	a	954	G
31	a	955	A
31	a	956	G
31	a	958	A
31	a	959	U
31	a	960	G
31	a	961	U
31	a	964	U
31	a	966	U
31	a	967	A
31	a	969	U
31	a	970	U
31	a	971	C
31	a	973	A
31	a	975	G
31	a	977	A
31	a	978	A
31	a	980	G
31	a	981	C
31	a	983	A
31	a	984	A
31	a	985	G
31	a	986	A
31	a	987	A
31	a	988	C
31	a	989	C
31	a	990	U
31	a	991	U
31	a	992	A
31	a	993	C
31	a	996	A
31	a	997	A
31	a	998	U
31	a	1000	U

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Mol	Chain	Res	Type
31	a	1001	U
31	a	1002	G
31	a	1003	A
31	a	1006	U
31	a	1008	C
31	a	1011	U
31	a	1012	G
31	a	1013	A
31	a	1014	C
31	a	1015	A
31	a	1016	A
31	a	1017	C
31	a	1019	C
31	a	1022	G
31	a	1023	A
31	a	1024	G
31	a	1030	G
31	a	1031	C
31	a	1033	U
31	a	1036	C
31	a	1038	C
31	a	1039	U
31	a	1040	U
31	a	1041	C
31	a	1042	G
31	a	1046	G
31	a	1051	A
31	a	1052	G
31	a	1055	A
31	a	1057	A
31	a	1058	G
31	a	1060	U
31	a	1064	G
31	a	1065	C
31	a	1066	A
31	a	1069	G
31	a	1071	U
31	a	1072	G
31	a	1074	C
31	a	1076	U
31	a	1077	C
31	a	1078	A

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Mol	Chain	Res	Type
31	a	1080	C
31	a	1081	U
31	a	1083	G
31	a	1085	G
31	a	1089	U
31	a	1091	A
31	a	1094	U
31	a	1095	G
31	a	1096	U
31	a	1097	U
31	a	1098	G
31	a	1099	G
31	a	1100	G
31	a	1101	U
31	a	1102	U
31	a	1103	A
31	a	1104	A
31	a	1105	G
31	a	1106	U
31	a	1107	C
31	a	1108	C
31	a	1109	C
31	a	1110	G
31	a	1112	A
31	a	1113	A
31	a	1120	C
31	a	1122	A
31	a	1123	C
31	a	1124	C
31	a	1128	A
31	a	1129	A
31	a	1131	C
31	a	1133	U
31	a	1134	A
31	a	1135	G
31	a	1136	U
31	a	1137	U
31	a	1138	G
31	a	1139	C
31	a	1143	C
31	a	1144	A
31	a	1145	U

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Mol	Chain	Res	Type
31	a	1146	U
31	a	1148	A
31	a	1149	G
31	a	1150	U
31	a	1151	U
31	a	1152	G
31	a	1156	A
31	a	1157	C
31	a	1158	U
31	a	1160	U
31	a	1161	A
31	a	1164	U
31	a	1165	U
31	a	1167	A
31	a	1168	C
31	a	1169	U
31	a	1170	G
31	a	1171	C
31	a	1173	G
31	a	1175	U
31	a	1176	G
31	a	1177	A
31	a	1178	C
31	a	1179	A
31	a	1180	A
31	a	1185	G
31	a	1186	A
31	a	1187	G
31	a	1190	A
31	a	1191	G
31	a	1192	G
31	a	1196	G
31	a	1197	G
31	a	1198	A
31	a	1200	G
31	a	1201	A
31	a	1202	C
31	a	1203	G
31	a	1204	U
31	a	1205	C
31	a	1206	A
31	a	1208	A

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Mol	Chain	Res	Type
31	a	1210	C
31	a	1211	A
31	a	1212	U
31	a	1214	A
31	a	1215	U
31	a	1216	G
31	a	1218	C
31	a	1221	U
31	a	1222	U
31	a	1223	A
31	a	1224	U
31	a	1225	G
31	a	1226	A
31	a	1228	U
31	a	1229	U
31	a	1230	G
31	a	1231	G
31	a	1232	G
31	a	1234	U
31	a	1235	A
31	a	1236	C
31	a	1237	A
31	a	1238	C
31	a	1240	C
31	a	1241	G
31	a	1246	A
31	a	1247	C
31	a	1248	A
31	a	1249	A
31	a	1250	U
31	a	1251	G
31	a	1253	A
31	a	1255	A
31	a	1256	A
31	a	1257	U
31	a	1258	A
31	a	1260	A
31	a	1263	G
31	a	1266	C
31	a	1267	A
31	a	1269	C
31	a	1270	G

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Mol	Chain	Res	Type
31	a	1272	A
31	a	1273	A
31	a	1274	C
31	a	1275	C
31	a	1277	C
31	a	1278	G
31	a	1280	G
31	a	1281	G
31	a	1282	U
31	a	1283	C
31	a	1284	A
31	a	1285	A
31	a	1286	G
31	a	1288	A
31	a	1289	A
31	a	1290	A
31	a	1291	U
31	a	1294	C
31	a	1295	A
31	a	1296	U
31	a	1297	A
31	a	1300	G
31	a	1302	U
31	a	1303	G
31	a	1304	U
31	a	1305	U
31	a	1308	C
31	a	1309	A
31	a	1310	G
31	a	1311	U
31	a	1312	U
31	a	1314	G
31	a	1315	G
31	a	1317	U
31	a	1318	U
31	a	1319	G
31	a	1320	U
31	a	1321	A
31	a	1322	G
31	a	1323	U
31	a	1324	C
31	a	1325	U

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Mol	Chain	Res	Type
31	a	1326	G
31	a	1327	C
31	a	1328	A
31	a	1329	A
31	a	1330	C
31	a	1332	C
31	a	1333	G
31	a	1336	U
31	a	1337	A
31	a	1338	C
31	a	1339	A
31	a	1340	U
31	a	1341	G
31	a	1342	A
31	a	1343	A
31	a	1344	G
31	a	1345	C
31	a	1346	U
31	a	1348	G
31	a	1349	A
31	a	1354	C
31	a	1356	A
31	a	1357	G
31	a	1358	U
31	a	1362	C
31	a	1363	G
31	a	1370	A
31	a	1373	A
31	a	1374	U
31	a	1378	A
31	a	1381	G
31	a	1382	U
31	a	1383	G
31	a	1384	A
31	a	1387	A
31	a	1388	C
31	a	1389	G
31	a	1390	U
31	a	1391	U
31	a	1392	C
31	a	1393	C
31	a	1394	C

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Mol	Chain	Res	Type
31	a	1400	U
31	a	1401	U
31	a	1402	G
31	a	1403	U
31	a	1404	A
31	a	1406	A
31	a	1409	C
31	a	1410	C
31	a	1414	C
31	a	1415	G
31	a	1417	C
31	a	1419	C
31	a	1420	A
31	a	1421	C
31	a	1425	G
31	a	1427	G
31	a	1428	A
31	a	1429	G
31	a	1430	U
31	a	1433	G
31	a	1434	U
31	a	1435	A
31	a	1439	C
31	a	1445	G
31	a	1447	C
31	a	1448	G
31	a	1449	G
31	a	1450	U
31	a	1451	G
31	a	1452	G
31	a	1454	G
31	a	1455	U
31	a	1456	A
31	a	1457	A
31	a	1458	C
31	a	1459	C
31	a	1460	U
31	a	1461	U
31	a	1463	U
31	a	1464	A
31	a	1465	G
31	a	1466	G

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Mol	Chain	Res	Type
31	a	1467	A
31	a	1468	G
31	a	1469	C
31	a	1470	U
31	a	1474	C
31	a	1476	U
31	a	1478	G
31	a	1479	A
31	a	1483	U
31	a	1490	A
31	a	1492	U
31	a	1494	A
31	a	1495	U
31	a	1496	U
31	a	1497	G
31	a	1498	G
31	a	1500	G
31	a	1503	A
31	a	1504	A
31	a	1507	C
31	a	1508	G
31	a	1509	U
31	a	1511	A
31	a	1513	A
31	a	1514	A
31	a	1515	G
31	a	1517	U
31	a	1519	G
31	a	1522	G
31	a	1526	C
31	a	1528	G
31	a	1529	A
31	a	1530	A
31	a	1531	G
31	a	1532	G
31	a	1534	G
31	a	1536	G
31	a	1537	G
31	a	1540	G
31	a	1541	G
31	a	1542	A
31	a	1543	U

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	69	C
1	A	233	U
1	A	267	G
1	A	282	A
1	A	291	G
1	A	320	U
1	A	327	G
1	A	385	U
1	A	396	G
1	A	416	G
1	A	432	G
1	A	433	U
1	A	576	U
1	A	657	U
1	A	688	A
1	A	690	U
1	A	697	U
1	A	748	U
1	A	759	U
1	A	809	A
1	A	812	U
1	A	835	U
1	A	840	C
1	A	1024	A
1	A	1026	C
1	A	1075	G
1	A	1077	U
1	A	1092	A
1	A	1108	C
1	A	1190	A
1	A	1198	G
1	A	1460	U
1	A	1489	A
1	A	1496	G
1	A	1503	U
1	A	1520	A
1	A	1521	A
1	A	1626	A
1	A	1632	A
1	A	1658	A
1	A	1707	U
1	A	1823	U

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Mol	Chain	Res	Type
1	A	1975	G
1	A	2117	A
1	A	2127	G
1	A	2237	U
1	A	2302	C
1	A	2323	U
1	A	2428	U
1	A	2450	U
1	A	2455	G
1	A	2608	G
1	A	2749	G
1	A	2783	U
1	A	2816	C

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
1	A	8
31	a	2
52	v	1

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Mol	Chain	Number of breaks
43	m	1
37	g	1
38	h	1
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:GLN	C	131:ILE	N	30.98
1	A	2207:U	O3'	2208:A	P	12.82
1	A	1939:A	O3'	1944:U	P	12.52
1	a	465:U	O3'	466:G	P	11.00
1	A	929:C	O3'	937:G	P	9.63
1	A	1096:C	O3'	1097:U	P	7.26
1	m	93:ARG	C	94:GLY	N	6.43
1	A	1153:C	O3'	1154:G	P	5.83
1	g	1:MET	C	2:PRO	N	4.64
1	A	2217:G	O3'	2218:G	P	4.18
1	A	770:G	O3'	771:G	P	4.05
1	A	1448:U	O3'	1449:A	P	3.78
1	h	89:ALA	C	90:LYS	N	2.12
1	a	36:G	O3'	37:C	P	2.00
1	E	132:GLU	C	133:ALA	N	1.17

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10079. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.