Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:16 PM BST

PDB ID	:	4DR7
Title	:	Crystal structure of the Thermus thermophilus (HB8) 30S ribosomal subunit with codon, crystallographically disordered near-cognate transfer RNA anti-codon stem-loop mismatched at the second codon position, and streptomycin bound
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-16
Resolution	:	3.75 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

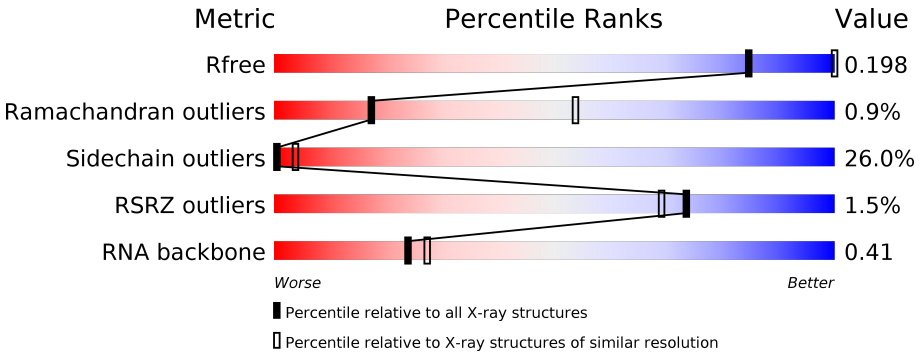
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)
RNA backbone	3102	1035 (4.52-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	41% 45% 13%
2	B	256	% 70% 23% 8%
3	C	239	2% 68% 18% 13%
4	D	209	2% 76% 23%
5	E	162	65% 28% 7%
6	F	101	% 70% 30%

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Mol	Chain	Length	Quality of chain
7	G	156	2% 78% 22%
8	H	138	70% 28%
9	I	128	2% 78% 21%
10	J	105	4% 71% 23% 6%
11	K	129	78% 13% 9%
12	L	135	4% 69% 23% 7%
13	M	126	4% 70% 23% 6%
14	N	61	2% 74% 25%
15	O	89	2% 76% 20%
16	P	88	69% 26% 5%
17	Q	105	71% 24% 5%
18	R	88	64% 17% 19%
19	S	93	2% 69% 16% 13%
20	T	106	67% 24% 7%
21	U	27	7% 78% 15% 7%
22	V	4	100% 75% 25%
23	W	11	91% 73% 27%
24	a	8	13% 38% 25% 38%
25	b	3	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1622	-	-	-	X
26	MG	A	1624	-	-	-	X
26	MG	A	1665	-	-	-	X
26	MG	A	1675	-	-	-	X
26	MG	A	1711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1724	-	-	-	X
26	MG	A	1729	-	-	-	X
26	MG	A	1730	-	-	-	X
26	MG	A	1734	-	-	-	X
26	MG	A	1759	-	-	-	X
26	MG	A	1760	-	-	-	X
26	MG	A	1769	-	-	-	X
26	MG	A	1770	-	-	-	X
26	MG	A	1774	-	-	-	X
26	MG	A	1808	-	-	-	X
26	MG	A	1813	-	-	-	X
26	MG	A	1877	-	-	-	X
26	MG	A	1880	-	-	-	X
26	MG	A	1886	-	-	-	X
26	MG	A	1887	-	-	-	X
26	MG	A	1904	-	-	-	X
26	MG	A	1912	-	-	-	X
26	MG	A	1913	-	-	-	X
26	MG	A	1914	-	-	-	X
26	MG	A	1917	-	-	-	X
26	MG	A	1923	-	-	-	X
26	MG	A	1926	-	-	-	X
26	MG	D	304	-	-	-	X
26	MG	G	201	-	-	-	X
26	MG	N	102	-	-	-	X
26	MG	P	103	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1513	32707	14570	6056	10561	1520	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1896	1211	337	343	5	0	0	1

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O	0	0	0
			585	373	116	96			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*CP*CP*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 24 is a RNA chain called 5'-R(P*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	8	Total	C	N	O	P	0	0	0
			175	78	34	55	8			

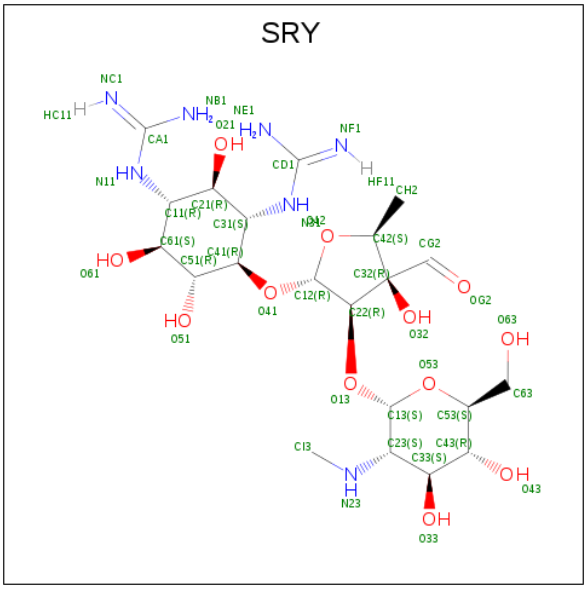
- Molecule 25 is a RNA chain called 5'-R(P*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	3	Total	C	N	O	P	0	0	0
			60	27	6	24	3			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	3	Total Mg 3 3	0	0
26	G	1	Total Mg 1 1	0	0
26	J	1	Total Mg 1 1	0	0
26	Q	1	Total Mg 1 1	0	0
26	D	3	Total Mg 3 3	0	0
26	E	4	Total Mg 4 4	0	0
26	H	1	Total Mg 1 1	0	0
26	A	326	Total Mg 326 326	0	0
26	N	1	Total Mg 1 1	0	0
26	S	2	Total Mg 2 2	0	0
26	F	1	Total Mg 1 1	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C N O 40 21 7 12	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	1	Total Zn 1 1	0	0
28	N	1	Total Zn 1 1	0	0

- Molecule 29 is water.

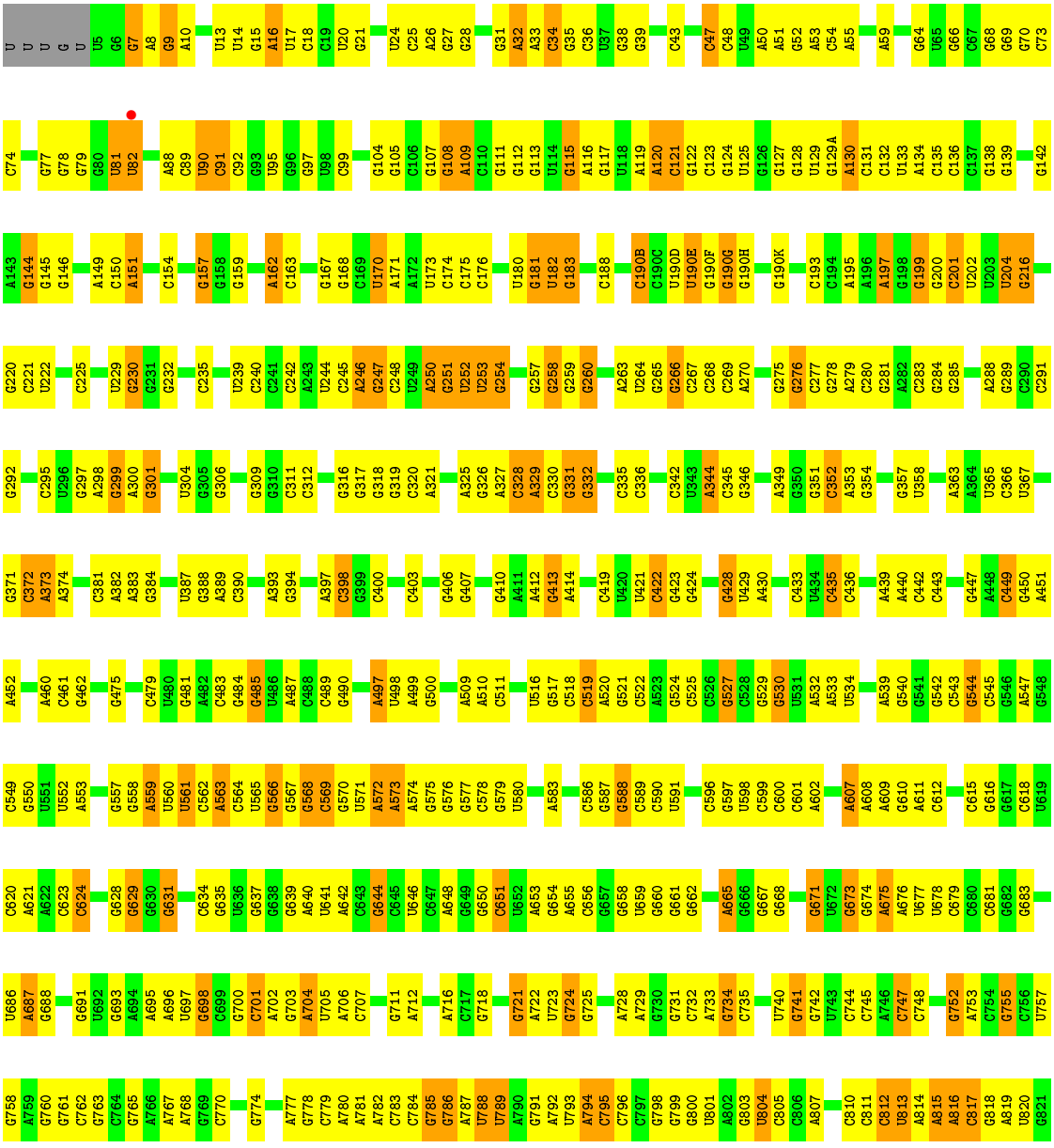
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	866	Total O 866 866	0	0
29	C	1	Total O 1 1	0	0
29	D	7	Total O 7 7	0	0
29	E	5	Total O 5 5	0	0
29	L	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	T	3	Total O 3 3	0	0
29	U	4	Total O 4 4	0	0
29	W	1	Total O 1 1	0	0

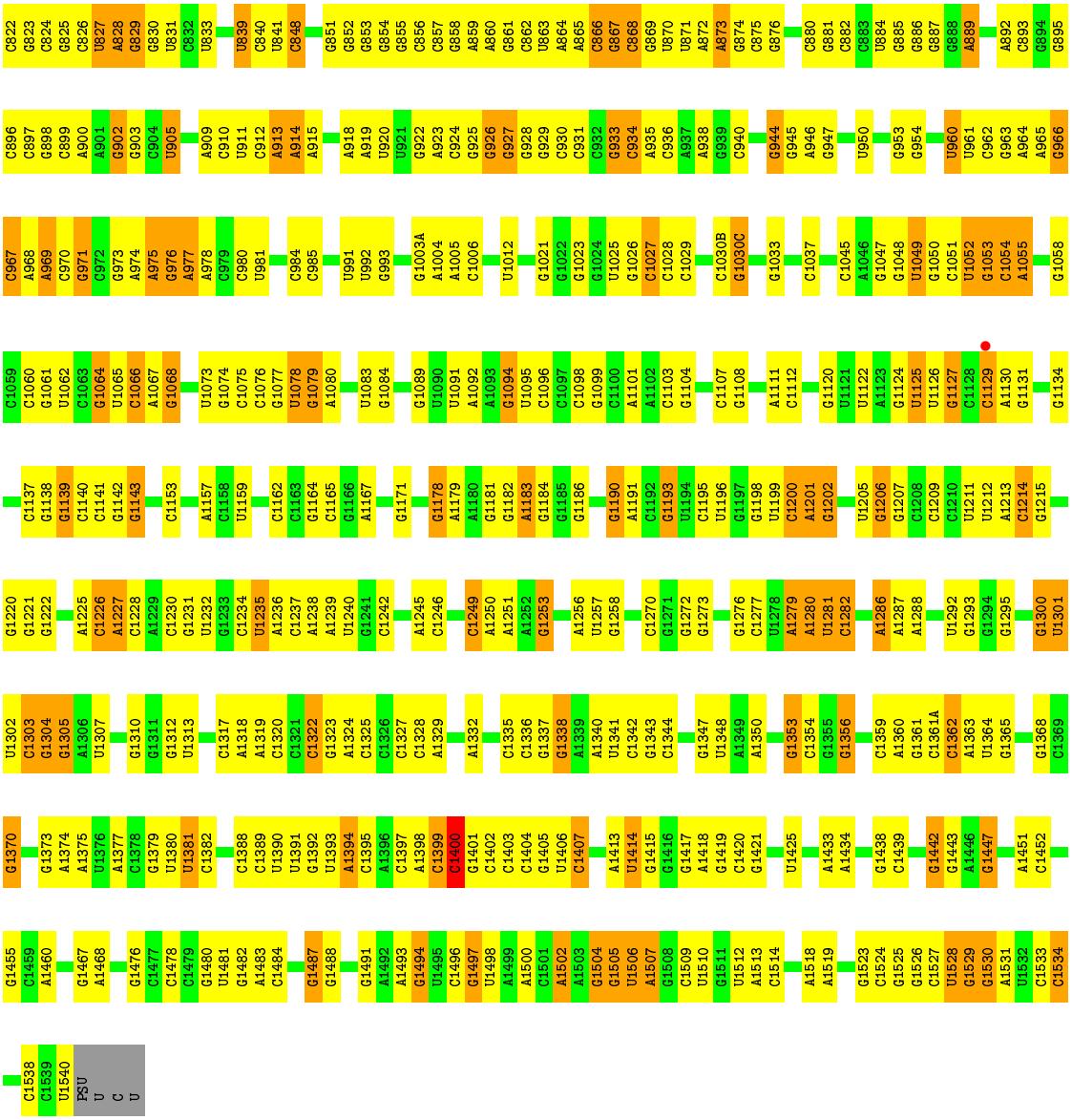
3 Residue-property plots (i)

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

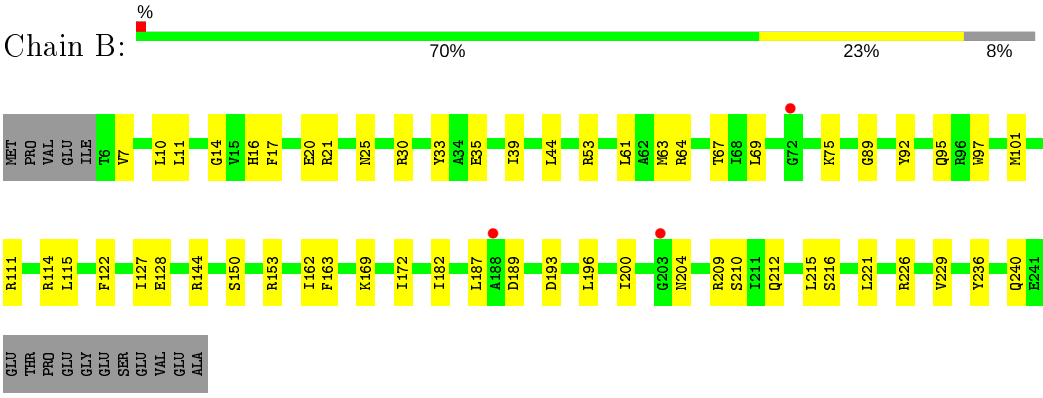
- Molecule 1: 16S rRNA

Chain A:



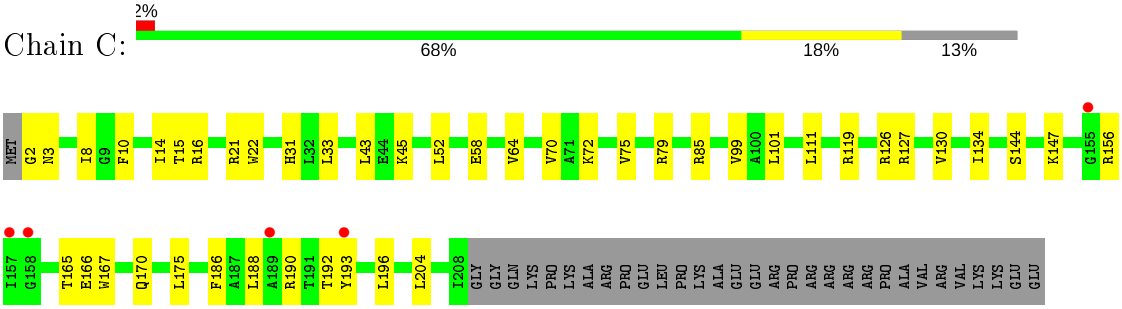


• Molecule 2: 30S ribosomal protein S2



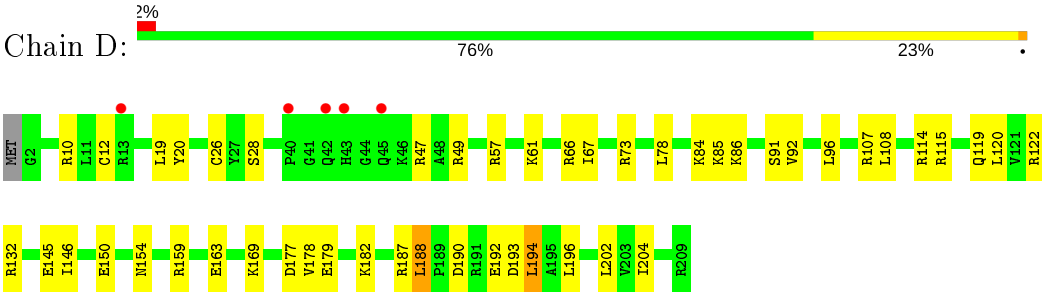
• Molecule 3: 30S ribosomal protein S3

Chain C:



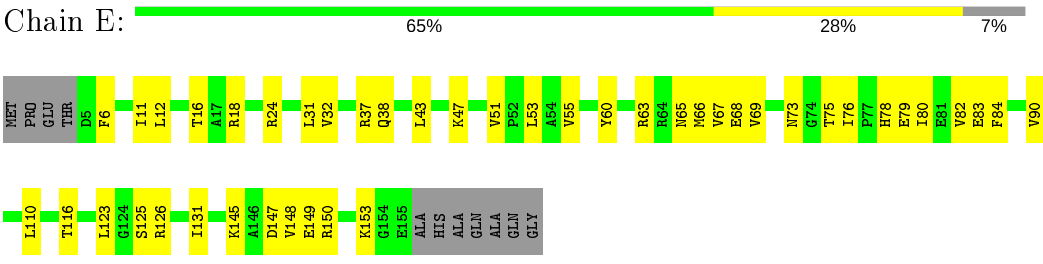
• Molecule 4: 30S ribosomal protein S4

Chain D:



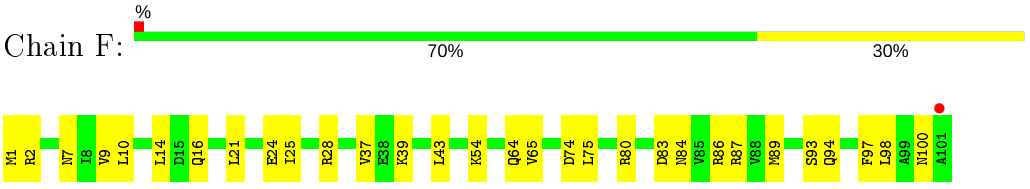
• Molecule 5: 30S ribosomal protein S5

Chain E:



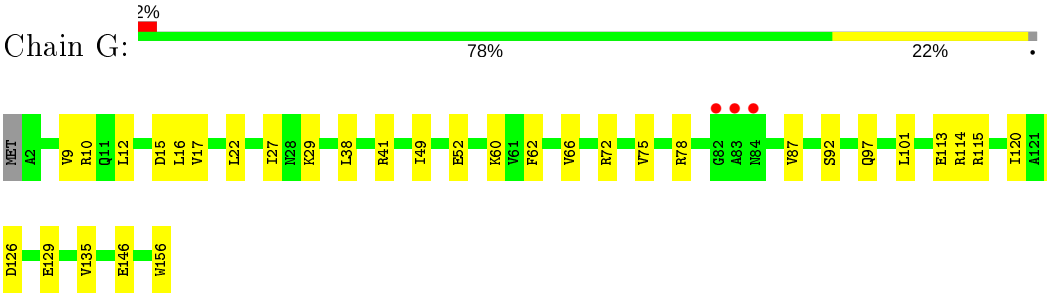
• Molecule 6: 30S ribosomal protein S6

Chain F:



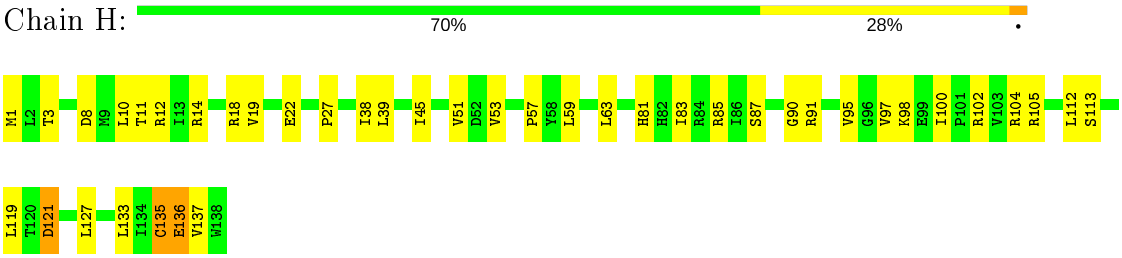
• Molecule 7: 30S ribosomal protein S7

Chain G:



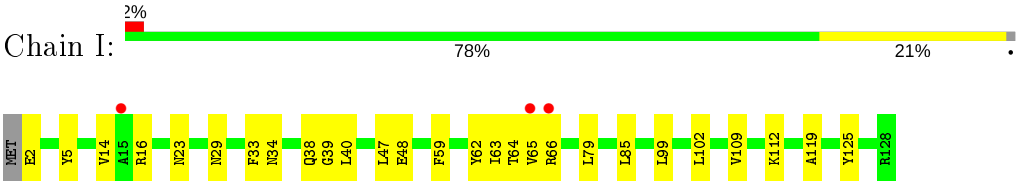
• Molecule 8: 30S ribosomal protein S8

Chain H:



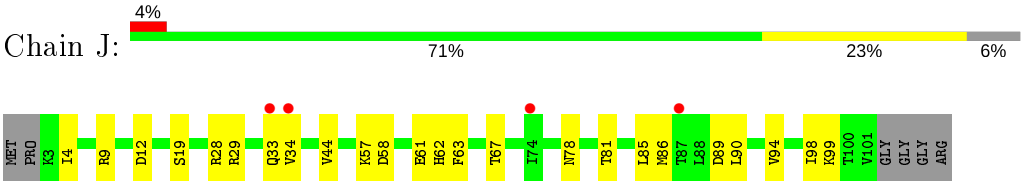
- Molecule 9: 30S ribosomal protein S9

Chain I:



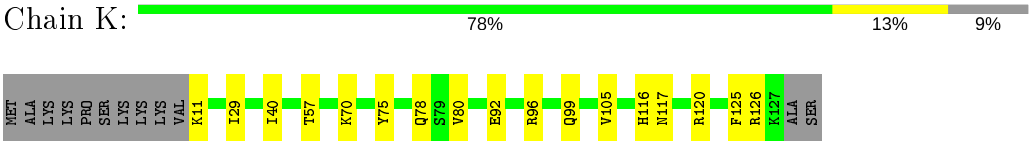
- Molecule 10: 30S ribosomal protein S10

Chain J:



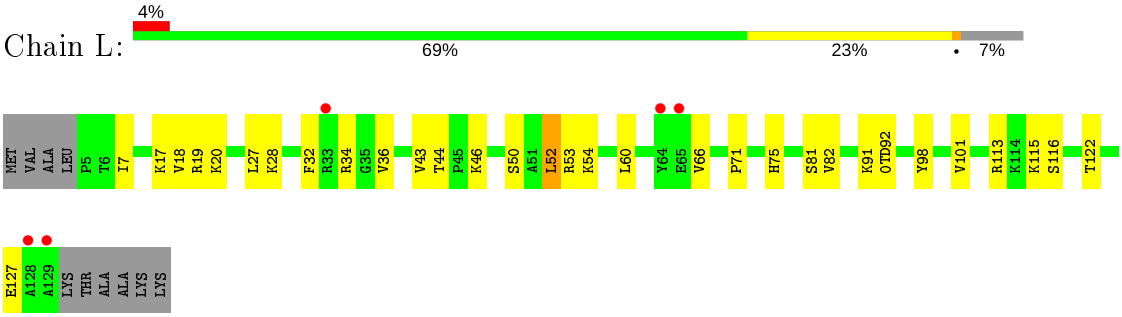
- Molecule 11: 30S ribosomal protein S11

Chain K:



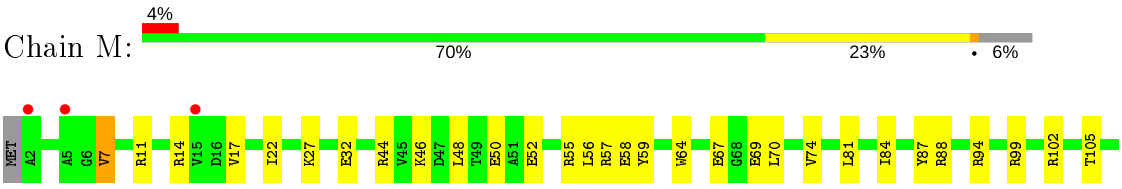
- Molecule 12: 30S ribosomal protein S12

Chain L:



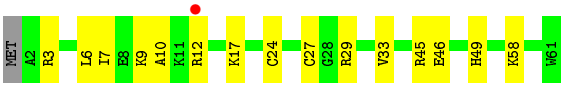
- Molecule 13: 30S ribosomal protein S13

Chain M:



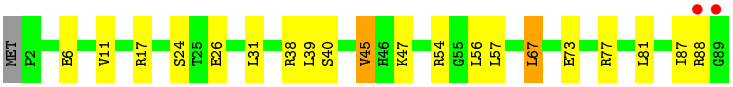
- Molecule 14: 30S ribosomal protein S14

Chain N:



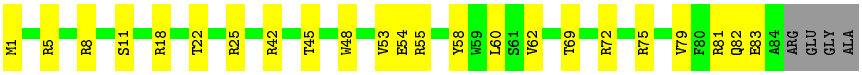
- Molecule 15: 30S ribosomal protein S15

Chain O:



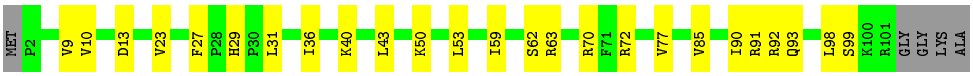
- Molecule 16: 30S ribosomal protein S16

Chain P:



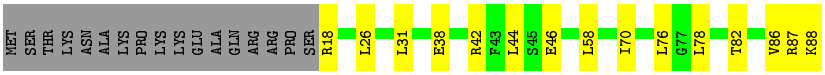
- Molecule 17: 30S ribosomal protein S17

Chain Q:



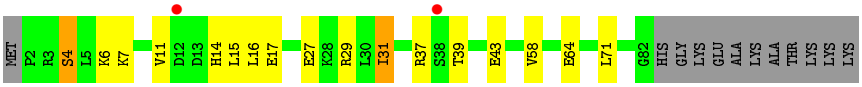
- Molecule 18: 30S ribosomal protein S18

Chain R:



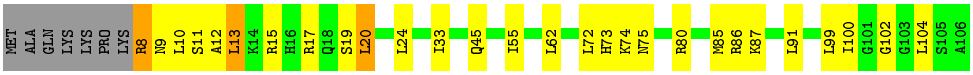
- Molecule 19: 30S ribosomal protein S19

Chain S:



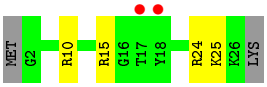
- Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein THX

Chain U:

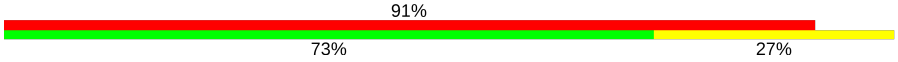


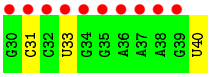
• Molecule 22: 5'-R(*UP*UP*UP*U)-3'

Chain V:

• Molecule 23: 5'-R(*GP*CP*CP*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'

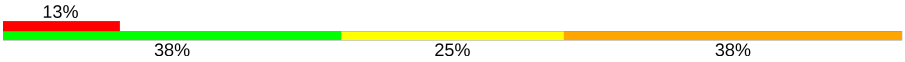
Chain W:

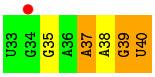




• Molecule 24: 5'-R(P*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'

Chain a:





• Molecule 25: 5'-R(P*UP*UP*U)-3'

Chain b:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.49Å 402.49Å 174.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.75 49.65 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.75) 100.0 (49.65-3.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.148 , 0.201 0.146 , 0.198	Depositor DCC
R_{free} test set	7304 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	130.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 102.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	53659	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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	1.21	135/36234 (0.4%)	1.90	1769/56547 (3.1%)
2	B	0.74	0/1931	0.93	2/2607 (0.1%)
3	C	0.62	0/1637	0.83	0/2207
4	D	0.73	1/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	1.04	1/1163 (0.1%)	1.17	3/1566 (0.2%)
6	F	0.65	0/856	0.86	0/1154
7	G	0.68	0/1276	0.87	0/1709
8	H	1.11	2/1136 (0.2%)	1.18	4/1527 (0.3%)
9	I	0.65	0/1029	0.88	2/1379 (0.1%)
10	J	0.71	1/806 (0.1%)	0.95	2/1084 (0.2%)
11	K	0.76	0/888	0.97	0/1198
12	L	0.90	0/978	1.08	3/1308 (0.2%)
13	M	0.68	0/947	0.94	0/1270
14	N	0.68	0/501	0.85	1/664 (0.2%)
15	O	0.86	0/745	1.02	3/992 (0.3%)
16	P	0.93	0/717	1.08	3/965 (0.3%)
17	Q	1.08	1/847 (0.1%)	1.25	4/1131 (0.4%)
18	R	0.76	0/590	1.00	1/782 (0.1%)
19	S	0.57	0/662	0.77	0/892
20	T	0.87	0/765	1.18	4/1007 (0.4%)
21	U	0.69	0/213	0.87	0/279
22	V	0.53	0/84	0.98	0/128
23	W	0.62	0/241	0.92	0/375
24	a	0.85	0/174	1.89	10/270 (3.7%)
25	b	0.76	0/65	1.31	2/98 (2.0%)
All	All	1.08	141/56218 (0.3%)	1.66	1817/83457 (2.2%)

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
2	B	0	3
3	C	0	2
4	D	0	1
8	H	0	2
9	I	0	1
10	J	0	2
12	L	0	2
16	P	0	1
19	S	0	1
20	T	0	2
21	U	0	1
All	All	0	18

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	A	N9-C4	-10.24	1.31	1.37
1	A	1513	A	N9-C4	-9.49	1.32	1.37
1	A	266	G	N7-C5	-9.34	1.33	1.39
1	A	573	A	N7-C5	-9.28	1.33	1.39
8	H	135	CYS	CB-SG	-9.04	1.66	1.82
1	A	1227	A	N9-C4	-8.41	1.32	1.37
1	A	1502	A	N3-C4	-8.37	1.29	1.34
1	A	860	A	N3-C4	-8.21	1.29	1.34
1	A	1502	A	N9-C4	-8.06	1.33	1.37
1	A	788	U	C2-N3	7.67	1.43	1.37
1	A	151	A	N9-C4	-7.36	1.33	1.37
1	A	868	C	N1-C6	-7.28	1.32	1.37
1	A	1509	C	N3-C4	-7.25	1.28	1.33
1	A	814	A	N9-C4	-7.15	1.33	1.37
1	A	1066	C	N1-C6	-7.12	1.32	1.37
1	A	787	A	N9-C4	-6.99	1.33	1.37
1	A	109	A	N9-C4	-6.97	1.33	1.37
1	A	130	A	N9-C4	-6.87	1.33	1.37
1	A	563	A	N3-C4	-6.87	1.30	1.34
1	A	366	C	N1-C2	6.81	1.47	1.40
1	A	1502	A	C5-C6	-6.80	1.34	1.41
1	A	1079	G	N7-C5	-6.78	1.35	1.39
1	A	920	U	C4-O4	6.69	1.28	1.23
1	A	868	C	C4-C5	-6.67	1.37	1.43
1	A	1080	A	N3-C4	-6.54	1.30	1.34
1	A	1525	G	C6-N1	-6.52	1.34	1.39
1	A	266	G	C5-C6	-6.52	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	882	C	N3-C4	-6.52	1.29	1.33
1	A	926	G	N9-C4	6.47	1.43	1.38
1	A	691	G	N7-C5	-6.45	1.35	1.39
1	A	298	A	N3-C4	-6.38	1.31	1.34
1	A	767	A	N3-C4	-6.38	1.31	1.34
1	A	26	A	N9-C4	-6.38	1.34	1.37
1	A	1076	C	N1-C6	-6.37	1.33	1.37
1	A	279	A	N9-C4	-6.36	1.34	1.37
1	A	780	A	N9-C4	-6.34	1.34	1.37
1	A	828	A	N7-C5	-6.34	1.35	1.39
1	A	798	G	C5-C4	-6.32	1.33	1.38
1	A	600	C	N1-C6	-6.28	1.33	1.37
1	A	858	G	C6-O6	6.28	1.29	1.24
1	A	26	A	N3-C4	-6.27	1.31	1.34
1	A	574	A	C5-C4	-6.22	1.34	1.38
1	A	1500	A	C6-N1	-6.16	1.31	1.35
1	A	892	A	N9-C4	-6.00	1.34	1.37
1	A	1487	G	N3-C4	-5.98	1.31	1.35
1	A	572	A	C5-C4	-5.97	1.34	1.38
1	A	938	A	N9-C4	-5.97	1.34	1.37
1	A	144	G	N1-C2	5.91	1.42	1.37
1	A	1340	A	N9-C4	-5.88	1.34	1.37
1	A	1239	A	N9-C4	-5.86	1.34	1.37
1	A	1513	A	N3-C4	-5.85	1.31	1.34
1	A	1500	A	N3-C4	-5.85	1.31	1.34
17	Q	9	VAL	CA-CB	-5.85	1.42	1.54
1	A	722	A	C5-C6	-5.84	1.35	1.41
1	A	242	C	N1-C6	-5.82	1.33	1.37
1	A	1528	U	C3'-O3'	5.81	1.50	1.42
1	A	934	C	C2-O2	5.79	1.29	1.24
1	A	644	G	N1-C2	-5.79	1.33	1.37
1	A	913	A	C3'-O3'	5.76	1.50	1.42
1	A	266	G	C3'-C2'	5.75	1.59	1.52
1	A	817	C	N1-C6	-5.75	1.33	1.37
1	A	1487	G	N7-C5	-5.75	1.35	1.39
1	A	1527	C	C4-C5	-5.73	1.38	1.43
1	A	1064	G	N3-C4	-5.73	1.31	1.35
1	A	807	A	N3-C4	-5.72	1.31	1.34
1	A	567	G	C5-C4	-5.71	1.34	1.38
1	A	572	A	C6-N1	-5.69	1.31	1.35
1	A	246	A	C5-C4	-5.67	1.34	1.38
4	D	12	CYS	CB-SG	5.67	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	C	N3-C4	-5.67	1.29	1.33
8	H	137	VAL	CB-CG2	-5.65	1.41	1.52
1	A	325	A	N3-C4	-5.62	1.31	1.34
1	A	698	G	N7-C5	-5.60	1.35	1.39
1	A	868	C	N3-C4	-5.57	1.30	1.33
1	A	1103	C	N1-C6	-5.57	1.33	1.37
1	A	863	U	N1-C2	-5.55	1.33	1.38
1	A	926	G	C5-C6	5.53	1.47	1.42
1	A	609	A	N9-C4	-5.52	1.34	1.37
1	A	298	A	N9-C4	-5.52	1.34	1.37
1	A	320	C	N1-C6	-5.50	1.33	1.37
1	A	915	A	N7-C5	-5.50	1.35	1.39
1	A	566	G	N7-C5	-5.47	1.35	1.39
1	A	577	G	N9-C4	-5.46	1.33	1.38
1	A	144	G	C5-C4	5.46	1.42	1.38
1	A	602	A	N3-C4	-5.46	1.31	1.34
1	A	1377	A	N9-C4	-5.43	1.34	1.37
1	A	107	G	C5-C6	-5.42	1.36	1.42
1	A	601	C	N1-C6	-5.42	1.33	1.37
1	A	1078	U	C4-O4	-5.42	1.19	1.23
1	A	642	A	N9-C4	-5.41	1.34	1.37
1	A	1530	G	C2-N3	-5.41	1.28	1.32
1	A	599	C	N1-C6	-5.41	1.33	1.37
1	A	81	U	N1-C2	5.40	1.43	1.38
1	A	611	A	N9-C4	-5.39	1.34	1.37
1	A	858	G	N3-C4	-5.36	1.31	1.35
1	A	1507	A	C6-N1	-5.34	1.31	1.35
1	A	881	G	N9-C8	-5.33	1.34	1.37
1	A	655	A	N9-C4	-5.33	1.34	1.37
1	A	1487	G	N9-C8	-5.31	1.34	1.37
1	A	1514	C	N3-C4	-5.29	1.30	1.33
5	E	90	VAL	CB-CG1	-5.29	1.41	1.52
1	A	574	A	C6-N1	-5.27	1.31	1.35
1	A	1512	U	C4-O4	5.26	1.27	1.23
1	A	1350	A	N7-C5	-5.25	1.36	1.39
1	A	926	G	C5-C4	5.23	1.42	1.38
1	A	1507	A	N3-C4	-5.22	1.31	1.34
1	A	1513	A	C5-C4	-5.22	1.35	1.38
1	A	266	G	C2-N3	5.22	1.36	1.32
1	A	811	C	N1-C6	-5.22	1.34	1.37
1	A	1502	A	N7-C5	-5.20	1.36	1.39
1	A	704	A	N3-C4	-5.19	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	A	N9-C4	5.18	1.41	1.37
1	A	327	A	C5-C6	-5.18	1.36	1.41
1	A	1053	G	N7-C5	5.15	1.42	1.39
1	A	574	A	N3-C4	-5.15	1.31	1.34
1	A	1080	A	C6-N1	-5.12	1.31	1.35
1	A	1375	A	C6-N6	-5.12	1.29	1.33
1	A	134	A	N3-C4	-5.12	1.31	1.34
1	A	1084	G	C5-C6	5.12	1.47	1.42
1	A	855	G	N3-C4	-5.12	1.31	1.35
1	A	819	A	N3-C4	-5.11	1.31	1.34
1	A	813	U	N1-C6	-5.10	1.33	1.38
1	A	325	A	N9-C4	-5.09	1.34	1.37
1	A	828	A	N3-C4	-5.08	1.31	1.34
1	A	853	G	N7-C5	-5.08	1.36	1.39
1	A	117	G	N1-C2	5.07	1.41	1.37
1	A	640	A	N3-C4	-5.05	1.31	1.34
1	A	823	G	N3-C4	-5.05	1.31	1.35
1	A	117	G	C5-C4	5.05	1.41	1.38
1	A	781	A	N7-C5	-5.05	1.36	1.39
1	A	926	G	C2-N3	5.04	1.36	1.32
1	A	741	G	N9-C4	-5.04	1.33	1.38
1	A	120	A	C6-N1	-5.02	1.32	1.35
1	A	568	G	P-O5'	-5.01	1.54	1.59
1	A	1488	G	N9-C8	-5.01	1.34	1.37
1	A	1350	A	C5-C6	-5.01	1.36	1.41
1	A	239	U	C4-O4	-5.00	1.19	1.23
1	A	640	A	C6-N1	-5.00	1.32	1.35
1	A	74	C	N1-C6	5.00	1.40	1.37
1	A	654	G	C6-N1	-5.00	1.36	1.39
10	J	57	LYS	CB-CG	5.00	1.66	1.52

All (1817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	G	C6-C5-N7	-19.86	118.48	130.40
1	A	366	C	N1-C2-O2	17.84	129.60	118.90
1	A	117	G	N1-C6-O6	15.21	129.03	119.90
1	A	1200	C	C2-N1-C1'	15.12	135.43	118.80
1	A	573	A	C8-N9-C4	-15.02	99.79	105.80
1	A	266	G	N1-C6-O6	14.91	128.85	119.90
1	A	1403	C	N3-C2-O2	14.11	131.78	121.90
1	A	1200	C	N1-C2-O2	14.05	127.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	858	G	C5-C6-N1	-13.71	104.64	111.50
1	A	366	C	N3-C2-O2	-13.36	112.55	121.90
1	A	1524	C	N3-C4-C5	-13.31	116.58	121.90
1	A	266	G	C5-C6-O6	-12.74	120.95	128.60
1	A	117	G	N9-C4-C5	-12.34	100.46	105.40
1	A	266	G	C4-C5-C6	12.10	126.06	118.80
1	A	1524	C	C6-N1-C2	-12.09	115.46	120.30
1	A	1092	A	N1-C6-N6	12.09	125.85	118.60
1	A	863	U	C2-N1-C1'	-12.03	103.27	117.70
1	A	1403	C	N1-C2-O2	-11.95	111.73	118.90
1	A	366	C	C2-N1-C1'	11.95	131.94	118.80
1	A	481	G	N1-C6-O6	11.95	127.07	119.90
1	A	1281	U	C5-C4-O4	11.94	133.06	125.90
1	A	624	C	C6-N1-C2	11.88	125.05	120.30
1	A	117	G	C6-C5-N7	-11.85	123.29	130.40
1	A	117	G	C2-N3-C4	-11.83	105.98	111.90
1	A	104	G	N1-C6-O6	11.73	126.94	119.90
1	A	144	G	N1-C6-O6	11.73	126.94	119.90
1	A	762	C	C6-N1-C2	11.70	124.98	120.30
1	A	579	G	N1-C6-O6	11.67	126.90	119.90
1	A	266	G	C4-C5-N7	11.64	115.45	110.80
1	A	873	A	C8-N9-C4	-11.51	101.20	105.80
1	A	1200	C	C5-C6-N1	11.48	126.74	121.00
1	A	1234	C	C6-N1-C2	11.42	124.87	120.30
1	A	1084	G	N3-C4-C5	-11.26	122.97	128.60
1	A	1079	G	C8-N9-C4	-11.20	101.92	106.40
1	A	1200	C	C6-N1-C1'	-11.19	107.38	120.80
1	A	586	C	C6-N1-C2	11.14	124.76	120.30
1	A	570	G	N3-C4-C5	-10.99	123.11	128.60
1	A	283	C	C2-N1-C1'	10.97	130.87	118.80
1	A	295	C	C6-N1-C2	10.96	124.68	120.30
1	A	117	G	C8-N9-C1'	-10.95	112.77	127.00
1	A	634	C	C6-N1-C2	-10.87	115.95	120.30
1	A	1084	G	C4-C5-N7	-10.80	106.48	110.80
1	A	788	U	N3-C4-O4	10.76	126.93	119.40
1	A	920	U	N3-C4-C5	-10.65	108.21	114.60
1	A	572	A	N1-C6-N6	-10.62	112.23	118.60
1	A	863	U	C5-C4-O4	10.58	132.25	125.90
1	A	868	C	N1-C2-O2	-10.58	112.55	118.90
1	A	732	C	N3-C4-C5	10.56	126.12	121.90
1	A	144	G	C5-C6-N1	-10.54	106.23	111.50
1	A	266	G	N7-C8-N9	10.54	118.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	572	A	C5-C6-N1	10.33	122.86	117.70
1	A	824	C	C6-N1-C2	10.31	124.42	120.30
1	A	449	C	C6-N1-C2	-10.25	116.20	120.30
1	A	572	A	N9-C4-C5	10.25	109.90	105.80
1	A	1502	A	C2-N3-C4	-10.24	105.48	110.60
1	A	248	C	C5-C6-N1	-10.22	115.89	121.00
1	A	644	G	C4-C5-N7	10.20	114.88	110.80
1	A	873	A	C2-N3-C4	10.20	115.70	110.60
1	A	863	U	C6-N1-C1'	10.18	135.45	121.20
1	A	248	C	C6-N1-C2	10.17	124.37	120.30
1	A	884	U	C5-C6-N1	-10.15	117.62	122.70
1	A	820	U	N1-C2-N3	10.05	120.93	114.90
1	A	1329	A	N1-C6-N6	10.02	124.61	118.60
1	A	860	A	C8-N9-C4	-10.00	101.80	105.80
1	A	703	G	C4-C5-N7	-9.97	106.81	110.80
1	A	176	C	C6-N1-C2	9.96	124.28	120.30
1	A	559	A	C6-N1-C2	-9.95	112.63	118.60
1	A	856	C	N1-C2-O2	-9.94	112.94	118.90
1	A	283	C	C5-C6-N1	9.94	125.97	121.00
1	A	1190	G	C4-N9-C1'	9.93	139.41	126.50
1	A	691	G	C8-N9-C4	-9.92	102.43	106.40
1	A	90	U	C5-C4-O4	9.90	131.84	125.90
1	A	117	G	C5-C6-N1	-9.90	106.55	111.50
1	A	770	C	C5-C6-N1	-9.90	116.05	121.00
1	A	648	A	C8-N9-C4	9.89	109.76	105.80
1	A	859	A	N1-C6-N6	9.89	124.53	118.60
1	A	266	G	C4-N9-C1'	9.87	139.33	126.50
1	A	729	A	N1-C6-N6	9.86	124.51	118.60
1	A	1530	G	N3-C4-C5	9.81	133.50	128.60
1	A	920	U	C5-C4-O4	9.76	131.75	125.90
1	A	866	C	C6-N1-C2	-9.75	116.40	120.30
1	A	1370	G	C8-N9-C4	-9.75	102.50	106.40
1	A	635	G	C2-N3-C4	-9.75	107.03	111.90
1	A	1381	U	N1-C2-O2	9.74	129.62	122.80
1	A	864	A	N1-C6-N6	-9.70	112.78	118.60
1	A	563	A	C8-N9-C4	-9.67	101.93	105.80
1	A	722	A	N1-C6-N6	9.67	124.40	118.60
1	A	825	G	C8-N9-C4	9.67	110.27	106.40
1	A	117	G	C8-N9-C4	9.66	110.26	106.40
1	A	1524	C	N1-C2-O2	-9.61	113.14	118.90
1	A	266	G	N3-C4-N9	9.58	131.75	126.00
1	A	146	G	N1-C6-O6	9.57	125.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	G	C4-C5-C6	9.54	124.52	118.80
1	A	139	G	C5-C6-N1	-9.53	106.74	111.50
1	A	232	G	C6-C5-N7	-9.51	124.69	130.40
1	A	1335	C	C6-N1-C2	9.51	124.10	120.30
1	A	563	A	N9-C4-C5	9.49	109.59	105.80
1	A	366	C	C6-N1-C1'	-9.48	109.43	120.80
1	A	1232	U	N1-C2-O2	-9.47	116.17	122.80
1	A	1066	C	C6-N1-C1'	-9.47	109.44	120.80
1	A	874	G	N1-C6-O6	9.47	125.58	119.90
1	A	703	G	C5-C6-O6	9.44	134.26	128.60
1	A	1528	U	C2-N1-C1'	9.43	129.02	117.70
1	A	91	C	C2-N1-C1'	9.43	129.17	118.80
1	A	481	G	C6-C5-N7	-9.43	124.75	130.40
1	A	266	G	C5-N7-C8	-9.42	99.59	104.30
1	A	768	A	C8-N9-C4	9.41	109.57	105.80
1	A	283	C	N1-C2-O2	9.40	124.54	118.90
1	A	328	C	N3-C4-N4	-9.38	111.44	118.00
1	A	732	C	C2-N3-C4	-9.36	115.22	119.90
1	A	621	A	C8-N9-C4	-9.32	102.07	105.80
1	A	815	A	C8-N9-C4	9.31	109.53	105.80
1	A	867	G	N1-C6-O6	9.31	125.49	119.90
1	A	1514	C	N1-C2-O2	-9.31	113.31	118.90
1	A	648	A	N7-C8-N9	-9.31	109.15	113.80
1	A	867	G	C8-N9-C1'	-9.30	114.90	127.00
1	A	698	G	C4-N9-C1'	9.29	138.58	126.50
1	A	795	C	N3-C2-O2	9.25	128.38	121.90
1	A	721	G	C6-C5-N7	-9.24	124.86	130.40
1	A	864	A	C5-C6-N6	9.21	131.07	123.70
1	A	90	U	N3-C4-O4	-9.20	112.96	119.40
1	A	1239	A	C8-N9-C4	9.20	109.48	105.80
1	A	529	G	N1-C6-O6	9.17	125.40	119.90
1	A	269	C	C5-C6-N1	-9.13	116.43	121.00
1	A	860	A	N9-C4-C5	9.13	109.45	105.80
1	A	722	A	C2-N3-C4	-9.10	106.05	110.60
1	A	1507	A	N1-C6-N6	-9.09	113.15	118.60
1	A	1200	C	C6-N1-C2	-9.08	116.67	120.30
1	A	559	A	C8-N9-C4	-9.08	102.17	105.80
1	A	644	G	C6-C5-N7	-9.06	124.96	130.40
1	A	577	G	C2-N3-C4	-9.06	107.37	111.90
1	A	940	C	C6-N1-C2	9.04	123.92	120.30
1	A	283	C	C2-N3-C4	9.02	124.41	119.90
1	A	818	G	N1-C6-O6	9.02	125.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	729	A	C5-N7-C8	-9.02	99.39	103.90
1	A	1381	U	N3-C2-O2	-9.00	115.90	122.20
1	A	635	G	C6-C5-N7	-8.99	125.00	130.40
1	A	481	G	C5-C6-N1	-8.98	107.01	111.50
1	A	1108	G	N3-C4-C5	-8.98	124.11	128.60
1	A	623	C	C6-N1-C2	8.97	123.89	120.30
1	A	1392	G	C6-C5-N7	-8.97	125.02	130.40
1	A	1107	C	C6-N1-C2	-8.96	116.72	120.30
1	A	881	G	C8-N9-C4	8.93	109.97	106.40
1	A	635	G	C5-C6-N1	-8.92	107.04	111.50
1	A	788	U	N3-C2-O2	8.91	128.44	122.20
1	A	975	A	N1-C6-N6	8.86	123.92	118.60
1	A	232	G	N1-C6-O6	8.86	125.22	119.90
1	A	284	G	N1-C6-O6	8.86	125.22	119.90
1	A	1186	G	N3-C4-C5	8.86	133.03	128.60
1	A	1068	G	C8-N9-C4	-8.84	102.86	106.40
1	A	1392	G	N1-C6-O6	8.83	125.20	119.90
1	A	91	C	C6-N1-C2	-8.82	116.77	120.30
1	A	783	C	C6-N1-C2	8.80	123.82	120.30
1	A	885	G	C2-N3-C4	-8.80	107.50	111.90
1	A	570	G	C8-N9-C4	-8.78	102.89	106.40
1	A	1524	C	C4-C5-C6	8.78	121.79	117.40
1	A	909	A	C5-C6-N6	-8.77	116.69	123.70
1	A	651	C	C6-N1-C2	8.73	123.79	120.30
1	A	698	G	C6-C5-N7	-8.73	125.16	130.40
1	A	529	G	C4-N9-C1'	8.73	137.85	126.50
1	A	621	A	N7-C8-N9	8.73	118.17	113.80
1	A	144	G	C2-N3-C4	-8.72	107.54	111.90
1	A	1053	G	C8-N9-C4	8.72	109.89	106.40
1	A	244	U	N1-C2-O2	8.72	128.90	122.80
1	A	91	C	N1-C2-O2	8.71	124.13	118.90
1	A	926	G	N3-C4-C5	-8.71	124.25	128.60
1	A	700	G	C4-C5-N7	8.70	114.28	110.80
1	A	700	G	N3-C4-N9	8.69	131.22	126.00
1	A	1066	C	C6-N1-C2	8.69	123.78	120.30
1	A	259	G	N1-C2-N3	8.68	129.11	123.90
1	A	1228	C	N1-C2-O2	8.68	124.11	118.90
1	A	741	G	N3-C4-N9	-8.68	120.80	126.00
1	A	814	A	C2-N3-C4	-8.67	106.27	110.60
1	A	1186	G	C2-N3-C4	-8.66	107.57	111.90
1	A	529	G	C8-N9-C1'	-8.64	115.77	127.00
1	A	50	A	C8-N9-C4	8.61	109.24	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	579	G	C5-C6-O6	-8.61	123.44	128.60
1	A	277	C	C6-N1-C2	8.60	123.74	120.30
1	A	1468	A	C8-N9-C4	8.59	109.24	105.80
1	A	795	C	N1-C2-O2	-8.58	113.75	118.90
1	A	1388	C	N3-C2-O2	8.55	127.89	121.90
1	A	266	G	C8-N9-C4	-8.55	102.98	106.40
1	A	868	C	C6-N1-C2	-8.55	116.88	120.30
1	A	618	C	C2-N1-C1'	-8.54	109.41	118.80
1	A	971	G	N1-C6-O6	8.53	125.02	119.90
1	A	909	A	N1-C6-N6	8.53	123.72	118.60
1	A	573	A	C4-C5-C6	8.52	121.26	117.00
1	A	1202	G	N1-C6-O6	-8.52	114.79	119.90
1	A	735	C	C6-N1-C2	8.52	123.71	120.30
1	A	858	G	N1-C6-O6	8.51	125.00	119.90
1	A	525	C	C6-N1-C2	8.50	123.70	120.30
1	A	127	G	C8-N9-C4	8.47	109.79	106.40
1	A	928	G	N1-C6-O6	8.47	124.98	119.90
1	A	232	G	C4-C5-N7	8.46	114.18	110.80
1	A	283	C	C6-N1-C2	-8.46	116.92	120.30
1	A	884	U	C4-C5-C6	8.46	124.77	119.70
1	A	1200	C	N3-C2-O2	-8.45	115.98	121.90
1	A	650	G	C8-N9-C4	8.45	109.78	106.40
1	A	780	A	C8-N9-C4	8.44	109.17	105.80
1	A	1080	A	N1-C6-N6	-8.43	113.54	118.60
1	A	382	A	C8-N9-C4	-8.42	102.43	105.80
1	A	656	C	C6-N1-C2	8.41	123.67	120.30
1	A	268	C	N1-C2-O2	8.40	123.94	118.90
1	A	519	C	N1-C2-O2	8.39	123.94	118.90
1	A	182	U	N3-C2-O2	-8.39	116.33	122.20
1	A	1083	U	N3-C2-O2	8.38	128.07	122.20
1	A	701	C	N1-C2-O2	8.37	123.92	118.90
1	A	721	G	N3-C4-N9	8.37	131.02	126.00
1	A	788	U	C5-C6-N1	8.37	126.88	122.70
1	A	872	A	C2-N3-C4	-8.36	106.42	110.60
1	A	572	A	C8-N9-C4	-8.36	102.46	105.80
1	A	874	G	C8-N9-C4	8.35	109.74	106.40
1	A	1527	C	C5-C4-N4	-8.34	114.36	120.20
1	A	111	G	N3-C4-N9	-8.34	121.00	126.00
1	A	763	G	C8-N9-C4	8.33	109.73	106.40
1	A	1202	G	C5-C6-O6	8.32	133.59	128.60
1	A	573	A	N7-C8-N9	8.32	117.96	113.80
1	A	1058	G	C8-N9-C4	8.31	109.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	716	A	N1-C6-N6	-8.29	113.63	118.60
1	A	8	A	C8-N9-C4	-8.28	102.49	105.80
1	A	175	C	C6-N1-C2	8.26	123.60	120.30
1	A	634	C	N3-C4-C5	-8.26	118.60	121.90
1	A	440	A	C2-N3-C4	-8.23	106.48	110.60
1	A	721	G	C4-C5-C6	8.23	123.74	118.80
1	A	810	C	N3-C4-N4	8.23	123.76	118.00
1	A	259	G	N1-C2-N2	-8.22	108.80	116.20
1	A	874	G	N9-C4-C5	-8.22	102.11	105.40
1	A	914	A	C8-N9-C4	-8.20	102.52	105.80
1	A	398	C	C6-N1-C2	8.19	123.58	120.30
1	A	559	A	N3-C4-C5	-8.18	121.08	126.80
1	A	814	A	N1-C2-N3	8.18	133.39	129.30
1	A	871	U	N1-C2-O2	8.18	128.53	122.80
1	A	1365	G	C8-N9-C4	-8.18	103.13	106.40
1	A	1054	C	N1-C2-O2	8.18	123.81	118.90
1	A	965	A	C8-N9-C4	8.17	109.07	105.80
1	A	721	G	C4-N9-C1'	8.16	137.11	126.50
1	A	132	C	C2-N3-C4	-8.15	115.82	119.90
1	A	283	C	N3-C4-C5	-8.14	118.64	121.90
1	A	867	G	C6-C5-N7	-8.12	125.53	130.40
1	A	1390	U	N3-C4-C5	-8.11	109.73	114.60
1	A	829	G	C8-N9-C4	8.11	109.64	106.40
1	A	1186	G	C5-C6-N1	-8.10	107.45	111.50
1	A	1392	G	C5-C6-N1	-8.10	107.45	111.50
1	A	266	G	C8-N9-C1'	-8.09	116.48	127.00
1	A	864	A	N9-C4-C5	8.08	109.03	105.80
1	A	1502	A	C5-N7-C8	-8.07	99.86	103.90
1	A	1512	U	N3-C4-C5	-8.07	109.76	114.60
1	A	873	A	C5-C6-N1	8.07	121.73	117.70
1	A	1190	G	N7-C8-N9	8.06	117.13	113.10
1	A	1530	G	N3-C4-N9	-8.05	121.17	126.00
1	A	816	A	N1-C6-N6	-8.05	113.77	118.60
1	A	1186	G	N3-C4-N9	-8.05	121.17	126.00
1	A	1452	C	N1-C2-O2	8.04	123.72	118.90
1	A	659	U	C5-C6-N1	-8.03	118.68	122.70
1	A	278	G	C4-C5-N7	-8.02	107.59	110.80
1	A	1083	U	C5-C4-O4	-8.02	121.09	125.90
1	A	32	A	C6-N1-C2	-8.01	113.80	118.60
1	A	1500	A	N1-C6-N6	-8.00	113.80	118.60
1	A	288	A	C2-N3-C4	-8.00	106.60	110.60
1	A	867	G	C4-N9-C1'	7.99	136.89	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1227	A	N1-C6-N6	7.99	123.39	118.60
1	A	788	U	N3-C4-C5	-7.99	109.81	114.60
1	A	481	G	C4-C5-C6	7.98	123.59	118.80
1	A	1279	A	C8-N9-C4	-7.98	102.61	105.80
1	A	91	C	N3-C2-O2	-7.97	116.32	121.90
1	A	940	C	C5-C6-N1	-7.97	117.02	121.00
1	A	807	A	N1-C2-N3	7.96	133.28	129.30
1	A	1092	A	N9-C4-C5	-7.96	102.62	105.80
1	A	1190	G	C8-N9-C1'	-7.96	116.66	127.00
1	A	479	C	N3-C4-C5	-7.95	118.72	121.90
1	A	820	U	N1-C2-O2	-7.95	117.23	122.80
1	A	885	G	N3-C4-C5	7.94	132.57	128.60
1	A	944	G	C5-C6-O6	7.94	133.36	128.60
1	A	1488	G	C8-N9-C4	7.94	109.58	106.40
1	A	265	G	N1-C2-N2	-7.93	109.06	116.20
1	A	1507	A	N9-C4-C5	7.93	108.97	105.80
1	A	1235	U	N1-C2-N3	7.93	119.66	114.90
1	A	704	A	C8-N9-C4	-7.93	102.63	105.80
1	A	609	A	C2-N3-C4	-7.92	106.64	110.60
1	A	815	A	N7-C8-N9	-7.92	109.84	113.80
1	A	853	G	C6-C5-N7	-7.92	125.65	130.40
1	A	1322	C	C2-N1-C1'	7.92	127.51	118.80
1	A	674	G	C8-N9-C4	7.92	109.57	106.40
1	A	970	C	N1-C2-O2	7.92	123.65	118.90
1	A	43	C	C6-N1-C2	7.91	123.47	120.30
1	A	299	G	N1-C6-O6	7.91	124.65	119.90
1	A	1528	U	C6-N1-C1'	-7.91	110.13	121.20
1	A	732	C	C5-C6-N1	-7.91	117.05	121.00
1	A	628	G	N3-C4-N9	7.91	130.74	126.00
1	A	721	G	C8-N9-C1'	-7.90	116.73	127.00
1	A	1064	G	N9-C4-C5	7.90	108.56	105.40
1	A	232	G	N9-C4-C5	-7.88	102.25	105.40
1	A	117	G	C4-N9-C1'	7.88	136.74	126.50
9	I	39	GLY	N-CA-C	-7.88	93.41	113.10
1	A	729	A	C5-C6-N6	-7.87	117.40	123.70
1	A	874	G	C5-C6-O6	-7.87	123.88	128.60
1	A	117	G	C4-C5-C6	7.87	123.52	118.80
1	A	852	G	N1-C6-O6	7.85	124.61	119.90
1	A	104	G	C6-C5-N7	-7.85	125.69	130.40
1	A	1344	C	C6-N1-C2	7.85	123.44	120.30
1	A	1493[A]	A	C5-N7-C8	-7.84	99.98	103.90
1	A	1493[B]	A	C5-N7-C8	-7.84	99.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1488	G	N7-C8-N9	-7.84	109.18	113.10
1	A	559	A	C5-C6-N1	7.84	121.62	117.70
1	A	813	U	C2-N1-C1'	7.84	127.10	117.70
24	a	39	G	N1-C6-O6	7.83	124.60	119.90
1	A	487	A	C8-N9-C4	7.83	108.93	105.80
1	A	522	C	C5-C6-N1	-7.83	117.09	121.00
20	T	20	LEU	CA-CB-CG	-7.83	97.30	115.30
1	A	266	G	N3-C4-C5	-7.82	124.69	128.60
1	A	1222	G	C5-C6-N1	-7.81	107.60	111.50
1	A	635	G	N1-C6-O6	7.80	124.58	119.90
1	A	858	G	C4-C5-C6	7.79	123.47	118.80
1	A	529	G	C5-C6-N1	-7.78	107.61	111.50
1	A	819	A	C4-C5-C6	7.78	120.89	117.00
1	A	596	C	C6-N1-C2	7.77	123.41	120.30
1	A	963	G	N1-C6-O6	7.75	124.55	119.90
1	A	135	C	N3-C4-C5	-7.75	118.80	121.90
1	A	383	A	N1-C6-N6	-7.74	113.96	118.60
1	A	580	U	N3-C4-C5	-7.74	109.96	114.60
1	A	570	G	C4-N9-C1'	7.74	136.56	126.50
1	A	400	C	N3-C4-C5	7.73	124.99	121.90
1	A	918	A	N1-C2-N3	7.73	133.16	129.30
1	A	1528	U	P-O3'-C3'	7.73	128.97	119.70
1	A	1092	A	C6-C5-N7	-7.72	126.89	132.30
1	A	190(G)	G	C5-C6-N1	-7.71	107.65	111.50
1	A	1414	U	N3-C2-O2	-7.71	116.81	122.20
1	A	1074	G	C5-C6-N1	-7.71	107.65	111.50
1	A	867	G	N3-C4-N9	7.70	130.62	126.00
1	A	522	C	C2-N1-C1'	-7.70	110.33	118.80
1	A	783	C	N3-C4-C5	7.69	124.98	121.90
1	A	1277	C	C6-N1-C2	-7.69	117.22	120.30
1	A	1099	G	N9-C4-C5	7.69	108.47	105.40
1	A	109	A	C2-N3-C4	-7.68	106.76	110.60
1	A	753	A	N9-C4-C5	7.68	108.87	105.80
1	A	813	U	C5-C4-O4	-7.67	121.30	125.90
1	A	1394	A	C5-C6-N6	-7.67	117.56	123.70
1	A	570	G	C2-N3-C4	7.67	115.74	111.90
1	A	128	G	N1-C6-O6	7.66	124.49	119.90
1	A	805	C	N3-C4-C5	7.66	124.96	121.90
1	A	770	C	C6-N1-C2	7.66	123.36	120.30
1	A	1108	G	C8-N9-C4	-7.66	103.34	106.40
1	A	783	C	N3-C4-N4	-7.65	112.64	118.00
1	A	55	A	N1-C6-N6	-7.63	114.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	G	C8-N9-C4	7.62	109.45	106.40
1	A	700	G	C6-C5-N7	-7.61	125.83	130.40
1	A	779	C	N1-C2-O2	-7.61	114.34	118.90
1	A	1230	C	N3-C4-N4	7.61	123.32	118.00
1	A	946	A	C6-N1-C2	-7.60	114.04	118.60
1	A	1390	U	N1-C2-N3	7.60	119.46	114.90
1	A	529	G	C6-C5-N7	-7.60	125.84	130.40
1	A	591	U	C5-C6-N1	-7.60	118.90	122.70
1	A	1496	C	N3-C4-C5	-7.60	118.86	121.90
1	A	697	U	C5-C6-N1	-7.59	118.90	122.70
1	A	1525	G	N1-C6-O6	-7.59	115.34	119.90
1	A	722	A	C6-C5-N7	-7.59	126.99	132.30
1	A	1353	G	N3-C4-C5	-7.59	124.81	128.60
1	A	1240	U	C5-C4-O4	7.58	130.45	125.90
1	A	1053	G	N7-C8-N9	-7.58	109.31	113.10
1	A	242	C	C4-C5-C6	7.58	121.19	117.40
1	A	326	G	C5-C6-N1	-7.57	107.72	111.50
1	A	858	G	N3-C2-N2	-7.57	114.60	119.90
1	A	32	A	C4-N9-C1'	7.57	139.92	126.30
1	A	572	A	C2-N3-C4	7.57	114.38	110.60
1	A	782	A	C8-N9-C4	-7.56	102.78	105.80
1	A	618	C	N3-C2-O2	7.56	127.19	121.90
1	A	297	G	N3-C4-C5	-7.55	124.82	128.60
1	A	1190	G	C8-N9-C4	-7.54	103.38	106.40
1	A	1403	C	N3-C4-N4	7.53	123.27	118.00
1	A	981	U	N3-C4-O4	7.52	124.67	119.40
1	A	1525	G	C5-C6-N1	7.52	115.26	111.50
1	A	579	G	C4-C5-N7	7.52	113.81	110.80
1	A	782	A	N9-C4-C5	7.52	108.81	105.80
1	A	400	C	N1-C2-O2	7.52	123.41	118.90
1	A	693	G	N1-C6-O6	7.52	124.41	119.90
1	A	1487	G	N3-C4-C5	-7.51	124.84	128.60
1	A	667	G	C2-N3-C4	-7.51	108.15	111.90
1	A	784	C	N3-C2-O2	-7.51	116.65	121.90
1	A	107	G	C4-C5-N7	7.49	113.80	110.80
1	A	928	G	C5-C6-O6	-7.49	124.10	128.60
1	A	1084	G	C5-N7-C8	7.49	108.05	104.30
1	A	1202	G	C4-C5-N7	-7.49	107.80	110.80
1	A	874	G	C8-N9-C1'	-7.49	117.26	127.00
1	A	698	G	C8-N9-C1'	-7.48	117.27	127.00
1	A	16	A	C8-N9-C4	7.48	108.79	105.80
1	A	1055	A	N1-C6-N6	-7.48	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	C	C6-N1-C2	-7.47	117.31	120.30
1	A	648	A	C5-N7-C8	7.46	107.63	103.90
1	A	27	G	C5-C6-O6	-7.46	124.13	128.60
1	A	893	C	N1-C2-O2	7.45	123.37	118.90
1	A	230	G	C8-N9-C1'	-7.45	117.32	127.00
1	A	859	A	C5-C6-N6	-7.44	117.75	123.70
1	A	881	G	C8-N9-C1'	-7.44	117.33	127.00
1	A	332	G	C5-C6-O6	-7.43	124.14	128.60
1	A	1281	U	N3-C4-O4	-7.42	114.20	119.40
1	A	781	A	C8-N9-C4	-7.42	102.83	105.80
1	A	923	A	C2-N3-C4	-7.42	106.89	110.60
1	A	920	U	C4-C5-C6	7.42	124.15	119.70
1	A	382	A	N9-C4-C5	7.40	108.76	105.80
1	A	628	G	N3-C4-C5	-7.40	124.90	128.60
1	A	637	G	C5-C6-N1	-7.39	107.80	111.50
1	A	698	G	N3-C4-C5	-7.39	124.91	128.60
1	A	1232	U	N3-C2-O2	7.38	127.37	122.20
1	A	760	G	C8-N9-C1'	-7.36	117.43	127.00
1	A	573	A	N9-C4-C5	7.36	108.75	105.80
1	A	1305	G	C5-C6-N1	-7.36	107.82	111.50
1	A	328	C	C5-C4-N4	7.36	125.35	120.20
1	A	1092	A	C5-C6-N6	-7.36	117.81	123.70
1	A	852	G	C5-C6-N1	-7.35	107.82	111.50
1	A	134	A	N1-C2-N3	7.33	132.97	129.30
1	A	745	C	C6-N1-C2	7.33	123.23	120.30
1	A	1094	G	C4-C5-N7	7.33	113.73	110.80
1	A	816	A	C5-C6-N6	7.33	129.56	123.70
1	A	946	A	N1-C6-N6	-7.32	114.21	118.60
1	A	436	C	C6-N1-C2	7.32	123.23	120.30
1	A	1068	G	N7-C8-N9	7.32	116.76	113.10
1	A	1199	U	N3-C2-O2	-7.31	117.08	122.20
1	A	251	G	N1-C2-N2	-7.31	109.62	116.20
1	A	447	G	N3-C4-N9	7.31	130.38	126.00
1	A	1370	G	N7-C8-N9	7.30	116.75	113.10
1	A	1084	G	N1-C6-O6	-7.30	115.52	119.90
1	A	635	G	N1-C2-N3	7.29	128.28	123.90
1	A	1092	A	C4-C5-N7	7.29	114.34	110.70
1	A	139	G	N1-C6-O6	7.29	124.27	119.90
1	A	38	G	N3-C4-N9	-7.28	121.63	126.00
1	A	1193	G	C5-C6-N1	-7.28	107.86	111.50
1	A	27	G	C8-N9-C4	-7.28	103.49	106.40
1	A	1080	A	N9-C4-C5	7.28	108.71	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	C	N3-C4-C5	7.27	124.81	121.90
1	A	823	G	C2-N3-C4	-7.27	108.26	111.90
1	A	1353	G	C8-N9-C4	-7.27	103.49	106.40
1	A	787	A	C5-N7-C8	-7.27	100.27	103.90
1	A	597	G	N3-C4-N9	7.26	130.36	126.00
1	A	1301	U	C6-N1-C2	-7.26	116.64	121.00
1	A	250	A	C5-C6-N1	-7.25	114.08	117.70
1	A	1205	U	N3-C2-O2	-7.24	117.13	122.20
1	A	1447	G	N1-C6-O6	7.24	124.25	119.90
1	A	1350	A	C5-N7-C8	-7.24	100.28	103.90
1	A	830	G	C2-N3-C4	-7.23	108.28	111.90
1	A	1143	G	N1-C6-O6	7.22	124.23	119.90
1	A	7	G	N9-C4-C5	-7.22	102.51	105.40
15	O	67	LEU	CA-CB-CG	-7.22	98.70	115.30
1	A	635	G	C4-C5-C6	7.20	123.12	118.80
1	A	577	G	N3-C4-C5	7.19	132.20	128.60
1	A	867	G	C4-C5-C6	7.19	123.11	118.80
1	A	1403	C	C6-N1-C2	7.19	123.18	120.30
1	A	254	G	C2-N3-C4	-7.19	108.31	111.90
1	A	451	A	C2-N3-C4	-7.19	107.00	110.60
1	A	586	C	C2-N1-C1'	-7.19	110.89	118.80
1	A	929	G	N1-C6-O6	7.18	124.21	119.90
1	A	1231	G	C8-N9-C1'	-7.18	117.66	127.00
1	A	868	C	N3-C4-C5	-7.18	119.03	121.90
1	A	32	A	C8-N9-C1'	-7.18	114.78	127.70
1	A	1530	G	C8-N9-C4	7.18	109.27	106.40
1	A	760	G	C6-C5-N7	-7.17	126.10	130.40
1	A	854	G	N1-C2-N2	-7.17	109.75	116.20
1	A	722	A	C4-C5-N7	7.16	114.28	110.70
1	A	197	A	N1-C6-N6	-7.16	114.30	118.60
1	A	1338	G	C5-C6-O6	7.16	132.90	128.60
1	A	109	A	N3-C4-N9	-7.16	121.67	127.40
1	A	522	C	C6-N1-C2	7.16	123.16	120.30
1	A	703	G	N9-C4-C5	7.16	108.26	105.40
1	A	732	C	C6-N1-C2	7.16	123.16	120.30
1	A	283	C	C6-N1-C1'	-7.15	112.22	120.80
1	A	20	U	C5-C6-N1	-7.15	119.12	122.70
1	A	783	C	C2-N1-C1'	-7.14	110.94	118.80
1	A	1399	C	C5-C4-N4	-7.14	115.20	120.20
1	A	183	G	C8-N9-C4	-7.14	103.54	106.40
1	A	583	A	N1-C6-N6	7.14	122.89	118.60
24	a	38	A	C5-C6-N1	-7.13	114.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	G	N1-C6-O6	7.13	124.18	119.90
1	A	718	G	N1-C6-O6	7.12	124.17	119.90
1	A	1230	C	C5-C4-N4	-7.11	115.22	120.20
1	A	813	U	N3-C4-O4	7.11	124.37	119.40
1	A	1227	A	C5-N7-C8	-7.10	100.35	103.90
1	A	365	U	C2-N1-C1'	7.10	126.22	117.70
1	A	1230	C	N3-C2-O2	7.10	126.87	121.90
1	A	50	A	N1-C2-N3	-7.10	125.75	129.30
1	A	1375	A	C5-C6-N1	7.10	121.25	117.70
1	A	729	A	C4-C5-N7	7.09	114.25	110.70
1	A	1310	G	C8-N9-C1'	-7.09	117.78	127.00
1	A	1276	G	N1-C6-O6	7.09	124.15	119.90
1	A	68	G	C8-N9-C4	7.08	109.23	106.40
1	A	91	C	C5-C6-N1	7.08	124.54	121.00
1	A	371	G	N1-C6-O6	-7.08	115.65	119.90
1	A	934	C	N1-C2-N3	-7.08	114.25	119.20
1	A	828	A	C2-N3-C4	-7.08	107.06	110.60
1	A	701	C	N3-C2-O2	-7.07	116.95	121.90
1	A	8	A	N9-C4-C5	7.07	108.63	105.80
1	A	856	C	N3-C4-C5	-7.07	119.07	121.90
1	A	698	G	N3-C4-N9	7.07	130.24	126.00
1	A	1190	G	C6-C5-N7	-7.07	126.16	130.40
1	A	120	A	N1-C6-N6	-7.06	114.36	118.60
1	A	895	G	C8-N9-C4	-7.06	103.58	106.40
1	A	945	G	C5-C6-N1	7.06	115.03	111.50
1	A	36	C	N3-C2-O2	-7.06	116.96	121.90
1	A	1388	C	C6-N1-C2	7.06	123.12	120.30
1	A	1507	A	C8-N9-C4	-7.05	102.98	105.80
1	A	365	U	N3-C4-O4	7.05	124.34	119.40
1	A	259	G	C2-N3-C4	-7.05	108.38	111.90
1	A	912	C	N3-C4-C5	7.05	124.72	121.90
1	A	1061	G	C2-N3-C4	-7.04	108.38	111.90
1	A	1380	U	N3-C2-O2	-7.04	117.27	122.20
1	A	269	C	C2-N3-C4	-7.04	116.38	119.90
1	A	1341	U	C5-C4-O4	7.04	130.12	125.90
1	A	799	G	N1-C6-O6	7.03	124.12	119.90
1	A	700	G	C5-C6-O6	-7.03	124.38	128.60
1	A	621	A	C5-N7-C8	-7.02	100.39	103.90
1	A	975	A	C4-C5-N7	7.01	114.21	110.70
1	A	681	C	C6-N1-C2	-7.01	117.50	120.30
1	A	190(G)	G	N1-C6-O6	7.01	124.11	119.90
1	A	104	G	C5-C6-N1	-7.01	108.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	G	C8-N9-C4	7.01	109.20	106.40
1	A	1322	C	N3-C4-C5	-7.01	119.10	121.90
1	A	250	A	C2-N3-C4	-7.00	107.10	110.60
1	A	1061	G	C5-C6-N1	-7.00	108.00	111.50
1	A	181	G	C4-N9-C1'	6.99	135.59	126.50
1	A	774	G	N1-C6-O6	6.99	124.09	119.90
1	A	940	C	C2-N3-C4	-6.99	116.41	119.90
1	A	552	U	C2-N3-C4	-6.98	122.81	127.00
1	A	1438	G	N1-C6-O6	6.98	124.09	119.90
1	A	1047	G	C8-N9-C4	6.98	109.19	106.40
1	A	117	G	C5-C6-O6	-6.98	124.41	128.60
1	A	316	G	N1-C6-O6	-6.98	115.71	119.90
1	A	329	A	C2-N3-C4	-6.98	107.11	110.60
1	A	1399	C	N3-C4-N4	6.97	122.88	118.00
1	A	674	G	N9-C4-C5	-6.97	102.61	105.40
1	A	278	G	N9-C4-C5	6.96	108.19	105.40
1	A	590	C	C6-N1-C2	6.96	123.09	120.30
1	A	817	C	C6-N1-C1'	-6.96	112.44	120.80
1	A	753	A	N1-C6-N6	-6.96	114.42	118.60
1	A	1403	C	C5-C4-N4	-6.96	115.33	120.20
1	A	552	U	N3-C2-O2	-6.96	117.33	122.20
1	A	854	G	C8-N9-C1'	-6.96	117.95	127.00
1	A	127	G	N1-C6-O6	6.96	124.07	119.90
1	A	447	G	C8-N9-C1'	-6.95	117.96	127.00
1	A	580	U	C5-C4-O4	6.95	130.07	125.90
1	A	722	A	C5-N7-C8	-6.95	100.42	103.90
1	A	1493[A]	A	N7-C8-N9	6.95	117.28	113.80
1	A	1493[B]	A	N7-C8-N9	6.95	117.28	113.80
1	A	27	G	C4-C5-N7	6.95	113.58	110.80
4	D	202	LEU	CA-CB-CG	-6.94	99.34	115.30
1	A	703	G	N1-C6-O6	-6.94	115.74	119.90
1	A	1421	G	C8-N9-C4	-6.94	103.62	106.40
1	A	686	U	C5-C4-O4	6.93	130.06	125.90
1	A	235	C	C6-N1-C2	6.93	123.07	120.30
1	A	946	A	C8-N9-C4	-6.93	103.03	105.80
1	A	1373	G	N9-C4-C5	6.93	108.17	105.40
1	A	295	C	C5-C6-N1	-6.92	117.54	121.00
1	A	755	G	C5-C6-O6	-6.92	124.45	128.60
10	J	58	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	182	U	N1-C2-O2	6.91	127.64	122.80
1	A	824	C	N3-C4-C5	6.91	124.66	121.90
1	A	549	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	863	U	N3-C4-O4	-6.91	114.57	119.40
1	A	260	G	C5-C6-N1	-6.90	108.05	111.50
1	A	1442	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1525	G	N9-C4-C5	6.89	108.16	105.40
1	A	635	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1228	C	C2-N1-C1'	6.89	126.38	118.80
1	A	246	A	C2-N3-C4	6.88	114.04	110.60
1	A	975	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1530	G	N7-C8-N9	-6.88	109.66	113.10
1	A	487	A	N7-C8-N9	-6.88	110.36	113.80
1	A	113	G	N1-C6-O6	6.87	124.02	119.90
1	A	758	G	C2-N3-C4	-6.87	108.46	111.90
1	A	1066	C	N1-C2-O2	6.86	123.02	118.90
1	A	919	A	N1-C6-N6	6.86	122.71	118.60
1	A	1323	G	C2-N3-C4	-6.86	108.47	111.90
1	A	167	G	C5-C6-N1	6.85	114.92	111.50
1	A	90	U	C2-N1-C1'	-6.85	109.48	117.70
1	A	700	G	N3-C2-N2	6.85	124.69	119.90
1	A	830	G	N1-C2-N3	6.85	128.01	123.90
1	A	787	A	C2-N3-C4	-6.85	107.18	110.60
1	A	1336	C	N3-C4-C5	-6.84	119.16	121.90
1	A	357	G	C4-C5-N7	-6.84	108.06	110.80
1	A	741	G	C4-N9-C1'	-6.84	117.61	126.50
1	A	852	G	C2-N3-C4	-6.84	108.48	111.90
24	a	39	G	C5-C6-O6	-6.84	124.50	128.60
1	A	729	A	C6-C5-N7	-6.83	127.52	132.30
1	A	884	U	N3-C2-O2	-6.83	117.42	122.20
1	A	1202	G	N3-C4-C5	-6.83	125.19	128.60
1	A	874	G	C6-C5-N7	-6.83	126.31	130.40
1	A	857	C	C6-N1-C2	6.82	123.03	120.30
1	A	881	G	N9-C4-C5	-6.82	102.67	105.40
1	A	104	G	C2-N3-C4	-6.82	108.49	111.90
1	A	188	C	N3-C4-C5	-6.82	119.17	121.90
1	A	1178	G	C8-N9-C4	-6.81	103.68	106.40
1	A	398	C	N3-C4-C5	6.81	124.62	121.90
1	A	1200	C	C2-N3-C4	6.80	123.30	119.90
1	A	1337	G	C5-C6-N1	-6.80	108.10	111.50
1	A	1338	G	N1-C6-O6	-6.79	115.83	119.90
1	A	193	C	C5-C6-N1	-6.78	117.61	121.00
25	b	3	U	N1-C2-O2	6.78	127.55	122.80
1	A	644	G	N3-C2-N2	6.78	124.64	119.90
1	A	1292	U	N3-C2-O2	6.78	126.94	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	39	G	N9-C4-C5	-6.78	102.69	105.40
1	A	947	G	C4-C5-N7	6.77	113.51	110.80
1	A	788	U	N1-C2-O2	-6.77	118.06	122.80
1	A	1310	G	N3-C4-N9	6.77	130.06	126.00
1	A	1343	G	C6-C5-N7	-6.77	126.34	130.40
1	A	1447	G	C4-C5-N7	6.77	113.51	110.80
1	A	677	U	N1-C2-N3	6.76	118.96	114.90
1	A	168	G	C5-C6-N1	-6.76	108.12	111.50
1	A	765	G	N1-C6-O6	6.75	123.95	119.90
1	A	285	G	N3-C4-C5	6.75	131.98	128.60
1	A	706	A	C2-N3-C4	-6.75	107.22	110.60
1	A	1195	C	N3-C4-N4	6.75	122.72	118.00
1	A	1249	C	C6-N1-C2	-6.75	117.60	120.30
1	A	133	U	C5-C4-O4	6.75	129.95	125.90
1	A	1202	G	N9-C4-C5	6.75	108.10	105.40
1	A	677	U	N3-C2-O2	-6.74	117.48	122.20
1	A	973	G	C8-N9-C4	6.74	109.10	106.40
1	A	1054	C	C2-N3-C4	6.74	123.27	119.90
1	A	32	A	N3-C4-C5	-6.73	122.09	126.80
1	A	563	A	N1-C6-N6	-6.73	114.56	118.60
1	A	27	G	C5-N7-C8	-6.73	100.94	104.30
1	A	1338	G	N9-C4-C5	6.72	108.09	105.40
1	A	383	A	N9-C4-C5	6.72	108.49	105.80
1	A	1329	A	C5-C6-N6	-6.71	118.33	123.70
1	A	400	C	N3-C4-N4	-6.71	113.30	118.00
1	A	662	G	N1-C6-O6	6.71	123.92	119.90
17	Q	63	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	73	C	C5-C6-N1	6.70	124.35	121.00
1	A	644	G	N1-C2-N2	-6.70	110.17	116.20
1	A	964	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1066	C	N1-C2-N3	-6.70	114.51	119.20
1	A	623	C	C5-C6-N1	-6.70	117.65	121.00
1	A	157	G	N1-C6-O6	6.69	123.92	119.90
1	A	615	C	C6-N1-C2	-6.69	117.62	120.30
1	A	824	C	C5-C6-N1	-6.68	117.66	121.00
1	A	1442	G	C4-N9-C1'	6.68	135.18	126.50
1	A	762	C	N3-C4-C5	6.68	124.57	121.90
1	A	64	G	N1-C6-O6	6.67	123.91	119.90
1	A	885	G	N1-C6-O6	6.67	123.90	119.90
1	A	275	G	N9-C4-C5	-6.67	102.73	105.40
24	a	39	G	C4-C5-N7	6.67	113.47	110.80
1	A	1447	G	C5-C6-O6	-6.67	124.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	G	N7-C8-N9	6.66	116.43	113.10
1	A	747	C	C6-N1-C2	6.66	122.96	120.30
1	A	975	A	N9-C4-C5	-6.66	103.14	105.80
1	A	285	G	C2-N3-C4	-6.66	108.57	111.90
1	A	586	C	C5-C6-N1	-6.66	117.67	121.00
1	A	687	A	P-O3'-C3'	6.66	127.69	119.70
1	A	1077	G	C6-C5-N7	-6.66	126.41	130.40
1	A	28	G	N9-C4-C5	6.65	108.06	105.40
1	A	1405	G	N3-C4-C5	6.65	131.93	128.60
1	A	729	A	N7-C8-N9	6.65	117.12	113.80
1	A	16	A	C2-N3-C4	-6.64	107.28	110.60
1	A	1234	C	N1-C2-N3	-6.64	114.55	119.20
1	A	14	U	C6-N1-C2	-6.64	117.02	121.00
1	A	275	G	C8-N9-C1'	-6.64	118.37	127.00
1	A	795	C	N3-C4-C5	-6.64	119.24	121.90
1	A	782	A	N1-C2-N3	6.64	132.62	129.30
1	A	18	C	C6-N1-C2	6.64	122.95	120.30
1	A	109	A	N9-C4-C5	6.64	108.45	105.80
1	A	828	A	C5-N7-C8	-6.64	100.58	103.90
1	A	1282	C	C6-N1-C2	-6.63	117.65	120.30
1	A	171	A	N1-C6-N6	-6.62	114.63	118.60
1	A	873	A	N7-C8-N9	6.62	117.11	113.80
1	A	247	G	C8-N9-C4	6.62	109.05	106.40
1	A	873	A	N3-C4-C5	-6.62	122.17	126.80
1	A	117	G	N1-C2-N3	6.61	127.87	123.90
1	A	529	G	N3-C4-N9	6.61	129.97	126.00
1	A	1483	A	N1-C6-N6	-6.61	114.63	118.60
17	Q	9	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	275	G	C8-N9-C4	6.60	109.04	106.40
1	A	47	C	N3-C4-C5	6.59	124.54	121.90
1	A	700	G	N9-C4-C5	-6.59	102.76	105.40
1	A	1073	U	C5-C6-N1	-6.59	119.41	122.70
1	A	1107	C	C5-C6-N1	6.59	124.29	121.00
1	A	818	G	N3-C2-N2	-6.58	115.29	119.90
1	A	1226	C	C6-N1-C2	6.58	122.93	120.30
1	A	529	G	N3-C4-C5	-6.58	125.31	128.60
1	A	934	C	N1-C2-O2	6.58	122.85	118.90
1	A	784	C	C6-N1-C2	-6.58	117.67	120.30
1	A	824	C	C2-N1-C1'	-6.57	111.57	118.80
1	A	130	A	C2-N3-C4	-6.57	107.31	110.60
1	A	620	C	N1-C2-O2	6.57	122.84	118.90
1	A	1322	C	N3-C4-N4	6.57	122.60	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	G	N1-C2-N2	6.57	122.11	116.20
1	A	1079	G	N7-C8-N9	6.57	116.38	113.10
1	A	449	C	N3-C4-N4	6.56	122.59	118.00
1	A	543	C	C6-N1-C2	-6.56	117.67	120.30
1	A	644	G	C5-N7-C8	-6.56	101.02	104.30
1	A	7	G	N3-C4-N9	6.56	129.94	126.00
1	A	818	G	C5-C6-N1	-6.56	108.22	111.50
1	A	559	A	N1-C2-N3	6.56	132.58	129.30
1	A	563	A	C2-N3-C4	6.56	113.88	110.60
1	A	1227	A	C4-C5-N7	6.56	113.98	110.70
1	A	1227	A	C2-N3-C4	-6.56	107.32	110.60
1	A	521	G	N1-C6-O6	-6.56	115.97	119.90
1	A	784	C	N3-C4-C5	-6.56	119.28	121.90
1	A	1524	C	N3-C4-N4	6.55	122.59	118.00
1	A	734	G	N1-C6-O6	6.55	123.83	119.90
1	A	365	U	C5-C4-O4	-6.55	121.97	125.90
1	A	251	G	N3-C4-N9	6.55	129.93	126.00
1	A	676	A	C8-N9-C4	6.55	108.42	105.80
1	A	525	C	N3-C2-O2	6.55	126.48	121.90
1	A	1094	G	N9-C4-C5	-6.55	102.78	105.40
1	A	170	U	C5-C6-N1	-6.54	119.43	122.70
1	A	265	G	C2-N3-C4	-6.54	108.63	111.90
1	A	1033	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1414	U	C5-C6-N1	-6.54	119.43	122.70
1	A	403	C	C5-C6-N1	-6.54	117.73	121.00
1	A	1500	A	N9-C4-C5	6.54	108.42	105.80
1	A	620	C	C6-N1-C2	6.53	122.91	120.30
1	A	854	G	C6-C5-N7	-6.53	126.48	130.40
1	A	1249	C	N3-C4-C5	-6.53	119.29	121.90
1	A	1341	U	C2-N1-C1'	-6.53	109.86	117.70
1	A	372	C	C6-N1-C1'	-6.53	112.97	120.80
1	A	1058	G	N7-C8-N9	-6.53	109.84	113.10
1	A	971	G	C5-C6-N1	-6.52	108.24	111.50
1	A	32	A	N3-C4-N9	6.52	132.62	127.40
1	A	770	C	C2-N3-C4	-6.52	116.64	119.90
1	A	742	G	N3-C4-N9	-6.52	122.09	126.00
1	A	859	A	N9-C4-C5	-6.51	103.19	105.80
1	A	1060	C	C2-N1-C1'	6.51	125.97	118.80
1	A	745	C	N3-C4-C5	6.51	124.50	121.90
1	A	1502	A	C4-C5-N7	6.51	113.96	110.70
1	A	885	G	C5-C6-N1	-6.51	108.25	111.50
1	A	365	U	C6-N1-C1'	-6.51	112.09	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	A	C5-N7-C8	-6.51	100.65	103.90
1	A	651	C	N3-C2-O2	6.51	126.45	121.90
1	A	889	A	N1-C2-N3	6.50	132.55	129.30
1	A	918	A	C6-N1-C2	-6.50	114.70	118.60
1	A	698	G	C4-C5-C6	6.50	122.70	118.80
1	A	229	U	N1-C2-O2	-6.50	118.25	122.80
1	A	1084	G	C6-N1-C2	-6.49	121.20	125.10
1	A	1051	C	N3-C4-C5	-6.49	119.30	121.90
1	A	1390	U	C4-C5-C6	6.48	123.59	119.70
1	A	963	G	C5-C6-N1	-6.48	108.26	111.50
1	A	268	C	C6-N1-C2	6.48	122.89	120.30
1	A	1053	G	C5-N7-C8	6.47	107.54	104.30
1	A	534	U	N3-C2-O2	6.47	126.73	122.20
1	A	760	G	C4-N9-C1'	6.47	134.91	126.50
1	A	111	G	N3-C4-C5	6.46	131.83	128.60
1	A	774	G	N9-C4-C5	-6.46	102.81	105.40
1	A	13	U	N3-C4-O4	6.46	123.92	119.40
1	A	181	G	N3-C4-C5	-6.46	125.37	128.60
1	A	276	G	N1-C6-O6	-6.46	116.03	119.90
1	A	1341	U	N3-C4-O4	-6.46	114.88	119.40
1	A	725	G	C5-C6-N1	6.45	114.73	111.50
1	A	693	G	C5-C6-O6	-6.45	124.73	128.60
1	A	1301	U	N3-C4-C5	-6.45	110.73	114.60
1	A	597	G	N1-C2-N2	-6.44	110.40	116.20
1	A	108	G	N1-C6-O6	6.44	123.76	119.90
1	A	258	G	N1-C6-O6	6.44	123.76	119.90
1	A	644	G	C4-N9-C1'	6.43	134.87	126.50
1	A	77	G	N3-C4-N9	6.43	129.86	126.00
1	A	761	G	C2-N3-C4	-6.43	108.69	111.90
1	A	867	G	N9-C4-C5	-6.42	102.83	105.40
1	A	867	G	N1-C2-N3	6.42	127.75	123.90
1	A	654	G	N1-C2-N2	-6.42	110.42	116.20
1	A	798	G	N1-C2-N2	6.42	121.98	116.20
1	A	825	G	N7-C8-N9	-6.42	109.89	113.10
1	A	561	U	N3-C4-O4	6.42	123.89	119.40
1	A	789	U	C5-C6-N1	6.42	125.91	122.70
1	A	248	C	C2-N3-C4	-6.41	116.69	119.90
1	A	1350	A	C8-N9-C4	-6.41	103.23	105.80
1	A	204	U	C2-N1-C1'	6.41	125.39	117.70
1	A	522	C	N3-C4-N4	-6.41	113.51	118.00
1	A	15	G	N1-C6-O6	6.41	123.74	119.90
1	A	1199	U	C6-N1-C2	-6.40	117.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1390	U	C6-N1-C2	-6.40	117.16	121.00
1	A	92	C	C6-N1-C1'	-6.39	113.13	120.80
1	A	1433	A	N1-C2-N3	6.39	132.50	129.30
1	A	635	G	N9-C4-C5	-6.39	102.84	105.40
1	A	807	A	N7-C8-N9	-6.39	110.61	113.80
1	A	1092	A	C5-N7-C8	-6.39	100.71	103.90
1	A	868	C	N3-C4-N4	6.39	122.47	118.00
1	A	870	U	C5-C6-N1	-6.38	119.51	122.70
1	A	721	G	N1-C2-N2	-6.38	110.46	116.20
1	A	1183	A	N1-C6-N6	6.38	122.43	118.60
1	A	390	C	N3-C4-N4	6.38	122.47	118.00
1	A	1099	G	C4-C5-N7	-6.38	108.25	110.80
1	A	32	A	C4-C5-C6	6.38	120.19	117.00
1	A	90	U	C6-N1-C1'	6.38	130.13	121.20
1	A	679	C	N1-C2-O2	-6.38	115.07	118.90
1	A	297	G	C8-N9-C4	-6.38	103.85	106.40
1	A	866	C	N1-C2-N3	6.37	123.66	119.20
1	A	1340	A	C2-N3-C4	-6.37	107.42	110.60
1	A	123	C	N3-C4-C5	-6.37	119.35	121.90
1	A	928	G	C6-C5-N7	-6.37	126.58	130.40
1	A	9	G	C4-C5-N7	6.36	113.34	110.80
1	A	129	U	N1-C2-N3	6.36	118.72	114.90
1	A	618	C	C6-N1-C2	6.36	122.84	120.30
1	A	946	A	N9-C4-C5	6.36	108.34	105.80
1	A	1073	U	C6-N1-C2	6.36	124.82	121.00
1	A	1107	C	N3-C4-C5	-6.36	119.36	121.90
1	A	447	G	N9-C4-C5	-6.36	102.86	105.40
1	A	77	G	C4-C5-N7	6.36	113.34	110.80
1	A	524	G	C5-C6-N1	-6.36	108.32	111.50
1	A	789	U	C6-N1-C2	-6.35	117.19	121.00
1	A	902	G	C8-N9-C4	6.35	108.94	106.40
1	A	639	G	C5-C6-O6	-6.35	124.79	128.60
1	A	269	C	C4-C5-C6	6.34	120.57	117.40
1	A	703	G	C5-N7-C8	6.34	107.47	104.30
1	A	230	G	C4-N9-C1'	6.34	134.74	126.50
1	A	1237	C	C4-C5-C6	6.33	120.57	117.40
1	A	960	U	N1-C2-O2	6.33	127.23	122.80
1	A	28	G	C4-C5-N7	-6.33	108.27	110.80
1	A	671	G	C5-C6-N1	-6.33	108.34	111.50
1	A	839	U	N1-C2-O2	6.33	127.23	122.80
1	A	579	G	C5-N7-C8	-6.32	101.14	104.30
1	A	874	G	C4-C5-N7	6.32	113.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	194	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	721	G	C5-C6-N1	-6.32	108.34	111.50
9	I	47	LEU	CA-CB-CG	-6.32	100.77	115.30
1	A	924	C	N3-C2-O2	6.32	126.32	121.90
1	A	407	G	C2-N3-C4	-6.31	108.75	111.90
1	A	962	C	C6-N1-C2	6.31	122.82	120.30
1	A	616	G	C5-C6-N1	-6.31	108.35	111.50
1	A	741	G	N3-C4-C5	6.31	131.75	128.60
1	A	154	C	C5-C4-N4	-6.30	115.79	120.20
1	A	830	G	N1-C6-O6	6.30	123.68	119.90
1	A	881	G	N3-C4-N9	6.30	129.78	126.00
1	A	1487	G	C8-N9-C4	-6.30	103.88	106.40
1	A	1497	G	N3-C4-N9	6.29	129.78	126.00
1	A	372	C	C6-N1-C2	6.29	122.82	120.30
1	A	428	G	C8-N9-C4	-6.29	103.88	106.40
1	A	91	C	N3-C4-N4	6.29	122.40	118.00
1	A	342	C	C6-N1-C2	-6.29	117.79	120.30
1	A	1279	A	N7-C8-N9	6.29	116.94	113.80
1	A	1205	U	C2-N1-C1'	6.28	125.24	117.70
1	A	597	G	C6-C5-N7	-6.28	126.63	130.40
1	A	1530	G	C5-C6-N1	-6.28	108.36	111.50
1	A	77	G	N9-C4-C5	-6.28	102.89	105.40
1	A	557	G	N9-C4-C5	6.28	107.91	105.40
1	A	810	C	C5-C4-N4	-6.28	115.81	120.20
1	A	1389	C	C6-N1-C2	6.28	122.81	120.30
1	A	1350	A	N7-C8-N9	6.27	116.94	113.80
1	A	250	A	C8-N9-C4	6.27	108.31	105.80
1	A	297	G	C4-N9-C1'	6.27	134.65	126.50
1	A	721	G	N3-C4-C5	-6.27	125.46	128.60
1	A	774	G	C4-C5-N7	6.27	113.31	110.80
1	A	1074	G	C2-N3-C4	-6.27	108.77	111.90
1	A	1362	C	C6-N1-C2	-6.27	117.79	120.30
1	A	91	C	C5-C4-N4	-6.26	115.81	120.20
1	A	691	G	N7-C8-N9	6.26	116.23	113.10
1	A	788	U	C2-N3-C4	6.26	130.76	127.00
1	A	927	G	N1-C6-O6	6.26	123.66	119.90
1	A	285	G	C5-C6-N1	-6.26	108.37	111.50
1	A	246	A	N1-C2-N3	-6.26	126.17	129.30
1	A	1342	C	N1-C2-O2	-6.26	115.15	118.90
1	A	125	U	N1-C2-N3	6.25	118.65	114.90
1	A	1531	A	N7-C8-N9	6.25	116.92	113.80
1	A	637	G	N1-C6-O6	6.25	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	C	C2-N1-C1'	6.24	125.67	118.80
1	A	795	C	C6-N1-C2	6.24	122.80	120.30
1	A	252	U	C5-C6-N1	-6.24	119.58	122.70
1	A	1327	C	C4-C5-C6	6.24	120.52	117.40
1	A	32	A	C5-C6-N6	-6.23	118.71	123.70
1	A	947	G	N9-C4-C5	-6.23	102.91	105.40
1	A	1068	G	N3-C4-C5	-6.23	125.49	128.60
1	A	1281	U	N1-C2-N3	6.23	118.64	114.90
1	A	981	U	C5-C6-N1	6.22	125.81	122.70
1	A	665	A	C5-N7-C8	-6.22	100.79	103.90
1	A	969	A	N1-C6-N6	6.22	122.33	118.60
1	A	1310	G	C4-N9-C1'	6.22	134.59	126.50
1	A	598	U	N1-C2-O2	-6.22	118.45	122.80
1	A	260	G	N1-C2-N3	6.22	127.63	123.90
1	A	928	G	C4-C5-N7	6.21	113.28	110.80
1	A	1329	A	C6-C5-N7	-6.21	127.95	132.30
1	A	162	A	C8-N9-C4	-6.21	103.32	105.80
1	A	1157	A	C5-C6-N6	6.21	128.67	123.70
1	A	1228	C	C6-N1-C1'	-6.21	113.35	120.80
1	A	1338	G	C4-C5-N7	-6.21	108.32	110.80
1	A	199	G	C2-N3-C4	-6.20	108.80	111.90
1	A	828	A	N1-C6-N6	6.20	122.32	118.60
1	A	1178	G	N9-C4-C5	6.20	107.88	105.40
1	A	1512	U	C4-C5-C6	6.19	123.42	119.70
1	A	201	C	C2-N1-C1'	6.19	125.61	118.80
1	A	1157	A	N1-C6-N6	-6.19	114.89	118.60
1	A	232	G	C5-N7-C8	-6.18	101.21	104.30
1	A	400	C	N3-C2-O2	-6.18	117.57	121.90
1	A	7	G	C8-N9-C1'	-6.18	118.97	127.00
1	A	242	C	C5-C6-N1	-6.18	117.91	121.00
1	A	246	A	N7-C8-N9	-6.18	110.71	113.80
1	A	50	A	C4-C5-C6	-6.18	113.91	117.00
1	A	640	A	N1-C2-N3	6.17	132.39	129.30
1	A	884	U	N1-C2-O2	6.17	127.12	122.80
1	A	558	G	C4-C5-N7	6.16	113.27	110.80
1	A	887	G	N1-C2-N3	6.16	127.60	123.90
1	A	1066	C	C2-N1-C1'	6.16	125.58	118.80
1	A	859	A	C8-N9-C4	6.16	108.27	105.80
1	A	862	C	N3-C4-C5	6.16	124.36	121.90
1	A	673	G	C5-C6-O6	-6.16	124.90	128.60
1	A	1209	C	C6-N1-C2	-6.16	117.84	120.30
1	A	912	C	C4-C5-C6	-6.15	114.32	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190(E)	U	C2-N3-C4	-6.15	123.31	127.00
1	A	1064	G	N3-C2-N2	-6.15	115.59	119.90
1	A	1231	G	N3-C4-N9	6.15	129.69	126.00
24	a	39	G	C8-N9-C4	6.15	108.86	106.40
1	A	284	G	C6-C5-N7	-6.15	126.71	130.40
1	A	1235	U	N1-C2-O2	-6.15	118.50	122.80
1	A	898	G	N1-C2-N3	6.14	127.59	123.90
1	A	848	C	C5-C6-N1	6.14	124.07	121.00
1	A	1442	G	N3-C4-C5	-6.14	125.53	128.60
1	A	285	G	N1-C6-O6	6.14	123.58	119.90
1	A	897	C	N3-C4-C5	6.13	124.35	121.90
1	A	1103	C	C5-C6-N1	-6.13	117.93	121.00
1	A	1487	G	N9-C4-C5	6.13	107.85	105.40
1	A	109	A	C8-N9-C4	-6.13	103.35	105.80
1	A	181	G	C4-C5-C6	6.13	122.48	118.80
1	A	755	G	N1-C6-O6	6.13	123.58	119.90
1	A	900	A	C2-N3-C4	-6.13	107.54	110.60
1	A	257	G	C8-N9-C4	6.12	108.85	106.40
1	A	1493[A]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	1493[B]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	265	G	N9-C4-C5	-6.12	102.95	105.40
1	A	926	G	N3-C4-N9	6.12	129.67	126.00
1	A	970	C	N3-C2-O2	-6.12	117.62	121.90
1	A	1391	U	C5-C6-N1	-6.12	119.64	122.70
1	A	1500	A	C6-N1-C2	-6.12	114.93	118.60
1	A	524	G	N1-C6-O6	6.11	123.57	119.90
1	A	35	G	N1-C6-O6	6.11	123.56	119.90
1	A	1253	G	C6-C5-N7	-6.11	126.74	130.40
1	A	1300	G	N9-C4-C5	6.10	107.84	105.40
1	A	1487	G	C6-N1-C2	-6.10	121.44	125.10
1	A	540	G	N1-C6-O6	6.10	123.56	119.90
1	A	230	G	N1-C2-N2	-6.10	110.71	116.20
1	A	373	A	C5-C6-N6	6.10	128.58	123.70
1	A	1058	G	C6-C5-N7	6.10	134.06	130.40
1	A	1483	A	C5-N7-C8	6.09	106.95	103.90
1	A	782	A	N1-C6-N6	-6.09	114.94	118.60
1	A	130	A	C5-N7-C8	-6.09	100.86	103.90
1	A	976	G	C2-N3-C4	-6.09	108.86	111.90
1	A	910	C	C2-N3-C4	-6.08	116.86	119.90
1	A	1531	A	C5-C6-N6	-6.08	118.83	123.70
1	A	144	G	C6-C5-N7	-6.08	126.75	130.40
1	A	335	C	C5-C6-N1	-6.08	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	C	N3-C4-C5	6.07	124.33	121.90
1	A	768	A	N7-C8-N9	-6.07	110.77	113.80
8	H	38	ILE	CB-CA-C	-6.07	99.46	111.60
1	A	115	G	C5-C6-N1	6.07	114.53	111.50
1	A	654	G	N1-C2-N3	6.07	127.54	123.90
1	A	174	C	C5-C4-N4	-6.06	115.95	120.20
1	A	733	A	C2-N3-C4	-6.06	107.57	110.60
1	A	833	U	N3-C2-O2	-6.05	117.96	122.20
1	A	812	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1488	G	C5-N7-C8	6.05	107.32	104.30
1	A	127	G	N3-C4-C5	6.04	131.62	128.60
1	A	741	G	C4-C5-N7	-6.04	108.38	110.80
1	A	631	G	C4-N9-C1'	6.04	134.35	126.50
1	A	586	C	N3-C4-C5	6.03	124.31	121.90
1	A	1502	A	C6-C5-N7	-6.03	128.08	132.30
1	A	1237	C	N3-C4-C5	-6.03	119.49	121.90
1	A	742	G	N1-C2-N2	6.03	121.63	116.20
1	A	1079	G	N9-C4-C5	6.03	107.81	105.40
1	A	263	A	N1-C6-N6	-6.03	114.98	118.60
1	A	78	G	N1-C6-O6	6.03	123.52	119.90
1	A	1029	C	C6-N1-C2	-6.03	117.89	120.30
8	H	12	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	300	A	C4-C5-C6	6.02	120.01	117.00
1	A	868	C	N3-C2-O2	6.02	126.12	121.90
1	A	260	G	C4-C5-C6	6.02	122.41	118.80
1	A	363	A	C2-N3-C4	-6.02	107.59	110.60
1	A	1487	G	C4-N9-C1'	6.02	134.32	126.50
1	A	572	A	C6-N1-C2	-6.01	114.99	118.60
1	A	1505	G	N3-C2-N2	-6.01	115.69	119.90
1	A	1399	C	C6-N1-C2	-6.00	117.90	120.30
1	A	447	G	C6-C5-N7	-6.00	126.80	130.40
1	A	570	G	N9-C4-C5	6.00	107.80	105.40
1	A	1497	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	852	G	C8-N9-C4	6.00	108.80	106.40
1	A	1337	G	N1-C6-O6	5.99	123.50	119.90
1	A	854	G	C2-N3-C4	-5.99	108.91	111.90
1	A	873	A	N9-C4-C5	5.99	108.19	105.80
1	A	1084	G	C5-C6-O6	5.98	132.19	128.60
1	A	79	G	N7-C8-N9	5.98	116.09	113.10
1	A	145	G	N1-C6-O6	5.97	123.48	119.90
1	A	21	G	N3-C4-N9	5.97	129.58	126.00
1	A	607	A	C5-C6-N1	-5.97	114.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	893	C	C2-N3-C4	5.97	122.89	119.90
1	A	896	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1491	G	N3-C2-N2	-5.97	115.72	119.90
1	A	374	A	C8-N9-C4	5.97	108.19	105.80
1	A	1074	G	C4-C5-C6	5.97	122.38	118.80
1	A	1530	G	N3-C2-N2	-5.97	115.72	119.90
1	A	1325	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1353	G	C2-N3-C4	5.96	114.88	111.90
1	A	117	G	C4-C5-N7	5.96	113.19	110.80
1	A	944	G	N1-C6-O6	-5.96	116.32	119.90
1	A	259	G	C4-C5-C6	5.96	122.38	118.80
1	A	786	G	N1-C6-O6	5.96	123.47	119.90
1	A	1531	A	C8-N9-C4	-5.96	103.42	105.80
1	A	768	A	N1-C6-N6	5.96	122.17	118.60
1	A	774	G	C5-C6-O6	-5.95	125.03	128.60
1	A	856	C	C4-C5-C6	5.95	120.38	117.40
1	A	1094	G	C6-C5-N7	-5.95	126.83	130.40
1	A	349	A	N1-C6-N6	-5.95	115.03	118.60
1	A	651	C	N3-C4-C5	5.95	124.28	121.90
1	A	712	A	N1-C2-N3	5.95	132.27	129.30
1	A	767	A	N9-C4-C5	5.95	108.18	105.80
1	A	946	A	C5-C6-N1	5.95	120.67	117.70
1	A	1531	A	C5-N7-C8	-5.95	100.93	103.90
1	A	38	G	C8-N9-C1'	5.94	134.72	127.00
1	A	170	U	N1-C2-O2	-5.94	118.64	122.80
1	A	1089	G	C8-N9-C4	-5.94	104.03	106.40
1	A	1439	C	N3-C4-C5	-5.94	119.53	121.90
1	A	1307	U	N1-C2-O2	5.94	126.95	122.80
17	Q	31	LEU	CA-CB-CG	-5.94	101.65	115.30
1	A	15	G	N9-C4-C5	-5.93	103.03	105.40
1	A	250	A	N1-C6-N6	5.93	122.16	118.60
1	A	654	G	C2-N3-C4	-5.93	108.93	111.90
1	A	853	G	N3-C4-N9	5.93	129.56	126.00
1	A	807	A	C8-N9-C4	5.93	108.17	105.80
8	H	135	CYS	CA-CB-SG	-5.93	103.32	114.00
1	A	1234	C	N3-C4-C5	5.93	124.27	121.90
1	A	265	G	C6-C5-N7	-5.93	126.84	130.40
1	A	898	G	C2-N3-C4	-5.93	108.94	111.90
1	A	190(K)	G	C8-N9-C4	5.92	108.77	106.40
1	A	542	G	N1-C6-O6	-5.92	116.35	119.90
1	A	774	G	C6-C5-N7	-5.92	126.85	130.40
1	A	791	G	C5-C6-N1	-5.92	108.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	718	G	C5-C6-O6	-5.92	125.05	128.60
1	A	920	U	N1-C2-N3	5.92	118.45	114.90
1	A	618	C	N3-C4-N4	-5.92	113.86	118.00
1	A	674	G	C2-N3-C4	-5.92	108.94	111.90
1	A	1529	G	N3-C2-N2	-5.91	115.76	119.90
1	A	711	G	C2-N3-C4	-5.91	108.94	111.90
1	A	1084	G	N1-C2-N3	5.91	127.45	123.90
1	A	136	C	C6-N1-C2	-5.91	117.94	120.30
1	A	931	C	C5-C6-N1	-5.91	118.05	121.00
1	A	1335	C	N1-C2-N3	-5.91	115.06	119.20
1	A	1507	A	N1-C2-N3	5.91	132.25	129.30
1	A	38	G	C4-N9-C1'	-5.91	118.82	126.50
1	A	144	G	N3-C2-N2	-5.91	115.77	119.90
1	A	553	A	C8-N9-C4	5.91	108.16	105.80
1	A	1300	G	C4-C5-N7	-5.91	108.44	110.80
1	A	328	C	P-O3'-C3'	5.90	126.78	119.70
1	A	317	G	C2-N3-C4	-5.90	108.95	111.90
1	A	1529	G	N1-C2-N3	5.90	127.44	123.90
1	A	1530	G	N1-C2-N2	5.90	121.51	116.20
24	a	37	A	C2-N3-C4	-5.90	107.65	110.60
2	B	7	VAL	N-CA-C	5.90	126.93	111.00
1	A	447	G	C4-N9-C1'	5.90	134.17	126.50
1	A	610	G	N1-C6-O6	-5.90	116.36	119.90
1	A	799	G	C4-C5-N7	5.90	113.16	110.80
1	A	1301	U	N3-C4-O4	5.90	123.53	119.40
1	A	924	C	N3-C4-C5	-5.89	119.54	121.90
1	A	104	G	C5-C6-O6	-5.89	125.06	128.60
1	A	854	G	C4-N9-C1'	5.89	134.15	126.50
1	A	1214	C	C2-N1-C1'	5.88	125.27	118.80
24	a	37	A	C5-C6-N1	-5.88	114.76	117.70
1	A	1099	G	C8-N9-C4	-5.88	104.05	106.40
8	H	136	GLU	N-CA-C	-5.88	95.13	111.00
1	A	284	G	C2-N3-C4	-5.88	108.96	111.90
1	A	686	U	C5-C6-N1	-5.88	119.76	122.70
1	A	1534	C	N1-C2-O2	5.88	122.42	118.90
1	A	1530	G	C4-N9-C1'	-5.87	118.86	126.50
1	A	650	G	N1-C6-O6	5.87	123.42	119.90
1	A	963	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1253	G	N1-C6-O6	5.87	123.42	119.90
1	A	1467	G	C8-N9-C4	-5.87	104.05	106.40
1	A	90	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1502	A	N3-C4-C5	5.87	130.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	G	N1-C6-O6	5.86	123.42	119.90
1	A	400	C	C6-N1-C2	5.86	122.65	120.30
1	A	53	A	C6-N1-C2	-5.86	115.08	118.60
1	A	449	C	C2-N1-C1'	5.86	125.25	118.80
1	A	599	C	C2-N3-C4	-5.86	116.97	119.90
1	A	875	C	C2-N3-C4	-5.86	116.97	119.90
1	A	552	U	N3-C4-O4	-5.86	115.30	119.40
1	A	880	C	C6-N1-C2	5.85	122.64	120.30
1	A	1062	U	C5-C4-O4	5.85	129.41	125.90
1	A	1452	C	C6-N1-C2	5.85	122.64	120.30
1	A	658	G	N1-C2-N3	5.85	127.41	123.90
1	A	1310	G	N1-C2-N2	-5.85	110.93	116.20
1	A	1064	G	C6-N1-C2	-5.85	121.59	125.10
1	A	251	G	N3-C4-C5	-5.85	125.68	128.60
1	A	1414	U	C4-C5-C6	5.85	123.21	119.70
1	A	607	A	C6-N1-C2	5.84	122.11	118.60
1	A	1108	G	C4-N9-C1'	5.84	134.10	126.50
1	A	1527	C	N3-C4-N4	5.84	122.09	118.00
1	A	579	G	C6-C5-N7	-5.84	126.89	130.40
1	A	975	A	C6-N1-C2	5.84	122.10	118.60
1	A	796	C	C4-C5-C6	5.84	120.32	117.40
1	A	481	G	C4-N9-C1'	5.84	134.09	126.50
1	A	741	G	C6-C5-N7	5.84	133.90	130.40
1	A	1335	C	C5-C4-N4	-5.84	116.11	120.20
1	A	1483	A	C2-N3-C4	5.84	113.52	110.60
20	T	13	LEU	CB-CA-C	-5.84	99.11	110.20
1	A	1438	G	C8-N9-C4	5.83	108.73	106.40
1	A	1523	G	N3-C2-N2	-5.83	115.82	119.90
1	A	1487	G	C4-C5-C6	5.83	122.30	118.80
1	A	1190	G	C4-C5-C6	5.82	122.30	118.80
1	A	864	A	C4-C5-N7	-5.82	107.79	110.70
1	A	656	C	N3-C4-C5	5.82	124.23	121.90
1	A	852	G	N9-C4-C5	-5.82	103.07	105.40
1	A	190(G)	G	C4-C5-C6	5.82	122.29	118.80
1	A	679	C	C5-C6-N1	-5.82	118.09	121.00
1	A	1249	C	C5-C6-N1	5.82	123.91	121.00
1	A	1482	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1510	U	N1-C2-O2	5.82	126.87	122.80
1	A	129	U	C5-C4-O4	5.82	129.39	125.90
1	A	865	A	C5-C6-N1	5.82	120.61	117.70
1	A	344	A	N7-C8-N9	5.81	116.71	113.80
1	A	693	G	C6-C5-N7	-5.81	126.91	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	G	N9-C4-C5	-5.81	103.08	105.40
1	A	854	G	N1-C2-N3	5.81	127.39	123.90
1	A	297	G	C5-C6-O6	5.80	132.08	128.60
1	A	707	C	C2-N1-C1'	-5.80	112.42	118.80
1	A	38	G	N3-C4-C5	5.80	131.50	128.60
1	A	235	C	C5-C6-N1	-5.80	118.10	121.00
1	A	242	C	C6-N1-C2	5.80	122.62	120.30
1	A	259	G	C5-C6-N1	-5.80	108.60	111.50
1	A	565	U	C6-N1-C2	5.80	124.48	121.00
1	A	676	A	N7-C8-N9	-5.80	110.90	113.80
1	A	925	G	N3-C4-C5	-5.80	125.70	128.60
1	A	860	A	N1-C2-N3	5.79	132.20	129.30
1	A	1200	C	N3-C4-N4	5.79	122.06	118.00
1	A	142	G	N3-C4-C5	-5.79	125.70	128.60
1	A	251	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	1303	C	N3-C4-N4	-5.79	113.95	118.00
1	A	925	G	N3-C4-N9	5.79	129.47	126.00
1	A	519	C	C6-N1-C2	5.78	122.61	120.30
1	A	944	G	N9-C4-C5	5.78	107.71	105.40
1	A	1281	U	C6-N1-C1'	5.78	129.29	121.20
1	A	597	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	760	G	C4-C5-C6	5.78	122.27	118.80
1	A	258	G	C2-N3-C4	-5.78	109.01	111.90
1	A	332	G	C4-C5-N7	5.78	113.11	110.80
1	A	566	G	N3-C4-N9	5.78	129.47	126.00
1	A	552	U	N1-C2-N3	5.77	118.36	114.90
1	A	644	G	N7-C8-N9	5.77	115.99	113.10
1	A	831	U	C5-C4-O4	5.77	129.36	125.90
1	A	629	G	N3-C4-C5	-5.77	125.72	128.60
1	A	716	A	C5-C6-N1	5.77	120.58	117.70
1	A	779	C	C2-N3-C4	-5.77	117.02	119.90
1	A	945	G	C4-C5-C6	-5.77	115.34	118.80
1	A	1153	C	C6-N1-C2	5.77	122.61	120.30
1	A	910	C	C5-C6-N1	-5.76	118.12	121.00
1	A	180	U	C5-C4-O4	-5.76	122.44	125.90
1	A	259	G	C8-N9-C4	-5.76	104.10	106.40
1	A	68	G	N7-C8-N9	-5.76	110.22	113.10
1	A	752	G	N1-C6-O6	5.76	123.35	119.90
1	A	1231	G	C4-N9-C1'	5.75	133.98	126.50
1	A	73	C	C2-N3-C4	5.75	122.78	119.90
1	A	618	C	C6-N1-C1'	5.75	127.70	120.80
1	A	414	A	N1-C2-N3	5.75	132.17	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	799	G	C5-C6-O6	-5.74	125.15	128.60
1	A	1227	A	N3-C4-C5	5.74	130.82	126.80
1	A	15	G	C8-N9-C4	5.74	108.70	106.40
1	A	1129	C	C5-C6-N1	5.74	123.87	121.00
1	A	130	A	N1-C6-N6	5.74	122.04	118.60
1	A	181	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	292	G	N1-C6-O6	5.74	123.34	119.90
1	A	725	G	C5-C6-O6	-5.73	125.16	128.60
1	A	251	G	N3-C2-N2	5.73	123.91	119.90
1	A	1373	G	C8-N9-C4	-5.73	104.11	106.40
1	A	265	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	637	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	1055	A	C2-N3-C4	5.73	113.46	110.60
1	A	50	A	N7-C8-N9	-5.73	110.94	113.80
1	A	911	U	C2-N1-C1'	-5.73	110.83	117.70
1	A	635	G	N1-C2-N2	-5.72	111.05	116.20
1	A	875	C	C5-C6-N1	-5.72	118.14	121.00
1	A	905	U	C4-C5-C6	5.72	123.13	119.70
1	A	154	C	C6-N1-C1'	-5.72	113.94	120.80
1	A	558	G	C6-C5-N7	-5.72	126.97	130.40
1	A	693	G	N9-C4-C5	-5.72	103.11	105.40
1	A	745	C	C2-N3-C4	-5.72	117.04	119.90
1	A	326	G	N3-C4-N9	-5.72	122.57	126.00
1	A	21	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	125	U	N3-C2-O2	-5.71	118.20	122.20
1	A	32	A	C6-C5-N7	-5.71	128.30	132.30
1	A	373	A	N1-C6-N6	-5.71	115.17	118.60
1	A	674	G	N1-C6-O6	5.71	123.32	119.90
1	A	698	G	C8-N9-C4	-5.71	104.12	106.40
1	A	1221	G	C5-C6-N1	-5.71	108.65	111.50
1	A	1531	A	C4-C5-N7	5.71	113.55	110.70
1	A	711	G	C5-N7-C8	-5.70	101.45	104.30
1	A	540	G	C5-C6-O6	-5.70	125.18	128.60
1	A	127	G	C5-C6-O6	-5.70	125.18	128.60
1	A	704	A	N7-C8-N9	5.70	116.65	113.80
1	A	963	G	N7-C8-N9	5.70	115.95	113.10
1	A	631	G	N7-C8-N9	5.70	115.95	113.10
1	A	779	C	C6-N1-C2	5.70	122.58	120.30
1	A	407	G	N3-C4-C5	5.70	131.45	128.60
1	A	1134	G	C8-N9-C4	-5.70	104.12	106.40
1	A	144	G	N3-C4-C5	5.70	131.45	128.60
1	A	232	G	C8-N9-C1'	-5.70	119.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	677	U	C6-N1-C2	-5.69	117.58	121.00
1	A	920	U	C6-N1-C2	-5.69	117.58	121.00
1	A	240	C	C6-N1-C2	5.69	122.58	120.30
1	A	279	A	C2-N3-C4	-5.69	107.75	110.60
1	A	1415	G	C8-N9-C4	5.69	108.68	106.40
1	A	1062	U	C6-N1-C2	-5.69	117.59	121.00
1	A	673	G	C4-C5-N7	5.68	113.07	110.80
1	A	856	C	N1-C2-N3	5.68	123.18	119.20
1	A	440	A	N1-C2-N3	5.68	132.14	129.30
1	A	1092	A	C8-N9-C1'	-5.68	117.48	127.70
1	A	91	C	C6-N1-C1'	-5.67	113.99	120.80
1	A	1084	G	N9-C4-C5	5.67	107.67	105.40
1	A	1329	A	N9-C4-C5	-5.67	103.53	105.80
1	A	1504	G	N3-C4-N9	5.67	129.40	126.00
1	A	753	A	C4-C5-N7	-5.67	107.86	110.70
1	A	858	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1364	U	C6-N1-C2	5.67	124.40	121.00
1	A	1310	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1381	U	C2-N1-C1'	5.66	124.50	117.70
1	A	204	U	C5-C6-N1	5.66	125.53	122.70
1	A	121	C	C6-N1-C2	5.66	122.56	120.30
1	A	1074	G	N1-C6-O6	5.66	123.30	119.90
15	O	77	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	1388	C	N1-C2-O2	-5.66	115.51	118.90
1	A	597	G	C4-N9-C1'	5.66	133.85	126.50
1	A	1074	G	C6-C5-N7	-5.66	127.01	130.40
1	A	1524	C	N1-C2-N3	5.66	123.16	119.20
1	A	1058	G	C4-C5-N7	-5.65	108.54	110.80
1	A	637	G	C6-C5-N7	-5.65	127.01	130.40
1	A	971	G	C2-N3-C4	-5.65	109.08	111.90
1	A	1143	G	C4-C5-N7	5.65	113.06	110.80
1	A	830	G	N3-C2-N2	-5.65	115.95	119.90
1	A	21	G	N9-C4-C5	-5.65	103.14	105.40
1	A	330	C	N1-C2-O2	-5.65	115.51	118.90
1	A	1394	A	C5-C6-N1	5.64	120.52	117.70
1	A	1433	A	C6-N1-C2	-5.64	115.21	118.60
5	E	63	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	1442	G	N3-C4-N9	5.64	129.38	126.00
1	A	1505	G	C4-C5-N7	-5.64	108.55	110.80
1	A	902	G	N7-C8-N9	-5.64	110.28	113.10
1	A	1120	G	N3-C4-C5	-5.64	125.78	128.60
1	A	1286	A	C8-N9-C4	-5.63	103.55	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1438	G	C5-C6-O6	-5.63	125.22	128.60
1	A	111	G	C8-N9-C1'	5.63	134.32	127.00
1	A	393	A	C2-N3-C4	-5.62	107.79	110.60
1	A	1190	G	N3-C4-C5	-5.62	125.79	128.60
1	A	125	U	C4-C5-C6	5.62	123.07	119.70
1	A	435	C	N3-C4-C5	-5.62	119.65	121.90
1	A	933	G	C6-C5-N7	-5.62	127.03	130.40
1	A	1301	U	N1-C2-N3	5.62	118.27	114.90
1	A	1527	C	C2-N1-C1'	5.62	124.98	118.80
1	A	383	A	C8-N9-C4	-5.62	103.55	105.80
1	A	497	A	N1-C6-N6	-5.62	115.23	118.60
1	A	656	C	C5-C4-N4	-5.62	116.27	120.20
1	A	216	G	N1-C6-O6	-5.62	116.53	119.90
1	A	1077	G	C4-C5-C6	5.61	122.17	118.80
1	A	162	A	N1-C6-N6	-5.61	115.23	118.60
1	A	816	A	N7-C8-N9	-5.61	111.00	113.80
1	A	1531	A	C5-C6-N1	5.61	120.50	117.70
1	A	270	A	N1-C6-N6	5.61	121.96	118.60
1	A	190(G)	G	C6-C5-N7	-5.60	127.04	130.40
1	A	787	A	N7-C8-N9	5.60	116.60	113.80
1	A	588	G	C8-N9-C4	5.60	108.64	106.40
1	A	816	A	N3-C4-N9	-5.60	122.92	127.40
1	A	559	A	N7-C8-N9	5.60	116.60	113.80
1	A	1220	G	N1-C6-O6	5.60	123.26	119.90
1	A	1392	G	C4-C5-N7	5.60	113.04	110.80
1	A	21	G	N7-C8-N9	-5.59	110.30	113.10
1	A	120	A	N7-C8-N9	-5.59	111.00	113.80
1	A	1392	G	C4-N9-C1'	5.59	133.77	126.50
1	A	1343	G	C4-C5-N7	5.59	113.04	110.80
1	A	204	U	C6-N1-C1'	-5.59	113.38	121.20
24	a	39	G	N3-C4-C5	5.59	131.40	128.60
1	A	38	G	C5-C6-N1	-5.59	108.71	111.50
1	A	831	U	N3-C2-O2	-5.59	118.29	122.20
1	A	122	G	C2-N3-C4	-5.59	109.11	111.90
1	A	497	A	C4-C5-N7	-5.59	107.91	110.70
1	A	675	A	C2-N3-C4	-5.59	107.81	110.60
1	A	767	A	N1-C6-N6	-5.58	115.25	118.60
1	A	113	G	C6-C5-N7	-5.58	127.05	130.40
1	A	146	G	C5-C6-O6	-5.58	125.25	128.60
1	A	741	G	C8-N9-C1'	5.58	134.26	127.00
1	A	1186	G	N1-C6-O6	5.58	123.25	119.90
1	A	634	C	C5-C4-N4	5.58	124.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	G	C4-C5-C6	5.58	122.15	118.80
1	A	190(B)	C	C6-N1-C2	-5.58	118.07	120.30
17	Q	99	SER	N-CA-C	5.58	126.06	111.00
1	A	1075	C	C6-N1-C2	5.57	122.53	120.30
1	A	761	G	C6-C5-N7	-5.57	127.06	130.40
1	A	644	G	N3-C4-N9	5.57	129.34	126.00
1	A	696	A	N1-C6-N6	5.57	121.94	118.60
1	A	1112	C	N3-C2-O2	-5.57	118.00	121.90
1	A	79	G	C8-N9-C4	-5.56	104.17	106.40
1	A	265	G	N1-C2-N3	5.56	127.24	123.90
1	A	1253	G	C8-N9-C4	-5.56	104.18	106.40
1	A	332	G	N3-C2-N2	-5.56	116.01	119.90
1	A	373	A	N1-C2-N3	5.56	132.08	129.30
1	A	1425	U	C5-C4-O4	5.56	129.23	125.90
1	A	252	U	C4-C5-C6	5.55	123.03	119.70
1	A	1068	G	C6-C5-N7	-5.55	127.07	130.40
1	A	863	U	N1-C2-O2	-5.55	118.92	122.80
1	A	931	C	C2-N3-C4	-5.55	117.12	119.90
1	A	201	C	N1-C2-O2	5.55	122.23	118.90
1	A	52	G	N1-C2-N2	-5.55	111.21	116.20
1	A	55	A	C6-N1-C2	-5.55	115.27	118.60
1	A	580	U	C4-C5-C6	5.55	123.03	119.70
1	A	1500	A	C8-N9-C4	-5.54	103.58	105.80
1	A	389	A	C4-C5-C6	5.54	119.77	117.00
1	A	577	G	C8-N9-C4	5.54	108.62	106.40
1	A	811	C	C6-N1-C1'	-5.54	114.15	120.80
1	A	881	G	N7-C8-N9	-5.54	110.33	113.10
20	T	13	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	1415	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	747	C	N1-C2-O2	-5.54	115.58	118.90
1	A	1322	C	C6-N1-C2	-5.54	118.08	120.30
1	A	9	G	N9-C4-C5	-5.54	103.19	105.40
1	A	422	C	N1-C2-N3	-5.54	115.32	119.20
1	A	1322	C	C6-N1-C1'	-5.54	114.16	120.80
1	A	232	G	N3-C4-N9	5.54	129.32	126.00
1	A	893	C	N1-C2-N3	-5.54	115.33	119.20
1	A	190(B)	C	C5-C6-N1	5.53	123.77	121.00
1	A	650	G	N7-C8-N9	-5.53	110.33	113.10
1	A	811	C	C5-C4-N4	-5.53	116.33	120.20
1	A	1293	G	N3-C4-N9	-5.53	122.68	126.00
1	A	924	C	C2-N3-C4	5.53	122.67	119.90
1	A	1529	G	C4-N9-C1'	5.53	133.69	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	A	N1-C2-N3	5.53	132.06	129.30
1	A	926	G	C4-C5-N7	-5.53	108.59	110.80
1	A	829	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1157	A	N9-C4-C5	5.53	108.01	105.80
1	A	27	G	N1-C6-O6	5.53	123.22	119.90
1	A	135	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	889	A	C8-N9-C4	-5.53	103.59	105.80
1	A	1394	A	N1-C6-N6	5.53	121.92	118.60
1	A	1084	G	N3-C4-N9	5.52	129.31	126.00
1	A	628	G	C4-N9-C1'	5.52	133.68	126.50
1	A	283	C	N3-C4-N4	5.52	121.86	118.00
1	A	357	G	C5-C6-O6	5.52	131.91	128.60
1	A	650	G	C2-N3-C4	-5.52	109.14	111.90
1	A	711	G	C8-N9-C4	-5.52	104.19	106.40
1	A	864	A	C8-N9-C4	-5.52	103.59	105.80
1	A	867	G	C5-C6-N1	-5.51	108.74	111.50
1	A	245	C	C5-C4-N4	-5.51	116.34	120.20
1	A	761	G	N1-C2-N3	5.51	127.21	123.90
1	A	962	C	N3-C4-C5	5.51	124.10	121.90
1	A	969	A	C6-C5-N7	-5.51	128.44	132.30
1	A	281	G	C4-C5-N7	5.51	113.00	110.80
1	A	778	G	N1-C2-N3	-5.51	120.60	123.90
1	A	1249	C	N3-C4-N4	5.51	121.85	118.00
1	A	142	G	C5-C6-N1	5.50	114.25	111.50
1	A	767	A	C5-C6-N6	5.50	128.10	123.70
1	A	1280	A	N9-C4-C5	5.50	108.00	105.80
1	A	117	G	N3-C4-N9	5.50	129.30	126.00
16	P	58	TYR	CB-CA-C	-5.50	99.40	110.40
1	A	145	G	C5-C6-N1	-5.50	108.75	111.50
1	A	973	G	N7-C8-N9	-5.50	110.35	113.10
1	A	264	U	C5-C4-O4	5.50	129.20	125.90
1	A	1392	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	1140	C	C6-N1-C2	-5.49	118.10	120.30
1	A	107	G	N1-C6-O6	5.49	123.19	119.90
1	A	583	A	C8-N9-C4	5.49	108.00	105.80
1	A	583	A	C2-N3-C4	-5.49	107.85	110.60
1	A	175	C	C5-C6-N1	-5.49	118.26	121.00
1	A	1083	U	C6-N1-C2	5.49	124.29	121.00
1	A	372	C	N3-C4-N4	5.49	121.84	118.00
1	A	1322	C	C5-C6-N1	5.49	123.74	121.00
1	A	976	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1417	G	N3-C4-C5	-5.49	125.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	675	A	C5-C6-N6	5.48	128.09	123.70
1	A	77	G	C5-C6-O6	-5.48	125.31	128.60
1	A	279	A	N1-C2-N3	5.48	132.04	129.30
1	A	301	G	C4-N9-C1'	5.48	133.62	126.50
1	A	20	U	C4-C5-C6	5.48	122.99	119.70
1	A	1373	G	C4-C5-N7	-5.48	108.61	110.80
1	A	1083	U	N3-C4-O4	5.47	123.23	119.40
1	A	73	C	N3-C2-O2	5.47	125.73	121.90
1	A	1235	U	C6-N1-C2	-5.47	117.72	121.00
1	A	1374	A	C8-N9-C4	-5.47	103.61	105.80
1	A	570	G	C6-N1-C2	-5.47	121.82	125.10
1	A	686	U	C4-C5-C6	5.47	122.98	119.70
1	A	260	G	C2-N3-C4	-5.47	109.17	111.90
1	A	678	U	C5-C4-O4	-5.47	122.62	125.90
1	A	132	C	C5-C6-N1	-5.46	118.27	121.00
1	A	1199	U	N1-C2-N3	5.46	118.18	114.90
1	A	300	A	C8-N9-C4	-5.46	103.61	105.80
1	A	745	C	C5-C6-N1	-5.46	118.27	121.00
1	A	816	A	C2-N3-C4	-5.46	107.87	110.60
1	A	860	A	C4-C5-C6	5.46	119.73	117.00
1	A	335	C	C6-N1-C2	5.46	122.48	120.30
1	A	734	G	N7-C8-N9	5.46	115.83	113.10
1	A	59	A	C5-C6-N1	5.46	120.43	117.70
1	A	419	C	C6-N1-C2	5.45	122.48	120.30
1	A	1368	G	N3-C4-C5	-5.45	125.87	128.60
1	A	174	C	C2-N1-C1'	5.45	124.80	118.80
1	A	180	U	C6-N1-C1'	-5.45	113.57	121.20
1	A	366	C	C6-N1-C2	-5.45	118.12	120.30
1	A	853	G	C4-N9-C1'	5.45	133.59	126.50
4	D	12	CYS	CA-CB-SG	5.45	123.81	114.00
1	A	34	C	N1-C2-O2	-5.45	115.63	118.90
1	A	43	C	C5-C6-N1	-5.45	118.28	121.00
1	A	1434	A	C8-N9-C4	5.45	107.98	105.80
1	A	32	A	N1-C6-N6	5.45	121.87	118.60
1	A	232	G	C4-N9-C1'	5.45	133.58	126.50
1	A	280	C	N3-C4-N4	-5.45	114.19	118.00
1	A	1098	C	C6-N1-C2	5.45	122.48	120.30
1	A	1240	U	N3-C2-O2	-5.45	118.39	122.20
1	A	1354	C	C6-N1-C2	-5.45	118.12	120.30
1	A	1494	G	N3-C4-N9	5.45	129.27	126.00
1	A	70	G	N3-C4-C5	5.45	131.32	128.60
1	A	394	G	C5-C6-O6	5.44	131.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	953	G	N9-C4-C5	-5.44	103.22	105.40
1	A	1323	G	C5-C6-N1	-5.44	108.78	111.50
1	A	1506	U	C5-C4-O4	-5.44	122.64	125.90
1	A	26	A	N1-C2-N3	5.44	132.02	129.30
1	A	265	G	N3-C2-N2	5.43	123.70	119.90
1	A	1055	A	N9-C4-C5	5.43	107.97	105.80
1	A	1527	C	C6-N1-C1'	-5.43	114.28	120.80
1	A	111	G	N3-C2-N2	-5.43	116.10	119.90
1	A	1493[A]	A	C4-C5-N7	5.43	113.41	110.70
1	A	1493[B]	A	C4-C5-N7	5.43	113.41	110.70
1	A	552	U	N3-C4-C5	5.43	117.86	114.60
1	A	250	A	N9-C4-C5	-5.42	103.63	105.80
1	A	278	G	C5-C6-O6	5.42	131.85	128.60
1	A	1502	A	N3-C4-N9	-5.42	123.06	127.40
1	A	608	A	C2-N3-C4	-5.42	107.89	110.60
1	A	648	A	C6-N1-C2	-5.42	115.35	118.60
1	A	724	G	N1-C6-O6	5.42	123.15	119.90
1	A	924	C	N1-C2-O2	-5.42	115.65	118.90
1	A	120	A	C5-N7-C8	5.42	106.61	103.90
1	A	317	G	N3-C4-C5	5.42	131.31	128.60
1	A	628	G	C8-N9-C1'	-5.42	119.96	127.00
1	A	675	A	C5-C6-N1	-5.42	114.99	117.70
1	A	230	G	N3-C4-N9	5.42	129.25	126.00
1	A	530	G	N1-C6-O6	-5.42	116.65	119.90
1	A	1343	G	N7-C8-N9	5.42	115.81	113.10
1	A	1405	G	N3-C4-N9	-5.42	122.75	126.00
1	A	107	G	C6-C5-N7	-5.42	127.15	130.40
18	R	76	LEU	CA-CB-CG	-5.41	102.85	115.30
1	A	259	G	C4-N9-C1'	5.41	133.53	126.50
1	A	874	G	C2-N3-C4	-5.41	109.19	111.90
1	A	881	G	N1-C6-O6	5.41	123.15	119.90
1	A	400	C	C5-C6-N1	-5.41	118.30	121.00
1	A	671	G	N1-C6-O6	5.41	123.14	119.90
1	A	1125	U	N3-C2-O2	5.41	125.99	122.20
1	A	107	G	N9-C4-C5	-5.41	103.24	105.40
1	A	283	C	N3-C2-O2	-5.41	118.12	121.90
1	A	817	C	C2-N1-C1'	5.41	124.75	118.80
1	A	589	C	C2-N3-C4	-5.40	117.20	119.90
1	A	1242	C	N3-C4-C5	5.40	124.06	121.90
1	A	304	U	C5-C6-N1	-5.40	120.00	122.70
1	A	16	A	N7-C8-N9	-5.39	111.10	113.80
1	A	124	G	N1-C2-N3	5.39	127.14	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1202	G	C8-N9-C4	-5.39	104.24	106.40
1	A	641	U	N1-C2-N3	5.38	118.13	114.90
1	A	826	C	N3-C4-N4	5.38	121.77	118.00
1	A	20	U	C2-N3-C4	-5.38	123.77	127.00
1	A	1143	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1276	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1395	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1413	A	N1-C2-N3	5.38	131.99	129.30
1	A	1231	G	N9-C4-C5	-5.38	103.25	105.40
16	P	60	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	631	G	C8-N9-C4	-5.37	104.25	106.40
1	A	1375	A	N1-C6-N6	-5.37	115.38	118.60
1	A	197	A	C5-C6-N6	5.37	128.00	123.70
1	A	264	U	N1-C2-N3	5.37	118.12	114.90
1	A	413	G	C4-C5-N7	-5.37	108.65	110.80
1	A	490	G	C5-C6-O6	-5.37	125.38	128.60
5	E	69	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	931	C	N3-C4-C5	5.37	124.05	121.90
1	A	1023	G	N3-C4-C5	-5.37	125.92	128.60
1	A	1332	A	C5-C6-N6	5.37	127.99	123.70
1	A	1053	G	C4-C5-N7	-5.37	108.65	110.80
1	A	1108	G	N3-C4-N9	5.37	129.22	126.00
1	A	92	C	C5-C4-N4	-5.36	116.44	120.20
1	A	279	A	C4-C5-C6	5.36	119.68	117.00
1	A	497	A	N9-C4-C5	5.36	107.95	105.80
1	A	1054	C	C5-C6-N1	5.36	123.68	121.00
1	A	1206	G	C5-C6-N1	-5.36	108.82	111.50
1	A	1350	A	C4-C5-N7	5.36	113.38	110.70
1	A	566	G	C6-C5-N7	-5.36	127.19	130.40
1	A	200	G	C5-C6-N1	-5.36	108.82	111.50
1	A	800	G	C4-N9-C1'	5.36	133.46	126.50
1	A	854	G	N9-C4-C5	-5.35	103.26	105.40
1	A	524	G	N3-C2-N2	-5.35	116.15	119.90
1	A	779	C	C5-C6-N1	-5.35	118.32	121.00
1	A	1304	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1338	G	N1-C2-N3	5.35	127.11	123.90
1	A	1460	A	N1-C6-N6	5.35	121.81	118.60
1	A	10	A	N1-C2-N3	5.35	131.97	129.30
1	A	358	U	N1-C2-N3	5.35	118.11	114.90
1	A	1165	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1399	C	N1-C2-O2	-5.35	115.69	118.90
1	A	204	U	N1-C2-N3	-5.35	111.69	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	934	C	C2-N3-C4	5.35	122.57	119.90
1	A	1125	U	C5-C4-O4	-5.35	122.69	125.90
1	A	1080	A	C5-C6-N6	5.35	127.98	123.70
1	A	558	G	N1-C6-O6	5.34	123.11	119.90
4	D	188	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	77	G	C6-C5-N7	-5.34	127.19	130.40
1	A	277	C	C5-C6-N1	-5.34	118.33	121.00
1	A	291	C	N3-C4-C5	5.34	124.04	121.90
1	A	1068	G	C4-N9-C1'	5.34	133.44	126.50
1	A	1433	A	N1-C6-N6	-5.34	115.39	118.60
1	A	786	G	C5-C6-N1	-5.34	108.83	111.50
1	A	1530	G	N1-C6-O6	5.34	123.10	119.90
1	A	483	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	644	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	1246	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	55	A	C5-C6-N1	5.33	120.37	117.70
1	A	281	G	C5-N7-C8	-5.33	101.64	104.30
1	A	767	A	C4-C5-N7	-5.33	108.03	110.70
1	A	871	U	N3-C2-O2	-5.33	118.47	122.20
1	A	1167	A	C8-N9-C4	-5.33	103.67	105.80
20	T	102	GLY	N-CA-C	-5.33	99.78	113.10
1	A	635	G	C4-N9-C1'	5.33	133.43	126.50
1	A	557	G	C4-C5-N7	-5.33	108.67	110.80
1	A	351	G	N1-C2-N3	5.32	127.09	123.90
1	A	403	C	C4-C5-C6	5.32	120.06	117.40
1	A	288	A	N1-C6-N6	5.32	121.79	118.60
1	A	1055	A	C5-C6-N1	5.32	120.36	117.70
1	A	1286	A	N7-C8-N9	5.32	116.46	113.80
1	A	780	A	N7-C8-N9	-5.32	111.14	113.80
1	A	1092	A	C4-N9-C1'	5.32	135.87	126.30
1	A	317	G	N1-C6-O6	5.31	123.09	119.90
1	A	1324	A	C8-N9-C4	-5.31	103.67	105.80
1	A	423	G	N3-C4-N9	5.31	129.19	126.00
1	A	479	C	C2-N3-C4	5.31	122.55	119.90
1	A	876	G	C5-N7-C8	-5.31	101.64	104.30
1	A	1480	G	C5-C6-N1	-5.31	108.84	111.50
1	A	980	C	C5-C4-N4	-5.31	116.48	120.20
1	A	936	C	C5-C6-N1	-5.30	118.35	121.00
1	A	1481	U	C5-C4-O4	5.30	129.08	125.90
2	B	25	ASN	C-N-CD	5.30	139.54	128.40
1	A	17	U	N1-C2-N3	5.30	118.08	114.90
1	A	70	G	N1-C6-O6	5.29	123.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	783	C	C5-C6-N1	-5.29	118.35	121.00
1	A	895	G	N7-C8-N9	5.29	115.75	113.10
1	A	963	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1415	G	N9-C4-C5	-5.29	103.28	105.40
1	A	607	A	N1-C6-N6	5.29	121.77	118.60
1	A	69	G	C8-N9-C4	5.29	108.52	106.40
1	A	389	A	N1-C2-N3	5.29	131.94	129.30
1	A	732	C	N3-C2-O2	-5.29	118.20	121.90
1	A	752	G	C8-N9-C4	5.29	108.52	106.40
1	A	822	C	C2-N3-C4	-5.29	117.26	119.90
1	A	947	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1091	U	N3-C4-C5	-5.29	111.43	114.60
1	A	534	U	C6-N1-C2	5.29	124.17	121.00
1	A	820	U	C6-N1-C1'	5.29	128.60	121.20
1	A	947	G	N3-C2-N2	5.29	123.60	119.90
1	A	705	U	C5-C6-N1	-5.28	120.06	122.70
1	A	1295	G	C8-N9-C4	-5.28	104.29	106.40
1	A	861	G	C5-C6-N1	5.28	114.14	111.50
1	A	920	U	C6-N1-C1'	5.28	128.59	121.20
1	A	1201	A	N3-C4-C5	-5.28	123.11	126.80
1	A	259	G	C6-C5-N7	-5.27	127.24	130.40
14	N	10	ALA	N-CA-C	-5.27	96.76	111.00
1	A	577	G	N1-C2-N3	5.27	127.06	123.90
1	A	721	G	N3-C2-N2	5.27	123.59	119.90
1	A	1350	A	C6-C5-N7	-5.27	128.61	132.30
1	A	820	U	C2-N3-C4	-5.27	123.84	127.00
1	A	934	C	C6-N1-C2	5.27	122.41	120.30
1	A	827	U	C2-N1-C1'	5.27	124.02	117.70
1	A	54	C	C2-N3-C4	-5.26	117.27	119.90
1	A	635	G	C8-N9-C4	5.26	108.51	106.40
1	A	644	G	N9-C4-C5	-5.26	103.29	105.40
1	A	800	G	C6-C5-N7	-5.26	127.24	130.40
1	A	819	A	N1-C2-N3	5.26	131.93	129.30
12	L	66	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	919	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1077	G	N1-C2-N2	-5.26	111.46	116.20
1	A	1380	U	C5-C4-O4	5.26	129.06	125.90
10	J	58	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	1033	G	N9-C4-C5	5.26	107.50	105.40
1	A	1281	U	N3-C2-O2	-5.26	118.52	122.20
1	A	221	C	C5-C6-N1	-5.25	118.37	121.00
1	A	565	U	N1-C2-N3	-5.25	111.75	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	964	A	C2-N3-C4	-5.25	107.97	110.60
1	A	1505	G	N9-C4-C5	5.25	107.50	105.40
1	A	1512	U	N1-C2-N3	5.25	118.05	114.90
1	A	1487	G	N3-C2-N2	-5.25	116.22	119.90
1	A	1494	G	C6-C5-N7	-5.25	127.25	130.40
1	A	248	C	C4-C5-C6	5.25	120.03	117.40
1	A	1249	C	C2-N1-C1'	5.25	124.58	118.80
1	A	112	G	C8-N9-C4	5.25	108.50	106.40
1	A	119	A	N1-C6-N6	5.25	121.75	118.60
1	A	244	U	N1-C2-N3	-5.24	111.75	114.90
1	A	1058	G	N3-C4-C5	5.24	131.22	128.60
15	O	45	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	573	A	C6-C5-N7	-5.24	128.63	132.30
1	A	1392	G	C4-C5-C6	5.24	121.94	118.80
1	A	711	G	N7-C8-N9	5.24	115.72	113.10
1	A	740	U	C5-C6-N1	-5.24	120.08	122.70
1	A	1099	G	N3-C4-N9	-5.24	122.86	126.00
1	A	440	A	C5-C6-N1	-5.23	115.08	117.70
1	A	1200	C	C5-C4-N4	-5.23	116.54	120.20
1	A	801	U	N3-C4-C5	5.23	117.74	114.60
1	A	831	U	N1-C2-N3	5.23	118.04	114.90
1	A	946	A	N1-C2-N3	5.23	131.92	129.30
1	A	149	A	N1-C6-N6	-5.23	115.46	118.60
1	A	650	G	N3-C2-N2	-5.23	116.24	119.90
1	A	668	G	C8-N9-C4	5.23	108.49	106.40
1	A	489	C	C6-N1-C2	5.23	122.39	120.30
1	A	1497	G	N3-C4-C5	-5.22	125.99	128.60
1	A	309	G	C4-C5-N7	5.22	112.89	110.80
1	A	544	G	N3-C4-C5	-5.22	125.99	128.60
1	A	816	A	N3-C4-C5	5.22	130.46	126.80
1	A	122	G	N3-C4-C5	5.22	131.21	128.60
1	A	352	C	N1-C2-O2	-5.22	115.77	118.90
1	A	965	A	N9-C4-C5	-5.22	103.71	105.80
1	A	1096	C	C6-N1-C2	-5.22	118.21	120.30
1	A	975	A	C2-N3-C4	-5.22	107.99	110.60
1	A	1305	G	C4-C5-C6	5.22	121.93	118.80
1	A	641	U	C2-N3-C4	-5.21	123.87	127.00
1	A	1027	C	N3-C4-C5	-5.21	119.81	121.90
1	A	1525	G	C6-N1-C2	-5.21	121.97	125.10
1	A	744	C	C5-C6-N1	-5.21	118.39	121.00
1	A	823	G	N1-C2-N3	5.21	127.03	123.90
1	A	190(E)	U	N1-C2-N3	5.21	118.03	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	931	C	N3-C4-N4	-5.21	114.35	118.00
1	A	1507	A	C5-C6-N6	5.21	127.87	123.70
1	A	1134	G	N9-C4-C5	5.21	107.48	105.40
1	A	331	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	1484	C	N1-C2-O2	-5.21	115.78	118.90
1	A	15	G	C4-C5-N7	5.20	112.88	110.80
1	A	781	A	N7-C8-N9	5.20	116.40	113.80
1	A	781	A	C4-C5-C6	5.20	119.60	117.00
1	A	782	A	C5-C6-N6	5.20	127.86	123.70
1	A	953	G	N1-C6-O6	5.20	123.02	119.90
1	A	1421	G	N7-C8-N9	5.20	115.70	113.10
1	A	900	A	N1-C2-N3	5.20	131.90	129.30
1	A	679	C	C6-N1-C2	5.20	122.38	120.30
1	A	964	A	N7-C8-N9	5.19	116.40	113.80
1	A	436	C	C2-N1-C1'	-5.19	113.09	118.80
1	A	830	G	C5-C6-N1	-5.19	108.90	111.50
1	A	1049	U	C2-N1-C1'	5.19	123.93	117.70
12	L	17	LYS	CD-CE-NZ	5.19	123.64	111.70
1	A	25	C	C6-N1-C2	5.19	122.38	120.30
1	A	104	G	C4-C5-C6	5.19	121.91	118.80
1	A	481	G	C8-N9-C1'	-5.19	120.25	127.00
1	A	1108	G	C4-C5-C6	5.19	121.91	118.80
1	A	540	G	C4-C5-N7	5.19	112.88	110.80
1	A	804	U	C4-C5-C6	5.19	122.81	119.70
1	A	1037	C	C6-N1-C2	-5.18	118.23	120.30
1	A	882	C	N1-C2-N3	5.18	122.83	119.20
5	E	63	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	760	G	N9-C4-C5	-5.18	103.33	105.40
1	A	497	A	C5-C6-N6	5.18	127.84	123.70
1	A	1322	C	C2-N3-C4	5.18	122.49	119.90
1	A	1293	G	N3-C4-C5	5.18	131.19	128.60
1	A	1272	G	N3-C4-C5	-5.18	126.01	128.60
1	A	232	G	C5-C6-N1	-5.17	108.91	111.50
1	A	691	G	C6-C5-N7	-5.17	127.30	130.40
1	A	311	C	C5-C6-N1	-5.17	118.42	121.00
1	A	969	A	C5-N7-C8	-5.17	101.31	103.90
1	A	1030(C)	G	C8-N9-C4	-5.17	104.33	106.40
1	A	816	A	C6-C5-N7	5.17	135.92	132.30
1	A	558	G	C5-N7-C8	-5.17	101.72	104.30
1	A	811	C	C2-N3-C4	-5.17	117.32	119.90
1	A	816	A	C8-N9-C4	5.17	107.87	105.80
1	A	134	A	C2-N3-C4	-5.16	108.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	G	C5-C6-O6	-5.16	125.50	128.60
1	A	190(H)	G	C4-C5-N7	-5.16	108.74	110.80
1	A	648	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1253	G	C4-N9-C1'	5.16	133.21	126.50
1	A	700	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1493[A]	A	N1-C6-N6	5.16	121.69	118.60
1	A	1493[B]	A	N1-C6-N6	5.16	121.69	118.60
1	A	824	C	C2-N3-C4	-5.16	117.32	119.90
1	A	190(B)	C	C2-N1-C1'	5.16	124.47	118.80
1	A	667	G	N3-C4-C5	5.16	131.18	128.60
1	A	566	G	N3-C4-C5	-5.15	126.02	128.60
1	A	280	C	C5-C6-N1	-5.15	118.42	121.00
1	A	701	C	N3-C4-N4	-5.15	114.39	118.00
1	A	705	U	N1-C2-N3	5.15	117.99	114.90
1	A	976	G	N3-C2-N2	-5.15	116.30	119.90
1	A	1390	U	C5-C4-O4	5.15	128.99	125.90
1	A	97	G	C8-N9-C4	-5.15	104.34	106.40
1	A	596	C	N3-C2-O2	5.15	125.50	121.90
1	A	193	C	C6-N1-C2	5.15	122.36	120.30
1	A	1052	U	C6-N1-C2	-5.14	117.91	121.00
1	A	596	C	C2-N1-C1'	-5.14	113.14	118.80
1	A	220	G	N1-C6-O6	5.14	122.98	119.90
1	A	306	G	N3-C4-C5	5.14	131.17	128.60
1	A	785	G	C8-N9-C4	5.14	108.46	106.40
1	A	1377	A	N1-C6-N6	-5.14	115.52	118.60
1	A	1395	C	C5-C4-N4	5.14	123.80	120.20
1	A	612	C	C5-C6-N1	-5.14	118.43	121.00
1	A	1484	C	N3-C2-O2	5.14	125.50	121.90
1	A	109	A	C5-C6-N6	5.13	127.81	123.70
1	A	357	G	N9-C4-C5	5.13	107.45	105.40
1	A	246	A	C8-N9-C4	5.13	107.85	105.80
1	A	881	G	C6-C5-N7	-5.13	127.32	130.40
1	A	558	G	C5-C6-O6	-5.13	125.52	128.60
1	A	796	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1186	G	N3-C2-N2	-5.13	116.31	119.90
1	A	618	C	C5-C4-N4	5.13	123.79	120.20
1	A	120	A	C5-C6-N6	5.13	127.80	123.70
1	A	435	C	C6-N1-C2	-5.13	118.25	120.30
1	A	805	C	C4-C5-C6	-5.13	114.84	117.40
12	L	52	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	683	G	C8-N9-C4	-5.12	104.35	106.40
1	A	390	C	N3-C4-C5	-5.12	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	758	G	N1-C2-N3	5.12	126.97	123.90
1	A	1030(C)	G	N3-C4-C5	-5.12	126.04	128.60
1	A	1365	G	N9-C4-C5	5.12	107.45	105.40
1	A	201	C	C6-N1-C1'	-5.12	114.65	120.80
1	A	539	A	C2-N3-C4	5.12	113.16	110.60
1	A	570	G	N3-C4-N9	5.12	129.07	126.00
1	A	812	C	N3-C2-O2	-5.12	118.31	121.90
1	A	889	A	C4-C5-C6	5.12	119.56	117.00
1	A	1332	A	C8-N9-C4	-5.12	103.75	105.80
1	A	1077	G	N1-C2-N3	5.12	126.97	123.90
1	A	828	A	C6-C5-N7	-5.12	128.72	132.30
1	A	109	A	N1-C2-N3	5.12	131.86	129.30
1	A	1139	G	N3-C4-C5	-5.12	126.04	128.60
1	A	317	G	C4-C5-N7	5.11	112.84	110.80
1	A	621	A	C6-C5-N7	-5.11	128.72	132.30
1	A	910	C	N1-C2-N3	5.11	122.78	119.20
1	A	919	A	C4-C5-N7	5.11	113.26	110.70
1	A	1370	G	C4-N9-C1'	5.11	133.14	126.50
1	A	47	C	C6-N1-C2	5.11	122.34	120.30
1	A	316	G	C6-C5-N7	5.11	133.46	130.40
1	A	803	G	N1-C2-N2	-5.11	111.60	116.20
1	A	823	G	C6-C5-N7	-5.11	127.33	130.40
1	A	10	A	N1-C6-N6	-5.11	115.54	118.60
1	A	530	G	N3-C2-N2	5.11	123.47	119.90
1	A	120	A	C4-C5-N7	-5.10	108.15	110.70
1	A	266	G	N9-C4-C5	-5.10	103.36	105.40
1	A	284	G	C5-C6-N1	-5.10	108.95	111.50
1	A	521	G	C6-C5-N7	5.10	133.46	130.40
1	A	660	G	N9-C4-C5	-5.10	103.36	105.40
1	A	1344	C	C5-C6-N1	-5.10	118.45	121.00
1	A	181	G	N3-C4-N9	5.10	129.06	126.00
1	A	66	G	C2-N3-C4	-5.10	109.35	111.90
1	A	485	G	C5-C6-N1	-5.10	108.95	111.50
1	A	741	G	N9-C4-C5	5.10	107.44	105.40
1	A	1341	U	C6-N1-C1'	5.10	128.34	121.20
1	A	757	U	N1-C2-O2	-5.10	119.23	122.80
1	A	253	U	N1-C2-O2	-5.09	119.23	122.80
1	A	930	C	C2-N3-C4	-5.09	117.35	119.90
1	A	1084	G	C4-C5-C6	5.09	121.86	118.80
1	A	1504	G	N9-C4-C5	-5.09	103.36	105.40
1	A	190(F)	G	C4-C5-N7	-5.09	108.76	110.80
1	A	259	G	N7-C8-N9	5.09	115.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	570	G	C8-N9-C1'	-5.09	120.39	127.00
1	A	1078	U	C4-C5-C6	-5.09	116.65	119.70
1	A	1222	G	N1-C6-O6	5.09	122.95	119.90
1	A	796	C	N3-C4-C5	-5.09	119.86	121.90
1	A	306	G	N1-C6-O6	5.09	122.95	119.90
1	A	853	G	N7-C8-N9	5.09	115.64	113.10
1	A	909	A	C4-C5-N7	5.09	113.24	110.70
1	A	1277	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1012	U	C6-N1-C2	-5.08	117.95	121.00
1	A	947	G	N1-C2-N2	-5.08	111.62	116.20
1	A	1310	G	N9-C4-C5	-5.08	103.37	105.40
24	a	37	A	N1-C2-N3	5.08	131.84	129.30
1	A	336	C	N3-C4-N4	5.08	121.56	118.00
1	A	903	G	N9-C4-C5	5.08	107.43	105.40
1	A	1195	C	C5-C4-N4	-5.08	116.64	120.20
1	A	1236	A	C5-C6-N6	-5.08	119.64	123.70
1	A	393	A	N1-C6-N6	5.08	121.65	118.60
1	A	814	A	C8-N9-C4	5.07	107.83	105.80
1	A	597	G	N1-C2-N3	5.07	126.94	123.90
1	A	933	G	C4-C5-N7	5.07	112.83	110.80
1	A	977	A	N3-C4-C5	-5.07	123.25	126.80
1	A	1405	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	1494	G	C4-C5-N7	5.07	112.83	110.80
1	A	92	C	N1-C2-O2	5.07	121.94	118.90
1	A	344	A	C5-N7-C8	-5.07	101.37	103.90
1	A	183	G	N7-C8-N9	5.06	115.63	113.10
1	A	544	G	C4-N9-C1'	5.06	133.08	126.50
1	A	579	G	N3-C4-C5	5.06	131.13	128.60
1	A	190(D)	U	N3-C2-O2	-5.06	118.66	122.20
1	A	292	G	C8-N9-C4	5.06	108.42	106.40
1	A	794	A	N1-C2-N3	-5.06	126.77	129.30
1	A	795	C	C2-N1-C1'	-5.06	113.23	118.80
1	A	1127	G	N1-C6-O6	-5.06	116.86	119.90
1	A	858	G	C4-N9-C1'	5.06	133.08	126.50
1	A	886	G	C5-C6-N1	-5.06	108.97	111.50
1	A	433	C	N3-C2-O2	-5.05	118.36	121.90
1	A	50	A	C6-N1-C2	5.05	121.63	118.60
1	A	149	A	N1-C2-N3	5.05	131.83	129.30
1	A	642	A	N1-C2-N3	5.05	131.83	129.30
1	A	600	C	C4-C5-C6	5.05	119.92	117.40
1	A	658	G	N1-C2-N2	-5.05	111.66	116.20
1	A	1356	G	C8-N9-C4	-5.05	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	U	C2-N3-C4	-5.05	123.97	127.00
1	A	903	G	N1-C6-O6	-5.05	116.87	119.90
1	A	1324	A	N1-C6-N6	5.05	121.63	118.60
1	A	403	C	C2-N1-C1'	-5.04	113.25	118.80
1	A	1232	U	C2-N3-C4	-5.04	123.97	127.00
1	A	16	A	C5-C6-N1	-5.04	115.18	117.70
1	A	288	A	N3-C4-C5	5.04	130.33	126.80
1	A	447	G	N3-C2-N2	5.04	123.43	119.90
1	A	910	C	C4-C5-C6	5.04	119.92	117.40
1	A	1279	A	C4-C5-C6	5.04	119.52	117.00
1	A	637	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1434	A	C5-C6-N6	-5.04	119.67	123.70
1	A	1476	G	C8-N9-C4	-5.04	104.38	106.40
1	A	521	G	C4-C5-N7	-5.03	108.79	110.80
1	A	964	A	N9-C4-C5	5.03	107.81	105.80
25	b	3	U	N3-C2-O2	-5.03	118.68	122.20
1	A	64	G	C6-C5-N7	-5.03	127.38	130.40
1	A	646	U	C5-C4-O4	5.03	128.92	125.90
1	A	330	C	N3-C4-C5	-5.03	119.89	121.90
1	A	800	G	N1-C6-O6	5.03	122.92	119.90
1	A	899	C	C2-N1-C1'	5.03	124.33	118.80
1	A	250	A	C6-N1-C2	5.03	121.62	118.60
1	A	558	G	C8-N9-C4	-5.03	104.39	106.40
1	A	1488	G	C4-C5-N7	-5.03	108.79	110.80
1	A	142	G	C2-N3-C4	5.03	114.41	111.90
1	A	826	C	C2-N1-C1'	5.03	124.33	118.80
1	A	135	C	C6-N1-C1'	5.02	126.83	120.80
1	A	1055	A	C4-C5-N7	-5.02	108.19	110.70
1	A	828	A	C4-C5-N7	5.02	113.21	110.70
1	A	1099	G	N3-C2-N2	-5.02	116.39	119.90
1	A	1303	C	N3-C4-C5	5.02	123.91	121.90
1	A	712	A	C2-N3-C4	-5.02	108.09	110.60
1	A	651	C	N1-C2-O2	-5.02	115.89	118.90
1	A	859	A	N3-C4-N9	5.02	131.41	127.40
1	A	357	G	N1-C6-O6	-5.02	116.89	119.90
1	A	21	G	N3-C2-N2	5.01	123.41	119.90
16	P	5	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	276	G	C5-C6-O6	5.01	131.60	128.60
1	A	611	A	N1-C6-N6	5.01	121.61	118.60
1	A	786	G	N3-C4-C5	5.01	131.10	128.60
1	A	125	U	C5-C6-N1	-5.01	120.20	122.70
1	A	673	G	N1-C6-O6	5.01	122.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1303	C	C6-N1-C2	5.00	122.30	120.30
1	A	266	G	P-O3'-C3'	5.00	125.70	119.70
1	A	1179	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	75	LYS	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
3	C	2	GLY	Peptide
4	D	154	ASN	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
9	I	38	GLN	Peptide
10	J	61	GLU	Peptide
10	J	85	LEU	Peptide
12	L	46	LYS	Peptide
12	L	91	LYS	Peptide
16	P	82	GLN	Peptide
19	S	4	SER	Peptide
20	T	12	ALA	Peptide
20	T	8	ARG	Peptide
21	U	24	ARG	Peptide

5.2 Too-close contacts

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 X-ray entries followed by that with respect to entries of similar resolution.

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
2	B	234/256 (91%)	197 (84%)	34 (14%)	3 (1%)	12 48
3	C	205/239 (86%)	169 (82%)	35 (17%)	1 (0%)	29 65
4	D	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	29 65
5	E	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	22 59
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
7	G	153/156 (98%)	132 (86%)	21 (14%)	0	100 100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22 59
9	I	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19 56
10	J	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	4 33
11	K	115/129 (89%)	98 (85%)	17 (15%)	0	100 100
12	L	122/135 (90%)	110 (90%)	8 (7%)	4 (3%)	4 32
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	17 54
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100 100
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100 100
16	P	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	13 49
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100 100
18	R	69/88 (78%)	60 (87%)	9 (13%)	0	100 100
19	S	79/93 (85%)	68 (86%)	9 (11%)	2 (2%)	5 36
20	T	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	15 52
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
All	All	2349/2541 (92%)	2046 (87%)	283 (12%)	20 (1%)	17 54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR
9	I	119	ALA
12	L	28	LYS
16	P	83	GLU
19	S	31	ILE
10	J	81	THR
10	J	86	MET
19	S	6	LYS
12	L	115	LYS
20	T	73	HIS
2	B	21	ARG

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	229	VAL
5	E	153	LYS
8	H	121	ASP
12	L	27	LEU
10	J	34	VAL
12	L	71	PRO
13	M	7	VAL
4	D	67	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	B	201/220 (91%)	151 (75%)	50 (25%)	0	4
3	C	160/188 (85%)	119 (74%)	41 (26%)	0	4
4	D	180/181 (99%)	134 (74%)	46 (26%)	0	4
5	E	115/123 (94%)	75 (65%)	40 (35%)	0	1
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	1
7	G	126/127 (99%)	92 (73%)	34 (27%)	0	3
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	2
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	5
10	J	87/92 (95%)	70 (80%)	17 (20%)	1	9
11	K	89/99 (90%)	72 (81%)	17 (19%)	1	9
12	L	103/110 (94%)	80 (78%)	23 (22%)	1	6
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	1
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	2
15	O	79/80 (99%)	60 (76%)	19 (24%)	0	5
16	P	72/74 (97%)	54 (75%)	18 (25%)	0	4
17	Q	95/97 (98%)	74 (78%)	21 (22%)	1	6
18	R	62/77 (80%)	48 (77%)	14 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	71/80 (89%)	55 (78%)	16 (22%)	1 6
20	T	76/82 (93%)	51 (67%)	25 (33%)	0 1
21	U	19/22 (86%)	16 (84%)	3 (16%)	2 17
All	All	1985/2111 (94%)	1468 (74%)	517 (26%)	0 4

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	11	LEU
2	B	16	HIS
2	B	17	PHE
2	B	20	GLU
2	B	30	ARG
2	B	33	TYR
2	B	35	GLU
2	B	39	ILE
2	B	44	LEU
2	B	53	ARG
2	B	61	LEU
2	B	63	MET
2	B	64	ARG
2	B	67	THR
2	B	69	LEU
2	B	92	TYR
2	B	97	TRP
2	B	101	MET
2	B	107	THR
2	B	109	SER
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	122	PHE
2	B	127	ILE
2	B	128	GLU
2	B	144	ARG
2	B	150	SER
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	169	LYS

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Mol	Chain	Res	Type
2	B	172	ILE
2	B	182	ILE
2	B	187	LEU
2	B	189	ASP
2	B	193	ASP
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	209	ARG
2	B	210	SER
2	B	212	GLN
2	B	215	LEU
2	B	216	SER
2	B	221	LEU
2	B	226	ARG
2	B	236	TYR
2	B	240	GLN
3	C	3	ASN
3	C	8	ILE
3	C	10	PHE
3	C	14	ILE
3	C	16	ARG
3	C	21	ARG
3	C	22	TRP
3	C	31	HIS
3	C	33	LEU
3	C	43	LEU
3	C	45	LYS
3	C	52	LEU
3	C	58	GLU
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	75	VAL
3	C	79	ARG
3	C	85	ARG
3	C	99	VAL
3	C	101	LEU
3	C	111	LEU
3	C	119	ARG
3	C	126	ARG
3	C	127	ARG

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Mol	Chain	Res	Type
3	C	130	VAL
3	C	134	ILE
3	C	144	SER
3	C	147	LYS
3	C	156	ARG
3	C	165	THR
3	C	167	TRP
3	C	170	GLN
3	C	175	LEU
3	C	186	PHE
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	10	ARG
4	D	19	LEU
4	D	20	TYR
4	D	26	CYS
4	D	28	SER
4	D	47	ARG
4	D	49	ARG
4	D	57	ARG
4	D	61	LYS
4	D	66	ARG
4	D	73	ARG
4	D	78	LEU
4	D	84	LYS
4	D	85	LYS
4	D	86	LYS
4	D	91	SER
4	D	92	VAL
4	D	96	LEU
4	D	107	ARG
4	D	108	LEU
4	D	114	ARG
4	D	115	ARG
4	D	119	GLN
4	D	120	LEU
4	D	122	ARG
4	D	127	THR

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Mol	Chain	Res	Type
4	D	131	ARG
4	D	132	ARG
4	D	145	GLU
4	D	146	ILE
4	D	150	GLU
4	D	159	ARG
4	D	163	GLU
4	D	169	LYS
4	D	177	ASP
4	D	178	VAL
4	D	179	GLU
4	D	182	LYS
4	D	187	ARG
4	D	188	LEU
4	D	190	ASP
4	D	192	GLU
4	D	193	ASP
4	D	194	LEU
4	D	196	LEU
4	D	204	ILE
5	E	6	PHE
5	E	11	ILE
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	24	ARG
5	E	31	LEU
5	E	32	VAL
5	E	37	ARG
5	E	38	GLN
5	E	43	LEU
5	E	47	LYS
5	E	51	VAL
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	65	ASN
5	E	66	MET
5	E	67	VAL
5	E	68	GLU
5	E	75	THR
5	E	76	ILE

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Mol	Chain	Res	Type
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	83	GLU
5	E	84	PHE
5	E	100	VAL
5	E	105	VAL
5	E	110	LEU
5	E	116	THR
5	E	123	LEU
5	E	125	SER
5	E	126	ARG
5	E	131	ILE
5	E	145	LYS
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
6	F	1	MET
6	F	2	ARG
6	F	7	ASN
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	16	GLN
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	28	ARG
6	F	37	VAL
6	F	39	LYS
6	F	43	LEU
6	F	54	LYS
6	F	64	GLN
6	F	65	VAL
6	F	74	ASP
6	F	75	LEU
6	F	80	ARG
6	F	83	ASP
6	F	84	ASN
6	F	86	ARG
6	F	87	ARG

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Mol	Chain	Res	Type
6	F	89	MET
6	F	93	SER
6	F	94	GLN
6	F	97	PHE
6	F	98	LEU
6	F	100	ASN
7	G	9	VAL
7	G	10	ARG
7	G	12	LEU
7	G	15	ASP
7	G	16	LEU
7	G	17	VAL
7	G	22	LEU
7	G	27	ILE
7	G	29	LYS
7	G	38	LEU
7	G	41	ARG
7	G	49	ILE
7	G	52	GLU
7	G	60	LYS
7	G	62	PHE
7	G	66	VAL
7	G	72	ARG
7	G	75	VAL
7	G	78	ARG
7	G	87	VAL
7	G	92	SER
7	G	97	GLN
7	G	101	LEU
7	G	113	GLU
7	G	114	ARG
7	G	115	ARG
7	G	120	ILE
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	129	GLU
7	G	135	VAL
7	G	146	GLU
7	G	156	TRP
8	H	1	MET
8	H	3	THR

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Mol	Chain	Res	Type
8	H	8	ASP
8	H	10	LEU
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	22	GLU
8	H	39	LEU
8	H	45	ILE
8	H	51	VAL
8	H	53	VAL
8	H	57	PRO
8	H	59	LEU
8	H	63	LEU
8	H	81	HIS
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	113	SER
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
8	H	133	LEU
8	H	135	CYS
8	H	136	GLU
9	I	2	GLU
9	I	5	TYR
9	I	14	VAL
9	I	16	ARG
9	I	23	ASN
9	I	29	ASN
9	I	33	PHE
9	I	34	ASN

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Mol	Chain	Res	Type
9	I	40	LEU
9	I	48	GLU
9	I	59	PHE
9	I	62	TYR
9	I	63	ILE
9	I	64	THR
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	85	LEU
9	I	99	LEU
9	I	102	LEU
9	I	109	VAL
9	I	112	LYS
9	I	125	TYR
10	J	4	ILE
10	J	9	ARG
10	J	12	ASP
10	J	19	SER
10	J	28	ARG
10	J	29	ARG
10	J	33	GLN
10	J	44	VAL
10	J	62	HIS
10	J	63	PHE
10	J	67	THR
10	J	78	ASN
10	J	89	ASP
10	J	90	LEU
10	J	94	VAL
10	J	98	ILE
10	J	99	LYS
11	K	11	LYS
11	K	29	ILE
11	K	40	ILE
11	K	57	THR
11	K	70	LYS
11	K	75	TYR
11	K	78	GLN
11	K	80	VAL
11	K	92	GLU
11	K	96	ARG

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Mol	Chain	Res	Type
11	K	99	GLN
11	K	105	VAL
11	K	116	HIS
11	K	117	ASN
11	K	120	ARG
11	K	125	PHE
11	K	126	ARG
12	L	7	ILE
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	32	PHE
12	L	34	ARG
12	L	36	VAL
12	L	43	VAL
12	L	44	THR
12	L	50	SER
12	L	52	LEU
12	L	53	ARG
12	L	54	LYS
12	L	60	LEU
12	L	75	HIS
12	L	81	SER
12	L	82	VAL
12	L	98	TYR
12	L	101	VAL
12	L	113	ARG
12	L	116	SER
12	L	122	THR
12	L	127	GLU
13	M	7	VAL
13	M	11	ARG
13	M	14	ARG
13	M	17	VAL
13	M	22	ILE
13	M	27	LYS
13	M	32	GLU
13	M	44	ARG
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	52	GLU

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Mol	Chain	Res	Type
13	M	55	ARG
13	M	56	LEU
13	M	57	ARG
13	M	58	GLU
13	M	59	TYR
13	M	64	TRP
13	M	67	GLU
13	M	69	GLU
13	M	70	LEU
13	M	74	VAL
13	M	81	LEU
13	M	84	ILE
13	M	87	TYR
13	M	88	ARG
13	M	94	ARG
13	M	99	ARG
13	M	102	ARG
13	M	105	THR
14	N	3	ARG
14	N	6	LEU
14	N	7	ILE
14	N	9	LYS
14	N	12	ARG
14	N	17	LYS
14	N	24	CYS
14	N	27	CYS
14	N	29	ARG
14	N	33	VAL
14	N	45	ARG
14	N	46	GLU
14	N	49	HIS
14	N	58	LYS
15	O	6	GLU
15	O	11	VAL
15	O	17	ARG
15	O	24	SER
15	O	26	GLU
15	O	31	LEU
15	O	38	ARG
15	O	39	LEU
15	O	40	SER
15	O	45	VAL

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Mol	Chain	Res	Type
15	O	47	LYS
15	O	54	ARG
15	O	56	LEU
15	O	57	LEU
15	O	67	LEU
15	O	73	GLU
15	O	81	LEU
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	8	ARG
16	P	11	SER
16	P	18	ARG
16	P	22	THR
16	P	25	ARG
16	P	42	ARG
16	P	45	THR
16	P	48	TRP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	69	THR
16	P	72	ARG
16	P	75	ARG
16	P	79	VAL
16	P	81	ARG
17	Q	10	VAL
17	Q	13	ASP
17	Q	23	VAL
17	Q	27	PHE
17	Q	29	HIS
17	Q	36	ILE
17	Q	40	LYS
17	Q	43	LEU
17	Q	50	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	62	SER
17	Q	70	ARG
17	Q	72	ARG
17	Q	77	VAL

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Mol	Chain	Res	Type
17	Q	85	VAL
17	Q	90	ILE
17	Q	91	ARG
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
18	R	18	ARG
18	R	26	LEU
18	R	31	LEU
18	R	38	GLU
18	R	42	ARG
18	R	44	LEU
18	R	46	GLU
18	R	58	LEU
18	R	70	ILE
18	R	78	LEU
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	4	SER
19	S	7	LYS
19	S	11	VAL
19	S	14	HIS
19	S	15	LEU
19	S	16	LEU
19	S	17	GLU
19	S	27	GLU
19	S	29	ARG
19	S	31	ILE
19	S	37	ARG
19	S	39	THR
19	S	43	GLU
19	S	58	VAL
19	S	64	GLU
19	S	71	LEU
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	15	ARG

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Mol	Chain	Res	Type
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	33	ILE
20	T	45	GLN
20	T	55	ILE
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG
20	T	85	MET
20	T	86	ARG
20	T	87	LYS
20	T	91	LEU
20	T	99	LEU
20	T	100	ILE
20	T	104	LEU
21	U	10	ARG
21	U	15	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
4	D	125	HIS
5	E	65	ASN
7	G	37	ASN
9	I	73	GLN
12	L	75	HIS
13	M	101	GLN
15	O	42	HIS
16	P	16	HIS
19	S	23	ASN
19	S	57	HIS
20	T	9	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	377 (25%)	48 (3%)
22	V	3/4 (75%)	1 (33%)	0
23	W	10/11 (90%)	2 (20%)	0
24	a	7/8 (87%)	4 (57%)	0
25	b	2/3 (66%)	0	0
All	All	1525/1548 (98%)	384 (25%)	48 (3%)

All (384) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	16	A
1	A	31	G
1	A	32	A
1	A	33	A
1	A	34	C
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	81	U
1	A	82	U
1	A	88	A
1	A	89	C
1	A	90	U
1	A	91	C
1	A	95	U
1	A	99	C
1	A	105	G
1	A	108	G
1	A	109	A
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	138	G
1	A	144	G
1	A	151	A
1	A	157	G

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Mol	Chain	Res	Type
1	A	159	G
1	A	162	A
1	A	163	C
1	A	170	U
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(B)	C
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	216	G
1	A	222	U
1	A	225	C
1	A	230	G
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	258	G
1	A	260	G
1	A	266	G
1	A	267	C
1	A	276	G
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	345	C

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Mol	Chain	Res	Type
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	384	G
1	A	387	U
1	A	388	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	435	C
1	A	439	A
1	A	442	C
1	A	443	C
1	A	449	C
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	475	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C

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Mol	Chain	Res	Type
1	A	519	C
1	A	520	A
1	A	527	7MG
1	A	530	G
1	A	532	A
1	A	533	A
1	A	544	G
1	A	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	569	C
1	A	571	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	578	C
1	A	587	G
1	A	588	G
1	A	607	A
1	A	624	C
1	A	629	G
1	A	631	G
1	A	644	G
1	A	651	C
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	673	G
1	A	675	A
1	A	687	A
1	A	688	G
1	A	695	A

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Mol	Chain	Res	Type
1	A	698	G
1	A	701	C
1	A	702	A
1	A	704	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	734	G
1	A	741	G
1	A	747	C
1	A	748	C
1	A	752	G
1	A	755	G
1	A	777	A
1	A	785	G
1	A	786	G
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	804	U
1	A	812	C
1	A	813	U
1	A	815	A
1	A	816	A
1	A	817	C
1	A	827	U
1	A	828	A
1	A	829	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	866	C
1	A	867	G
1	A	868	C
1	A	869	G

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Mol	Chain	Res	Type
1	A	873	A
1	A	889	A
1	A	902	G
1	A	905	U
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	933	G
1	A	934	C
1	A	935	A
1	A	944	G
1	A	950	U
1	A	954	G
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	984	C
1	A	985	C
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1021	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1045	C
1	A	1048	G

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Mol	Chain	Res	Type
1	A	1050	G
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1079	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1111	A
1	A	1122	U
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1159	U
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1178	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1193	G

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Mol	Chain	Res	Type
1	A	1196	U
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1235	U
1	A	1238	A
1	A	1245	A
1	A	1249	C
1	A	1250	A
1	A	1251	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1312	G
1	A	1313	U
1	A	1317	C

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Mol	Chain	Res	Type
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1328	C
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1356	G
1	A	1359	C
1	A	1360	A
1	A	1361	G
1	A	1362	C
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1393	U
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1406	U
1	A	1407	5MC
1	A	1414	U
1	A	1418	A
1	A	1419	G
1	A	1420	C
1	A	1442	G
1	A	1443	G
1	A	1447	G
1	A	1451	A
1	A	1455	G
1	A	1478	C
1	A	1487	G
1	A	1494	G
1	A	1497	G
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1526	G
1	A	1529	G
1	A	1530	G
1	A	1534	C
1	A	1538	C
22	V	2	U
23	W	31	C
23	W	33	U
24	a	35	G
24	a	37	A
24	a	39	G
24	a	40	PSU

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	89	C
1	A	115	G
1	A	129(A)	G
1	A	150	C
1	A	181	G
1	A	204	U
1	A	246	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C
1	A	344	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	499	A
1	A	509	A
1	A	544	G
1	A	559	A
1	A	560	U
1	A	587	G
1	A	687	A

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Mol	Chain	Res	Type
1	A	701	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	991	U
1	A	1026	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1137	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1279	A
1	A	1281	U
1	A	1300	G
1	A	1319	A
1	A	1347	G
1	A	1360	A
1	A	1361(A)	C
1	A	1397	C
1	A	1528	U
1	A	1533	C

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	967	1	15,22,23	0.87	0	19,32,35	1.08	2 (10%)
1	5MC	A	1404	1	15,22,23	0.96	1 (6%)	19,32,35	1.16	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	7MG	A	527	1	22,26,27	2.79	9 (40%)	28,39,42	1.49	4 (14%)
1	M2G	A	966	1	20,27,28	1.36	3 (15%)	22,40,43	2.35	5 (22%)
1	2MG	A	1207	1	19,26,27	2.94	5 (26%)	21,38,41	2.35	2 (9%)
1	UR3	A	1498	1	14,22,23	0.88	1 (7%)	15,32,35	0.97	0
1	MA6	A	1518[A]	1	19,26,27	1.34	4 (21%)	18,38,41	0.70	0
1	5MC	A	1407	1	15,22,23	1.87	2 (13%)	19,32,35	1.14	1 (5%)
12	0TD	L	92	12	4,9,10	1.16	0	3,11,13	4.33	2 (66%)
23	PSU	W	40	23	17,21,22	1.06	2 (11%)	20,30,33	3.24	7 (35%)
1	PSU	A	516	1	17,21,22	1.37	2 (11%)	20,30,33	3.35	5 (25%)
1	4OC	A	1402	1	16,23,24	1.75	4 (25%)	17,32,35	1.31	1 (5%)
1	PSU	A	1540	1	17,21,22	1.08	1 (5%)	20,30,33	3.21	5 (25%)
1	MA6	A	1519[A]	1	19,26,27	1.14	2 (10%)	18,38,41	0.87	0
1	MA6	A	1518[B]	1	19,26,27	1.22	2 (10%)	18,38,41	0.80	0
1	MA6	A	1519[B]	1	19,26,27	1.98	5 (26%)	18,38,41	0.72	0
24	PSU	a	40	24,1	17,21,22	1.68	2 (11%)	20,30,33	3.60	6 (30%)
1	5MC	A	1400	1	15,22,23	1.55	4 (26%)	19,32,35	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	3/5/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	3/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	2/5/25/26	0/2/2/2
12	0TD	L	92	12	-	2/3/12/14	-
23	PSU	W	40	23	-	6/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	5/9/29/30	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	5/7/29/30	0/3/3/3
24	PSU	a	40	24,1	-	3/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	8.20	1.41	1.34
1	A	1207	2MG	C6-N1	7.15	1.45	1.33
1	A	527	7MG	C6-C5	6.68	1.50	1.41
1	A	1407	5MC	C5-C4	6.01	1.50	1.41
1	A	527	7MG	C8-N9	-5.72	1.32	1.45
24	a	40	PSU	C5-C1'	5.29	1.56	1.52
1	A	1519[B]	MA6	C6-N1	4.80	1.40	1.33
1	A	527	7MG	C2-N2	4.69	1.43	1.33
1	A	527	7MG	C4-N3	4.42	1.39	1.34
1	A	1402	4OC	C2-N3	4.28	1.46	1.38
1	A	1519[B]	MA6	C2-N1	4.26	1.41	1.33
1	A	966	M2G	C6-N1	4.16	1.40	1.33
1	A	1207	2MG	C6-C5	3.99	1.48	1.41
1	A	527	7MG	C5-N7	3.73	1.46	1.39
1	A	1519[B]	MA6	C2-N3	3.72	1.38	1.32
1	A	516	PSU	C4-N3	3.63	1.39	1.33
1	A	1207	2MG	C2-N1	3.55	1.45	1.34
1	A	1540	PSU	C4-N3	3.47	1.39	1.33
1	A	1400	5MC	C2-N3	3.22	1.44	1.38
1	A	1518[B]	MA6	C6-N1	3.18	1.37	1.33
1	A	1400	5MC	C5-C4	3.01	1.46	1.41
1	A	1400	5MC	C4-N4	2.97	1.41	1.34
1	A	516	PSU	C5-C1'	2.94	1.54	1.52
1	A	1402	4OC	CM4-N4	2.91	1.50	1.45
24	a	40	PSU	C4-N3	2.89	1.38	1.33
1	A	1519[B]	MA6	C4-N3	2.87	1.39	1.35
1	A	1518[A]	MA6	C2-N1	2.85	1.39	1.33
1	A	527	7MG	CM7-N7	-2.83	1.41	1.46
23	W	40	PSU	C4-N3	2.82	1.37	1.33
1	A	1518[B]	MA6	C2-N1	2.76	1.39	1.33
1	A	1407	5MC	C2-N3	2.57	1.43	1.38
1	A	1518[A]	MA6	C4-N3	2.56	1.39	1.35
1	A	1498	UR3	C6-N1	-2.53	1.32	1.35
1	A	1519[B]	MA6	C5-C4	2.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519[A]	MA6	C2-N1	2.44	1.38	1.33
1	A	527	7MG	O5'-C5'	-2.40	1.38	1.44
1	A	966	M2G	C2-N1	2.39	1.38	1.34
1	A	966	M2G	C4-N3	2.36	1.39	1.35
1	A	527	7MG	C5-C4	-2.34	1.34	1.39
1	A	1518[A]	MA6	C5-C4	2.33	1.47	1.40
1	A	1519[A]	MA6	C6-N1	2.20	1.36	1.33
1	A	1402	4OC	C4-N3	-2.17	1.30	1.34
23	W	40	PSU	C5-C1'	-2.15	1.50	1.52
1	A	527	7MG	C6-N1	2.14	1.36	1.33
1	A	1518[A]	MA6	C6-N1	2.13	1.36	1.33
1	A	1402	4OC	C4-N4	-2.11	1.31	1.36
1	A	1404	5MC	C5-C4	2.08	1.44	1.41
1	A	1207	2MG	C4-N3	2.08	1.38	1.35
1	A	1400	5MC	C4-N3	2.01	1.37	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	40	PSU	N1-C2-N3	-12.47	118.52	128.43
1	A	516	PSU	N1-C2-N3	-11.62	119.19	128.43
1	A	1540	PSU	N1-C2-N3	-11.41	119.36	128.43
23	W	40	PSU	N1-C2-N3	-10.37	120.19	128.43
1	A	1207	2MG	C5-C6-N1	-9.40	110.58	123.43
1	A	966	M2G	C5-C6-N1	-8.25	112.14	123.43
1	A	516	PSU	C4-N3-C2	6.73	120.82	115.14
23	W	40	PSU	C4-N3-C2	6.04	120.25	115.14
1	A	1540	PSU	C4-N3-C2	6.01	120.22	115.14
12	L	92	0TD	CB-CA-N	-5.99	96.33	109.10
24	a	40	PSU	C4-N3-C2	5.58	119.85	115.14
1	A	966	M2G	C6-N1-C2	5.48	122.71	116.18
24	a	40	PSU	C6-N1-C2	5.01	123.63	115.36
23	W	40	PSU	C5-C4-N3	-4.82	119.14	125.36
24	a	40	PSU	C5-C1'-C2'	4.68	123.66	115.32
1	A	1207	2MG	C6-N1-C2	4.25	122.80	115.18
12	L	92	0TD	CSB-SB-CB	-4.22	93.56	101.85
1	A	1402	4OC	CM4-N4-C4	-4.01	119.52	122.97
1	A	516	PSU	C5-C4-N3	-3.86	120.39	125.36
24	a	40	PSU	C5-C6-N1	-3.75	119.83	124.44
1	A	1540	PSU	C5-C4-N3	-3.59	120.74	125.36
23	W	40	PSU	C5-C6-N1	-3.44	120.20	124.44
1	A	1540	PSU	C6-N1-C2	3.36	120.91	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	C6-N1-C2	3.22	120.68	115.36
1	A	1407	5MC	N4-C4-N3	-3.19	112.52	117.03
1	A	527	7MG	C5-C4-N3	-3.17	121.31	126.49
1	A	1400	5MC	C2-N3-C4	3.16	119.83	116.02
23	W	40	PSU	C5-C1'-C2'	-3.12	109.75	115.32
23	W	40	PSU	C6-N1-C2	3.02	120.33	115.36
1	A	527	7MG	C2-N3-C4	2.85	121.76	113.89
1	A	527	7MG	N7-C8-N9	2.76	107.33	103.38
1	A	966	M2G	C2-N3-C4	-2.65	112.27	115.28
23	W	40	PSU	O4'-C1'-C5	-2.64	105.84	109.93
1	A	967	5MC	CM5-C5-C6	2.61	124.18	118.68
1	A	527	7MG	N3-C4-N9	2.54	130.18	126.91
1	A	966	M2G	N1-C2-N2	-2.47	114.69	117.19
1	A	967	5MC	C2-N3-C4	2.39	118.91	116.02
24	a	40	PSU	C5-C4-N3	-2.30	122.40	125.36
1	A	1540	PSU	C5-C6-N1	-2.29	121.62	124.44
1	A	1404	5MC	C5-C4-N3	2.24	124.79	121.26
1	A	516	PSU	O4'-C1'-C2'	2.16	108.16	104.66
1	A	966	M2G	CM1-N2-C2	-2.09	119.30	121.29
1	A	1404	5MC	N4-C4-N3	-2.05	114.13	117.03

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	967	5MC	C2'-C1'-N1-C6
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	1498	UR3	C2'-C1'-N1-C6
1	A	1518[A]	MA6	C5-C6-N6-C9
1	A	1518[A]	MA6	C5-C6-N6-C10
1	A	1407	5MC	O4'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
23	W	40	PSU	C2'-C1'-C5-C4
23	W	40	PSU	C2'-C1'-C5-C6
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	C2'-C1'-N1-C6
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
24	a	40	PSU	O4'-C1'-C5-C4
24	a	40	PSU	O4'-C1'-C5-C6
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1407	5MC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	N1-C6-N6-C9
1	A	1519[A]	MA6	N1-C6-N6-C9
24	a	40	PSU	C2'-C1'-C5-C6
23	W	40	PSU	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10
23	W	40	PSU	O4'-C4'-C5'-O5'
23	W	40	PSU	O4'-C1'-C5-C6
23	W	40	PSU	O4'-C1'-C5-C4
12	L	92	0TD	CA-CB-SB-CSB
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	0	1

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 347 ligands modelled in this entry, 346 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	SRY	A	1928	-	40,42,42	2.31	11 (27%)	49,63,63	2.56	17 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SRY	A	1928	-	-	6/20/87/87	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1928	SRY	CD1-N31	9.25	1.49	1.33
27	A	1928	SRY	CA1-N11	5.72	1.43	1.33
27	A	1928	SRY	O53-C53	-3.59	1.35	1.44
27	A	1928	SRY	C23-N23	-3.08	1.42	1.47
27	A	1928	SRY	C32-CG2	-2.96	1.47	1.52
27	A	1928	SRY	C11-N11	-2.61	1.41	1.45
27	A	1928	SRY	CD1-NE1	2.53	1.45	1.34
27	A	1928	SRY	C21-C11	-2.47	1.48	1.53
27	A	1928	SRY	CA1-NB1	2.37	1.44	1.34
27	A	1928	SRY	C21-C31	-2.09	1.49	1.53
27	A	1928	SRY	O51-C51	-2.04	1.38	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	1928	SRY	C43-C33-C23	-7.52	99.32	110.34
27	A	1928	SRY	C61-C11-N11	-6.41	98.51	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	1928	SRY	C12-O42-C42	-6.15	98.71	108.38
27	A	1928	SRY	C13-O13-C22	-5.45	106.79	116.25
27	A	1928	SRY	O53-C13-C23	4.39	119.15	110.58
27	A	1928	SRY	O53-C53-C43	3.95	116.86	109.69
27	A	1928	SRY	O41-C41-C51	3.65	116.99	107.28
27	A	1928	SRY	O32-C32-C22	3.51	119.76	111.62
27	A	1928	SRY	C51-C61-C11	3.22	115.05	110.34
27	A	1928	SRY	O21-C21-C31	3.00	115.72	109.66
27	A	1928	SRY	O51-C51-C61	-2.95	103.52	110.35
27	A	1928	SRY	OG2-CG2-C32	-2.84	117.71	124.27
27	A	1928	SRY	O53-C53-C63	-2.48	100.26	106.44
27	A	1928	SRY	O43-C43-C33	2.29	115.64	110.35
27	A	1928	SRY	C63-C53-C43	-2.17	107.92	113.00
27	A	1928	SRY	O63-C63-C53	-2.06	104.24	111.29
27	A	1928	SRY	CI3-N23-C23	-2.02	111.44	114.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

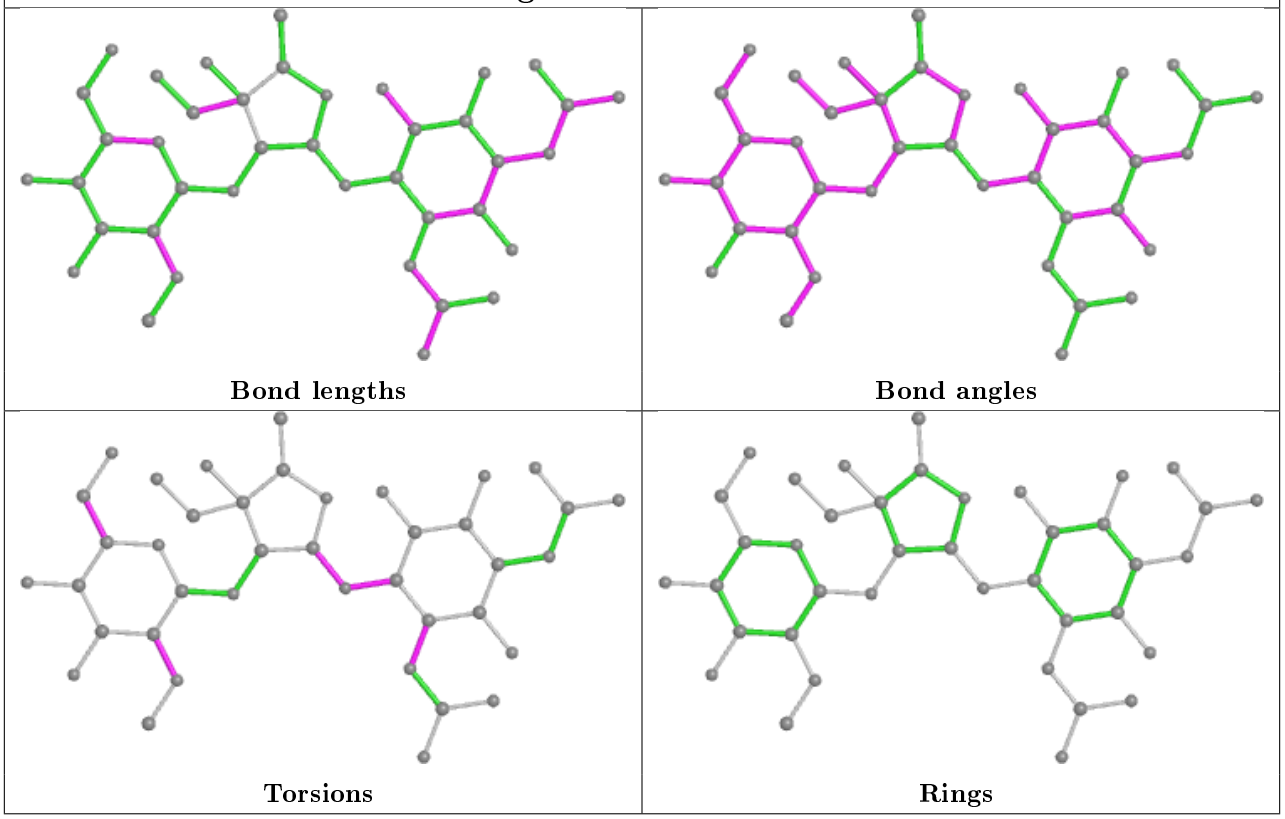
Mol	Chain	Res	Type	Atoms
27	A	1928	SRY	O53-C53-C63-O63
27	A	1928	SRY	C43-C53-C63-O63
27	A	1928	SRY	O42-C12-O41-C41
27	A	1928	SRY	C51-C41-O41-C12
27	A	1928	SRY	C13-C23-N23-CI3
27	A	1928	SRY	C21-C31-N31-CD1

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SRY A 1928



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1500/1522 (98%)	-0.49	2 (0%) 95 96	80, 129, 232, 327	0
2	B	236/256 (92%)	-0.17	3 (1%) 77 73	62, 153, 220, 247	0
3	C	207/239 (86%)	-0.25	5 (2%) 59 53	94, 191, 226, 244	0
4	D	208/209 (99%)	-0.24	5 (2%) 59 53	105, 149, 198, 214	0
5	E	151/162 (93%)	-0.46	0 100 100	80, 114, 166, 193	0
6	F	101/101 (100%)	-0.49	1 (0%) 82 79	110, 150, 182, 226	0
7	G	155/156 (99%)	-0.41	3 (1%) 66 62	121, 160, 223, 238	0
8	H	138/138 (100%)	-0.45	0 100 100	75, 104, 138, 155	0
9	I	127/128 (99%)	0.08	3 (2%) 59 53	125, 184, 217, 240	0
10	J	99/105 (94%)	0.14	4 (4%) 38 33	81, 203, 272, 295	0
11	K	117/129 (90%)	-0.42	0 100 100	88, 130, 160, 167	0
12	L	124/135 (91%)	0.03	5 (4%) 38 33	97, 136, 168, 247	0
13	M	118/126 (93%)	0.05	5 (4%) 36 31	127, 158, 192, 211	0
14	N	60/61 (98%)	-0.22	1 (1%) 70 65	144, 169, 210, 246	0
15	O	88/89 (98%)	-0.01	2 (2%) 60 55	94, 127, 182, 225	0
16	P	84/88 (95%)	-0.24	0 100 100	96, 126, 164, 239	0
17	Q	100/105 (95%)	-0.34	0 100 100	83, 111, 150, 189	0
18	R	71/88 (80%)	-0.32	0 100 100	95, 132, 178, 229	0
19	S	81/93 (87%)	0.16	2 (2%) 57 51	84, 184, 228, 234	0
20	T	99/106 (93%)	-0.28	0 100 100	95, 126, 167, 212	0
21	U	25/27 (92%)	0.40	2 (8%) 12 10	77, 163, 192, 220	0
22	V	4/4 (100%)	3.96	4 (100%) 0 0	263, 267, 272, 275	0
23	W	10/11 (90%)	7.09	10 (100%) 0 0	234, 291, 345, 387	5 (50%)
24	a	7/8 (87%)	0.68	1 (14%) 2 3	200, 217, 290, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	b	3/3 (100%)	1.05	0 100 100	172, 172, 206, 218	0
All	All	3913/4089 (95%)	-0.29	58 (1%) 73 69	62, 140, 222, 387	5 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	32	C	13.1
23	W	31	C	8.8
23	W	33	U	8.2
1	A	1129	C	7.9
23	W	30	G	7.6
23	W	35	G	7.6
12	L	129	ALA	7.0
15	O	89	GLY	7.0
23	W	37	A	6.1
23	W	38	A	6.0
22	V	2	U	5.1
23	W	36	A	5.0
22	V	3	U	4.9
23	W	34	G	4.9
21	U	18	TYR	4.6
10	J	33	GLN	4.2
10	J	34	VAL	3.8
23	W	39	G	3.7
9	I	15	ALA	3.5
12	L	65	GLU	3.5
22	V	4	U	3.4
6	F	101	ALA	3.1
7	G	83	ALA	3.1
13	M	2	ALA	3.0
7	G	84	ASN	3.0
12	L	33	ARG	2.9
13	M	117	VAL	2.9
7	G	82	GLY	2.9
3	C	157	ILE	2.9
3	C	158	GLY	2.9
12	L	128	ALA	2.8
3	C	155	GLY	2.8
14	N	12	ARG	2.7
4	D	42	GLN	2.7
1	A	82	U	2.6
10	J	74	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
19	S	38	SER	2.5
4	D	13	ARG	2.5
3	C	189	ALA	2.5
24	a	34	G	2.5
3	C	193	TYR	2.5
22	V	1	U	2.4
9	I	65	VAL	2.3
15	O	88	ARG	2.3
13	M	15	VAL	2.3
13	M	116	THR	2.3
2	B	72	GLY	2.3
10	J	87	THR	2.2
21	U	17	THR	2.2
19	S	12	ASP	2.2
12	L	64	TYR	2.2
4	D	43	HIS	2.2
9	I	66	ARG	2.2
13	M	5	ALA	2.1
2	B	188	ALA	2.0
2	B	203	GLY	2.0
4	D	45	GLN	2.0
4	D	40	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PSU	W	40	20/21	0.68	0.33	291,301,325,326	0
1	PSU	A	1540	20/21	0.71	0.35	253,269,289,293	0
24	PSU	a	40	20/21	0.81	0.32	208,236,258,262	0
1	4OC	A	1402	22/23	0.92	0.21	104,119,127,142	0
1	M2G	A	966	25/26	0.94	0.18	122,137,142,145	0
1	MA6	A	1518[B]	24/25	0.94	0.20	107,122,137,148	24
1	MA6	A	1518[A]	24/25	0.94	0.20	110,122,127,131	24
1	5MC	A	1404	21/22	0.95	0.17	102,129,148,149	0
1	UR3	A	1498	21/22	0.95	0.25	111,124,183,193	0
1	5MC	A	1400	21/22	0.95	0.17	103,130,148,159	0
1	MA6	A	1519[A]	24/25	0.96	0.30	100,115,125,126	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	516	20/21	0.96	0.10	123,147,168,168	0
1	MA6	A	1519[B]	24/25	0.96	0.30	101,116,129,130	24
1	5MC	A	1407	21/22	0.96	0.11	127,152,158,162	0
1	2MG	A	1207	24/25	0.96	0.15	154,167,200,202	0
1	5MC	A	967	21/22	0.97	0.12	117,131,145,146	0
1	7MG	A	527	24/25	0.97	0.17	91,114,123,126	0
12	0TD	L	92	10/11	0.99	0.22	113,121,127,289	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1886	1/1	-0.00	1.21	121,121,121,121	0
26	MG	A	1910	1/1	0.10	0.29	120,120,120,120	0
26	MG	A	1901	1/1	0.24	0.35	101,101,101,101	0
26	MG	D	304	1/1	0.35	0.54	455,455,455,455	0
26	MG	A	1794	1/1	0.42	0.27	518,518,518,518	0
26	MG	A	1624	1/1	0.43	1.10	147,147,147,147	0
26	MG	A	1926	1/1	0.50	0.58	116,116,116,116	0
26	MG	A	1675	1/1	0.53	1.12	122,122,122,122	0
26	MG	A	1846	1/1	0.54	0.33	449,449,449,449	0
26	MG	A	1892	1/1	0.54	0.38	92,92,92,92	0
26	MG	A	1729	1/1	0.59	0.55	101,101,101,101	0
26	MG	G	201	1/1	0.60	0.83	117,117,117,117	0
26	MG	A	1770	1/1	0.61	0.62	106,106,106,106	0
26	MG	A	1622	1/1	0.62	0.51	81,81,81,81	0
26	MG	A	1808	1/1	0.62	0.45	498,498,498,498	0
26	MG	A	1665	1/1	0.63	0.67	117,117,117,117	0
26	MG	A	1730	1/1	0.64	0.71	97,97,97,97	0
26	MG	A	1904	1/1	0.64	0.66	97,97,97,97	0
26	MG	A	1917	1/1	0.64	0.85	128,128,128,128	0
26	MG	A	1769	1/1	0.67	0.54	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	P	102	1/1	0.68	0.35	101,101,101,101	0
26	MG	A	1914	1/1	0.68	1.03	99,99,99,99	0
26	MG	A	1921	1/1	0.69	0.39	84,84,84,84	0
26	MG	A	1758	1/1	0.70	0.31	101,101,101,101	0
26	MG	A	1909	1/1	0.71	0.35	93,93,93,93	0
26	MG	A	1744	1/1	0.72	0.32	82,82,82,82	0
26	MG	A	1774	1/1	0.73	0.42	109,109,109,109	0
26	MG	A	1781	1/1	0.73	0.35	104,104,104,104	0
26	MG	A	1699	1/1	0.74	0.07	414,414,414,414	0
26	MG	A	1916	1/1	0.74	0.19	119,119,119,119	0
26	MG	A	1724	1/1	0.74	0.54	117,117,117,117	0
26	MG	A	1734	1/1	0.75	0.52	124,124,124,124	0
26	MG	P	103	1/1	0.75	0.47	96,96,96,96	0
26	MG	A	1912	1/1	0.75	0.55	104,104,104,104	0
26	MG	A	1891	1/1	0.75	0.16	127,127,127,127	0
26	MG	A	1760	1/1	0.76	0.60	88,88,88,88	0
26	MG	A	1793	1/1	0.76	0.27	483,483,483,483	0
26	MG	A	1813	1/1	0.76	0.67	471,471,471,471	0
26	MG	A	1880	1/1	0.77	0.48	508,508,508,508	0
26	MG	A	1877	1/1	0.77	0.43	456,456,456,456	1
26	MG	A	1899	1/1	0.77	0.33	68,68,68,68	0
26	MG	A	1711	1/1	0.77	1.00	133,133,133,133	0
26	MG	A	1759	1/1	0.78	0.86	86,86,86,86	0
26	MG	A	1632	1/1	0.78	0.33	248,248,248,248	0
26	MG	A	1913	1/1	0.78	0.78	108,108,108,108	0
26	MG	A	1923	1/1	0.79	0.78	86,86,86,86	0
26	MG	N	102	1/1	0.79	0.54	107,107,107,107	0
26	MG	A	1809	1/1	0.79	0.23	494,494,494,494	0
26	MG	A	1743	1/1	0.79	0.36	105,105,105,105	0
26	MG	A	1887	1/1	0.79	0.55	102,102,102,102	0
26	MG	A	1628	1/1	0.80	0.28	152,152,152,152	0
26	MG	A	1894	1/1	0.80	0.20	94,94,94,94	0
26	MG	E	204	1/1	0.80	0.26	128,128,128,128	0
26	MG	A	1852	1/1	0.80	0.34	450,450,450,450	0
26	MG	P	101	1/1	0.80	0.32	58,58,58,58	0
26	MG	A	1871	1/1	0.80	0.25	392,392,392,392	0
26	MG	A	1700	1/1	0.80	0.37	302,302,302,302	0
26	MG	A	1679	1/1	0.81	0.18	369,369,369,369	0
26	MG	A	1898	1/1	0.81	0.63	89,89,89,89	0
26	MG	D	302	1/1	0.81	0.39	104,104,104,104	0
26	MG	A	1893	1/1	0.82	0.44	114,114,114,114	0
26	MG	A	1618	1/1	0.82	0.39	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1728	1/1	0.82	0.86	114,114,114,114	0
26	MG	A	1884	1/1	0.82	1.05	119,119,119,119	0
26	MG	H	201	1/1	0.82	0.33	67,67,67,67	0
26	MG	A	1863	1/1	0.82	0.22	409,409,409,409	0
26	MG	A	1925	1/1	0.82	0.15	114,114,114,114	0
26	MG	A	1902	1/1	0.83	0.35	119,119,119,119	0
26	MG	A	1649	1/1	0.83	0.33	84,84,84,84	0
26	MG	A	1837	1/1	0.83	0.24	469,469,469,469	0
26	MG	A	1779	1/1	0.83	0.33	102,102,102,102	0
26	MG	A	1908	1/1	0.83	0.30	81,81,81,81	0
26	MG	A	1766	1/1	0.83	0.52	105,105,105,105	0
26	MG	A	1865	1/1	0.83	0.39	457,457,457,457	0
26	MG	A	1684	1/1	0.83	0.13	109,109,109,109	0
26	MG	A	1834	1/1	0.83	0.93	412,412,412,412	1
26	MG	A	1900	1/1	0.84	0.33	93,93,93,93	0
26	MG	A	1897	1/1	0.84	0.43	114,114,114,114	0
26	MG	A	1636	1/1	0.84	0.41	88,88,88,88	0
26	MG	A	1807	1/1	0.84	0.47	517,517,517,517	1
26	MG	A	1723	1/1	0.84	0.26	117,117,117,117	0
26	MG	A	1740	1/1	0.84	0.56	93,93,93,93	0
26	MG	A	1784	1/1	0.84	0.28	122,122,122,122	0
26	MG	A	1726	1/1	0.85	0.16	98,98,98,98	0
26	MG	A	1694	1/1	0.85	0.40	87,87,87,87	0
26	MG	A	1707	1/1	0.85	0.35	135,135,135,135	0
26	MG	A	1819	1/1	0.85	0.52	493,493,493,493	0
26	MG	A	1836	1/1	0.86	0.22	416,416,416,416	1
26	MG	A	1814	1/1	0.86	0.18	440,440,440,440	0
26	MG	A	1614	1/1	0.86	0.17	285,285,285,285	0
26	MG	A	1670	1/1	0.86	0.46	234,234,234,234	0
26	MG	A	1797	1/1	0.86	0.16	502,502,502,502	0
26	MG	A	1838	1/1	0.87	0.57	538,538,538,538	0
26	MG	A	1644	1/1	0.87	0.38	127,127,127,127	0
26	MG	A	1876	1/1	0.87	0.46	463,463,463,463	1
26	MG	A	1722	1/1	0.87	0.89	95,95,95,95	0
26	MG	A	1826	1/1	0.87	0.08	395,395,395,395	0
26	MG	A	1697	1/1	0.87	0.18	135,135,135,135	0
26	MG	A	1647	1/1	0.87	0.30	104,104,104,104	0
26	MG	F	601	1/1	0.87	0.06	102,102,102,102	0
26	MG	A	1682	1/1	0.87	0.07	242,242,242,242	0
26	MG	A	1678	1/1	0.88	0.11	217,217,217,217	0
26	MG	A	1881	1/1	0.88	0.13	414,414,414,414	0
26	MG	A	1737	1/1	0.88	0.70	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1889	1/1	0.88	0.22	95,95,95,95	0
26	MG	A	1732	1/1	0.88	0.20	100,100,100,100	0
26	MG	A	1639	1/1	0.88	0.19	87,87,87,87	0
26	MG	A	1879	1/1	0.89	0.28	438,438,438,438	0
26	MG	A	1657	1/1	0.89	0.33	220,220,220,220	0
26	MG	A	1617	1/1	0.89	0.22	85,85,85,85	0
26	MG	A	1762	1/1	0.89	0.43	82,82,82,82	0
26	MG	A	1720	1/1	0.89	0.25	74,74,74,74	0
26	MG	A	1727	1/1	0.89	0.66	84,84,84,84	0
26	MG	A	1745	1/1	0.89	0.47	92,92,92,92	0
26	MG	A	1660	1/1	0.89	0.23	224,224,224,224	0
26	MG	A	1717	1/1	0.89	0.22	152,152,152,152	0
26	MG	A	1655	1/1	0.89	0.29	125,125,125,125	0
26	MG	A	1878	1/1	0.89	0.20	346,346,346,346	0
26	MG	A	1772	1/1	0.89	0.12	93,93,93,93	0
26	MG	A	1804	1/1	0.89	0.50	447,447,447,447	0
26	MG	A	1785	1/1	0.90	0.21	108,108,108,108	0
26	MG	A	1829	1/1	0.90	0.28	489,489,489,489	0
26	MG	A	1673	1/1	0.90	0.92	91,91,91,91	0
26	MG	A	1890	1/1	0.90	0.18	112,112,112,112	0
26	MG	A	1788	1/1	0.90	0.10	285,285,285,285	0
26	MG	A	1905	1/1	0.90	0.20	105,105,105,105	0
26	MG	A	1676	1/1	0.90	0.28	158,158,158,158	0
26	MG	Q	201	1/1	0.90	0.47	145,145,145,145	0
26	MG	A	1782	1/1	0.90	0.59	87,87,87,87	0
26	MG	A	1795	1/1	0.90	1.11	359,359,359,359	0
26	MG	A	1725	1/1	0.90	0.26	92,92,92,92	0
26	MG	A	1796	1/1	0.90	0.22	416,416,416,416	0
26	MG	A	1799	1/1	0.90	0.21	426,426,426,426	0
26	MG	A	1629	1/1	0.90	0.26	223,223,223,223	0
26	MG	A	1856	1/1	0.91	0.06	478,478,478,478	0
26	MG	A	1907	1/1	0.91	0.27	120,120,120,120	0
26	MG	A	1661	1/1	0.91	0.28	244,244,244,244	0
26	MG	A	1920	1/1	0.91	0.07	138,138,138,138	0
26	MG	A	1895	1/1	0.91	0.18	106,106,106,106	0
26	MG	A	1748	1/1	0.91	0.14	110,110,110,110	0
26	MG	A	1919	1/1	0.91	0.18	78,78,78,78	0
26	MG	A	1767	1/1	0.91	0.32	111,111,111,111	0
26	MG	A	1839	1/1	0.91	0.05	467,467,467,467	0
26	MG	A	1751	1/1	0.91	0.46	76,76,76,76	0
26	MG	A	1739	1/1	0.91	0.17	78,78,78,78	0
26	MG	A	1742	1/1	0.91	0.35	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1777	1/1	0.91	0.15	94,94,94,94	0
26	MG	A	1810	1/1	0.91	0.37	474,474,474,474	0
26	MG	A	1756	1/1	0.91	0.15	126,126,126,126	0
26	MG	A	1688	1/1	0.91	0.41	186,186,186,186	0
26	MG	A	1869	1/1	0.91	0.27	431,431,431,431	0
26	MG	A	1845	1/1	0.91	0.31	410,410,410,410	0
26	MG	A	1815	1/1	0.91	0.22	506,506,506,506	0
26	MG	E	202	1/1	0.91	0.12	124,124,124,124	0
26	MG	A	1798	1/1	0.91	0.07	464,464,464,464	0
26	MG	A	1805	1/1	0.91	0.09	331,331,331,331	0
26	MG	A	1683	1/1	0.91	0.05	154,154,154,154	0
26	MG	A	1790	1/1	0.91	0.14	444,444,444,444	0
26	MG	A	1866	1/1	0.91	0.20	434,434,434,434	0
26	MG	A	1786	1/1	0.92	0.09	109,109,109,109	0
26	MG	A	1853	1/1	0.92	0.25	502,502,502,502	0
26	MG	A	1671	1/1	0.92	0.24	96,96,96,96	0
26	MG	A	1613	1/1	0.92	0.15	202,202,202,202	0
26	MG	A	1663	1/1	0.92	0.14	160,160,160,160	0
26	MG	A	1817	1/1	0.92	0.17	419,419,419,419	0
26	MG	A	1773	1/1	0.92	0.10	103,103,103,103	0
26	MG	A	1918	1/1	0.92	0.20	75,75,75,75	0
26	MG	A	1609	1/1	0.92	0.08	157,157,157,157	0
26	MG	A	1695	1/1	0.92	0.06	176,176,176,176	0
26	MG	A	1927	1/1	0.92	0.21	112,112,112,112	0
26	MG	A	1842	1/1	0.92	0.50	488,488,488,488	0
26	MG	A	1844	1/1	0.92	0.08	420,420,420,420	0
26	MG	S	101	1/1	0.92	0.11	115,115,115,115	0
26	MG	A	1621	1/1	0.92	0.16	131,131,131,131	0
26	MG	A	1765	1/1	0.92	0.16	104,104,104,104	0
26	MG	A	1763	1/1	0.92	0.27	120,120,120,120	0
26	MG	A	1792	1/1	0.92	0.17	415,415,415,415	0
26	MG	A	1816	1/1	0.92	0.44	454,454,454,454	0
26	MG	A	1646	1/1	0.93	0.17	136,136,136,136	0
26	MG	A	1757	1/1	0.93	0.21	88,88,88,88	0
26	MG	A	1709	1/1	0.93	0.21	245,245,245,245	0
26	MG	A	1857	1/1	0.93	0.33	308,308,308,308	0
26	MG	A	1753	1/1	0.93	0.24	109,109,109,109	0
26	MG	A	1888	1/1	0.93	0.31	89,89,89,89	0
26	MG	A	1714	1/1	0.93	0.24	108,108,108,108	0
26	MG	A	1903	1/1	0.93	0.21	78,78,78,78	0
26	MG	A	1840	1/1	0.93	0.17	467,467,467,467	1
26	MG	A	1752	1/1	0.93	0.22	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1841	1/1	0.93	0.26	496,496,496,496	0
26	MG	A	1640	1/1	0.93	0.23	172,172,172,172	0
26	MG	A	1860	1/1	0.93	0.21	460,460,460,460	0
26	MG	A	1855	1/1	0.93	0.18	401,401,401,401	0
26	MG	A	1820	1/1	0.93	0.22	373,373,373,373	0
26	MG	A	1718	1/1	0.93	0.24	326,326,326,326	0
26	MG	A	1848	1/1	0.93	0.21	407,407,407,407	0
26	MG	A	1806	1/1	0.93	0.20	505,505,505,505	0
26	MG	A	1850	1/1	0.93	0.07	236,236,236,236	0
26	MG	A	1875	1/1	0.93	0.20	460,460,460,460	0
26	MG	A	1915	1/1	0.93	0.68	117,117,117,117	0
26	MG	A	1883	1/1	0.93	0.26	443,443,443,443	0
26	MG	A	1823	1/1	0.93	0.12	422,422,422,422	0
26	MG	A	1712	1/1	0.94	0.20	170,170,170,170	0
26	MG	A	1681	1/1	0.94	0.03	256,256,256,256	0
26	MG	A	1642	1/1	0.94	0.28	78,78,78,78	0
26	MG	A	1755	1/1	0.94	0.50	74,74,74,74	0
26	MG	A	1825	1/1	0.94	0.19	436,436,436,436	0
26	MG	A	1861	1/1	0.94	0.11	443,443,443,443	0
26	MG	E	201	1/1	0.94	0.35	95,95,95,95	0
26	MG	A	1824	1/1	0.94	0.26	503,503,503,503	0
26	MG	A	1812	1/1	0.94	0.73	444,444,444,444	0
26	MG	A	1864	1/1	0.94	0.20	393,393,393,393	0
26	MG	A	1835	1/1	0.94	0.14	309,309,309,309	0
26	MG	A	1650	1/1	0.94	0.19	151,151,151,151	0
26	MG	A	1659	1/1	0.94	0.29	90,90,90,90	0
26	MG	A	1870	1/1	0.94	0.48	406,406,406,406	0
26	MG	A	1802	1/1	0.94	0.10	355,355,355,355	0
26	MG	A	1768	1/1	0.94	0.35	107,107,107,107	0
26	MG	A	1604	1/1	0.94	0.25	91,91,91,91	0
26	MG	J	201	1/1	0.94	0.42	109,109,109,109	0
26	MG	A	1746	1/1	0.94	0.15	104,104,104,104	0
26	MG	A	1922	1/1	0.95	0.34	110,110,110,110	0
26	MG	A	1641	1/1	0.95	0.17	102,102,102,102	0
26	MG	A	1822	1/1	0.95	0.13	293,293,293,293	0
26	MG	A	1702	1/1	0.95	0.13	279,279,279,279	0
26	MG	A	1637	1/1	0.95	0.29	228,228,228,228	0
26	MG	A	1691	1/1	0.95	0.21	186,186,186,186	0
26	MG	A	1741	1/1	0.95	0.16	105,105,105,105	0
26	MG	A	1706	1/1	0.95	0.13	190,190,190,190	0
26	MG	A	1612	1/1	0.95	0.44	281,281,281,281	0
26	MG	A	1801	1/1	0.95	0.20	464,464,464,464	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1731	1/1	0.95	0.19	68,68,68,68	0
26	MG	A	1849	1/1	0.95	0.31	471,471,471,471	0
26	MG	A	1854	1/1	0.95	0.52	418,418,418,418	0
26	MG	A	1680	1/1	0.95	0.23	214,214,214,214	0
26	MG	A	1643	1/1	0.95	0.08	71,71,71,71	0
26	MG	A	1831	1/1	0.95	0.18	395,395,395,395	0
26	MG	A	1696	1/1	0.95	0.31	263,263,263,263	0
26	MG	A	1735	1/1	0.95	0.12	106,106,106,106	0
26	MG	A	1783	1/1	0.95	0.13	110,110,110,110	0
26	MG	A	1874	1/1	0.96	0.09	467,467,467,467	0
26	MG	A	1780	1/1	0.96	0.32	119,119,119,119	0
26	MG	A	1620	1/1	0.96	0.21	166,166,166,166	0
27	SRY	A	1928	40/40	0.96	0.15	70,100,124,130	0
26	MG	D	303	1/1	0.96	0.21	104,104,104,104	0
26	MG	A	1896	1/1	0.96	0.13	114,114,114,114	0
26	MG	A	1885	1/1	0.96	0.08	84,84,84,84	0
26	MG	A	1906	1/1	0.96	0.12	64,64,64,64	0
26	MG	A	1771	1/1	0.96	0.58	102,102,102,102	0
26	MG	A	1721	1/1	0.96	0.26	92,92,92,92	0
26	MG	A	1800	1/1	0.96	0.32	415,415,415,415	1
26	MG	A	1821	1/1	0.96	0.29	428,428,428,428	0
26	MG	A	1658	1/1	0.96	0.17	115,115,115,115	0
26	MG	S	102	1/1	0.96	0.13	106,106,106,106	0
26	MG	A	1674	1/1	0.96	0.08	260,260,260,260	0
26	MG	A	1664	1/1	0.96	0.19	154,154,154,154	0
26	MG	A	1631	1/1	0.96	0.09	158,158,158,158	0
26	MG	A	1719	1/1	0.96	0.08	262,262,262,262	0
26	MG	A	1705	1/1	0.96	0.13	74,74,74,74	0
26	MG	A	1872	1/1	0.96	0.25	359,359,359,359	0
26	MG	A	1862	1/1	0.96	0.36	268,268,268,268	0
26	MG	A	1924	1/1	0.96	0.11	131,131,131,131	0
26	MG	A	1708	1/1	0.96	0.22	152,152,152,152	0
26	MG	A	1630	1/1	0.96	0.26	158,158,158,158	0
26	MG	A	1787	1/1	0.96	0.25	496,496,496,496	0
26	MG	A	1715	1/1	0.96	0.22	229,229,229,229	0
26	MG	A	1789	1/1	0.96	0.16	378,378,378,378	0
26	MG	E	203	1/1	0.96	0.12	101,101,101,101	0
26	MG	A	1868	1/1	0.96	0.43	380,380,380,380	0
26	MG	A	1776	1/1	0.96	0.17	96,96,96,96	0
26	MG	A	1747	1/1	0.97	0.15	115,115,115,115	0
26	MG	A	1615	1/1	0.97	0.09	147,147,147,147	0
26	MG	A	1775	1/1	0.97	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1710	1/1	0.97	0.13	253,253,253,253	0
26	MG	A	1668	1/1	0.97	0.25	173,173,173,173	0
26	MG	A	1689	1/1	0.97	0.14	126,126,126,126	0
26	MG	A	1602	1/1	0.97	0.47	66,66,66,66	1
26	MG	A	1754	1/1	0.97	0.16	85,85,85,85	0
26	MG	A	1603	1/1	0.97	0.13	277,277,277,277	0
26	MG	A	1811	1/1	0.97	1.55	468,468,468,468	0
26	MG	A	1645	1/1	0.97	0.41	227,227,227,227	0
26	MG	A	1606	1/1	0.97	0.41	87,87,87,87	0
26	MG	A	1634	1/1	0.97	0.08	107,107,107,107	0
26	MG	A	1701	1/1	0.97	0.22	108,108,108,108	0
26	MG	A	1698	1/1	0.97	0.18	124,124,124,124	0
26	MG	A	1830	1/1	0.97	0.27	480,480,480,480	0
26	MG	A	1693	1/1	0.97	0.10	108,108,108,108	0
28	ZN	N	101	1/1	0.97	0.16	164,164,164,164	0
26	MG	A	1685	1/1	0.97	0.50	126,126,126,126	0
26	MG	A	1828	1/1	0.97	0.13	432,432,432,432	0
26	MG	A	1778	1/1	0.97	0.11	119,119,119,119	1
26	MG	A	1791	1/1	0.97	0.19	283,283,283,283	0
26	MG	A	1851	1/1	0.97	0.28	328,328,328,328	0
26	MG	A	1669	1/1	0.97	0.09	123,123,123,123	0
26	MG	A	1672	1/1	0.98	0.10	166,166,166,166	0
26	MG	A	1803	1/1	0.98	0.20	345,345,345,345	0
26	MG	A	1666	1/1	0.98	0.08	149,149,149,149	0
26	MG	A	1761	1/1	0.98	0.59	105,105,105,105	0
26	MG	A	1651	1/1	0.98	0.17	110,110,110,110	0
26	MG	A	1750	1/1	0.98	0.18	74,74,74,74	0
26	MG	A	1847	1/1	0.98	0.18	441,441,441,441	0
26	MG	A	1736	1/1	0.98	0.15	123,123,123,123	0
26	MG	A	1716	1/1	0.98	0.25	132,132,132,132	0
26	MG	A	1654	1/1	0.98	0.09	161,161,161,161	0
26	MG	A	1662	1/1	0.98	0.12	123,123,123,123	0
26	MG	A	1677	1/1	0.98	0.23	235,235,235,235	0
26	MG	A	1843	1/1	0.98	0.68	357,357,357,357	0
26	MG	A	1867	1/1	0.98	0.54	413,413,413,413	1
28	ZN	D	301	1/1	0.98	0.29	138,138,138,138	0
26	MG	A	1667	1/1	0.98	0.18	119,119,119,119	0
26	MG	A	1605	1/1	0.98	0.09	254,254,254,254	0
26	MG	A	1764	1/1	0.98	0.45	78,78,78,78	0
26	MG	A	1832	1/1	0.98	0.09	278,278,278,278	0
26	MG	A	1873	1/1	0.98	0.12	361,361,361,361	0
26	MG	A	1619	1/1	0.98	0.12	64,64,64,64	0

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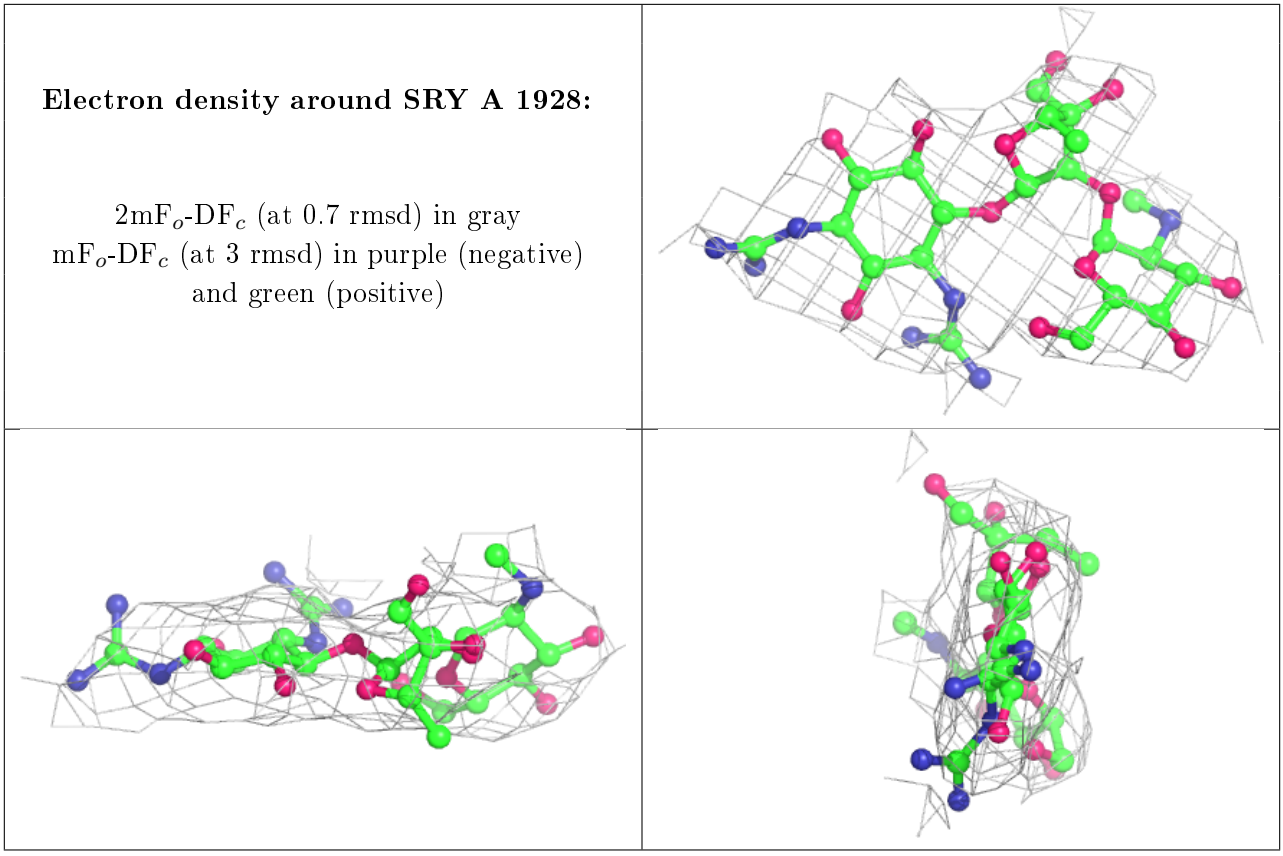
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1608	1/1	0.98	0.21	73,73,73,73	0
26	MG	A	1686	1/1	0.98	0.37	184,184,184,184	0
26	MG	A	1733	1/1	0.98	0.19	70,70,70,70	0
26	MG	A	1633	1/1	0.98	0.18	118,118,118,118	0
26	MG	A	1648	1/1	0.98	0.24	93,93,93,93	0
26	MG	A	1656	1/1	0.98	0.22	236,236,236,236	0
26	MG	A	1690	1/1	0.98	0.07	114,114,114,114	0
26	MG	A	1833	1/1	0.98	0.13	335,335,335,335	0
26	MG	A	1652	1/1	0.98	0.09	72,72,72,72	0
26	MG	A	1687	1/1	0.98	0.14	106,106,106,106	0
26	MG	A	1616	1/1	0.98	0.17	63,63,63,63	0
26	MG	A	1704	1/1	0.98	0.15	104,104,104,104	0
26	MG	A	1818	1/1	0.98	0.09	189,189,189,189	0
26	MG	A	1749	1/1	0.98	0.14	84,84,84,84	0
26	MG	A	1625	1/1	0.99	0.06	113,113,113,113	0
26	MG	A	1623	1/1	0.99	0.13	67,67,67,67	0
26	MG	A	1911	1/1	0.99	0.12	100,100,100,100	0
26	MG	A	1610	1/1	0.99	0.24	81,81,81,81	0
26	MG	A	1607	1/1	0.99	0.11	154,154,154,154	0
26	MG	A	1638	1/1	0.99	0.13	86,86,86,86	0
26	MG	A	1653	1/1	0.99	0.25	96,96,96,96	0
26	MG	A	1626	1/1	0.99	0.26	245,245,245,245	0
26	MG	A	1882	1/1	0.99	0.34	315,315,315,315	0
26	MG	A	1858	1/1	0.99	0.23	355,355,355,355	0
26	MG	A	1713	1/1	0.99	0.11	211,211,211,211	0
26	MG	A	1859	1/1	0.99	0.16	427,427,427,427	0
26	MG	A	1692	1/1	0.99	0.20	182,182,182,182	0
26	MG	A	1827	1/1	0.99	0.08	251,251,251,251	0
26	MG	A	1703	1/1	0.99	0.14	97,97,97,97	0
26	MG	A	1635	1/1	0.99	0.14	74,74,74,74	0
26	MG	A	1738	1/1	1.00	0.05	68,68,68,68	0
26	MG	A	1611	1/1	1.00	0.10	113,113,113,113	0
26	MG	A	1627	1/1	1.00	0.11	141,141,141,141	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SRY A 1928:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.