



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:09 AM GMT

PDB ID : 4DR4
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, cognate transfer RNA anticodon stem-loop and multiple copies of paromomycin molecules bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogle, G.
Deposited on : 2012-02-16
Resolution : 3.97 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

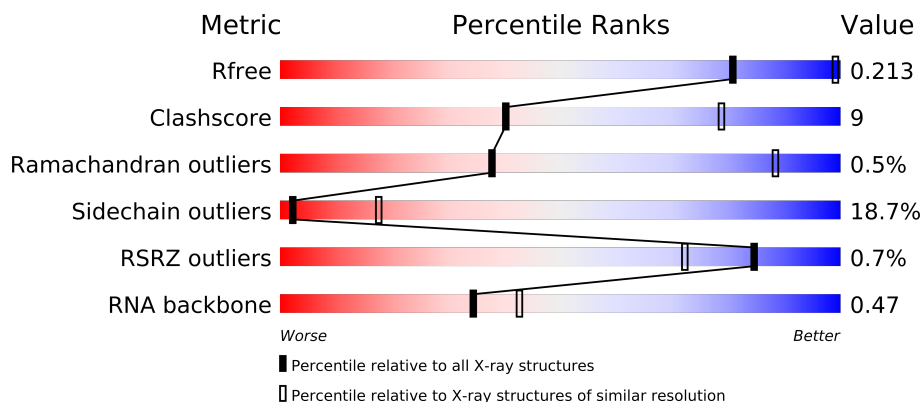
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.97 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}	66092	1005 (4.46-3.46)
Clashscore	79885	1195 (4.42-3.50)
Ramachandran outliers	78287	1137 (4.42-3.50)
Sidechain outliers	78261	1124 (4.42-3.50)
RSRZ outliers	66119	1005 (4.46-3.46)
RNA backbone	1838	1018 (5.00-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	3	
23	W	15	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53651 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

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
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

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

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

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

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

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

- 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	S	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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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	73	Total	C	N	O		0	0	0
			598	381	118	99				

- 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			

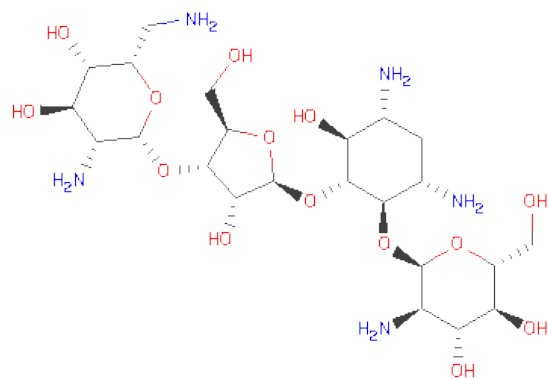
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	3	Total	C	N	O	P	0	0	0
			57	27	6	22	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	3	Total	Mg	0	0
			3	3		
25	Q	1	Total	Mg	0	0
			1	1		
25	D	2	Total	Mg	0	0
			2	2		
25	E	4	Total	Mg	0	0
			4	4		
25	H	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		
25	A	339	Total	Mg	0	8
			345	345		
25	T	1	Total	Mg	0	0
			1	1		
25	N	1	Total	Mg	0	0
			1	1		
25	O	1	Total	Mg	0	0
			1	1		
25	L	1	Total	Mg	0	0
			1	1		
25	S	2	Total	Mg	0	0
			2	2		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		

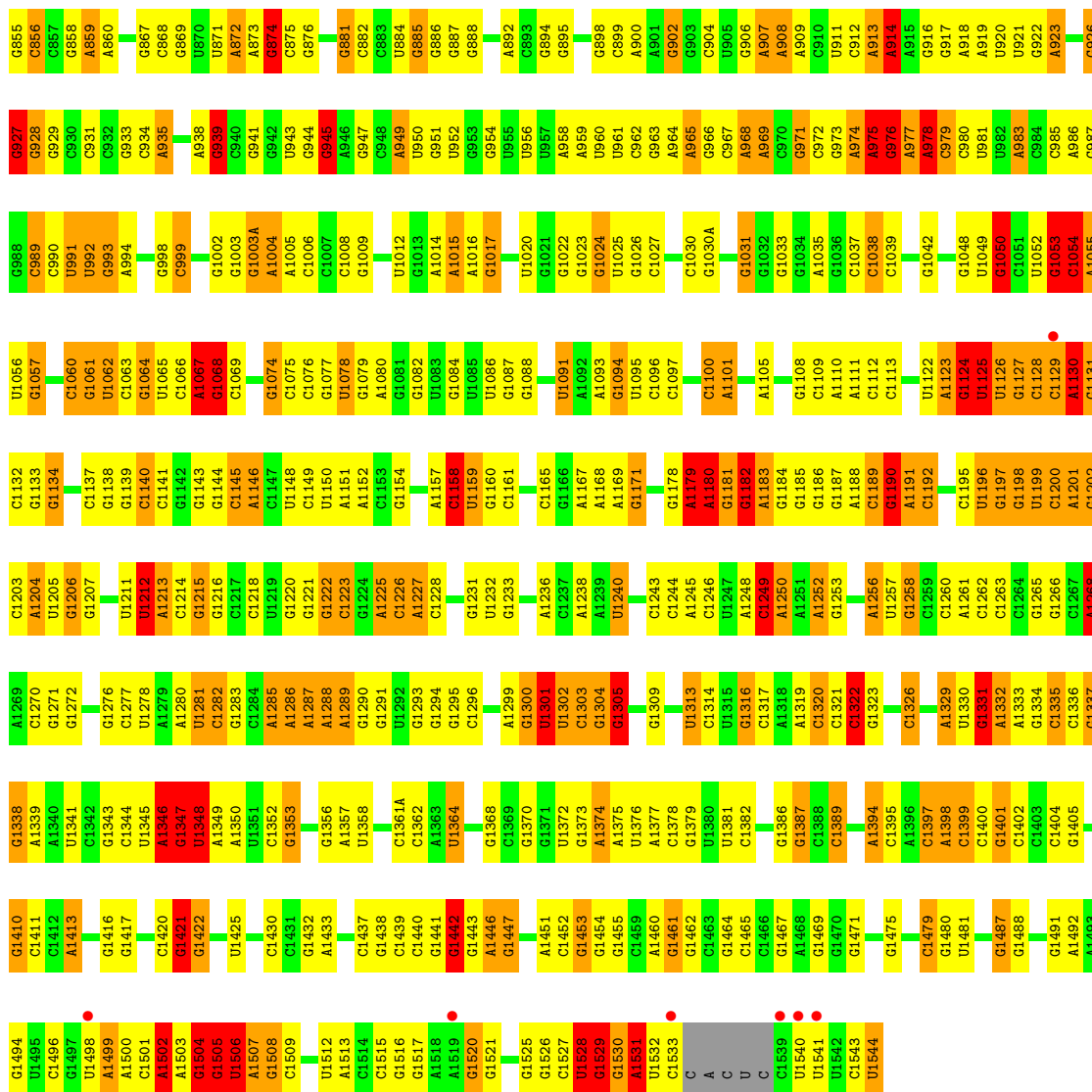
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	N	1	Total	Zn	0	0
			1	1		

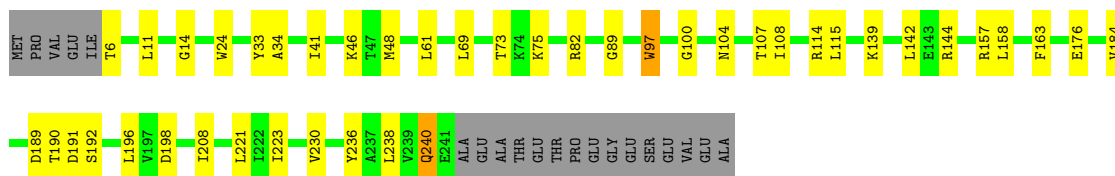
- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	480	Total	O	0	0
			480	480		
27	C	1	Total	O	0	0
			1	1		
27	D	2	Total	O	0	0
			2	2		
27	E	5	Total	O	0	0
			5	5		
27	K	1	Total	O	0	0
			1	1		
27	L	2	Total	O	0	0
			2	2		
27	N	2	Total	O	0	0
			2	2		
27	O	4	Total	O	0	0
			4	4		
27	V	1	Total	O	0	0
			1	1		



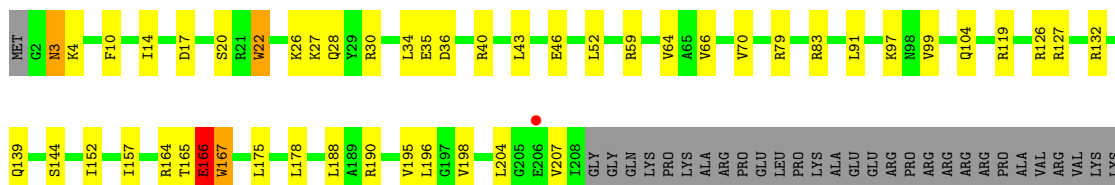
- Molecule 2: 30S ribosomal protein S2

Chain B:



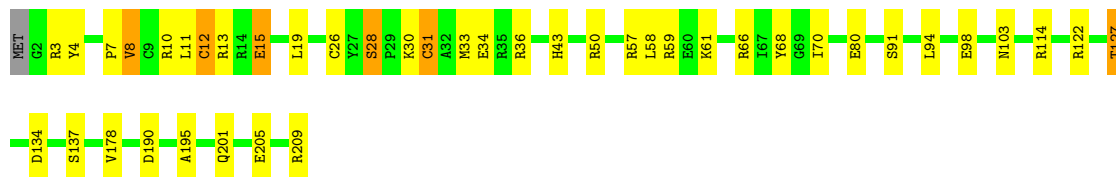
- Molecule 3: 30S ribosomal protein S3

Chain C:

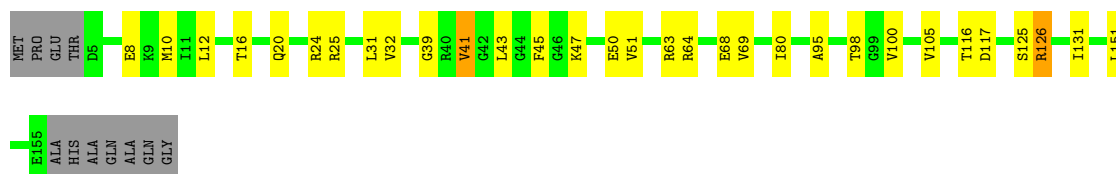


GLU
GLU

- Molecule 4: 30S ribosomal protein S4

Chain D: 

- Molecule 5: 30S ribosomal protein S5

Chain E: 

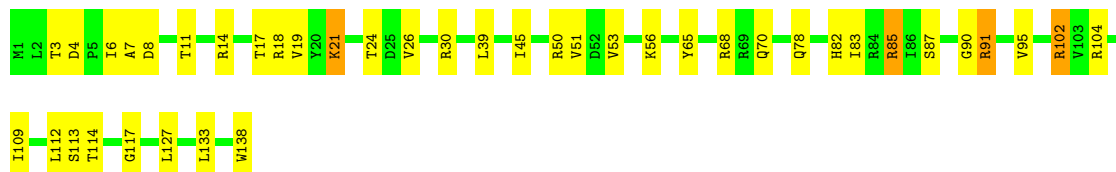
- Molecule 6: 30S ribosomal protein S6

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: 



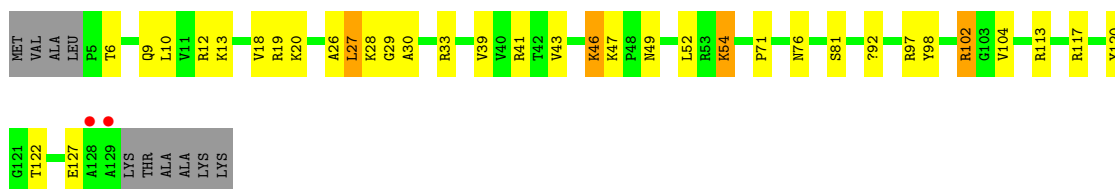
- Molecule 11: 30S ribosomal protein S11

Chain K: 



- Molecule 12: 30S ribosomal protein S12

Chain L: 



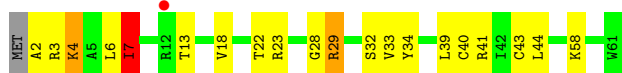
- Molecule 13: 30S ribosomal protein S13

Chain M: 



- Molecule 14: 30S ribosomal protein S14

Chain N: 



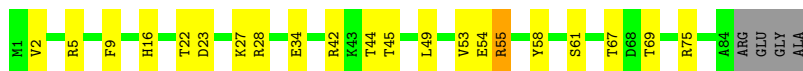
- Molecule 15: 30S ribosomal protein S15

Chain O: 



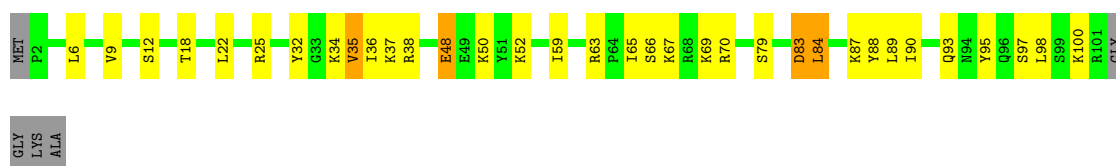
- Molecule 16: 30S ribosomal protein S16

Chain P: 



- Molecule 17: 30S ribosomal protein S17

Chain Q: 



- Molecule 18: 30S ribosomal protein S18

Chain R:



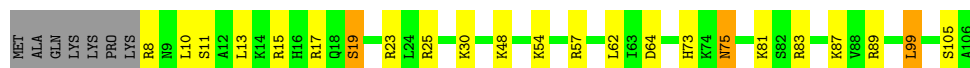
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein THX

Chain U:



- Molecule 22: 5'-R(*UP*UP*U)-3'

Chain V:



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

Chain W:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.95Å 400.95Å 176.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.97 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.73-3.97) 99.6 (49.73-3.97)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.153 , 0.212 0.153 , 0.213	Depositor DCC
R_{free} test set	6165 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123790 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	53651	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, MG, 0TD, PAR, 2MG, 5MC, UR3, 4OC, M2G, 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	1.11	67/36037 (0.2%)	1.84	1584/56239 (2.8%)
2	B	0.68	0/1931	0.86	3/2607 (0.1%)
3	C	0.71	1/1637 (0.1%)	0.86	1/2207 (0.0%)
4	D	0.74	2/1733 (0.1%)	0.92	4/2318 (0.2%)
5	E	0.79	0/1163	1.02	1/1566 (0.1%)
6	F	0.66	0/856	0.85	0/1154
7	G	0.68	1/1276 (0.1%)	0.84	1/1709 (0.1%)
8	H	0.77	0/1136	0.96	0/1527
9	I	0.68	0/1029	0.94	2/1379 (0.1%)
10	J	0.73	0/806	0.92	1/1084 (0.1%)
11	K	0.66	0/900	0.87	0/1213
12	L	0.90	1/978 (0.1%)	1.05	3/1308 (0.2%)
13	M	0.72	0/947	0.88	1/1270 (0.1%)
14	N	0.79	0/501	0.98	1/664 (0.2%)
15	O	0.67	0/745	0.88	0/992
16	P	0.82	0/717	0.95	0/965
17	Q	0.86	0/847	1.06	3/1131 (0.3%)
18	R	0.71	0/604	0.91	1/801 (0.1%)
19	S	0.62	0/662	0.84	0/892
20	T	0.77	0/765	1.04	1/1007 (0.1%)
21	U	0.70	0/213	0.82	0/279
22	V	1.12	0/62	2.13	6/94 (6.4%)
23	W	1.00	0/357	1.41	7/555 (1.3%)
All	All	0.99	72/55902 (0.1%)	1.60	1620/82961 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
4	D	0	1
8	H	0	1
12	L	0	1
13	M	0	1
14	N	0	1
17	Q	0	1
19	S	0	1
All	All	0	10

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1227	A	N9-C4	-8.38	1.32	1.37
1	A	116	A	N9-C4	-8.37	1.32	1.37
1	A	372	C	N3-C4	8.23	1.39	1.33
1	A	372	C	C2-O2	7.65	1.31	1.24
1	A	622	A	N9-C4	-7.50	1.33	1.37
1	A	792	A	C5-C6	-7.43	1.34	1.41
12	L	26	ALA	CA-CB	7.42	1.68	1.52
1	A	913	A	C6-N1	-6.99	1.30	1.35
1	A	817	C	N1-C6	-6.86	1.33	1.37
1	A	882	C	N3-C4	-6.83	1.29	1.33
1	A	975	A	N9-C4	-6.77	1.33	1.37
1	A	722	A	N9-C4	-6.62	1.33	1.37
1	A	372	C	N1-C2	6.55	1.46	1.40
4	D	12	CYS	CB-SG	6.48	1.93	1.82
1	A	1079	G	C6-O6	6.43	1.29	1.24
1	A	803	G	N3-C4	-6.40	1.30	1.35
1	A	733	A	N9-C4	-6.38	1.34	1.37
1	A	523	A	N9-C4	-6.37	1.34	1.37
1	A	1301	U	C3'-O3'	6.28	1.50	1.42
1	A	92	C	N1-C6	-6.22	1.33	1.37
1	A	1056	U	C2-N3	6.14	1.42	1.37
1	A	1124	G	N9-C4	6.11	1.42	1.38
1	A	130	A	N3-C4	-6.10	1.31	1.34
1	A	1346	A	N9-C4	-6.03	1.34	1.37
1	A	1339	A	N9-C4	-6.01	1.34	1.37
1	A	481	G	C6-N1	5.91	1.43	1.39
1	A	231	G	N7-C5	-5.90	1.35	1.39
1	A	329	A	N9-C4	-5.83	1.34	1.37
1	A	913	A	C6-N6	-5.82	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	A	N9-C4	-5.82	1.34	1.37
1	A	792	A	N7-C5	-5.81	1.35	1.39
1	A	279	A	N9-C4	-5.79	1.34	1.37
1	A	328	C	C3'-O3'	5.78	1.50	1.42
1	A	349	A	N9-C4	-5.78	1.34	1.37
1	A	105	G	C6-O6	5.76	1.29	1.24
1	A	828	A	N9-C4	-5.73	1.34	1.37
1	A	1401	G	C6-N1	-5.71	1.35	1.39
1	A	1394	A	N9-C4	-5.70	1.34	1.37
1	A	304	U	C4-O4	5.70	1.28	1.23
1	A	481	G	N1-C2	5.68	1.42	1.37
1	A	1227	A	N3-C4	-5.66	1.31	1.34
1	A	1303	C	N3-C4	-5.63	1.30	1.33
1	A	372	C	C2-N3	5.61	1.40	1.35
1	A	602	A	N9-C4	-5.59	1.34	1.37
1	A	559	A	N9-C4	5.58	1.41	1.37
7	G	47	CYS	CB-SG	-5.57	1.72	1.81
1	A	640	A	C5-C6	-5.53	1.36	1.41
1	A	908	A	N9-C4	-5.53	1.34	1.37
1	A	927	G	N9-C4	-5.52	1.33	1.38
1	A	298	A	N9-C4	-5.50	1.34	1.37
1	A	802	A	N3-C4	-5.50	1.31	1.34
1	A	1331	G	N9-C8	-5.49	1.34	1.37
1	A	1305	G	N3-C4	-5.44	1.31	1.35
1	A	975	A	C5-C4	5.43	1.42	1.38
4	D	31	CYS	CB-SG	5.43	1.91	1.82
1	A	266	G	N9-C4	-5.40	1.33	1.38
1	A	921	U	C4-O4	5.39	1.27	1.23
1	A	1394	A	C6-N1	-5.38	1.31	1.35
1	A	1101	A	N7-C5	5.32	1.42	1.39
1	A	1344	C	C2-O2	5.28	1.29	1.24
1	A	1054	C	C4-C5	-5.21	1.38	1.43
1	A	375	U	C4-O4	5.21	1.27	1.23
1	A	250	A	N9-C4	5.17	1.41	1.37
1	A	92	C	C2-N3	-5.17	1.31	1.35
1	A	646	U	C4-O4	5.17	1.27	1.23
1	A	1179	A	N9-C4	-5.16	1.34	1.37
3	C	167	TRP	CB-CG	-5.13	1.41	1.50
1	A	251	G	N9-C4	5.08	1.42	1.38
1	A	301	G	N9-C4	-5.05	1.33	1.38
1	A	257	G	C6-O6	5.04	1.28	1.24
1	A	804	U	C2-N3	-5.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	A	N3-C4	-5.01	1.31	1.34

All (1620) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	C	C4-C5-C6	-15.67	109.57	117.40
1	A	1054	C	C5-C6-N1	14.40	128.20	121.00
1	A	1054	C	N1-C2-N3	-13.92	109.46	119.20
1	A	1054	C	C2-N3-C4	13.81	126.80	119.90
1	A	1331	G	C5-N7-C8	13.48	111.04	104.30
1	A	1079	G	C5-C6-N1	-13.43	104.79	111.50
1	A	318	G	C5-C6-N1	-13.36	104.82	111.50
1	A	572	A	N1-C6-N6	-12.95	110.83	118.60
1	A	975	A	C2-N3-C4	-12.90	104.15	110.60
1	A	1331	G	N1-C6-O6	-12.85	112.19	119.90
1	A	1329	A	N1-C6-N6	12.84	126.30	118.60
1	A	372	C	C6-N1-C2	12.78	125.41	120.30
1	A	1331	G	C4-C5-N7	-12.69	105.72	110.80
1	A	28	G	N1-C6-O6	12.57	127.44	119.90
1	A	1200	C	N1-C2-O2	12.15	126.19	118.90
1	A	856	C	C6-N1-C2	-12.06	115.47	120.30
1	A	1331	G	N7-C8-N9	-11.85	107.17	113.10
1	A	266	G	N1-C6-O6	11.81	126.98	119.90
1	A	884	U	C5-C6-N1	-11.75	116.82	122.70
1	A	481	G	N1-C6-O6	11.71	126.93	119.90
1	A	117	G	N1-C6-O6	11.70	126.92	119.90
1	A	907	A	N1-C6-N6	-11.68	111.59	118.60
1	A	116	A	C2-N3-C4	-11.51	104.84	110.60
1	A	433	C	C5-C6-N1	11.46	126.73	121.00
1	A	820	U	N1-C2-O2	-11.43	114.80	122.80
1	A	105	G	C5-C6-N1	-11.40	105.80	111.50
1	A	856	C	N3-C4-C5	-11.38	117.35	121.90
1	A	232	G	N9-C4-C5	-11.36	100.86	105.40
1	A	1413	A	C5-C6-N1	-11.20	112.10	117.70
1	A	633	G	N1-C6-O6	11.16	126.60	119.90
1	A	818	G	C8-N9-C4	-11.03	101.99	106.40
1	A	853	G	N1-C6-O6	10.99	126.50	119.90
1	A	545	C	C6-N1-C2	-10.80	115.98	120.30
1	A	1064	G	N3-C2-N2	-10.73	112.39	119.90
1	A	372	C	N1-C2-N3	-10.66	111.74	119.20
1	A	885	G	N1-C6-O6	10.61	126.26	119.90
1	A	869	G	N1-C6-O6	10.51	126.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	975	A	N7-C8-N9	10.45	119.02	113.80
1	A	553	A	C8-N9-C4	10.42	109.97	105.80
1	A	818	G	N9-C4-C5	10.39	109.56	105.40
1	A	1054	C	N1-C2-O2	10.37	125.12	118.90
1	A	190(I)	G	C8-N9-C4	10.34	110.54	106.40
1	A	975	A	C5-C6-N1	-10.25	112.58	117.70
1	A	115	G	C8-N9-C4	10.24	110.50	106.40
1	A	1506	U	N1-C2-N3	-10.22	108.77	114.90
1	A	105	G	N1-C6-O6	10.20	126.02	119.90
1	A	1222	G	C5-C6-N1	-10.17	106.42	111.50
1	A	266	G	C2-N3-C4	-10.16	106.82	111.90
1	A	851	G	N1-C6-O6	10.15	125.99	119.90
1	A	117	G	C5-C6-N1	-10.14	106.43	111.50
1	A	373	A	C8-N9-C4	10.12	109.85	105.80
1	A	1206	G	N1-C6-O6	10.12	125.97	119.90
1	A	416	G	N1-C6-O6	10.06	125.94	119.90
1	A	226	G	C8-N9-C4	10.05	110.42	106.40
1	A	1064	G	N1-C2-N3	10.05	129.93	123.90
1	A	792	A	N1-C6-N6	10.05	124.63	118.60
1	A	623	C	C6-N1-C2	9.92	124.27	120.30
1	A	372	C	N1-C2-O2	9.85	124.81	118.90
1	A	19	C	C6-N1-C2	-9.84	116.36	120.30
1	A	348	G	N1-C6-O6	9.82	125.79	119.90
1	A	174	C	C5-C6-N1	9.79	125.90	121.00
1	A	378	G	N1-C6-O6	9.78	125.77	119.90
1	A	1079	G	C4-C5-C6	9.74	124.64	118.80
1	A	820	U	N3-C4-C5	-9.65	108.81	114.60
1	A	328	C	C2-N1-C1'	9.65	129.42	118.80
1	A	251	G	N3-C4-C5	-9.64	123.78	128.60
1	A	975	A	C5-N7-C8	-9.49	99.15	103.90
1	A	530	G	C8-N9-C4	9.47	110.19	106.40
1	A	1200	C	C5-C6-N1	9.46	125.73	121.00
1	A	525	C	C6-N1-C2	9.41	124.06	120.30
1	A	541	G	N1-C6-O6	9.35	125.51	119.90
1	A	231	G	N1-C6-O6	9.35	125.51	119.90
1	A	309	G	N1-C6-O6	9.34	125.50	119.90
1	A	266	G	C6-C5-N7	-9.32	124.81	130.40
1	A	325	A	N1-C6-N6	-9.32	113.01	118.60
1	A	1465	C	N1-C2-O2	9.24	124.44	118.90
1	A	633	G	N9-C4-C5	-9.23	101.71	105.40
1	A	231	G	C6-C5-N7	-9.19	124.89	130.40
1	A	1331	G	N3-C4-C5	-9.19	124.01	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1200	C	C2-N1-C1'	9.18	128.90	118.80
1	A	646	U	C5-C4-O4	9.10	131.36	125.90
1	A	1129	C	C6-N1-C2	-9.10	116.66	120.30
1	A	920	U	C5-C4-O4	9.07	131.34	125.90
1	A	220	G	C8-N9-C4	-9.04	102.79	106.40
1	A	804	U	N3-C2-O2	-9.02	115.89	122.20
1	A	1343	G	N1-C6-O6	8.99	125.30	119.90
1	A	509	A	N1-C6-N6	-8.97	113.22	118.60
1	A	1506	U	C5-C4-O4	-8.96	120.52	125.90
1	A	304	U	N3-C4-C5	-8.94	109.23	114.60
1	A	633	G	C4-C5-N7	8.91	114.36	110.80
1	A	1054	C	C6-N1-C1'	-8.91	110.11	120.80
1	A	640	A	N1-C6-N6	8.90	123.94	118.60
1	A	633	G	C5-C6-O6	-8.87	123.28	128.60
1	A	331	G	N1-C6-O6	8.84	125.20	119.90
1	A	1125	U	C6-N1-C2	8.84	126.30	121.00
1	A	1060	C	C6-N1-C2	-8.83	116.77	120.30
1	A	559	A	C4-C5-C6	8.81	121.41	117.00
1	A	1505	G	C8-N9-C4	-8.80	102.88	106.40
1	A	232	G	N3-C4-N9	8.80	131.28	126.00
1	A	522	C	C6-N1-C2	8.78	123.81	120.30
1	A	839	U	N1-C2-O2	8.77	128.94	122.80
1	A	1455	G	N1-C6-O6	8.77	125.16	119.90
1	A	43	C	C6-N1-C2	8.76	123.81	120.30
1	A	1313	U	N1-C2-N3	-8.76	109.64	114.90
1	A	116	A	C5-C6-N1	-8.73	113.33	117.70
1	A	257	G	C5-C6-N1	-8.71	107.14	111.50
1	A	1206	G	C5-C6-O6	-8.70	123.38	128.60
1	A	945	G	N1-C6-O6	8.67	125.10	119.90
1	A	1526	G	C4-C5-N7	8.65	114.26	110.80
1	A	772	U	N3-C2-O2	-8.64	116.15	122.20
1	A	190(F)	G	N9-C4-C5	8.63	108.85	105.40
1	A	318	G	N1-C6-O6	8.62	125.07	119.90
1	A	606	G	N3-C4-N9	8.62	131.17	126.00
1	A	1200	C	C2-N3-C4	8.62	124.21	119.90
1	A	907	A	N9-C4-C5	8.60	109.24	105.80
1	A	665	A	N1-C6-N6	-8.58	113.45	118.60
1	A	372	C	C6-N1-C1'	-8.57	110.51	120.80
1	A	1532	U	N3-C2-O2	-8.56	116.20	122.20
1	A	1276	G	C8-N9-C4	-8.56	102.98	106.40
1	A	990	C	C6-N1-C2	-8.55	116.88	120.30
1	A	1469	G	N1-C6-O6	8.55	125.03	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	G	C8-N9-C4	8.55	109.82	106.40
1	A	386	C	N1-C2-O2	-8.55	113.77	118.90
1	A	559	A	N3-C4-C5	-8.54	120.82	126.80
1	A	876	G	N3-C4-N9	-8.53	120.88	126.00
1	A	190(F)	G	C8-N9-C4	-8.53	102.99	106.40
1	A	1333	A	N1-C6-N6	-8.53	113.48	118.60
1	A	808	C	N1-C2-O2	-8.51	113.79	118.90
1	A	287	U	N3-C4-C5	-8.51	109.49	114.60
1	A	1331	G	C8-N9-C4	8.50	109.80	106.40
1	A	884	U	C4-C5-C6	8.49	124.79	119.70
1	A	15	G	N1-C6-O6	8.48	124.98	119.90
1	A	332	G	N1-C6-O6	8.46	124.98	119.90
1	A	309	G	C5-C6-O6	-8.44	123.53	128.60
1	A	1305	G	N1-C2-N3	8.43	128.96	123.90
1	A	1200	C	C6-N1-C1'	-8.42	110.70	120.80
1	A	299	G	N1-C6-O6	8.41	124.95	119.90
1	A	645	C	C6-N1-C2	-8.40	116.94	120.30
1	A	1054	C	C2-N1-C1'	8.40	128.04	118.80
1	A	1187	G	C6-C5-N7	-8.39	125.37	130.40
1	A	900	A	C2-N3-C4	-8.39	106.41	110.60
1	A	139	G	N1-C6-O6	8.39	124.93	119.90
1	A	1305	G	C2-N3-C4	-8.36	107.72	111.90
1	A	1302	U	N3-C2-O2	-8.34	116.36	122.20
1	A	761	G	C4-C5-N7	8.34	114.14	110.80
1	A	730	G	N3-C4-C5	-8.32	124.44	128.60
1	A	35	G	N1-C6-O6	8.29	124.88	119.90
1	A	1064	G	C2-N3-C4	-8.28	107.76	111.90
1	A	907	A	C5-C6-N6	8.27	130.32	123.70
1	A	433	C	C6-N1-C2	-8.25	117.00	120.30
1	A	852	G	N1-C6-O6	8.23	124.84	119.90
1	A	190(F)	G	N3-C4-N9	-8.23	121.06	126.00
1	A	48	C	C6-N1-C2	8.23	123.59	120.30
1	A	416	G	C6-C5-N7	-8.23	125.46	130.40
1	A	614	A	N1-C6-N6	8.22	123.53	118.60
1	A	564	C	C2-N3-C4	8.22	124.01	119.90
1	A	839	U	C2-N1-C1'	8.21	127.55	117.70
1	A	504	C	C6-N1-C2	-8.21	117.02	120.30
1	A	722	A	C5-N7-C8	-8.20	99.80	103.90
1	A	573	A	N9-C4-C5	8.20	109.08	105.80
1	A	318	G	C4-C5-C6	8.19	123.71	118.80
1	A	789	U	C5-C4-O4	8.16	130.80	125.90
1	A	852	G	C5-C6-N1	-8.16	107.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	G	C5-C6-O6	-8.15	123.71	128.60
1	A	331	G	C6-C5-N7	-8.15	125.51	130.40
1	A	867	G	N1-C6-O6	8.15	124.79	119.90
1	A	260	G	C5-C6-N1	-8.15	107.43	111.50
1	A	1087	G	N1-C6-O6	8.15	124.79	119.90
1	A	574	A	C8-N9-C4	8.14	109.06	105.80
1	A	1526	G	C5-C6-O6	-8.14	123.72	128.60
1	A	1212	U	C2-N1-C1'	8.14	127.47	117.70
1	A	971	G	N1-C6-O6	8.13	124.78	119.90
1	A	27	G	C4-C5-N7	8.13	114.05	110.80
1	A	144	G	N1-C6-O6	8.12	124.77	119.90
1	A	183	G	C8-N9-C4	-8.12	103.15	106.40
1	A	875	C	C6-N1-C2	8.10	123.54	120.30
1	A	780	A	N1-C6-N6	8.10	123.46	118.60
1	A	266	G	C4-C5-N7	8.10	114.04	110.80
1	A	1329	A	C6-C5-N7	-8.09	126.64	132.30
1	A	800	G	C8-N9-C4	-8.07	103.17	106.40
1	A	89	C	C6-N1-C2	-8.06	117.08	120.30
1	A	1086	U	C5-C6-N1	8.06	126.73	122.70
1	A	317	G	N1-C6-O6	8.06	124.73	119.90
1	A	284	G	N1-C6-O6	8.05	124.73	119.90
1	A	820	U	N3-C4-O4	8.04	125.03	119.40
1	A	1373	G	C5-C6-N1	-8.02	107.49	111.50
1	A	1146	A	C8-N9-C4	8.01	109.00	105.80
1	A	28	G	C4-C5-N7	8.00	114.00	110.80
1	A	1336	C	C6-N1-C2	7.99	123.50	120.30
1	A	541	G	C5-C6-N1	-7.99	107.51	111.50
1	A	518	C	C5-C4-N4	7.98	125.79	120.20
1	A	1054	C	C5-C4-N4	-7.98	114.61	120.20
1	A	981	U	N3-C4-O4	7.98	124.98	119.40
1	A	752	G	C5-C6-N1	-7.97	107.51	111.50
1	A	1410	G	C8-N9-C4	7.97	109.59	106.40
1	A	108	G	C4-N9-C1'	7.96	136.85	126.50
1	A	616	G	C5-C6-N1	-7.95	107.53	111.50
1	A	1531	A	C8-N9-C4	-7.94	102.62	105.80
1	A	564	C	N3-C4-N4	7.94	123.56	118.00
1	A	856	C	C4-C5-C6	7.93	121.37	117.40
1	A	854	G	C6-C5-N7	-7.92	125.65	130.40
1	A	1204	A	N1-C6-N6	-7.90	113.86	118.60
1	A	1394	A	C2-N3-C4	-7.90	106.65	110.60
1	A	1496	C	N1-C2-O2	-7.90	114.16	118.90
1	A	30	U	C5-C4-O4	-7.88	121.17	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1361(A)	C	C6-N1-C2	-7.88	117.15	120.30
1	A	1451	A	N1-C2-N3	-7.88	125.36	129.30
1	A	733	A	C2-N3-C4	-7.86	106.67	110.60
1	A	809	G	C8-N9-C4	7.86	109.54	106.40
1	A	1265	G	C8-N9-C4	-7.86	103.26	106.40
1	A	311	C	N3-C4-C5	-7.86	118.76	121.90
1	A	1286	A	C8-N9-C4	-7.86	102.66	105.80
1	A	650	G	N1-C6-O6	7.86	124.61	119.90
1	A	917	G	N1-C6-O6	7.85	124.61	119.90
1	A	397	A	C8-N9-C4	-7.85	102.66	105.80
1	A	27	G	C5-N7-C8	-7.85	100.38	104.30
1	A	481	G	C5-C6-N1	-7.82	107.59	111.50
1	A	979	C	N3-C4-C5	-7.81	118.77	121.90
22	V	3	U	N3-C2-O2	-7.81	116.73	122.20
1	A	147	G	C5-C6-N1	-7.81	107.60	111.50
1	A	685	G	C5-C6-N1	-7.81	107.60	111.50
1	A	1299	A	C5-N7-C8	-7.80	100.00	103.90
1	A	1200	C	N1-C2-N3	-7.80	113.74	119.20
1	A	645	C	C2-N1-C1'	7.79	127.37	118.80
1	A	1413	A	C2-N3-C4	-7.79	106.71	110.60
1	A	931	C	N3-C4-N4	-7.78	112.55	118.00
1	A	1438	G	N1-C6-O6	7.77	124.56	119.90
1	A	29	G	N9-C4-C5	7.77	108.51	105.40
1	A	232	G	C8-N9-C1'	-7.76	116.91	127.00
1	A	789	U	N3-C2-O2	-7.76	116.77	122.20
1	A	1187	G	C4-N9-C1'	7.76	136.58	126.50
1	A	1231	G	N1-C6-O6	7.75	124.55	119.90
1	A	394	G	C2-N3-C4	-7.75	108.02	111.90
1	A	1331	G	C6-C5-N7	7.75	135.05	130.40
1	A	772	U	N1-C2-N3	7.75	119.55	114.90
1	A	921	U	N3-C4-C5	-7.75	109.95	114.60
1	A	920	U	C5-C6-N1	-7.74	118.83	122.70
1	A	69	G	N1-C6-O6	7.74	124.54	119.90
1	A	614	A	C5-N7-C8	-7.72	100.04	103.90
1	A	36	C	N3-C2-O2	-7.71	116.50	121.90
1	A	1258	G	C8-N9-C4	-7.71	103.31	106.40
1	A	614	A	C5-C6-N6	-7.71	117.53	123.70
1	A	815	A	C5-C6-N1	-7.71	113.85	117.70
1	A	1442	G	N3-C4-C5	-7.70	124.75	128.60
1	A	792	A	C4-C5-N7	7.70	114.55	110.70
1	A	1502	A	C4-C5-N7	7.69	114.55	110.70
1	A	1520	G	C5-C6-O6	-7.68	123.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1199	U	C4-C5-C6	7.67	124.31	119.70
1	A	394	G	N1-C6-O6	7.67	124.50	119.90
1	A	523	A	C8-N9-C4	7.67	108.87	105.80
1	A	574	A	N1-C6-N6	7.67	123.20	118.60
1	A	606	G	C5-C6-O6	-7.67	124.00	128.60
1	A	1053	G	C8-N9-C4	7.67	109.47	106.40
1	A	1520	G	N1-C6-O6	7.67	124.50	119.90
1	A	232	G	N3-C2-N2	7.66	125.26	119.90
1	A	574	A	N9-C4-C5	-7.66	102.74	105.80
1	A	1465	C	N3-C2-O2	-7.66	116.54	121.90
1	A	545	C	C2-N1-C1'	7.65	127.22	118.80
1	A	780	A	C5-C6-N6	-7.65	117.58	123.70
1	A	661	G	N3-C2-N2	-7.64	114.55	119.90
1	A	820	U	N1-C2-N3	7.64	119.48	114.90
1	A	298	A	C2-N3-C4	-7.63	106.78	110.60
1	A	881	G	C2-N3-C4	-7.63	108.09	111.90
1	A	287	U	C6-N1-C2	-7.62	116.42	121.00
1	A	225	C	C6-N1-C2	7.62	123.35	120.30
1	A	876	G	N3-C4-C5	7.62	132.41	128.60
22	V	3	U	N1-C2-O2	7.61	128.13	122.80
1	A	1038	C	C6-N1-C2	-7.61	117.26	120.30
1	A	1382	C	C6-N1-C2	-7.61	117.26	120.30
1	A	631	G	C8-N9-C4	-7.60	103.36	106.40
1	A	30	U	N3-C2-O2	7.60	127.52	122.20
1	A	975	A	C6-C5-N7	-7.60	126.98	132.30
1	A	814	A	C2-N3-C4	-7.59	106.80	110.60
1	A	1061	G	N1-C6-O6	7.59	124.45	119.90
1	A	921	U	N3-C4-O4	7.59	124.71	119.40
1	A	1202	G	C5-C6-O6	7.58	133.15	128.60
4	D	12	CYS	CA-CB-SG	7.58	127.65	114.00
1	A	561	U	N3-C4-O4	7.58	124.70	119.40
1	A	299	G	C5-C6-N1	-7.57	107.71	111.50
1	A	1222	G	N1-C6-O6	7.57	124.44	119.90
1	A	1302	U	N1-C2-O2	7.57	128.10	122.80
1	A	945	G	C5-C6-O6	-7.56	124.06	128.60
1	A	232	G	C6-C5-N7	-7.56	125.86	130.40
1	A	820	U	C4-C5-C6	7.55	124.23	119.70
1	A	881	G	N1-C2-N3	7.55	128.43	123.90
1	A	1187	G	N1-C6-O6	7.55	124.43	119.90
1	A	939	G	N3-C4-C5	7.54	132.37	128.60
1	A	1420	C	C6-N1-C2	-7.54	117.28	120.30
1	A	1316	G	C8-N9-C4	7.54	109.42	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	869	G	C5-C6-N1	-7.52	107.74	111.50
1	A	70	G	C5-C6-N1	-7.51	107.74	111.50
1	A	876	G	C8-N9-C1'	7.50	136.75	127.00
1	A	1349	A	N1-C6-N6	-7.50	114.10	118.60
1	A	646	U	N3-C4-C5	-7.50	110.10	114.60
1	A	1064	G	N3-C4-N9	-7.49	121.50	126.00
1	A	722	A	C4-C5-N7	7.48	114.44	110.70
1	A	179	A	N1-C6-N6	7.47	123.08	118.60
1	A	785	G	C4-C5-N7	7.47	113.79	110.80
1	A	130	A	N1-C6-N6	7.46	123.08	118.60
1	A	1475	G	C8-N9-C4	-7.46	103.42	106.40
17	Q	35	VAL	CB-CA-C	-7.45	97.25	111.40
1	A	144	G	C5-C6-N1	-7.44	107.78	111.50
1	A	245	C	C5-C4-N4	-7.44	114.99	120.20
1	A	1231	G	C8-N9-C4	7.44	109.38	106.40
1	A	1331	G	C6-N1-C2	-7.43	120.64	125.10
1	A	372	C	N3-C4-N4	7.43	123.20	118.00
1	A	13	U	C5-C6-N1	-7.41	119.00	122.70
1	A	724	G	C5-C6-O6	-7.40	124.16	128.60
1	A	378	G	C2-N3-C4	-7.38	108.21	111.90
1	A	1252	A	N1-C6-N6	-7.38	114.17	118.60
1	A	1487	G	C5-C6-N1	-7.38	107.81	111.50
1	A	1171	G	N1-C6-O6	7.37	124.32	119.90
1	A	445	G	N1-C6-O6	7.37	124.32	119.90
1	A	232	G	C4-C5-N7	7.37	113.75	110.80
1	A	1467	G	N1-C6-O6	-7.37	115.48	119.90
1	A	375	U	N3-C4-C5	-7.36	110.18	114.60
1	A	876	G	C4-N9-C1'	-7.36	116.93	126.50
1	A	231	G	C4-C5-N7	7.36	113.74	110.80
1	A	523	A	C2-N3-C4	-7.36	106.92	110.60
1	A	10	A	C2-N3-C4	-7.35	106.92	110.60
1	A	875	C	C5-C6-N1	-7.35	117.32	121.00
1	A	1228	C	N1-C2-O2	7.35	123.31	118.90
1	A	781	A	N1-C2-N3	7.35	132.97	129.30
1	A	1528	U	C5-C6-N1	-7.35	119.03	122.70
1	A	566	G	N1-C6-O6	-7.34	115.50	119.90
1	A	614	A	C8-N9-C4	-7.34	102.86	105.80
1	A	1206	G	C6-C5-N7	-7.34	126.00	130.40
1	A	737	A	N1-C6-N6	7.33	123.00	118.60
1	A	216	G	N1-C6-O6	-7.32	115.51	119.90
1	A	183	G	N7-C8-N9	7.32	116.76	113.10
1	A	425	G	N1-C6-O6	-7.32	115.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	G	N7-C8-N9	7.31	116.76	113.10
1	A	573	A	C4-C5-N7	-7.29	107.06	110.70
1	A	1178	G	C8-N9-C4	-7.28	103.49	106.40
1	A	804	U	N1-C2-N3	7.28	119.27	114.90
1	A	564	C	N1-C2-N3	-7.28	114.11	119.20
1	A	1487	G	N1-C6-O6	7.28	124.27	119.90
1	A	309	G	N9-C4-C5	-7.27	102.49	105.40
1	A	1389	C	N3-C2-O2	7.27	126.99	121.90
1	A	614	A	N7-C8-N9	7.27	117.43	113.80
1	A	1231	G	N3-C4-C5	7.26	132.23	128.60
1	A	308	C	N3-C4-N4	7.26	123.08	118.00
1	A	1227	A	C2-N3-C4	-7.25	106.97	110.60
1	A	190(K)	G	C5-C6-N1	-7.24	107.88	111.50
1	A	1276	G	N7-C8-N9	7.24	116.72	113.10
1	A	577	G	N3-C4-C5	7.24	132.22	128.60
1	A	923	A	C2-N3-C4	-7.23	106.98	110.60
1	A	993	G	C8-N9-C4	-7.23	103.51	106.40
1	A	10	A	N1-C2-N3	7.23	132.91	129.30
1	A	232	G	N1-C6-O6	7.21	124.23	119.90
1	A	1320	C	C6-N1-C2	7.19	123.17	120.30
1	A	899	C	N3-C4-C5	-7.18	119.03	121.90
1	A	216	G	C6-C5-N7	7.17	134.70	130.40
1	A	648	A	C8-N9-C4	7.17	108.67	105.80
1	A	82	U	C6-N1-C2	-7.17	116.70	121.00
1	A	706	A	C5-N7-C8	-7.17	100.32	103.90
17	Q	9	VAL	CB-CA-C	-7.16	97.79	111.40
1	A	941	G	N3-C2-N2	-7.16	114.89	119.90
1	A	518	C	C6-N1-C2	-7.15	117.44	120.30
1	A	39	G	C5-C6-O6	-7.15	124.31	128.60
1	A	317	G	C5-C6-N1	-7.14	107.93	111.50
1	A	858	G	C4-N9-C1'	7.14	135.78	126.50
1	A	1057	G	N3-C4-N9	-7.14	121.72	126.00
1	A	645	C	N3-C4-C5	-7.14	119.05	121.90
1	A	373	A	N7-C8-N9	-7.13	110.23	113.80
1	A	699	C	C6-N1-C2	7.13	123.15	120.30
1	A	1195	C	C6-N1-C2	-7.13	117.45	120.30
1	A	301	G	C2-N3-C4	-7.12	108.34	111.90
1	A	1186	G	C2-N3-C4	-7.12	108.34	111.90
1	A	117	G	C2-N3-C4	-7.11	108.34	111.90
1	A	1140	C	C6-N1-C2	-7.11	117.46	120.30
1	A	572	A	C6-C5-N7	7.11	137.28	132.30
1	A	1243	C	C5-C6-N1	7.11	124.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	U	C4-C5-C6	7.10	123.96	119.70
1	A	744	C	C6-N1-C2	-7.10	117.46	120.30
1	A	818	G	C4-C5-N7	-7.10	107.96	110.80
1	A	816	A	C8-N9-C4	7.09	108.64	105.80
1	A	1543	C	N3-C4-C5	-7.08	119.07	121.90
1	A	93	G	C8-N9-C4	7.08	109.23	106.40
1	A	975	A	N1-C2-N3	7.08	132.84	129.30
1	A	1303	C	N3-C4-N4	-7.08	113.04	118.00
1	A	574	A	C6-N1-C2	7.08	122.84	118.60
1	A	991	U	N3-C4-O4	-7.08	114.45	119.40
1	A	1244	C	N3-C4-C5	-7.07	119.07	121.90
1	A	761	G	N9-C4-C5	-7.06	102.58	105.40
1	A	1421	G	C8-N9-C4	-7.06	103.58	106.40
1	A	836	G	C8-N9-C4	7.05	109.22	106.40
12	L	27	LEU	CA-CB-CG	7.05	131.52	115.30
1	A	764	C	N3-C4-C5	-7.05	119.08	121.90
1	A	504	C	N3-C4-C5	-7.04	119.08	121.90
1	A	614	A	C4-C5-N7	7.04	114.22	110.70
1	A	1331	G	C5-C6-O6	7.04	132.83	128.60
1	A	640	A	C6-C5-N7	-7.04	127.37	132.30
1	A	734	G	N1-C6-O6	7.04	124.12	119.90
1	A	917	G	C5-C6-O6	-7.04	124.38	128.60
1	A	220	G	N7-C8-N9	7.04	116.62	113.10
1	A	595	G	C8-N9-C4	7.03	109.21	106.40
1	A	899	C	C6-N1-C2	-7.03	117.49	120.30
1	A	328	C	C5-C6-N1	7.02	124.51	121.00
1	A	853	G	C5-C6-N1	-7.02	107.99	111.50
1	A	904	C	N1-C2-O2	-7.02	114.69	118.90
1	A	328	C	C6-N1-C1'	-7.02	112.38	120.80
1	A	251	G	N3-C4-N9	7.01	130.21	126.00
1	A	348	G	N3-C4-C5	7.01	132.11	128.60
1	A	1387	G	N3-C4-C5	7.01	132.10	128.60
1	A	928	G	N1-C6-O6	7.00	124.10	119.90
1	A	1344	C	N1-C2-O2	7.00	123.10	118.90
1	A	92	C	C6-N1-C2	6.99	123.10	120.30
1	A	530	G	N7-C8-N9	-6.98	109.61	113.10
1	A	509	A	C8-N9-C4	-6.98	103.01	105.80
1	A	397	A	N7-C8-N9	6.97	117.28	113.80
1	A	792	A	N9-C4-C5	-6.97	103.01	105.80
1	A	1113	C	C5-C6-N1	6.97	124.48	121.00
1	A	1338	G	C5-C6-O6	6.97	132.78	128.60
1	A	29	G	C8-N9-C4	-6.97	103.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	G	N1-C6-O6	6.97	124.08	119.90
1	A	1146	A	N7-C8-N9	-6.96	110.32	113.80
1	A	550	G	N3-C2-N2	-6.96	115.03	119.90
1	A	48	C	C5-C6-N1	-6.96	117.52	121.00
1	A	1331	G	C5-C6-N1	6.95	114.97	111.50
1	A	190(I)	G	N7-C8-N9	-6.95	109.63	113.10
1	A	1344	C	N1-C2-N3	-6.95	114.34	119.20
1	A	190(K)	G	N1-C6-O6	6.94	124.06	119.90
1	A	927	G	C5-C6-N1	-6.94	108.03	111.50
1	A	698	G	N1-C6-O6	6.94	124.06	119.90
1	A	772	U	C2-N3-C4	-6.93	122.84	127.00
1	A	1305	G	C5-C6-N1	-6.93	108.04	111.50
1	A	372	C	C5-C4-N4	-6.92	115.35	120.20
1	A	248	C	C6-N1-C2	6.92	123.07	120.30
1	A	670	G	C8-N9-C4	6.92	109.17	106.40
1	A	771	G	C8-N9-C4	-6.92	103.63	106.40
1	A	1202	G	N9-C4-C5	6.92	108.17	105.40
1	A	854	G	C4-N9-C1'	6.92	135.49	126.50
1	A	1544	U	C6-N1-C2	-6.92	116.85	121.00
1	A	574	A	N1-C2-N3	-6.91	125.84	129.30
1	A	27	G	C5-C6-O6	-6.91	124.45	128.60
1	A	1531	A	N7-C8-N9	6.91	117.25	113.80
1	A	1101	A	N1-C2-N3	-6.91	125.85	129.30
1	A	1074	G	N3-C4-N9	6.90	130.14	126.00
1	A	666	G	N1-C6-O6	6.89	124.04	119.90
1	A	606	G	C6-C5-N7	-6.89	126.27	130.40
1	A	872	A	C4-C5-N7	6.89	114.14	110.70
1	A	1479	C	C6-N1-C2	-6.88	117.55	120.30
1	A	1439	C	N3-C4-C5	-6.87	119.15	121.90
1	A	266	G	C5-N7-C8	-6.87	100.87	104.30
1	A	416	G	C4-C5-N7	6.86	113.55	110.80
1	A	544	G	N1-C6-O6	-6.85	115.79	119.90
1	A	1258	G	N3-C4-C5	-6.85	125.17	128.60
1	A	839	U	C6-N1-C1'	-6.85	111.61	121.20
1	A	376	G	N1-C6-O6	6.85	124.01	119.90
1	A	398	C	C6-N1-C2	6.85	123.04	120.30
1	A	1145	C	C6-N1-C2	-6.84	117.56	120.30
1	A	1350	A	N1-C6-N6	-6.84	114.50	118.60
1	A	545	C	N3-C2-O2	-6.83	117.12	121.90
1	A	139	G	C5-C6-N1	-6.83	108.08	111.50
1	A	1057	G	C8-N9-C1'	6.83	135.88	127.00
1	A	1187	G	C4-C5-C6	6.83	122.90	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	A	N7-C8-N9	6.83	117.21	113.80
1	A	446	G	N1-C6-O6	6.82	123.99	119.90
1	A	514	C	C6-N1-C2	-6.82	117.57	120.30
1	A	41	G	N1-C6-O6	6.82	123.99	119.90
1	A	610	G	N1-C6-O6	-6.82	115.81	119.90
1	A	927	G	N3-C4-C5	6.82	132.01	128.60
1	A	55	A	N1-C6-N6	-6.82	114.51	118.60
1	A	1331	G	C2-N3-C4	6.81	115.30	111.90
1	A	309	G	C8-N9-C4	6.80	109.12	106.40
1	A	913	A	N1-C6-N6	-6.80	114.52	118.60
1	A	355	C	C6-N1-C2	-6.79	117.58	120.30
1	A	1202	G	N3-C4-N9	-6.79	121.92	126.00
1	A	34	C	N3-C2-O2	6.79	126.65	121.90
1	A	16	A	C8-N9-C4	6.78	108.51	105.80
1	A	360	A	N1-C6-N6	6.78	122.67	118.60
1	A	231	G	C5-C6-O6	-6.78	124.53	128.60
1	A	308	C	C2-N3-C4	6.78	123.29	119.90
1	A	439	A	C8-N9-C4	-6.78	103.09	105.80
1	A	1504	G	N1-C6-O6	6.77	123.96	119.90
1	A	978	A	N1-C6-N6	6.77	122.66	118.60
1	A	1333	A	C5-C6-N1	6.77	121.09	117.70
1	A	973	G	C6-C5-N7	6.76	134.46	130.40
1	A	1506	U	C6-N1-C2	6.76	125.06	121.00
1	A	35	G	C6-C5-N7	-6.75	126.35	130.40
1	A	284	G	C5-C6-O6	-6.75	124.55	128.60
1	A	378	G	C4-C5-N7	6.75	113.50	110.80
1	A	241	C	N3-C4-C5	6.74	124.59	121.90
1	A	808	C	N3-C2-O2	6.74	126.62	121.90
1	A	332	G	C5-C6-O6	-6.74	124.56	128.60
1	A	525	C	N1-C2-N3	-6.74	114.49	119.20
1	A	668	G	C8-N9-C4	6.74	109.09	106.40
1	A	964	A	C5-C6-N1	-6.73	114.33	117.70
1	A	105	G	C2-N3-C4	-6.73	108.53	111.90
1	A	322	C	C6-N1-C2	6.73	122.99	120.30
1	A	372	C	C2-N3-C4	6.73	123.26	119.90
1	A	146	G	C8-N9-C4	-6.72	103.71	106.40
1	A	328	C	N1-C2-O2	6.72	122.93	118.90
1	A	378	G	C6-C5-N7	-6.72	126.37	130.40
1	A	818	G	C5-C6-O6	6.72	132.63	128.60
1	A	1374	A	C5-C6-N1	-6.72	114.34	117.70
1	A	856	C	N3-C2-O2	-6.71	117.20	121.90
1	A	1505	G	N3-C4-C5	-6.71	125.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	G	C5-C6-N1	-6.71	108.15	111.50
1	A	518	C	N3-C4-C5	-6.71	119.22	121.90
1	A	320	C	C6-N1-C2	-6.71	117.62	120.30
1	A	522	C	C5-C6-N1	-6.70	117.65	121.00
1	A	1410	G	N9-C4-C5	-6.70	102.72	105.40
1	A	16	A	N7-C8-N9	-6.70	110.45	113.80
1	A	318	G	N3-C2-N2	-6.70	115.21	119.90
1	A	761	G	C6-C5-N7	-6.70	126.38	130.40
1	A	89	C	N3-C4-C5	-6.70	119.22	121.90
1	A	614	A	C6-C5-N7	-6.70	127.61	132.30
1	A	1074	G	C6-C5-N7	-6.70	126.38	130.40
1	A	1190	G	N3-C4-N9	6.69	130.02	126.00
1	A	1455	G	C6-C5-N7	-6.69	126.39	130.40
1	A	962	C	C6-N1-C2	6.69	122.97	120.30
1	A	964	A	C4-C5-C6	6.69	120.34	117.00
1	A	1231	G	C2-N3-C4	-6.68	108.56	111.90
1	A	1395	C	N1-C2-O2	6.68	122.91	118.90
1	A	1464	G	C5-C6-N1	-6.68	108.16	111.50
1	A	521	G	N3-C4-N9	-6.68	121.99	126.00
1	A	920	U	N3-C4-O4	-6.68	114.73	119.40
1	A	329	A	N7-C8-N9	-6.67	110.46	113.80
1	A	907	A	C4-C5-N7	-6.67	107.36	110.70
1	A	979	C	C6-N1-C2	-6.67	117.63	120.30
1	A	401	C	C6-N1-C2	-6.67	117.63	120.30
1	A	907	A	N1-C2-N3	6.67	132.63	129.30
1	A	108	G	C6-C5-N7	-6.67	126.40	130.40
1	A	564	C	C5-C6-N1	6.66	124.33	121.00
1	A	926	G	N9-C4-C5	6.66	108.06	105.40
1	A	362	G	C5-C6-N1	-6.65	108.17	111.50
1	A	1338	G	N9-C4-C5	6.65	108.06	105.40
1	A	1350	A	C6-N1-C2	-6.65	114.61	118.60
1	A	318	G	C2-N3-C4	-6.65	108.58	111.90
1	A	1502	A	C6-C5-N7	-6.65	127.64	132.30
1	A	1502	A	C5-N7-C8	-6.64	100.58	103.90
1	A	266	G	C5-C6-O6	-6.64	124.61	128.60
1	A	1076	C	C5-C6-N1	6.64	124.32	121.00
1	A	1416	G	C2-N3-C4	-6.64	108.58	111.90
1	A	1134	G	C8-N9-C4	-6.63	103.75	106.40
1	A	425	G	C5-C6-N1	6.63	114.81	111.50
1	A	1502	A	N1-C6-N6	6.63	122.58	118.60
1	A	58	C	C5-C6-N1	6.62	124.31	121.00
1	A	973	G	N1-C2-N3	-6.62	119.93	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1057	G	C4-N9-C1'	-6.62	117.90	126.50
1	A	216	G	N7-C8-N9	-6.61	109.79	113.10
1	A	606	G	N3-C4-C5	-6.61	125.29	128.60
1	A	1101	A	C4-C5-C6	-6.61	113.70	117.00
1	A	1186	G	N1-C6-O6	6.61	123.86	119.90
1	A	115	G	N7-C8-N9	-6.60	109.80	113.10
1	A	525	C	N3-C2-O2	6.60	126.52	121.90
1	A	1505	G	N7-C8-N9	6.60	116.40	113.10
1	A	521	G	N1-C6-O6	-6.59	115.94	119.90
1	A	570	G	C8-N9-C4	-6.59	103.76	106.40
14	N	7	ILE	CB-CA-C	6.59	124.78	111.60
1	A	58	C	C6-N1-C2	-6.59	117.67	120.30
1	A	92	C	C5-C6-N1	-6.59	117.71	121.00
1	A	62	U	C5-C4-O4	6.58	129.85	125.90
1	A	858	G	C8-N9-C1'	-6.58	118.44	127.00
1	A	260	G	C4-C5-N7	-6.58	108.17	110.80
1	A	968	A	N9-C4-C5	-6.58	103.17	105.80
1	A	559	A	N3-C4-N9	6.58	132.66	127.40
1	A	76	C	C5-C6-N1	6.57	124.29	121.00
1	A	393	A	C8-N9-C4	6.57	108.43	105.80
1	A	854	G	N7-C8-N9	6.57	116.38	113.10
1	A	1343	G	C5-C6-O6	-6.57	124.66	128.60
1	A	928	G	C5-C6-N1	-6.56	108.22	111.50
1	A	111	G	N9-C4-C5	6.56	108.02	105.40
1	A	553	A	N7-C8-N9	-6.55	110.52	113.80
1	A	1037	C	C6-N1-C2	-6.55	117.68	120.30
1	A	886	G	C5-C6-N1	-6.55	108.23	111.50
1	A	1285	A	N1-C6-N6	-6.55	114.67	118.60
1	A	1212	U	N1-C2-O2	6.54	127.38	122.80
9	I	39	GLY	N-CA-C	-6.54	96.76	113.10
1	A	1378	C	C2-N1-C1'	6.53	125.99	118.80
1	A	867	G	N3-C2-N2	-6.53	115.33	119.90
1	A	1465	C	C2-N1-C1'	6.53	125.99	118.80
1	A	317	G	C2-N3-C4	-6.53	108.64	111.90
1	A	1329	A	C5-C6-N6	-6.53	118.48	123.70
1	A	1464	G	N1-C6-O6	6.53	123.82	119.90
1	A	108	G	C8-N9-C1'	-6.52	118.52	127.00
1	A	117	G	N9-C4-C5	-6.52	102.79	105.40
1	A	313	A	C8-N9-C4	6.52	108.41	105.80
1	A	576	G	C5-C6-N1	-6.52	108.24	111.50
1	A	509	A	N9-C4-C5	6.52	108.41	105.80
2	B	11	LEU	CA-CB-CG	6.51	130.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1343	G	C4-C5-N7	6.50	113.40	110.80
1	A	98	U	C5-C4-O4	6.50	129.80	125.90
1	A	324	G	C5-C6-O6	6.50	132.50	128.60
1	A	139	G	C2-N3-C4	-6.50	108.65	111.90
1	A	912	C	N3-C2-O2	6.50	126.45	121.90
1	A	980	C	C6-N1-C2	-6.49	117.70	120.30
1	A	674	G	N1-C6-O6	6.49	123.80	119.90
1	A	1056	U	N3-C4-O4	6.49	123.94	119.40
1	A	1337	G	C4-N9-C1'	-6.49	118.06	126.50
1	A	1442	G	C4-N9-C1'	6.49	134.94	126.50
9	I	56	LEU	CA-CB-CG	6.49	130.22	115.30
1	A	553	A	C2-N3-C4	-6.49	107.36	110.60
1	A	1397	C	N3-C2-O2	-6.48	117.37	121.90
1	A	389	A	C4-C5-C6	6.47	120.24	117.00
1	A	232	G	C8-N9-C4	6.47	108.99	106.40
1	A	329	A	C8-N9-C4	6.47	108.39	105.80
1	A	853	G	N9-C4-C5	-6.47	102.81	105.40
1	A	148	G	C6-C5-N7	-6.46	126.52	130.40
1	A	311	C	C6-N1-C2	-6.46	117.72	120.30
1	A	119	A	N1-C2-N3	6.46	132.53	129.30
23	W	37	A	C5-C6-N1	-6.46	114.47	117.70
1	A	430	A	N1-C6-N6	6.46	122.47	118.60
1	A	573	A	N1-C6-N6	-6.45	114.73	118.60
1	A	975	A	N1-C6-N6	6.45	122.47	118.60
1	A	800	G	N7-C8-N9	6.45	116.33	113.10
1	A	293	G	N1-C6-O6	6.45	123.77	119.90
1	A	1329	A	C4-C5-N7	6.45	113.92	110.70
1	A	444	C	C6-N1-C2	-6.44	117.72	120.30
1	A	939	G	N3-C4-N9	-6.44	122.13	126.00
1	A	1509	C	N3-C4-C5	6.44	124.48	121.90
1	A	572	A	N9-C4-C5	6.44	108.38	105.80
1	A	1068	G	C8-N9-C4	-6.44	103.82	106.40
1	A	781	A	C6-N1-C2	-6.42	114.75	118.60
1	A	660	G	N9-C4-C5	-6.42	102.83	105.40
1	A	1069	C	C2-N3-C4	6.42	123.11	119.90
1	A	189	G	C8-N9-C4	6.42	108.97	106.40
1	A	609	A	C2-N3-C4	-6.41	107.39	110.60
1	A	541	G	C6-C5-N7	-6.41	126.55	130.40
1	A	973	G	N1-C6-O6	-6.41	116.06	119.90
1	A	35	G	C5-C6-N1	-6.41	108.30	111.50
1	A	593	G	C5-C6-N1	-6.41	108.30	111.50
1	A	317	G	C6-C5-N7	-6.40	126.56	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	G	C8-N9-C4	6.40	108.96	106.40
1	A	1387	G	N3-C4-N9	-6.40	122.16	126.00
1	A	28	G	C6-C5-N7	-6.39	126.56	130.40
1	A	886	G	N1-C6-O6	6.38	123.73	119.90
1	A	851	G	C8-N9-C4	6.38	108.95	106.40
1	A	1196	U	N1-C2-O2	6.38	127.27	122.80
1	A	637	G	C4-C5-N7	6.38	113.35	110.80
1	A	1200	C	C4-C5-C6	-6.38	114.21	117.40
1	A	761	G	C5-C6-O6	-6.38	124.78	128.60
1	A	928	G	C8-N9-C4	6.37	108.95	106.40
1	A	328	C	P-O3'-C3'	6.37	127.34	119.70
1	A	931	C	C5-C6-N1	-6.37	117.82	121.00
1	A	872	A	C5-N7-C8	-6.36	100.72	103.90
1	A	544	G	C5-C6-N1	6.36	114.68	111.50
1	A	417	C	N3-C4-C5	-6.36	119.36	121.90
1	A	1344	C	N3-C4-C5	6.36	124.44	121.90
1	A	28	G	C5-N7-C8	-6.35	101.12	104.30
1	A	1143	G	C8-N9-C4	-6.35	103.86	106.40
1	A	116	A	N1-C2-N3	6.35	132.47	129.30
1	A	853	G	C6-C5-N7	-6.34	126.60	130.40
1	A	521	G	N3-C4-C5	6.33	131.77	128.60
1	A	1110	A	C5-N7-C8	-6.33	100.73	103.90
1	A	1416	G	C5-C6-N1	-6.33	108.33	111.50
1	A	945	G	C4-C5-N7	6.33	113.33	110.80
1	A	1206	G	C4-C5-N7	6.33	113.33	110.80
1	A	308	C	C5-C6-N1	6.33	124.16	121.00
1	A	1433	A	C8-N9-C4	-6.33	103.27	105.80
1	A	876	G	C4-C5-C6	-6.33	115.00	118.80
1	A	562	C	C4-C5-C6	-6.32	114.24	117.40
1	A	34	C	N3-C4-C5	6.32	124.43	121.90
1	A	27	G	N1-C6-O6	6.31	123.69	119.90
1	A	328	C	C4-C5-C6	-6.31	114.25	117.40
1	A	112	G	C8-N9-C4	6.31	108.92	106.40
1	A	345	C	C6-N1-C2	-6.31	117.78	120.30
1	A	1249	C	C5-C6-N1	6.31	124.15	121.00
1	A	92	C	N1-C2-O2	6.31	122.68	118.90
1	A	226	G	N7-C8-N9	-6.30	109.95	113.10
1	A	559	A	C6-N1-C2	-6.30	114.82	118.60
1	A	350	G	C2-N3-C4	-6.30	108.75	111.90
1	A	332	G	N3-C2-N2	-6.30	115.49	119.90
1	A	851	G	C5-C6-N1	-6.30	108.35	111.50
1	A	34	C	C6-N1-C2	6.30	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	A	C2-N3-C4	-6.29	107.45	110.60
20	T	99	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	529	G	N1-C6-O6	6.29	123.67	119.90
1	A	1057	G	N3-C4-C5	6.29	131.74	128.60
1	A	1266	G	N3-C4-N9	-6.29	122.23	126.00
1	A	833	U	C5-C4-O4	6.29	129.67	125.90
1	A	615	C	C6-N1-C2	-6.28	117.79	120.30
1	A	1088	G	N3-C4-C5	6.28	131.74	128.60
1	A	239	U	N3-C2-O2	6.28	126.59	122.20
1	A	518	C	N1-C2-N3	6.28	123.59	119.20
1	A	572	A	C5-C6-N1	6.28	120.84	117.70
1	A	1526	G	C6-C5-N7	-6.28	126.63	130.40
1	A	119	A	N1-C6-N6	-6.28	114.83	118.60
1	A	66	G	C2-N3-C4	-6.27	108.77	111.90
1	A	651	C	N3-C2-O2	6.27	126.29	121.90
22	V	3	U	C2-N1-C1'	6.26	125.22	117.70
1	A	484	G	N3-C4-C5	-6.26	125.47	128.60
1	A	505	G	N1-C6-O6	6.26	123.66	119.90
1	A	553	A	N9-C4-C5	-6.26	103.30	105.80
1	A	780	A	C4-C5-N7	6.26	113.83	110.70
1	A	792	A	C6-N1-C2	6.26	122.36	118.60
1	A	1186	G	C5-C6-N1	-6.26	108.37	111.50
1	A	633	G	C8-N9-C4	6.25	108.90	106.40
1	A	876	G	N1-C2-N2	6.25	121.83	116.20
1	A	1506	U	C6-N1-C1'	-6.25	112.44	121.20
1	A	856	C	N1-C2-N3	6.25	123.58	119.20
1	A	1348	U	C2-N1-C1'	6.25	125.20	117.70
1	A	482	A	C4-C5-C6	6.25	120.12	117.00
1	A	623	C	N3-C4-C5	6.25	124.40	121.90
1	A	117	G	C6-C5-N7	-6.25	126.65	130.40
1	A	449	C	N3-C4-C5	-6.25	119.40	121.90
1	A	949	A	C2-N3-C4	-6.24	107.48	110.60
1	A	398	C	N3-C2-O2	6.24	126.27	121.90
1	A	1353	G	N1-C6-O6	-6.24	116.16	119.90
1	A	92	C	N3-C2-O2	-6.24	117.53	121.90
1	A	1185	G	N3-C4-C5	6.24	131.72	128.60
1	A	1270	C	N3-C4-C5	-6.24	119.41	121.90
1	A	1079	G	C4-C5-N7	-6.23	108.31	110.80
1	A	28	G	N3-C4-C5	6.23	131.72	128.60
1	A	1530	G	N1-C6-O6	6.23	123.64	119.90
23	W	33	U	N1-C2-N3	6.23	118.64	114.90
1	A	79	G	N9-C4-C5	-6.23	102.91	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1334	G	N1-C6-O6	6.23	123.64	119.90
1	A	1331	G	N3-C4-N9	6.23	129.74	126.00
1	A	201	C	C6-N1-C2	6.22	122.79	120.30
1	A	283	C	C2-N1-C1'	6.22	125.65	118.80
1	A	374	A	C4-C5-C6	6.22	120.11	117.00
1	A	786	G	C6-C5-N7	-6.22	126.67	130.40
1	A	1113	C	C4-C5-C6	-6.21	114.29	117.40
1	A	1455	G	C5-C6-N1	-6.21	108.39	111.50
1	A	1057	G	N3-C2-N2	-6.21	115.55	119.90
1	A	620	C	N1-C2-N3	-6.21	114.85	119.20
1	A	886	G	N9-C4-C5	-6.21	102.92	105.40
1	A	50	A	C8-N9-C4	6.21	108.28	105.80
1	A	712	A	N1-C2-N3	6.21	132.40	129.30
1	A	1481	U	C5-C4-O4	6.21	129.62	125.90
1	A	1196	U	N3-C2-O2	-6.20	117.86	122.20
1	A	266	G	C5-C6-N1	-6.20	108.40	111.50
1	A	973	G	C5-C6-N1	6.20	114.60	111.50
1	A	1052	U	C6-N1-C2	-6.20	117.28	121.00
1	A	1061	G	C2-N3-C4	-6.20	108.80	111.90
1	A	1057	G	N1-C2-N2	6.19	121.77	116.20
1	A	109	A	C8-N9-C4	-6.19	103.32	105.80
1	A	186	C	N3-C4-C5	6.19	124.38	121.90
1	A	1199	U	N3-C4-C5	-6.19	110.89	114.60
1	A	873	A	C8-N9-C4	-6.18	103.33	105.80
1	A	310	G	C5-C6-O6	-6.18	124.89	128.60
1	A	592	G	C5-C6-N1	-6.18	108.41	111.50
1	A	646	U	C6-N1-C1'	6.18	129.85	121.20
1	A	542	G	C6-C5-N7	-6.18	126.69	130.40
1	A	364	A	C2-N3-C4	-6.17	107.51	110.60
1	A	1333	A	C6-N1-C2	-6.17	114.90	118.60
1	A	705	U	N3-C2-O2	-6.17	117.88	122.20
1	A	266	G	N3-C4-C5	6.17	131.69	128.60
1	A	1048	G	N3-C4-C5	6.17	131.68	128.60
1	A	129	U	C2-N1-C1'	-6.17	110.30	117.70
1	A	530	G	C4-N9-C1'	-6.16	118.49	126.50
1	A	1461	G	N3-C4-C5	6.16	131.68	128.60
1	A	518	C	C4-C5-C6	6.16	120.48	117.40
1	A	1266	G	C4-C5-N7	-6.16	108.34	110.80
1	A	574	A	C4-C5-N7	6.15	113.78	110.70
1	A	80	G	N3-C4-C5	-6.15	125.53	128.60
1	A	298	A	C5-N7-C8	-6.15	100.83	103.90
1	A	802	A	C8-N9-C4	-6.15	103.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1050	G	N1-C6-O6	6.15	123.59	119.90
1	A	722	A	C2-N3-C4	-6.14	107.53	110.60
1	A	1266	G	C5-C6-O6	6.14	132.29	128.60
1	A	1145	C	N3-C4-C5	-6.14	119.44	121.90
1	A	885	G	C6-C5-N7	-6.14	126.72	130.40
1	A	1411	C	C6-N1-C2	-6.14	117.84	120.30
1	A	816	A	N1-C6-N6	-6.13	114.92	118.60
1	A	561	U	C5-C4-O4	-6.13	122.22	125.90
1	A	1084	G	N3-C4-C5	-6.13	125.53	128.60
1	A	1301	U	P-O3'-C3'	6.13	127.06	119.70
1	A	119	A	N9-C4-C5	6.13	108.25	105.80
1	A	993	G	N7-C8-N9	6.13	116.17	113.10
1	A	391	G	N1-C6-O6	6.13	123.58	119.90
1	A	1303	C	N3-C4-C5	6.13	124.35	121.90
1	A	283	C	C2-N3-C4	6.12	122.96	119.90
1	A	968	A	C8-N9-C4	6.12	108.25	105.80
1	A	199	G	N1-C6-O6	6.12	123.57	119.90
1	A	547	A	C2-N3-C4	6.12	113.66	110.60
1	A	1322	C	C6-N1-C1'	-6.12	113.46	120.80
1	A	1299	A	C6-C5-N7	-6.12	128.02	132.30
1	A	190(F)	G	N3-C2-N2	-6.12	115.62	119.90
1	A	1186	G	N3-C4-C5	6.12	131.66	128.60
1	A	174	C	C6-N1-C2	-6.11	117.86	120.30
1	A	1248	A	N1-C6-N6	6.11	122.27	118.60
1	A	1347	G	C8-N9-C4	6.11	108.84	106.40
1	A	761	G	N1-C6-O6	6.11	123.57	119.90
1	A	1401	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	216	G	C4-N9-C1'	-6.11	118.56	126.50
1	A	1386	G	C4-C5-N7	-6.11	108.36	110.80
1	A	290	C	N1-C2-O2	-6.11	115.24	118.90
1	A	331	G	C4-C5-N7	6.11	113.24	110.80
1	A	782	A	C5-C6-N1	6.11	120.75	117.70
1	A	767	A	N1-C6-N6	-6.10	114.94	118.60
1	A	173	U	N3-C4-O4	-6.10	115.13	119.40
1	A	888	G	C8-N9-C1'	-6.10	119.07	127.00
1	A	377	G	C5-C6-N1	6.10	114.55	111.50
1	A	975	A	C4-C5-C6	6.10	120.05	117.00
1	A	869	G	C6-C5-N7	-6.10	126.74	130.40
1	A	401	C	N3-C4-N4	6.09	122.27	118.00
1	A	1299	A	C4-C5-N7	6.09	113.75	110.70
1	A	251	G	N1-C2-N2	-6.08	110.72	116.20
1	A	1248	A	C8-N9-C4	6.08	108.23	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	G	C8-N9-C4	-6.08	103.97	106.40
1	A	1506	U	N3-C4-O4	6.08	123.65	119.40
1	A	34	C	C5-C4-N4	-6.08	115.95	120.20
1	A	125	U	N1-C2-N3	6.08	118.55	114.90
1	A	923	A	N9-C4-C5	-6.07	103.37	105.80
1	A	181	G	N3-C4-C5	-6.07	125.56	128.60
1	A	1110	A	C4-C5-N7	6.07	113.74	110.70
1	A	108	G	C4-C5-N7	6.07	113.23	110.80
1	A	1442	G	C8-N9-C4	-6.07	103.97	106.40
1	A	42	G	C5-C6-N1	-6.07	108.47	111.50
1	A	931	C	C2-N1-C1'	-6.07	112.13	118.80
1	A	962	C	N3-C4-C5	6.06	124.32	121.90
1	A	1346	A	C2-N3-C4	-6.06	107.57	110.60
1	A	1502	A	N9-C4-C5	-6.06	103.38	105.80
12	L	102	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	576	G	C2-N3-C4	-6.05	108.87	111.90
1	A	304	U	C6-N1-C2	-6.05	117.37	121.00
1	A	391	G	C5-C6-O6	-6.05	124.97	128.60
1	A	190(I)	G	N3-C4-C5	6.05	131.62	128.60
1	A	730	G	C4-N9-C1'	6.04	134.36	126.50
1	A	775	G	C4-C5-N7	-6.04	108.38	110.80
1	A	433	C	C2-N3-C4	6.04	122.92	119.90
1	A	1187	G	C8-N9-C1'	-6.04	119.15	127.00
1	A	1337	G	C8-N9-C1'	6.04	134.85	127.00
1	A	378	G	C5-C6-O6	-6.04	124.98	128.60
1	A	807	A	C6-N1-C2	-6.04	114.98	118.60
1	A	1246	C	C6-N1-C2	6.04	122.72	120.30
1	A	860	A	C2-N3-C4	-6.03	107.58	110.60
1	A	1250	A	N1-C6-N6	6.03	122.22	118.60
1	A	416	G	C5-C6-O6	-6.02	124.99	128.60
1	A	392	G	C8-N9-C4	6.02	108.81	106.40
1	A	786	G	N7-C8-N9	6.02	116.11	113.10
1	A	898	G	C8-N9-C4	6.02	108.81	106.40
1	A	803	G	C5-C6-N1	-6.02	108.49	111.50
1	A	521	G	C5-C6-O6	6.02	132.21	128.60
1	A	780	A	N9-C4-C5	-6.02	103.39	105.80
1	A	360	A	C6-C5-N7	-6.02	128.09	132.30
1	A	1520	G	C4-C5-N7	6.02	113.21	110.80
1	A	578	C	N3-C4-C5	-6.01	119.50	121.90
1	A	390	C	N3-C2-O2	6.01	126.11	121.90
1	A	755	G	C4-C5-N7	6.01	113.20	110.80
1	A	297	G	C4-C5-N7	-6.01	108.40	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	N9-C4-C5	-6.00	103.00	105.40
1	A	852	G	C4-C5-C6	6.00	122.40	118.80
1	A	259	G	C6-C5-N7	-6.00	126.80	130.40
1	A	542	G	C4-N9-C1'	6.00	134.30	126.50
1	A	698	G	C6-C5-N7	-6.00	126.80	130.40
1	A	975	A	C8-N9-C4	-6.00	103.40	105.80
1	A	308	C	N1-C2-N3	-6.00	115.00	119.20
1	A	606	G	C4-N9-C1'	6.00	134.29	126.50
1	A	724	G	C4-C5-N7	6.00	113.20	110.80
1	A	724	G	N1-C6-O6	5.99	123.50	119.90
1	A	1374	A	C5-C6-N6	5.99	128.50	123.70
1	A	529	G	C5-C6-O6	-5.99	125.00	128.60
1	A	1063	C	N1-C2-O2	-5.99	115.31	118.90
1	A	1347	G	N7-C8-N9	-5.99	110.11	113.10
1	A	856	C	C2-N1-C1'	5.98	125.38	118.80
1	A	1438	G	C8-N9-C4	5.98	108.79	106.40
1	A	853	G	C8-N9-C4	5.98	108.79	106.40
1	A	888	G	C4-N9-C1'	5.98	134.28	126.50
1	A	108	G	C5-N7-C8	-5.98	101.31	104.30
1	A	560	U	C5-C4-O4	5.98	129.49	125.90
1	A	1180	A	C8-N9-C4	-5.98	103.41	105.80
1	A	36	C	N1-C2-O2	5.97	122.48	118.90
1	A	299	G	C8-N9-C4	5.97	108.79	106.40
1	A	768	A	N1-C6-N6	5.97	122.19	118.60
1	A	818	G	C5-C6-N1	-5.97	108.51	111.50
1	A	1397	C	C6-N1-C2	-5.97	117.91	120.30
1	A	670	G	C5-C6-O6	-5.97	125.02	128.60
1	A	733	A	N1-C2-N3	5.97	132.28	129.30
1	A	818	G	N7-C8-N9	5.97	116.08	113.10
1	A	1432	G	C5-C6-O6	5.96	132.18	128.60
1	A	730	G	C8-N9-C4	-5.96	104.02	106.40
1	A	1329	A	N9-C4-C5	-5.96	103.42	105.80
1	A	611	A	C8-N9-C4	5.96	108.18	105.80
1	A	1231	G	C5-C6-N1	-5.96	108.52	111.50
1	A	82	U	C5-C6-N1	5.95	125.68	122.70
1	A	304	U	N3-C4-O4	5.95	123.57	119.40
1	A	367	U	C6-N1-C1'	-5.95	112.87	121.20
1	A	1421	G	N3-C4-C5	-5.95	125.62	128.60
1	A	200	G	N1-C6-O6	5.95	123.47	119.90
1	A	575	G	C8-N9-C4	5.95	108.78	106.40
1	A	785	G	N1-C6-O6	5.94	123.46	119.90
1	A	971	G	N3-C4-C5	5.94	131.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	G	C5-C6-O6	-5.94	125.04	128.60
1	A	293	G	C5-C6-O6	-5.93	125.04	128.60
1	A	324	G	C4-C5-N7	-5.93	108.43	110.80
1	A	645	C	N3-C4-N4	5.93	122.15	118.00
1	A	959	A	C8-N9-C4	5.93	108.17	105.80
1	A	1526	G	N1-C6-O6	5.93	123.46	119.90
1	A	626	U	N3-C4-C5	5.93	118.16	114.60
1	A	1113	C	N3-C2-O2	5.93	126.05	121.90
1	A	518	C	C6-N1-C1'	5.93	127.91	120.80
1	A	1373	G	C4-C5-C6	5.93	122.36	118.80
1	A	672	U	C5-C4-O4	5.93	129.46	125.90
1	A	812	C	P-O3'-C3'	5.92	126.81	119.70
1	A	816	A	C4-C5-C6	-5.92	114.04	117.00
1	A	923	A	C8-N9-C4	5.92	108.17	105.80
1	A	884	U	C6-N1-C2	5.92	124.55	121.00
23	W	33	U	N1-C2-O2	-5.92	118.66	122.80
1	A	1452	C	C6-N1-C2	5.92	122.67	120.30
1	A	875	C	C2-N3-C4	-5.92	116.94	119.90
1	A	29	G	N3-C4-N9	-5.91	122.45	126.00
1	A	646	U	C2-N1-C1'	-5.91	110.61	117.70
1	A	1243	C	C2-N3-C4	5.91	122.86	119.90
1	A	1525	G	N3-C4-C5	-5.91	125.64	128.60
1	A	15	G	C5-C6-O6	-5.91	125.06	128.60
1	A	1048	G	N1-C6-O6	5.90	123.44	119.90
1	A	1079	G	C5-C6-O6	5.90	132.14	128.60
1	A	16	A	C5-N7-C8	5.90	106.85	103.90
1	A	147	G	N1-C6-O6	5.90	123.44	119.90
1	A	913	A	P-O3'-C3'	5.90	126.78	119.70
1	A	1056	U	C5-C6-N1	5.90	125.65	122.70
1	A	1338	G	C8-N9-C4	-5.90	104.04	106.40
1	A	1348	U	C5-C6-N1	5.90	125.65	122.70
1	A	836	G	N9-C4-C5	-5.90	103.04	105.40
1	A	837	G	C5-C6-N1	-5.90	108.55	111.50
1	A	303	A	C2-N3-C4	-5.90	107.65	110.60
1	A	1487	G	C6-N1-C2	5.89	128.64	125.10
23	W	37	A	N1-C6-N6	5.89	122.14	118.60
1	A	785	G	N3-C4-C5	5.89	131.55	128.60
1	A	886	G	N3-C4-C5	5.89	131.55	128.60
1	A	412	A	C8-N9-C4	5.89	108.16	105.80
1	A	288	A	N3-C4-C5	5.89	130.92	126.80
1	A	160	A	N1-C6-N6	5.88	122.13	118.60
1	A	817	C	C6-N1-C2	5.88	122.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	A	C8-N9-C4	5.88	108.15	105.80
1	A	1068	G	N7-C8-N9	5.88	116.04	113.10
1	A	1245	A	N7-C8-N9	-5.88	110.86	113.80
1	A	654	G	N1-C2-N3	5.88	127.43	123.90
1	A	297	G	N1-C6-O6	-5.88	116.37	119.90
1	A	648	A	N7-C8-N9	-5.88	110.86	113.80
1	A	887	G	C8-N9-C4	5.88	108.75	106.40
1	A	1192	C	N1-C2-O2	5.88	122.43	118.90
1	A	482	A	N1-C2-N3	5.88	132.24	129.30
1	A	324	G	C5-C6-N1	-5.88	108.56	111.50
1	A	1064	G	C6-N1-C2	-5.87	121.58	125.10
1	A	1296	C	N1-C2-O2	-5.87	115.38	118.90
1	A	640	A	C4-C5-N7	5.87	113.64	110.70
1	A	105	G	C4-C5-C6	5.87	122.32	118.80
1	A	712	A	C8-N9-C4	-5.87	103.45	105.80
1	A	1461	G	C4-N9-C1'	-5.87	118.87	126.50
1	A	675	A	C5-C6-N1	-5.86	114.77	117.70
1	A	731	G	C5-C6-O6	-5.86	125.08	128.60
1	A	852	G	C6-C5-N7	-5.86	126.88	130.40
1	A	378	G	C5-N7-C8	-5.86	101.37	104.30
1	A	1064	G	N9-C4-C5	5.86	107.74	105.40
1	A	606	G	C4-C5-N7	5.86	113.14	110.80
1	A	1475	G	C5-C6-N1	-5.86	108.57	111.50
1	A	111	G	C8-N9-C4	-5.85	104.06	106.40
1	A	348	G	C5-C6-O6	-5.85	125.09	128.60
1	A	446	G	C5-C6-N1	-5.85	108.58	111.50
1	A	1543	C	C6-N1-C2	-5.85	117.96	120.30
1	A	76	C	C4-C5-C6	-5.84	114.48	117.40
1	A	573	A	C2-N3-C4	5.84	113.52	110.60
1	A	542	G	N1-C6-O6	5.84	123.40	119.90
1	A	1245	A	C8-N9-C4	5.84	108.14	105.80
1	A	529	G	C4-C5-N7	5.84	113.13	110.80
1	A	262	A	C8-N9-C4	-5.83	103.47	105.80
1	A	991	U	C5-C6-N1	-5.83	119.78	122.70
1	A	300	A	N1-C6-N6	5.83	122.10	118.60
1	A	268	C	N1-C2-O2	5.83	122.40	118.90
1	A	573	A	C8-N9-C4	-5.83	103.47	105.80
1	A	147	G	C4-C5-C6	5.83	122.30	118.80
1	A	661	G	N3-C4-N9	-5.83	122.50	126.00
1	A	1286	A	N7-C8-N9	5.83	116.71	113.80
1	A	1338	G	N3-C4-N9	-5.83	122.50	126.00
1	A	900	A	N1-C2-N3	5.82	132.21	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	G	N1-C6-O6	5.82	123.39	119.90
1	A	1416	G	N1-C6-O6	5.82	123.39	119.90
1	A	1283	G	N7-C8-N9	5.82	116.01	113.10
1	A	688	G	C2-N3-C4	-5.82	108.99	111.90
1	A	698	G	C2-N3-C4	-5.81	108.99	111.90
5	E	41	VAL	CB-CA-C	-5.81	100.36	111.40
1	A	25	C	C6-N1-C2	5.81	122.62	120.30
1	A	387	U	C5-C6-N1	-5.81	119.80	122.70
1	A	871	U	N1-C2-O2	5.81	126.87	122.80
1	A	1326	C	N3-C4-C5	-5.81	119.58	121.90
1	A	108	G	C5-C6-O6	-5.81	125.12	128.60
1	A	885	G	C5-C6-O6	-5.81	125.12	128.60
1	A	69	G	N3-C4-C5	5.80	131.50	128.60
1	A	409	G	C8-N9-C4	5.80	108.72	106.40
1	A	1222	G	C6-N1-C2	5.80	128.58	125.10
1	A	792	A	C6-C5-N7	-5.80	128.24	132.30
1	A	935	A	C8-N9-C4	5.80	108.12	105.80
1	A	1377	A	N1-C2-N3	5.80	132.20	129.30
1	A	682	G	N3-C4-C5	5.79	131.50	128.60
1	A	642	A	C2-N3-C4	-5.79	107.70	110.60
1	A	1087	G	C6-C5-N7	-5.79	126.93	130.40
1	A	201	C	N1-C2-O2	5.78	122.37	118.90
1	A	572	A	C5-C6-N6	5.78	128.33	123.70
1	A	260	G	N9-C4-C5	5.78	107.71	105.40
1	A	605	U	N3-C4-O4	5.78	123.44	119.40
1	A	1335	C	C6-N1-C2	5.78	122.61	120.30
1	A	47	C	C5-C6-N1	-5.78	118.11	121.00
1	A	1295	G	N1-C6-O6	5.78	123.37	119.90
1	A	854	G	C8-N9-C4	-5.77	104.09	106.40
1	A	1290	G	N3-C2-N2	-5.77	115.86	119.90
1	A	1361(A)	C	N3-C2-O2	-5.77	117.86	121.90
1	A	109	A	N9-C4-C5	5.77	108.11	105.80
1	A	640	A	C5-N7-C8	-5.77	101.02	103.90
1	A	765	G	C8-N9-C4	5.77	108.71	106.40
1	A	1543	C	C2-N3-C4	5.77	122.78	119.90
1	A	174	C	N1-C2-O2	5.76	122.36	118.90
1	A	398	C	C4-C5-C6	-5.76	114.52	117.40
1	A	859	A	C2-N3-C4	-5.76	107.72	110.60
1	A	876	G	C6-C5-N7	5.76	133.86	130.40
1	A	885	G	C5-C6-N1	-5.76	108.62	111.50
1	A	1513	A	C8-N9-C4	5.76	108.11	105.80
4	D	57	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	G	C6-C5-N7	-5.76	126.94	130.40
1	A	1266	G	N9-C4-C5	5.76	107.70	105.40
1	A	131	C	N1-C2-O2	5.75	122.35	118.90
1	A	1455	G	C8-N9-C4	-5.75	104.10	106.40
1	A	978	A	C6-C5-N7	-5.75	128.27	132.30
1	A	258	G	C5-C6-N1	-5.75	108.62	111.50
1	A	688	G	N1-C6-O6	5.75	123.35	119.90
2	B	196	LEU	CA-CB-CG	-5.75	102.08	115.30
1	A	637	G	N1-C6-O6	5.75	123.35	119.90
1	A	401	C	C5-C6-N1	5.75	123.87	121.00
1	A	561	U	C2-N1-C1'	5.74	124.59	117.70
1	A	1451	A	C2-N3-C4	5.74	113.47	110.60
1	A	148	G	N1-C6-O6	5.74	123.34	119.90
1	A	1131	G	C5-C6-O6	-5.74	125.16	128.60
23	W	33	U	C6-N1-C2	-5.74	117.56	121.00
1	A	1216	G	C8-N9-C4	5.74	108.69	106.40
1	A	825	G	C8-N9-C4	5.74	108.69	106.40
1	A	616	G	N1-C6-O6	5.74	123.34	119.90
1	A	170	U	N3-C4-C5	-5.73	111.16	114.60
1	A	1471	G	N1-C6-O6	5.73	123.34	119.90
1	A	1113	C	C5-C4-N4	-5.73	116.19	120.20
1	A	888	G	C5-C6-N1	-5.73	108.64	111.50
1	A	301	G	C5-C6-N1	-5.72	108.64	111.50
1	A	1417	G	N1-C6-O6	5.72	123.33	119.90
1	A	174	C	C4-C5-C6	-5.72	114.54	117.40
1	A	393	A	C2-N3-C4	-5.72	107.74	110.60
1	A	1437	C	C6-N1-C2	5.71	122.59	120.30
1	A	232	G	C4-N9-C1'	5.71	133.92	126.50
1	A	1206	G	N9-C4-C5	-5.71	103.12	105.40
1	A	1053	G	N7-C8-N9	-5.71	110.25	113.10
1	A	639	G	C5-C6-O6	-5.71	125.17	128.60
1	A	216	G	C4-C5-N7	-5.71	108.52	110.80
1	A	1101	A	C6-C5-N7	5.71	136.29	132.30
1	A	874	G	N3-C4-N9	5.70	129.42	126.00
1	A	126	G	N1-C6-O6	5.70	123.32	119.90
1	A	60	A	C4-C5-N7	-5.70	107.85	110.70
1	A	574	A	N3-C4-C5	5.70	130.79	126.80
1	A	1015	A	N1-C6-N6	-5.70	115.18	118.60
1	A	1125	U	N1-C2-N3	-5.70	111.48	114.90
1	A	1205	U	C2-N3-C4	-5.70	123.58	127.00
1	A	572	A	C4-C5-C6	-5.69	114.16	117.00
1	A	809	G	N1-C6-O6	5.69	123.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1223	C	C5-C6-N1	5.69	123.85	121.00
1	A	1252	A	C2-N3-C4	5.69	113.44	110.60
1	A	1290	G	N1-C6-O6	5.69	123.31	119.90
1	A	895	G	N3-C2-N2	-5.69	115.92	119.90
1	A	674	G	C2-N3-C4	-5.69	109.06	111.90
1	A	1447	G	N1-C6-O6	5.69	123.31	119.90
1	A	158	G	C8-N9-C4	-5.68	104.13	106.40
1	A	162	A	N1-C6-N6	-5.68	115.19	118.60
1	A	216	G	C5-N7-C8	5.68	107.14	104.30
1	A	533	A	N1-C2-N3	5.68	132.14	129.30
1	A	1012	U	C6-N1-C2	-5.68	117.59	121.00
1	A	348	G	C4-C5-N7	5.68	113.07	110.80
12	L	10	LEU	CA-CB-CG	-5.68	102.24	115.30
1	A	1227	A	C5-N7-C8	-5.68	101.06	103.90
1	A	296	U	N1-C2-N3	5.67	118.31	114.90
1	A	654	G	N1-C6-O6	-5.67	116.50	119.90
1	A	309	G	C4-C5-N7	5.67	113.07	110.80
1	A	734	G	C6-C5-N7	-5.67	127.00	130.40
1	A	690	G	C8-N9-C4	5.67	108.67	106.40
1	A	1182	G	N1-C6-O6	5.67	123.30	119.90
1	A	109	A	N1-C6-N6	-5.67	115.20	118.60
1	A	285	G	C2-N3-C4	-5.67	109.07	111.90
1	A	380	G	C5-C6-N1	-5.66	108.67	111.50
1	A	676	A	C2-N3-C4	-5.66	107.77	110.60
1	A	286	G	N1-C6-O6	5.66	123.30	119.90
1	A	730	G	C4-C5-C6	5.66	122.20	118.80
1	A	1187	G	N7-C8-N9	5.66	115.93	113.10
1	A	804	U	C4-C5-C6	5.65	123.09	119.70
1	A	146	G	N7-C8-N9	5.65	115.93	113.10
1	A	650	G	C5-C6-O6	-5.65	125.21	128.60
1	A	911	U	N3-C4-C5	-5.65	111.21	114.60
1	A	927	G	C2-N3-C4	-5.65	109.08	111.90
1	A	1455	G	N3-C2-N2	-5.65	115.95	119.90
1	A	1290	G	N1-C2-N2	5.65	121.28	116.20
1	A	194	C	N1-C2-O2	5.64	122.29	118.90
1	A	606	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	782	A	C5-N7-C8	-5.64	101.08	103.90
1	A	1084	G	C4-C5-C6	5.64	122.18	118.80
1	A	1532	U	C6-N1-C2	-5.64	117.62	121.00
1	A	705	U	N1-C2-N3	5.64	118.28	114.90
1	A	514	C	N3-C4-N4	5.63	121.94	118.00
1	A	902	G	C2-N3-C4	-5.63	109.08	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1467	G	N9-C4-C5	5.63	107.65	105.40
1	A	809	G	C2-N3-C4	-5.63	109.08	111.90
1	A	599	C	N3-C4-N4	5.63	121.94	118.00
1	A	1314	C	N3-C4-C5	-5.63	119.65	121.90
1	A	187	C	C6-N1-C2	-5.63	118.05	120.30
1	A	1236	A	C5-N7-C8	-5.63	101.08	103.90
1	A	254	G	C5-C6-N1	-5.63	108.69	111.50
1	A	1258	G	C2-N3-C4	5.63	114.71	111.90
1	A	15	G	C6-C5-N7	-5.62	127.03	130.40
1	A	190(F)	G	C8-N9-C1'	5.62	134.31	127.00
1	A	613	C	N3-C4-N4	5.62	121.94	118.00
1	A	377	G	C6-N1-C2	-5.62	121.73	125.10
1	A	457	C	C6-N1-C2	5.62	122.55	120.30
1	A	135	C	N3-C4-C5	-5.61	119.66	121.90
1	A	515	G	C4-C5-N7	5.61	113.05	110.80
1	A	1526	G	N9-C4-C5	-5.61	103.15	105.40
1	A	577	G	C5-N7-C8	-5.61	101.49	104.30
1	A	170	U	C6-N1-C2	-5.61	117.63	121.00
1	A	1187	G	C8-N9-C4	-5.61	104.16	106.40
1	A	1515	C	N3-C4-N4	5.61	121.93	118.00
1	A	363	A	C5-N7-C8	-5.61	101.10	103.90
1	A	575	G	N7-C8-N9	-5.61	110.30	113.10
1	A	1197	G	C8-N9-C4	-5.61	104.16	106.40
1	A	325	A	N9-C4-C5	5.61	108.04	105.80
1	A	410	G	C4-C5-N7	5.61	113.04	110.80
1	A	1012	U	N3-C4-C5	-5.61	111.24	114.60
1	A	1346	A	N3-C4-N9	-5.61	122.92	127.40
1	A	829	G	C4-C5-N7	5.60	113.04	110.80
1	A	931	C	C5-C4-N4	5.60	124.12	120.20
1	A	294	U	N3-C2-O2	5.60	126.12	122.20
1	A	902	G	N3-C4-C5	5.59	131.40	128.60
1	A	378	G	N3-C4-C5	5.59	131.40	128.60
1	A	1131	G	N1-C6-O6	5.59	123.26	119.90
1	A	1192	C	N3-C2-O2	-5.59	117.98	121.90
1	A	410	G	C6-C5-N7	-5.59	127.05	130.40
1	A	620	C	C6-N1-C2	5.59	122.53	120.30
1	A	804	U	C5-C6-N1	-5.59	119.91	122.70
1	A	1078	U	C5-C6-N1	5.59	125.49	122.70
1	A	1079	G	C6-C5-N7	-5.59	127.05	130.40
1	A	668	G	C8-N9-C1'	-5.59	119.74	127.00
1	A	867	G	C5-C6-O6	-5.59	125.25	128.60
1	A	993	G	C4-N9-C1'	5.59	133.76	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1258	G	N7-C8-N9	5.59	115.89	113.10
1	A	685	G	C2-N3-C4	-5.58	109.11	111.90
1	A	706	A	C4-C5-N7	5.58	113.49	110.70
1	A	1061	G	C5-C6-O6	-5.58	125.25	128.60
1	A	35	G	N7-C8-N9	5.58	115.89	113.10
1	A	389	A	C8-N9-C4	-5.58	103.57	105.80
1	A	174	C	C2-N1-C1'	5.58	124.93	118.80
1	A	869	G	N3-C4-C5	5.58	131.39	128.60
1	A	1150	U	C6-N1-C2	-5.58	117.66	121.00
1	A	1421	G	N7-C8-N9	5.58	115.89	113.10
1	A	1128	C	N1-C2-O2	-5.57	115.56	118.90
1	A	1364	U	C5-C6-N1	-5.57	119.92	122.70
1	A	329	A	C5-C6-N6	5.57	128.16	123.70
1	A	576	G	N1-C6-O6	5.57	123.24	119.90
18	R	78	LEU	CA-CB-CG	-5.57	102.50	115.30
1	A	1054	C	N3-C4-C5	5.57	124.13	121.90
1	A	13	U	C4-C5-C6	5.56	123.04	119.70
1	A	1079	G	C4-N9-C1'	5.56	133.73	126.50
1	A	1212	U	C6-N1-C1'	-5.56	113.41	121.20
1	A	459	G	C6-C5-N7	-5.56	127.06	130.40
1	A	1198	G	C8-N9-C4	5.56	108.62	106.40
1	A	1516	G	C8-N9-C1'	5.56	134.22	127.00
1	A	1074	G	C8-N9-C1'	-5.56	119.78	127.00
1	A	434	U	N1-C2-N3	-5.55	111.57	114.90
1	A	675	A	C2-N3-C4	-5.55	107.82	110.60
1	A	1526	G	C5-N7-C8	-5.55	101.53	104.30
1	A	1130	A	N7-C8-N9	5.54	116.57	113.80
1	A	806	C	C6-N1-C2	5.54	122.52	120.30
1	A	1266	G	C6-C5-N7	5.54	133.72	130.40
1	A	1192	C	C2-N1-C1'	5.54	124.89	118.80
1	A	568	G	C8-N9-C4	-5.53	104.19	106.40
1	A	190(K)	G	C6-C5-N7	-5.53	127.08	130.40
1	A	688	G	C8-N9-C4	5.53	108.61	106.40
1	A	394	G	N3-C4-C5	5.53	131.36	128.60
1	A	14	U	N1-C2-O2	-5.53	118.93	122.80
1	A	289	G	N1-C6-O6	5.53	123.22	119.90
1	A	367	U	C5-C4-O4	-5.52	122.59	125.90
1	A	66	G	N3-C4-C5	5.52	131.36	128.60
1	A	859	A	N1-C2-N3	5.52	132.06	129.30
1	A	577	G	C4-C5-N7	5.52	113.01	110.80
1	A	1361(A)	C	N1-C2-O2	5.52	122.21	118.90
1	A	1313	U	C2-N3-C4	5.52	130.31	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	G	C8-N9-C1'	-5.51	119.83	127.00
1	A	387	U	N3-C2-O2	-5.51	118.34	122.20
1	A	1467	G	C5-C6-O6	5.51	131.91	128.60
1	A	246	A	C8-N9-C4	5.51	108.00	105.80
1	A	431	A	N1-C6-N6	5.51	121.91	118.60
1	A	9	G	C8-N9-C4	5.51	108.60	106.40
1	A	564	C	C5-C4-N4	-5.51	116.34	120.20
1	A	367	U	C2-N1-C1'	5.51	124.31	117.70
1	A	542	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	1227	A	C5-C6-N1	-5.50	114.95	117.70
1	A	767	A	N7-C8-N9	-5.50	111.05	113.80
1	A	947	G	C4-C5-N7	5.50	113.00	110.80
1	A	1304	G	C4-C5-N7	-5.50	108.60	110.80
1	A	459	G	N7-C8-N9	5.50	115.85	113.10
22	V	2	U	C5-C6-N1	-5.50	119.95	122.70
1	A	886	G	C6-N1-C2	5.49	128.40	125.10
1	A	108	G	N1-C6-O6	5.49	123.19	119.90
1	A	35	G	C8-N9-C4	-5.49	104.20	106.40
1	A	648	A	C5-C6-N1	5.49	120.44	117.70
1	A	245	C	N3-C4-C5	5.49	124.09	121.90
1	A	1323	G	N3-C4-C5	5.49	131.34	128.60
1	A	139	G	N3-C2-N2	-5.48	116.06	119.90
1	A	479	C	N3-C4-C5	-5.48	119.71	121.90
1	A	117	G	C6-N1-C2	5.48	128.39	125.10
1	A	550	G	N3-C4-C5	5.48	131.34	128.60
1	A	328	C	N3-C2-O2	-5.48	118.07	121.90
1	A	904	C	C5-C6-N1	-5.48	118.26	121.00
1	A	1188	A	C8-N9-C4	5.47	107.99	105.80
1	A	1353	G	C5-C6-N1	5.47	114.24	111.50
1	A	1146	A	N1-C6-N6	-5.47	115.32	118.60
1	A	19	C	C5-C6-N1	5.46	123.73	121.00
1	A	818	G	N3-C4-N9	-5.46	122.72	126.00
1	A	1165	C	C6-N1-C2	-5.46	118.11	120.30
1	A	300	A	C5-C6-N6	-5.46	119.33	123.70
1	A	651	C	N1-C2-O2	-5.46	115.62	118.90
1	A	1405	G	N1-C6-O6	5.46	123.18	119.90
1	A	386	C	N3-C2-O2	5.46	125.72	121.90
1	A	125	U	C2-N3-C4	-5.46	123.72	127.00
1	A	303	A	N1-C2-N3	5.46	132.03	129.30
1	A	431	A	N9-C4-C5	-5.46	103.62	105.80
1	A	1113	C	N1-C2-N3	-5.46	115.38	119.20
1	A	661	G	N1-C2-N2	5.46	121.11	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	36	A	C4-C5-C6	5.45	119.73	117.00
1	A	964	A	N1-C2-N3	5.45	132.03	129.30
1	A	559	A	C4-N9-C1'	5.45	136.11	126.30
1	A	64	G	N3-C2-N2	-5.45	116.09	119.90
1	A	255	G	N1-C6-O6	5.45	123.17	119.90
1	A	1076	C	C6-N1-C2	-5.45	118.12	120.30
1	A	721	G	N3-C4-C5	-5.44	125.88	128.60
1	A	610	G	N9-C4-C5	5.44	107.58	105.40
1	A	261	U	N1-C2-N3	5.44	118.17	114.90
1	A	459	G	C8-N9-C4	-5.44	104.22	106.40
1	A	1465	C	C6-N1-C2	-5.44	118.12	120.30
1	A	429	U	N1-C2-N3	5.44	118.16	114.90
1	A	254	G	N3-C4-N9	-5.44	122.74	126.00
1	A	971	G	N3-C2-N2	-5.44	116.09	119.90
1	A	618	C	C6-N1-C2	5.43	122.47	120.30
1	A	1192	C	C6-N1-C2	-5.43	118.13	120.30
1	A	384	G	C5-C6-N1	5.43	114.22	111.50
1	A	621	A	N1-C6-N6	5.43	121.86	118.60
1	A	1074	G	C4-N9-C1'	5.43	133.56	126.50
1	A	1128	C	N3-C4-C5	-5.43	119.73	121.90
1	A	976	G	N9-C4-C5	-5.43	103.23	105.40
1	A	665	A	C4-C5-N7	-5.43	107.99	110.70
1	A	1243	C	C6-N1-C2	-5.42	118.13	120.30
1	A	658	G	N1-C6-O6	5.42	123.15	119.90
1	A	752	G	N1-C6-O6	5.42	123.15	119.90
1	A	907	A	C8-N9-C4	-5.42	103.63	105.80
1	A	785	G	C5-C6-O6	-5.41	125.35	128.60
1	A	916	G	C4-C5-N7	-5.41	108.63	110.80
1	A	981	U	N3-C2-O2	5.41	125.99	122.20
1	A	542	G	N3-C4-N9	5.41	129.25	126.00
1	A	1100	C	C6-N1-C2	5.41	122.46	120.30
1	A	190(K)	G	C8-N9-C4	-5.41	104.24	106.40
1	A	1283	G	C5-N7-C8	-5.41	101.60	104.30
1	A	1505	G	C4-C5-C6	5.41	122.04	118.80
1	A	251	G	N1-C6-O6	-5.40	116.66	119.90
1	A	523	A	N3-C4-C5	5.40	130.58	126.80
1	A	1061	G	C4-C5-N7	5.40	112.96	110.80
1	A	431	A	C4-C5-N7	5.40	113.40	110.70
1	A	174	C	C5-C4-N4	-5.39	116.43	120.20
1	A	655	A	N1-C6-N6	5.39	121.83	118.60
1	A	820	U	C6-N1-C2	-5.39	117.77	121.00
1	A	1161	C	C6-N1-C2	-5.39	118.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1232	U	N1-C2-O2	-5.39	119.03	122.80
1	A	615	C	C4-C5-C6	5.38	120.09	117.40
1	A	665	A	C5-C6-N6	5.38	128.01	123.70
1	A	722	A	N9-C4-C5	-5.38	103.65	105.80
1	A	976	G	C8-N9-C4	5.38	108.55	106.40
1	A	1195	C	C4-C5-C6	5.38	120.09	117.40
1	A	323	U	C6-N1-C2	-5.38	117.77	121.00
1	A	973	G	C4-C5-C6	-5.38	115.57	118.80
1	A	1201	A	P-O3'-C3'	5.38	126.16	119.70
1	A	1236	A	C4-C5-N7	5.38	113.39	110.70
1	A	116	A	C4-C5-C6	5.38	119.69	117.00
1	A	625	G	C8-N9-C1'	-5.38	120.01	127.00
1	A	1543	C	C5-C6-N1	5.38	123.69	121.00
1	A	249	U	C5-C6-N1	-5.38	120.01	122.70
1	A	752	G	C8-N9-C4	5.37	108.55	106.40
1	A	802	A	N1-C2-N3	5.37	131.99	129.30
1	A	328	C	C6-N1-C2	-5.37	118.15	120.30
1	A	703	G	C5-C6-N1	-5.37	108.81	111.50
1	A	1389	C	C6-N1-C2	5.37	122.45	120.30
4	D	57	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	685	G	C8-N9-C4	5.37	108.55	106.40
1	A	1067	A	C2-N3-C4	5.37	113.28	110.60
10	J	40	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	257	G	N1-C6-O6	5.36	123.12	119.90
1	A	613	C	C5-C4-N4	-5.36	116.44	120.20
1	A	1124	G	C8-N9-C4	-5.36	104.25	106.40
1	A	1052	U	N3-C4-C5	-5.36	111.39	114.60
1	A	682	G	N3-C4-N9	-5.35	122.79	126.00
1	A	1252	A	C5-C6-N1	5.35	120.38	117.70
1	A	128	G	N3-C4-N9	-5.35	122.79	126.00
1	A	301	G	N3-C4-C5	5.35	131.28	128.60
1	A	308	C	C5-C4-N4	-5.35	116.45	120.20
1	A	542	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1074	G	N1-C6-O6	5.35	123.11	119.90
1	A	1516	G	C4-N9-C1'	-5.35	119.54	126.50
1	A	1411	C	N3-C2-O2	-5.35	118.15	121.90
1	A	297	G	N1-C2-N3	5.35	127.11	123.90
1	A	1516	G	N3-C4-N9	-5.35	122.79	126.00
1	A	260	G	N3-C2-N2	-5.35	116.16	119.90
1	A	259	G	C5-C6-N1	-5.35	108.83	111.50
1	A	312	C	C6-N1-C2	-5.35	118.16	120.30
1	A	69	G	N3-C2-N2	-5.34	116.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	G	N3-C4-C5	5.34	131.27	128.60
1	A	487	A	C8-N9-C4	5.34	107.94	105.80
1	A	1299	A	C8-N9-C4	-5.34	103.66	105.80
1	A	1442	G	C2-N3-C4	5.34	114.57	111.90
1	A	1505	G	C4-N9-C1'	5.34	133.44	126.50
1	A	660	G	C8-N9-C4	5.34	108.54	106.40
1	A	665	A	N9-C4-C5	5.34	107.94	105.80
1	A	873	A	N1-C6-N6	-5.34	115.40	118.60
1	A	1496	C	N3-C2-O2	5.33	125.63	121.90
1	A	814	A	N1-C2-N3	5.33	131.97	129.30
1	A	115	G	N9-C4-C5	-5.33	103.27	105.40
1	A	860	A	N1-C2-N3	5.33	131.97	129.30
1	A	107	G	N3-C2-N2	5.33	123.63	119.90
1	A	1074	G	N9-C4-C5	-5.33	103.27	105.40
1	A	1401	G	C4-N9-C1'	5.33	133.42	126.50
1	A	119	A	C6-N1-C2	-5.32	115.41	118.60
1	A	228	A	N9-C4-C5	5.32	107.93	105.80
1	A	360	A	N7-C8-N9	5.32	116.46	113.80
1	A	655	A	C2-N3-C4	-5.32	107.94	110.60
1	A	902	G	N1-C6-O6	5.32	123.09	119.90
1	A	1236	A	C5-C6-N6	-5.32	119.44	123.70
1	A	1091	U	N1-C2-N3	5.32	118.09	114.90
1	A	633	G	C6-C5-N7	-5.32	127.21	130.40
1	A	658	G	C4-N9-C1'	5.32	133.41	126.50
1	A	410	G	C4-N9-C1'	5.31	133.41	126.50
1	A	631	G	N7-C8-N9	5.31	115.76	113.10
1	A	1231	G	N9-C4-C5	-5.31	103.28	105.40
1	A	670	G	N9-C4-C5	-5.31	103.28	105.40
1	A	384	G	N1-C6-O6	-5.31	116.72	119.90
1	A	403	C	N3-C4-N4	5.31	121.72	118.00
1	A	631	G	N3-C4-C5	-5.31	125.94	128.60
1	A	116	A	C8-N9-C4	5.31	107.92	105.80
1	A	434	U	C5-C4-O4	-5.31	122.72	125.90
1	A	1111	A	C2-N3-C4	5.31	113.25	110.60
1	A	181	G	C4-C5-N7	-5.31	108.68	110.80
1	A	1531	A	C5-N7-C8	-5.31	101.25	103.90
1	A	666	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1529	G	C5-C6-O6	-5.30	125.42	128.60
1	A	28	G	C5-C6-N1	-5.30	108.85	111.50
1	A	411	A	N1-C6-N6	-5.30	115.42	118.60
1	A	1333	A	N9-C4-C5	5.30	107.92	105.80
1	A	773	G	C8-N9-C4	-5.30	104.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	A	N9-C4-C5	-5.30	103.68	105.80
1	A	1205	U	N3-C4-C5	5.30	117.78	114.60
22	V	2	U	C6-N1-C2	5.30	124.18	121.00
1	A	550	G	C2-N3-C4	-5.29	109.25	111.90
1	A	858	G	C6-C5-N7	-5.29	127.22	130.40
1	A	331	G	C5-N7-C8	-5.29	101.65	104.30
1	A	1339	A	C2-N3-C4	-5.29	107.95	110.60
1	A	416	G	C5-N7-C8	-5.29	101.66	104.30
1	A	1438	G	C2-N3-C4	-5.28	109.26	111.90
1	A	610	G	N3-C4-N9	-5.28	122.83	126.00
1	A	241	C	C6-N1-C2	5.28	122.41	120.30
1	A	27	G	N7-C8-N9	5.28	115.74	113.10
1	A	962	C	C4-C5-C6	-5.28	114.76	117.40
1	A	144	G	C6-C5-N7	-5.28	127.23	130.40
1	A	658	G	C6-C5-N7	-5.28	127.23	130.40
1	A	1372	U	C5-C4-O4	-5.28	122.73	125.90
1	A	281	G	C6-N1-C2	-5.27	121.94	125.10
1	A	326	G	N1-C6-O6	5.27	123.06	119.90
1	A	1079	G	N1-C6-O6	5.27	123.06	119.90
1	A	9	G	N1-C6-O6	5.27	123.06	119.90
1	A	715	A	N1-C2-N3	5.27	131.93	129.30
1	A	482	A	C5-C6-N1	-5.26	115.07	117.70
1	A	666	G	C4-C5-N7	5.26	112.91	110.80
1	A	1265	G	N7-C8-N9	5.26	115.73	113.10
1	A	64	G	N1-C6-O6	5.26	123.06	119.90
1	A	789	U	C5-C6-N1	-5.26	120.07	122.70
1	A	62	U	N3-C4-C5	-5.26	111.44	114.60
1	A	987	G	C2-N3-C4	-5.26	109.27	111.90
1	A	190(G)	G	C4-C5-N7	5.26	112.90	110.80
1	A	284	G	N3-C2-N2	-5.25	116.22	119.90
1	A	783	C	C2-N3-C4	-5.25	117.27	119.90
1	A	1062	U	C5-C4-O4	5.25	129.05	125.90
1	A	1487	G	N1-C2-N2	5.25	120.93	116.20
1	A	802	A	N9-C4-C5	5.25	107.90	105.80
1	A	60	A	C5-N7-C8	5.25	106.52	103.90
1	A	447	G	N3-C4-C5	-5.25	125.98	128.60
1	A	768	A	C5-C6-N6	-5.25	119.50	123.70
1	A	621	A	C2-N3-C4	-5.25	107.98	110.60
1	A	816	A	N7-C8-N9	-5.25	111.18	113.80
1	A	15	G	N9-C4-C5	-5.24	103.30	105.40
1	A	329	A	C2-N3-C4	-5.24	107.98	110.60
1	A	730	G	N1-C2-N3	5.24	127.05	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	981	U	N3-C4-C5	-5.24	111.46	114.60
1	A	1064	G	C8-N9-C4	-5.24	104.30	106.40
1	A	1244	C	N3-C4-N4	5.24	121.67	118.00
1	A	1442	G	N3-C4-N9	5.24	129.14	126.00
1	A	620	C	C2-N3-C4	5.23	122.52	119.90
1	A	789	U	C4-C5-C6	5.23	122.84	119.70
1	A	1469	G	C2-N3-C4	-5.23	109.28	111.90
1	A	296	U	C6-N1-C2	-5.23	117.86	121.00
1	A	1417	G	C5-C6-N1	-5.23	108.88	111.50
1	A	494	G	C8-N9-C4	-5.23	104.31	106.40
1	A	731	G	N1-C6-O6	5.23	123.04	119.90
1	A	119	A	C4-C5-N7	-5.23	108.09	110.70
1	A	1014	A	N7-C8-N9	5.23	116.41	113.80
1	A	869	G	C2-N3-C4	-5.22	109.29	111.90
1	A	1189	C	C6-N1-C2	5.22	122.39	120.30
1	A	1268	A	N3-C4-C5	-5.22	123.14	126.80
1	A	1348	U	N3-C2-O2	-5.22	118.54	122.20
1	A	1544	U	N1-C2-N3	5.22	118.03	114.90
1	A	1481	U	C4-C5-C6	5.22	122.83	119.70
1	A	28	G	C2-N3-C4	-5.22	109.29	111.90
1	A	1151	A	C5-N7-C8	5.22	106.51	103.90
1	A	318	G	C6-C5-N7	-5.22	127.27	130.40
1	A	434	U	N3-C2-O2	5.22	125.85	122.20
1	A	515	G	N7-C8-N9	5.22	115.71	113.10
1	A	963	G	N1-C6-O6	5.21	123.03	119.90
1	A	1212	U	C5-C6-N1	5.21	125.31	122.70
1	A	1258	G	N3-C4-N9	5.21	129.13	126.00
1	A	561	U	C6-N1-C1'	-5.21	113.90	121.20
1	A	567	G	N3-C4-N9	-5.21	122.87	126.00
1	A	26	A	N1-C6-N6	-5.21	115.47	118.60
1	A	1196	U	C2-N1-C1'	5.21	123.95	117.70
1	A	1377	A	C6-N1-C2	-5.21	115.47	118.60
1	A	284	G	N1-C2-N2	5.21	120.89	116.20
1	A	929	G	N3-C2-N2	-5.21	116.25	119.90
1	A	283	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	549	C	C6-N1-C2	5.21	122.38	120.30
1	A	1061	G	N3-C4-C5	5.21	131.21	128.60
1	A	1101	A	C8-N9-C4	5.21	107.88	105.80
1	A	398	C	N1-C2-N3	-5.21	115.56	119.20
1	A	259	G	C4-N9-C1'	5.20	133.26	126.50
1	A	1425	U	C5-C4-O4	5.20	129.02	125.90
1	A	29	G	C8-N9-C1'	5.20	133.76	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1178	G	N3-C4-C5	-5.20	126.00	128.60
1	A	376	G	N3-C4-N9	5.20	129.12	126.00
1	A	481	G	C5-C6-O6	-5.20	125.48	128.60
1	A	933	G	N1-C6-O6	5.20	123.02	119.90
1	A	1268	A	C4-C5-N7	-5.20	108.10	110.70
1	A	1341	U	C5-C6-N1	-5.20	120.10	122.70
1	A	1513	A	N7-C8-N9	-5.20	111.20	113.80
1	A	552	U	C5-C6-N1	-5.20	120.10	122.70
1	A	839	U	C5-C6-N1	5.20	125.30	122.70
1	A	860	A	C4-C5-C6	5.19	119.60	117.00
1	A	66	G	N3-C4-N9	-5.19	122.89	126.00
1	A	190(K)	G	N7-C8-N9	5.19	115.69	113.10
1	A	1345	U	N3-C4-O4	5.19	123.03	119.40
1	A	573	A	N3-C4-C5	-5.19	123.17	126.80
1	A	785	G	C5-N7-C8	-5.19	101.71	104.30
1	A	110	C	N3-C2-O2	5.19	125.53	121.90
1	A	429	U	C5-C6-N1	-5.19	120.11	122.70
1	A	432	A	P-O3'-C3'	5.19	125.92	119.70
1	A	481	G	C6-C5-N7	-5.19	127.29	130.40
1	A	331	G	C5-C6-O6	-5.18	125.49	128.60
1	A	423	G	C4-N9-C1'	5.18	133.24	126.50
1	A	566	G	C5-C6-O6	5.18	131.71	128.60
1	A	1303	C	N3-C2-O2	-5.18	118.27	121.90
1	A	867	G	C6-C5-N7	-5.18	127.29	130.40
1	A	433	C	C4-C5-C6	-5.18	114.81	117.40
1	A	1276	G	C6-C5-N7	-5.18	127.29	130.40
1	A	1451	A	C4-C5-C6	-5.18	114.41	117.00
1	A	1528	U	C6-N1-C2	5.18	124.11	121.00
1	A	1528	U	P-O3'-C3'	5.18	125.91	119.70
1	A	552	U	N3-C4-O4	-5.18	115.78	119.40
1	A	623	C	C5-C6-N1	-5.18	118.41	121.00
1	A	1199	U	N3-C4-O4	5.18	123.02	119.40
1	A	373	A	C2-N3-C4	-5.17	108.01	110.60
1	A	563	A	C5-N7-C8	-5.17	101.31	103.90
1	A	1077	G	C8-N9-C4	5.17	108.47	106.40
1	A	1368	G	N1-C6-O6	5.17	123.00	119.90
1	A	595	G	N1-C6-O6	5.17	123.00	119.90
1	A	894	G	N1-C6-O6	5.17	123.00	119.90
1	A	283	C	N1-C2-O2	5.17	122.00	118.90
1	A	722	A	N3-C4-C5	5.17	130.42	126.80
23	W	32	U	C6-N1-C2	-5.17	117.90	121.00
1	A	1091	U	C4-C5-C6	5.17	122.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	A	C3'-C2'-C1'	-5.16	97.37	101.50
1	A	917	G	C5-N7-C8	-5.16	101.72	104.30
1	A	1039	C	N3-C4-C5	-5.16	119.83	121.90
1	A	30	U	C6-N1-C2	5.16	124.09	121.00
1	A	660	G	C4-C5-N7	5.16	112.86	110.80
1	A	697	U	C4-C5-C6	5.16	122.79	119.70
1	A	724	G	C5-N7-C8	-5.16	101.72	104.30
1	A	282	A	C8-N9-C4	5.15	107.86	105.80
1	A	874	G	C8-N9-C1'	-5.15	120.30	127.00
1	A	1520	G	C6-C5-N7	-5.15	127.31	130.40
1	A	1285	A	N9-C4-C5	5.15	107.86	105.80
1	A	449	C	C2-N3-C4	5.15	122.47	119.90
1	A	591	U	C5-C4-O4	-5.15	122.81	125.90
1	A	791	G	C4-N9-C1'	5.15	133.19	126.50
1	A	926	G	C4-C5-N7	-5.14	108.74	110.80
1	A	1329	A	C5-N7-C8	-5.14	101.33	103.90
1	A	853	G	C5-C6-O6	-5.14	125.51	128.60
1	A	1123	A	N1-C6-N6	5.14	121.69	118.60
1	A	1158	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1350	A	C5-C6-N1	5.14	120.27	117.70
1	A	952	U	C6-N1-C2	-5.14	117.92	121.00
1	A	971	G	C8-N9-C4	5.14	108.46	106.40
1	A	1128	C	N3-C2-O2	5.14	125.50	121.90
1	A	125	U	N3-C4-O4	5.14	123.00	119.40
1	A	927	G	C8-N9-C4	5.14	108.45	106.40
1	A	968	A	N1-C6-N6	5.14	121.68	118.60
1	A	297	G	C5-C6-O6	5.13	131.68	128.60
1	A	825	G	N9-C4-C5	-5.13	103.35	105.40
1	A	977	A	C2-N3-C4	5.13	113.17	110.60
1	A	712	A	N9-C4-C5	5.13	107.85	105.80
1	A	1215	G	N1-C6-O6	5.13	122.98	119.90
1	A	1508	G	C5-C6-O6	-5.13	125.52	128.60
1	A	375	U	C4-C5-C6	5.13	122.78	119.70
1	A	328	C	N3-C4-C5	5.12	123.95	121.90
1	A	1082	G	N1-C6-O6	5.12	122.97	119.90
1	A	279	A	N1-C2-N3	5.12	131.86	129.30
1	A	541	G	C2-N3-C4	-5.12	109.34	111.90
1	A	1101	A	C2-N3-C4	5.12	113.16	110.60
17	Q	22	LEU	CA-CB-CG	-5.12	103.53	115.30
1	A	172	A	C4-C5-C6	5.12	119.56	117.00
1	A	331	G	N9-C4-C5	-5.12	103.35	105.40
1	A	1294	G	C8-N9-C4	-5.12	104.35	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1422	G	N1-C6-O6	5.12	122.97	119.90
1	A	1295	G	N3-C2-N2	-5.11	116.32	119.90
4	D	94	LEU	CA-CB-CG	-5.11	103.54	115.30
7	G	61	VAL	CB-CA-C	-5.11	101.69	111.40
1	A	749	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1171	G	N9-C4-C5	-5.11	103.36	105.40
1	A	32	A	C8-N9-C4	-5.10	103.76	105.80
1	A	923	A	N3-C4-C5	5.10	130.37	126.80
1	A	1131	G	C4-C5-N7	5.10	112.84	110.80
1	A	275	G	C6-C5-N7	-5.10	127.34	130.40
1	A	550	G	C5-C6-O6	-5.10	125.54	128.60
1	A	216	G	C8-N9-C4	5.10	108.44	106.40
1	A	584	G	N1-C2-N2	5.10	120.79	116.20
1	A	648	A	C2-N3-C4	5.09	113.15	110.60
1	A	425	G	C8-N9-C4	-5.09	104.36	106.40
1	A	45	U	C5-C6-N1	-5.09	120.16	122.70
1	A	152	A	N1-C6-N6	-5.09	115.55	118.60
1	A	820	U	C6-N1-C1'	5.09	128.32	121.20
1	A	45	U	C4-C5-C6	5.08	122.75	119.70
1	A	310	G	N1-C6-O6	5.08	122.95	119.90
1	A	610	G	C5-C6-O6	5.08	131.65	128.60
1	A	836	G	N1-C6-O6	5.08	122.95	119.90
1	A	1532	U	N1-C2-O2	5.08	126.36	122.80
1	A	950	U	C5-C4-O4	5.08	128.95	125.90
1	A	1004	A	C2-N3-C4	5.08	113.14	110.60
1	A	1356	G	C8-N9-C4	-5.08	104.37	106.40
1	A	20	U	N3-C2-O2	5.08	125.75	122.20
1	A	1188	A	N1-C2-N3	5.08	131.84	129.30
1	A	1268	A	N1-C6-N6	-5.08	115.55	118.60
1	A	307	C	N1-C2-N3	-5.07	115.65	119.20
1	A	128	G	N3-C4-C5	5.07	131.13	128.60
1	A	276	G	N3-C4-C5	5.07	131.14	128.60
1	A	1248	A	N9-C4-C5	-5.07	103.77	105.80
1	A	350	G	N1-C2-N3	5.07	126.94	123.90
1	A	515	G	C6-C5-N7	-5.07	127.36	130.40
1	A	288	A	C2-N3-C4	-5.07	108.07	110.60
1	A	854	G	C8-N9-C1'	-5.07	120.41	127.00
1	A	1343	G	C6-C5-N7	-5.07	127.36	130.40
1	A	251	G	C6-N1-C2	-5.07	122.06	125.10
1	A	387	U	N1-C2-N3	5.07	117.94	114.90
1	A	375	U	N3-C4-O4	5.06	122.94	119.40
1	A	964	A	C2-N3-C4	-5.06	108.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	G	C8-N9-C4	5.06	108.42	106.40
1	A	1077	G	N7-C8-N9	-5.06	110.57	113.10
1	A	1521	G	C5-C6-N1	5.06	114.03	111.50
1	A	595	G	C2-N3-C4	-5.06	109.37	111.90
1	A	615	C	N3-C2-O2	-5.05	118.36	121.90
1	A	1283	G	C8-N9-C4	-5.05	104.38	106.40
1	A	444	C	N3-C4-C5	-5.05	119.88	121.90
1	A	1158	C	N1-C2-O2	5.05	121.93	118.90
1	A	926	G	C5-C6-O6	5.05	131.63	128.60
1	A	1252	A	N9-C4-C5	5.05	107.82	105.80
22	V	1	U	C4-C5-C6	-5.05	116.67	119.70
1	A	317	G	C4-C5-C6	5.05	121.83	118.80
1	A	729	A	C8-N9-C4	5.05	107.82	105.80
1	A	943	U	C5-C6-N1	-5.05	120.18	122.70
1	A	1346	A	N3-C4-C5	5.05	130.33	126.80
1	A	806	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	881	G	C5-C6-N1	-5.04	108.98	111.50
1	A	1337	G	C6-C5-N7	5.04	133.43	130.40
1	A	1421	G	C4-N9-C1'	5.04	133.06	126.50
1	A	1504	G	C5-C6-N1	-5.04	108.98	111.50
1	A	931	C	C2-N3-C4	-5.04	117.38	119.90
1	A	1125	U	N3-C2-O2	5.04	125.73	122.20
1	A	767	A	C5-N7-C8	5.04	106.42	103.90
1	A	914	A	N7-C8-N9	-5.04	111.28	113.80
1	A	1268	A	N9-C4-C5	5.04	107.81	105.80
1	A	1344	C	C4-C5-C6	-5.04	114.88	117.40
1	A	1469	G	C5-C6-O6	-5.03	125.58	128.60
1	A	918	A	C8-N9-C4	5.03	107.81	105.80
1	A	964	A	C6-C5-N7	-5.03	128.78	132.30
1	A	992	U	C6-N1-C2	5.03	124.02	121.00
1	A	1053	G	N1-C6-O6	5.03	122.92	119.90
1	A	89	C	C5-C6-N1	5.03	123.51	121.00
1	A	125	U	C5-C4-O4	-5.03	122.88	125.90
1	A	1105	A	C4-C5-C6	5.03	119.51	117.00
1	A	1202	G	C4-C5-N7	-5.03	108.79	110.80
1	A	795	C	N1-C2-O2	5.03	121.92	118.90
1	A	1100	C	C2-N1-C1'	-5.03	113.27	118.80
1	A	262	A	N7-C8-N9	5.02	116.31	113.80
1	A	62	U	C4-C5-C6	5.02	122.71	119.70
1	A	809	G	N9-C4-C5	-5.02	103.39	105.40
1	A	820	U	N3-C2-O2	5.02	125.72	122.20
1	A	835	U	N3-C4-C5	-5.02	111.59	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	837	G	C2-N3-C4	-5.02	109.39	111.90
3	C	198	VAL	CB-CA-C	-5.02	101.86	111.40
1	A	129	U	C5-C4-O4	5.02	128.91	125.90
1	A	791	G	C6-C5-N7	-5.02	127.39	130.40
1	A	1374	A	N1-C2-N3	5.02	131.81	129.30
1	A	1430	C	N1-C2-O2	5.02	121.91	118.90
1	A	20	U	C6-N1-C2	5.02	124.01	121.00
1	A	69	G	N3-C4-N9	-5.02	122.99	126.00
1	A	1067	A	C8-N9-C4	-5.02	103.79	105.80
1	A	1487	G	C8-N9-C4	-5.01	104.39	106.40
1	A	706	A	N7-C8-N9	5.01	116.31	113.80
1	A	1227	A	N3-C4-N9	-5.01	123.39	127.40
1	A	39	G	N1-C6-O6	5.01	122.91	119.90
1	A	156	G	C4-N9-C1'	-5.01	119.99	126.50
1	A	559	A	N1-C2-N3	5.01	131.80	129.30
1	A	1054	C	N3-C2-O2	5.01	125.41	121.90
1	A	1293	G	C5-C6-O6	-5.01	125.59	128.60
2	B	158	LEU	CA-CB-CG	-5.01	103.78	115.30
13	M	99	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	73	C	N1-C2-O2	-5.01	115.89	118.90
1	A	325	A	C5-C6-N6	5.01	127.70	123.70
1	A	1455	G	N7-C8-N9	5.01	115.60	113.10
1	A	1214	C	N3-C2-O2	-5.00	118.40	121.90
1	A	165	C	C6-N1-C2	-5.00	118.30	120.30
1	A	1249	C	C6-N1-C2	-5.00	118.30	120.30
1	A	391	G	N9-C4-C5	-5.00	103.40	105.40
1	A	550	G	C4-N9-C1'	-5.00	120.00	126.50
1	A	653	A	N7-C8-N9	5.00	116.30	113.80
1	A	911	U	C2-N1-C1'	-5.00	111.70	117.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
4	D	195	ALA	Peptide
8	H	90	GLY	Peptide
12	L	46	LYS	Peptide
13	M	62	ASN	Peptide
14	N	7	ILE	Peptide

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Mol	Chain	Res	Type	Group
17	Q	79	SER	Peptide
19	S	6	LYS	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	0	310	0
2	B	1896	0	0	9	0
3	C	1613	0	0	9	0
4	D	1703	0	0	19	0
5	E	1147	0	0	5	0
6	F	843	0	0	2	0
7	G	1257	0	0	4	0
8	H	1116	0	0	14	0
9	I	1010	0	0	5	0
10	J	793	0	0	6	0
11	K	885	0	0	5	0
12	L	973	0	0	13	0
13	M	937	0	0	4	0
14	N	492	0	0	9	0
15	O	734	0	0	1	0
16	P	701	0	0	7	0
17	Q	834	0	0	10	0
18	R	598	0	0	3	0
19	S	648	0	0	3	0
20	T	763	0	0	6	0
21	U	209	0	0	2	0
22	V	57	0	0	3	0
23	W	319	0	0	2	0
24	A	756	0	810	60	0
25	A	345	0	0	0	0
25	D	2	0	0	0	0
25	E	4	0	0	0	0
25	H	1	0	0	0	0
25	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	N	1	0	0	0	0
25	O	1	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	S	2	0	0	0	0
25	T	1	0	0	0	0
25	V	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	480	0	0	6	0
27	C	1	0	0	0	0
27	D	2	0	0	0	0
27	E	5	0	0	0	0
27	K	1	0	0	0	0
27	L	2	0	0	0	0
27	N	2	0	0	1	0
27	O	4	0	0	0	0
27	V	1	0	0	0	0
All	All	53651	0	810	432	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (432) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:983:A:O2'	1:A:1050:G:OP2	1.91	0.87
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.10	0.84
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.10	0.84
24:A:1608:PAR:O43	24:A:1608:PAR:N21	2.10	0.84
1:A:1271:G:OP1	24:A:1616:PAR:N32	2.11	0.83
1:A:537:G:OP1	12:L:113:ARG:NH2	2.11	0.83
5:E:95:ALA:O	5:E:98:THR:OG1	1.96	0.82
1:A:1061:G:OP1	24:A:1608:PAR:O44	1.97	0.82
24:A:1605:PAR:N21	24:A:1605:PAR:O53	2.14	0.80
24:A:1608:PAR:H531	24:A:1608:PAR:HN22	1.48	0.79
1:A:1212:U:O2'	1:A:1213:A:O5'	2.02	0.78
1:A:424:G:N7	24:A:1611:PAR:N21	2.30	0.77
1:A:625:G:O6	24:A:1606:PAR:N24	2.19	0.75
14:N:4:LYS:NZ	27:N:202:HOH:O	2.18	0.75
10:J:49:VAL:O	10:J:61:GLU:N	2.20	0.74
1:A:951:G:OP2	13:M:102:ARG:NH2	2.21	0.74
1:A:927:G:O2'	1:A:1503:A:N7	2.21	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:972:C:OP1	10:J:57:LYS:NZ	2.22	0.73
1:A:51:A:OP2	24:A:1604:PAR:H24	1.89	0.73
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.22	0.72
1:A:1387:G:O2'	27:A:2274:HOH:O	2.07	0.72
8:H:85:ARG:NH1	8:H:87:SER:O	2.21	0.72
1:A:47:C:OP1	24:A:1604:PAR:N32	2.23	0.72
12:L:47:LYS:NZ	22:V:3:U:OP1	2.23	0.72
1:A:413:G:N2	1:A:429:U:OP2	2.23	0.71
8:H:17:THR:O	8:H:78:GLN:NE2	2.24	0.71
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.23	0.70
1:A:1023:G:O6	1:A:1024:G:N2	2.24	0.70
1:A:642:A:N3	8:H:113:SER:OG	2.25	0.70
1:A:329:A:O2'	1:A:332:G:N7	2.25	0.70
24:A:1613:PAR:N21	24:A:1613:PAR:O23	2.25	0.70
1:A:414:A:P	24:A:1611:PAR:H122	2.15	0.69
1:A:61:G:O2'	27:A:2002:HOH:O	2.10	0.69
24:A:1616:PAR:O53	24:A:1616:PAR:N24	2.26	0.69
24:A:1602:PAR:O44	24:A:1602:PAR:N24	2.24	0.69
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.27	0.68
2:B:189:ASP:O	2:B:192:SER:OG	2.09	0.68
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.26	0.68
12:L:49:ASN:ND2	12:L:92:OTD:SB	2.67	0.68
4:D:8:VAL:O	4:D:11:LEU:N	2.25	0.68
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.25	0.68
9:I:29:ASN:ND2	9:I:65:VAL:O	2.26	0.68
24:A:1612:PAR:N21	24:A:1612:PAR:H42	2.09	0.68
1:A:414:A:OP2	24:A:1611:PAR:N12	2.27	0.67
1:A:1505:G:O2'	1:A:1506:U:OP2	2.12	0.67
1:A:928:G:O2'	1:A:1533:C:OP1	2.11	0.67
1:A:1528:U:O2'	1:A:1529:G:OP2	2.12	0.67
1:A:1008:C:N3	1:A:1022:G:N2	2.42	0.66
1:A:1256:A:N6	1:A:1278:U:O4'	2.28	0.66
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.29	0.66
1:A:1182:G:O2'	1:A:1183:A:OP2	2.13	0.66
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.29	0.66
17:Q:18:THR:OG1	17:Q:69:LYS:NZ	2.29	0.65
1:A:217:C:O2'	1:A:461:C:N4	2.30	0.65
1:A:983:A:OP1	14:N:3:ARG:NH2	2.30	0.65
1:A:542:G:OP1	4:D:10:ARG:NH2	2.30	0.65
24:A:1610:PAR:O44	24:A:1610:PAR:N24	2.30	0.64
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.14	0.64
24:A:1603:PAR:H532	24:A:1603:PAR:HN61	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1009:G:N2	1:A:1020:U:O2	2.32	0.63
24:A:1616:PAR:O44	24:A:1616:PAR:N64	2.30	0.62
1:A:1192:C:O2	5:E:25:ARG:NH2	2.32	0.62
1:A:1347:G:N2	1:A:1374:A:OP2	2.33	0.62
3:C:35:GLU:OE1	3:C:97:LYS:NZ	2.33	0.62
1:A:559:A:OP1	5:E:126:ARG:NH2	2.33	0.61
1:A:1494:G:OP1	24:A:1601:PAR:N32	2.34	0.61
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.34	0.61
1:A:976:G:OP1	14:N:32:SER:N	2.33	0.61
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.34	0.60
1:A:109:A:C6	1:A:326:G:C6	2.89	0.60
1:A:103:C:OP1	20:T:17:ARG:NH1	2.33	0.60
1:A:226:G:N7	24:A:1617:PAR:O31	2.34	0.60
1:A:1127:G:N2	1:A:1145:C:N3	2.50	0.60
1:A:1158:C:O2	1:A:1181:G:N2	2.34	0.60
1:A:1240:U:OP2	7:G:116:ALA:N	2.34	0.59
1:A:958:A:N3	1:A:985:C:O2'	2.35	0.59
1:A:362:G:N2	1:A:365:U:OP2	2.36	0.59
1:A:438:G:O2'	1:A:495:U:O4	2.20	0.59
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	0.59
24:A:1618:PAR:HN21	24:A:1618:PAR:H322	1.51	0.59
1:A:985:C:C2	1:A:1221:G:N2	2.71	0.59
2:B:184:VAL:N	2:B:198:ASP:OD2	2.36	0.59
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.35	0.59
1:A:978:A:O2'	1:A:1322:C:N3	2.36	0.59
1:A:928:G:N2	1:A:1389:C:O2	2.36	0.58
1:A:427:U:OP2	4:D:36:ARG:NH2	2.36	0.58
1:A:1159:U:O4'	1:A:1182:G:N2	2.36	0.58
1:A:656:C:O2'	15:O:28:GLN:OE1	2.21	0.58
1:A:318:G:N2	1:A:335:C:O2	2.36	0.58
1:A:989:C:O2'	1:A:1017:G:O2'	2.21	0.57
1:A:974:A:OP2	14:N:29:ARG:NH1	2.38	0.57
1:A:1288:A:N3	1:A:1352:C:O2'	2.36	0.57
1:A:1097:C:O2'	1:A:1168:A:N3	2.38	0.57
1:A:1179:A:O2'	1:A:1180:A:OP1	2.22	0.57
1:A:998:G:N2	1:A:999:C:N3	2.53	0.57
12:L:52:LEU:O	12:L:54:LYS:NZ	2.38	0.57
1:A:1125:U:O2'	1:A:1281:U:O2	2.22	0.57
4:D:28:SER:O	4:D:30:LYS:N	2.38	0.56
1:A:161:A:N1	1:A:347:G:O2'	2.38	0.56
24:A:1605:PAR:N64	24:A:1605:PAR:O44	2.36	0.56
1:A:872:A:C8	1:A:874:G:C8	2.93	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:619:U:N3	4:D:134:ASP:OD2	2.39	0.56
1:A:355:C:OP1	24:A:1604:PAR:N21	2.39	0.56
1:A:830:G:N2	1:A:856:C:O2	2.39	0.56
20:T:15:ARG:O	20:T:19:SER:N	2.39	0.56
1:A:502:G:OP1	12:L:117:ARG:N	2.38	0.56
1:A:409:G:N2	1:A:433:C:N3	2.53	0.56
1:A:532:A:N6	1:A:1206:G:O2'	2.39	0.55
1:A:1261:A:N6	1:A:1262:C:O2	2.38	0.55
1:A:1124:G:O2'	1:A:1145:C:N4	2.40	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.55
1:A:28:G:O2'	1:A:296:U:OP1	2.24	0.55
1:A:235:C:N4	27:A:2126:HOH:O	2.39	0.55
1:A:756:C:N4	27:A:2114:HOH:O	2.39	0.55
1:A:986:A:C2	1:A:1220:G:C2	2.95	0.54
1:A:812:C:O2'	1:A:813:U:OP2	2.24	0.54
1:A:279:A:OP2	17:Q:95:TYR:OH	2.25	0.54
1:A:64:G:C2	1:A:67:C:N4	2.75	0.54
1:A:772:U:OP1	24:A:1615:PAR:H222	2.08	0.54
1:A:1347:G:O2'	1:A:1348:U:P	2.65	0.54
1:A:1054:C:P	1:A:1197:G:OP2	2.65	0.54
1:A:427:U:OP1	4:D:13:ARG:NH2	2.41	0.54
1:A:855:G:C5	1:A:856:C:C5	2.96	0.54
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.41	0.54
1:A:775:G:N2	1:A:804:U:O4	2.41	0.54
3:C:20:SER:OG	3:C:40:ARG:NH2	2.41	0.54
8:H:4:ASP:OD1	8:H:7:ALA:N	2.41	0.54
14:N:34:TYR:N	14:N:39:LEU:O	2.41	0.54
1:A:1128:C:O2'	1:A:1130:A:C8	2.61	0.53
1:A:1316:G:N2	1:A:1319:A:OP2	2.41	0.53
1:A:1544:U:O3'	22:V:1:U:O5'	2.26	0.53
2:B:100:GLY:O	2:B:104:ASN:N	2.41	0.53
1:A:1346:A:N6	1:A:1375:A:OP2	2.42	0.53
1:A:836:G:C6	1:A:851:G:C6	2.96	0.53
1:A:410:G:N1	1:A:429:U:O2	2.42	0.53
1:A:216:G:O2'	1:A:217:C:O4'	2.27	0.53
11:K:54:ARG:O	11:K:57:THR:OG1	2.27	0.53
1:A:1313:U:O4	19:S:4:SER:OG	2.26	0.53
1:A:1347:G:O2'	1:A:1348:U:O5'	2.27	0.53
24:A:1615:PAR:H11	24:A:1615:PAR:O52	2.08	0.53
1:A:660:G:C2	1:A:746:A:C2	2.97	0.53
1:A:1190:G:O2'	1:A:1191:A:P	2.67	0.53
1:A:636:U:O4	24:A:1610:PAR:H54	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:A:P	24:A:1611:PAR:N12	2.82	0.52
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.57	0.52
12:L:27:LEU:O	12:L:30:ALA:N	2.42	0.52
1:A:8:A:N6	4:D:205:GLU:O	2.42	0.52
1:A:644:G:C5	1:A:645:C:C5	2.97	0.52
1:A:1331:G:O2'	1:A:1332:A:P	2.68	0.52
1:A:1206:G:C6	1:A:1207:2MG:C5	2.98	0.52
1:A:343:U:O2'	1:A:346:G:O6	2.27	0.52
16:P:22:THR:OG1	16:P:23:ASP:N	2.43	0.52
1:A:131:C:O2'	1:A:262:A:O2'	2.26	0.52
1:A:190(E):U:O2	17:Q:63:ARG:NH2	2.43	0.52
1:A:578:C:O2'	1:A:728:A:N3	2.42	0.52
6:F:70:ASP:N	6:F:70:ASP:OD1	2.42	0.52
1:A:885:G:O2'	1:A:914:A:N1	2.43	0.51
14:N:40:CYS:SG	14:N:43:CYS:N	2.83	0.51
1:A:1413:A:C2	1:A:1488:G:C2	2.98	0.51
1:A:1223:C:OP1	19:S:78:ARG:NH1	2.42	0.51
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.44	0.51
1:A:1003(A):G:N2	1:A:1038:C:O2	2.43	0.51
1:A:390:C:O3'	16:P:28:ARG:NH2	2.44	0.51
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.51
1:A:355:C:O2'	1:A:388:G:N3	2.43	0.51
24:A:1610:PAR:H33	24:A:1610:PAR:N24	2.23	0.51
1:A:246:A:N1	1:A:278:G:O2'	2.44	0.51
8:H:21:LYS:O	8:H:65:TYR:OH	2.29	0.51
1:A:377:G:OP1	16:P:5:ARG:NH1	2.43	0.51
24:A:1610:PAR:O54	24:A:1610:PAR:O34	2.27	0.51
1:A:262:A:C6	1:A:263:A:C6	2.99	0.51
1:A:1167:A:C6	1:A:1168:A:C6	2.98	0.51
1:A:324:G:N2	1:A:327:A:C8	2.79	0.51
1:A:771:G:N2	1:A:808:C:O2	2.44	0.51
21:U:17:THR:O	21:U:22:ARG:NH1	2.44	0.51
7:G:140:ASP:OD2	7:G:143:ARG:NH2	2.44	0.51
1:A:1226:C:O2'	13:M:103:THR:O	2.28	0.51
1:A:892:A:C2	1:A:907:A:C4	2.99	0.51
1:A:1213:A:C6	1:A:1215:G:C4	2.99	0.50
1:A:106:C:O2'	1:A:379:C:OP1	2.29	0.50
1:A:377:G:N2	1:A:387:U:O2	2.44	0.50
1:A:838:G:N2	1:A:849:C:C2	2.80	0.50
1:A:668:G:N2	1:A:738:C:O2	2.44	0.50
4:D:127:THR:OG1	4:D:127:THR:O	2.29	0.50
1:A:345:C:O2	1:A:346:G:N2	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:G:C6	1:A:36:C:N4	2.80	0.50
1:A:1060:C:O2'	10:J:56:HIS:ND1	2.43	0.49
24:A:1603:PAR:C53	24:A:1603:PAR:HN61	2.24	0.49
11:K:27:ASN:OD1	11:K:28:THR:N	2.45	0.49
1:A:410:G:O6	1:A:429:U:O2'	2.30	0.49
1:A:949:A:C2	1:A:1233:G:N3	2.81	0.49
1:A:1213:A:N6	1:A:1215:G:N3	2.60	0.49
24:A:1602:PAR:N24	24:A:1602:PAR:H33	2.27	0.49
12:L:76:ASN:O	12:L:76:ASN:CG	2.51	0.49
1:A:533:A:C6	1:A:536:C:C2	3.01	0.49
1:A:1347:G:O6	9:I:10:ARG:NH2	2.45	0.49
1:A:922:G:O2'	1:A:1398:A:N1	2.46	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49
1:A:587:G:O2'	1:A:588:G:OP2	2.30	0.49
1:A:1263:C:N3	1:A:1272:G:N2	2.61	0.48
1:A:1061:G:C6	1:A:1062:U:N3	2.80	0.48
3:C:3:ASN:N	3:C:3:ASN:OD1	2.46	0.48
1:A:670:G:OP2	24:A:1613:PAR:N24	2.45	0.48
1:A:836:G:OP1	18:R:61:LYS:NZ	2.46	0.48
1:A:511:C:O3'	4:D:43:HIS:NE2	2.45	0.48
1:A:1288:A:C6	1:A:1289:A:C5	3.02	0.48
1:A:1054:C:N3	23:W:34:G:O4'	2.46	0.48
12:L:117:ARG:O	12:L:120:TYR:N	2.47	0.48
1:A:1128:C:N3	1:A:1144:G:N2	2.61	0.48
1:A:956:U:C2	1:A:1225:A:C2	3.01	0.48
1:A:1068:G:N7	1:A:1094:G:O2'	2.46	0.48
1:A:131:C:OP1	1:A:190(F):G:N2	2.46	0.48
1:A:1030:C:N3	1:A:1031:G:N2	2.62	0.48
1:A:1126:U:C2	1:A:1127:G:C8	3.02	0.48
1:A:1168:A:C6	1:A:1169:A:C6	3.01	0.48
1:A:157:G:C2	1:A:158:G:C8	3.02	0.48
1:A:340:U:C2	1:A:350:G:N2	2.82	0.48
1:A:592:G:N2	1:A:648:A:C4	2.81	0.48
24:A:1613:PAR:H322	24:A:1613:PAR:H11	1.78	0.48
1:A:1287:A:C6	1:A:1288:A:C6	3.01	0.48
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.48
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.48
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.46	0.47
1:A:1190:G:O2'	1:A:1191:A:O5'	2.32	0.47
1:A:1074:G:C6	1:A:1075:C:C4	3.03	0.47
1:A:1441:G:O2'	1:A:1460:A:N6	2.46	0.47
1:A:123:C:OP1	1:A:311:C:O2'	2.31	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:662:G:O6	24:A:1605:PAR:H62	2.14	0.47
1:A:803:G:OP1	24:A:1615:PAR:O41	2.31	0.47
18:R:17:SER:OG	18:R:17:SER:O	2.32	0.47
1:A:1442:G:C5	1:A:1446:A:N6	2.83	0.47
13:M:86:CYS:SG	13:M:87:TYR:N	2.88	0.47
1:A:187:C:O2	20:T:105:SER:OG	2.33	0.47
1:A:1002:G:C6	1:A:1003:G:C6	3.03	0.47
1:A:1122:U:O4	1:A:1123:A:N6	2.48	0.47
12:L:49:ASN:ND2	12:L:92:OTD:OD2	2.48	0.47
1:A:781:A:C8	1:A:802:A:C2	3.02	0.47
1:A:919:A:O2'	1:A:1080:A:N1	2.48	0.47
24:A:1608:PAR:H531	24:A:1608:PAR:N21	2.24	0.47
1:A:352:C:O2'	1:A:354:G:OP1	2.32	0.47
1:A:506:G:C6	1:A:507:C:C4	3.03	0.47
24:A:1614:PAR:H52	24:A:1614:PAR:H11	1.68	0.47
24:A:1605:PAR:H322	24:A:1605:PAR:C51	2.27	0.47
1:A:1091:U:O2	1:A:1093:A:C8	2.67	0.47
1:A:1503:A:OP1	1:A:1531:A:O2'	2.33	0.47
8:H:82:HIS:ND1	8:H:138:TRP:CD1	2.83	0.47
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.48	0.47
24:A:1603:PAR:H532	24:A:1603:PAR:N64	2.28	0.46
1:A:1222:G:OP2	1:A:1322:C:N4	2.48	0.46
1:A:432:A:C8	1:A:433:C:C6	3.03	0.46
1:A:1501:C:N4	1:A:1504:G:C2	2.83	0.46
1:A:1182:G:O2'	1:A:1183:A:P	2.74	0.46
1:A:661:G:N2	1:A:745:C:C2	2.83	0.46
1:A:1015:A:C6	1:A:1016:A:C6	3.03	0.46
1:A:1112:C:N3	3:C:178:LEU:N	2.62	0.46
20:T:75:ASN:N	20:T:75:ASN:OD1	2.49	0.46
1:A:297:G:N2	1:A:300:A:OP2	2.48	0.46
1:A:1309:G:C6	1:A:1329:A:C2	3.04	0.46
1:A:716:A:N7	24:A:1613:PAR:O41	2.47	0.46
1:A:965:A:C2	1:A:969:A:C2	3.04	0.46
1:A:583:A:N6	1:A:758:G:O2'	2.49	0.46
1:A:768:A:O2'	1:A:1512:U:O2'	2.34	0.46
20:T:89:ARG:NH2	20:T:105:SER:O	2.48	0.46
1:A:378:G:N2	1:A:385:C:O2	2.48	0.46
1:A:1055:A:C6	1:A:1206:G:C5	3.04	0.46
24:A:1603:PAR:O52	24:A:1603:PAR:H11	2.16	0.46
5:E:8:GLU:OE1	5:E:63:ARG:NH2	2.49	0.46
1:A:1133:G:N2	1:A:1141:C:O2	2.48	0.46
8:H:104:ARG:NE	8:H:138:TRP:CZ2	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1442:G:O6	1:A:1461:G:N2	2.50	0.45
1:A:786:G:C2	1:A:797:C:C2	3.04	0.45
1:A:1057:G:C5	1:A:1204:A:C2	3.04	0.45
1:A:231:G:N7	24:A:1612:PAR:H612	2.31	0.45
17:Q:48:GLU:OE1	17:Q:50:LYS:NZ	2.49	0.45
1:A:908:A:C2	1:A:909:A:C4	3.04	0.45
1:A:1330:U:O4	1:A:1331:G:N1	2.50	0.45
1:A:527:7MG:O2'	1:A:535:A:N1	2.49	0.45
1:A:391:G:C6	1:A:392:G:C5	3.04	0.45
1:A:1134:G:N2	1:A:1140:C:O2	2.49	0.45
24:A:1613:PAR:H23	24:A:1613:PAR:H52	1.65	0.45
24:A:1610:PAR:N21	24:A:1610:PAR:O43	2.50	0.45
1:A:165:C:C2	1:A:166:G:C8	3.05	0.45
4:D:15:GLU:OE2	4:D:59:ARG:NE	2.49	0.45
1:A:1148:U:C5	1:A:1149:C:C4	3.04	0.45
1:A:355:C:C4	1:A:356:A:N7	2.85	0.45
1:A:1157:A:C2	1:A:1181:G:C4	3.05	0.45
1:A:1300:G:O2'	1:A:1301:U:O5'	2.35	0.45
14:N:23:ARG:NH1	14:N:28:GLY:O	2.50	0.45
1:A:1268:A:N3	1:A:1326:C:O2'	2.50	0.44
1:A:496:A:C2	1:A:497:A:C4	3.05	0.44
12:L:27:LEU:O	12:L:29:GLY:N	2.50	0.44
1:A:1054:C:O2'	1:A:1055:A:O5'	2.34	0.44
1:A:1321:C:C5	1:A:1322:C:C2	3.04	0.44
1:A:1375:A:C2	1:A:1376:U:C2	3.05	0.44
1:A:298:A:N6	27:A:2267:HOH:O	2.50	0.44
1:A:837:G:C2	1:A:850:U:O2	2.70	0.44
1:A:1030(A):G:N2	1:A:1031:G:O6	2.50	0.44
1:A:1127:G:N2	1:A:1145:C:C2	2.86	0.44
1:A:945:G:C2	1:A:1337:G:C2	3.06	0.44
1:A:684:A:O2'	11:K:39:PRO:O	2.36	0.44
16:P:9:PHE:N	16:P:16:HIS:O	2.51	0.44
1:A:1357:A:C5	1:A:1358:U:C4	3.06	0.44
8:H:114:THR:OG1	8:H:117:GLY:O	2.36	0.44
1:A:976:G:N7	1:A:1358:U:C2	2.86	0.44
1:A:116:A:OP1	27:A:2017:HOH:O	2.21	0.44
1:A:1256:A:C2	1:A:1277:C:N4	2.86	0.44
3:C:22:TRP:NE1	3:C:36:ASP:OD1	2.50	0.44
1:A:1440:C:C2	1:A:1462:G:C2	3.06	0.44
24:A:1616:PAR:HN21	24:A:1616:PAR:H42	1.83	0.44
1:A:378:G:C2	1:A:386:C:O2	2.71	0.44
11:K:129:SER:O	11:K:129:SER:OG	2.36	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:4:TYR:OH	4:D:7:PRO:O	2.36	0.44
1:A:439:A:C4	1:A:497:A:C2	3.06	0.43
1:A:1281:U:O2'	1:A:1282:C:OP1	2.35	0.43
1:A:1093:A:N3	1:A:1109:C:O2'	2.51	0.43
1:A:396:G:O2'	1:A:398:C:OP1	2.35	0.43
1:A:635:G:N7	24:A:1610:PAR:O34	2.40	0.43
1:A:120:A:OP2	24:A:1603:PAR:O53	2.28	0.43
4:D:31:CYS:SG	4:D:31:CYS:O	2.77	0.43
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.43
24:A:1602:PAR:H51	24:A:1602:PAR:H322	1.82	0.43
1:A:1055:A:C8	1:A:1206:G:C2	3.06	0.43
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.71	0.43
1:A:938:A:N6	1:A:939:G:C6	2.86	0.43
1:A:1421:G:C6	1:A:1480:G:N1	2.86	0.43
1:A:410:G:N1	1:A:429:U:C2	2.86	0.43
4:D:15:GLU:OE1	4:D:66:ARG:NH1	2.52	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
1:A:190(C):C:C5	1:A:190(D):U:C5	3.07	0.43
1:A:382:A:C2	1:A:383:A:C4	3.06	0.43
1:A:575:G:C5	1:A:881:G:C2	3.06	0.43
1:A:975:A:C5'	1:A:975:A:C8	3.01	0.43
1:A:690:G:C6	1:A:691:G:C6	3.07	0.43
2:B:198:ASP:OD1	8:H:68:ARG:NH2	2.51	0.43
1:A:1331:G:O2'	1:A:1332:A:O5'	2.37	0.43
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.36	0.43
1:A:476:G:C2	1:A:477:G:C4	3.07	0.43
1:A:216:G:O2'	1:A:217:C:O5'	2.36	0.43
1:A:200:G:N2	1:A:218:C:C2	2.87	0.43
1:A:255:G:C2	1:A:272:C:C2	3.07	0.43
1:A:1404:5MC:O4'	1:A:1499:A:C2	2.71	0.43
1:A:553:A:O2'	12:L:29:GLY:O	2.36	0.43
2:B:189:ASP:OD2	2:B:190:THR:N	2.52	0.43
24:A:1601:PAR:O52	24:A:1601:PAR:H11	2.19	0.43
1:A:1304:G:N1	1:A:1332:A:OP2	2.52	0.43
1:A:9:G:C4	1:A:26:A:N1	2.87	0.43
1:A:181:G:N2	1:A:195:A:C4	2.87	0.43
12:L:9:GLN:O	12:L:13:LYS:N	2.52	0.43
1:A:75:G:C6	1:A:96:G:C6	3.07	0.43
1:A:197:A:N1	1:A:220:G:O2'	2.51	0.43
1:A:736:C:OP2	18:R:68:LYS:NZ	2.51	0.42
2:B:238:LEU:C	2:B:240:GLN:N	2.72	0.42
1:A:1053:G:O2'	1:A:1199:U:C5	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:58:TYR:CD1	16:P:58:TYR:C	2.91	0.42
1:A:315:A:O2'	1:A:330:C:O2'	2.37	0.42
1:A:128:G:N7	24:A:1612:PAR:N32	2.63	0.42
1:A:1304:G:C5	1:A:1305:G:N1	2.88	0.42
17:Q:90:ILE:O	17:Q:93:GLN:N	2.51	0.42
1:A:130:A:OP2	1:A:190(E):U:O2'	2.36	0.42
1:A:252:U:C4	1:A:253:U:O4	2.72	0.42
1:A:147:G:C2	1:A:148:G:C8	3.08	0.42
5:E:39:GLY:O	5:E:69:VAL:N	2.51	0.42
1:A:239:U:O4	24:A:1603:PAR:H642	2.20	0.42
1:A:285:G:C2	1:A:286:G:C8	3.08	0.42
1:A:1422:G:N2	1:A:1479:C:C2	2.87	0.42
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.52	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.42
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.52	0.42
1:A:45:U:OP1	1:A:307:C:O2'	2.36	0.42
1:A:403:C:OP1	4:D:137:SER:OG	2.38	0.42
1:A:397:A:C6	1:A:548:G:N7	2.88	0.42
1:A:1402:4OC:O2	1:A:1500:A:N1	2.52	0.42
1:A:1054:C:OP1	1:A:1197:G:OP2	2.37	0.42
13:M:37:THR:O	13:M:55:ARG:NH1	2.53	0.42
1:A:410:G:OP1	4:D:30:LYS:NZ	2.53	0.42
1:A:1375:A:N1	1:A:1376:U:C2	2.88	0.42
1:A:815:A:N3	1:A:1527:C:O2'	2.53	0.42
1:A:367:U:C6	1:A:394:G:N2	2.88	0.42
1:A:192:U:C2	1:A:193:C:C6	3.08	0.42
1:A:157:G:N3	1:A:158:G:C8	2.88	0.41
1:A:122:G:C2	1:A:123:C:C2	3.08	0.41
1:A:837:G:N2	1:A:850:U:O2	2.53	0.41
2:B:34:ALA:O	2:B:41:ILE:N	2.53	0.41
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.53	0.41
1:A:1453:G:N2	1:A:1454:G:C5	2.89	0.41
8:H:102:ARG:N	8:H:102:ARG:CD	2.83	0.41
24:A:1609:PAR:H33	24:A:1609:PAR:H24	1.74	0.41
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
4:D:31:CYS:C	4:D:33:MET:N	2.73	0.41
1:A:102:G:O2'	1:A:151:A:N3	2.53	0.41
12:L:71:PRO:O	12:L:102:ARG:NH1	2.53	0.41
11:K:34:ASP:N	11:K:34:ASP:OD1	2.53	0.41
2:B:73:THR:O	2:B:75:LYS:N	2.54	0.41
1:A:1160:G:O6	1:A:1181:G:O6	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:321:A:C2	1:A:333:G:C2	3.08	0.41
24:A:1613:PAR:H11	24:A:1613:PAR:N32	2.35	0.41
1:A:504:C:C2	1:A:542:G:C2	3.09	0.41
1:A:325:A:N6	1:A:326:G:C2	2.88	0.41
1:A:1447:G:C6	1:A:1460:A:C2	3.08	0.41
8:H:6:ILE:CD1	8:H:6:ILE:N	2.84	0.41
1:A:1127:G:C2	1:A:1145:C:N3	2.88	0.41
22:V:1:U:N3	23:W:37:A:C2	2.89	0.41
1:A:1401:G:C2	1:A:1402:4OC:C1'	3.04	0.41
1:A:1067:A:O2'	1:A:1093:A:O3'	2.39	0.41
1:A:190(I):G:C6	1:A:190(J):U:C4	3.09	0.41
6:F:15:ASP:OD1	6:F:17:SER:N	2.54	0.41
1:A:338:A:C2	1:A:339:C:C2	3.08	0.41
1:A:1348:U:N3	1:A:1374:A:N7	2.69	0.41
1:A:127:G:C6	24:A:1612:PAR:H221	2.56	0.41
24:A:1603:PAR:H43	24:A:1603:PAR:O54	2.20	0.41
1:A:590:C:OP1	8:H:30:ARG:N	2.54	0.41
1:A:1410:G:N2	1:A:1491:G:C4	2.89	0.41
24:A:1616:PAR:H11	24:A:1616:PAR:H32	1.87	0.41
1:A:1055:A:N6	1:A:1206:G:C5	2.89	0.41
1:A:98:U:O4	24:A:1618:PAR:H12	2.21	0.41
1:A:855:G:C4	1:A:856:C:C6	3.09	0.41
1:A:1203:C:OP1	14:N:2:ALA:N	2.54	0.41
1:A:397:A:N7	1:A:547:A:O2'	2.54	0.41
1:A:474:G:OP2	16:P:75:ARG:NH1	2.54	0.41
1:A:557:G:N1	1:A:558:G:C2	2.89	0.41
1:A:1501:C:C5	1:A:1504:G:C4	3.09	0.40
1:A:37:U:O2'	1:A:547:A:N1	2.53	0.40
1:A:289:G:C6	1:A:290:C:N4	2.89	0.40
1:A:410:G:C2	1:A:429:U:C2	3.09	0.40
1:A:544:G:C6	1:A:545:C:C4	3.09	0.40
1:A:597:G:C6	1:A:644:G:C6	3.10	0.40
1:A:1442:G:N7	1:A:1446:A:N6	2.70	0.40
1:A:415:A:OP1	24:A:1611:PAR:N64	2.55	0.40
1:A:745:C:OP1	1:A:851:G:O2'	2.40	0.40
1:A:1190:G:O6	24:A:1608:PAR:N64	2.54	0.40
24:A:1602:PAR:O34	24:A:1602:PAR:O54	2.35	0.40

There are no symmetry-related clashes.

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%)	204 (87%)	30 (13%)	0	100	100
3	C	205/239 (86%)	184 (90%)	20 (10%)	1 (0%)	38	88
4	D	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	149/162 (92%)	144 (97%)	5 (3%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	27	83
10	J	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	7	58
11	K	117/129 (91%)	105 (90%)	11 (9%)	1 (1%)	25	81
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	27	83
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	19	77
16	P	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	65 (92%)	6 (8%)	0	100	100
19	S	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	9	62
20	T	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	22	80
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2145 (91%)	197 (8%)	11 (0%)	38	88

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE

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Mol	Chain	Res	Type
20	T	99	LEU
9	I	38	GLN
19	S	6	LYS
10	J	34	VAL
10	J	83	GLU
10	J	85	LEU
11	K	95	ILE
15	O	87	ILE
3	C	66	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	176 (88%)	25 (12%)	7 40
3	C	160/188 (85%)	121 (76%)	39 (24%)	1 8
4	D	180/181 (99%)	159 (88%)	21 (12%)	8 43
5	E	115/123 (94%)	91 (79%)	24 (21%)	1 13
6	F	90/90 (100%)	66 (73%)	24 (27%)	1 7
7	G	126/127 (99%)	105 (83%)	21 (17%)	3 24
8	H	119/119 (100%)	94 (79%)	25 (21%)	1 12
9	I	98/99 (99%)	75 (76%)	23 (24%)	1 9
10	J	87/92 (95%)	69 (79%)	18 (21%)	2 13
11	K	90/99 (91%)	78 (87%)	12 (13%)	6 37
12	L	103/110 (94%)	86 (84%)	17 (16%)	3 25
13	M	94/101 (93%)	75 (80%)	19 (20%)	2 14
14	N	49/50 (98%)	39 (80%)	10 (20%)	2 14
15	O	79/80 (99%)	63 (80%)	16 (20%)	2 14
16	P	72/74 (97%)	60 (83%)	12 (17%)	3 24
17	Q	95/97 (98%)	75 (79%)	20 (21%)	1 12
18	R	64/77 (83%)	56 (88%)	8 (12%)	7 40
19	S	71/80 (89%)	53 (75%)	18 (25%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	76/82 (93%)	60 (79%)	16 (21%)	1	12
21	U	19/22 (86%)	16 (84%)	3 (16%)	4	28
All	All	1988/2111 (94%)	1617 (81%)	371 (19%)	2	17

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	6	THR
2	B	24	TRP
2	B	33	TYR
2	B	46	LYS
2	B	48	MET
2	B	61	LEU
2	B	69	LEU
2	B	82	ARG
2	B	97	TRP
2	B	107	THR
2	B	108	ILE
2	B	114	ARG
2	B	115	LEU
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	157	ARG
2	B	163	PHE
2	B	191	ASP
2	B	208	ILE
2	B	221	LEU
2	B	223	ILE
2	B	230	VAL
2	B	236	TYR
2	B	240	GLN
3	C	3	ASN
3	C	4	LYS
3	C	10	PHE
3	C	14	ILE
3	C	17	ASP
3	C	22	TRP
3	C	26	LYS
3	C	27	LYS
3	C	28	GLN

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Mol	Chain	Res	Type
3	C	30	ARG
3	C	34	LEU
3	C	43	LEU
3	C	46	GLU
3	C	52	LEU
3	C	64	VAL
3	C	70	VAL
3	C	79	ARG
3	C	83	ARG
3	C	91	LEU
3	C	99	VAL
3	C	104	GLN
3	C	119	ARG
3	C	126	ARG
3	C	127	ARG
3	C	132	ARG
3	C	139	GLN
3	C	144	SER
3	C	152	ILE
3	C	157	ILE
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	175	LEU
3	C	188	LEU
3	C	190	ARG
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
3	C	207	VAL
4	D	3	ARG
4	D	8	VAL
4	D	12	CYS
4	D	15	GLU
4	D	19	LEU
4	D	26	CYS
4	D	28	SER
4	D	34	GLU
4	D	50	ARG
4	D	58	LEU
4	D	61	LYS
4	D	70	ILE

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Mol	Chain	Res	Type
4	D	80	GLU
4	D	91	SER
4	D	114	ARG
4	D	122	ARG
4	D	127	THR
4	D	178	VAL
4	D	190	ASP
4	D	201	GLN
4	D	209	ARG
5	E	10	MET
5	E	12	LEU
5	E	16	THR
5	E	20	GLN
5	E	24	ARG
5	E	31	LEU
5	E	32	VAL
5	E	41	VAL
5	E	43	LEU
5	E	45	PHE
5	E	47	LYS
5	E	50	GLU
5	E	51	VAL
5	E	64	ARG
5	E	68	GLU
5	E	80	ILE
5	E	100	VAL
5	E	105	VAL
5	E	116	THR
5	E	117	ASP
5	E	125	SER
5	E	126	ARG
5	E	131	ILE
5	E	151	LEU
6	F	3	ARG
6	F	6	VAL
6	F	10	LEU
6	F	11	ASN
6	F	14	LEU
6	F	16	GLN
6	F	24	GLU
6	F	25	ILE
6	F	36	ARG

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Mol	Chain	Res	Type
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU
6	F	46	ARG
6	F	54	LYS
6	F	55	ASP
6	F	61	LEU
6	F	65	VAL
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	83	ASP
6	F	86	ARG
6	F	92	LYS
6	F	98	LEU
7	G	3	ARG
7	G	10	ARG
7	G	12	LEU
7	G	21	VAL
7	G	27	ILE
7	G	38	LEU
7	G	47	CYS
7	G	48	LYS
7	G	50	ILE
7	G	52	GLU
7	G	67	GLU
7	G	79	ARG
7	G	92	SER
7	G	94	ARG
7	G	97	GLN
7	G	113	GLU
7	G	114	ARG
7	G	118	VAL
7	G	124	LEU
7	G	149	ARG
7	G	156	TRP
8	H	3	THR
8	H	8	ASP
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL

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Mol	Chain	Res	Type
8	H	21	LYS
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	45	ILE
8	H	50	ARG
8	H	51	VAL
8	H	53	VAL
8	H	56	LYS
8	H	70	GLN
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	95	VAL
8	H	102	ARG
8	H	109	ILE
8	H	112	LEU
8	H	127	LEU
8	H	133	LEU
9	I	2	GLU
9	I	3	GLN
9	I	12	GLU
9	I	14	VAL
9	I	23	ASN
9	I	27	THR
9	I	47	LEU
9	I	54	ASP
9	I	56	LEU
9	I	66	ARG
9	I	79	LEU
9	I	86	VAL
9	I	95	LYS
9	I	99	LEU
9	I	102	LEU
9	I	108	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	125	TYR

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Mol	Chain	Res	Type
10	J	4	ILE
10	J	9	ARG
10	J	16	LEU
10	J	21	GLN
10	J	23	ILE
10	J	33	GLN
10	J	38	ILE
10	J	50	ILE
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	63	PHE
10	J	65	LEU
10	J	73	ASP
10	J	80	LYS
10	J	83	GLU
10	J	89	ASP
10	J	99	LYS
11	K	11	LYS
11	K	21	ILE
11	K	29	ILE
11	K	48	ILE
11	K	79	SER
11	K	80	VAL
11	K	84	VAL
11	K	91	ARG
11	K	116	HIS
11	K	119	CYS
11	K	120	ARG
11	K	127	LYS
12	L	6	THR
12	L	12	ARG
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	33	ARG
12	L	39	VAL
12	L	41	ARG
12	L	43	VAL
12	L	46	LYS
12	L	54	LYS
12	L	81	SER

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Mol	Chain	Res	Type
12	L	97	ARG
12	L	98	TYR
12	L	104	VAL
12	L	122	THR
12	L	127	GLU
13	M	3	ARG
13	M	4	ILE
13	M	11	ARG
13	M	14	ARG
13	M	44	ARG
13	M	56	LEU
13	M	62	ASN
13	M	64	TRP
13	M	79	LYS
13	M	93	ARG
13	M	98	VAL
13	M	99	ARG
13	M	101	GLN
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	114	ARG
13	M	115	LYS
14	N	4	LYS
14	N	6	LEU
14	N	7	ILE
14	N	13	THR
14	N	18	VAL
14	N	22	THR
14	N	29	ARG
14	N	33	VAL
14	N	41	ARG
14	N	44	LEU
15	O	9	GLN
15	O	10	LYS
15	O	22	THR
15	O	32	LEU
15	O	38	ARG
15	O	40	SER
15	O	45	VAL
15	O	47	LYS

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Mol	Chain	Res	Type
15	O	65	ARG
15	O	66	LEU
15	O	68	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
15	O	87	ILE
15	O	88	ARG
16	P	2	VAL
16	P	27	LYS
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	49	LEU
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	61	SER
16	P	67	THR
16	P	69	THR
17	Q	6	LEU
17	Q	12	SER
17	Q	25	ARG
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	37	LYS
17	Q	38	ARG
17	Q	48	GLU
17	Q	52	LYS
17	Q	59	ILE
17	Q	65	ILE
17	Q	83	ASP
17	Q	84	LEU
17	Q	87	LYS
17	Q	88	TYR
17	Q	89	LEU
17	Q	97	SER
17	Q	98	LEU
17	Q	100	LYS
18	R	26	LEU
18	R	31	LEU

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Mol	Chain	Res	Type
18	R	47	THR
18	R	53	ARG
18	R	59	SER
18	R	75	ILE
18	R	84	LYS
18	R	88	LYS
19	S	3	ARG
19	S	4	SER
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	13	ASP
19	S	14	HIS
19	S	15	LEU
19	S	18	LYS
19	S	28	LYS
19	S	30	LEU
19	S	31	ILE
19	S	36	ARG
19	S	60	VAL
19	S	62	ILE
19	S	63	THR
19	S	70	LYS
19	S	81	ARG
20	T	8	ARG
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	19	SER
20	T	23	ARG
20	T	25	ARG
20	T	30	LYS
20	T	48	LYS
20	T	54	LYS
20	T	57	ARG
20	T	62	LEU
20	T	73	HIS
20	T	75	ASN
20	T	83	ARG
20	T	87	LYS
21	U	13	ILE
21	U	15	ARG

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Mol	Chain	Res	Type
21	U	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	318 (21%)	46 (3%)
22	V	2/3 (66%)	1 (50%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1523/1540 (98%)	323 (21%)	46 (3%)

All (323) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	51	A
1	A	54	C
1	A	58	C
1	A	60	A
1	A	61	G
1	A	62	U
1	A	82	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	143	A
1	A	144	G
1	A	163	C
1	A	182	U
1	A	183	G

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Mol	Chain	Res	Type
1	A	190(E)	U
1	A	190(F)	G
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	270	A
1	A	289	G
1	A	298	A
1	A	299	G
1	A	308	C
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	378	G
1	A	384	G
1	A	390	C
1	A	397	A

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Mol	Chain	Res	Type
1	A	398	C
1	A	402	G
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	432	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	453	A
1	A	460	A
1	A	461	C
1	A	463	A
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C

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Mol	Chain	Res	Type
1	A	563	A
1	A	564	C
1	A	568	G
1	A	570	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	587	G
1	A	588	G
1	A	597	G
1	A	607	A
1	A	618	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	667	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	748	C
1	A	755	G
1	A	766	A
1	A	773	G
1	A	777	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	798	G
1	A	812	C

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Mol	Chain	Res	Type
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	868	C
1	A	874	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	944	G
1	A	945	G
1	A	954	G
1	A	960	U
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	979	C
1	A	983	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A

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Mol	Chain	Res	Type
1	A	999	C
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1017	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1031	G
1	A	1033	G
1	A	1035	A
1	A	1042	G
1	A	1050	G
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	1094	G
1	A	1095	U
1	A	1096	C
1	A	1100	C
1	A	1101	A
1	A	1108	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	1132	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1154	G
1	A	1158	C

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1171	G
1	A	1179	A
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1218	C
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1252	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1268	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1291	G
1	A	1300	G
1	A	1301	U

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Mol	Chain	Res	Type
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1421	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1540	PSU
1	A	1541	PSU
22	V	3	U

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Mol	Chain	Res	Type
23	W	30	G
23	W	33	U
23	W	36	A
23	W	42	C

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	266	G
1	A	328	C
1	A	329	A
1	A	353	A
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	509	A
1	A	559	A
1	A	560	U
1	A	687	A
1	A	701	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1124	G
1	A	1129	C
1	A	1179	A
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U

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Mol	Chain	Res	Type
1	A	1225	A
1	A	1256	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1505	G
1	A	1528	U

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

15 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	2MG	A	1207	1	24,26,27	1.88	4 (16%)	32,38,41	10.95	3 (9%)
1	5MC	A	1400	1	20,22,23	1.89	4 (20%)	26,32,35	2.20	4 (15%)
1	4OC	A	1402	1	21,23,24	1.15	2 (9%)	26,32,35	1.08	2 (7%)
1	5MC	A	1404	1	20,22,23	1.52	3 (15%)	26,32,35	1.21	4 (15%)
1	5MC	A	1407	1	20,22,23	1.03	1 (5%)	26,32,35	1.52	6 (23%)
1	UR3	A	1498	1	20,22,23	1.16	1 (5%)	23,32,35	1.22	1 (4%)
1	MA6	A	1518	1	26,26,27	1.19	4 (15%)	37,38,41	1.15	5 (13%)
1	MA6	A	1519	1	26,26,27	1.13	4 (15%)	37,38,41	1.04	1 (2%)
1	PSU	A	1540	1	19,21,22	1.15	1 (5%)	23,30,33	1.47	3 (13%)
1	PSU	A	1541	1	19,21,22	1.12	1 (5%)	23,30,33	1.69	4 (17%)
1	PSU	A	516	1	19,21,22	1.50	1 (5%)	23,30,33	0.93	1 (4%)
1	7MG	A	527	1,25	24,26,27	4.11	7 (29%)	34,39,42	1.47	9 (26%)
1	M2G	A	966	1	25,27,28	0.97	2 (8%)	34,40,43	8.31	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	967	1	20,22,23	1.81	3 (15%)	26,32,35	1.45	3 (11%)
12	0TD	L	92	12	9,9,10	7.25	2 (22%)	9,11,13	3.19	4 (44%)

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	2MG	A	1207	1	-	0/10/27/28	0/1/3/3
1	5MC	A	1400	1	-	1/6/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/10/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/6/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/6/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/6/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519	1	-	0/13/29/30	0/1/3/3
1	PSU	A	1540	1	-	0/8/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1	-	0/8/25/26	0/2/2/2
1	7MG	A	527	1,25	-	1/8/37/38	0/1/3/3
1	M2G	A	966	1	-	0/12/29/30	0/1/3/3
1	5MC	A	967	1	-	0/6/25/26	0/2/2/2
12	0TD	L	92	12	-	0/10/12/14	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	20.63	1.25	1.11
1	A	527	7MG	C8-N9	-15.61	1.33	1.46
1	A	527	7MG	C2-N2	8.36	1.45	1.32
12	L	92	0TD	CA-C	6.43	1.60	1.48
1	A	967	5MC	C2-N1	6.05	1.44	1.38
1	A	1207	2MG	C6-N1	5.90	1.47	1.37
1	A	1400	5MC	C2-N1	5.73	1.44	1.38
1	A	516	PSU	C6-N1	5.34	1.37	1.32
1	A	1404	5MC	C2-N1	5.03	1.43	1.38
1	A	527	7MG	C4-N3	5.00	1.41	1.34
1	A	527	7MG	C8-N7	-4.87	1.31	1.45
1	A	527	7MG	CM7-N7	-4.09	1.39	1.46
1	A	1541	PSU	C6-N1	4.07	1.36	1.32
1	A	1540	PSU	C6-N1	3.86	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	O6-C6	3.60	1.31	1.24
1	A	967	5MC	P-OP1	3.59	1.50	1.46
1	A	1207	2MG	C2-N1	3.55	1.45	1.36
1	A	1498	UR3	C2-N3	3.46	1.42	1.38
1	A	1402	4OC	C2-N1	3.37	1.41	1.38
1	A	1400	5MC	C4-N3	3.08	1.37	1.32
1	A	1207	2MG	C8-N9	3.03	1.41	1.36
1	A	1518	MA6	C6-C5	-2.92	1.38	1.44
1	A	527	7MG	O6-C6	-2.76	1.19	1.24
1	A	1518	MA6	C2'-C1'	-2.75	1.49	1.53
1	A	1407	5MC	C2-N1	2.50	1.41	1.38
1	A	1400	5MC	P-OP1	2.43	1.49	1.46
1	A	1404	5MC	C2-N3	2.38	1.42	1.35
1	A	1400	5MC	C2-N3	2.36	1.41	1.35
1	A	527	7MG	C4-N9	-2.31	1.33	1.37
1	A	1519	MA6	C2-N1	2.30	1.38	1.33
1	A	1519	MA6	C6-N6	2.30	1.43	1.37
1	A	1518	MA6	C4-N9	-2.28	1.34	1.37
1	A	1402	4OC	P-OP1	2.27	1.49	1.46
1	A	967	5MC	C2-N3	2.24	1.41	1.35
1	A	1404	5MC	C6-C5	-2.22	1.34	1.40
1	A	1519	MA6	C4-N3	2.21	1.39	1.35
1	A	966	M2G	C2-N2	-2.16	1.32	1.34
1	A	1519	MA6	C6-N1	2.14	1.38	1.32
1	A	1518	MA6	C10-N6	2.12	1.51	1.45
1	A	966	M2G	C4-N9	2.00	1.40	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-61.71	125.83	134.14
1	A	966	M2G	C6-C5-N7	-47.85	127.70	134.14
1	A	1400	5MC	C6-N1-C2	9.32	123.22	118.62
1	A	1541	PSU	O4'-C1'-C5	6.06	117.09	109.55
12	L	92	0TD	CSB-SB-CB	-5.41	92.10	101.48
1	A	1540	PSU	C5-C1'-C2'	-5.16	106.50	115.61
12	L	92	0TD	C-CA-N	-5.11	103.62	111.94
12	L	92	0TD	CG-CB-SB	-4.88	102.16	108.74
1	A	967	5MC	C2-N3-C4	4.43	119.43	115.41
1	A	1400	5MC	C2-N3-C4	4.14	119.16	115.41
1	A	1407	5MC	C2-N3-C4	4.13	119.15	115.41
1	A	966	M2G	N1-C2-N2	-3.97	113.44	118.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	967	5MC	C6-N1-C2	3.73	120.45	118.62
1	A	1404	5MC	C2-N3-C4	3.48	118.56	115.41
1	A	966	M2G	C6-N1-C2	3.33	122.63	120.28
1	A	1407	5MC	CM5-C5-C6	3.17	125.33	118.59
12	L	92	0TD	CB-CA-N	-3.11	103.44	109.55
1	A	527	7MG	N7-C8-N9	3.00	107.05	103.08
1	A	1519	MA6	C2-N1-C6	2.95	117.93	111.53
1	A	1402	4OC	C2-N3-C4	2.86	118.74	115.27
1	A	527	7MG	N2-C2-N1	2.84	120.98	117.86
1	A	1407	5MC	N4-C4-N3	-2.82	113.86	118.73
1	A	1402	4OC	C6-C5-C4	-2.78	116.29	117.45
1	A	1518	MA6	C1'-N9-C4	-2.70	121.96	126.64
1	A	527	7MG	C4-N9-C1'	-2.67	119.65	126.00
1	A	527	7MG	C6-C5-N7	2.60	137.38	131.87
1	A	1541	PSU	C4-N3-C2	-2.58	120.12	125.36
1	A	527	7MG	C5-C4-N3	-2.58	121.96	126.61
1	A	1518	MA6	N1-C6-N6	-2.57	114.33	117.04
1	A	527	7MG	N3-C4-N9	2.55	131.09	127.06
1	A	1407	5MC	CM5-C5-C4	-2.51	118.90	121.43
1	A	527	7MG	C8-N9-C1'	2.49	129.01	121.94
1	A	1404	5MC	C2-N1-C1'	2.46	122.37	119.03
1	A	1518	MA6	N3-C2-N1	2.42	130.73	128.71
1	A	1407	5MC	C5-C4-N3	2.33	125.10	121.21
1	A	527	7MG	C5-C6-N1	2.28	121.69	115.25
1	A	1400	5MC	N4-C4-N3	-2.28	114.81	118.73
1	A	516	PSU	C5-C6-N1	2.25	123.97	120.68
1	A	1407	5MC	C6-N1-C2	2.24	119.72	118.62
1	A	1540	PSU	C3'-C2'-C1'	-2.25	99.22	101.85
1	A	1540	PSU	C4-N3-C2	-2.24	120.82	125.36
1	A	1207	2MG	C5-C6-N1	-2.20	108.97	115.39
1	A	1400	5MC	CM5-C5-C6	2.18	123.22	118.59
1	A	967	5MC	N4-C4-N3	-2.17	114.98	118.73
1	A	1518	MA6	C8-N9-C1'	2.17	130.66	126.38
1	A	966	M2G	N1-C2-N3	2.16	128.17	123.44
1	A	1498	UR3	C3'-C2'-C1'	2.15	104.27	100.91
1	A	527	7MG	CM7-N7-C8	2.12	124.49	119.23
1	A	1404	5MC	N4-C4-N3	-2.10	115.12	118.73
1	A	1541	PSU	C5-C1'-C2'	-2.09	111.92	115.61
1	A	1404	5MC	C6-N1-C2	2.08	119.64	118.62
1	A	1207	2MG	CM2-N2-C2	-2.08	120.36	123.73
1	A	966	M2G	C8-N9-C4	-2.08	105.31	106.90
1	A	1518	MA6	C2-N1-C6	2.05	115.97	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	C4-C5-C1'	2.02	124.93	120.95
1	A	966	M2G	C2-N3-C4	-2.01	112.30	115.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	OP2-P-O5'-C5'
1	A	1400	5MC	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 383 ligands modelled in this entry, 365 are monoatomic - leaving 18 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$
24	PAR	A	1601	-	45,45,45	1.36	6 (13%)	67,67,67	1.55	13 (19%)
24	PAR	A	1602	-	45,45,45	1.62	9 (20%)	67,67,67	1.70	11 (16%)
24	PAR	A	1603	-	45,45,45	1.48	8 (17%)	67,67,67	1.64	13 (19%)
24	PAR	A	1604	-	45,45,45	1.43	6 (13%)	67,67,67	1.61	13 (19%)
24	PAR	A	1605	-	45,45,45	1.29	7 (15%)	67,67,67	1.49	12 (17%)
24	PAR	A	1606	-	45,45,45	1.49	8 (17%)	67,67,67	1.62	12 (17%)
24	PAR	A	1607	-	45,45,45	1.72	9 (20%)	67,67,67	1.64	15 (22%)
24	PAR	A	1608	25	45,45,45	1.49	8 (17%)	67,67,67	1.63	13 (19%)
24	PAR	A	1609	-	45,45,45	1.80	14 (31%)	67,67,67	1.66	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PAR	A	1610	-	45,45,45	1.69	12 (26%)	67,67,67	1.69	14 (20%)
24	PAR	A	1611	-	45,45,45	1.64	8 (17%)	67,67,67	1.63	12 (17%)
24	PAR	A	1612	-	45,45,45	1.57	8 (17%)	67,67,67	1.61	12 (17%)
24	PAR	A	1613	-	45,45,45	1.71	10 (22%)	67,67,67	1.66	13 (19%)
24	PAR	A	1614	-	45,45,45	1.75	13 (28%)	67,67,67	1.57	12 (17%)
24	PAR	A	1615	-	45,45,45	2.12	11 (24%)	67,67,67	1.71	14 (20%)
24	PAR	A	1616	-	45,45,45	2.00	12 (26%)	67,67,67	1.64	14 (20%)
24	PAR	A	1617	25	45,45,45	2.15	14 (31%)	67,67,67	1.67	13 (19%)
24	PAR	A	1618	-	45,45,45	2.30	17 (37%)	67,67,67	1.61	13 (19%)

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
24	PAR	A	1601	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1602	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1603	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1604	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1605	-	-	0/18/94/94	1/4/4/4
24	PAR	A	1606	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1607	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1608	25	-	0/18/94/94	0/4/4/4
24	PAR	A	1609	-	-	1/18/94/94	0/4/4/4
24	PAR	A	1610	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1611	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1612	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1613	-	-	2/18/94/94	1/4/4/4
24	PAR	A	1614	-	-	0/18/94/94	1/4/4/4
24	PAR	A	1615	-	-	1/18/94/94	0/4/4/4
24	PAR	A	1616	-	-	0/18/94/94	2/4/4/4
24	PAR	A	1617	25	-	0/18/94/94	0/4/4/4
24	PAR	A	1618	-	-	1/18/94/94	1/4/4/4

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1615	PAR	C13-C23	6.52	1.61	1.52
24	A	1617	PAR	C52-C42	6.17	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1618	PAR	C13-C23	5.83	1.60	1.52
24	A	1618	PAR	C34-C24	5.61	1.61	1.53
24	A	1608	PAR	C22-C12	5.59	1.56	1.52
24	A	1602	PAR	C14-C24	5.52	1.63	1.52
24	A	1616	PAR	C13-C23	5.40	1.59	1.52
24	A	1618	PAR	C52-C42	5.39	1.63	1.52
24	A	1617	PAR	C13-C23	5.38	1.59	1.52
24	A	1613	PAR	C34-C24	4.95	1.60	1.53
24	A	1604	PAR	C52-C42	4.88	1.62	1.52
24	A	1615	PAR	O43-C13	4.70	1.50	1.41
24	A	1611	PAR	C34-C24	4.66	1.59	1.53
24	A	1610	PAR	O43-C13	4.61	1.49	1.41
24	A	1611	PAR	O43-C13	4.57	1.49	1.41
24	A	1603	PAR	C52-C42	4.47	1.61	1.52
24	A	1617	PAR	C34-C24	4.44	1.59	1.53
24	A	1607	PAR	C52-C42	4.43	1.61	1.52
24	A	1615	PAR	C52-C42	4.36	1.61	1.52
24	A	1618	PAR	C42-C32	4.29	1.59	1.52
24	A	1615	PAR	O52-C52	4.26	1.54	1.43
24	A	1612	PAR	C13-C23	4.23	1.58	1.52
24	A	1618	PAR	O43-C13	4.22	1.49	1.41
24	A	1609	PAR	C14-C24	4.13	1.60	1.52
24	A	1616	PAR	C52-C42	4.10	1.60	1.52
24	A	1617	PAR	C42-C32	4.01	1.58	1.52
24	A	1616	PAR	C34-C24	3.99	1.59	1.53
24	A	1609	PAR	C22-C32	-3.92	1.49	1.52
24	A	1602	PAR	C31-C21	3.92	1.58	1.53
24	A	1604	PAR	C42-C32	3.88	1.58	1.52
24	A	1614	PAR	C14-C24	3.86	1.59	1.52
24	A	1606	PAR	O43-C13	3.84	1.48	1.41
24	A	1614	PAR	C52-C42	3.83	1.59	1.52
24	A	1610	PAR	C14-C24	3.77	1.59	1.52
24	A	1607	PAR	O43-C13	3.73	1.48	1.41
24	A	1614	PAR	C34-C24	3.73	1.58	1.53
24	A	1606	PAR	C52-C42	3.72	1.59	1.52
24	A	1615	PAR	O52-C13	3.71	1.51	1.41
24	A	1616	PAR	C14-C24	3.70	1.59	1.52
24	A	1606	PAR	C34-C24	3.69	1.58	1.53
24	A	1607	PAR	C22-C32	-3.68	1.49	1.52
24	A	1610	PAR	C11-C21	3.63	1.59	1.52
24	A	1607	PAR	C62-C52	3.61	1.62	1.52
24	A	1612	PAR	C14-C24	3.59	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1612	PAR	O43-C13	3.58	1.48	1.41
24	A	1609	PAR	C34-C24	3.58	1.58	1.53
24	A	1613	PAR	C14-C24	3.56	1.59	1.52
24	A	1616	PAR	O43-C13	3.56	1.47	1.41
24	A	1618	PAR	C14-C24	3.51	1.59	1.52
24	A	1618	PAR	O33-C14	3.45	1.51	1.41
24	A	1609	PAR	O43-C13	3.38	1.47	1.41
24	A	1601	PAR	C13-C23	3.38	1.57	1.52
24	A	1601	PAR	C31-C21	3.37	1.58	1.53
24	A	1614	PAR	C42-C32	3.37	1.57	1.52
24	A	1611	PAR	C52-C42	3.27	1.58	1.52
24	A	1617	PAR	O52-C52	3.27	1.52	1.43
24	A	1617	PAR	O33-C14	3.24	1.50	1.41
24	A	1615	PAR	C22-C12	3.23	1.54	1.52
24	A	1615	PAR	C42-C32	3.21	1.57	1.52
24	A	1609	PAR	C13-C23	3.21	1.57	1.52
24	A	1613	PAR	C52-C42	3.15	1.58	1.52
24	A	1616	PAR	C42-C32	3.11	1.57	1.52
24	A	1612	PAR	C52-C42	3.11	1.58	1.52
24	A	1601	PAR	C11-C21	3.09	1.58	1.52
24	A	1604	PAR	C22-C32	3.08	1.54	1.52
24	A	1616	PAR	C31-C21	3.06	1.57	1.53
24	A	1613	PAR	C13-C23	3.06	1.56	1.52
24	A	1603	PAR	C13-C23	3.06	1.56	1.52
24	A	1601	PAR	C52-C42	3.06	1.58	1.52
24	A	1617	PAR	C14-C24	3.01	1.58	1.52
24	A	1618	PAR	C31-C21	2.97	1.57	1.53
24	A	1602	PAR	C52-C42	2.95	1.58	1.52
24	A	1603	PAR	C33-C43	2.92	1.61	1.52
24	A	1613	PAR	C62-C52	2.88	1.60	1.52
24	A	1610	PAR	C31-C21	2.87	1.57	1.53
24	A	1618	PAR	O52-C52	2.85	1.51	1.43
24	A	1616	PAR	O52-C52	2.84	1.50	1.43
24	A	1607	PAR	C62-C12	2.84	1.60	1.52
24	A	1609	PAR	C44-C54	2.84	1.59	1.53
24	A	1617	PAR	C62-C52	2.84	1.60	1.52
24	A	1614	PAR	C13-C23	2.83	1.56	1.52
24	A	1607	PAR	C44-C54	2.83	1.59	1.53
24	A	1618	PAR	C62-C52	2.81	1.60	1.52
24	A	1610	PAR	O54-C14	2.80	1.49	1.41
24	A	1609	PAR	C52-C42	2.80	1.57	1.52
24	A	1611	PAR	C42-C32	2.80	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1602	PAR	O43-C13	2.80	1.46	1.41
24	A	1603	PAR	C22-C12	2.80	1.54	1.52
24	A	1606	PAR	O52-C52	2.78	1.50	1.43
24	A	1610	PAR	C41-C51	2.76	1.59	1.53
24	A	1607	PAR	C13-C23	2.75	1.56	1.52
24	A	1609	PAR	O33-C14	2.74	1.49	1.41
24	A	1614	PAR	C31-C21	2.74	1.57	1.53
24	A	1606	PAR	C13-C23	2.72	1.56	1.52
24	A	1613	PAR	O33-C14	2.72	1.49	1.41
24	A	1616	PAR	C62-C52	2.68	1.60	1.52
24	A	1606	PAR	C22-C12	2.65	1.54	1.52
24	A	1610	PAR	O54-C54	2.65	1.51	1.44
24	A	1613	PAR	O52-C52	2.63	1.50	1.43
24	A	1617	PAR	O43-C13	2.61	1.46	1.41
24	A	1611	PAR	C31-C21	2.61	1.57	1.53
24	A	1618	PAR	O52-C13	2.60	1.48	1.41
24	A	1608	PAR	C62-C12	2.60	1.59	1.52
24	A	1616	PAR	C11-C21	2.59	1.57	1.52
24	A	1605	PAR	O43-C13	2.59	1.46	1.41
24	A	1612	PAR	C11-C21	2.58	1.57	1.52
24	A	1603	PAR	C62-C52	2.58	1.59	1.52
24	A	1602	PAR	O33-C14	2.56	1.48	1.41
24	A	1605	PAR	O33-C14	2.53	1.48	1.41
24	A	1611	PAR	C14-C24	2.52	1.57	1.52
24	A	1614	PAR	O52-C52	2.50	1.50	1.43
24	A	1609	PAR	C41-C51	2.50	1.58	1.53
24	A	1609	PAR	C62-C52	2.50	1.59	1.52
24	A	1612	PAR	C41-C51	2.50	1.58	1.53
24	A	1610	PAR	C52-C42	2.50	1.57	1.52
24	A	1605	PAR	O54-C14	2.49	1.48	1.41
24	A	1608	PAR	C11-C21	2.49	1.57	1.52
24	A	1616	PAR	O52-C13	2.48	1.48	1.41
24	A	1615	PAR	C31-C21	2.46	1.56	1.53
24	A	1601	PAR	C33-C43	2.45	1.60	1.52
24	A	1618	PAR	C11-C21	2.44	1.57	1.52
24	A	1603	PAR	O43-C13	2.44	1.46	1.41
24	A	1617	PAR	O11-C11	2.42	1.48	1.41
24	A	1602	PAR	O54-C14	2.41	1.48	1.41
24	A	1615	PAR	C23-C33	2.41	1.58	1.53
24	A	1608	PAR	O43-C13	2.40	1.45	1.41
24	A	1602	PAR	C22-C32	-2.39	1.50	1.52
24	A	1614	PAR	O33-C14	2.37	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1617	PAR	O33-C33	2.37	1.49	1.43
24	A	1603	PAR	C11-C21	2.35	1.57	1.52
24	A	1615	PAR	C62-C12	2.34	1.58	1.52
24	A	1608	PAR	C14-C24	2.34	1.57	1.52
24	A	1605	PAR	C33-C43	2.33	1.59	1.52
24	A	1614	PAR	C62-C52	2.33	1.59	1.52
24	A	1616	PAR	O33-C14	2.31	1.48	1.41
24	A	1613	PAR	O52-C13	2.30	1.47	1.41
24	A	1604	PAR	C33-C43	2.29	1.59	1.52
24	A	1617	PAR	C22-C12	-2.28	1.50	1.52
24	A	1605	PAR	C34-C24	2.28	1.56	1.53
24	A	1611	PAR	C22-C32	2.25	1.54	1.52
24	A	1617	PAR	C44-C54	2.24	1.58	1.53
24	A	1614	PAR	C33-C43	2.24	1.59	1.52
24	A	1618	PAR	O11-C11	2.23	1.47	1.41
24	A	1618	PAR	C22-C32	2.22	1.53	1.52
24	A	1615	PAR	O11-C11	2.21	1.47	1.41
24	A	1611	PAR	O33-C14	2.21	1.47	1.41
24	A	1614	PAR	C22-C12	2.21	1.53	1.52
24	A	1604	PAR	O43-C13	2.21	1.45	1.41
24	A	1610	PAR	O11-C11	2.20	1.47	1.41
24	A	1618	PAR	C44-C34	2.20	1.58	1.52
24	A	1612	PAR	C22-C32	2.17	1.53	1.52
24	A	1607	PAR	O52-C52	2.17	1.49	1.43
24	A	1608	PAR	C34-C24	2.17	1.56	1.53
24	A	1603	PAR	C14-C24	2.17	1.56	1.52
24	A	1612	PAR	C34-C24	2.15	1.56	1.53
24	A	1605	PAR	C13-C23	2.15	1.55	1.52
24	A	1607	PAR	O33-C14	2.15	1.47	1.41
24	A	1609	PAR	O52-C52	2.15	1.49	1.43
24	A	1604	PAR	C13-C23	2.14	1.55	1.52
24	A	1606	PAR	C33-C43	2.13	1.59	1.52
24	A	1617	PAR	O52-C13	2.13	1.47	1.41
24	A	1613	PAR	C22-C12	2.13	1.53	1.52
24	A	1606	PAR	C62-C52	2.12	1.58	1.52
24	A	1608	PAR	C62-C52	2.11	1.58	1.52
24	A	1609	PAR	C31-C21	2.11	1.56	1.53
24	A	1601	PAR	C62-C52	2.10	1.58	1.52
24	A	1618	PAR	O33-C33	2.09	1.49	1.43
24	A	1614	PAR	O54-C14	2.09	1.47	1.41
24	A	1610	PAR	O33-C14	2.07	1.47	1.41
24	A	1609	PAR	C11-C21	2.07	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1613	PAR	C42-C32	2.05	1.55	1.52
24	A	1614	PAR	C24-N24	2.04	1.50	1.47
24	A	1609	PAR	C24-N24	2.04	1.50	1.47
24	A	1610	PAR	C13-C23	2.03	1.55	1.52
24	A	1618	PAR	O54-C14	2.03	1.47	1.41
24	A	1608	PAR	C52-C42	2.03	1.56	1.52
24	A	1610	PAR	C62-C52	2.03	1.58	1.52
24	A	1602	PAR	C44-C34	-2.02	1.47	1.52
24	A	1602	PAR	C11-C21	2.01	1.56	1.52
24	A	1605	PAR	C31-C21	2.01	1.56	1.53

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1602	PAR	O33-C14-C24	7.09	122.12	108.09
24	A	1610	PAR	O33-C14-C24	6.54	121.04	108.09
24	A	1609	PAR	O33-C14-C24	6.00	119.96	108.09
24	A	1607	PAR	O33-C14-C24	5.97	119.90	108.09
24	A	1618	PAR	O33-C14-C24	5.88	119.72	108.09
24	A	1612	PAR	O33-C14-C24	5.82	119.60	108.09
24	A	1616	PAR	O33-C14-C24	5.71	119.39	108.09
24	A	1611	PAR	O33-C14-C24	5.69	119.36	108.09
24	A	1613	PAR	O33-C14-C24	5.67	119.31	108.09
24	A	1617	PAR	O33-C14-C24	5.59	119.16	108.09
24	A	1606	PAR	O33-C14-C24	5.56	119.09	108.09
24	A	1608	PAR	O33-C14-C24	5.49	118.94	108.09
24	A	1614	PAR	O33-C14-C24	5.29	118.56	108.09
24	A	1615	PAR	O33-C14-C24	5.21	118.39	108.09
24	A	1605	PAR	O33-C14-C24	5.13	118.24	108.09
24	A	1603	PAR	O52-C13-C23	4.94	116.32	107.50
24	A	1604	PAR	O33-C14-C24	4.87	117.72	108.09
24	A	1601	PAR	O52-C13-C23	4.83	116.12	107.50
24	A	1603	PAR	O33-C14-C24	4.83	117.65	108.09
24	A	1615	PAR	O52-C13-C23	4.78	116.03	107.50
24	A	1601	PAR	O33-C14-C24	4.71	117.42	108.09
24	A	1613	PAR	O52-C13-C23	4.68	115.86	107.50
24	A	1617	PAR	O52-C13-C23	4.45	115.44	107.50
24	A	1616	PAR	O52-C13-C23	4.42	115.38	107.50
24	A	1606	PAR	O52-C13-C23	4.22	115.04	107.50
24	A	1614	PAR	O52-C13-C23	3.98	114.61	107.50
24	A	1612	PAR	O11-C11-O51	3.93	120.49	110.69
24	A	1604	PAR	O52-C13-C23	3.88	114.42	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1602	PAR	O52-C13-O43	-3.87	107.81	111.51
24	A	1602	PAR	C34-C24-N24	-3.86	103.27	110.91
24	A	1615	PAR	O11-C11-O51	3.85	120.30	110.69
24	A	1607	PAR	O52-C13-C23	3.84	114.35	107.50
24	A	1612	PAR	O52-C13-C23	3.81	114.30	107.50
24	A	1618	PAR	O11-C11-O51	3.77	120.10	110.69
24	A	1604	PAR	C22-C32-C42	3.77	116.52	109.83
24	A	1617	PAR	C13-C23-C33	3.74	107.07	102.05
24	A	1617	PAR	O11-C11-O51	3.71	119.95	110.69
24	A	1618	PAR	O52-C13-C23	3.70	114.11	107.50
24	A	1608	PAR	O52-C13-C23	3.70	114.11	107.50
24	A	1609	PAR	O52-C13-C23	3.63	113.99	107.50
24	A	1611	PAR	O52-C13-O43	-3.61	108.05	111.51
24	A	1605	PAR	O52-C13-C23	3.61	113.94	107.50
24	A	1609	PAR	C11-O51-C51	3.59	120.71	113.73
24	A	1616	PAR	C13-C23-C33	3.51	106.76	102.05
24	A	1603	PAR	C34-C24-N24	-3.49	104.00	110.91
24	A	1610	PAR	O52-C13-O43	-3.49	108.17	111.51
24	A	1610	PAR	C34-C24-N24	-3.49	104.01	110.91
24	A	1609	PAR	O52-C13-O43	-3.43	108.22	111.51
24	A	1615	PAR	C13-C23-C33	3.42	106.65	102.05
24	A	1608	PAR	C22-C12-C62	3.41	115.26	110.06
24	A	1608	PAR	C14-O33-C33	-3.40	109.33	117.99
24	A	1607	PAR	O34-C34-C44	-3.39	102.76	110.35
24	A	1606	PAR	O11-C11-O51	3.38	119.13	110.69
24	A	1602	PAR	O34-C34-C44	-3.34	102.86	110.35
24	A	1613	PAR	O34-C34-C44	-3.33	102.88	110.35
24	A	1614	PAR	O11-C11-O51	3.32	118.97	110.69
24	A	1612	PAR	C34-C24-N24	-3.30	104.39	110.91
24	A	1607	PAR	C14-O33-C33	-3.29	109.60	117.99
24	A	1603	PAR	O11-C11-O51	3.28	118.87	110.69
24	A	1610	PAR	O34-C34-C44	-3.28	103.00	110.35
24	A	1610	PAR	O52-C13-C23	3.26	113.33	107.50
24	A	1604	PAR	O11-C11-O51	3.26	118.83	110.69
24	A	1613	PAR	O52-C13-O43	-3.23	108.42	111.51
24	A	1605	PAR	C34-C24-N24	-3.19	104.60	110.91
24	A	1602	PAR	O52-C13-C23	3.18	113.18	107.50
24	A	1606	PAR	C34-C24-N24	-3.18	104.62	110.91
24	A	1611	PAR	C14-O33-C33	-3.17	109.91	117.99
24	A	1611	PAR	O11-C11-O51	3.16	118.56	110.69
24	A	1608	PAR	C34-C24-N24	-3.15	104.69	110.91
24	A	1601	PAR	C34-C24-N24	-3.14	104.69	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1609	PAR	C34-C24-N24	-3.14	104.70	110.91
24	A	1618	PAR	C14-O33-C33	-3.13	110.00	117.99
24	A	1613	PAR	C13-C23-C33	3.12	106.25	102.05
24	A	1615	PAR	C22-C12-C62	3.10	114.79	110.06
24	A	1604	PAR	C13-C23-C33	3.09	106.20	102.05
24	A	1610	PAR	O11-C11-O51	3.08	118.37	110.69
24	A	1615	PAR	C14-O33-C33	-3.08	110.14	117.99
24	A	1611	PAR	C22-C32-C42	3.07	115.28	109.83
24	A	1608	PAR	O11-C11-O51	3.05	118.29	110.69
24	A	1612	PAR	O52-C13-O43	-3.02	108.61	111.51
24	A	1616	PAR	O11-C11-O51	3.02	118.22	110.69
24	A	1614	PAR	O34-C34-C44	-3.01	103.59	110.35
24	A	1612	PAR	C14-O33-C33	-2.97	110.40	117.99
24	A	1605	PAR	C13-C23-C33	2.97	106.03	102.05
24	A	1615	PAR	C34-C24-N24	-2.94	105.09	110.91
24	A	1606	PAR	C14-O33-C33	-2.93	110.52	117.99
24	A	1617	PAR	C34-C24-N24	-2.93	105.12	110.91
24	A	1609	PAR	C22-C12-C62	2.92	114.50	110.06
24	A	1607	PAR	O11-C11-O51	2.91	117.96	110.69
24	A	1615	PAR	O34-C34-C44	-2.91	103.83	110.35
24	A	1612	PAR	C13-C23-C33	2.83	105.86	102.05
24	A	1616	PAR	O34-C34-C44	-2.83	104.01	110.35
24	A	1608	PAR	C13-C23-C33	2.83	105.85	102.05
24	A	1616	PAR	C34-C24-N24	-2.83	105.31	110.91
24	A	1603	PAR	O34-C34-C44	-2.83	104.02	110.35
24	A	1605	PAR	O34-C34-C44	-2.82	104.03	110.35
24	A	1617	PAR	O34-C34-C44	-2.81	104.05	110.35
24	A	1611	PAR	C11-O51-C51	2.81	119.19	113.73
24	A	1613	PAR	O11-C11-O51	2.80	117.68	110.69
24	A	1604	PAR	C13-O52-C52	-2.80	110.84	117.99
24	A	1611	PAR	C34-C24-N24	-2.80	105.38	110.91
24	A	1601	PAR	O34-C34-C44	-2.79	104.10	110.35
24	A	1603	PAR	C13-O52-C52	-2.79	110.88	117.99
24	A	1603	PAR	C22-C12-C62	2.78	114.30	110.06
24	A	1614	PAR	C34-C24-N24	-2.78	105.42	110.91
24	A	1615	PAR	O52-C52-C42	2.77	114.52	107.41
24	A	1604	PAR	C34-C24-N24	-2.74	105.49	110.91
24	A	1608	PAR	O34-C34-C44	-2.74	104.22	110.35
24	A	1616	PAR	C14-O33-C33	-2.73	111.04	117.99
24	A	1604	PAR	C14-O33-C33	-2.72	111.05	117.99
24	A	1609	PAR	O11-C11-O51	2.72	117.48	110.69
24	A	1608	PAR	O52-C13-O43	-2.72	108.91	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1607	PAR	C34-C24-N24	-2.71	105.55	110.91
24	A	1601	PAR	C13-O52-C52	-2.71	111.09	117.99
24	A	1607	PAR	O52-C13-O43	-2.69	108.93	111.51
24	A	1607	PAR	C22-C12-C62	2.69	114.15	110.06
24	A	1611	PAR	O34-C34-C44	-2.68	104.34	110.35
24	A	1617	PAR	O54-C54-C44	2.67	114.71	109.76
24	A	1609	PAR	C14-O33-C33	-2.67	111.18	117.99
24	A	1611	PAR	O52-C13-C23	2.67	112.26	107.50
24	A	1604	PAR	O34-C34-C44	-2.67	104.37	110.35
24	A	1618	PAR	O34-C34-C44	-2.66	104.40	110.35
24	A	1605	PAR	O11-C11-O51	2.65	117.30	110.69
24	A	1601	PAR	O11-C11-O51	2.64	117.28	110.69
24	A	1618	PAR	C34-C24-N24	-2.63	105.70	110.91
24	A	1618	PAR	O51-C51-C61	2.63	112.81	106.34
24	A	1606	PAR	O34-C34-C44	-2.63	104.45	110.35
24	A	1609	PAR	O51-C51-C61	2.63	112.80	106.34
24	A	1615	PAR	O52-C13-O43	-2.62	109.00	111.51
24	A	1602	PAR	O51-C51-C61	2.60	112.73	106.34
24	A	1612	PAR	O34-C34-C44	-2.57	104.59	110.35
24	A	1602	PAR	O11-C11-O51	2.56	117.09	110.69
24	A	1606	PAR	C22-C12-C62	2.55	113.95	110.06
24	A	1607	PAR	C52-C62-C12	2.54	116.54	109.53
24	A	1613	PAR	C14-O33-C33	-2.54	111.52	117.99
24	A	1613	PAR	C34-C24-N24	-2.53	105.91	110.91
24	A	1618	PAR	O52-C13-O43	-2.53	109.09	111.51
24	A	1617	PAR	C14-O33-C33	-2.52	111.57	117.99
24	A	1614	PAR	C13-C23-C33	2.51	105.42	102.05
24	A	1609	PAR	O34-C34-C44	-2.51	104.73	110.35
24	A	1604	PAR	C11-O51-C51	2.50	118.59	113.73
24	A	1603	PAR	O51-C51-C61	2.50	112.49	106.34
24	A	1613	PAR	C22-C12-C62	2.48	113.84	110.06
24	A	1601	PAR	C22-C32-C42	2.48	114.23	109.83
24	A	1602	PAR	O54-C54-C44	2.47	114.33	109.76
24	A	1606	PAR	C11-O51-C51	2.46	118.52	113.73
24	A	1614	PAR	C22-C12-C62	2.46	113.81	110.06
24	A	1601	PAR	O52-C13-O43	-2.45	109.16	111.51
24	A	1614	PAR	O43-C13-C23	-2.45	101.57	104.92
24	A	1601	PAR	O43-C13-C23	-2.44	101.58	104.92
24	A	1605	PAR	C14-O33-C33	-2.44	111.77	117.99
24	A	1615	PAR	O11-C42-C52	2.43	113.65	107.41
24	A	1605	PAR	C13-O52-C52	-2.42	111.82	117.99
24	A	1610	PAR	C22-C12-C62	2.41	113.73	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1604	PAR	O52-C13-O43	-2.41	109.20	111.51
24	A	1601	PAR	O51-C51-C61	2.41	112.27	106.34
24	A	1610	PAR	C14-O33-C33	-2.40	111.86	117.99
24	A	1617	PAR	C22-C32-C42	2.40	114.09	109.83
24	A	1601	PAR	C14-O33-C33	-2.40	111.88	117.99
24	A	1604	PAR	O51-C51-C61	2.39	112.22	106.34
24	A	1612	PAR	C13-O52-C52	-2.38	111.91	117.99
24	A	1602	PAR	C22-C12-C62	2.38	113.69	110.06
24	A	1616	PAR	O51-C51-C61	2.39	112.20	106.34
24	A	1609	PAR	O51-C51-C41	2.38	114.17	109.76
24	A	1612	PAR	O51-C51-C61	2.38	112.18	106.34
24	A	1614	PAR	O51-C51-C61	2.38	112.18	106.34
24	A	1605	PAR	O52-C13-O43	-2.37	109.24	111.51
24	A	1603	PAR	C11-O51-C51	2.37	118.34	113.73
24	A	1616	PAR	C22-C12-C62	2.37	113.67	110.06
24	A	1616	PAR	O52-C52-C42	2.37	113.48	107.41
24	A	1608	PAR	C13-O52-C52	-2.35	112.00	117.99
24	A	1614	PAR	C14-O33-C33	-2.33	112.04	117.99
24	A	1610	PAR	O34-C34-C24	-2.33	106.09	110.06
24	A	1607	PAR	O34-C34-C24	-2.33	106.10	110.06
24	A	1615	PAR	O54-C54-C44	2.32	114.05	109.76
24	A	1601	PAR	O33-C14-O54	-2.31	104.93	110.69
24	A	1610	PAR	C31-C41-C51	2.30	114.32	110.20
24	A	1608	PAR	O51-C51-C61	2.30	112.00	106.34
24	A	1605	PAR	O51-C51-C61	2.30	111.98	106.34
24	A	1611	PAR	O51-C51-C61	2.29	111.98	106.34
24	A	1618	PAR	O52-C52-C42	2.29	113.29	107.41
24	A	1607	PAR	C13-O52-C52	-2.29	112.15	117.99
24	A	1615	PAR	O51-C51-C61	2.28	111.94	106.34
24	A	1608	PAR	O33-C14-O54	-2.28	105.01	110.69
24	A	1608	PAR	C11-O51-C51	2.26	118.12	113.73
24	A	1610	PAR	O54-C54-C44	2.26	113.94	109.76
24	A	1616	PAR	C13-O52-C52	-2.26	112.23	117.99
24	A	1617	PAR	C13-O52-C52	-2.25	112.25	117.99
24	A	1616	PAR	O52-C13-O43	-2.23	109.37	111.51
24	A	1612	PAR	O33-C14-O54	-2.23	105.14	110.69
24	A	1606	PAR	O33-C14-O54	-2.22	105.17	110.69
24	A	1618	PAR	C22-C32-C42	2.21	113.75	109.83
24	A	1603	PAR	C14-O33-C33	-2.21	112.36	117.99
24	A	1607	PAR	O51-C51-C61	2.20	111.75	106.34
24	A	1609	PAR	O54-C54-C44	2.20	113.83	109.76
24	A	1603	PAR	O52-C13-O43	-2.18	109.42	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1618	PAR	C22-C12-C62	2.18	113.38	110.06
24	A	1617	PAR	O51-C51-C61	2.17	111.68	106.34
24	A	1614	PAR	O43-C43-C53	2.17	113.79	109.15
24	A	1607	PAR	O54-C54-C44	2.17	113.78	109.76
24	A	1602	PAR	C14-O33-C33	-2.16	112.47	117.99
24	A	1606	PAR	O51-C51-C61	2.16	111.65	106.34
24	A	1604	PAR	O33-C14-O54	-2.16	105.32	110.69
24	A	1613	PAR	O51-C51-C61	2.14	111.59	106.34
24	A	1617	PAR	O52-C52-C42	2.13	112.88	107.41
24	A	1610	PAR	O51-C51-C61	2.13	111.57	106.34
24	A	1603	PAR	O34-C34-C24	-2.12	106.46	110.06
24	A	1618	PAR	C44-C34-C24	2.11	115.20	111.31
24	A	1616	PAR	C11-O51-C51	2.11	117.83	113.73
24	A	1607	PAR	C13-C23-C33	2.11	104.88	102.05
24	A	1611	PAR	O54-C54-C44	2.10	113.65	109.76
24	A	1610	PAR	C13-O52-C52	-2.10	112.63	117.99
24	A	1605	PAR	O54-C54-C44	2.10	113.65	109.76
24	A	1606	PAR	O54-C54-C44	2.10	113.64	109.76
24	A	1601	PAR	O34-C34-C24	-2.09	106.50	110.06
24	A	1612	PAR	C22-C32-C42	2.09	113.54	109.83
24	A	1613	PAR	C22-C32-C42	2.08	113.51	109.83
24	A	1613	PAR	O52-C52-C42	2.08	112.74	107.41
24	A	1615	PAR	O34-C34-C24	-2.07	106.54	110.06
24	A	1611	PAR	O33-C14-O54	-2.07	105.53	110.69
24	A	1606	PAR	C13-O52-C52	-2.07	112.72	117.99
24	A	1605	PAR	C22-C32-C42	2.05	113.47	109.83
24	A	1618	PAR	O54-C54-C44	2.05	113.56	109.76
24	A	1603	PAR	O33-C14-O54	-2.05	105.58	110.69
24	A	1602	PAR	O33-C14-O54	-2.04	105.60	110.69
24	A	1613	PAR	C13-O52-C52	-2.03	112.82	117.99
24	A	1609	PAR	C13-O52-C52	-2.03	112.82	117.99
24	A	1614	PAR	C22-C32-C42	2.01	113.40	109.83
24	A	1617	PAR	O52-C13-O43	-2.01	109.58	111.51
24	A	1607	PAR	C62-C52-C42	2.01	115.76	111.39
24	A	1610	PAR	O33-C14-O54	-2.00	105.70	110.69
24	A	1616	PAR	O54-C54-C44	2.00	113.47	109.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1609	PAR	C33-O33-C14-C24

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Mol	Chain	Res	Type	Atoms
24	A	1613	PAR	C52-O52-C13-C23
24	A	1610	PAR	C33-O33-C14-C24
24	A	1602	PAR	C33-O33-C14-C24
24	A	1612	PAR	C42-O11-C11-C21
24	A	1615	PAR	C33-O33-C14-C24
24	A	1613	PAR	C42-O11-C11-C21
24	A	1618	PAR	C33-O33-C14-C24

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1605	PAR	C14-C24-C34-C44-C54-O54
24	A	1612	PAR	C12-C22-C32-C42-C52-C62
24	A	1614	PAR	C12-C22-C32-C42-C52-C62
24	A	1618	PAR	C12-C22-C32-C42-C52-C62
24	A	1610	PAR	C14-C24-C34-C44-C54-O54
24	A	1602	PAR	C14-C24-C34-C44-C54-O54
24	A	1616	PAR	C12-C22-C32-C42-C52-C62
24	A	1616	PAR	C14-C24-C34-C44-C54-O54
24	A	1613	PAR	C12-C22-C32-C42-C52-C62

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, 95th 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	1511/1522 (99%)	-0.36	7 (0%) 88 77	49, 88, 175, 339	0
2	B	236/256 (92%)	-0.03	0 100 100	70, 114, 159, 187	0
3	C	207/239 (86%)	-0.01	1 (0%) 88 77	80, 108, 146, 160	0
4	D	208/209 (99%)	-0.12	0 100 100	56, 92, 128, 166	0
5	E	151/162 (93%)	-0.16	0 100 100	47, 73, 107, 151	0
6	F	101/101 (100%)	-0.19	1 (0%) 79 65	68, 108, 134, 160	0
7	G	155/156 (99%)	-0.24	0 100 100	66, 106, 162, 193	0
8	H	138/138 (100%)	-0.16	0 100 100	47, 74, 104, 132	0
9	I	127/128 (99%)	0.19	1 (0%) 83 70	69, 112, 142, 158	0
10	J	99/105 (94%)	0.18	1 (1%) 79 65	75, 127, 185, 199	0
11	K	119/129 (92%)	-0.09	1 (0%) 83 70	54, 94, 132, 210	0
12	L	124/135 (91%)	0.09	2 (1%) 68 54	55, 80, 124, 185	0
13	M	118/126 (93%)	0.24	1 (0%) 83 70	78, 108, 137, 149	0
14	N	60/61 (98%)	-0.14	1 (1%) 67 52	75, 99, 139, 181	0
15	O	88/89 (98%)	0.11	2 (2%) 57 43	56, 90, 123, 172	0
16	P	84/88 (95%)	-0.02	0 100 100	58, 77, 107, 151	0
17	Q	100/105 (95%)	0.31	0 100 100	63, 81, 120, 155	0
18	R	73/88 (82%)	0.27	0 100 100	68, 100, 153, 221	0
19	S	81/93 (87%)	-0.06	0 100 100	89, 124, 151, 179	0
20	T	99/106 (93%)	0.11	0 100 100	65, 85, 130, 168	0
21	U	25/27 (92%)	0.34	0 100 100	87, 113, 132, 139	0
22	V	3/3 (100%)	0.67	0 100 100	99, 99, 103, 105	0
23	W	15/15 (100%)	0.82	1 (6%) 17 18	127, 144, 218, 227	0
All	All	3922/4081 (96%)	-0.14	19 (0%) 84 77	47, 96, 156, 339	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1540	PSU	6.3
12	L	129	ALA	5.8
1	A	1539	C	4.8
1	A	1541	PSU	4.3
11	K	128	ALA	3.6
14	N	12	ARG	3.4
1	A	1498	UR3	3.0
12	L	128	ALA	2.9
1	A	1533	C	2.9
1	A	1519	MA6	2.7
6	F	101	ALA	2.6
1	A	1129	C	2.6
15	O	89	GLY	2.5
23	W	40	C	2.3
3	C	206	GLU	2.3
13	M	5	ALA	2.2
15	O	88	ARG	2.2
10	J	98	ILE	2.1
9	I	128	ARG	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	5MC	A	1407	21/22	0.13	-	61,67,72,74	0
1	MA6	A	1519	24/25	0.28	-	55,57,64,67	0
1	M2G	A	966	25/26	0.18	-	66,100,115,127	0
1	PSU	A	1541	20/21	0.49	-	228,249,272,273	0
1	7MG	A	527	24/25	0.18	-	63,69,82,84	0
1	PSU	A	516	20/21	0.25	-	83,94,105,108	0
1	PSU	A	1540	20/21	0.64	-	210,258,270,270	0
12	0TD	L	92	10/11	0.35	-	55,83,98,428	0
1	5MC	A	967	21/22	0.13	-	59,75,118,121	0
1	UR3	A	1498	21/22	0.18	-	63,71,81,88	0
1	2MG	A	1207	24/25	0.13	-	91,106,114,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	5MC	A	1400	21/22	0.20	-	44,73,95,101	0
1	MA6	A	1518	24/25	0.21	-	58,69,75,78	0
1	4OC	A	1402	22/23	0.21	-	57,63,67,91	0
1	5MC	A	1404	21/22	0.14	-	55,64,71,72	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1642	1/1	0.17	-	70,70,70,70	0
25	MG	A	1821	1/1	0.28	-	33,33,33,33	0
25	MG	A	1729	1/1	0.03	-	73,73,73,73	0
25	MG	A	1660	1/1	0.23	-	84,84,84,84	0
25	MG	A	1639	1/1	0.38	-	55,55,55,55	0
25	MG	A	1677	1/1	0.53	-	118,118,118,118	0
25	MG	A	1906	1/1	0.21	-	73,73,73,73	0
25	MG	A	1897[B]	1/1	0.60	-	0,0,0,0	1
25	MG	A	1745	1/1	0.32	-	64,64,64,64	0
24	PAR	A	1615	42/42	0.32	-	149,149,149,149	0
24	PAR	A	1612	42/42	0.23	-	131,131,131,131	0
25	MG	A	1708	1/1	0.08	-	55,55,55,55	0
25	MG	A	1809	1/1	1.03	-	76,76,76,76	0
25	MG	A	1681	1/1	0.35	-	30,30,30,30	0
25	MG	A	1813	1/1	0.74	-	53,53,53,53	0
25	MG	A	1730	1/1	0.11	-	118,118,118,118	0
25	MG	A	1800[B]	1/1	0.68	-	7,7,7,7	1
25	MG	A	1953	1/1	0.13	-	179,179,179,179	0
25	MG	A	1874	1/1	0.35	-	13,13,13,13	0
25	MG	A	1762	1/1	0.12	-	63,63,63,63	0
25	MG	A	1773	1/1	0.18	-	74,74,74,74	0
25	MG	N	102	1/1	0.50	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1892	1/1	0.20	-	46,46,46,46	0
25	MG	A	1633	1/1	0.06	-	54,54,54,54	0
25	MG	A	1879	1/1	0.15	-	56,56,56,56	0
25	MG	E	201	1/1	0.19	-	92,92,92,92	0
25	MG	A	1912	1/1	0.38	-	51,51,51,51	0
25	MG	A	1638	1/1	0.36	-	56,56,56,56	0
25	MG	A	1791	1/1	0.27	-	30,30,30,30	0
25	MG	A	1890	1/1	0.55	-	59,59,59,59	0
25	MG	A	1767	1/1	0.13	-	72,72,72,72	0
25	MG	A	1929	1/1	0.76	-	44,44,44,44	0
25	MG	A	1764	1/1	0.14	-	65,65,65,65	0
25	MG	A	1838	1/1	0.61	-	50,50,50,50	0
25	MG	A	1644	1/1	0.09	-	40,40,40,40	0
25	MG	A	1801	1/1	0.86	-	57,57,57,57	0
25	MG	A	1679	1/1	0.19	-	47,47,47,47	0
25	MG	A	1781	1/1	0.14	-	67,67,67,67	0
25	MG	A	1713	1/1	0.41	-	63,63,63,63	0
25	MG	A	1652[A]	1/1	0.65	-	11,11,11,11	1
25	MG	A	1915	1/1	0.25	-	59,59,59,59	0
25	MG	A	1657	1/1	0.23	-	101,101,101,101	0
25	MG	A	1692	1/1	0.13	-	74,74,74,74	0
25	MG	A	1925	1/1	0.17	-	42,42,42,42	0
25	MG	E	202	1/1	0.37	-	45,45,45,45	0
25	MG	A	1854	1/1	0.12	-	40,40,40,40	0
25	MG	A	1935	1/1	0.36	-	57,57,57,57	0
25	MG	A	1655	1/1	0.12	-	78,78,78,78	0
25	MG	A	1747	1/1	0.22	-	108,108,108,108	0
25	MG	A	1626	1/1	0.07	-	100,100,100,100	0
25	MG	A	1715	1/1	0.31	-	82,82,82,82	0
25	MG	A	1911	1/1	0.14	-	49,49,49,49	0
26	ZN	N	101	1/1	0.14	-	88,88,88,88	0
25	MG	A	1861	1/1	0.08	-	57,57,57,57	0
25	MG	A	1690	1/1	0.14	-	100,100,100,100	0
25	MG	A	1683	1/1	0.23	-	102,102,102,102	0
25	MG	A	1717	1/1	0.10	-	110,110,110,110	0
25	MG	A	1857	1/1	0.98	-	54,54,54,54	0
25	MG	A	1943	1/1	0.23	-	178,178,178,178	0
25	MG	A	1852	1/1	0.39	-	47,47,47,47	0
25	MG	A	1706	1/1	0.26	-	52,52,52,52	0
25	MG	A	1702	1/1	0.11	-	104,104,104,104	0
25	MG	A	1876	1/1	0.95	-	69,69,69,69	0
25	MG	A	1760	1/1	0.17	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1845	1/1	0.26	-	64,64,64,64	0
25	MG	A	1667	1/1	0.12	-	56,56,56,56	0
25	MG	A	1826	1/1	0.17	-	44,44,44,44	0
25	MG	E	204	1/1	0.20	-	70,70,70,70	0
25	MG	A	1636	1/1	0.29	-	68,68,68,68	0
25	MG	A	1903	1/1	0.31	-	74,74,74,74	0
25	MG	A	1830	1/1	0.24	-	70,70,70,70	0
25	MG	A	1749	1/1	0.15	-	72,72,72,72	0
25	MG	A	1949	1/1	0.22	-	228,228,228,228	0
25	MG	A	1731	1/1	0.09	-	121,121,121,121	0
25	MG	D	302	1/1	0.53	-	71,71,71,71	0
25	MG	A	1736	1/1	0.14	-	88,88,88,88	0
25	MG	A	1707	1/1	0.15	-	80,80,80,80	0
25	MG	A	1643	1/1	0.45	-	40,40,40,40	0
24	PAR	A	1601	42/42	0.16	-	64,64,64,64	0
25	MG	A	1733	1/1	0.31	-	61,61,61,61	0
25	MG	A	1663	1/1	0.09	-	36,36,36,36	0
25	MG	A	1728	1/1	0.11	-	103,103,103,103	0
25	MG	A	1849	1/1	0.47	-	40,40,40,40	0
25	MG	A	1665	1/1	0.29	-	57,57,57,57	0
25	MG	A	1848	1/1	0.08	-	42,42,42,42	0
25	MG	A	1648	1/1	0.20	-	64,64,64,64	0
25	MG	A	1880	1/1	0.26	-	60,60,60,60	0
25	MG	A	1910	1/1	0.11	-	45,45,45,45	0
25	MG	A	1840	1/1	0.34	-	22,22,22,22	0
25	MG	A	1654	1/1	0.11	-	75,75,75,75	0
25	MG	A	1913	1/1	0.30	-	49,49,49,49	0
25	MG	A	1919[A]	1/1	0.25	-	9,9,9,9	1
25	MG	A	1664	1/1	0.36	-	74,74,74,74	0
25	MG	A	1756	1/1	0.08	-	93,93,93,93	0
25	MG	A	1955	1/1	0.12	-	179,179,179,179	0
25	MG	A	1723	1/1	0.10	-	94,94,94,94	0
25	MG	A	1888	1/1	0.57	-	71,71,71,71	0
24	PAR	A	1614	42/42	0.20	-	174,174,174,174	0
25	MG	A	1738	1/1	0.14	-	59,59,59,59	0
25	MG	A	1742	1/1	0.18	-	72,72,72,72	0
25	MG	A	1950	1/1	0.11	-	177,177,177,177	0
25	MG	A	1904	1/1	0.20	-	49,49,49,49	0
25	MG	A	1918	1/1	0.31	-	39,39,39,39	0
25	MG	A	1926	1/1	0.09	-	58,58,58,58	0
24	PAR	A	1613	42/42	0.24	-	120,120,120,120	0
25	MG	A	1780	1/1	0.50	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1957	1/1	0.11	-	103,103,103,103	0
25	MG	A	1770	1/1	0.23	-	90,90,90,90	0
25	MG	A	1862	1/1	0.25	-	38,38,38,38	0
25	MG	A	1882[B]	1/1	0.75	-	0,0,0,0	1
25	MG	A	1775	1/1	0.07	-	75,75,75,75	0
25	MG	A	1886	1/1	0.43	-	50,50,50,50	0
25	MG	A	1779	1/1	0.18	-	55,55,55,55	0
24	PAR	A	1610	42/42	0.30	-	144,144,144,144	0
25	MG	A	1788	1/1	0.36	-	95,95,95,95	0
25	MG	A	1686	1/1	0.15	-	91,91,91,91	0
25	MG	A	1753	1/1	0.09	-	94,94,94,94	0
25	MG	E	203	1/1	0.09	-	80,80,80,80	0
25	MG	A	1632	1/1	0.10	-	65,65,65,65	0
25	MG	S	101	1/1	0.27	-	22,22,22,22	0
25	MG	A	1778	1/1	0.46	-	59,59,59,59	0
25	MG	A	1836	1/1	0.32	-	75,75,75,75	0
25	MG	A	1768	1/1	0.18	-	103,103,103,103	0
25	MG	A	1732	1/1	0.11	-	84,84,84,84	0
25	MG	A	1649	1/1	0.19	-	47,47,47,47	0
25	MG	A	1931	1/1	0.83	-	58,58,58,58	0
25	MG	S	102	1/1	0.22	-	73,73,73,73	0
25	MG	A	1894	1/1	0.35	-	66,66,66,66	0
24	PAR	A	1611	42/42	0.27	-	131,131,131,131	0
25	MG	A	1952	1/1	0.11	-	148,148,148,148	0
25	MG	A	1843	1/1	0.09	-	35,35,35,35	0
25	MG	A	1951	1/1	0.29	-	110,110,110,110	0
25	MG	A	1803	1/1	0.41	-	71,71,71,71	0
25	MG	A	1905	1/1	0.89	-	83,83,83,83	0
25	MG	A	1823	1/1	0.41	-	57,57,57,57	0
24	PAR	A	1618	42/42	0.34	-	166,166,166,166	0
25	MG	A	1721	1/1	0.99	-	43,43,43,43	0
25	MG	A	1769	1/1	0.18	-	114,114,114,114	0
25	MG	A	1835	1/1	0.32	-	71,71,71,71	0
25	MG	A	1709	1/1	0.11	-	94,94,94,94	0
25	MG	A	1670	1/1	0.15	-	64,64,64,64	0
25	MG	A	1869	1/1	1.07	-	59,59,59,59	0
25	MG	A	1898	1/1	0.37	-	61,61,61,61	0
25	MG	A	1676	1/1	0.31	-	75,75,75,75	0
25	MG	A	1817	1/1	0.80	-	54,54,54,54	0
25	MG	A	1855	1/1	0.18	-	24,24,24,24	0
25	MG	A	1893	1/1	0.57	-	53,53,53,53	0
25	MG	A	1700	1/1	0.42	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1662	1/1	0.60	-	77,77,77,77	0
25	MG	A	1635	1/1	0.26	-	45,45,45,45	0
25	MG	A	1882[A]	1/1	0.75	-	0,0,0,0	1
25	MG	A	1622	1/1	0.07	-	106,106,106,106	0
25	MG	A	1766	1/1	0.10	-	97,97,97,97	0
25	MG	A	1956	1/1	0.13	-	193,193,193,193	0
25	MG	A	1630	1/1	0.07	-	83,83,83,83	0
25	MG	A	1703	1/1	0.22	-	57,57,57,57	0
25	MG	A	1916	1/1	0.34	-	51,51,51,51	0
25	MG	A	1704	1/1	0.14	-	83,83,83,83	0
25	MG	A	1739	1/1	0.32	-	85,85,85,85	0
25	MG	A	1883	1/1	0.36	-	62,62,62,62	0
25	MG	A	1873	1/1	0.47	-	29,29,29,29	0
25	MG	P	103	1/1	0.28	-	44,44,44,44	0
25	MG	A	1798	1/1	0.17	-	70,70,70,70	0
25	MG	A	1867	1/1	0.61	-	29,29,29,29	0
24	PAR	A	1604	42/42	0.20	-	64,64,64,64	0
25	MG	A	1800[A]	1/1	0.68	-	7,7,7,7	1
25	MG	A	1727	1/1	0.07	-	101,101,101,101	0
25	MG	A	1802	1/1	0.29	-	46,46,46,46	0
25	MG	A	1827	1/1	0.25	-	78,78,78,78	0
25	MG	A	1833	1/1	0.22	-	59,59,59,59	0
25	MG	A	1656	1/1	0.18	-	67,67,67,67	0
25	MG	A	1786	1/1	0.21	-	97,97,97,97	0
25	MG	A	1831	1/1	0.14	-	40,40,40,40	0
25	MG	A	1792	1/1	0.27	-	32,32,32,32	0
25	MG	A	1674	1/1	0.27	-	18,18,18,18	0
25	MG	A	1941	1/1	0.08	-	145,145,145,145	0
25	MG	A	1696	1/1	0.05	-	136,136,136,136	0
25	MG	A	1806	1/1	0.73	-	91,91,91,91	0
25	MG	A	1917	1/1	0.45	-	61,61,61,61	0
25	MG	A	1641	1/1	0.18	-	56,56,56,56	0
25	MG	A	1814	1/1	0.16	-	26,26,26,26	0
25	MG	A	1909	1/1	0.77	-	68,68,68,68	0
25	MG	H	201	1/1	0.56	-	53,53,53,53	0
25	MG	A	1695	1/1	0.13	-	94,94,94,94	0
25	MG	A	1799	1/1	0.23	-	59,59,59,59	0
25	MG	A	1868	1/1	0.39	-	68,68,68,68	0
26	ZN	D	301	1/1	0.31	-	141,141,141,141	0
25	MG	A	1899	1/1	0.34	-	18,18,18,18	0
25	MG	A	1637	1/1	0.19	-	29,29,29,29	0
25	MG	A	1818	1/1	0.23	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1750	1/1	0.62	-	67,67,67,67	0
25	MG	A	1922	1/1	0.61	-	76,76,76,76	0
25	MG	A	1705	1/1	0.10	-	57,57,57,57	0
25	MG	A	1841	1/1	0.39	-	64,64,64,64	0
25	MG	A	1712	1/1	0.21	-	34,34,34,34	0
25	MG	A	1812	1/1	0.84	-	65,65,65,65	0
25	MG	A	1653[B]	1/1	0.83	-	11,11,11,11	1
25	MG	A	1711	1/1	0.09	-	64,64,64,64	0
25	MG	A	1924	1/1	0.46	-	54,54,54,54	0
25	MG	A	1684	1/1	0.08	-	25,25,25,25	0
25	MG	P	101	1/1	0.22	-	13,13,13,13	0
25	MG	A	1938	1/1	0.05	-	43,43,43,43	0
25	MG	A	1737	1/1	0.10	-	63,63,63,63	0
25	MG	A	1751	1/1	0.10	-	95,95,95,95	0
25	MG	A	1853	1/1	0.64	-	44,44,44,44	0
25	MG	A	1860	1/1	0.21	-	55,55,55,55	0
25	MG	A	1881	1/1	0.42	-	63,63,63,63	0
25	MG	A	1693	1/1	0.25	-	96,96,96,96	0
25	MG	A	1797	1/1	0.57	-	47,47,47,47	0
25	MG	A	1620	1/1	0.10	-	70,70,70,70	0
25	MG	A	1825	1/1	0.29	-	59,59,59,59	0
25	MG	A	1627	1/1	0.12	-	30,30,30,30	0
25	MG	A	1744	1/1	0.22	-	62,62,62,62	0
25	MG	A	1901[A]	1/1	0.25	-	16,16,16,16	1
25	MG	A	1946	1/1	0.10	-	146,146,146,146	0
25	MG	V	101	1/1	0.66	-	75,75,75,75	0
25	MG	A	1640	1/1	0.12	-	59,59,59,59	0
25	MG	A	1629	1/1	0.10	-	60,60,60,60	0
25	MG	A	1631	1/1	0.06	-	75,75,75,75	0
25	MG	A	1834	1/1	0.19	-	57,57,57,57	0
25	MG	A	1675	1/1	0.44	-	74,74,74,74	0
25	MG	A	1872	1/1	0.28	-	30,30,30,30	0
25	MG	A	1933	1/1	0.12	-	82,82,82,82	0
25	MG	A	1947	1/1	0.09	-	133,133,133,133	0
25	MG	A	1682	1/1	0.12	-	104,104,104,104	0
25	MG	A	1685	1/1	0.12	-	57,57,57,57	0
25	MG	A	1936	1/1	0.37	-	68,68,68,68	0
25	MG	A	1896	1/1	0.36	-	57,57,57,57	0
25	MG	A	1908	1/1	0.84	-	66,66,66,66	0
24	PAR	A	1607	42/42	0.22	-	99,99,99,99	42
25	MG	A	1740	1/1	0.19	-	113,113,113,113	0
25	MG	A	1805	1/1	0.35	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1746	1/1	0.30	-	146,146,146,146	0
25	MG	A	1804	1/1	0.17	-	62,62,62,62	0
25	MG	A	1858	1/1	0.16	-	37,37,37,37	0
24	PAR	A	1608	42/42	0.24	-	81,81,81,81	42
25	MG	A	1659	1/1	0.26	-	87,87,87,87	0
25	MG	A	1698	1/1	0.09	-	56,56,56,56	0
25	MG	T	201	1/1	0.30	-	88,88,88,88	0
25	MG	A	1923	1/1	0.11	-	29,29,29,29	0
24	PAR	A	1606	42/42	0.22	-	113,113,113,113	0
25	MG	A	1680	1/1	0.13	-	67,67,67,67	0
25	MG	A	1944	1/1	0.11	-	74,74,74,74	0
25	MG	A	1757	1/1	0.08	-	133,133,133,133	0
25	MG	A	1954	1/1	0.47	-	150,150,150,150	0
25	MG	A	1863	1/1	0.27	-	53,53,53,53	0
25	MG	A	1719	1/1	0.43	-	72,72,72,72	0
25	MG	A	1794	1/1	0.39	-	61,61,61,61	0
25	MG	A	1666	1/1	0.15	-	91,91,91,91	0
25	MG	A	1820	1/1	0.39	-	70,70,70,70	0
25	MG	A	1694	1/1	0.23	-	108,108,108,108	0
25	MG	A	1720	1/1	0.32	-	89,89,89,89	0
25	MG	A	1901[B]	1/1	0.25	-	16,16,16,16	1
25	MG	A	1672	1/1	0.21	-	56,56,56,56	0
25	MG	A	1714	1/1	0.27	-	66,66,66,66	0
25	MG	D	303	1/1	0.10	-	73,73,73,73	0
25	MG	A	1864[B]	1/1	0.41	-	11,11,11,11	1
25	MG	A	1777	1/1	0.39	-	60,60,60,60	0
25	MG	A	1759	1/1	0.23	-	121,121,121,121	0
25	MG	A	1691	1/1	0.31	-	111,111,111,111	0
25	MG	A	1789	1/1	0.28	-	127,127,127,127	0
25	MG	A	1839	1/1	0.15	-	56,56,56,56	0
25	MG	A	1932	1/1	1.43	-	71,71,71,71	0
25	MG	A	1765	1/1	0.13	-	113,113,113,113	0
25	MG	A	1851	1/1	0.45	-	57,57,57,57	0
25	MG	A	1754	1/1	0.22	-	67,67,67,67	0
25	MG	A	1811	1/1	0.32	-	56,56,56,56	0
25	MG	A	1647	1/1	0.22	-	72,72,72,72	0
25	MG	A	1646	1/1	0.09	-	69,69,69,69	0
25	MG	A	1687	1/1	0.19	-	53,53,53,53	0
25	MG	A	1846	1/1	0.24	-	49,49,49,49	0
25	MG	A	1871	1/1	0.22	-	63,63,63,63	0
25	MG	A	1808	1/1	0.25	-	31,31,31,31	0
25	MG	A	1725	1/1	0.24	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	Q	201	1/1	0.12	-	60,60,60,60	0
25	MG	A	1793	1/1	0.25	-	22,22,22,22	0
25	MG	A	1919[B]	1/1	0.25	-	9,9,9,9	1
25	MG	O	101	1/1	0.20	-	112,112,112,112	0
24	PAR	A	1609	42/42	0.29	-	121,121,121,121	42
25	MG	A	1891	1/1	0.83	-	50,50,50,50	0
25	MG	A	1900	1/1	0.23	-	27,27,27,27	0
25	MG	A	1819	1/1	0.43	-	64,64,64,64	0
25	MG	A	1902	1/1	0.23	-	64,64,64,64	0
25	MG	A	1741	1/1	0.20	-	52,52,52,52	0
25	MG	A	1748	1/1	0.23	-	87,87,87,87	0
25	MG	A	1837	1/1	0.36	-	54,54,54,54	0
25	MG	A	1701	1/1	0.16	-	85,85,85,85	0
25	MG	A	1625	1/1	0.15	-	30,30,30,30	0
25	MG	A	1787	1/1	0.23	-	66,66,66,66	0
25	MG	A	1621	1/1	0.25	-	69,69,69,69	0
25	MG	A	1865	1/1	0.72	-	58,58,58,58	0
25	MG	A	1697	1/1	0.20	-	77,77,77,77	0
25	MG	A	1669	1/1	0.54	-	76,76,76,76	0
25	MG	A	1658	1/1	0.11	-	57,57,57,57	0
25	MG	A	1832	1/1	0.36	-	77,77,77,77	0
25	MG	A	1671	1/1	0.07	-	66,66,66,66	0
25	MG	A	1822	1/1	0.29	-	63,63,63,63	0
25	MG	A	1628	1/1	0.23	-	48,48,48,48	0
25	MG	A	1619	1/1	0.35	-	69,69,69,69	0
25	MG	A	1885	1/1	0.36	-	45,45,45,45	0
25	MG	A	1877	1/1	0.12	-	59,59,59,59	0
25	MG	A	1673	1/1	0.18	-	73,73,73,73	0
25	MG	A	1795	1/1	0.15	-	57,57,57,57	0
25	MG	L	201	1/1	0.17	-	57,57,57,57	0
24	PAR	A	1602	42/42	0.17	-	71,71,71,71	0
25	MG	A	1755	1/1	0.21	-	74,74,74,74	0
24	PAR	A	1605	42/42	0.23	-	94,94,94,94	42
25	MG	A	1942	1/1	0.11	-	143,143,143,143	0
25	MG	A	1771	1/1	0.51	-	89,89,89,89	0
25	MG	A	1807	1/1	0.57	-	83,83,83,83	0
25	MG	A	1624	1/1	0.20	-	58,58,58,58	0
25	MG	A	1847	1/1	0.64	-	85,85,85,85	0
25	MG	A	1870	1/1	0.26	-	35,35,35,35	0
25	MG	A	1785	1/1	0.12	-	51,51,51,51	0
25	MG	A	1651	1/1	0.24	-	48,48,48,48	0
25	MG	A	1716	1/1	0.22	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1940	1/1	0.48	-	82,82,82,82	0
25	MG	A	1688	1/1	0.19	-	60,60,60,60	0
25	MG	A	1920	1/1	0.57	-	50,50,50,50	0
25	MG	A	1726	1/1	0.09	-	93,93,93,93	0
24	PAR	A	1617	42/42	0.29	-	189,189,189,189	0
25	MG	A	1782	1/1	0.10	-	68,68,68,68	0
25	MG	A	1699	1/1	0.15	-	79,79,79,79	0
25	MG	A	1689	1/1	0.11	-	75,75,75,75	0
25	MG	A	1844	1/1	0.17	-	35,35,35,35	0
25	MG	A	1772	1/1	0.68	-	61,61,61,61	0
25	MG	A	1824	1/1	0.46	-	64,64,64,64	0
25	MG	A	1668	1/1	0.47	-	66,66,66,66	0
25	MG	A	1815	1/1	0.41	-	45,45,45,45	0
25	MG	A	1945	1/1	0.10	-	156,156,156,156	0
25	MG	A	1816	1/1	1.11	-	53,53,53,53	0
25	MG	A	1790	1/1	0.16	-	162,162,162,162	0
25	MG	A	1850	1/1	0.31	-	71,71,71,71	0
25	MG	A	1884	1/1	0.44	-	55,55,55,55	0
25	MG	A	1934	1/1	0.17	-	69,69,69,69	0
25	MG	A	1907	1/1	0.17	-	53,53,53,53	0
25	MG	A	1661	1/1	0.09	-	90,90,90,90	0
25	MG	A	1743	1/1	0.13	-	71,71,71,71	0
25	MG	A	1914	1/1	0.82	-	44,44,44,44	0
25	MG	A	1722	1/1	0.09	-	43,43,43,43	0
25	MG	A	1897[A]	1/1	0.60	-	0,0,0,0	1
25	MG	A	1783	1/1	0.82	-	41,41,41,41	0
25	MG	A	1829	1/1	0.14	-	37,37,37,37	0
25	MG	A	1927	1/1	0.12	-	62,62,62,62	0
24	PAR	A	1603	42/42	0.20	-	103,103,103,103	3
25	MG	A	1678	1/1	0.23	-	48,48,48,48	0
25	MG	A	1939	1/1	0.21	-	57,57,57,57	0
25	MG	A	1735	1/1	0.38	-	67,67,67,67	0
25	MG	A	1796	1/1	0.76	-	58,58,58,58	0
24	PAR	A	1616	42/42	0.24	-	216,216,216,216	0
25	MG	A	1864[A]	1/1	0.41	-	11,11,11,11	1
25	MG	A	1842	1/1	0.79	-	43,43,43,43	0
25	MG	A	1761	1/1	0.21	-	155,155,155,155	0
25	MG	A	1774	1/1	0.08	-	71,71,71,71	0
25	MG	A	1875	1/1	0.16	-	14,14,14,14	0
25	MG	A	1887	1/1	0.75	-	64,64,64,64	0
25	MG	A	1948	1/1	0.09	-	122,122,122,122	0
25	MG	A	1650	1/1	0.20	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1784	1/1	0.33	-	89,89,89,89	0
25	MG	A	1776	1/1	0.21	-	65,65,65,65	0
25	MG	A	1734	1/1	0.46	-	63,63,63,63	0
25	MG	A	1634	1/1	0.14	-	42,42,42,42	0
25	MG	A	1856	1/1	0.25	-	59,59,59,59	0
25	MG	A	1645	1/1	0.30	-	53,53,53,53	0
25	MG	A	1866	1/1	1.94	-	53,53,53,53	0
25	MG	A	1895	1/1	0.39	-	44,44,44,44	0
25	MG	A	1758	1/1	0.28	-	85,85,85,85	0
25	MG	A	1930	1/1	0.46	-	79,79,79,79	0
25	MG	A	1928	1/1	0.96	-	93,93,93,93	0
25	MG	A	1937	1/1	0.40	-	61,61,61,61	0
25	MG	A	1763	1/1	0.16	-	65,65,65,65	0
25	MG	A	1752	1/1	0.14	-	147,147,147,147	0
25	MG	A	1921	1/1	0.35	-	48,48,48,48	0
25	MG	A	1889	1/1	0.53	-	66,66,66,66	0
25	MG	A	1828	1/1	0.46	-	107,107,107,107	0
25	MG	A	1724	1/1	0.14	-	82,82,82,82	0
25	MG	A	1859	1/1	0.55	-	73,73,73,73	0
25	MG	A	1878	1/1	0.27	-	13,13,13,13	0
25	MG	P	102	1/1	0.22	-	51,51,51,51	0
25	MG	A	1710	1/1	0.36	-	82,82,82,82	0
25	MG	A	1810	1/1	0.79	-	71,71,71,71	0
25	MG	A	1623	1/1	0.52	-	64,64,64,64	0
25	MG	A	1718	1/1	1.15	-	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.